SciCADE 2024

International Conference on Scientific Computation and Differential Equations

July 15 - 19, 2024 @ National University of Singapore, Singapore

Webpage

Program

Conference Venue

ConfTool

Invited Plenary Speakers

Ann Almgren, Lawrence Berkeley National Laboratory, USA
Elena Celledoni, Norwegian University of Science and Technology, Norway
Qianxiao Li, National University of Singapore, Singapore
Jianfeng Lu, Duke University, USA
Carola-Bibiane Schönlieb, University of Cambridge, UK
Jie Shen, Eastern Institute of Technology, Ningbo, China
Gilles Vilmart, University of Geneva, Switzerland
Lei Zhang, Peking University, China

Scientific Committee

Weizhu Bao, National University of Singapore, Singapore (Chair)
Qiang Du, Columbia University, United States
Erwan Faou, Ecole Normale Superieure de Rennes, France
Benedict Leimkuhler, University of Edinburgh, United Kingdom
Christian Lubich, Universitat Tubingen, Germany
Alexander Ostermann, University of Innsbruck, Austria
Linda Petzold, University of California Santa Barbara, United States
Tao Tang, Beijing Normal University-Hong Kong Baptist University United International College (UIC), China
Carol Woodward, Lawrence Livermore National Laboratory, United States

Local Organizing Committee

Co-Chairs:
Weizhu Bao, National University of Singapore, Singapore
Weiqing Ren, National University of Singapore, Singapore
Li-Lian Wang, Nanyang Technological University, Singapore

Members:
Zhenning Cai, National University of Singapore, Singapore
Qianxiao Li, National University of Singapore, Singapore
Xin Tong, National University of Singapore, Singapore

Secretary

Jiamin Ong, National University of Singapore, Singapore

National University of Singapore Wi-Fi Instructions

1. Connect to "NUS_Guest" wireless network
2. Select "Event Login" at the login page
3. Enter the Wi-Fi PIN that's provided below

Wi-Fi PIN: 478YKL
Event Name: SciCADE 2024
Event Venue: LT27

	July 14, Sunday	July 15, Monday	July 16, Tuesday	July 17, Wednesday	July 18, Thursday	July 19, Friday
8.00 – 8.30		Registration				
8.30 – 9.00		Opening (8.50 – 9.00)	Registration	Registration	Registration	Registration
9.00 – 9.30		Plenary Lecture 1 **Jie SHEN** (Chair: Li-Lian WANG)	Plenary Lecture 3 **Gilles VILMART** (Chair: Alexander OSTERMANN)	New Talent Award Lecture **Gianluca CERUTI** (Chair: Weiqing REN)	Plenary Lecture 5 **Jianfeng LU** (Chair: Zhenning CAI)	Plenary Lecture 7 **Qianxiao LI** (Chair: Christian LUBICH)
9.30 – 10.00						
10.00 – 10.30		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
10.30 – 11.00		MS01, MS02, MS04, MS13, MS19, MS25, MS29, MS36, MS43, MS50, MS54, MS55, PCT01, PCT02	MS05, MS06, MS14, MS21, MS23, MS26, MS37, MS40, MS50, MS52, MS54, MS55, PCT05, PCT06	MS06, MS11, MS12, MS17, MS18, MS20, MS30, MS33, MS35, MS41, MS46, MS49, PCT09, PCT10	MS03, MS07, MS08, MS10, MS11, MS15, MS22, MS34, MS45, MS48, MS54, MS55, PCT11, PCT12	MS08, MS10, MS12, MS30, MS31, MS33, MS35, MS48, MS49, MS51, MS53, MS54
11.00 – 11.30						
11.30 – 12.00						Plenary Lecture 8 **Ann ALMGREN** (Chair: Weizhu BAO)
12.00 – 12.30						
12.30 – 13.00		Lunch (by SciCADE)	Lunch (by SciCADE)		Lunch (on Own)	Closing & Farewell (12.30 - 12.40)
13.00 – 13.30				Lunch (on Own)		
13.30 – 14.00						
14.00 – 14.30	Registration *Venue: Medicine Science Library (MSL) Level 1, National University of Singapore*	Plenary Lecture 2 **Elena CELLEDONI** (Chair: Benedict LEIMKUHLER)	Plenary Lecture 4 **Lei ZHANG** (Chair: Qiang DU)	Free Discussion & Self-Excursion	Plenary Lecture 6 **Carola-Bibiane SCHÖNLIEB** (Chair: Xin TONG)	
14.30 – 15.00						
15.00 – 15.30		Coffee Break	Coffee Break		Coffee Break	
15.30 – 16.00		MS01, MS05, MS14, MS24, MS25, MS26, MS36, MS40, MS43, MS47, MS54, MS55, PCT03, PCT04	MS04, MS08, MS11, MS17, MS18, MS20, MS23, MS28, MS37, MS38, MS44, MS55, PCT07, PCT08		MS09, MS15, MS16, MS20, MS27, MS30, MS31, MS32, MS41, MS42, MS53, MS54, PCT13, PCT14	
16.00 – 16.30						
16.30 – 17.00						
17.00 – 17.30						
17.30 – 18.00		Reception			Poster Session	
18.00 – 18.30						
18.30 – 19.00		Dahlquist Prize Lecture **Yingda CHENG** (Chair: Carol WOODWARD)			Banquet (19.00 – 21.00) *Venue: Marina Bay Sands, Sands Expo and Convention Centre (Hibiscus Ballroom)*	
19.00 – 19.30						

July 15, Monday

8:00 - 8:50	**Registration** @Medicine Science Library (MSL) Level 1													
8:50 - 9:00	**Opening** @LT27													
9:00 - 10:00	**Plenary Lecture 1** @LT27 (Chair: Li-Lian WANG) **Title**: A new class of higher-order stiffly stable schemes with application to the Navier-Stokes equations **Speaker**: **Jie SHEN** (Eastern Institute of Technology)													
10:00 - 10:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS04-1)	S16-02-02 (MS36-1)	S16-02-03 (MS01-1)	S16-0304 (MS25-1)	S16-03-05/06 (MS19)	S16-0307 (MS55-1)	S16-0309 (MS50-1)	S17-04-04 (MS02)	S17-04-05 (MS13)	S17-05-11 (MS43-1)	S17-05-12 (MS54-1)	S17-06-11 (MS29)	MSL-01-01 (PCT01)	MSL-01-02 (PCT02)
10:30 - 11:00	Limin Ma	Daniel Paulin	Zewen Shen	Yan Xu	René Wittmann	Lyudmila Grigoryeva	Zhongyi Huang	Kengo Kamatani	Dimitri Breda	Xin Guo	Ji Lin	Matthieu Darcy	Lishan Fang	Wensheng Zhang
11:00 - 11:30	Beibei Zhu	Fernando Casas	Hai Zhu	Giulia Bertaglia	Jie Xu	Davide Murari	Xiang Zhou	Pierre Alquier	Mihály Kovács	Lei Shi	XingBiao Hu	Edoardo Calvello	Zeyu Xia	Yunyun Yang
11:30 - 12:00	Qian Zhang	Ramona Häberli	Mohan Zhao	Tao Xiong	Umberto Zerbinati	Xiaofeng Xu	Liu Liu	Erik von Schwerin	Muhammad Tanveer	Jeremie Houssineau	Man Jia	Niklas Baumgarten	Ying Liu	Justin Wan
12:00 - 12:30	Xinran Ruan	Q. M. Wargnier	Bowei Wu	Hyung Ju Hwang	Ning Jiang	Takaharu Yaguchi	Tan Zhang	Edwin Fong	Qian Guo	Colin Fox	Liming Ling	Anastasia Istratuca	Weiwei Zhang	Changqing Teng
12:30 - 14:00	Lunch (provided by SciCADE) @MSL Level 1													
14:00 - 15:00	**Plenary Lecture 2** @LT27 (Chair: Benedict LEIMKUHLER) **Title:** Deep learning of diffeomorphisms with application to shape analysis **Speaker:** **Elena CELLEDONI** (Norwegian University of Science and Technology)													
15:00 - 15:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS14-1)	S16-02-02 (MS36-2)	S16-02-03 (MS01-2)	S16-0304 (MS25-2)	S16-03-0506 (MS05-1)	S16-0307 (MS55-2)	S16-0309 (MS24)	S17-04-04 (MS47)	S17-04-05 (MS26-1)	S17-05-11 (MS43-2)	S17-05-12 (MS54-2)	S17-06-11 (MS40-1)	MSL-01-01 (PCT03)	MSL-01-02 (PCT04)
15:30 - 16:00	Guillaume Bal	Benedict Leimkuhler	Dhairya Malhotra	Zhicheng Hu	Genming Bai	Ferdia John Sherry	Yiqiu Dong	Eric Chung	Lukas Einkemmer	Santiago Badia	Junchao Chen	Jemima M. Tabeart	Xuanzhao Gao	Sandeep Kumar
16:00 - 16:30	Buyang Li	Eugen Bronasco	Tristan Goodwill	Mattia Zanella	Xinlong Feng	Brynjulf Owren	Ji Hui	Moritz Hauck	Fabio Zoccolan	Yiming Ying	Yong Chen	Christoph Hansknecht	Ilham Asmouh	Tobias Jahnke
16:30 - 17:00	Yifei Wu	Michela Ottobre	Shidong Jiang	Bertram Düring	Harald Garcke	Richard Tsai	Bin Dong	Guanglian Li	Stefan Schnake	Zhongjian Wang	LiYuan Ma	Sean Hon	Robert Altmann	Shubham Kumar
17:00 - 17:30	Yue Feng	Florian Rossmannek	Daniel Fortunato	Andrea Medaglia	Elena Bachini	Sofya Maslovskaya	Xiaoqun Zhang	Chen Hui Pang	Dominik Sulz	Jakob Zech	Lin Luo	Bernhard Heinzelreiter	Kwanghyuk Park	Ram Surendra Singh
17:30 - 18:30	Reception @MSL Level 1 & LT27 Foyer													
18:30 - 19:30	**Dahlquist Prize Lecture** @LT27 (Chair: Carol WOODWARD) **Title**: Sparse grid discontinuous Galerkin (DG) methods for high dimensional PDEs **Speaker**: **Yingda CHENG** (Virginia Polytechnic Institute and State University)													

July 16, Tuesday

8:30 - 9:00	**Registration** @MSL Level 1													
9:00 - 10:00	**Plenary Lecture 3** @LT27 (Chair: Alexander OSTERMANN) **Title**: Explicit stabilized integrators for stiff problems: the interplay of geometric integration and stochastic integration **Speaker**: **Gilles VILMART** (University of Geneva)													
10:00 - 10:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS14-2)	S16-02-02 (MS06-1)	S16-02-03 (MS37-1)	S16-0304 (MS21)	S16-03-0506 (MS05-2)	S16-0307 (MS55-3)	S16-0309 (MS50-2)	S17-04-04 (MS23-1)	S17-04-05 (MS26-2)	S17-05-11 (MS52)	S17-05-12 (MS54-3)	S17-06-11 (MS40-2)	MSL-01-01 (PCT05)	MSL-01-02 (PCT06)
10:30 - 11:00	Pranav Singh	Weizhu Bao	Peijun Li	Wei Guo	Ana Djurdjevac	Juan-Pablo Ortega	Wei Zhu	Yibao Li	Benjamin Carrel	Christian Offen	Shi-Hao Li	Tim Sucha	Daisuke Inoue	Weihang Gao
11:00 - 11:30	Lun Ji	Bin Wang	Xiaolong Zhang	Juntao Huang	Joyce Ghantous	Jianyu Hu	Yuehaw Khoo	Weidan Ni	Steffen Schotthoefer	Benedikt Brantner	Xiang-Ke Chang	Estefania L. Romero	Haruki Takemura	Jiaxi Zhao
11:30 - 12:00	Chushan Wang	Yanyan Shi	Zhiguo Yang	Haizhao Yang	Michael Lantelme	Katarzyna Michalowska	Yifan Chen	Haibiao Zheng	Pia Katharina Stammer	Philipp Horn	Zuonong Zhu	Tan Minh Nguyen	Tianyu Jin	Rakesh Kumar
12:00 - 12:30	Hang Li	Johanna Mödl	Xue Jiang	Zhichao Peng	Hailong Guo	Moshe Eliasof	Yue Xie	Chaozhen Wei	Stanislav Budzinskiy	Tomasz Michal Tyranowski	Ruomeng Li	A. Miniguano-Trujillo	Jingfeng Wang	Faranak Pahlevani
12:30 - 14:00	Lunch (provided by SciCADE) @MSL Level 1													
14:00 - 15:00	**Plenary Lecture 4** @LT27 (Chair: Qiang DU) **Title:** Construction of solution landscape for complex systems **Speaker:** **Lei ZHANG** (Peking University)													
15:00 - 15:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS04-2)	S16-02-02 (MS08-1)	S16-02-03 (MS37-2)	S16-0304 (MS18-1)	S16-03-05/06 (MS20-1)	S16-0307 (MS55-4)	S16-0309 (MS11-1)	S17-04-04 (MS23-2)	S17-04-05 (MS38)	S17-05-11 (MS28)	S17-05-12 (MS17-1)	S17-06-11 (MS44)	MSL-01-01 (PCT07)	MSL-01-02 (PCT08)
15:30 - 16:00	Zhiwen Zhang	Yajuan Sun	Zhenli Xu	Qi Wang	Tiezheng Qian	Måns Williamson	Jianliang Qian	Yaning Xie	Xu Yang	Chengcheng Ling	Shuyu Sun	Jan ten Thije Boonkkamp	Chinmay Patwardhan	Karolina Benkova
16:00 - 16:30	Zhizhang Wu	Balázs Kovács	Bo Wang	Jizu Huang	Guijin Zou	Gautam Pai	Huibin Chang	Meng Zhao	Guozhi Dong	Helena K. Kremp	Tao Zhou	Rinki Rawat	Jajati Keshari Sahoo	Razvan-Andrei Lascu
16:30 - 17:00	Wei Liu	Ruili Zhang	Maohui Lyu	Qing Cheng	Yakun Li	James Jackaman	Tao Yin	Min-Jhe Lu	Lihui Chai	Christian Bayer	Qin Sheng	Hanz Martin Cheng	Yibo Wang	Fraser J. W. O'Brien
17:00 - 17:30	Na Liu	Naoki Ishii	Hongfei Zhan	Chuan Fan	Zhixuan Li	Eldad Haber	Hao Liu	Wenjun Ying	Haibo Li	Joscha Diehl	Chaoyu Liu	Chitranjan Pandey	Khaled Hariz	Jens Lang
17:30 - 18:00	Jilu Wang		Teng Zhang	Bo Lin	Brendan Harding		Feifei Jing	Xihua Xu	Ping Tong		Sanah Suri	B.V. Rathish Kumar	Georg Maierhofer	Tuo Liu

July 17, Wednesday

8:30 - 9:00	**Registration** @MSL Level 1													
9:00 - 10:00	**New Talent Award Lecture** @LT27 (Chair: Weiqing REN) **Title**: Geometry-driven approach to low-rank dynamics **Speaker**: **Gianluca CERUTI** (University of Innsbruck)													
10:00 - 10:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS46)	S16-02-02 (MS06-2)	S16-02-03 (MS33-1)	S16-0304 (MS18-2)	S16-03-05/06 (MS20-2)	S16-0307 (MS41-1)	S16-0309 (MS11-2)	S17-04-04 (MS30-1)	S17-04-05 (MS35-1)	S17-05-11 (MS12-1)	S17-05-12 (MS17-2)	S17-06-11 (MS49-1)	MSL-01-01 (PCT09)	MSL-01-02 (PCT10)
10:30 - 11:00	Can Huang	Karolina Kropielnicka	David George Shirokoff	Qinglin Tang	Xianmin Xu	Lei Wu	Kei Fong Lam	Xiaoquan Yang	Benjamin Dörich	Yiwen Lin	Xiaoping Wang	Kaido Lätt	Fei Xu	Zecheng Gan
11:00 - 11:30	Xia Cui	Yongyong Cai	David Gardner	Xiaoli Li	Dong Wang	Zhiping Mao	Jianbo Cui	Guanghui Hu	Chupeng Ma	Xiaodong Liu	Michael Günther	Mikk Vikerpuur	Yuhan Chen	Xinpeng Xu
11:30 - 12:00	Sheng Chen	Michael Kirn	Jia Yin	Zhaohui Fu	Meng Li	Hongqiao Wang	Shingyu Leung	Shucheng Pan	José Carlos Garay	Wangtao Lu	Qiumei Huang	Huiting Yang	Maosheng Jiang	Na Wang
12:00 - 12:30	Huajie Chen	Xiaofei Zhao	Sebastian Bleecke	Yanrong Zhang	Xufeng Xiao	Yifei Duan	Chong Chen	Xing Ji	Florian Schaefer	Haibing Wang	Yunzhuo Guo	Yin Yang	Micol Bassanini	Sougata Mandal
12:30 - 13:00	Changhui Tan		Kiera Eloise Harmatz-Kean	Fukeng Huang	Jiashun Hu	Zhiqiang Cai	Huangxin Chen	Hualin Liu	Timo Sprekeler	Yunwen Yin	Zhonghua Qiao	Yanni Gao	Amit Kumar Pal	Hariharan Soundararajan
13:00 - 14:00	Lunch (on Own)													
14:00 - 18:00	Free Discussion & Self-Excursion													

July 18, Thursday

8:30 - 9:00	**Registration** @MSL Level 1													
9:00 - 10:00	**Plenary Lecture 5** @LT27 (Chair: Zhenning CAI) **Title**: Convergence analysis of classical and quantum dynamics via hypocoercivity **Speaker**: **Jianfeng LU** (Duke University)													
10:00 - 10:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS15-1)	S16-02-02 (MS08-2)	S16-02-03 (MS48-1)	S16-0304 (MS45)	S16-03-0506 (MS07)	S16-0307 (MS55-5)	S16-0309 (MS11-3)	S17-04-04 (MS22)	S17-04-05 (MS34)	S17-05-11 (MS10-1)	S17-05-12 (MS54-4)	S17-06-11 (MS03)	MSL-01-01 (PCT11)	MSL-01-02 (PCT012)
10:30 - 11:00	Hanquan Wang	Michael Kraus	Jing Gao	Michael Lindsey	Carol S. Woodward	Chao Wang	Jun Lai	Neil Kumar Chada	Xin Tong	Christian Lubich	Xianguo Geng	Youjun Deng	Devang Sinha	Shu Ma
11:00 - 11:30	Yong Zhang	Yuto Miyatake	Yujian Jiao	Siyao Yang	Alexander Ostermann	Andy Wan	Roy Yuchen He	Sam Power	Tiangang Cui	Cecilia Pagliantini	Xiaochuan Liu	Yukun Guo	Jhuma Sen Gupta	Xiaoqin Shen
11:30 - 12:00	Yongjun Yuan	Aiqing Zhu	Junjie Ma	Yingzhou Li	Sergio Blanes	Jian Liu	Xiang Xu	Adrien Laurent	Zhidi Lin	Lee Forrest Ricketson	Jing Kang	Yuliang Wang	Shin-Hwa Wang	Dehami Kiryu
12:00 - 12:30	Xianzhe Chen	Qifeng Zhang	Lijun Yi	Fabian M. Faulstich	Uri Michael Ascher	Daisuke Furihata	Luchan Zhang	René Lohmann	C. Moriarty-Osborne	Julian Mangott	Dafeng Zuo	Shiqi Ma	Deb Narayan Barik	Baige Xu
12:30 - 14:00	Lunch (on Own)													
14:00 - 15:00	**Plenary Lecture 6** @LT27 (Chair: Xin TONG) **Title:** Mathematical imaging: From geometric PDEs and variational modelling to deep learning for images **Speaker: Carola-Bibiane SCHÖNLIEB** (University of Cambridge)													
15:00 - 15:30	Coffee Break @MSL Level 1 & LT27 Foyer													
	S16-02-01 (MS15-2)	S16-02-02 (MS16)	S16-02-03 (MS53-1)	S16-0304 (MS31-1)	S16-03-05/06 (MS20-3)	S16-0307 (MS41-2)	S16-0309 (MS42)	S17-04-04 (MS30-2)	S17-04-05 (MS27)	S17-05-11 (MS32)	S17-05-12 (MS54-5)	S17-06-11 (MS09)	MSL-01-01 (PCT13)	MSL-01-02 (PCT14)
15:30 - 16:00	Yali Gao	Tommaso Buvoli	Soeren Bartels	Junxiong Jia	Jiang Yang	Peijie Zhou	Qiaolin He	Zhijun Shen	Peter A. Whalley	Natesan Srinivasan	Chengfa Wu	Xianchao Wang	Dohyun Kim	Guanyu Zhou
16:00 - 16:30	Wenfan Yi	Markus Neher	Robert Nürnberg	Lei Ma	Lifang Pei	Haijun Yu	Qiang Ma	Fan Zhang	Akash Sharma	Jugal Mohapatra	Di Yang	Jian Zhai	Jewel Howlader	Maria Lopez-Fernandez
16:30 - 17:00	Ying Ma	Jitse Niesen	Shuo Yang	Kejun Tang	Yifei Li	Jiayu Zhai	Yangshuai Wang	Liang Pan	Lei Li	Shuo Zhang	Zhiwei Wu	Fenglin Sun	Reema Jain	Ruoxia Yao
17:00 - 17:30	Jiong-Yue Li	Tanya V. Tafolla	Rong Tang	Li Zeng	Wei Jiang	Ting Gao	Kuang Huang	Loïc Balazi	Xuefeng Gao	Guru Prem P. Mahalingam	Zhenya Yan	Giovanni Covi	Ashish Poonia	Caiqin Song
17:30 - 18:30	Poster Session @MSL Level 1													
19:00 - 21:00	Banquet Venue: Marina Bay Sands Expo and Convention Centre (Hibiscus Ballroom) Free Shuttle Bus (provided by SciCADE) @NUS LT27 Bus Stop to Banquet Venue: 6.00pm, 6.05pm, 6.10pm, 6.15pm, 6.20pm													

July 19, Friday

8:30 - 9:00	**Registration** @MSL Level 1											
9:00 - 10:00	**Plenary Lecture 7** @LT27 (Chair: Christian LUBICH) **Title**: Learning, approximation and control **Speaker**: **Qianxiao LI** (National University of Singapore)											
10:00 - 10:30	Coffee Break @MSL Level 1 & LT27 Foyer											
	S16-02-01 (MS33-2)	S16-02-02 (MS08-3)	S16-02-03 (MS48-2)	S16-0304 (MS31-2)	S16-03-05/06 (MS53-2)	S16-0307 (MS10-2)	S16-0309 (MS51)	S17-04-04 (MS30-3)	S17-04-05 (MS35-2)	S17-05-11 (MS12-2)	S17-05-12 (MS54-6)	S17-06-11 (MS49-2)
10:30 - 11:00	Steven Byram Roberts	Anjiao Gu	Zhaoxiang Li	Zihao Yang	Michael Feischl	Jonas Kusch	Anil Rathi	Bin Xie	Michał Wichrowski	Jue Wang	Jian Xu	Huifang Yuan
11:00 - 11:30	Abhijit Biswas	Yihan Shen	Jing Zhang	Yue Qiu	Tokuhiro Eto	Thomas Trigo Trindade	Dipak Kumar Sahoo	Kun Wang	Andreas Rupp	Lei Zhang	Haiqiong Zhao	Hui Liang
11:30 - 12:30	**Plenary Lecture 8** @LT27 (Chair: Weizhu BAO) **Title:** Adaptive mesh refinement: Algorithms and applications **Speaker:** **Ann ALMGREN** (Lawrence Berkeley National Laboratory)											
12:30 - 12:40	Closing & Farewell											

SciCADE 2024 **Location: LT27** (LT27 is located at Blk S16)

Date: Monday, 15/July/2024

8:50am - 9:00am	**Opening Session** Location: **LT27**
9:00am - 10:00am	**Jie SHEN, A new class of higher-order stiffly stable schemes with application to the Navier-Stokes equations** Location: **LT27** Chair: **Li-Lian Wang**
2:00pm - 3:00pm	**Elena CELLEDONI, Deep learning of diffeomorphisms with application to shape analysis** Location: **LT27** Chair: **Benedict Leimkuhler**
6:30pm - 7:30pm	**Yingda CHENG, Sparse grid discontinuous Galerkin (DG) methods for high dimensional PDEs** Location: **LT27** Chair: **Carol S. Woodward**

Date: Tuesday, 16/July/2024

9:00am - 10:00am	**Gilles VILMART, Explicit stabilized integrators for stiff problems: the interplay of geometric integration and stochastic integration** Location: **LT27** Chair: **Alexander Ostermann**
2:00pm - 3:00pm	**Lei ZHANG, Construction of solution landscape for complex systems** Location: **LT27** Chair: **Qiang Du**

Date: Wednesday, 17/July/2024

9:00am - 10:00am	**Gianluca CERUTI, Geometry-driven approach to low-rank dynamics** Location: **LT27** Chair: **Weiqing Ren**

Date: Thursday, 18/July/2024

9:00am - 10:00am	**Jianfeng LU, Analysis of flow-based generative models** Location: **LT27** Chair: **Zhenning Cai**
2:00pm - 3:00pm	**Carola-Bibiane SCHÖNLIEB, Mathematical imaging: From geometric PDEs and variational modelling to deep learning for images** Location: **LT27** Chair: **Xin Tong**

Date: Friday, 19/July/2024

9:00am - 10:00am	**Qianxiao LI, Learning, approximation and control** Location: **LT27** Chair: **Christian Lubich**
11:30am - 12:30pm	**Ann ALMGREN, Adaptive Mesh Refinement: Algorithms and Applications** Location: **LT27** Chair: **Weizhu Bao**

SciCADE 2024 Location: MSL-01-01（**Medicine Science Library Level 1 Room 1**）

Date: Monday, 15/July/2024

8:00am - 8:50am

Registration
Location: **MSL-01-01**

10:30am - 12:30pm

Parallel Contributed Talks 01
Location: **MSL-01-01**

10:30am - 11:00am

Data-based adaptive mesh refinement of finite element thin plate spline
Lishan Fang

11:00am - 11:30am

Optimal Error Estimates of a Crank-Nicolson Finite Element Projection Method for Magnetohydrodynamic Equations
Zeyu Xia

11:30am - 12:00pm

Recovery-based a posteriori error estimate for the weak Galerkin finite element method
Ying Liu, Yufeng Nie

12:00pm - 12:30pm

Node-based adaptive local mesh generation method and its application
Weiwei Zhang, Yuqing Zhou

3:30pm - 5:30pm

Parallel Contributed Talks 03
Location: **MSL-01-01**

3:30pm - 4:00pm

Fast Algorithm for Quasi-2D Coulomb Systems
Xuanzhao Gao, Zecheng Gan, Jiuyang Liang, Zhenli Xu

4:00pm - 4:30pm

An L^2-projection isogeometric analysis based on Strang splitting for nonlinear systems of convection-diffusion-reaction
Ilham Asmouh, Alexander Ostermann

4:30pm - 5:00pm

Bulk-surface splitting for parabolic problems with dynamic boundary conditions
Robert Altmann

5:00pm - 5:30pm

A THIRD-ORDER FINITE DIFFERENCE WENO SCHEME WITH SHALLOW NEURAL NETWORK
Kwanghyuk Park, Xinjuan Chen, Dongjin Lee, Jiaxi Gu, Jae-Hun Jung

SciCADE 2024 Location: MSL-01-01 (**Medicine Science Library Level 1 Room 1**)

Date: Tuesday, 16/July/2024

8:30am - 9:00am

Check-in
Location: **MSL-01-01**

10:30am - 12:30pm

Parallel Contributed Talks 05
Location: **MSL-01-01**

10:30am - 11:00am
An Uncertainty-aware Mesh-free Numerical Method for Kolmogorov PDEs
Daisuke Inoue, Yuji Ito, Takahito Kashiwabara, Norikazu Saito, Hiroaki Yoshida

---

11:00am - 11:30am
Error estimates of the CIP scheme for one-dimensional advection equations
Haruki Takemura, Takahito Kashiwabara

11:30am - 12:00pm
Fast implicit hybrid solvers for stiff time-evolution equations
Tianyu Jin, Georg Maierhofer, Katharina Schratz

12:00pm - 12:30pm
Towards the calculation generalized target functional with multi-mesh approach
Jingfeng Wang, Guanghui Hu

3:30pm - 6:00pm

Parallel Contributed Talks 07
Location: **MSL-01-01**

3:30pm - 4:00pm
A multi-scale low-rank integrator for Marshak waves
Chinmay Patwardhan, Jonas Kusch, Martin Frank

4:00pm - 4:30pm
Two-Step iterative method for solving singular tensor equations $\mathcal{A}*_M\mathcal{X}=\mathcal{B}$ under M-product
Jajati Keshari Sahoo

4:30pm - 5:00pm
Exponential integrator for stochastic strongly damped wave equation based on the Wong-Zakai approximation
Yibo Wang

5:00pm - 5:30pm
Fractional variational integrators based on convolution quadrature
Khaled Hariz, Fernando Jimenez, Sina Ober-Blöbaum

5:30pm - 6:00pm
Runge–Kutta resonance-based methods and symplectic low-regularity integrators
Georg Maierhofer, Katharina Schratz

SciCADE 2024 Location: MSL-01-01（**Medicine Science Library Level 1 Room 1**）

Date: Wednesday, 17/July/2024

8:30am - 9:00am

Check-in
Location: **MSL-01-01**

10:30am - 1:00pm

Parallel Contributed Talks 09
Location: **MSL-01-01**

10:30am - 11:00am
Acceleration of self-consistent field iteration for electronic structure calculations
Fei Xu

11:00am - 11:30am
Enhancing Modeling Accuracy via Discriminating Hamiltonian Systems
Yuhan Chen, Takaharu Yaguchi

11:30am - 12:00pm
Linear Relaxation Method with Regularized Energy Quadratization for Phase Field Model
Maosheng Jiang

12:00pm - 12:30pm
Energy-preserving discretizations of anisotropic waves applied to plasma physics
Micol Bassanini, Simone Deparis, Paolo Ricci

12:30pm - 1:00pm
Weak Galerkin Mixed FEM for the Crank-Nicolson Scheme of Parabolic Interface Problems
Amit Kumar Pal, Jhuma Sen Gupta

SciCADE 2024 Location: MSL-01-01 (**Medicine Science Library Level 1 Room 1**)

Date: Thursday, 18/July/2024

8:30am - 9:00am

Check-in
Location: **MSL-01-01**

10:30am - 12:30pm

Parallel Contributed Talks 11
Location: **MSL-01-01**

10:30am - 11:00am
Efficient Multilevel Importance Sampling in Derivative Pricing
Devang Sinha, Siddhartha Pratim Chakrabarty

11:00am - 11:30am
On the weak Galerkin mixed FEM for parabolic interface problems
Jhuma Sen Gupta, Amit Kumar Pal, Rajen Kumar Sinha

11:30am - 12:00pm
Evolutionary bifurcation diagrams of a multiparameter generalized logistic problem
KUO-CHIH HUNG, SHIN-HWA WANG

12:00pm - 12:30pm
Impact of Liquidity Risk and Limited Liability in Loan Portfolio Management
DEB NARAYAN BARIK, S IDDHARTHA P. C HAKRABARTY

3:30pm - 5:30pm

Parallel Contributed Talks 13
Location: **MSL-01-01**

3:30pm - 4:00pm
Asymptotic convergence of heterogeneous first-order aggregation models: from the sphere to the unitary group
Dohyun Kim, Hansol Park

4:00pm - 4:30pm
Parameter Uniform Numerical Methods Based on OSCM for The Singularly Perturbed Differential Equations with Delay in Time
Jewel Howlader, pankaj Mishra, Kapil K. Sharma

4:30pm - 5:00pm
Study of Soret Effect in Magnetized Dissipative Chemically Reactive Sisko Nanofluid Flow: A Numerical Insight
Reema Jain, Yogesh Dadhich

5:00pm - 5:30pm
HIV Community Transmission under Treatment: A Two-strain Modelling Approach
Ashish Poonia, Siddhartha Pratim Chakrabarty

SciCADE 2024 Location: MSL-01-02（Medicine Science Library Level 1 Room 2）

Date: Monday, 15/July/2024

10:30am - 12:30pm

Parallel Contributed Talks 02
Location: **MSL-01-02**

10:30am - 11:00am
Elastic full-waveform inversion as training a neural network
Wensheng Zhang

11:00am - 11:30am
WITS: Weakly-supervised individual tooth segmentation model trained on box-level labels
Ruicheng Xie, Yunyun Yang, Zhaoyang Chen

11:30am - 12:00pm
Self-Attention Network for Solving HJB Equation arising from Optimal Trade Execution
Andrew Na, Justin Wan

12:00pm - 12:30pm
Neural Option Pricing for Rough Bergomi Model
Changqing Teng, Guanglian Li

3:30pm - 5:30pm

Parallel Contributed Talks 04
Location: **MSL-01-02**

3:30pm - 4:00pm
Recent progress on the Schrödinger map equation
Sandeep Kumar

4:00pm - 4:30pm
On error bounds for approximations to high-frequency wave propagation in nonlinear dispersive media
Julian Baumstark, Tobias Jahnke

4:30pm - 5:00pm
Unique Solvability conditions for the absolute value equations and absolute value matrix equations
Shubham Kumar, Deepmala --

5:00pm - 5:30pm
Synchronous cycles in migrating population dynamics
Ram Surendra Singh, Yogesh Trivedi, Anushaya Mohapatra

SciCADE 2024 Location: MSL-01-02（**Medicine Science Library Level 1 Room 2**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

Parallel Contributed Talks 06
Location: **MSL-01-02**

10:30am - 11:00am

RBMD: Random Batch Molecular Dynamics on Heterogeneous Computing Architectures
Weihang Gao

11:00am - 11:30am

Mitigating distribution shift in machine learning-augmented hybrid simulation
Jiaxi Zhao, Qianxiao Li

11:30am - 12:00pm

Superconvergent Jacobi Spectral Methods for System of Nonlinear Volterra- Integro-Differential Equations
Rakesh Kumar, BV Rathish Kumar

12:00pm - 12:30pm

A Time Filtered Scheme for Non-linear Hyperbolic Equations Motivated by Modeling DNA Transcription Process
Faranak Pahlevani, Kevin Courtney, Lisa Davis

3:30pm - 6:00pm

Parallel Contributed Talks 08
Location: **MSL-01-02**

3:30pm - 4:00pm

PDE-constrained optimization with flux-correction in mathematical biology
Karolina Benkova, John Pearson, Mariya Ptashnyk

4:00pm - 4:30pm

Mirror Descent-Ascent for mean-field min-max problems
Razvan-Andrei Lascu

4:30pm - 5:00pm

A Model Independent Approach for Empirically Identifying the Optimal Control Strategy of a Power Storage Facility
Fraser John Wilkinson O'Brien

5:00pm - 5:30pm

Implicit Peer Triplets in Gradient-Based Solution Algorithms for ODE Constrained Optimal Control
Jens Lang, Bernhard A. Schmitt

5:30pm - 6:00pm

Explicit Runge-Kutta methods for quadratic optimization with optimal rates
Tuo Liu, David Ketcheson

SciCADE 2024 Location: MSL-01-02（**Medicine Science Library Level 1 Room 2**）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

Parallel Contributed Talks 10
Location: **MSL-01-02**

10:30am - 11:00am

Modeling and Fast Algorithms for the Dynamics of Auto-Chemotactic Chiral Active Droplets
Zecheng Gan

11:00am - 11:30am

Simulation Method of Microscale Fluid-Structure Interactions: Diffuse-Resistance-Domain Approach
Xinpeng Xu

11:30am - 12:00pm

Optimal-order convergence of the linearly extrapolated Crank–Nicolson method and the two-step BDF method for the Navier–Stokes equations with H^1 initial data
Na Wang

12:00pm - 12:30pm

Nonclassical Symmetry Analysis to Find out Analytical Solution of a Porous Media Flow Model
Sougata Mandal, **Sukhendu Ghosh**

12:30pm - 1:00pm

Study on dynamical behaviour of reaction-diffusion epidemic model
Hariharan Soundararajan, **Shangerganesh Lingeshwaran**

SciCADE 2024 Location: MSL-01-02（**Medicine Science Library Level 1 Room 2**）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

Parallel Contributed Talks 12
Location: **MSL-01-02**
Chair: **Buyang Li**

10:30am - 11:00am
Optimal convergence of the arbitrary Lagrangian–Eulerian interface tracking method for two-phase Navier–Stokes flow
Buyang Li, Shu Ma, Weifeng Qiu

11:00am - 11:30am
Stable and efficient methods for 2D-3C clamped plate and shallow shell models
Xiaoqin Shen

11:30am - 12:00pm
Improved estimate of the number of input points of DeepONet
Dehami Kiryu, Baige Xu, Takaharu Yaguchi

12:00pm - 12:30pm
Operator Learning of Hamiltonian Density for Modeling Nonlinear Waves
Baige Xu, Yusuke Tanaka, Takashi Matsubara, Takaharu Yaguchi

3:30pm - 5:30pm

Parallel Contributed Talks 14
Location: **MSL-01-02**

3:30pm - 4:00pm
Numerical method for the crack problem with a Signorini-type contact condition on a linear combination of displacement and velocity
Guanyu Zhou

4:00pm - 4:30pm
Generalized Convolution Quadrature for non smooth sectorial problems
Jing Guo, Maria Lopez-Fernandez

4:30pm - 5:00pm
Supersymmerties with Arbitrary Functions of a New Supersymmetric Dispersionless System and the classifications
Ruoxia Yao

5:00pm - 5:30pm
Nonlocal Yajima–Oikawa system: binary Darboux transformation, exact solutions and dynamic properties
Caiqin Song, Hai-qiong Zhao, Zuo-nong Zhu

SciCADE 2024 Location: S16-02-01 (Blk S16 Level 2 Room 1)

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS04-1 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion
Location: **S16-02-01**

10:30am - 11:00am
An energy stable and maximum bound principle preserving scheme for the dynamic Ginzburg Landau equations
Limin Ma

11:00am - 11:30am
Explicit K-symplectic methods for nonseparable non-canonical Hamiltonian systems
Beibei Zhu, Lun Ji, Aiqing Zhu, Yifa Tang

11:30am - 12:00pm
Space-time discontinuous Galerkin methods for Korteweg-de Vries type equations
Qian Zhang, Xia Yinhua

12:00pm - 12:30pm
Numerical methods for ground states of Bose-Einstein condensate with higher-order interactions
Xinran Ruan

3:30pm - 5:30pm

MS14-1 Numerical Integration for Dispersive Problems
Location: **S16-02-01**

3:30pm - 4:00pm
Simulation of asymmetric interface transport in topological insulators
Guillaume Bal

4:00pm - 4:30pm
Numerical approximation of discontinuous solutions of the semilinear wave equation
Jiachuan Cao, Buyang Li, Yanping Lin, Fangyan Yao

4:30pm - 5:00pm
The non-relativistic limits of nonlinear quantum field equations
Yifei Wu

5:00pm - 5:30pm
Improved Uniform Error Bounds on Time-splitting Methods for Long-time Dynamics of Dispersive PDEs
Yue Feng

SciCADE 2024 *Location:* S16-02-01 (Blk S16 Level 2 Room 1)

Date: Tuesday, 16/July/2024

10:30am -

MS14-2 Numerical Integration for Dispersive Problems
Location: **S16-02-01**

12:30pm

10:30am - 11:00am

Unitary rational approximations for the matrix exponential

Tobias Jawecki, Pranav Singh

11:00am - 11:30am

Bourgain techniques for low regularity error estimates

Lun Ji, Alexander Ostermann, Frédéric Rousset, Katharina Schratz

11:30am - 12:00pm

An explicit and symmetric exponential wave integrator for the nonlinear Schr\"{o}dinger equation with low regularity potential and nonlinearity

Weizhu Bao, Chushan Wang

12:00pm - 12:30pm

Filtered Lie-Trotter splitting for the “good” Boussinesq equation: low regularity estimates

Lun Ji, Hang Li, Alexander Ostermann, Chunmei Su

3:30pm - 6:00pm

MS04-2 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Location: S16-02-01

3:30pm - 4:00pm

A Novel Stochastic Interacting Particle-Field Algorithm for 3D Parabolic-Parabolic Keller-Segel Chemotaxis System

Zhongjian Wang, Jack Xin, Zhiwen Zhang

4:00pm - 4:30pm

An iterative algorithm for POD basis adaptation in solving parametric convection-diffusion equations

Zhizhang Wu, Zhiwen Zhang

4:30pm - 5:00pm

Computation of two types of ground state solutions for nonlinear Schrödinger equations

Wei Liu

5:00pm - 5:30pm

A 3-D High-order Spectral Element Time-Domain Method for Quantum Device Simulations

Na Liu, Kangshuai Du

5:30pm - 6:00pm

Optimal L^2 error estimates of unconditionally stable FE schemes for the Cahn-Hilliard-Navier-Stokes system

Jilu Wang

SciCADE 2024 *Location:* S16-02-01 (**Blk S16 Level 2 Room 1**)

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems
Location: **S16-02-01**

10:30am - 11:00am
An unconditionally stable IMEX scheme for Allen-Cahn/Cahn-Hilliard equation perturbed by multiplicative noise
Can Huang

11:00am - 11:30am
Analysis for a high accuracy nonlinear scheme for strong nonlinear diffusion problem
Xia Cui, Yu-Jie Gong, Guang-Wei Yuan

11:30am - 12:00pm
Spectral Methods for Partial Differential Equations on Complex Geometries
Sheng Chen

12:00pm - 12:30pm
Stability of the Minimal Energy Path
Huajie Chen

12:30pm - 1:00pm
The sticky particle system with alignment interactions
Changhui Tan

SciCADE 2024 *Location:* S16-02-01 (**Blk S16 Level 2 Room 1**)

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS15-1 Efficient and High-order Numerical Methods for Problems in Quantum Physics
Location: **S16-02-01**

10:30am - 11:00am
An asymptotic preserving scheme for the defocusing Davey-Stewartson II equation in the semiclassical limit
Hanquan Wang

11:00am - 11:30am
A Spectrally Accurate Numerical Method For Computing The Bogoliubov-De Gennes Excitations Of Dipolar Bose-Einstein Condensates
Yong ZHANG

11:30am - 12:00pm
An accurate and efficient numerical method to compute the ground states of the rotating spin-orbit coupled spin-1 Bose-Einstein condensates
Yongjun Yuan

12:00pm - 12:30pm
A fourth-order compact time-splitting method for the Dirac equation
Jia Yin, Weizhu Bao, Xianzhe Chen

3:30pm - 5:30pm

MS15-2 Efficient and High-order Numerical Methods for Problems in Quantum Physics
Location: **S16-02-01**

3:30pm - 4:00pm
Numerical methods for Bogoliubov-de Gennes excitations of Bose-Einstein condensates
Yali Gao

4:00pm - 4:30pm
Numerical methods for the logarithmic Dirac equation
Wenfan Yi

4:30pm - 5:00pm
Error estimates of numerical methods for the Dirac equation
Ying Ma

5:00pm - 5:30pm
Radiation fields for semilinear Dirac equations with spinor null forms
Jiong-Yue Li

Date: Friday, 19/July/2024

10:30am - 11:30am

MS33-2 Challenges and Innovations for the Time-Stepping of PDEs
Location: **S16-02-01**

10:30am - 11:00am
On the order of Runge-Kutta methods applied to stiff, semilinear ODEs
Steven Byram Roberts, David George Shirokoff, Abhijit Biswas, David Isaac Ketcheson, Benjamin Seibold

---

11:00am - 11:30am
Accurate Solution of the NLS Equation via Conservative Multiple-Relaxation ImEx Methods
Abhijit Biswas, David I. Ketcheson

SciCADE 2024 Location: S16-02-02（Blk S16 Level 2 Room 2）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS36-1 Geometric and Multiscale Methods for High-Dimensional Dynamics
Location: **S16-02-02**

10:30am - 11:00am
Unbiased Kinetic Langevin Monte Carlo with Inexact Gradients
Neil Chada, Benedict Leimkuhler, <u>Daniel Paulin</u>, Peter Whalley

---

11:00am - 11:30am
Splitting methods with modified potentials for certain classes of nonlinear evolution equations
<u>Fernando Casas</u>

11:30am - 12:00pm
Overcoming the order barrier two in splitting methods when applied to semilinear parabolic problems with non-periodic boundary conditions
<u>Ramona Häberli</u>

12:00pm - 12:30pm
Advanced Time-Adaptive PIROCK Method with Error Control for Magnetic Reconnection Simulations in Chromospheric Environments
<u>Q. M. Wargnier</u>, G. Vilmart, J. Martinez-Sykora, V. H. Hansteen, B. De Pontieu

3:30pm - 5:30pm

MS36-2 Geometric and Multiscale Methods for High-Dimensional Dynamics
Location: **S16-02-02**

3:30pm - 4:00pm
Numerical methods for stochastic collisional dynamics
<u>Benedict Leimkuhler</u>, Akash Sharma, Michael Tretyakov

4:00pm - 4:30pm
Exotic aromatic forests for high-order sampling of the invariant measure
<u>Eugen Bronasco</u>

4:30pm - 5:00pm
Uniform in time numerical approximations of (multiscale) SDEs
<u>Michela Ottobre</u>

5:00pm - 5:30pm
State-Space Systems as Dynamic Generative Models
<u>Florian Rossmannek</u>

SciCADE 2024 Location: S16-02-02（**Blk S16 Level 2 Room 2**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS06-1 Numerical Methods for Highly Oscillatory ODEs and PDEs
Location: **S16-02-02**

10:30am - 11:00am
Uniform error bounds on numerical methods for long-time dynamics of dispersive PDEs
Weizhu Bao, Yongyong Cai, Yue Feng, Chunmei Su

11:00am - 11:30am
Solving long-time nonlinear Schr\"{o}dinger equation by a class of oscillation-relaxation integrators
Kai Liu, Bin Wang, Xiaofei Zhao

11:30am - 12:00pm
Filtered finite difference methods for highly oscillatory semilinear hyperbolic systems
Christian Lubich, Yanyan Shi

12:00pm - 12:30pm
Time integration method for wave propagation with spatio-temporal oscillations
Tobias Jahnke, Johanna Mödl

3:30pm - 6:00pm

MS08-1 Recent Advances on Structure-preserving Algorithms with Applications
Location: **S16-02-02**
Chair: **Bin Wang**

3:30pm - 4:00pm
Geometric numerical integration for the linear-gradient system
Yajuan Sun

4:00pm - 4:30pm
Error estimates for backward difference formulae for the transient Stokes problem
Alessandro Contri, André Massing, Balázs Kovács

4:30pm - 5:00pm
Structure-preserving algorithms and their error estimates for the relativistic dynamics of charged particle
Ruili Zhang

5:00pm - 5:30pm
Aggressive Splitting in Structure-Preserving Numerical Methods
Naoki Ishii, Toyohiro Aso, Shun Sato, Takayasu Matsuo

SciCADE 2024 Location: S16-02-02（**Blk S16 Level 2 Room 2**）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS06-2 Numerical Methods for Highly Oscillatory ODEs and PDEs
Location: **S16-02-02**

10:30am - 11:00am

Asymptotic expansions for the linear PDEs with oscillatory input terms: Analytical form and error analysis
Karolina Kropielnicka

11:00am - 11:30am

A uniformly accurate method for the Klein-Gordon-Dirac system in the nonrelativistic regime
Yongyong Cai, Wenfan Yi

11:30am - 12:00pm

Using non-resonant step sizes to improve efficiency of time integrators for oscillatory non-linear Dirac equations
Tobias Jahnke, Michael Kirn

12:00pm - 12:30pm

Numerical methods for disordered NLS
Xiaofei Zhao

SciCADE 2024 Location: S16-02-02（Blk S16 Level 2 Room 2）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS08-2 Recent Advances on Structure-preserving Algorithms with Applications
Location: **S16-02-02**
Chair: **Ruili Zhang**

10:30am - 11:00am
Crossroads between Geometric Numerical Integration and Machine Learning
Michael Kraus

11:00am - 11:30am
Splitting algorithms for total variation imaging via SAV approach
Raymond H. Chan, Yuto Miyatake

11:30am - 12:00pm
Learning stochastic differential equations from data
Aiqing Zhu, Qianxiao Li

12:00pm - 12:30pm
Invariant-preserving difference schemes for the R2CH system
Qifeng Zhang

3:30pm - 5:30pm

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms
Location: **S16-02-02**

3:30pm - 4:00pm
Parallelism and Exponential Integration
Tommaso Buvoli

4:00pm - 4:30pm
Computation of phi functions for exponential integrators
Markus Neher

4:30pm - 5:00pm
A Krylov subspace exponential integrator based on the Adams-Bashforth method
Jitse Niesen

5:00pm - 5:30pm
Low Synchronization Arnoldi Methods with Application to Exponential Integrators
Tanya Vanessa Tafolla, Stephane Gaudreault, Mayya Tokman

Date: Friday, 19/July/2024

10:30am - 11:30am

MS08-3 Recent Advances on Structure-preserving Algorithms with Applications
Location: **S16-02-02**

10:30am - 11:00am
Hamiltonian Particle-in-Cell methods for Vlasov-Poisson equations
Anjiao Gu, Yang He, Yajuan Sun

11:00am - 11:30am
Variational integrators for the Lagrangian quadratic in velocities
Yihan Shen

SciCADE 2024 Location: S16-02-03 (Blk S16 Level 2 Room 3)

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS01-1 Recent Advances in Fast Algorithms and Integral Equation Methods
Location: **S16-02-03**

10:30am - 11:00am
Rapid evaluation of Newtonian potentials on planar domains
Zewen Shen, Kirill Serkh

11:00am - 11:30am
High-order quadrature for the evaluation of layer potentials on surfaces in three dimensions via exterior extension and complete reduction
Hai Zhu, Shidong Jiang

11:30am - 12:00pm
The Approximation of Singular Functions by Series of Non-integer Powers
Mohan Zhao, Kirill Serkh

12:00pm - 12:30pm
A panel based trapezoidal quadrature for surface integral operators
Bowei Wu, Joar Bagge

3:30pm - 5:30pm

MS01-2 Recent Advances in Fast Algorithms and Integral Equation Methods
Location: **S16-02-03**

3:30pm - 4:00pm
Fast and accurate simulation of close-to-touching discs in 2D Stokes flow
Dhairya Malhotra, Mariana Martinez Aguilar, Dan Fortunato

4:00pm - 4:30pm
A fast integral equation solver for surface PDEs.
Tristan Goodwill, Michael O'Neil, Jeremy Hoskins

4:30pm - 5:00pm
A Dual-space Multilevel Kernel-splitting Framework for Discrete and Continuous Convolution
Shidong Jiang, Leslie Greengard

5:00pm - 5:30pm
Fast algorithms for bulk-surface diffusion
Daniel Fortunato

SciCADE 2024 Location: S16-02-03 (**Blk S16 Level 2 Room 3**)

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS37-1 High-Order Methods for Linear and Nonlinear Wave Propagation
Location: **S16-02-03**
Chair: **Li-Lian Wang**

10:30am - 11:00am
Cavity scattering problems for the biharmonic wave equation
Peijun Li

11:00am - 11:30am
Low regularity estimates of the Lie-Trotter time-splitting Fourier spectral method for the logarithmic Schrödinger equation
Xiaolong Zhang, **Li-Lian Wang**

11:30am - 12:00pm
Structure-preserving spectral and spectral-element methods for Vlasov-Maxwell equations
Zhiguo Yang

12:00pm - 12:30pm
A perfectly matched layer method for signal-propagation problems in axon
Xue Jiang

3:30pm - 6:00pm

MS37-2 High-Order Methods for Linear and Nonlinear Wave Propagation
Location: **S16-02-03**
Chair: **Zhiguo Yang**

3:30pm - 4:00pm
Structure-preserving particle-in-cell method for plasma simulations
Zhenli Xu

4:00pm - 4:30pm
Fast boundary element method for scattering problem in layered media
Bo Wang

4:30pm - 5:00pm
Numerical simulation of nonlocal effects in metallic nanostructures using generalized HD model
Maohui Lyu

5:00pm - 5:30pm
A general tetrahedral spectral element method and its implementation to Kohn-Sham equation
Hongfei Zhan, **Guanghui Hu**

5:30pm - 6:00pm
Numerical methods for the biharmonic nonlinear Schrödinger equation
Teng Zhang

SciCADE 2024 Location: S16-02-03 (**Blk S16 Level 2 Room 3**)

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS33-1 Challenges and Innovations for the Time-Stepping of PDEs
Location: **S16-02-03**

10:30am - 11:00am

Explicit Runge-Kutta Methods that Avoid Order Reduction with an Optimal Number of Stages

David George Shirokoff, Abhijit Biswas, David Isaac Ketcheson, Steven Byram Roberts, Benjamin Seibold

---

11:00am - 11:30am

Adaptive methods for the two-time Kadanoff-Baym equations

David Gardner, Thomas Blommel, Emanuel Gull, Carol Woodward

11:30am - 12:00pm

Accelerating non-equilibrium Green's function computation through dynamic mode decomposition and recurrent neural networks

Jia Yin, Yang-hao Chan, Felipe Jornada, Diana Qiu, Steven Louie, Chao Yang

---

12:00pm - 12:30pm

On the rate of error growth in time for numerical solutions for chosen PDE problems

Sebastian Bleecke

12:30pm - 1:00pm

Leveraging Unconditional Stability Theory to Advance Index-1 Differential-Algebraic Equations Without Inverting Constraints

Kiera Eloise Harmatz-Kean, Benjamin Seibold, Rujeko Chinomona, David Shirokoff

SciCADE 2024 Location: S16-02-03 (**Blk S16 Level 2 Room 3**)

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS48-1 Recent Advances on Spectral and High-Order Methods
Location: **S16-02-03**

10:30am - 11:00am
A framework for stable spectral methods in d-dimensional unit balls
Jing GAO

11:00am - 11:30am
Finite-difference method on the surface of the helical pipes
Yujian Jiao

11:30am - 12:00pm
A convolution quadrature using derivatives and its application
Junjie Ma

12:00pm - 12:30pm
A unified superconvergent postprocessing technique for Galerkin time-stepping methods
Lijun Yi

3:30pm - 5:30pm

MS53-1 Surface Evolution and Harmonic Maps
Location: **S16-02-03**

3:30pm - 4:00pm
Error estimates for inextensible elastic curves
Soeren Bartels

4:00pm - 4:30pm
Numerical analysis for fourth order geometric curve evolutions based on the DeTurck trick
Robert Nürnberg, Klaus Deckelnick

4:30pm - 5:00pm
Accelerated gradient flows for large bending deformations of nonlinear plates
Guozhi Dong, Hailong Guo, Shuo Yang

5:00pm - 5:30pm
Convergence of an evolving finite element method for surface evolution with tangential motion by harmonic map heat flow
Guangwei Gao, Buyang Li, Rong Tang

Date: Friday, 19/July/2024

10:30am - 11:30am

MS48-2 Recent Advances on Spectral and High-Order Methods
Location: **S16-02-03**

10:30am - 11:00am
Spectral collocation method for numerical solution to the fully nonlinear Monge-Amp\`{e}re equation
Zhaoxiang LI

11:00am - 11:30am
Novel spectral methods for maxwell eigenvalue problem using divergence free curl-orthogonal polynomials
Jing Zhang

SciCADE 2024 Location: S16-03-04 （**Blk S16 Level 3 Room 4**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS25-1 Analysis and Numerical Computations for Kinetic Models
Location: **S16-03-04**

10:30am - 11:00am
Discontinuous Galerkin Finite Element Methods for Port-Hamiltonian Dynamical Systems
Yan Xu

11:00am - 11:30am
Kinetic modeling of infectious viral dynamics based on mutual utility functions
Giulia Bertaglia, Lorenzo Pareschi, Giuseppe Toscani

11:30am - 12:00pm
Efficient asymptotic preserving SL-DG methods for multiscale kinetic transport equations
Tao Xiong

12:00pm - 12:30pm
Neural PDE Solvers toward Digital Twin: Theory and Applications
Hyung Ju Hwang, Hwi Jae Son, Jaeyong Lee, Hyuntae Jo

3:30pm - 5:30pm

MS25-2 Analysis and Numerical Computations for Kinetic Models
Location: **S16-03-04**

3:30pm - 4:00pm
A fast iteration for the moment model of the Boltzmann-BGK equation in near-continuum regimes
Zhicheng Hu

4:00pm - 4:30pm
Reduced Variance Random Batch Methods for nonlocal meanfield equations
Mattia Zanella

4:30pm - 5:00pm
On a kinetic Elo rating model for players with dynamical strength
Bertram Düring

5:00pm - 5:30pm
Stochastic Galerkin Particle Methods for Kinetic Equations of Plasmas with Uncertainties
Andrea Medaglia

SciCADE 2024 Location: S16-03-04 （Blk S16 Level 3 Room 4）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems
Location: **S16-03-04**

10:30am - 11:00am
A symplectic deep autoencoder for Hamiltonian systems
Wei Guo

11:00am - 11:30am
Hyperbolic machine learning moment closure models for the radiative transfer equation
Juntao Huang

11:30am - 12:00pm
Finite Expression Method: A Symbolic Approach for Scientific Machine Learning
Haizhao Yang

12:00pm - 12:30pm
A Reduced Order Model Enhanced Iterative Solver for Parametric Radiative Transfer Equation
Zhichao Peng

3:30pm - 6:00pm

MS18-1 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems
Location: **S16-03-04**

3:30pm - 4:00pm
A Thermodynamically Consistent Nonisothermal Hydrodynamical Model for Binary Fluids with Cross-Coupling
Qi Wang

4:00pm - 4:30pm
APTT: An accuracy-preserved tensor-train method for the Boltzmann-BGK equation
Zhitao Zhu, Chuanfu Xiao, Kejun tang, Jizu Huang, Chao Yang

4:30pm - 5:00pm
A new flow dynamic approach for Wasserstein gradient flows
Qing Cheng

5:00pm - 5:30pm
Structure-preserving Oscillation-Eliminating Hermite WENO Method for Hyperbolic Systems
Chuan Fan

5:30pm - 6:00pm
A structure-preserving method to the Boltzmann equation
Bo Lin, Zhenning Cai

SciCADE 2024 Location: S16-03-04 （Blk S16 Level 3 Room 4）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS18-2 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems
Location: **S16-03-04**

10:30am - 11:00am

A linearly implicit energy-preserving method for the logarithmic Klein-Gordon equation

Qingzhou Shu, Chunmei Su, Qinglin Tang

11:00am - 11:30am

New fully decoupled and high-order algorithms with optimal energy approximationfor the Cahn-Hilliard-Navier-Stokes phase field model

Xiaoli Li

11:30am - 12:00pm

STURCTURE PRESERVING IMPLICIT-EXPLICIT RUNGE-KUTTA METHODS FOR GRADIENT FLOWS

Zhaohui Fu

12:00pm - 12:30pm

Highly Efficient Numerical Methods for Energy Dissipative/Conservative Nonlinear Systems

Yanrong Zhang

12:30pm - 1:00pm

New unconditionally stable higher-order consistent splitting schemes for the Navier-Stokes equations

Fukeng Huang, Jie Shen

SciCADE 2024 Location: S16-03-04 （**Blk S16 Level 3 Room 4**）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS45 Numerical Methods for Quantum Many-Body Problems
Location: **S16-03-04**

10:30am - 11:00am
Adaptive diagonal basis sets for electronic structure theory
Michael Lindsey

11:00am - 11:30am
Density Estimation via Sketching and its Applications in Solving Fokker-Planck Equation
Siyao Yang

11:30am - 12:00pm
Parallel Coordinate Descent Full Configuration Interaction
Weiguo Gao, Yingzhou Li, Yuejia Zhang

12:00pm - 12:30pm
Augmented Lagrangian method for coupled-cluster
Fabian Maximilian Faulstich

3:30pm - 5:30pm

MS31-1 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification
Location: **S16-03-04**

3:30pm - 4:00pm
Learning prediction function of prior measures for statistical inverse problems
Junxiong Jia

4:00pm - 4:30pm
On theoretical understanding of generative distribution learning through the lens of infinite-dimensional statistics
Lin Liu, Ling Guo, Lei Ma, Sihui Zhao

4:30pm - 5:00pm
Deep adaptive sampling for surrogate modeling without labeled data
Kejun Tang

5:00pm - 5:30pm
Deep adaptive density approximation for Fokker-Planck type equations
Li Zeng

Date: Friday, 19/July/2024

10:30am - 11:30am

MS31-2 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification
Location: **S16-03-04**

10:30am - 11:00am
Phase Field Smoothing-PINN: a neural network solver for partial differential equations with discontinuous coefficients
Zihao Yang, Rui He, Jizu Huang, Xiaofei Guan

11:00am - 11:30am
Resolution invariant deep operator network for PDEs with complex geometries
Yue Qiu

SciCADE 2024 Location: S16-03-05/06（**Blk S16 Level 3 Room 5/6**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS19 Recent Advances in Theories and Computations of Liquid Crystals
Location: **S16-03-05/06**

10:30am - 11:00am
Classical density functional theory for colloidal liquid crystals: predicting phase behavior and topological defects from first principles
René Wittmann

11:00am - 11:30am
Quasi-entropy
Jie Xu

11:30am - 12:00pm
From Polyatomic Gas to Liquid Crystals: A Kinetic Approach
Umberto Zerbinati, Patrick E. Farrell, Giovanni Russo

12:00pm - 12:30pm
Recent progress on the hyperbolic Ericksen-Leslie system for liquid crystals
Ning Jiang

3:30pm - 5:30pm

MS05-1 Numerical Methods for Geometric PDEs and Interface Problems
Location: **S16-03-05/06**

3:30pm - 4:00pm
A convergent evolving finite element method with artificial tangential motion for surface evolution under a prescribed velocity field.
Genming Bai

4:00pm - 4:30pm
An ALE meshfree method for surface PDEs coupling with forced mean curvature flow
Xinlong Feng

4:30pm - 5:00pm
Parametric finite element approximation of two-phase Navier–Stokes flow with viscoelasticity
Harald Garcke, Robert Nürnberg, Denni Trautweins

5:00pm - 5:30pm
Including low-dimensional features in 2D surface models
Elena Bachini, Antonia Larese, Mario Putti, Guglielmo Scovazzi

SciCADE 2024 Location: S16-03-05/06（**Blk S16 Level 3 Room 5/6**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS05-2 Numerical Methods for Geometric PDEs and Interface Problems
Location: **S16-03-05/06**

10:30am - 11:00am
Multilevel Representations of Isotropic Gaussian Random Fields on the Sphere
Ana Djurdjevac

11:00am - 11:30am
Numerical analysis of a spectral problem with Ventcel boundary conditions on curved meshes
Joyce Ghantous

11:30am - 12:00pm
Space-time adaptivity for parabolic PDEs on stationary surfaces
Michael Lantelme, Balázs Kovács

12:00pm - 12:30pm
Parametric polynomial preserving recovery on manifolds and its application
Hailong Guo

3:30pm - 6:00pm

MS20-1 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows
Location: **S16-03-05/06**

3:30pm - 4:00pm
A Variational Approach to the Modelling of Evaporating Droplets
Tiezheng Qian

4:00pm - 4:30pm
Mechanics at Nano-Bio interface: Cellular Packing of Flexible Nanomaterials and Membrane Targeting Antimicrobials
Guijin Zou, Xin Yi, Huajian Gao

4:30pm - 5:00pm
Hydrodynamics of a thin film of active nematic fluid
Yakun LI

5:00pm - 5:30pm
Capillary Folding of Thin Elastic Sheets
Zhixuan Li

5:30pm - 6:00pm
Modeling inertial migration of particles in curved duct flow
Brendan Harding

SciCADE 2024 Location: S16-03-05/06（**Blk S16 Level 3 Room 5/6**）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS20-2 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows
Location: **S16-03-05/06**

10:30am - 11:00am

Transformed Model Reduction for Partial Differential Equations with Sharp Inner Layers
Tianyou Tang, Xianmin Xu

11:00am - 11:30am

Efficient methods for interface related optimization problems
Dong Wang

11:30am - 12:00pm

Parametric finite element methods for anisotropic axisymmetric flows
Meng Li

12:00pm - 12:30pm

Numerical investigations on solving surface interface problems
Xufeng Xiao

12:30pm - 1:00pm

Evolving finite element methods with an artificial tangential velocity for mean curvature flow and Willmore flow
Jiashun Hu, Buyang Li

SciCADE 2024 Location: S16-03-05/06（**Blk S16 Level 3 Room 5/6**）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls
Location: **S16-03-05/06**

10:30am - 11:00am
Solving the Real-Time Boltzmann Transport Equation with Adaptive and Multirate Time Integration Methods
Jia Yao, Ivan Maliyov, Carol S. Woodward, David Gardner, Marco Bernardi

---

11:00am - 11:30am
Splitting for low regularity problems
Alexander Ostermann

11:30am - 12:00pm
Numerical integration of the Schödinger equation: Polynomial versus splitting methods
Sergio Blanes

12:00pm - 12:30pm
Wrong solutions for differential systems
Uri Michael Ascher

3:30pm - 5:30pm

MS20-3 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows
Location: **S16-03-05/06**

3:30pm - 4:00pm
Original Energy Dissipation Preserving Exponential Time Differencing Runge--Kutta methods for Phase-field Gradient Flows
Jiang Yang

4:00pm - 4:30pm
Structure-preserving parametric finite element method for some curvature flows with nonlocal terms
Lifang Pei

4:30pm - 5:00pm
A Structure-Preserving Parametric Finite Element Method of Anisotropic Geometric Flows
Yifei Li

5:00pm - 5:30pm
High order in time, BGN-based parametric finite element methods for solving geometric flows
Wei Jiang, Chunmei Su, Ganghui Zhang

Date: Friday, 19/July/2024

10:30am - 11:30am

MS53-2 Surface Evolution and Harmonic Maps
Location: **S16-03-05/06**

10:30am - 11:00am
Numerics of the stochastic Landau-Lifshitz-Gilbert equation
Michael Feischl

11:00am - 11:30am
Stability and Volume Conservation in the Multi-Phase Mullins-Sekerka Problem: A Finite Element Perspective
Tokuhiro Eto

SciCADE 2024 Location: S16-03-07（**Blk S16 Level 3 Room 7**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS55-1 Dynamical Systems, Structure Preservation and Deep Learning
Location: **S16-03-07**

10:30am - 11:00am

Nearest Neighbors GParareal: Improving Scalability of Gaussian Processes for Parallel-in-Time Solvers
Lyudmila Grigoryeva, Guglielmo Gattiglio, Massimiliano Tamborrino

---

11:00am - 11:30am

Neural network aided simulation of ordinary differential equations
Marta Betcke, Priscilla Canizares, Lisa Kreusser, Davide Murari, Ferdia Sherry, Zak Shumaylov

---

11:30am - 12:00pm

Greedy algorithm with randomized dictionaries in application to ReLU^k shallow neural network approximation
Jongho Park, Xiaofeng Xu, Jinchao Xu

12:00pm - 12:30pm

An error bound of PINNs for solving differential equations
Takashi Matsubara, Takaharu Yaguchi

3:30pm - 5:30pm

MS55-2 Dynamical Systems, Structure Preservation and Deep Learning
Location: **S16-03-07**

3:30pm - 4:00pm

Designing Stable Neural Networks using Convex Analysis and ODEs
Ferdia John Sherry, Elena Celledoni, Matthias Joachim Ehrhardt, Davide Murari, Brynjulf Owren, Carola-Bibiane Schönlieb

---

4:00pm - 4:30pm

Stability of numerical methods on Riemannian manifolds with applications to neural networks.
Brynjulf Owren, Elena Celledoni

4:30pm - 5:00pm

Deep learning and oscillatory dynamical systems
Richard Tsai

5:00pm - 5:30pm

Reversible numerical methods in deep learning
Sofya Maslovskaya, Sina Ober-Blöbaum, Christian Offen, Pranav Singh, Boris Wembe

SciCADE 2024 Location: S16-03-07（**Blk S16 Level 3 Room 7**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS55-3 Dynamical Systems, Structure Preservation and Deep Learning
Location: **S16-03-07**

10:30am - 11:00am
A Structure-Preserving Kernel Method for Learning Hamiltonian Systems
Jianyu Hu, Juan-Pablo Ortega, Daiying Yin

11:00am - 11:30am
Kernel-based techniques for the learning of Poisson systems
Jianyu Hu, Juan-Pablo Ortega, Daiying Yin

11:30am - 12:00pm
Multi-Resolution Learning of Partial Differential Equations with Deep Operators and Long Short-Term Memory Networks
Katarzyna Michalowska

12:00pm - 12:30pm
On The Temporal Domain of Differential Equation Inspired Graph Neural Networks
Moshe Eliasof

3:30pm - 6:00pm

MS55-4 Dynamical Systems, Structure Preservation and Deep Learning
Location: **S16-03-07**

3:30pm - 4:00pm
Almost sure convergence of stochastic Hamiltonian descent methods
Måns Williamson

4:00pm - 4:30pm
Geometric Learning with Group Convolutions: PDE-Based Equivariant Neural Networks and Optimal Transport.
Gautam Pai

4:30pm - 5:00pm
Convolving dynamics between scales
James Jackaman

5:00pm - 5:30pm
Stochastic interpolation, score matching and generative models
Eldad Haber

SciCADE 2024 Location: S16-03-07（**Blk S16 Level 3 Room 7**）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS41-1 Machine Learning and Novel Numerical Methods for Dynamical Systems

Location: **S16-03-07**

10:30am - 11:00am

Theoretical Insights into the Structure of SGD Noise

Lei Wu

11:00am - 11:30am

SAV-based optimization methods for the training in deep learning

Zhiping Mao

11:30am - 12:00pm

Gaussian process for parameter estimation in dynamic systems

Hongqiao Wang

12:00pm - 12:30pm

A Minimal Control Family of Dynamical Syetem for Universal Approximation

Yifei Duan, Yongqiang Cai

12:30pm - 1:00pm

Weak Generative Sampler to Efficiently Sample Invariant Distribution of Stochastic Differential Equation

Zhiqiang Cai, Yu Cao, Yuanfei Huang, Xiang Zhou

SciCADE 2024 Location: S16-03-07 (Blk S16 Level 3 Room 7)

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS55-5 Dynamical Systems, Structure Preservation and Deep Learning
Location: **S16-03-07**

10:30am - 11:00am
PiLocNet: Physics-informed neural network on 3D localization with rotating point spread function
Mingda Lu, Zitian Ao, Chao Wang, Sudhakar Prasad, Raymond Chan

---

11:00am - 11:30am
Compositional Physics Informed Neural Network
Pratham Lalwani, Andy Wan

11:30am - 12:00pm
Surrogate Simulations of Charged Particle Dynamics Using Structure-Preserving Neural Networks
Jian Liu

12:00pm - 12:30pm
An attempt to apply particle method for the Cahn-Hilliard equation to preserve some invariant properties
Daisuke Furihata

3:30pm - 5:30pm

MS41-2 Machine Learning and Novel Numerical Methods for Dynamical Systems
Location: **S16-03-07**

3:30pm - 4:00pm
Bridging data and dynamics in single-cell transcriptomics analysis through machine learning
Peijie Zhou

4:00pm - 4:30pm
Thermodynamically Consistent Model Reduction of Polymeric Fluid Dynamics using OnsagerNet
Haijun Yu

4:30pm - 5:00pm
A hybrid adaptive sampling for solving Fokker-Planck equations
Jiayu Zhai

5:00pm - 5:30pm
Functional Tipping Indicators via Schrödinger Bridge
Jin Guo, Ting Gao

Date: Friday, 19/July/2024

10:30am - 11:30am

MS10-2 Recent Advances in Complexity Reduction for High-dimensional Problems
Location: **S16-03-07**

10:30am - 11:00am
High-order parallel time integrators for dynamical low-rank approximation
Jonas Kusch

11:00am - 11:30am
Generalised Petrov-Galerkin Dynamical Low Rank Approximations
Thomas Trigo Trindade, Fabio Nobile

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS50-1 Recent Development of Generative Models in Computational Mathematics and Data Sciences
Location: **S16-03-09**

10:30am - 11:00am
Generalization of DeepONets for Learning Operators Arising from a Class of Singularly Perturbed Problems
Zhongyi Huang

11:00am - 11:30am
Exploring the Optimal Choice for Generative Processes in Diffusion Models
Yu Cao, Jingrun Chen, Yixin Luo, Xiang Zhou

11:30am - 12:00pm
On Asymptotic-Preserving Neural Networks for the Semiconductor Boltzmann Equation
Liu Liu

12:00pm - 12:30pm
A convergent interacting particle method for computing KPP front speeds in random flows
Tan Zhang, Zhongjian Wang, Jack Xin, Zhiwen Zhang

3:30pm - 5:30pm

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems
Location: **S16-03-09**

3:30pm - 4:00pm
Sampling Strategies in Sparse Bayesian Inference
Yiqiu Dong

4:00pm - 4:30pm
Neural Expectation Maximization for Self-supervised Blind Image Deblurring
Ji Hui

4:30pm - 5:00pm
PDEformer: Towards a Foundation Model for Solving Parametric PDEs and Beyond
Bin Dong

5:00pm - 5:30pm
Bi-modality Images Transfer with a Discrete Process Matching Method
Zhe Xiong, Qiaoqiao Ding, Xiaoqun Zhang

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS50-2 Recent Development of Generative Models in Computational Mathematics and Data Sciences
Location: **S16-03-09**

10:30am - 11:00am
Structure-preserving generative models and their statistical guarantees
Wei Zhu

11:00am - 11:30am
Convex Relaxation for Fokker-Planck
Yian Chen, Yuehaw Khoo, Lek-Heng Lim

11:30am - 12:00pm
Probabilistic Forecasting with Stochastic Interplants and Follmer Processes
Yifan Chen

12:00pm - 12:30pm
Randomized methods for computing optimal transport without regularization and their convergence analysis
Yue Xie, Zhongjian Wang, Zhiwen Zhang

3:30pm - 6:00pm

MS11-1 Recent Advances in Scientific Computing and Learning
Location: **S16-03-09**

3:30pm - 4:00pm
Fast Butterfly-compressed Hadamard-Babich Integrator for High-Frequency Helmholtz Equations in Inhomogeneous Media
Jianliang Qian, Yang Liu, Jian Song, Robert Burridge

4:00pm - 4:30pm
Fast minimization for curvature based regularization models based on bilinear decomposition
Huibin Chang

4:30pm - 5:00pm
Mathematical and numerical study of the signal-propagation problem in axon
Tao Yin

5:00pm - 5:30pm
Deep neural networks with mathematical background for image segmentation
Hao Liu

5:30pm - 6:00pm
Well-posedness and numerical analysis of a class of hemivariational inequalities governed by fluid-fluid coupled flow
Feifei Jing

SciCADE 2024 Location: S16-03-09 (Blk S16 Level 3 Room 9)

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS11-2 Recent Advances in Scientific Computing and Learning
Location: **S16-03-09**

10:30am - 11:00am

Phase field topology optimization in 3D and 4D printing

Harald Garcke, Kei Fong Lam, Robert Nurnberg, Andrea Signori

11:00am - 11:30am

Wasserstein Hamiltonian Flow and Its Structure Preserving Numerical Schemes.

Jianbo Cui

11:30am - 12:00pm

Spherical Essentially Non-Oscillatory (SENO) Interpolation

Shingyu Leung

12:00pm - 12:30pm

Convergence Analysis of Nonlinear Kaczmarz Method for Systems of Nonlinear Equations with Component-wise Convex Mapping

Chong Chen

12:30pm - 1:00pm

Efficient threshold dynamics methods for topology optimization for fluids and heat transfer problems

Huangxin Chen

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS11-3 Recent Advances in Scientific Computing and Learning
Location: **S16-03-09**

10:30am - 11:00am
Fast and accurate solvers for three dimensional wave scattering problems
Jun Lai

11:00am - 11:30am
Rigidity of PDE operators on model identification from scarce data
Roy Yuchen He

11:30am - 12:00pm
Numerical Algorithms for Inverse Spectral Problems Based on Trace Formulas
Xiang Xu

12:00pm - 12:30pm
Modeling Randomness Effects in High-Entropy Alloys
Luchan Zhang

3:30pm - 5:30pm

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems
Location: **S16-03-09**

3:30pm - 4:00pm
Moving Sampling Physics-informed Neural Networks induced by Moving Mesh PDE
Qiaolin He

4:00pm - 4:30pm
High order asymptotic computations for the Dirichlet eigenvalue problem in perforated domain with multiscale cavities.
Qiang Ma

4:30pm - 5:00pm
A Framework for Generalization Analysis of Machine-Learned Interatomic Potentials: A Case Study on Crystalline Defects
Yangshuai Wang

5:00pm - 5:30pm
Automated discovery of fundamental variables hidden in experimental data
Kuang Huang

Date: Friday, 19/July/2024

10:30am - 11:30am

MS51 Recent Trends in Stabilized FE Methods for Fluid Flows
Location: **S16-03-09**

10:30am - 11:00am
Variational Multiscale FEM for Cahn-Hillard-Navier-Stokes Model
Anil Rathi, B. V. Rathish Kumar

11:00am - 11:30am
Variational multiscale Stabilized FEM for unified FSI model
DIPAK KUMAR SAHOO, B V RATHISH KUMAR

SciCADE 2024 Location: S17-04-04（**Blk S17 Level 4 Seminar Room 3**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS02 Advances in Markov chain Sampling Methods
Location: **S17-04-04**

10:30am - 11:00am
Non-reversible guided Metropolis kernel
Kengo Kamatani, Xiaolin Song

11:00am - 11:30am
Optimistic Estimation of Convergence in Markov Chains with the Average Mixing Time
Geoffrey Wolfer, Pierre Alquier

11:30am - 12:00pm
Importance Sampling for Rare Event Tracking in Ensemble Kalman Filters
Nadhir Ben Rached, Erik von Schwerin, Gaukhar Shaimerdenova, Raúl Tempone

---

12:00pm - 12:30pm
Predictive Resampling for Martingale Posteriors
Edwin Fong

3:30pm - 5:30pm

MS47 Recent Advances in Numerical Homogenization
Location: **S17-04-04**

3:30pm - 4:00pm
An efficient exponential integrator for generalized multiscale finite element methods
Eric Chung

4:00pm - 4:30pm
Reliable coarse-scale approximation of spatial network models
Moritz Hauck, Axel Målqvist, Roland Maier

4:30pm - 5:00pm
Wavelet-based Edge Multiscale Parareal Algorithm for subdiffusion equations with heterogeneous coefficients in a large time domain
Guanglian Li

5:00pm - 5:30pm
Numerical Methods for Multiscale Equations with Discontinuous Coefficients
Chen Hui Pang, Viet Ha Hoang

SciCADE 2024 Location: S17-04-04（**Blk S17 Level 4 Seminar Room 3**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS23-1 Modeling and Simulations for Multiphase Interface Problem
Location: **S17-04-04**

10:30am - 11:00am
Multiscale topology optimization method for lattice materials
Yibao Li, Binhu Xia

11:00am - 11:30am
A novel steepness-adjustable harmonic volume-of-fluid method for interface capturing
Weidan Ni, Qinghong Zeng, Yucang Ruan, Zhiwei He

11:30am - 12:00pm
Decoupled multiscale finite element methods for the Stokes-Darcy model
Haibiao Zheng

12:00pm - 12:30pm
Structure preserving primal dual methods for free interface dynamics as gradient flows with respect to transport distances
Chaozhen Wei

3:30pm - 6:00pm

MS23-2 Modeling and Simulations for Multiphase Interface Problem
Location: **S17-04-04**

3:30pm - 4:00pm
A fourth-order kernel-free boundary integral method for variable coefficients elliptic PDEs
Yaning Xie

4:00pm - 4:30pm
Three-layer Hele-Shaw problem driven by a sink
Meng Zhao

4:30pm - 5:00pm
Exploring Cancer Mechanisms: Mechanical and Chemical Interactions in Tumor Growth
Min-Jhe Lu

5:00pm - 5:30pm
A Cartesian grid method for nonhomogeneous elliptic interface problems on unbounded domains
Wenjun Ying

5:30pm - 6:00pm
A parameter-free staggered-grid Lagrangian scheme for two-dimensional compressible flow problems
Xihua Xu

SciCADE 2024 Location: S17-04-04（Blk S17 Level 4 Seminar Room 3）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS30-1 Advanced Numerical Methods for CFD with Applications
Location: **S17-04-04**

10:30am - 11:00am
Robust and Efficient Unstructured Finite Volume Method for Compressible Flow Simulations
Xiaoquan Yang, Jia Yan, Jue Ding

11:00am - 11:30am
A mechanism-informed reinforcement learning framework for shape optimization of airfoils
Jingfeng Wang, Guanghui Hu

11:30am - 12:00pm
A compact fully-discrete high-order schemes for complex flow simulation
Shucheng Pan, Tong Zhou

12:00pm - 12:30pm
A discontinutiy feedback factor for compressible flow simulation
Xing Ji

12:30pm - 1:00pm
Numerical Simulation of High Enthalpy Flows using Gas-Kinetic Scheme with Multi-Temperature Model
Hualin Liu, Xing Ji

SciCADE 2024 Location: S17-04-04 (Blk S17 Level 4 Seminar Room 3)

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS22 Stochastic Numerics with Applications to Sampling
Location: **S17-04-04**

10:30am - 11:00am
Unbiased Kinetic Langevin Monte Carlo Methods
Neil Kumar Chada, Benedict Leimkuhler, Daniel Paulin, Peter Whalley

---

11:00am - 11:30am
Enhanced Gradient Flows of Parameters and Probability Measures for Statistical Inference
Sam Power, Rocco Caprio, Adam Johansen, Jen Ning Lim, Juan Kuntz

---

11:30am - 12:00pm
Application of the Hopf algebra structures of exotic aromatic series to stochastic numerical analysis
Adrien Laurent, Eugen Bronasco

12:00pm - 12:30pm
Collective Behavior in Interacting Particle Systems
Benedict Leimkuhler, René Lohmann, Greg Pavliotis, Peter Whalley

3:30pm - 5:30pm

MS30-2 Advanced Numerical Methods for CFD with Applications
Location: **S17-04-04**

3:30pm - 4:00pm
A staggered Lagrangian MHD method based on subcell Riemann solver
Zhijun Shen

4:00pm - 4:30pm
Physical-constraint-preserving high-order DG method for compressible multi-medium flows
Fan Zhang

4:30pm - 5:00pm
Multiple-GPU accelerated high-order gas-kinetic scheme for direct numerical simulation of compressible turbulence
Liang Pan

5:00pm - 5:30pm
Multi-scale finite element method (MsFEM) for incompressible flows
Loïc Balazi, Grégoire Allaire, Pascal Omnes

Date: Friday, 19/July/2024

10:30am - 11:30am

MS30-3 Advanced Numerical Methods for CFD with Applications
Location: **S17-04-04**

10:30am - 11:00am
High-fidelity simulation based on multi-moment finite volume method on hybrid unstructured grids
Bin Xie, Feng Xiao

11:00am - 11:30am
Advanced computing process in HODG framework
Kun Wang, Tiegang Liu

SciCADE 2024 Location: S17-04-05（**Blk S17 Level 4 Seminar Room 2**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations
Location: **S17-04-05**

10:30am - 11:00am
On the Euler method for stochastic delay differential equations
Dimitri Breda, Stefano Maset

11:00am - 11:30am
Regularity and numerics for fractional stochastic elliptic PDEs on graphs
David Bolin, Mihály Kovács, Vivek Kumar, Alexandre B. Simas

11:30am - 12:00pm
Sparse identification of stochastic delay differential equations
Dimitri Breda, Dajana Conte, Raffaele D'Ambrosio, Muhammad Tanveer, Ida Santaniello

---

12:00pm - 12:30pm
Unified Framework for Momentum Stochastic Gradient Descent: Insights from Linear Multistep Methods
Qian Guo

3:30pm - 5:30pm

MS26-1 Dynamical Low Rank Approximation: From Theory to Applications
Location: **S17-04-05**

3:30pm - 4:00pm
An overview of dynamical low-rank techniques for hyperbolic problems
Lukas Einkemmer

4:00pm - 4:30pm
Dynamical Low-Rank Approximation of SDEs
Yoshihito Kazashi, Fabio Nobile, Fabio Zoccolan

4:30pm - 5:00pm
Semi-Implicit Dynamical Low Rank Approximation: Convergence to Equilibrium
Stefan Schnake, Eirik Endeve, Cory Hauck, Peiming Yin

5:00pm - 5:30pm
Dynamical low-rank tensor methods for quantum simulations
Dominik Sulz, Christian Lubich, Gianluca Ceruti, Jonas Kusch

SciCADE 2024 Location: S17-04-05（**Blk S17 Level 4 Seminar Room 2**）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS26-2 Dynamical Low Rank Approximation: From Theory to Applications
Location: **S17-04-05**

10:30am - 11:00am
Dynamical low-rank approximation accelerated by the discrete empirical interpolation method
Benjamin Carrel, Bart Vandereycken

11:00am - 11:30am
Neural Network Training with Dynamical Low-Rank Inspired Optimizers
Steffen Schotthoefer, Jonas Kusch, Gianluca Ceruti, Emanuele Zangrando, Francesco Tudisco

---

11:30am - 12:00pm
Multi-level dynamical low-rank approximations for stochastic problems in radiation therapy
Pia Katharina Stammer, Jonas Kusch, Danny Lathouwers, Chinmay Patwardhan, Niklas Wahl

---

12:00pm - 12:30pm
Parametric PDEs and low-rank approximation of function-valued matrices
Stanislav Budzinskiy

12:30pm - 1:00pm
Cost-Effective Time Integration of Nonlinear Tensor Differential Equations on Low-Rank Tucker Tensor and Tensor Train Manifolds
Behzad Ghahremani, Hessam Babaee

3:30pm - 6:00pm

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications
Location: **S17-04-05**

3:30pm - 4:00pm
Machine Learning and Seismic Tomography
Xu Yang

4:00pm - 4:30pm
A class of second-order dissipative hyperbolic PDEs and their applications in variational problems
Guozhi Dong

4:30pm - 5:00pm
Seismic tomography with random batch gradient reconstruction
Yixiao Hu, Lihui Chai, Xu Yang, Zhongyi Huang

5:00pm - 5:30pm
Scalable Iterative Data-Adaptive RKHS Regularization
Haibo Li, Jinchao Feng, Fei Lu

5:30pm - 6:00pm
Adjoint method for elliptically anisotropic wave equations with application in medical and seismic imaging
Ping Tong

SciCADE 2024 Location: S17-04-05（**Blk S17 Level 4 Seminar Room 2**）

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS35-1 Discretization Methods Involving Multiple Levels and Scales
Location: **S17-04-05**

10:30am - 11:00am
Error bounds for discrete minimizers of the Ginzburg-Landau energy in the high-κ regime
Benjamin Dörich, Patrick Henning

11:00am - 11:30am
A multicale generalized FEM based on locally optimal spectral approximations for high-frequency wave problems
Chupeng Ma, Christian Alber, Robert Scheichl

11:30am - 12:00pm
Hierarchical Super-Localized Orthogonal Decomposition Methods for Multiscale Elliptic Problems
José Carlos Garay, Hannah Mohr, Daniel Peterseim

12:00pm - 12:30pm
Information Geometric Regularization of the Barotropic Euler Equation
Ruijia Cao, Florian Schaefer

12:30pm - 1:00pm
Numerical homogenization of nondivergence-form PDEs in a Cordes framework
Timo Sprekeler

SciCADE 2024 Location: S17-04-05（**Blk S17 Level 4 Seminar Room 2**）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS34 Computational Techniques for Bayesian Data Assimilation
Location: **S17-04-05**

10:30am - 11:00am
Ensemble Kalman Inversion in high dimension
Xin Tong

11:00am - 11:30am
Tensor-Train Methods for Sequential State and Parameter Estimation in State-Space Models
Tiangang Cui, Yiran Zhao

11:30am - 12:00pm
Ensemble Kalman Filtering Meets Gaussian Process State-Space Models
Zhidi Lin

12:00pm - 12:30pm
Convergence rates of non-stationary and deep Gaussian process regression
Conor Moriarty-Osborne, Aretha Teckentrup

3:30pm - 5:30pm

MS27 SDE Methods and Data Science Applications
Location: **S17-04-05**

3:30pm - 4:00pm
Wasserstein convergence and bias estimates for kinetic Langevin integrators
Peter Archibald Whalley

4:00pm - 4:30pm
Sampling on manifolds via SDEs
Karthik Bharath, Alexander Lewis, Akash Sharma, Michael Tretyakov

---

4:30pm - 5:00pm
On the ergodicity and sharp error estimates of the stochastic gradient Langevin dynamics
Lei Li, Jian-Guo Liu, Yuliang Wang

5:00pm - 5:30pm
Wasserstein Convergence Guarantees for a General Class of Score-Based Generative Models
Xuefeng Gao

Date: Friday, 19/July/2024

10:30am - 11:30am

MS35-2 Discretization Methods Involving Multiple Levels and Scales
Location: **S17-04-05**

10:30am - 11:00am
Solving Jump-Coefficient Problems with High Accuracy Using Immersed Three-Field Formulation
Michał Wichrowski

11:00am - 11:30am
Homogeneous multigrid for hybrid discretizations: application to HHO methods
Daniele A. Di Pietro, Zhaonan Dong, Guido Kanschat, Peipei Lu, Pierre Matalon, Andreas Rupp

SciCADE 2024 Location: S17-05-11 (**Blk S17 Level 5 Seminar Room 5**)

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS43-1 Mathematical Methods for Scientific Machine Learning
Location: **S17-05-11**

10:30am - 11:00am
Convergence of the Randomized Kaczmarz Algorithm in Hilbert Spaces
Xin Guo, Junhong Lin, Dingxuan Zhou

11:00am - 11:30am
Classification with Deep Neural Networks
Lei Shi

11:30am - 12:00pm
Ensemble Kalman filtering for epistemic uncertainty
Chatchuea Kimchaiwong, Jeremie Houssineau, Adam Johansen

12:00pm - 12:30pm
Deterministic Sampling Algorithms
Colin Fox, Li-Jen Hsiao, Jeong-Eun {Kate} Lee

3:30pm - 5:30pm

MS43-2 Mathematical Methods for Scientific Machine Learning
Location: **S17-05-11**

3:30pm - 4:00pm
Adaptive Finite Element Interpolated Neural Networks
Santiago Badia, Wei Li, Alberto F. Martin

4:00pm - 4:30pm
Interplay between Machine Learning and Optimisation via Algorithmic Stability
Yiming Ying

4:30pm - 5:00pm
Global Well-posedness and Convergence Analysis of Score-based Generative Models via Sharp Lipschitz Estimates
Zhongjian Wang

5:00pm - 5:30pm
Nonparametric Distribution Learning via Neural ODEs
Jakob Zech

SciCADE 2024 Location: S17-05-11 (Blk S17 Level 5 Seminar Room 5)

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning
Location: **S17-05-11**

10:30am - 11:00am
Learning of Lagrangian odes and pdes from data with UQ
Christian Offen

11:00am - 11:30am
Time Series-Aware Structure-Preserving Neural Networks
Benedikt Brantner

11:30am - 12:00pm
Generalized Hamiltonian Neural Networks for Parameter-dependent Hamiltonian Systems
Philipp Horn, Barry Koren

12:00pm - 12:30pm
Autoencoders for structure-preserving model reduction of stochastic Hamiltonian systems
Tomasz Michal Tyranowski

3:30pm - 6:00pm

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning
Location: **S17-05-11**

3:30pm - 4:00pm
Numerics on regualarization by noise
Chengcheng Ling

4:00pm - 4:30pm
Optimal rate of convergence for approximations of nonlinear SPDEs with additive space-time white noise
Helena Katharina Kremp

4:30pm - 5:00pm
Primal and dual optimal stopping with signatures
Christian Bayer, Luca Pelizzari, John Schoenmakers

5:00pm - 5:30pm
A multiplicative surface signature through its Magnus expansion
Joscha Diehl, Ilya Chevyrev, Kurusch Ebrahimi-Fard, Nikolas Tapia

SciCADE 2024 Location: S17-05-11 (**Blk S17 Level 5 Seminar Room 5**)

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS12-1 Recent Advances in Inverse Problems and Imaging
Location: **S17-05-11**

10:30am - 11:00am

A priori bounds and a reconstruction method for scattering and inverse scattering by random structures
Gang Bao, Yiwen Lin, Tianjiao Wang, Xiang Xu

11:00am - 11:30am

Inverse scattering with multi-frequency sparse data
Xiaodong Liu

11:30am - 12:00pm

Mathematical Theory for Electromagnetic Scattering Resonances and Field Enhancement in a Subwavelength Annular Gap
Wangtao Lu

12:00pm - 12:30pm

The forward and inverse problems for the time-domain wave equation in three dimensions
Haibing Wang

12:30pm - 1:00pm

Deep decomposition method for the limited aperture inverse obstacle scattering problem
Yunwen Yin, Liang Yan

SciCADE 2024 Location: S17-05-11 (**Blk S17 Level 5 Seminar Room 5**)

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS10-1 Recent Advances in Complexity Reduction for High-dimensional Problems
Location: **S17-05-11**

10:30am - 11:00am
Regularized dynamical parametric approximation
Christian Lubich, Caroline Lasser, Joerg Nick, Michael Feischl

---

11:00am - 11:30am
Dynamical approximation and sensor placement for the state estimation of transport problems
Cecilia Pagliantini, Olga Mula, Federico Vismara

11:30am - 12:00pm
Sparse grid techniques for particle-in-cell simulation of kinetic plasmas
Lee Forrest Ricketson

12:00pm - 12:30pm
A hierarchical low-rank algorithm for the kinetic chemical master equation
Lukas Einkemmer, Julian Mangott, Martina Prugger

3:30pm - 5:30pm

MS32 Advances on Numerical Methods for Singular Perturbation Problems
Location: **S17-05-11**

3:30pm - 4:00pm
Error Analysis of Weak Galerkin FEM for Singularly Perturbed Fourth–order Parabolic PDEs
Natesan Srinivasan, Aayushman Raina

4:00pm - 4:30pm
Numerical solution for singularly perturbed time-delayed parabolic problems involving two small parameters
Jugal Mohapatra, Sushree Priyadashana

4:30pm - 5:00pm
On simple numerical scheme for interface problem
Shuo Zhang

5:00pm - 5:30pm
Fractal cubic spline method for nonself-adjoint singularly perturbed boundary-value problems
Guru Prem Prasad Mahalingam, Balasubramani N, Natesan S

Date: Friday, 19/July/2024

10:30am - 11:30am

MS12-2 Recent Advances in Inverse Problems and Imaging
Location: **S17-05-11**

10:30am - 11:00am
Some results for the equivalent characterization of non-radiating sources
Jue Wang

11:00am - 11:30am
Obstacle scattering and inverse scattering in complex backgrounds
Lei Zhang

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS54-1 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

10:30am - 11:00am
Nondegenerate N-soliton solutions for coupling PDEs
Ji Lin

11:00am - 11:30am
Some New Results on Integrable Integro-differential Equations
XingBiao Hu

11:30am - 12:00pm
Symmetry study of a novel integrable supersymmetric dispersionless system
Man Jia

12:00pm - 12:30pm
The general rogue wave patterns of nonlinear Schrödinger equation
Liming Ling

3:30pm - 5:30pm

MS54-2 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

3:30pm - 4:00pm
Localized waves solutions of the massive Thirring model via bilinear KP-hierarchy reduction and PINN deep learning
Junchao Chen

4:00pm - 4:30pm
Lax pairs informed neural networks solving integrable systems.
Yong Chen

4:30pm - 5:00pm
The spatial structure, discrete solitons and stability analysis of the non-integrable discrete Hirota equation
LiYuan Ma

5:00pm - 5:30pm
Darboux transformation of generalized Camassa-Holm equation
Lin Luo

SciCADE 2024 *Location:* S17-05-12 (**Blk S17 Level 5 Seminar Room 4**)

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS54-3 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

10:30am - 11:00am
Applications of non-intersecting paths to integrable systems
Shi-Hao Li

11:00am - 11:30am
Analytic and numerical aspects of Novikov-type equations and their multipeakons
Xiang-Ke Chang

11:30am - 12:00pm
On the Coupled Modified Complex Short Pulse Equation
Hongqian Sun, Shoufeng Shen, Zuonong Zhu

12:00pm - 12:30pm
Solutions to semi-discrete integrable equations on theta-function periodic backgrounds
Ruomeng Li

3:30pm - 6:00pm

MS17-1 Recent Advances in Structure Preserving Numerical Methods
Location: **S17-05-12**

3:30pm - 4:00pm
Unconditionally energy-stable algorithms for porous media flow: From the Darcy scale to the Pore Scale
Shuyu Sun

4:00pm - 4:30pm
Deep adaptive density approximation for Fokker-Plank type equations
Tao Zhou

4:30pm - 5:00pm
A nonconventional stability analysis for a Crank-Nicolson scheme solving degenerate quenching equations
Qin Sheng

5:00pm - 5:30pm
Data Augmentation for Neural Operator-Based PDE Solvers through Inverse Evolution
Chaoyu Liu

5:30pm - 6:00pm
Functional Equivariance and Modified Vector Fields
Sanah Suri

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS17-2 Recent Advances in Structure Preserving Numerical Methods
Location: **S17-05-12**

10:30am - 11:00am

Recent progress on topology optimization
Xiaoping Wang

11:00am - 11:30am

Operator splitting schemes for port-Hamiltonian differential-algebraic equations
Michael Günther, Andreas Bartel, Andreas Frommer, Malak Diab, Nicole Marheineke

---

11:30am - 12:00pm

Exponential time differencing-Padé finite element method for nonlinear convection diffusion reaction equations with time constant delay
Qiumei Huang

12:00pm - 12:30pm

Convergence analysis of a positivity-preserving numerical scheme for the Cahn-Hilliard-Stokes system with Flory-Huggins energy potential
Yunzhuo Guo, Cheng Wang, Steven M. Wise, Zhengru Zhang

12:30pm - 1:00pm

Energy stable and maximum bound principle preserving schemes for the Q-tensor flow of liquid crystals
Zhonghua Qiao

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS54-4 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

10:30am - 11:00am
Application of tetragonal curves to coupled Boussinesq equations
Xianguo Geng

11:00am - 11:30am
Dynamics of higher-order peaked and smooth solitary waves
Xiaochuan Liu

11:30am - 12:00pm
New revival phenomena for the Kadomtsev-Petviashvili equation
Jing Kang

12:00pm - 12:30pm
Dubrovin-Frobenius manifolds and the extended Weyl group of type B
Dafeng Zuo

3:30pm - 5:30pm

MS54-5 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

3:30pm - 4:00pm
On the coupled Sasa-Satsuma equation
Bao-Feng Feng, Chengfa Wu

4:00pm - 4:30pm
Large genus asymptotics for a class of enumerative invariants
Di Yang

4:30pm - 5:00pm
Darboux transformations for the nonlinear Schrodinger and derivative nonlinear Schrodinger type systems
Zhiwei Wu

5:00pm - 5:30pm
Solitons in the integrable and nearly-integrable fractional nonlinear wave equations
Zhenya Yan

Date: Friday, 19/July/2024

10:30am - 11:30am

MS54-6 Theoretical and Numerical Aspects of Integrable Systems
Location: **S17-05-12**

10:30am - 11:00am
Asymptotics of the integrable equations with WKI-type spectral problem
Jian Xu

11:00am - 11:30am
Some properties of spatially discrete Boussinesq hierarchy and their continuous counterparts
Haiqiong Zhao

SciCADE 2024 Location: S17-06-11（**Blk S16 Level 6 Seminar Room 6**）

Date: Monday, 15/July/2024

10:30am - 12:30pm

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations
Location: **S17-06-11**

10:30am - 11:00am
Kernel methods for solving rough nonlinear partial differential equations
Ricardo Baptista, Edoardo Calvello, Matthieu Darcy, Houman Owhadi, Andrew Stuart, Xianjin Yang

---

11:00am - 11:30am
"The Mean-Field Ensemble Kalman Filter: From Analysis to Algorithms"
Edoardo Calvello

11:30am - 12:00pm
A Budgeted Multi-Level Monte Carlo Method for Estimates on the Full Spatial Domain
Niklas Baumgarten

12:00pm - 12:30pm
Multilevel Monte Carlo Methods with Smoothing
Anastasia Istratuca, Aretha Teckentrup

3:30pm - 5:30pm

MS40-1 Iterative Numerical Methods for Optimization and Control
Location: **S17-06-11**

3:30pm - 4:00pm
Saddle Point Preconditioners for PDE-constrained optimisation: a case study from Data assimilation
Jemima M. Tabeart, John W. Pearson

4:00pm - 4:30pm
Solving tree-coupled linear systems
Christoph Hansknecht

4:30pm - 5:00pm
Parallel-in-time Preconditioner for Parabolic Optimal Control Problems
Po Yin Fung, Sean Hon

5:00pm - 5:30pm
A Diagonalization-Based Parallel-in-Time Preconditioner for Instationary Flow Control Problems
Bernhard Heinzelreiter, John Pearson

SciCADE 2024 Location: S17-06-11（Blk S16 Level 6 Seminar Room 6）

Date: Tuesday, 16/July/2024

10:30am - 12:30pm

MS40-2 Iterative Numerical Methods for Optimization and Control
Location: **S17-06-11**

10:30am - 11:00am
Non-smooth shape optimization with applications for fluid-mechanical problems under uncertainty
Tim Suchan, Caroline Geiersbach, Volker Schulz, Kathrin Welker

---

11:00am - 11:30am
Multi-level Optimal Control with Neural Surrogate Models
Estefania Loayza Romero, Dante Kalise, Kirsten A. Morris, Zhengang Zhong

---

11:30am - 12:00pm
Transformers Meet Image Denoising: Mitigating Over-smoothing in Transformers via Regularized Nonlocal Functionals
Tam Nguyen, Tan Minh Nguyen, Richard Baraniuk

12:00pm - 12:30pm
Self isolation or social distancing: a nonlocal PDE-constrained optimisation approach for disease containment
Andrés Miniguano-Trujillo

3:30pm - 6:00pm

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models
Location: **S17-06-11**

3:30pm - 4:00pm
Mathematical and numerical modelling of multi-component diffusion
Jan ten Thije Boonkkamp, Jan van Dijk

4:00pm - 4:30pm
Complete Flux Scheme for time Fractional ADR Equation
Rinki Rawat, Chitranjan Pandey, B.V. Rathish Kumar, J.H.M ten Thije Boonkkamp

---

4:30pm - 5:00pm
A complete flux scheme for anisotropic advection-diffusion equations
Hanz Martin Cheng, Jan ten Thije Boonkkamp

5:00pm - 5:30pm
Finite volume Complete Flux Scheme for the Incompressible Navier-Stokes Equations
Chitranjan Pandey, J.H.M ten Thije Boonkkamp, B.V. Rathish Kumar

---

5:30pm - 6:00pm
A Novel Finite Volume Complete-Flux Scheme for Boussinesq Model
B.V. Rathish Kumar, Chitranjan Pandey, Thije Boonkkamp, . Jan ten

Date: Wednesday, 17/July/2024

10:30am - 1:00pm

MS49-1 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations
Location: **S17-06-11**
Chair: **Hui Liang**

10:30am - 11:00am

Numerical solution of fractional integro-differential equations with singularities

Kaido Latt, **Arvet Pedas**

11:00am - 11:30am

A collocation method based on central part interpolation for fractional integro-differential equations

Mikk Vikerpuur

11:30am - 12:00pm

Implicitly linear Jacobi spectral-collocation methods for two-dimensional weakly singular Volterra-Hammerstein integral equations

Qiumei Huang, **Huiting Yang**

12:00pm - 12:30pm

Multiscale Model Reduction for Heterogeneous Perforated Domains based on CEM-GMsFEM

Yin Yang, **Wei Xie**, **Yunqing Huang**, **Eric Chung**

12:30pm - 1:00pm

An efficient second-order discontinuous finite volume element scheme for the three-dimensional neutron transport equations

Yanni Gao, **Xueding Hang**, **Guangwei Yuan**

SciCADE 2024 Location: S17-06-11（Blk S16 Level 6 Seminar Room 6）

Date: Thursday, 18/July/2024

10:30am - 12:30pm

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering
Location: **S17-06-11**

10:30am - 11:00am
Theories and applications for multi-layered medium
Youjun Deng

11:00am - 11:30am
A novel Newton method for inverse elastic scattering problems
Yan Chang, Yukun Guo, Hongyu Liu, Deyue Zhang

11:30am - 12:00pm
Computational imaging of small-amplitude biperiodic surfaces with double negative material
Yuliang Wang

12:00pm - 12:30pm
Inverse medium problems with single measurement
Shiqi Ma

3:30pm - 5:30pm

MS09 Theory and Numerics of Inverse Problems
Location: **S17-06-11**

3:30pm - 4:00pm
A novel quantitative inverse scattering scheme using interior resonant modes
Xianchao Wang

4:00pm - 4:30pm
Inverting the local transverse and mixed ray transforms
Jian Zhai

4:30pm - 5:00pm
Reconstruction of acoustic sources from multi-frequency phaseless far-field data
Sun Fenglin

5:00pm - 5:30pm
Fractional random walks on graphs
Giovanni Covi

Date: Friday, 19/July/2024

10:30am - 11:30am

MS49-2 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations
Location: **S17-06-11**
Chair: **Qiumei Huang**

10:30am - 11:00am
Solving fractional differential equations in unbounded domains via rational approximation
Huifang Yuan

11:00am - 11:30am
A general collocation analysis for weakly singular Volterra integral equations with variable exponent
Hui Liang, Martin Stynes

Book of Abstracts

Contents

Part I Plenary Lectures

Title: Adaptive Mesh Refinement: Algorithms and Applications

Speaker: Ann ALMGREN, Lawrence Berkeley National Laboratory, USA

Abstract: Adaptive mesh refinement (AMR) is one of several techniques for dynamically modifying the spatial resolution of a simulation in particular regions of the spatial domain. Block-structured AMR specifically refines the mesh by defining locally structured regions with finer spatial, and possibly temporal, resolution. This combination of locally structured meshes within an irregular global hierarchy is in some sense the best of both worlds in that it enables regular local data access while enabling greater flexibility in the overall computation.

Originally, block-structured AMR was designed for solving hyperbolic conservation laws with explicit time-stepping; in this case the changes to solution methodology in transforming a single-level solver to an AMR-based solver are relatively straightforward. AMR has come a long way, however, and the more complex the simulation, the more complex the changes required to effectively use AMR. One can even consider whether to use different physical models at different levels of resolution. In this talk I will give an overview of block-structured AMR for different types of applications and will focus on a few key exemplars for how to think about adaptivity for multiphysics simulations.

Biography: Ann Almgren is a Senior Scientist and the Department Head of the Applied Mathematics Department in the Applied Mathematics and Computational Research (AMCR) Division of Lawrence Berkeley National Laboratory. Her primary research interest is in computational algorithms for solving partial differential equations (PDEs) in a variety of application areas. Her current projects include the development and implementation of new multiphysics algorithms in high-resolution adaptive mesh codes that are designed for the latest hybrid architectures. She is a SIAM Fellow, the Deputy Director of the ECP AMReX Co-Design Center, and serves on the editorial boards of CAMCoS and IJHPCA. In 2023 she was awarded the LBNL Director's Award for Exceptional Scientific Achievement. Prior to coming to LBL she worked at the Institute for Advanced Study in Princeton, NJ, and at Lawrence Livermore National Lab.

Title: Deep Learning of Diffeomorphisms with Application to Shape Analysis

Speaker: Elena CELLEDONI, Norwegian University of Science and Technology, Norway

Abstract: In this talk we discuss structure preservation and deep learning with applications to shape analysis. This is a framework for treating complex data and obtain metrics on spaces of data. Examples are spaces of unparametrized curves, time-signals, surfaces and images. A computationally demanding task for estimating distances between shapes, e.g. in object recognition, is the computation of optimal reparametrizations. This is an optimisation problem on the infinite dimensional group of orientation preserving diffeomorphisms.

We approximate diffeomorphisms with neural networks and use the optimal control and dynamical systems point of view to deep learning. We will discuss useful geometric properties in this context e.g. reparametrization invariance of the distance function, invertibility and contractivity of the neural networks. We will consider theory and applications of these ideas.

Biography: Elena Celledoni is a professor at the Department of Mathematical Sciences at the Norwegian University of Science and Technology (NTNU). She completed her undergraduate studies at the University of Trieste, Italy and her PhD at the University of Padua, Italy. She was a postdoctoral fellow at Department of Applied Mathematics and Theoretical Physics, Cambridge, UK, at the Mathematical Sciences Research Institute, Berkeley, California and at NTNU. She works on numerical analysis of differential equations and in particular the theory and applications of structure preserving algorithms. These methods are of use in industry for the simulation and control of rigid body dynamics, of slender structures, and of mechanical systems in general. She is also interested in the analysis and design of neural networks and their interplay with numerical analysis. This includes methods of shape analysis on Lie groups applied to activity recognition, with techniques both for curves and surfaces.

Title: Learning, approximation and control

Speaker: Qianxiao LI, National University of Singapore, Singapore

Abstract: In this talk, we discuss some interesting problems and recent results on the interface of deep learning, approximation theory and control theory. Through a dynamical system viewpoint of deep residual architectures, the study of model complexity in deep learning can be formulated as approximation or interpolation problems that can be studied using control theory, but with a mean-field twist. In a similar vein, training deep architectures can be formulated as optimal control problems in the mean-field sense. We provide some basic mathematical results on these new control problems that so arise, and discuss some applications in improving efficiency, robustness and adaptability of deep learning models.

Biography: Qianxiao Li is an assistant professor in the Department of Mathematics, and a principal investigator in the Institute for Functional Intelligent Materials, National University of Singapore.

He graduated with a BA in mathematics from the University of Cambridge and a PhD in applied mathematics from Princeton University.

His research interests include the interplay of machine learning and dynamical systems, control theory, stochastic optimisation algorithms and data-driven methods for science and engineering.

Title: Convergence analysis of classical and quantum dynamics via hypocoercivity

Speaker: Jianfeng LU, Duke University, USA

Abstract: In this talk we will review some recent developments in the framework of hypocoervicity to obtain quantitative convergence estimate of classical and quantum dynamics, with focus on underdamped Langevin dynamics for sampling and Lindblad dynamics for open quantum systems.

Biography: Jianfeng Lu is a Professor of Mathematics, Physics, and Chemistry at Duke University. Before joining Duke University, he obtained his PhD in Applied Mathematics from Princeton University in 2009 and was a Courant Instructor at New York University from 2009 to 2012. He works on mathematical analysis and algorithm development for problems and challenges arising from computational physics, theoretical chemistry, materials science, high-dimensional PDEs, and machine learning. He is a fellow of AMS. His work has been recognized by a Sloan Fellowship, an NSF Career Award, the IMA Prize in Mathematics and its Applications, and the Feng Kang Prize.

Title: Mathematical Imaging: From Geometric PDEs and Variational Modelling to Deep Learning for Images

Speaker: Carola-Bibiane SCHÖNLIEB, University of Cambridge, UK

Abstract: Images are a rich source of beautiful mathematical formalism and analysis. Associated mathematical problems arise in functional and non-smooth analysis, the theory and numerical analysis of nonlinear partial differential equations, inverse problems, harmonic, stochastic and statistical analysis, and optimisation.

In this talk we will learn about some of these mathematical problems, about variational models and PDEs for image analysis and inverse imaging problems as well as recent advances where such mathematical models are complemented by deep neural networks.

The talk is furnished with applications to art restoration, forest conservation and cancer research.

Biography: Carola-Bibiane Schönlieb is Professor of Applied Mathematics at the University of Cambridge. There, she is head of the Cambridge Image Analysis group and co-Director of the EPSRC Cambridge Mathematics of Information in Healthcare Hub. Since 2011 she is a fellow of Jesus College Cambridge and since 2016 a fellow of the Alan Turing Institute, London. She also holds the Chair of the Committee for Applications and Interdisciplinary Relations (CAIR) of the EMS. Her current research interests focus on variational methods, partial differential equations and machine learning for image analysis, image processing and inverse imaging problems. She has active interdisciplinary collaborations with clinicians, biologists and physicists on biomedical imaging topics, chemical engineers and plant scientists on image sensing, as well as collaborations with artists and art conservators on digital art restoration.

Her research has been acknowledged by scientific prizes, among them the LMS Whitehead Prize 2016, the Philip Leverhulme Prize in 2017, the Calderon Prize 2019, a Royal Society Wolfson fellowship in 2020, a doctorate honoris causa from the University of Klagenfurt in 2022, and by invitations to give plenary lectures at several renowned applied mathematics conferences, among them the SIAM conference on Imaging Science in 2014, the SIAM conference on Partial Differential Equations in 2015, the SIAM annual meeting in 2017, the Applied Inverse Problems Conference in 2019, the FOCM 2020 and the GAMM 2021.

Carola graduated from the Institute for Mathematics, University of Salzburg (Austria) in 2004. From 2004 to 2005 she held a teaching position in Salzburg. She received her PhD degree from the University of Cambridge (UK) in 2009. After one year of postdoctoral activity at the University of Göttingen (Germany), she became a Lecturer at Cambridge in 2010, promoted to Reader in 2015 and promoted to Professor in 2018.

Title: A New Class of Higher-order Stiffly Stable Schemes with Application to the Navier-Stokes Equations

Speaker: Jie SHEN, Eastern Institute of Technology, Ningbo, China

Abstract: How to construct higher-order decoupled, and stable schemes for the Navier-Stokes equations has been a long-standing problem. More precisely, only the decoupled schemes with first-order pressure extrapolation have been proven to be stable and convergent.

To overcome this difficulty, we first construct a new class of higher-order stiffly stable schemes for parabolic equations. Different from traditional time discretization schemes which are usually based on Taylor expansions at $t_{n+\beta}$ with $\beta\in [0,1]$ and whose stability regions decrease as their order of accuracy increase, we construct new schemes based on Taylor expansion at $t_{n+\beta}$ with $\beta>1$ as a parameter, and show that their stability regions increase with β, thus allowing us to choose β according to the stability and accuracy requirement. We shall provide a rigorous stability and error analysis for this new class of schemes.

Then, we show that by choosing suitable β, we can construct unconditionally stable (in H^1 norm), decoupled consistent splitting schemes up to fourth-order for the time-dependent Stokes problem. Finally, by combining the generalized SAV approach with the new consistent splitting schemes, we can construct

unconditionally stable and totally decoupled schemes of second- to fourth order for the Navier-Stokes equations and derive uniform optimal error estimates. We shall also present ample numerical results to show the computational advantages of these schemes.

Biography: Professor Jie Shen received his B.S. in Computational Mathematics from Peking University in 1982, and his PhD in Mathematics from Universite de Paris-Sud (currently Paris Saclay) at Orsay in 1987. He worked at Indiana University (1987-1991), Penn State University (1991-2001), University of Central Florida (2001-2002) and Purdue University (2002-2023). He served as the Director of Center for Computational and Applied Mathematics at Purdue University from 2012 to 2022, and was ratified as Distinguished Professor of Mathematics at Purdue University in 2023. In May 2023, he joined Eastern Institute of Technology, Ningbo, China, as a Chair Professor and Dean of School of Mathematical Science.

He is a recipient of the Fulbright "Research Chair" Award in 2008 and the Inaugural Research Award of the College of Science at Purdue University in 2013, and an elected Fellow of AMS and SIAM.

He serves on editorial boards for several leading international research journals and has authored/coauthored over 250 peer-reviewed research articles and two books with over 25,000 citations in Google Scholar.

His main research interests are numerical analysis, spectral methods and scientific computing with applications in computational fluid dynamics and materials science.

Title: Explicit Stabilized Integrators for Stiff Problems: The Interplay of Geometric Integration and Stochastic Integration

Speaker: Gilles VILMART, University of Geneva, Switzerland

Abstract: The preservation of geometric structures by numerical methods, such as the symplecticity of the flow for the long-time solution of deterministic Hamiltonian systems, often reveals essential for an accurate numerical integration, and this is the objective of geometric numerical integration.

In this talk, we highlight the role that some key geometric integration tools originally introduced in the deterministic setting, such as modified differential equations, processing techniques, Butcher trees, B-series and their generalizations, play in the design of high-order stochastic integrators, in particular for sampling the invariant distribution of ergodic stochastic partial differential equations or high-dimensional ergodic stochastic systems that typically arise in Langevin dynamics in the context of molecular dynamics simulations.

We show that this approach reveals decisive in particular for the construction of efficient explicit stabilized integrators for stiff stochastic problems, which are a popular alternative to implicit methods to avoid the severe timestep restrictions faced by standard explicit integrators.

Geometric numerical integration, high-dimensional ergodic stochastic systems, Butcher trees, B-series, explicit stabilized integrators.

Biography: Gilles Vilmart is a Senior Lecturer at the University of Geneva (Switzerland), Section of Mathematics. He received his PhD in Mathematics in 2008 from the University of Rennes 1 (France, National Institute for Research in Digital Science and Technology) and the University of Geneva (double doctorate program). Before joining the University of Geneva in 2013, he was a post-doctoral researcher at the Swiss Federal Institute of Technology, Lausanne and agrégé-préparateur at the École Normale Supérieure de Rennes where he obtained his Research Habilitation in 2013.

His research focuses on the numerical analysis of geometric and multiscale methods for deterministic or stochastic (partial) differential equations, with special emphasis on geometric numerical integration methods with related algebraic structures, and numerical homogenization methods for highly oscillatory problems.

He received the Mathematics Young Researcher First Prize 2013 of the Region Bretagne (France).

Title: Construction of Solution Landscape for Complex Systems

Speaker: Lei ZHANG, Peking University, China

Abstract: Energy landscape has been widely applied to many physical and biological systems. A long-standing problem in computational mathematics and physics is how to search for the entire family tree of possible stationary states on the energy landscape without unwanted random guesses? Here we introduce a novel concept “Solution Landscape”, which is a pathway map consisting of all stationary points and their connections. We develop a generic and efficient saddle dynamics method to construct the solution landscape, which not only identifies all possible minima, but also advances our understanding of how a complex system moves on the energy landscape. We then apply the solution landscape approach to study two problems: One is construction of the defect landscapes of confined nematic liquid crystals, and the other one is to find the transition pathways connecting crystalline and quasicrystalline phases.

Biography: Lei Zhang is Boya Distinguished Professor at Beijing International Center for Mathematical Research, Peking University. He is also a Principal Investigator at Center for Quantitative Biology, Center for Machine Learning Research. He obtained his PhD in Mathematics at Penn State University in 2009. His research is in the area of computational and applied mathematics and interdisciplinary science in biology, materials, and machine learning. He has published the papers in Phys. Rev. Lett., PNAS, Acta Numerica, Science journals, Cell journals, SIAM journals. He was awarded/funded by NSFC Innovation Research Group, NSFC Outstanding Youth Award, National Key Research and Development Program of China, NSFC Excellent Youth Award, Royal Society Newton Advanced Fellowship, etc. He serves as an Associate Editor for SIAM J. Appl. Math, Science China Mathematics, CSIAM Trans. Appl. Math, DCDS-B, The Innovation, and Mathematica Numerica Sinica.

Part II Prize Lectures

Germund Dahlquist Prize Lecture

Title: Sparse grid discontinuous Galerkin (DG) methods for high dimensional PDEs

Speaker: Yingda CHENG, Virginia Polytechnic Institute and State University, USA

Abstract: In this talk, I will introduce adaptive sparse grid DG methods, and discuss their applications in solving high dimensional PDEs, including kinetic equations, Hamilton-Jacobi equations, etc. The methods, which combines the advantages of sparse grid and DG approach, are shown to be particularly effective for high dimensional transport equations.The methods are constructed using multiwavelets of various kinds. We prove stability and accuracy for model equations. Adaptivity is incorporated for time evolution problems. Benchmark test results are shown.

Biography: Yingda Cheng is currently professor of mathematics and an affiliate faculty with computational modeling & data analytics program at Virginia Polytechnic Institute and State University (Virginia Tech). She was born in Hefei, China in 1983 and received her B.S. degree from the University of Science and Technology of China in 2003. She graduated with a Ph.D. degree in applied mathematics from Brown University in 2007. After a postdoctoral position at the University of Texas at Austin, Dr. Cheng was a faculty member at Michigan State University before the recent move to Virginia Tech.

Dr. Cheng's area of research is in scientific computing, numerical analysis, applied mathematics and data-driven modeling and computation, with applications in plasma physics, semiconductor devices, fluid mechanics, etc. She is interested in developing numerical schemes for PDEs governing complex physical behaviors in science and engineering. She has worked extensively on the construction and analysis of discontinuous Galerkin schemes and structure-preserving numerical schemes that tackles the curse of dimensionality for kinetic transport equations.

New Talent Award Lecture

Title: Geometry-driven Approach to Low-Rank Dynamics

Speaker: Gianluca CERUTI, University of Innsbruck, Austria

Abstract: In this contribution, we explore the low-rank approximability of large-dimensional systems, particularly those arising from discretized PDEs. Given the challenges of directly handling high-dimensional problems, we present an alternative approach known as Dynamical Low-Rank Approximation (DLRA). DLRA tackles the problem's dimensionality by dynamically projecting the system of interest onto a manifold of reduced computational complexity, with the projected dynamics intricately bound to the manifold's nuances. Thus, our discussion will focus on the recently introduced Basis-Update and Galerkin (BUG) integrator and its extensions that not only address these challenges but also preserves the structural properties of the dynamics involved.

Biography: Gianluca Ceruti completed his Master of Science at the University of Rome, Italy, in 2016. He then pursued his PhD at the University of Tuebingen, Germany, under the supervision of Prof. Dr. Christian Lubich, where he graduated in July 2021. His doctoral research focused on advanced computational methods, particularly in dynamical low-rank approximation. Following his PhD, Gianluca joined EPFL as a postdoctoral researcher under the guidance of Prof. Daniel Kressner. At EPFL, he further developed his expertise in numerical analysis and high-performance computing. He is now a postdoc at the University of Innsbruck, Austria, working in the research group of Prof. Lukas Einkemmer.

Part III Mini-symposium Talks

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

Organizers: Shidong Jiang (sjiang@flatironinstitute.org), Dhairya Malhotra (dmalhotra@flatironinstitute.org)

ID: 225 / MS01-1: 1

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

Rapid evaluation of Newtonian potentials on planar domains

Zewen Shen, **Kirill Serkh**

University of Toronto, Canada; zewen.shen@mail.utoronto.ca

In this talk, we present a high-order algorithm for the efficient evaluation of Newtonian potentials over general 2-D domains. The algorithm is based on the use of Green's third identity for transforming the Newtonian potential into a collection of layer potentials over the boundaries of the mesh elements, which can be easily evaluated by the Helsing-Ojala method. One important component of our algorithm is the use of high-order (up to order 20) bivariate polynomial interpolation in the monomial basis, for which we provide extensive justification. We will also discuss some extensions and generalizations of this work.

ID: 361 / MS01-1: 4

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

A panel based trapezoidal quadrature for surface integral operators

Bowei Wu[1], **Joar Bagge**[2]

[1]University of Massachusetts Lowell, USA; [2]University of Texas at Austin, USA; Bowei_Wu@uml.edu

The accuracy and stability of an integral equation solver crucially depend on its underlying quadrature method. Developing efficient quadrature schemes for surface integral operators in 3D has been a key challenge in integral equation method. We investigate a simple surface quadrature scheme that combines a simple domain decomposition technique with corrected trapezoidal quadrature rules for singular and near-singular integrals. The performance of this scheme on different surfaces will be presented and comparisons will be made with existing related methods.

ID: 386 / MS01-1: 3

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

The Approximation of Singular Functions by Series of Non-integer Powers

Mohan Zhao, **Kirill Serkh**

University of Toronto, Canada; mohan.zhao@mail.utoronto.ca

In this talk, we describe an algorithm for approximating functions of the form f(x) = <σ(μ), x^μ> over the interval [0,1], where σ(μ) is some distribution supported on [a,b], with $0<a<b<\infty$. Given a desired accuracy and the values of a and b, our method determines a priori a collection of non-integer powers, so that functions of this form are approximated by expansions in these powers, and a set of collocation points, such that the expansion coefficients can be found by collocating a given function at these points. Our method has a small uniform approximation error which is proportional to the desired accuracy multiplied by some small constants, and the number of singular powers and collocation points grows logarithmically with the desired accuracy. This method has applications to the solution of partial differential equations on domains with corners.

ID: 483 / MS01-1: 2

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

High-order quadrature for the evaluation of layer potentials on surfaces in three dimensions via exterior extension and complete reduction

Hai Zhu, Shidong Jiang

Center for Computational Mathematics, Flatiron Institute, United States of America;

hzhu@flatironinstitute.org

We present an improved high-order nearly-singular layer potential evaluation scheme on curved patches. This method utilizes a combination of quaternionic harmonic polynomial approximation/extension of the layer potential density, along with a complete reduction from nearly-singular surface integrals to a set of endpoint evaluations at the vertices of the patch. Unlike its predecessor, this improved quadrature scheme relies on a cleaner representation of the intermediate line integrals derived from applying Stokes theorem on manifolds, and provides a more robust solution especially for targets located in close proximity to the patch boundary.

ID: 570 / MS01-2: 1

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

Fast and accurate simulation of close-to-touching discs in 2D Stokes flow

Dhairya Malhotra[1], Mariana Martinez Aguilar[2], Dan Fortunato[1]

[1]Flatiron Institute, United States of America; [2]EPFL, Switzerland; dmalhotra@flatironinstitute.org

We introduce a high-order boundary integral method for simulating dense suspensions of rigid discs in a Stokesian fluid in 2D. Our method efficiently handles close-to-touching interactions down to distances of 1e-10 with only a coarse discretization of the boundary. Additionally, we present a preconditioner that significantly reduces the number of GMRES iterations required for solving the Stokes mobility problem at each time step. Coupled with high-order, adaptive time-stepping using spectral deferred correction, we are able to take larger time steps, mitigating the temporal stiffness resulting from close-to-touching interactions.

ID: 648 / MS01-2: 2

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

A fast integral equation solver for surface PDEs.

Tristan Goodwill[1], Michael O'Neil[2], Jeremy Hoskins[1]

[1]University of Chicago, United States of America; [2]New York University, United States of America;

tgoodwill@uchicago.edu

Elliptic PDEs on a surface embedded in three dimensions occur frequently in many areas of physics and computer graphics. In this talk, we show how planar Green's functions can be used to convert elliptic PDEs on a general smooth surface into second kind Fredholm integral equations. We will also discuss how the simplicity of the resulting integral equation can be leveraged to build a fast direct solver for the discretized linear system.

ID: 649 / MS01-2: 3

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

A Dual-space Multilevel Kernel-splitting Framework for Discrete and Continuous Convolution

Shidong Jiang, Leslie Greengard

Flatiron Institute, Simons Foundation, United States of America; sjiang@flatironinstitute.org

We introduce a new class of multilevel, adaptive, dual-space methods for computing fast convolutional transforms. The DMK (dual-space multilevel kernel-splitting) framework uses a hierarchy of grids, computing a smoothed interaction at the coarsest level, followed by a sequence of corrections at finer and finer scales until the problem is entirely local, at which point direct summation is applied. The DMK framework unifies the FMM, Ewald summation, and multilevel summation, achieving speeds comparable to the FFT in work per gridpoint, even in a fully adaptive context.

ID: 651 / MS01-2: 4

MS01 Recent Advances in Fast Algorithms and Integral Equation Methods

Fast algorithms for bulk-surface diffusion

Daniel Fortunato

Flatiron Institute, United States of America; dfortunato@flatironinstitute.org

We present a hybrid numerical asymptotic scheme for bulk-surface diffusion processes in the limit of large but finite bulk diffusivity. The method achieves arbitrary order accuracy in the reciprocal of bulk diffusivity via asymptotic corrections to a quasistatic solution, based on elliptic solves. We apply the scheme to a bulk-surface model of cell polarization.

MS02 Advances in Markov chain Sampling Methods

Organizers: Michael Choi (mchchoi@nus.edu.sg), Ajay Jasra (ajay.jasra0@gmail.com)

ID: 185 / MS02-1: 2

MS02 Advances in Markov chain Sampling Methods

Optimistic Estimation of Convergence in Markov Chains with the Average Mixing Time

Geoffrey Wolfer[1], Pierre Alquier[2]

[1]RIKEN AIP, Tokyo; [2]ESSEC Business School, Singapore; alquier@essec.edu

The convergence rate of a Markov chain to its stationary distribution is typically assessed using the concept of total variation mixing time. However, this worst-case measure often yields pessimistic estimates and is challenging to infer from observations. In this paper, we advocate for the use of the average-mixing time as a more optimistic and demonstrably easier-to-estimate alternative. We further illustrate its applicability across a range of settings, from two-point to countable spaces, and discuss some practical implications.

ID: 204 / MS02-1: 1

MS02 Advances in Markov chain Sampling Methods

Non-reversible guided Metropolis kernel

Kengo Kamatani[1], Xiaolin Song[2]

[1]Institute of Statistical Mathematics, Japan; [2]Osaka University, Japan; kamatani@ism.ac.jp

We introduce a novel class of non-reversible Metropolis kernels, extending the guided-walk kernel through a projection to a totally ordered group. Utilizing Haar measure, we develop the Haar-mixture kernel, notable for its unique Markov kernel construction by instilling a topological structure within the group. Our Delta-

guided Metropolis--Haar kernel, leveraging this Haar-mixture kernel for proposals, significantly outperforms traditional random-walk Metropolis and Hamiltonian Monte Carlo kernels in logistic regression and discretely observed stochastic processes, enhancing effective sample size per second by a factor of at least 10.

ID: 287 / MS02-1: 4

MS02 Advances in Markov chain Sampling Methods

Predictive Resampling for Martingale Posteriors

Edwin Fong

University of Hong Kong, Hong Kong S.A.R. (China); chefong@hku.hk

While the prior distribution is the usual starting point for Bayesian uncertainty, recent work has reframed Bayesian inference as the predictive imputation of missing observations. In particular, the martingale posterior arises when the Bayesian model is a chosen sequence of predictive distributions on future observables, which then induces a posterior distribution on the parameter of interest without the need for a likelihood and prior. This talk will introduce the framework and focus on posterior computation, which is substantially different to traditional Bayes.

ID: 661 / MS02-1: 3

MS02 Advances in Markov chain Sampling Methods

Importance Sampling for Rare Event Tracking in Ensemble Kalman Filters

Nadhir Ben Rached[2], Erik von Schwerin[1], Gaukhar Shaimerdenova[1], Raúl Tempone[1,3]

[1]King Abdullah University of Science and Technology, Saudi Arabia; [2]University of Leeds, Great Britain; [3]RWTH Aachen, Germany; erik.vonschwerin@kaust.edu.sa

We discuss importance sampling (IS) techniques for tracking an unlikely event's probability within ensemble Kalman filtering (EnKF). The low-probability event is characterized by the solution of a stochastic differential equation (SDE) crossing a plane. Between observations, we use IS with respect to the initial condition of the SDE and, via a stochastic optimal control formulation, the Wiener process. The strategy requires approximate solutions to a Kolmogorov Backward equation (KBE). In multi-dimensional settings, we base the IS on a KBE associated with a lower-dimensional SDE obtained by Markovian projection. In simple test problems, the proposed ideas result in significant variance reduction.

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering

Organizers: Hongjie Li (hongjieli@tsinghua.edu.cn), Xianchao Wang (xcwang@hit.edu.cn)

ID: 404 / MS03-1: 4

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering

Inverse medium problems with single measurement

Shiqi Ma

Jilin University, China, People's Republic of; mashiqi@jlu.edu.cn

We study the fixed angle inverse scattering problem of determining a sound speed from scattering measurements corresponding to a single incident wave. The main result shows that a sound speed close to constant can be stably determined by just one measurement. Our method is based on studying the linearized

problem, which turns out to be related to the acoustic problem in photoacoustic imaging. We adapt the modified time-reversal method from existing work to solve the linearized problem in a stable way, and we use this to give a local uniqueness result for the nonlinear inverse problem.

ID: 460 / MS03-1: 1

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering

Theories and applications for multi-layered medium

Youjun Deng

Central South University, China, People's Republic of; youjundeng@csu.edu.cn

In this talk, we shall present some recent work on multi-layered medium. We shall first show some asymptotic results for inhomogeneous medium, and then multi-layered medium, which is a special case of inhomogeneous medium. On the other hand, we shall show how to design multi-layer structures of metamaterials which may greatly increase the resonance modes.

ID: 496 / MS03-1: 2

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering

A novel Newton method for inverse elastic scattering problems

Yan Chang[1], Yukun Guo[1], Hongyu Liu[2], Deyue Zhang[3]

[1]Harbin Institute of Technology, People's Republic of China; [2]City University of Hong Kong, People's Republic of China; [3]Jilin University, People's Republic of China; ykguo@hit.edu.cn

This talk concerns the time-harmonic inverse elastic scattering problem of reconstructing the unknown rigid obstacle embedded in an open space filled with a homogeneous and isotropic elastic medium. Utilizing the near-field data and the boundary condition, a Newton-type iteration scheme is designed to identify the boundary curve of the obstacle. Based on the Helmholtz decomposition and the Fourier-Bessel expansion, we explicitly derive the approximate scattered field and its derivative on each iterative curve. Mathematical justifications for the convergence of the proposed method will be discussed. Numerical examples will be also presented to illustrate the validity of the proposed method.

ID: 525 / MS03-1: 3

MS03 Applications and Scientific Computing on PDE-based Inverse Scattering

Computational imaging of small-amplitude biperiodic surfaces with double negative material

Yuliang Wang

Beijing Normal University, China, People's Republic of; jadelightking@gmail.com

We consider the problem of imaging a periodic surface by acoustic waves. A slab of double negative metamaterial is placed above the surface and the scattered field is measured on the top boundary of the slab. The imaged surface is assumed to be a small perturbation of the flat surface so that we can make a transformed field expansion to linearize the problem and obtain a simple reconstruction formula. We show by analysis of the formula and numerical experiments that the resolution of the reconstruction can be greatly enhanced due to the double negative slab.

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Organizers: Xiaofei Zhao (matzhxf@whu.edu.cn), Limin Ma (limin18@whu.edu.cn)

ID: 153 / MS04-1: 4

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Numerical methods for ground states of Bose-Einstein condensate with higher-order interactions

Xinran Ruan

Capital Normal University, China, People's Republic of China; xinran.ruan@cnu.edu.cn

In a classical mean-field model of Bose-Einstein condensate (BEC), only the binary Fermi contact interaction is considered. However, in the case of higher particle densities, a modification is necessary and one choice is to include a higher-order interaction (HOI) term.

In the talk, I will introduce two numerical methods, namely the normalized gradient flow method and an optimization method based on density function formulation, to compute ground states of BEC with HOI. Specific techniques will be needed to overcome numerical instability issues caused by the HOI term.

ID: 244 / MS04-1: 1

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

An energy stable and maximum bound principle preserving scheme for the dynamic Ginzburg Landau equations

Limin Ma

Wuhan University, China, People's Republic of; limin18@whu.edu.cn

This talk considers a decoupled numerical scheme of the time-dependent Ginzburg-Landau equations under the temporal gauge. The maximum bound principle (MBP) of the order parameter and the energy dissipation law in the discrete sense are proved. The discrete energy stability and MBP-preservation can guarantee the stability and validity of the numerical simulations, and further facilitate the adoption of adaptive time-stepping strategy, which often plays an important role in long-time simulations of vortex dynamics, especially when the applied magnetic field is strong. An optimal error estimate of the proposed scheme is also given.

ID: 245 / MS04-1: 3

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Space-time discontinuous Galerkin methods for Korteweg-de Vries type equations

Qian Zhang, Xia Yinhua

Harbin Institute of Technology, Shenzhen, China; zhang.qian@hit.edu.cn

In this talk, we employ the high-order and structure-preserving space-time Galerkin method for discretization with a discontinuous basis function in space and a discontinuous or continuous basis function in time following a thorough examination of the equation structure and solution. The unified finite element method in terms of a fully discretization perspective can improve the theoretical study of fully discretization for KdV equation. In numerical implement, the spectral deferred correction method is used to simplify the computation. The numerical and the theoretical results demonstrates the capability of our proposed methods.

ID: 278 / MS04-1: 2

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Explicit K-symplectic methods for nonseparable non-canonical Hamiltonian systems

Beibei Zhu, Lun Ji, Aiqing Zhu, Yifa Tang

University of Science and Technology Beijing, China, People's Republic of; zhubeibei@ustb.edu.cn

We propose efficient numerical methods for nonseparable non-canonical Hamiltonian systems which are explicit, K-symplectic in the extended phase space with long time energy conservation properties. They are based on extending the original phase space to several copies of the phase space and imposing a mechanical restraint on the copies of the phase space. Explicit K-symplectic methods are constructed for the guiding center system and the Ablowitz-Ladik model of nonlinear Schrodinger equation. Numerical tests show that the proposed methods exhibit good numerical performance in preserving the phase orbit and the energy of the system over long time.

ID: 291 / MS04-2: 1

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

A Novel Stochastic Interacting Particle-Field Algorithm for 3D Parabolic-Parabolic Keller-Segel Chemotaxis System

Zhongjian Wang, Jack Xin, Zhiwen Zhang

The University of Hong Kong, China, People's Republic of; zhangzw@hku.hk

We propose an efficient stochastic interacting particle-field (SIPF) algorithm for computing aggregation patterns and near singular solutions of the parabolic-parabolic Keller-Segel (KS) chemotaxis system in 3D. Our approach approximates KS solutions using empirical measures of particles coupled with a smoother field variable computed through the spectral method. Numerical experiments confirm the convergence and self-adaptive nature of the SIPF algorithm to high gradient regions, which provides a low-cost approach to studying the emergence of finite time blowup in 3D using a small number of Fourier modes and varying initial mass.

ID: 294 / MS04-2: 2

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

An iterative algorithm for POD basis adaptation in solving parametric convection-diffusion equations

Zhizhang Wu, Zhiwen Zhang

The University of Hong Kong, Hong Kong S.A.R. (China); wuzz@hku.hk

We introduce an iterative algorithm for proper orthogonal decomposition (POD) basis adaptation in solving convection-diffusion equations with diffusivity as a parameter. To construct POD basis, we need fine-grid solvers to obtain accurate solution snapshots for small diffusivity, while coarse-grid solvers are sufficient for large diffusivity. By exploiting the implicit dependence of solutions on diffusivity, our method adapts the POD basis extracted from solution snapshots of large diffusivity for the construction of a reduced-order model at small diffusivity without resorting to fine-grid solvers. We provide convergence results for our method and numerical examples to show the feasibility of our method.

ID: 333 / MS04-2: 3

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Computation of two types of ground state solutions for nonlinear Schrödinger equations

Wei LIU

National University of Singapore, Singapore; wliu.hunnu@foxmail.com

This talk aims to present some recent advances on the computation and analysis of two types of ground state solutions, i.e., the energy ground state and the action ground state, for the nonlinear Schrödinger equation with possible rotation. Three specific topics will be mainly focused on: (i) novel normalized gradient flow and second-order flow methods for computing the energy ground state; (ii) minimization algorithms based on suitable variational characterizations for computing the action ground state; (iii) theoretical and numerical results on the relationship between these two types of solutions.

ID: 588 / MS04-2: 4

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

A 3-D High-order Spectral Element Time-Domain Method for Quantum Device Simulations

NA LIU, KANGSHUAI DU

Xiamen University, China, People's Republic of; liuna@xmu.edu.cn

A spectral element time-domain (SETD) method with perfectly matched layers (PML) is proposed to simulate the behavior of electron waves in three-dimensional (3-D) quantum devices. By utilizing Gauss-Lobatto-Legendre (GLL) polynomials and GLL quadrature, diagonal mass matrix is obtained which is meaningful in the time-stepping process. Several illustrative numerical examples are given to verify that the SETD-PML has spectral accuracy and is effective in addressing the challenges posed by open boundary conditions.

ID: 613 / MS04-2: 5

MS04 Communication of Structure-preserving Techniques for Computing Diffusion and Dispersion

Optimal L^2 error estimates of unconditionally stable FE schemes for the Cahn-Hilliard-Navier-Stokes system

Jilu Wang

Harbin Institute of Technology (Shenzhen), China, People's Republic of; wangjilu@hit.edu.cn

The paper is concerned with the analysis of a popular convex-splitting finite element method for the Cahn-Hilliard-Navier-Stokes system. Here we first present an optimal error estimate in L2-norm for the convex-splitting FEMs. We also show that optimal error estimates in the traditional (interpolation) sense may not always hold for all components in the coupled system due to the nature of the pollution/influence from lower-order approximations. Our analysis is based on two newly introduced elliptic quasi-projections and the superconvergence of negative norm estimates for the corresponding projection errors. Numerical examples are also presented to illustrate our theoretical results.

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Organizers: Balázs Kovács (balazs.kovacs@math.uni-paderborn.de), Thomas Ranner (T.Ranner@leeds.ac.uk), Quan Zhao (quanzhao@ustc.edu.cn)

ID: 264 / MS05-2: 4

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Parametric polynomial preserving recovery on manifolds and its application

Hailong Guo

The University of Melbourne, Australia; hailong.guo@unimelb.edu.au

We will introduce gradient recovery schemes for data defined on discretized manifolds. The proposed method, Parametric Polynomial Preserving Recovery (PPPR), does not require the tangent spaces of the exact manifolds, which have been assumed in some significant gradient recovery methods in the literature. We will also discuss several applications, including adaptive computation, discretizing the Vector-Laplacian equation, designing new finite element methods for fourth-order PDEs on surfaces, and a new geometric error analysis framework.

ID: 385 / MS05-1: 2

MS05 Numerical Methods for Geometric PDEs and Interface Problems

An ALE meshfree method for surface PDEs coupling with forced mean curvature flow

Xinlong Feng

Xinjiang University, PR China; fxlmath@xju.edu.cn

In this work, we propose an ALE mesh-free method for solving diffusion-reaction equations on evolving surfaces. The surface evolution law is determined by a forced mean curvature flow (FMCF). We develop a parametric RBF-FD method to solving FMCF and it's advantage is that it utilizes a suitable tangential velocity in the equation to maintain a fairly uniform distribution of nodes. Moreover, we discuss how to deal with the boundary conditions for PDEs on surfaces. Finally,numerical experiments are shown to demonstrate the effectiveness of the proposed method.

ID: 408 / MS05-2: 2

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Numerical analysis of a spectral problem with Ventcel boundary conditions on curved meshes

Joyce Ghantous

Université de Pau et des Pays de l'Adour (UPPA), France; joyce.ghantous@univ-pau.fr

We consider a spectral problem with Ventcel boundary conditions. The focus is on obtaining error estimations for the eigenvalues and the eigenfunctions expressed with respect to the finite element degree and to the mesh order. A crucial point concerns the construction of high order curved meshes for the discretization of the physical domain and on the definition of the lift operator, which is aimed to transform a function defined on the mesh domain into a function defined on the physical one. Once the theoretical a priori error estimates have been obtained, we perform numerical experiments in 2D and 3D validating these results.

ID: 485 / MS05-1: 4

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Including low-dimensional features in 2D surface models

Elena Bachini[1], Antonia Larese[1,2], Mario Putti[3], Guglielmo Scovazzi[4]

[1]Dept. of Mathematics "Tullio Levi-Civita", University of Padua, Italy; [2]Institute for Advanced Study, Technical University of Munich, Germany; [3]Dept. of Agronomy, Food, Natural resources, Animals and Environment, University of Padua, Italy; [4]Dept. of Civil and Environmental Engineering and Dept. of Mechanical Engineering and Materials Science, Duke University, USA; elena.bachini@unipd.it

We consider a two-dimensional surface PDE in its geometrically intrinsic formulation and discretized using a Galerkin finite element scheme also adapted to the geometric setting (ISFEM), forced by a low-dimensional feature. We are interested in using an unfitted mesh and try to counterbalance the loss of accuracy that occurs in this situation. We tackle this problem by extending the Shifted Interface approach to our geometrically intrinsic framework. We present numerical results obtained first considering simple surface models, such as the heat equation, to arrive finally at the solution of more complex models with internal interfaces.

ID: 519 / MS05-2: 3

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Space-time adaptivity for parabolic PDEs on stationary surfaces

Michael Lantelme, Balázs Kovács

Universität Paderborn, Germany; lantelme@math.uni-paderborn.de

In this talk we will discuss an adaptive algorithm for solving parabolic surface partial differential equations on closed stationary surfaces. The method uses surface finite elements in space and backward Euler method in time. The proposed error indicator bounds the error quantities globally in space from above and below, and in time globally from above and locally from below. An adaptive algorithm will be discussed using the derived error indicator, including refining and coarsening.

We will present numerical experiments to illustrate and complement the theory, showing the asymptotic behaviour of the error and reasonable refining and coarsening.

ID: 626 / MS05-2: 1

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Multilevel Representations of Isotropic Gaussian Random Fields on the Sphere

Ana Djurdjevac

Freie Universität Berlin, Germany; adjurdjevac@zedat.fu-berlin.de

We will construct series expansion of isotropic Gaussian random field on a sphere with independent Gaussian coefficients and localized basis functions. We will illustrate the application of such expansions to elliptic PDEs on the sphere with lognormal coefficients. In addition, we will comment on the extension of the presented results to other surfaces, which is the work in progress. This is a joint work with M. Bachmayr.

ID: 671 / MS05-1: 1

MS05 Numerical Methods for Geometric PDEs and Interface Problems

A convergent evolving finite element method with artificial tangential motion for surface evolution under a prescribed velocity field.

Genming Bai

University of Michigan / The Hong Kong Polytechnic University (PolyU), Hong Kong S.A.R. (China); gbai@umich.edu

A novel evolving surface finite element method, based on a novel equivalent formulation of the continuous problem, is proposed for computing the evolution of a closed hypersurface moving under a prescribed velocity field. The method improves the mesh quality of the approximate surface by minimizing the rate of deformation using an artificial tangential motion. The transport evolution equations of the normal vector and the extrinsic Weingarten matrix are derived and coupled with the surface evolution equations to ensure stability and convergence of the numerical approximations. Optimal-order convergence of the semi-discrete PFEM is proved for finite elements of degree $k \geqslant 2$.

ID: 701 / MS05-1: 3

MS05 Numerical Methods for Geometric PDEs and Interface Problems

Parametric finite element approximation of two-phase Navier–Stokes flow with viscoelasticity

Harald Garcke[1], Robert Nürnberg[2], Denni Trautweins[1]

[1]Universität Regensburg, Germany; [2]Universita di Trento, Italy; harald.garcke@ur.de

We present parametric finite element approximations of the two-phase Navier–Stokes flow with viscoelasticity. The free boundary problem is given by the viscoelastic Navier–Stokes equations in the two phases, which are connected with jump conditions across the interface. The elasticity in the fluids is described with the Oldroyd-B model for the left Cauchy-Green tensor.

We approximate a variational formulation for the mean curvature of the interface and for the interface evolution with a parametric finite element method.

The two-phase Navier–Stokes–Oldroyd-B system in the bulk is discretized in a way that unconditional solvability and stability for the coupled bulk-interface system is guaranteed.

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Organizers: Christian Lubich (lubich@na.uni-tuebingen.de), Tobias Jahnke (tobias.jahnke@kit.edu)

ID: 209 / MS06-1: 1

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Uniform error bounds on numerical methods for long-time dynamics of dispersive PDEs

Weizhu Bao[1], Yongyong Cai[2], Yue Feng[3], Chunmei Su[4]

[1]National University of Singapore, Singapore; [2]Beijing Normal University, China; [3]Xi'an Jiaotong University, China; [4]Tsinghua Univerisity, China; matbaowz@nus.edu.sg

In this talk, I report our recent work of error estimates on different numerical methods for the long-time dynamics of dispersive PDEs with small potential or weak nonlinearity, such as the Schroedinger equation with small potential, the nonlinear Schroedinger equation with weak nonlinearity, the nonlinear Klein-Gordon equation with weak nonlinearity, the Dirac equation with small electromagnetic potential, and the nonlinear Dirac equation with weak nonlinearity, etc. By introducing a new technique of regularity compensation oscillatory (RCO), we can establish improved uniform error bounds on time-splitting methods for dispersive PDEs with small potentials and/or weak nonlinearity.

ID: 224 / MS06-1: 2

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Solving long-time nonlinear Schr\"{o}dinger equation by a class of oscillation-relaxation integrators

Kai Liu[1], **Bin Wang**[2], **Xiaofei Zhao**[3]

[1]Nanjing Audit University, China; [2]Xi'an Jiaotong University, China; [3]Wuhan University, China; wangbinmaths@xjtu.edu.cn

In this talk, we numerically solve the long-time nonlinear Schr\"{o}dinger equation (NLSE) by using an oscillation-relaxation formulation. Such formulation allow us to propose a class of numerical methods named oscillation-relaxation integrators (ORIs). By convergence analysis, they are shown to offer nice error bounds. Long-term near-conservation laws of symmetric ORIs are also established and tested.

ID: 243 / MS06-2: 4

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Numerical methods for disordered NLS

Xiaofei Zhao

Wuhan University, China, People's Republic of; matzhxf@whu.edu.cn

The Schrödinger equation with a spatial random potential function will produce localization effects and has important applications in physics. In numerical simulations, the main difficulties come from the roughness and randomness of the potential function. From these two perspectives, the report will introduce some numerical methods for the relevant nonlinear Schrödinger equation and give convergence results.

ID: 327 / MS06-2: 3

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Using non-resonant step sizes to improve efficiency of time integrators for oscillatory non-linear Dirac equations

Tobias Jahnke, Michael Kirn

Karlsruhe Institute of Technology, Germany; michael.kirn@kit.edu

In the non-relativistic limit, solutions of non-linear Dirac equations exhibit rapid oscillations in time. Therefore, standard time integration methods only provide accurate approximations when tiny step sizes are used. We present a tailor-made time integrator without this restriction. The basic principle is to iterate Duhamel's formula, integrate highly-oscillatory phases exactly, and only approximate slowly varying parts. The resulting method is then significantly simplified by omitting numerous terms which would be relevant for the local error order, but do not affect the global error order if non-resonant step sizes are used. This is due to cancellations in the error accumulation.

ID: 412 / MS06-1: 3

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Filtered finite difference methods for highly oscillatory semilinear hyperbolic systems

Christian Lubich, Yanyan Shi

Universität Tübingen, Germany; shi@na.uni-tuebingen.de

This talk explores the numerical approximation of fast oscillating solutions to semilinear hyperbolic systems with a trilinear nonlinearity and fast oscillating initial condition. We propose two filtered finite difference schemes based on the leapfrog method. By comparing modulated Fourier expansions of numerical approximation and exact solution, the error analysis of large step sizes and mesh widths is obtained. Numerical experiments are conducted to validate the theoretical results.

ID: 480 / MS06-1: 4

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Time integration method for wave propagation with spatio-temporal oscillations

Tobias Jahnke, Johanna Mödl

Karlsruhe Institute of Technology, Germany; johanna.moedl@kit.edu

For nonlinear Friedrichs systems with solutions that oscillate rapidly in space and time, it is a major challenge to compute reasonable approximations efficiently. We tackle this problem by a fusion of analytical and numerical approximation techniques. First, we replace the original PDE system with a fine-tuned modification of the slowly varying envelope approximation. In the second step, we devise an efficient and uniformly accurate time integration method tailored to our novel modified PDE system. Central to this is the analysis of interactions between oscillatory and non-oscillatory parts of the solution.

ID: 482 / MS06-2: 2

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

A uniformly accurate method for the Klein-Gordon-Dirac system in the nonrelativistic regime

Yongyong Cai, Wenfan Yi

Beijing Normal University, China, People's Republic of; yongyong.cai@bnu.edu.cn

In this talk, we present a multiscale time integrator Fourier pseudospectral (MTI-FP) method for discretizing the massive Klein-Gordon-Dirac (KGD) system which involves a small dimensionless parameter $0<\varepsilon\leq 1$. In the nonrelativistic limit regime, the KGD system admits rapid oscillations in time as $\varepsilon\rightarrow 0^+$. In addition, the nonlinear Yukawa interaction and the indefinite Dirac operator bring other significant difficulties.

The main idea of the MTI-FP method is to construct a precise multiscale decomposition by the frequency (MDF) to the solution of the KGD system at each time step and then employ the Fourier pseudospectral discretization for the spatial derivatives

followed with the exponential wave integrator (EWI) for the time marching. This approach is explicit, easy to implement and preforms significantly better than the classical methods in the literature. More specifically, we rigorously establish the uniform error bounds at $O(\tau+h^{m_0-1})$ for all $\varepsilon\in(0,1]$ and optimal quadratic temporal error bounds at $O(\tau^2)$ in the $\varepsilon=O(1)$ regime, where τ is the time step size, h is mesh size and m_0 depends on the regularity of the solution.

Extensive numerical results demonstrate that our error bounds are optimal and sharp.

Finally, we apply the MTI-FP method to numerically study the nonrelativistic limit behaviors of the KGD system when $\varepsilon\rightarrow 0^+$.

ID: 549 / MS06-2: 1

MS06 Numerical Methods for Highly Oscillatory ODEs and PDEs

Asymptotic expansions for the linear PDEs with oscillatory input terms: Analytical form and error analysis

Karolina Kropielnicka

Polish Academy of Sciences, Poland; kkropielnicka@impan.pl

Partial differential equations with highly oscillatory input term are hardly ever solvable analytically and they are difficult to treat numerically. Modulated Fourier expansion used as an ansatz is a well known and extensively investigated tool in asymptotic numerical approach for this kind of problems.

In this talk I will consider input term with single frequency and will show that the ansatz need not be assumed – it can be derived naturally while developing formulas for expansion coefficients. Moreover I will present the formula describing the error term and its estimates. Theoretical investigations will be illustrated by results of the computational simulations.

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls

Organizers: Uri Michael Ascher (ascher@cs.ubc.ca), Raymond Spiteri (spiteri@cs.usask.ca)

ID: 191 / MS07-1: 4

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls

Wrong solutions for differential systems

Uri Michael Ascher

University of BC, Canada; ascher@cs.ubc.ca

We discuss situations where subtle reasons lead to wrong numerical solutions for differential equations. Such unhappy events often occur in the context of fractional step methods, especially when using conservative time discretizations, and there are some well-known examples for that. But other, rather different situations may give rise to similar phenomena as well. These will be demonstrated by computational examples, including the simulation of friction, damping and contact effects in deformable object motion arising in computer graphics animation and robotics.

ID: 349 / MS07-1: 1

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls

Solving the Real-Time Boltzmann Transport Equation with Adaptive and Multirate Time Integration Methods

Jia Yao[2], Ivan Maliyov[3], Carol S. Woodward[1], David Gardner[1], Marco Bernardi[2]

[1]Lawrence Livermore National Laboratory, United States of America; [2]California Institute of Technology; [3]CNRS; woodward6@llnl.gov

Electron dynamics can be modeled by the electron real-time Boltzmann transport equation (rt-BTE) with first-principles electron-phonon (e-ph) collisions. Solving the lattice (phonon) rt-BTE with e-ph and phonon-phonon (ph-ph) collisions remains challenging due to the different timescales of e-ph and ph-ph interactions. This presentation will overview multirate time integration capabilities in the SUNDIALS library and then describe interfacing between the PERTURBO code and SUNDIALS to efficiently advance coupled electron and phonon rt-BTEs in time. We show results indicating a significant speed-up using adaptive step size and multirate infinitesimal (MRI) methods from SUNDIALS.

Prepared by LLNL under Contract DE-AC52-07NA27344.

ID: 381 / MS07-1: 2

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls

Splitting for low regularity problems

Alexander Ostermann

University of Innsbruck, Austria; alexander.ostermann@uibk.ac.at

Splitting methods are a well-established tool for the integration of nonlinear evolution equations. In the case of dispersive equations, however, the schemes have serious problems with low regularity solutions. Appropriate frequency decomposition techniques combined with a step size related filtering in Fourier space help to stabilize the occurring numerical resonances. For the nonlinear Schrödinger equation (NLS), the required condition is $\tau N^2 \lesssim 1$, where τ denotes the step size and N the number of Fourier modes employed. Note that a similar constraint is also required for splitting methods to show near-preservation of energy for NLS.

ID: 667 / MS07-1: 3

MS07 Recent Advances in Fractional-step Methods: Advances and Pitfalls

Numerical integration of the Schödinger equation: Polynomial versus splitting methods

Sergio Blanes

Universitat Politècnica de València, Spain; serblaza@imm.upv.es

We consider the numerical integration of the semidiscretised Schrödinger equation which requires the computation of the exponential of a skew-Hermitian matrix acting on a vector. This can be achieved by considering polynomial methods like Taylor, Krylov or Chebyshev methods which are conditionally stable. Usually the matrix is separable into solvable parts and tailored splitting methods can be used which are unconditioanally stable and can be used for time-dependent potentials as well as for non-linear SEs, but can suffer from resonances for some values of the time step. Pros and cons of both families of methods are analysed in this talk.

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Organizers: Ruili Zhang (zhangrl@bjtu.edu.cn), Bin Wang (wangbinmaths@xjtu.edu.cn)

ID: 203 / MS08-2: 4

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Invariant-preserving difference schemes for the R2CH system

Qifeng Zhang

Zhejiang Sci-Tech University, China, People's Republic of; zhangqifeng0504@163.com

In this talk, we develop, analyze and numerically test two classes of invariant-preserving difference schemes for a rotation-two-component Camassa-Holm system (R2CH), which contains strongly nonlinear terms and high-order derivative terms. One of them is linearized one and another one is fully nonlinear. We prove that both the numerical schemes are uniquely solvable and second-order convergent for the spatial and temporal discretizations. Optimal error estimates for the velocity in the infinite norm and for the surface elevation in the L2-norm are obtained. Extensive numerical experiments verify the convergence results as well as conservation.

ID: 284 / MS08-1: 4

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Structure-preserving algorithms and their error estimates for the relativistic dynamics of charged particle

Ruili Zhang

Beijing Jiaotong University, China, People's Republic of; zhangrl@bjtu.edu.cn

In this talk, we investigate the numerical algorithms and their error estimates for the dynamics of relativistic charged particles. To maintain the fundamental principles of relativistic dynamics, we construct structure-preserving algorithms using the splitting scheme. These algorithm ensure the preservation of volume, energy, and the Lorentz invariant property exactly. Specifically, we establish an uniform and optimal error bound in both 4-position and 4-velocity for the algorithm under a strong magnetic field. Numerical experiments are also presented to demonstrate their advantages in both uniform error estimate and conservation of energy, compared to other numerical methods.

ID: 285 / MS08-2: 3

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Learning stochastic differential equations from data

Aiqing Zhu, Qianxiao Li

National University of Singapore, Singapore; zaq@nus.edu.sg

Learning unknown stochastic differential equations (SDEs) from observed data is a significant task with applications in various fields. Current approaches often rely on one-step stochastic numerical schemes, necessitating data with sufficiently high time resolution. In this talk, we will introduce novel approximations to the transition density of the parameterized SDE. Benefiting from the robust density approximation, our method exhibits superior accuracy compared to baseline methods in learning the fully unknown drift and diffusion functions and computing the invariant distribution from trajectory data. We then show several experiment results to verify the advantages and robustness of the proposed method.

ID: 319 / MS08-1: 2

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Error estimates for backward difference formulae for the transient Stokes problem

Alessandro Contri[2], André Massing[2], Balázs Kovács[1]

[1]Paderborn University, Germany; [2]NTNU, Norway; balazs.kovacs@math.uni-paderborn.de

In this talk we will present a new stability and error analysis of fully discrete approximation schemes for the transient Stokes equation.

The numerical method uses BDF methods of order 1 to 6 in time and a wide class of Galerkin finite element methods including both inf-sup stable spaces and symmetric pressure stabilized formulations.

We perform a unified error analysis for the above method, prove stability, and show optimal-order error estimates for both the velocity and the pressure. The main tools in our stability analysis is the G-stability theory of Dahlquist together with the multiplier technique introduced by Nevanlinna and Odeh.

ID: 419 / MS08-1: 3

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Structure-preserving Properties of Dynamical Low-Rank Integrators

Gianluca Ceruti

University of Innsbruck, Austria; Gianluca.Ceruti@uibk.ac.at

In this contribution, we explore the low-rank approximability of large-dimensional systems, particularly those arising from discretized PDEs. Given the challenges of directly handling high-dimensional problems, we present an alternative approach known as Dynamical Low-Rank Approximation (DLRA). DLRA tackles the problem's dimensionality by dynamically projecting the system of interest onto a manifold of reduced computational complexity, with the projected dynamics intricately bound to the manifold's nuances. Thus, our discussion will focus on the recently introduced Basis-Update and Galerkin (BUG) integrator and its extensions that not only addresses these challenges but also preserves the structural properties of the dynamics involved.

ID: 443 / MS08-2: 2

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Splitting algorithms for total variation imaging via SAV approach

Raymond H. Chan[1], **Yuto Miyatake**[2]

[1]City University of Hong Kong; [2]Osaka University; yuto.miyatake.cmc@osaka-u.ac.jp

This work introduces new algorithms for total variation imaging, employing a Scalar Auxiliary Variable (SAV) approach to enhance computational efficiency. By reformulating the gradient flow with a scalar auxiliary variable, we decompose the system into two subflows. These subflows are linearized for each time step, and subsequently integrated by using a Successive Overrelaxation (SOR) type method. This integration strategy makes the algorithms fully explicit, independently of boundary condition choices.

ID: 508 / MS08-2: 1

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Crossroads between Geometric Numerical Integration and Machine Learning

Michael Kraus

Max Planck Institute for Plasma Physics, Germany; michael.kraus@ipp.mpg.de

Many dynamical systems in physics and other fields possess some form of geometric structure, such as Lagrangian or Hamiltonian structure, symmetries and conservation laws. Geometric numerical integration algorithms which preserve these structures usually show greatly reduced errors and better long-time stability compared to algorithms that do not preserve these structures.

In this talk, we will show how the ideas of geometric numerical integration can be brought forward to the realms of scientific machine learning, where neural networks are used to solve differential equations.

ID: 614 / MS08-3: 2

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Variational integrators for the Lagrangian quadratic in velocities

Yihan Shen

Chinese Academy of Science, Academy of Mathematics and Systems Science, China, People's Republic of; shenyihan@lsec.cc.ac.cn

In this talk, we are confronted with the Lagrangian systems whose form of $L = M\dot q^2 + A(q)\dot q - U(q)$ and thus quadratic in velocities. We construct the variational integrators for the systems which is equivalent to a compostion methods. The numerical methods are long-time stable and have good behaviour in preserving the invariants like energy, momentum and so on. In the numerical experiments, we consider the charged paricle systems.

ID: 657 / MS08-1: 1

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Geometric numerical integration for the linear-gradient system

Yajuan Sun

Academy of Mathematics and Systems Science, CAS, China, People's Republic of; sunyj@lsec.cc.ac.cn

In this talk, the geometric integrators are presented for the linear-gradient system by a dimension-expansion technique. By introducing a vector-valued function, we embed a given linear-gradient system into a higher-dimensional space to achieve an equivalent extended system. Some numerical examples are provided to illustrate the accuracy, efficiency, and long-term stability of the new proposed schemes.

ID: 663 / MS08-3: 1

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Hamiltonian Particle-in-Cell methods for Vlasov-Poisson equations

Anjiao Gu[1], Yang He[2], Yajuan Sun[3]

[1]Shanghai Jiao Tong University, China; [2]School of Mathematics and Physics, University of Science and Technology Beijing, China; [3]LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China; School of Mathematical Sciences, University of Chinese Academy of Sciences, China; gaj2023@sjtu.edu.cn

In this talk, Particle-in-Cell algorithms for the Vlasov-Poisson system will be presented based on its Poisson bracket structure. The Poisson equation is solved by finite element methods, in which the appropriate finite element spaces are taken to guarantee that the semi-discretized system possesses a well defined discrete Poisson bracket structure. Then, splitting methods are applied to the semi-discretized system by decomposing the Hamiltonian function. The resulting discretizations are proved to be Poisson bracket preserving. Moreover, the conservative quantities of the system are also well preserved.

ID: 665 / MS08-1: 5

MS08 Recent Advances on Structure-preserving Algorithms with Applications

Aggressive Splitting in Structure-Preserving Numerical Methods

Naoki Ishii, Toyohiro Aso, Shun Sato, Takayasu Matsuo

The University of Tokyo, Japan; ishii-naoki@g.ecc.u-tokyo.ac.jp

Splitting methods are numerical methods where the operator is split into several parts to reduce computational cost. Inspired by stochastic gradient descent in the field of machine learning, we propose splitting the operator aggresively, that is, into as many parts as the problem size. We demonstrate that this approach is compatible with structure-preserving methods such as symplectic methods and the discrete gradient method. This method allows parallel computing, which enhances the practicality of structure-preserving methods.

MS09 Theory and Numerics of Inverse Problems

Organizers: Shiqi Ma (mashiqi@jlu.edu.cn), Minghui Song (songmh@hit.edu.cn)

ID: 214 / MS09-1: 2

MS09 Theory and Numerics of Inverse Problems

Inverting the local transverse and mixed ray transforms

Jian Zhai

Fudan University, China, People's Republic of; jianzhai@fudan.edu.cn

We consider the transverse and mixed ray transforms on a compact Riemannian manifold with smooth boundary. We show that the transverse ray transform and the mixed ray transform are invertible, up to natural obstructions, near a boundary point. When the manifold admits a strictly convex function, this local invertibility result leads to a global result by a layer stripping argument.

ID: 406 / MS09-1: 1

MS09 Theory and Numerics of Inverse Problems

A novel quantitative inverse scattering scheme using interior resonant modes

Xianchao Wang

Harbin Institute of Technology, China, People's Republic of; xcwang@hit.edu.cn

This talk is devoted to a novel quantitative imaging scheme of identifying

impenetrable obstacles in time-harmonic acoustic scattering from the associated far-field data. In the first phase, we determine the interior eigenvalues of the underlying unknown obstacle from the far-field data via the indicating behavior of the linear sampling method. In the second phase, we propose a novel iteration scheme of Newton's type to identify the boundary surface of the obstacle. Numerical experiments in both 2D and 3D are conducted, which confirm the promising features of the proposed imaging scheme.

ID: 700 / MS09-1: 3

MS09 Theory and Numerics of Inverse Problems

Reconstruction of acoustic sources from multi-frequency phaseless far-field data

Sun Fenglin

Tianjin Normal University, China, People's Republic of; fenglinsun@tjnu.edu.cn

This talk mainly focusing on the problem of determining an acoustic source from multi-frequency phaseless far-field data. By supplementing two reference sources in the inverse source model, we developed a novel strategy to recovering the phase information of far-field data. Mathematically, the stability of the phase retrieval approach is rigorously justified. Then we employ the Fourier method to deal with the multi-frequency inverse source problem with recovered phase information. This talk is based on a joint work with Xianchao Wang.

ID: 735 / MS09-1: 4

MS09 Theory and Numerics of Inverse Problems

Fractional random walks on graphs

Giovanni Covi

University of Helsinki, Finland; giovanni.covi@helsinki.fi

We study an inverse problem for a fractional random walk on a finite graph. We show that the edge structure of the graph and a conductivity function defined on the vertices of the graph can both be recovered from partial fractional random walk data. The data is partial in the sense that it is only accessible on part of the graph. Moreover, we completely characterize the random walk data. Our technique is based on purely algebraic methods. This is part of an ongoing work with Professor Matti Lassas.

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

Organizers: Lukas Einkemmer (lukas.einkemmer@uibk.ac.at)

ID: 106 / MS10-1: 4

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

A hierarchical low-rank algorithm for the kinetic chemical master equation

Lukas Einkemmer, Julian Mangott, Martina Prugger

Universität Innsbruck, Austria; julian.mangott@uibk.ac.at

In this talk a dynamical low-rank algorithm for the kinetic chemical master equation (CME) is presented. The stochastic description of chemical reaction networks with the kinetic CME is important for studying biological cells, but it suffers from the curse of dimensionality. We reduce the dimensionality of the problem by dividing the reaction network into partitions. Only reactions that cross partitions are subject to an approximation error. This method, compared to the commonly used stochastic simulation algorithm (SSA), is completely noise-free and in some cases it can drastically reduce memory consumption and run time and provide a better accuracy than SSA.

ID: 281 / MS10-2: 2

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

Generalised Petrov-Galerkin Dynamical Low Rank Approximations

Thomas Trigo Trindade, Fabio Nobile

EPFL, Switzerland; thomas.trigotrindade@epfl.ch

We present a generalised Petrov-Galerkin Dynamical Low Rank Approximations (PG-DLRA) framework in the Uncertainty Quantification context.

It aims to solve time-dependent random PDEs efficiently, by exploiting the low-rank structure of the solution random field.

To cancel or at least alleviate the numerical artifacts arising from the discretisation of PDEs, the PG-DLRA framework allows to import any stabilisation technique expressed as a generalised Galerkin or a Petrov-Galerkin method.

We apply the framework to stabilise advection-dominated problems discretised by the Finite Element method (using, e.g., the Streamline Upwind Petrov-Galerkin method) and analyse the resulting systems.

Numerical experiments validate the theoretical predictions.

ID: 454 / MS10-1: 2

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

Dynamical approximation and sensor placement for the state estimation of transport problems

Cecilia Pagliantini[1], **Olga Mula**[2], **Federico Vismara**[2]

[1]University of Pisa, Italy; [2]Eindhoven University of Technology, Netherlands; cecilia.pagliantini@unipi.it

We consider the inverse problem of reconstructing an unknown function u from a finite set of measurements, under the assumption that u is the trajectory of a transport problem with unknown input parameters. We propose an algorithm based on the Parameterized Background Data-Weak method (PBDW) where dynamical sensor placement is combined with approximation spaces that evolve in time. We prove that the method ensures an accurate reconstruction at all times and allows to incorporate relevant physical properties in the reconstructed solutions by suitably evolving the approximation space. As an application of this strategy we consider Hamiltonian systems modeling wave-type phenomena.

ID: 599 / MS10-2: 1

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

High-order parallel time integrators for dynamical low-rank approximation

Jonas Kusch

Norwegian University of Life Sciences, Norway; jonas.kusch1@gmail.com

A core challenge in dynamical low-rank approximation (DLRA) is the construction of efficient and robust time integrators. Recently, a first-order parallel robust time integrator for DLRA that permits dynamic rank adaptation and enables a fully parallel update of all low-rank factors was introduced. In this talk, an extension to second order is presented. Second order is achieved by a careful basis augmentation before solving the matrix differential equations of the factorized solution. The integrator fulfills a robust error bound with an improved dependence on normal components of the vector field while only requiring solving differential equations of rank 2r.

ID: 664 / MS10-1: 1

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

Regularized dynamical parametric approximation

Christian Lubich[1], **Caroline Lasser**[2], **Joerg Nick**[3], **Michael Feischl**[4]

[1]U Tuebingen; [2]TU Muenchen; [3]ETH Zurich; [4]TU Wien; lubich@na.uni-tuebingen.de

This talk is about the numerical approximation of evolution problems by nonlinear parametrizations u(t)=\Phi(q(t)) with time-dependent parameters q(t), which are to be determined in the computation. The motivation comes from approximations by multiple Gaussians and by tensor networks and by neural networks in various dynamical problems. The parametrization is typically irregular: the derivative \Phi'(q) can have arbitrarily small singular values and may have varying rank. We derive approximation results for a regularized approach in the time-continuous case as well as in time-discretized cases.

ID: 706 / MS10-1: 3

MS10 Recent Advances in Complexity Reduction for High-dimensional Problems

Sparse grid techniques for particle-in-cell simulation of kinetic plasmas

Lee Forrest Ricketson

Lawrence Livermore National Laboratory, United States of America; ricketson1@llnl.gov

The Vlasov model of plasmas is six-dimensional in general. The most prevalent method combatting this high dimensionality is particle-in-cell (PIC), which represents the system via particles interacting with fields on a spatial mesh. Use of particles introduces slow-converging sampling errors, while the spatial mesh permits only partial mitigation of the curse of dimensionality. We show that using sparse grids with PIC gives complexity depending only logarithmically on dimension, dramatically reducing sampling noise. We report progress combining sparse PIC with symplectic and implicit methods, then discuss ongoing work toward adaptive coordinate selection for sparse grids.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

MS11 Recent Advances in Scientific Computing and Learning

Organizers: Dong Wang (wangdong@cuhk.edu.cn), Roy He (royhe2@cityu.edu.hk), Hao Liu (haoliu@hkbu.edu.hk)

ID: 248 / MS11-1: 4

MS11 Recent Advances in Scientific Computing and Learning

Deep neural networks with mathematical background for image segmentation

Hao Liu

Hong Kong Baptist University, Hong Kong S.A.R. (China); haoliu@hkbu.edu.hk

For problems in image processing and many other fields, a large class of effective neural networks has encoder-decoder-based architectures. Although these networks have made impressive performances, mathematical explanations of their architectures are still underdeveloped. In this paper, we study the encoder-decoder-based network architecture from the algorithmic perspective and provide a mathematical explanation. Our PottsMGNet, an operator splitting scheme, incorporates the Potts model, control variables, multigrid method and operator splitting methods. We show that PottsMGNet is equivalent to an encoder-decoder-based network. It is shown that a number of the popular encoderdecoder-based neural networks are just instances of the proposed PottsMGNet.

ID: 249 / MS11-1: 3

MS11 Recent Advances in Scientific Computing and Learning

Mathematical and numerical study of the signal-propagation problem in axon

Tao Yin

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; yintao@lsec.cc.ac.cn

This talk will introduce our works on the modelling and analysis for the problem of signal propagation in myelinated axons to characterize the functions of the myelin sheath in the neural structure which is related to the wave scattering problems in open waveguids. Both the two-dimensional model in cylindrical coordinates and the three-dimensional model of full Maxwell's equations will be considered. The wellposedness and convergence analysis of the PML truncation will be discussed. Numerical experiments based on finite element discretization will also be presented. Some future works on the direct and inverse problems will be introduced.

ID: 250 / MS11-1: 1

MS11 Recent Advances in Scientific Computing and Learning

Fast Butterfly-compressed Hadamard-Babich Integrator for High-Frequency Helmholtz Equations in Inhomogeneous Media

Jianliang Qian[1], Yang Liu[2], Jian Song[1], Robert Burridge[3]

[1]Michigan State University, United States of America; [2]Lawrence Berkeley National Lab, Berkeley, CA, USA; [3]University of New Mexico, NM, USA; jqian@msu.edu

We present a butterfly-compressed representation of the Hadamard-Babich (HB) ansatz for the Green's function of the high-frequency Helmholtz equation in smooth inhomogeneous media. The resulting algorithm has almost linear complexity in both CPU time and memory. As a result, it can solve wave-propagation problems well beyond the capability of existing solvers. Remarkably, the proposed scheme can accurately model wave propagation in 2D domains with 640 wavelengths per direction and in 3D domains with 54 wavelengths per direction on a state-the-art supercomputer at Lawrence Berkeley National Laboratory.

ID: 251 / MS11-1: 2

MS11 Recent Advances in Scientific Computing and Learning

Fast minimization for curvature based regularization models based on bilinear decomposition

Huibin Chang

Tianjin Normal University, China, People's Republic of; changhuibin@tjnu.edu.cn

The curvature based regularization models can generate artifact-free results compared with the traditional total variation regularization model in image processing. However, strong nonlinearity and singularity due to the curvature term pose a great challenge for one to design fast and stable algorithms for the EE model. We propose a new, fast, hybrid alternating minimization (HALM) algorithm based on a bilinear decomposition of the gradient of the underlying image and prove the global convergence of the minimizing sequence generated by the algorithm under mild conditions.

ID: 252 / MS11-1: 5

MS11 Recent Advances in Scientific Computing and Learning

Well-posedness and numerical analysis of a class of hemivariational inequalities governed by fluid-fluid coupled flow

Feifei Jing

Northwestern Polytechnical University, China, People's Republic of; ffjing@nwpu.edu.cn

In this work, we explore the well-posedness and conduct numerical analysis of hemivariational inequalities for the coupled stationary Navier-Stokes/Navier-Stokes system. The interface condition involves the Clark subgradient and serves as a generalization of various interface interaction relations, including nonlinear transmission conditions and friction-type conditions.

We present an existence and uniqueness result for a solution of the continuous model. We propose a domain decomposition approach to solve the coupled system and examine the convergence of iterations.

Moreover, we use the finite element approximation to discretize the hemivariational inequality and derive error estimates. Numerical results are reported to illustrate the theoretical analysis.

ID: 255 / MS11-2: 1

MS11 Recent Advances in Scientific Computing and Learning

Phase field topology optimization in 3D and 4D printing

Harald Garcke[1], Kei Fong Lam[2], Robert Nurnberg[3], Andrea Signori[4]

[1]University of Regensburg, Germany; [2]Hong Kong Baptist University, Hong Kong S.A.R. (China); [3]University of Trento, Italy; [4]Politecnico di Milano, Italy; akflam@hkbu.edu.hk

3D printing refers to methodologies fabricating objects in a layer-by-layer fashion. Despite being able to build highly intricate and complex designs, one recurring issue relates to overhangs, which are regions that extend outwards without underlying support. This has led to the development of self-supporting designs that minimizes the regions where a so-called overhang angle constraint is violated. In this talk we extend previous phase-field topology optimization approaches to realize an overhang angle constraint with the help of a non-differentiable anisotropic perimeter functional. Subdifferential calculus is used to derive optimality conditions, and if time permits, we shall also discuss 4D printing.

ID: 259 / MS11-2: 2

MS11 Recent Advances in Scientific Computing and Learning

Wasserstein Hamiltonian Flow and Its Structure Preserving Numerical Schemes.

Jianbo Cui

Hong Kong Polytechnic University, China, People's Republic of; jianbo.cui@polyu.edu.hk

We study discretizations of Hamiltonian systems on the probability density manifold equipped with the L2-Wasserstein metric. Based on discrete optimal transport theory, several Hamiltonian systems, such as the Wasserstein geodesic equation and Schrodinger equation, on graph with different weights are derived. We prove the consistency and provide the approximate orders for those discretizations. By regularizing the system using Fisher information, we deduce an explicit lower bound for the density function, which guarantees that symplectic schemes can be used to discretize in time. Moreover, we show desirable long time behavior of these schemes, and demonstrate their performance on several numerical examples.

ID: 268 / MS11-2: 3

MS11 Recent Advances in Scientific Computing and Learning

Spherical Essentially Non-Oscillatory (SENO) Interpolation

Shingyu Leung

Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); masyleung@ust.hk

We will present the development of two new interpolation methods for S^2. In the first part of the talk, we will introduce a simple interpolation method called Spherical Interpolation of orDER-n (SIDER-n). This method generalizes the construction of Bezier curves developed for R. In the second part, we will incorporate the ENO philosophy and develop a new interpolation method called Spherical Essentially Non-Oscillatory (SENO). This method is specifically designed to address situations where the underlying curve on S^2 contains kinks or sharp discontinuities in the higher derivatives. Our proposed approach aims to reduce spurious oscillations in the high-order reconstruction.

ID: 399 / MS11-2: 4

MS11 Recent Advances in Scientific Computing and Learning

Convergence Analysis of Nonlinear Kaczmarz Method for Systems of Nonlinear Equations with Component-wise Convex Mapping

Chong Chen

Chinese Academy of Sciences, China, People's Republic of; chench@lsec.cc.ac.cn

Motivated by a class of nonlinear imaging inverse problems, for instance, multispectral computed tomography (MSCT), we study the convergence theory of the nonlinear Kaczmarz method (NKM) for solving the system of nonlinear equations with component-wise convex mapping, namely, the function corresponding to each equation being convex. However, such kind of nonlinear mapping may not satisfy the commonly used component-wise tangential cone condition (TCC). For this purpose, we propose a novel condition named relative gradient discrepancy condition (RGDC), and make use of it to prove the convergence and even the convergence rate of the NKM with several general index selection strategies.

ID: 423 / MS11-2: 5

MS11 Recent Advances in Scientific Computing and Learning

Efficient threshold dynamics methods for topology optimization for fluids and heat transfer problems

Huangxin Chen

Xiamen University, China, People's Republic of; chx@xmu.edu.cn

In this talk, we will introduce an efficient threshold dynamics method for topology optimization for fluids modeled with the Stokes equation. A one-domain approach is applied to solve the problem in the whole domain and the minimization problem can be solved with an iterative scheme. The total energy decaying property of the iterative algorithm can be obtained. The extensions of the iterative thresholding method will also be introduced for topology optimization for the Navier-Stokes flow and the heat transfer problems.

ID: 539 / MS11-3: 1

MS11 Recent Advances in Scientific Computing and Learning

Fast and accurate solvers for three dimensional wave scattering problems

Jun Lai

Zhejiang University, China, People's Republic of; laijun6@zju.edu.cn

The scattering problems for waves, including acoustics, electromagnetics and elastics, have recently received ever increasing attentions in both the engineering and mathematical communities for their important applications in geophysics, seismology and imaging. In this talk we will discuss some spectral accurate solvers for wave scattering problems in three dimensions via boundary integral equations. Their applications to the multi-particle scattering and inverse wave scattering will also be discussed.

ID: 633 / MS11-3: 2

MS11 Recent Advances in Scientific Computing and Learning

Rigidity of PDE operators on model identification from scarce data

Roy Yuchen He

City University of Hong Kong, Hong Kong S.A.R. (China); royhe2@cityu.edu.hk

Data-driven PDE identification is a rising research field and many algorithmic developments have been witnessed in recent years. Considering the sampling cost, it is often desirable to explore robust methods for scarce data, and mathematically, it is necessary to understand how this is possible. In this talk, we illustrate the problem of feasibility by arguing that PDE operators come with rigidity, which we characterize rigorously using microlocal analysis and dimension theory. Moreover, we propose an effective algorithm for learning PDEs from scarce data and demonstrate its performance in a series of experiments.

ID: 647 / MS11-3: 3

MS11 Recent Advances in Scientific Computing and Learning

Numerical Algorithms for Inverse Spectral Problems Based on Trace Formulas

XIANG XU

Zhejiang University, China, People's Republic of China; xxu@zju.edu.cn

In this talk, we will discuss some recent progress on numerical algorithms for inverse spectral problems for the Sturm-Liouville, Euler-Bernoulli and damped wave operator. Instead of inverting the map from spectral data to unknown coefficients directly, we propose a novel method to reconstruct the coefficients based on inverting a sequence of trace formulas which bridge the spectral and geometry information in terms of a series of nonlinear Fredholm integral equations. Numerical examples are presented to verify the validity and effectiveness of the proposed numerical algorithm. The impact of different parameters involved in the algorithm is also discussed.

ID: 710 / MS11-3: 4

MS11 Recent Advances in Scientific Computing and Learning

Modeling Randomness Effects in High-Entropy Alloys

Luchan Zhang

Shenzhen University, China, People's Republic of; zhanglc@szu.edu.cn

High-entropy alloys (HEAs) have novel mechanical properties. We propose a stochastic Peierls-Nabarro model to understand how random site occupancy affects intrinsic strength. The stochastic Peierls-Nabarro model accounts for the randomness in the composition, characterized by both the standard deviation of the randomness and the short range order. We find that compositional randomness induces an intrinsic strength. We also derive stochastic continuum models for HEAs from atomistic models that incorporate the atomic level randomness and the short-range order. These stochastic continuum models theoretically validate the randomness incorporation in our stochastic Peierls-Nabarro model.

MS12 Recent Advances in Inverse Problems and Imaging

Organizers: Liang Yan (yanliang@seu.edu.cn), Xiang Xu (xxu@zju.edu.cn)

ID: 241 / MS12-1: 1

MS12 Recent Advances in Inverse Problems and Imaging

A priori bounds and a reconstruction method for scattering and inverse scattering by random structures

Gang Bao[2], Yiwen Lin[1], Tianjiao Wang[2], Xiang Xu[2]

[1]Shanghai Jiao Tong University, People's Republic of China; [2]Zhejiang University, People's Republic of China; linyiwen@sjtu.edu.cn

In this talk, we will present a framework for the proof of a priori bounds explicitly with respect to frequencies for random surface scattering problems. By introducing a variable transform, the variational formulation in a random domain is reduced to that in a definite domain with random medium. Combining the stability result for the deterministic case, Pettis measurability theorem and Bochner's Theorem further yield the stability for random scattering problems. Besides, an MCCUQ reconstruction method is proposed for solving the inverse random surface scattering problem. Numerical results will demonstrate the reliability and efficiency of the proposed method.

ID: 296 / MS12-1: 2

MS12 Recent Advances in Inverse Problems and Imaging

Inverse scattering with multi-frequency sparse data

Xiaodong Liu

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, People's Republic of China; xdliu@amt.ac.cn

We present some mathematical theories and numerical algorithms for inverse scattering with multi-frequency sparse data. Precisely, we give a characterization of the number of the measurement sensors to uniquely determine the known objects. Some numerical algorithms arise based on the theoretical analyses. We will present the numerical simulations to verify the robustness and effectiveness of the proposed algorithms.

ID: 307 / MS12-1: 5

MS12 Recent Advances in Inverse Problems and Imaging

Deep decomposition method for the limited aperture inverse obstacle scattering problem

Yunwen Yin, Liang Yan

Southeast University, China, People's Republic of; yunwenyin@seu.edu.cn, yanliang@seu.edu.cn

It is well known that traditional deep learning relies solely on data, which may limit its performance for the inverse problem without ground truth labels. A fundamental question arises in light of these limitations: is it possible to enable deep learning to work on inverse problems without labeled data and to be aware of what it is learning? This work proposes a deep decomposition method (DDM) for such purposes. It accomplishes this by providing physical operators associated with the scattering model to the neural network architecture. Additionally, a deep learning based data completion scheme is implemented in DDM.

ID: 356 / MS12-2: 2

MS12 Recent Advances in Inverse Problems and Imaging

Obstacle scattering and inverse scattering in complex backgrounds

Lei Zhang

Zhejiang University of Technology, China; zhanglei@zjut.edu.cn

Extensive investigations into the scattering of electromagnetic waves by various composite targets have been conducted by numerous researchers over the past few decades. We analyze the rough surface inversion to the obstacle inverse scattering problem in large-scale surfaces and briefly introduce the theoretical and algorithmic research progress for the problems. Especially for the inverse obstacle scattering problems under a large-scale rough surface background. We proposed a numerical algorithm to achieve efficient inversion of the targets, and numerical examples also verified the effectiveness of the algorithm. Finally, we briefly introduce the research work we are currently carrying out.

ID: 357 / MS12-2: 1

MS12 Recent Advances in Inverse Problems and Imaging

Some results for the equivalent characterization of non-radiating sources

Jue Wang

Hangzhou Normal University, China; wangjue@hznu.edu.cn

This work offers an extensive exploration of non-radiating sources for the two- and three-dimensional biharmonic wave equations. Various equivalent characterizations are derived to reveal the nature of a non-radiating source. Additionally, we establish the connection between non-radiating sources in the biharmonic wave equation and those in the Helmholtz equation as well as the modified Helmholtz equation. Several illustrative examples are explicitly constructed to showcase the existence of non-radiating sources. One significant implication of the existence of non-radiating sources is that it undermines the uniqueness of the inverse source problem when utilizing boundary data at a fixed frequency.

ID: 368 / MS12-1: 3

MS12 Recent Advances in Inverse Problems and Imaging

Mathematical Theory for Electromagnetic Scattering Resonances and Field Enhancement in a Subwavelength Annular Gap

Wangtao Lu

Zhejiang University, China, People's Republic of; wangtaolu@zju.edu.cn

We present a mathematical theory for electromagnetic scattering resonances in a subwavelength annular hole embedded in a metallic slab, with the annulus width $h\ll1$. We develop a multiscale framework for the underlying scattering problem based upon a combination of the integral equation in the exterior domain and the waveguide mode expansion inside the tiny hole. It is shown that the resonances are associated with the TE/TEM waveguide modes in the annular hole, and they are close to the real axis with the imaginary parts of order ${\cal O}(h)$. Such a resonance structure can be used to realize super-resolution imaging.

ID: 484 / MS12-1: 4

MS12 Recent Advances in Inverse Problems and Imaging

The forward and inverse problems for the time-domain wave equation in three dimensions

Haibing Wang[1,2]

[1]Southeast University, China, People's Republic of; [2]Nanjing Center for Applied Mathematics, China, People's Republic of; hbwang@seu.edu.cn

In this talk, we will show our recent results on the forward and inverse problems for the time-domain wave equation in three dimensions. First, we consider an acoustic obstacle scattering problem and develop an efficient algorithm for solving it via a time-domain boundary intergral equation method. Then, we consider a time-domain multiple scattering problem and propose a decomposition method for efficiently solving it.

Finally, we study an inverse problem of recovering both the source and wave speed and propose a novel approach by injecting high contrast droplets.

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations

Organizers: Dimitri Breda (dimitri.breda@uniud.it), Dajana Conte (dajconte@unisa.it), Raffaele D'Ambrosio (raffaele.dambrosio@univaq.it)

ID: 290 / MS13-1: 3

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations

Sparse identification of stochastic delay differential equations

Dimitri Breda[1], Dajana Conte[2], Raffaele D'Ambrosio[3], Muhammad Tanveer[1], Ida Santaniello[2]

[1]University of Udine, Italy; [2]University of Salerno, Italy; [3]University of L'Aquila, Italy; tanveer.muhammad@spes.uniud.it

Recently, data-driven model discovery has emerged as a powerful approach to recover governing equations of dynamical systems from temporal data series. In particular, the SINDy algorithm, initially proposed for learning the right-hand side of ordinary differential equations, has been extended and applied to diverse classes of problems, including delay differential equations and stochastic (ordinary) differential equations. In this talk we present a further development by proposing a new SINDy algorithm to address the case of stochastic delay differential equations. A relevant MATLAB implementation is tested on several examples, including stochastic models with delay used to describe and investigate supply chains.

ID: 360

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations

Unified Framework for Momentum Stochastic Gradient Descent: Insights from Linear Multistep Methods

Qian Guo

Shanghai Normal University, China; qguo@shnu.edu.cn

This talk presents a novel analytical framework, derived from the linear multistep method for stochastic differential equations, to analyze the convergence behavior of momentum stochastic gradient descent methods. Our framework establishes connections between existing methods, like the stochastic heavy ball and Nesterov's accelerated methods, and the linear two-step method, demonstrating that they can be expressed as specific instances of the latter. This work offers valuable insights for analyzing and potentially improving stochastic gradient descent algorithms.

ID: 514 / MS13-1: 2

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations

Regularity and numerics for fractional stochastic elliptic PDEs on graphs

David Bolin[2], Mihály Kovács[1], Vivek Kumar[2], Alexandre B. Simas[3]

[1]Pázmány Péter Catholic University, Budapest University of Technology and Economics, Chalmers University of Technology; [2]King Abdullah University of Science and Technology; [3]Indian Statistical Institute; kovacs.mihaly@itk.ppke.hu

We consider fractional order elliptic problems on compact metric graphs and demonstrate the existence and uniqueness of solutions for a general class of vertex conditions. We determine the regularity of the solution in the specific case of Kirchhoff vertex conditions. We also consider a stochastic setting where the deterministic forcing is replaced by Gaussian white noise to define Gaussian Whittle–Matern fields on compact metric graphs as solutions. For the deterministic and stochastic settings, under generalized Kirchhoff vertex conditions, we propose and analyse a numerical method based on finite element approximation combined with a rational approximation of fractional powers of operators.

ID: 522 / MS13-1: 1

MS13 Numerical and Data-driven Tools for Stochastic Delay and Nonlocal Equations

On the Euler method for stochastic delay differential equations

Dimitri Breda[1], **Stefano Maset**[2]

[1]University of Udine, Italy; [2]University of Trieste, Italy; dimitri.breda@uniud.it

In this talk we investigate the use of the Euler method to integrate in time the initial value problem for stochastic delay differential equations (SDDEs). By considering a generic delay dependence, we focus on two possible methodologies which can extend the classic adaptation of the Euler-Maruyama scheme to SDDEs beyond the case of a single constant delay and a submultiple of such delay as constant stepsize. The first technique extends to the stochastic case a functional version of the Euler method. The second technique corresponds to an Euler semi-discretization of the associated abstract Cauchy problem.

MS14 Numerical Integration for Dispersive Problems

Organizers: Chunmei Su (sucm@tsinghua.edu.cn), Alexander Osterman (Alexander.Ostermann@uibk.ac.at)

ID: 282 / MS14-2: 2

MS14 Numerical Integration for Dispersive Problems

Bourgain techniques for low regularity error estimates

Lun Ji[1], **Alexander Ostermann**[1], **Frédéric Rousset**[2], **Katharina Schratz**[3]

[1]University of Innsbruck, Austria; [2]Université Paris-Saclay; [3]Sorbonne Université; Lun.Ji@uibk.ac.at

Standard time stepping techniques require a regularity constraint on the initial data u_0 for dispersive equations. We introduce a class of filtered integrators for problems where certain constraints are not satisfied. Moreover, when the regularity is critically low ($u_0\in H^s$ with $s\leq d/2$), the classical stability argument based on Sobolev spaces does not hold. We have developed a framework of Bourgain spaces that overcomes this problem. In this talk, I will summarize how these techniques are applied.

ID: 303 / MS14-2: 3

MS14 Numerical Integration for Dispersive Problems

An explicit and symmetric exponential wave integrator for the nonlinear Schr\"{o}dinger equation with low regularity potential and nonlinearity

Weizhu Bao, **Chushan Wang**

Department of Mathematics, National University of Singapore, Singapore; chushanwang@u.nus.edu

We propose and analyze a novel symmetric exponential wave integrator (sEWI) for the nonlinear Schr\"odinger equation (NLSE) with low regularity potential and nonlinearity. The sEWI is explicit and stable under a time step size restriction independent of the mesh size. We rigorously establish error estimates of the sEWI under various regularity assumptions on potential and nonlinearity. Extensive numerical results are reported to confirm our error estimates and to demonstrate the superiority of the sEWI, including much weaker regularity requirements on potential and nonlinearity and excellent long-time behavior with near conservation of mass and energy.

ID: 313 / MS14-1: 4

MS14 Numerical Integration for Dispersive Problems

Improved Uniform Error Bounds on Time-splitting Methods for Long-time Dynamics of Dispersive PDEs

Yue Feng

Xi'an Jiaotong University, China, People's Republic of; fengyue@u.nus.edu

In this talk, I begin with the nonlinear Klein-Gordon equation (NKGE) with weak nonlinearity, which is characterized by with a dimensionless parameter. Different numerical methods are applied to discretize the NKGE including finite difference methods, exponential wave integrators and time-splitting methods. By introducing a new technique—Regularity Compensation Oscillation (RCO) which controls the high frequency modes by the regularity of the exact solution and analyzes the low frequency modes by phase cancellation and energy method, we carry out the improved uniform error bounds for the time-splitting methods. The results have been extended to other dispersive PDEs including the (nonlinear) Schrodinger equation and Dirac equation.

ID: 315 / MS14-1: 2

MS14 Numerical Integration for Dispersive Problems

Numerical approximation of discontinuous solutions of the semilinear wave equation

Jiachuan Cao, Buyang Li, Yanping Lin, Fangyan Yao

The Hong Kong Polytechnic University; buyang.li@polyu.edu.hk

A high-frequency recovered fully discrete low-regularity integrator is constructed to approximate rough and possibly discontinuous solutions of the semilinear wave equation. The proposed method, with high-frequency recovery techniques, can capture the discontinuities of the solutions correctly without spurious oscillations and approximate rough and discontinuous solutions with a higher convergence rate than pre-existing methods. The proposed method is proved to have almost first-order convergence under the stepsize condition $\Delta t=O(1/N)$ for approximating discontinuous solutions of bounded variation in one dimension (which allow jump discontinuities), where Δt and N denote the time stepsize and the number of Fourier terms in the space discretization, respectively.

ID: 472 / MS14-1: 3

MS14 Numerical Integration for Dispersive Problems

The non-relativistic limits of nonlinear quantum field equations

Yifei Wu

Tianjin University, China, People's Republic of; yerfmath@gmail.com

In this talk, we will present some of the recent developments on the non-relativistic limits of nonlinear quantum field equations, including theoretical and numerical analysis works.

ID: 492 / MS14-2: 1

MS14 Numerical Integration for Dispersive Problems

Unitary rational approximations for the matrix exponential

Tobias Jawecki[1], **Pranav Singh**[2]

[1]TU Wien, Austria; [2]University of Bath, United Kingdom; ps2106@bath.ac.uk

Approximation to the matrix exponential is an important tool for solving a large class of linear, non-linear and non-autonomous ODEs and PDEs with oscillatory-in-time behaviour, prominent examples being Schrodinger equations and related equations of quantum mechanics such as Dirac, Pauli and Liouville--von Neumann equations, among others. In this talk, I will discuss some recent results on unitary rational approximations for the matrix exponential, including the surprising geometric numerical integration properties of AAA and AAA—Lawson methods, as well as existence, uniqueness, characterization and convergence rates for unitary rational best approximations, and their application to the matrix exponential.

ID: 593 / MS15-2: 3

MS14 Numerical Integration for Dispersive Problems

Error estimates of numerical methods for the Dirac equation

YING MA

Beijing University of Technology; maying@bjut.edu.cn

We present various numerical methods including the finite difference methods, symmetric and asymmetric exponential wave integrator Fourier pseudospectral methods, and establish error estimates for fully discrete schemes of the Dirac equation in the massless and nonrelativistic regime. This regime involves a small dimensionless parameter that is inversely proportional to the speed of light. The solution exhibits highly oscillatory behavior in time and rapid propagation waves in space in this regime. Extensive numerical results are reported to support our error estimates.

ID: 598 / MS15-2: 4

MS14 Numerical Integration for Dispersive Problems

Radiation fields for semilinear Dirac equations with spinor null forms

Jiong-Yue Li

Sun Yat-sen University, China, People's Republic of; lijiongyue@mail.sysu.edu.cn

We will talk about the scattering theory of half spin waves by the means of the radiation fields. We first define the radiation fields for semilinear Dirac equations with spinor null forms. Then we prove a nonlinear isomorphism between the weighted energy space of initial data and the weighted energy space of radiation fields. The proof is based on a careful study of the linear Dirac radiation fields combined with a functional framework. In the last, we also present a rigidity result. This is a joint with JIN JIA.

ID: 623 / MS14-1: 1

MS14 Numerical Integration for Dispersive Problems

Simulation of asymmetric interface transport in topological insulators

Guillaume Bal

University of Chicago, United States of America; guillaumebal@uchicago.edu

The surprising robustness to perturbation of the asymmetric transport observed along interfaces separating distinct insulating bulks affords a topological origin. This talk briefly reviews the classification of partial differential operators modeling such systems and the bulk-edge correspondence describing the non-trivial interface topology. We then present a scattering theory characterizing it quantitatively as well as integral formulations allowing us to compute such interface transport numerically. The theory is illustrated with examples of application in condensed matter physics and geophysics.

ID: 709 / MS14-2: 4

MS14 Numerical Integration for Dispersive Problems

Filtered Lie-Trotter splitting for the "good" Boussinesq equation: low regularity estimates

Lun Ji, Hang Li, Alexander Ostermann, Chunmei Su

Tsinghua University, China, People's Republic of; lihang20@mails.tsinghua.edu.cn

We investigate a filtered Lie-Trotter splitting scheme for the "good" Boussinesq equation and derive an error estimate for initial data with very low regularity. Through the use of discrete Bourgain spaces, our analysis extends to initial data in H^s for $0 < s \leqslant 2$, overcoming the constraint of $s > 1/2$ imposed by the bilinear estimate in smooth Sobolev spaces. We establish con- vergence rates of order $\tau^{\frac{s}{2}}$ in L^2 for such levels of regularity. Our analytical findings are supported by numerical experiments.

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

Organizers: Hanquan Wang (wang_hanquan@hotmail.com), Yan Wang (wang.yan@ccnu.edu.cn)

ID: 189 / MS15-2: 1

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

Numerical methods for Bogoliubov-de Gennes excitations of Bose-Einstein condensates

Yali Gao

Northwestern Polytechnical University, China; gaoylimath@nwpu.edu.cn

In this talk, we present the analytical properties and the numerical methods for the Bogoliubov-de Gennes equations, which describe the elementary excitation of Bose-Einstein condensates around the mean-field ground state. Derived analytical properties of the BdGEs can serve as benchmark tests for numerical algorithms, and efficient numerical methods are proposed to solve the BdGEs. Extensive numerical tests are performed to validate the effectiveness of the algorithms. Finally, the sine-spectral method is extended to study elementary excitations under the optical lattice potential and to solve the BdGEs around the first excited states of the GPE.

ID: 318 / MS15-2: 2

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

Numerical methods for the logarithmic Dirac equation

Wenfan Yi

Hunan University, China, People's Republic of; wfyi@hnu.edu.cn

In this talk, we consider numerical methods to tackle numerical challenges for solving the logarithmic Dirac equation (LogDiracE). To address this, we propose a regularized LogDiracE with the linear convergence to

the LogDiracE concerning a small regularization parameter for the bounded domain case. Then, a semi-implicit finite difference method, the physical information-based neural network method and the Fourier neural operator method are introduced to consider the regularized LogDiracE. These approaches guarantee a controlled solution that facilitates reliable simulations without succumbing to the logarithmic nonlinearity challenges for the LogDiracE. Numerical results demonstrate the effectiveness of these approaches for the LogDiracE.

ID: 363 / MS15-1: 4

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

A fourth-order compact time-splitting method for the Dirac equation

Jia Yin[1], Weizhu Bao[2], Chen Xianzhe

[1]Lawrence Berkeley National Laboratory; [2]National University of Singapore; cordelia_jia@outlook.com

We propose a new fourth-order compact time-splitting (S_{4c}) Fourier pseudospectral method for the Dirac equation by splitting the Dirac equation into two parts together with using the double commutator between them to integrate the Dirac equation at each time interval. The method is explicit, fourth-order in time and spectral order in space. At each time step, the number of substeps in S_{4c} is much less than those of the standard fourth-order splitting method and the fourth-order partitioned Runge-Kutta splitting method. We also extend the proposed method to the Dirac equation with time-dependent potentials.

ID: 538 / MS15-1: 1

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

An asymptotic preserving scheme for the defocusing Davey-Stewartson II equation in the semiclassical limit

Hanquan Wang

Yunnan University of Finance and Economics, China, People's Republic of; hanquan.wang@gmail.com

We devote to introducing a modified Madelung transform for the semiclassical limit of the defocusing DS II equation.Meanwhile,adding some asymptotically vanishing viscosity to obtain approximatively the solution on arbitrary time intervals for $\varepsilon>0$.In order to avoid the singular symbol appears in the Fourier space,we apply Sine spectral method to the non-local potential.Moreover, we demonstrate the system is always locally well-posed in a class of Sobolev spaces, and indeed asymptotic preserving. Before the formation time of oscillations,numerous experiments corroborate the fact that the time-splitting spectral method is uniformly accurate with order 2 in time and with spectral in space accuracy.

ID: 558 / MS15-1: 3

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

An accurate and efficient numerical method to compute the ground states of the rotating spin-orbit coupled spin-1 Bose-Einstein condensates

Yongjun Yuan

Hunan Normal University, China, People's Republic of; yuanyongjun0301@163.com

In this talk, an efficient and accurate preconditioned nonlinear conjugate gradient (PCG) method is designed to solve the ground states of rotating spin-orbit coupled spin-1 Bose-Einstein condensates (SOC spin-1 BECs) with an explicit approximate optimal step size for each iteration and a cascadic multigrid acceleration strategy. Based on extensive numerical experiments, the ground states of SOC spin-1 BECs under different parameters are demonstrated and some interesting physical phenomena are discovered.

ID: 576 / MS15-1: 2

MS15 Efficient and High-order Numerical Methods for Problems in Quantum Physics

A Spectrally Accurate Numerical Method For Computing The Bogoliubov-De Gennes Excitations Of Dipolar Bose-Einstein Condensates

Yong ZHANG

Tianjin University, China, People's Republic of; sunny5zhang@163.com

we introduce an efficient and robust numerical method to study the elementary excitation of dipolar Bose-Einstein condensates (BEC) around the mean field ground state. To evaluate the nonlocal interactions accurately and efficiently, we propose a new Simple Fourier Spectral Convolution method (SFSC). Then, integrating SFSC with the stan- dard Fourier spectral method for spatial discretization and Implicitly Restarted Arnoldi Methods (IRAM) for the eigenvalue problem, we derive an efficient and spectrally accurate method, named as SFSC-IRAM method, for the BdGEs. Finally, we apply the new method to study systematically the excitation spectrum and Bogoliubov amplitudes .

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms

Organizers: Pranab J Deka (pranab.deka@kuleuven.be)

ID: 430 / MS16-1: 2

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms

Computation of phi functions for exponential integrators

Markus Neher

KIT, Germany; markus.neher@kit.edu

Exponential integrators rely on the computation of phi functions for matrix arguments. Our talk is concerned with the computation of $\varphi_k(A)$ or $\varphi_k(A)b$, where A is a square matrix and b is a vector, both of moderate size.

The traditional scaling and squaring method for $\varphi_k(A)$ works as follows: When the norm of A is sufficiently small, $\varphi_k(A)$ is computed from a Padé approximation of φ_k. Otherwise, $\varphi_k(A)$ is computed recursively from function values $\varphi_j(A/2)$, $j = 0,\dots,k$.

In our talk, we develop new recurrence schemes for the phi functions. Numerical experiments show that these are competitive with existing formulas.

ID: 436 / MS16-1: 4

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms

Low Synchronization Arnoldi Methods with Application to Exponential Integrators

Tanya Vanessa Tafolla[1], Stephane Gaudreault[2], Mayya Tokman[1]

[1]University of California, Merced, United States of America; [2]Environment and Climate Change Canada; ttafolla@ucmerced.edu

Krylov subspace methods have a long history with exponential integrators due to their efficiency for computing exponetial-like functions for problems involving large matrices that are difficult to compute explicitly or store due to memory issues, or when obtaining information about the spectrum of a matrix is expensive. However, Krylov methods rely on the Arnoldi decomposition, which does not scale well in parallel due to the global communication from the inner products in the orthogonalization and vector normalization. We improve the parallel scalability of efficiency of exponential integators by introducing low-synchronization Arnoldi methods and demonstrate the improved performance on geophysical applications.

ID: 526 / MS16-1: 3

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms

A Krylov subspace exponential integrator based on the Adams-Bashforth method

Jitse Niesen

University of Leeds, United Kingdom; j.niesen@leeds.ac.uk

Exponential integrators are methods for the solution of ordinary differential equations which use the matrix exponential in some form. These methods are well suited for stiff ordinary differential equations where the stiffness is concentrated in the linear part. Over ten years ago, Will Wright and the speaker wrote some code called phipm for the computing the matrix exponential with Krylov methods. This talk will discuss how to embed this in an Adams-Bashforth exponential integrator and evaluate the resulting method against recent developments.

ID: 552 / MS16-1: 1

MS16 Recent Advances in Time Integration: Exponential Integrators and Algorithms

Parallelism and Exponential Integration

Tommaso Buvoli

Tulane University, New Orleans, LA, USA; tbuvoli@tulane.edu

Exponential integrators are a class of time integration methods for efficiently solving stiff ordinary differential equations. A key characteristic of these methods is that they treat a linear component exactly and approximate all remaining terms explicitly. In this talk I will discuss different strategies for incorporating parallelism into exponential integrators. Specifically, I will discuss exponential integrators that incorporate parallelism within the method (i.e., parallel function evaluations and output computations), and larger-scale exponential parallel-in-time methods that parallelize across multiple timesteps. I will highlight the performance of these methods compared to serial integrators, and broadly highlight the advantages of exponential integration over other method families.

MS17 Recent Advances in Structure Preserving Numerical Methods

Organizers: Alexander Ostermann (alexander.ostermann@uibk.ac.at), Zhonghua Qiao (zqiao@polyu.edu.hk)

ID: 179 / MS17-1: 3

MS17 Recent Advances in Structure Preserving Numerical Methods

A nonconventional stability analysis for a Crank-Nicolson scheme solving degenerate quenching equations

QIN SHENG

Baylor University, United States of America; qin_sheng@baylor.edu

Conventionally, the numerical stability of finite difference approximations of a semi-linear quenching equation is shown via frozen source terms, that is, ignoring potential jeopardization from quenching nonlinearities. The approach leaves an inadequacy

behind even in the sense of localized stability analysis. This talk introduces a much improved analysis of the numerical stability without freezing nonlinear source terms of the underlying equation. The strategy implemented can be extended for the numerical solution of similar singular partial differential equations. Simulation experiments will be presented.

ID: 390 / MS17-1: 1

MS17 Recent Advances in Structure Preserving Numerical Methods

Unconditionally energy-stable algorithms for porous media flow: From the Darcy scale to the Pore Scale

Shuyu Sun

King Abdullah University of Science and Technology (KAUST), Saudi Arabia; shuyu.sun@kaust.edu.sa

In this work, we present our work in unconditionally energy-stable algorithms for porous media flow at various scales. First, a novel, efficient and structure-preserving Smoothed Particle Hydrodynamics (SPH) method is proposed for pore-scale two-phase flow modeled by the Navier–Stokes–Cahn–Hilliard (NSCH) system. In addition to preserve the conservation of mass, the conservation of linear momentum and the conservation of angular momentum in the discrete solution, our scheme is unconditionally energy-stable. Second, we present new semi-implicit algorithms for Darcy two-phase flow with multiple capillary pressure functions. A few interesting examples are presented to demonstrate the efficiency and robustness of the new algorithms.

ID: 391 / MS17-1: 2

MS17 Recent Advances in Structure Preserving Numerical Methods

Deep adaptive density approximation for Fokker-Plank type equations

Tao Zhou

Chinese Academy of Sciences, China, People's Republic of; tzhou@lsec.cc.ac.cn

We propose adaptive deep learning method based on normalizing flow for Fokker-Planck equations. The solution of such equation is a probability density function. Traditional mesh-based methods may across difficulties since the dimension of spatial variable can be very high. To this end, we represent the solution by a flow-based generative model which constructs a mapping from a simple distribution to the target distribution. An adaptive procedure for choosing the training set is presented. Numerical examples are presented to show the effectiveness of the proposed approach. Finally, we design bounded KRnet and show applications to Keller-Segel equations and kinetic Fokker-Planck equations.

ID: 392 / MS17-2: 5

MS17 Recent Advances in Structure Preserving Numerical Methods

Energy stable and maximum bound principle preserving schemes for the Q-tensor flow of liquid crystals

Zhonghua Qiao

The Hong Kong Polytechnic University, Hong Kong S.A.R. (China); zqiao@polyu.edu.hk

We propose two efficient fully-discrete schemes for Q-tensor flow of liquid crystals by using the first- and second-order stabilized exponential scalar auxiliary variable (sESAV) approach in time and the finite difference method for spatial discretization. The modified discrete energy dissipation laws are unconditionally satisfied for both two constructed schemes. A particular feature is that, for two-dimensional and a kind of three-dimensional Q-tensor flows, the unconditional maximum-bound-principle (MBP) preservation of the constructed first-order scheme is successfully established, and the proposed second-order scheme preserves the discrete MBP property with a mild restriction on the time-step sizes.

ID: 417 / MS17-2: 3

MS17 Recent Advances in Structure Preserving Numerical Methods

Exponential time differencing-Padé finite element method for nonlinear convection diffusion reaction equations with time constant delay

Qiumei Huang

Beijing University of Technology, China, People's Republic of China; qmhuang@bjut.edu.cn

In this talk, ETD3-Padé and ETD4-Padé Galerkin finite element methods are proposed and analyzed for nonlinear delayed convection-diffusion-reaction equations with Dirichlet boundary conditions. An ETD-based RK is used for time integration of the corresponding equation. To overcome a well-known difficulty of numerical instability associated with the computation of the exponential operator, the Padé approach is used for such an exponential operator approximation, which in turn leads to the corresponding ETD-Padé schemes. An unconditional L2 numerical stability and convergence are proved for the proposed numerical schemes. Numerical experiments are presented to demonstrate the robustness of the proposed numerical schemes.

ID: 497 / MS17-2: 4

MS17 Recent Advances in Structure Preserving Numerical Methods

Convergence analysis of a positivity-preserving numerical scheme for the Cahn-Hilliard-Stokes system with Flory-Huggins energy potential

Yunzhuo Guo[1], Cheng Wang[2], Steven M. Wise[3], Zhengru Zhang[4]

[1]Beijing Normal University, China, People's Republic of; [2]The University of Massachusetts, USA; [3]The University of Tennessee, USA; [4]Beijing Normal University, P.R. China; yunzguo@mail.bnu.edu.cn

A convex-splitting finite difference scheme is proposed for the Cahn-Hilliard-Stokes system with Flory-Huggins energy. The positivity-preservation and unique solvability are justified, utilizing the singular nature of the logarithmic term as the phase variable approaches the singular limit values. An unconditional energy stability analysis is standard, as an outcome of the convex-concave decomposition technique. The convergence analysis is provided. In particular, a higher-order consistency analysis is performed to ensure the separation property of the numerical solution. In turn, using the approach of rough and refined error estimates, an optimal rate convergence is derived.

ID: 687 / MS17-1: 4

MS17 Recent Advances in Structure Preserving Numerical Methods

Data Augmentation for Neural Operator-Based PDE Solvers through Inverse Evolution

Chaoyu Liu

University of Cambridge, United Kingdom; cl920@cam.ac.uk

Neural networks have emerged as promising tools for solving partial differential equations (PDEs), particularly through the efficacy of neural operators. In this talk, we introduce a novel data augmentation method tailored to training neural operators for evolution equations, leveraging insights from their inverse processes. This attribute significantly economizes computational memory. Experiments demonstrate a substantial improvement in the performance of neural operator-based PDE solvers, especially when the data size is small.

ID: 689 / MS17-1: 5

MS17 Recent Advances in Structure Preserving Numerical Methods

Functional Equivariance and Modified Vector Fields

Sanah Suri

Washington University in St. Louis, United States of America; s.sanah@wustl.edu

Certain numerical integrators preserve geometric properties of the flow of differential equations. McLachlan and Stern introduced the idea of F-functional equivariance, a new framework generalizing the preservation of first integrals and other notable observables of a system. This talk will extend the idea of F-functional equivariance to backward error analysis and modified vector fields. We generalize results on invariant preservation, describe the numerical evolution of non-invariant observables, and show algebraic characterizations of F-functionally equivariant B-series.

ID: 719 / MS17-2: 1

MS17 Recent Advances in Structure Preserving Numerical Methods

Recent progress on topology optimization

Xiaoping Wang[1,2]

[1]The Chinese University of Hong Kong, Shenzhen, China, People's Republic of; [2]Shenzhen International Center on Industrial and Applied Mathematics,; wangxiaoping@cuhk.edu.cn

In this talk, I will give an introduction on a new method for topology optimization based on threshold dynamics method. Applications to linear elasticity, fluid network and porous media problems will be discussed. The method is also combined with diffusion model (generative machine model) to enhance the efficiency of the method.

ID: 725 / MS17-2: 2

MS17 Recent Advances in Structure Preserving Numerical Methods

Operator splitting schemes for port-Hamiltonian differential-algebraic equations

Michael Günther[1], **Andreas Bartel**[1], **Andreas Frommer**[1], **Malak Diab**[1], **Nicole Marheineke**[2]

[1]Bergische Universität Wuppertal, Germany; [2]Universität Trier, Germany; guenther@uni-wuppertal.de

The energy-based formulation of port-Hamiltonian differential algebraic systems (pH-DAEs) encodes physical properties directly into the equations. This paper focuses on operator-splitting techniques that preserve the structure in the port-Hamiltonian framework. The study explores two decomposition strategies:

one considering the underlying coupled subsystem structure and the other addressing energy-associated properties such as conservation and dissipation. The effectiveness of both strategies is evaluated using port-Hamiltonian benchmark examples from electric circuits.

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

Organizers: Qing Cheng (qingcheng@tongji.edu.cn), Fukeng Huang (hfkeng@nus.edu.sg), Jie Shen (jshen@eitech.edu.cn), Jiang Yang (yangj7@sustech.edu.cn)

ID: 183 / MS18-2: 2

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

New fully decoupled and high-order algorithms with optimal energy approximationfor the Cahn-Hilliard-Navier-Stokes phase field model

Xiaoli Li

Shandong University; xiaolimath@sdu.edu.cn

In this talk we present new fully decoupled and high-order implicit-explicit (IMEX) schemes for the Cahn-Hilliard-Navier-Stokes phase field model. These schemes are linear, fully decoupled, unconditionally energy stable, only require solving a sequence of elliptic equations with constant coefficients at each time step, and provide a new technique to preserve the consistency between original energy and modified energy. We carry out a rigorous error analysis for the first-order scheme and establish optimal global error estimates for the phase function, velocity and pressure in two and three-dimensional cases.

ID: 253 / MS18-2: 5

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

New unconditionally stable higher-order consistent splitting schemes for the Navier-Stokes equations

Fukeng Huang[1], Jie Shen[2]

[1]National University of Singapore, Singapore; [2]Eastern Institute of Technology Ningbo, China; hfkeng@nus.edu.sg

The consistent splitting schemes for the Navier-Stokes equations decouple the computation of pressure and velocity. However, only the first-order version of the consistent splitting schemes is proven to be unconditionally stable for the time dependent Stokes equations. We construct a new class of consistent splitting schemes of orders two to four for Navier-Stokes equations based on Taylor expansions at time t_{n+k} with $k\ge 1$. By choosing suitable k, we construct, for the first time, unconditionally stable and totally decoupled schemes of orders two to four for the velocity and pressure, and provide rigorous optimal error estimates.

ID: 254 / MS18-1: 5

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

A structure-preserving method to the Boltzmann equation

Bo Lin, Zhenning Cai

National University of Singapore, Singapore; matbl@nus.edu.sg

The Boltzmann equation is fundamental in kinetic theory, embodying conservation laws for mass, momentum, and energy, along with entropy dissipation. We propose a spectral method that ensures these properties are preserved and rigorously demonstrate its spectral accuracy. Our numerical experiments confirm the validity of our approach.

ID: 440 / MS18-1: 3

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

A new flow dynamic approach for Wasserstein gradient flows

Qing Cheng

Tongji University, China, People's Republic of; qingcheng@tongji.edu.cn

We develop a new flow dynamic approach for Wasserstein gradient flows. Motivatied by the classic JKO scheme, we develop a new class of Lagrangian schemes which only need to solve minimization problems with respective to displacement instead of density and velocity. The new approach can effectively capture the movement of the trajectory of meshes, and also can automatically preserve the nice properties of Wasserstein gradient flow structure,for example, positivitypreserving, mass conserving and energy dissipation. Numerical experiments are shown in 1D and 2D for Keller-Segel equations, Focker-Planck equations, Porous medium equations.

ID: 456 / MS18-2: 3

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

STURCTURE PRESERVING IMPLICIT-EXPLICIT RUNGE-KUTTA METHODS FOR GRADIENT FLOWS

Zhaohui Fu

National University of Singapore, Singapore; fuzhmath@nus.edu.sg

In this work, we construct and analyze a class of high-order implicit-explicit (IMEX)

Runge–Kutta (RK) methods for the time discretization of gradient flows with Lipschitz continuous nonlinear term. We show that these IMEX-RK schemes preserve the original energy dissipation property with no constraint on the time-step size. We also provide the rigorous estimate of the optimal convergence rate. To the best of our knowledge, this is the first linear high-order single-step scheme which guarantees the unconditional original energy stability for general gradient flows. Moreover, numerical examples are provided to illustrate the discrete energy decay and accuracy of the proposed methods.

ID: 569 / MS18-1: 1

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

A Thermodynamically Consistent Nonisothermal Hydrodynamical Model for Binary Fluids with Cross-Coupling

Qi Wang

University of south Carolina, United States of America; qwang@math.sc.edu

We present a general thermodynamically consistent nonisothermal hydrodynamical model for binary fluids, incorporating cross-coupling effects between the materials' phase, velocity, and temperature. Guided by the entropy quadratization method in time, we introduce a theoretical paradigm to derive second-order, entropy-production-rate preserving numerical algorithms for the general model. Mesh refinement tests are conducted to confirm the convergence of the scheme, and numerical results for three distinct cases of the

model, corresponding to three distinct types of phases and temperature coupling, are investigated to showcase the potential cross-coupling effects in describing relevant interface dynamics.

ID: 595 / MS18-2: 1

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

A linearly implicit energy-preserving method for the logarithmic Klein-Gordon equation

Qingzhou Shu[1], Chunmei Su[2], Qinglin Tang[1]

[1]Sichuan University, China, People's Republic of; [2]Tsinghua University, China, People's Republic of; qinglin_tang@163.com

In this talk, we will propose a linearly implicit energy-preserving method for the logarithmic Klein-Gordon equation. We will first propose a local Lagrangian regularization (LLR) method to regularize the logarithmic Klein-Gordon equation (LogKGE) to avoid singularity caused by the logarithmic nonlinearity, which leading to a LLR logarithmic Klein-Gordon equation (LLRLogKGE) with a small regularization parameter $0 < \varepsilon \ll 1$. A linearly implicit energy-preserving Fourier pseudo-spectral scheme via a numerical Lagrange multiplier (LagM- CNLF) is then proposed to discretize the LLRLogKGE. Ample numerical examples are then given to validate the method. Stability and interaction of solitons under different setups are also presented.

ID: 728 / MS18-1: 2

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

APTT: An accuracy-preserved tensor-train method for the Boltzmann-BGK equation

Zhitao Zhu, Chuanfu Xiao, Kejun tang, Jizu Huang, Chao Yang

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; huangjz@lsec.cc.ac.cn

In this talk, we propose a novel accuracy-preserved tensor-train (APTT) method to solve the Boltzmann-BGK equation. At each time step, the linear system is constructed with the tensor-train (TT) format, where the matrix, the right-hand side, and the collision term involved in the linear system are all represented using the low-rank TT format. Based on such a representation, an efficient and effective iterative solver can be implemented for solving the linear system, which can reduce two orders of magnitude in terms of both time and memory costs compared with classical methods.

ID: 736 / MS18-2: 4

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

Highly Efficient Numerical Methods for Energy Dissipative/Conservative Nonlinear Systems

Yanrong Zhang

Southern University of Science and Technology, China; yanrongzhang_math@163.com

In this talk, the first part introduces the application of the relaxed Scalar Auxiliary Variable (SAV) method to solve general dissipative systems. This involves using relaxation factor techniques to adjust the SAV, thereby ensuring that the revised modified energy closely approximates the original energy. Then we focus on the preservation of constraints, encompassing both global and local constraints. The second part will discuss the application of the Lagrange multipliers method to maintain global constraints. Next will explore strategies for preserving local constraints, specifically through the development of numerical schemes that preserve a lower density bound in variable-density Navier-Stokes equations.

ID: 739 / MS18-1: 4

MS18 Recent Advances in Structure-preserving Numerical Methods for Complex Nonlinear Systems

Structure-preserving Oscillation-Eliminating Hermite WENO Method for Hyperbolic Systems

Chuan Fan

Southern university of Science and technology, China, People's Republic of; fanc@sustech.edu.cn

In this presentation, we first propose high-order accurate, oscillation-eliminating, Hermite weighted essentially non-oscillatory (OE-HWENO) finite volume schemes for hyperbolic conservation laws. The OE-HWENO schemes incorporate an oscillation-eliminating (OE) procedure after each Runge--Kutta stage, by damping the first-order moments of the HWENO solution to suppress spurious oscillations without any problem-dependent parameter. To achieve the well-balanced and positivity-preserving properties simultaneously, then we design the structure-preserving OE-HWENO method to solve a class of hyperbolic systems with source terms. Extensive benchmarks validate the accuracy, efficiency, high resolution, and robustness of the OE-HWENO method.

MS19 Recent Advances in Theories and Computations of Liquid Crystals

Organizers: Lei Zhang (pkuzhangl@pku.edu.cn), Jingmin Xia (jingmin.xia@nudt.edu.cn)

ID: 238 / MS19-1: 1

MS19 Recent Advances in Theories and Computations of Liquid Crystals

Classical density functional theory for colloidal liquid crystals: predicting phase behavior and topological defects from first principles

René Wittmann

Heinrich-Heine-Universität Düsseldorf, Germany; rene.wittmann@hhu.de

Fundamental-measure based classical density functional theory (DFT) allows to predict the phase behavior and the structure of anisotropic colloidal model fluids with hard-core excluded-volume interactions only from the particle shape. In this presentation, I provide a general introduction to the versatile framework of DFT and present results for colloidal liquid crystals, ranging from the analytic investigation of biaxial nematic order to resolving the fine structure of topological defects in two-dimensional confined smectics.

ID: 308 / MS19-1: 2

MS19 Recent Advances in Theories and Computations of Liquid Crystals

Quasi-entropy

Jie Xu

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; xujie@lsec.cc.ac.cn

Local anisotropy in liquid crystals is usually described by angular moment tensors. The free energy needs a stabilizing entropy term. When non-axisymmetric molecules are involved, two classical approaches to write down an entropy term, quartic polynomial and maximum entropy state, become too complicated. We propose an elementary-function substitution of the original entropy (by maximum entropy state), called quasi-entropy, maintaining the essential properties: strict convexity; positive-definiteness of covariance matrix; rotational invariance; consistency in symmetry reduction. Homogeneous phase diagrams of several

representative cases match well with classical results. A preliminary application is deriving biaxial frame hydrodynamics from tensor model.

ID: 631 / MS19-1: 3

MS19 Recent Advances in Theories and Computations of Liquid Crystals

From Polyatomic Gas to Liquid Crystals: A Kinetic Approach

Umberto Zerbinati[1], **Patrick E. Farrell**[1], **Giovanni Russo**[2]

[1]University of Oxford, UK; [2]University of Catania, Italy; zerbinati@maths.ox.ac.uk

Presenting a novel kinetic model for calamitic fluids, we diverge from traditional Curtiss theory by incorporating nematic ordering. Through a kinetic point of view, we derive an energy functional akin to the Oseen-Frank energy, enhancing understanding of anisotropic effects. Employing the Noll-Coleman procedure we obtain a novel expression for stress and couple-stress tensors. Additionally, we explore nematoacoustic phenomena and develop an existence and uniqueness theory for stationary solutions of modified Leslie-Eriksen equations with a prescribed nematic field, utilizing Muckenhoupt weighted Sobolev spaces.

ID: 692 / MS19-1: 4

MS19 Recent Advances in Theories and Computations of Liquid Crystals

Recent progress on the hyperbolic Ericksen-Leslie system for liquid crystals

Ning Jiang

Wuhan University; njiang@whu.edu.cn

We review some recent progrss on the Ericksen-Leslie system for liquid crystals, in which we keep the inertial effect. This makes the system as the coupling of incompressible Navier-Stokes system and wave map type equtions with target manifold two dimentional sphere. This geometric dispersive equations includes second material derivetives transported by fluid equations. This make the analytical studies quite challenging. We employ techniques from both fluid equations and geometric dispersion equations to obtain some well-posedness results and long time behavior. This project is joint with Jiaxi Huang and Lifeng Zhao.

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Organizers: Weizhu Bao (matbaowz@nus.edu.sg), Wei Jiang (jiangwei1007@whu.edu.cn), Chunmei Su (sucm@tsinghua.edu.cn), Zhen Zhang (zhangz@sustech.edu.cn)

ID: 305 / MS20-2: 3

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Parametric finite element methods for anisotropic axisymmetric flows

Meng Li

Zhengzhou University, China, People's Republic of; limeng@zzu.edu.cn

This report considers parametric finite element methods for anisotropic flows in axisymmetric settings, including surface diffusion, conserved mean curvature, power mean curvature and intermediate evolution

flows. We introduce novel weak formulations, and different approximating methods are constructed and studied. Computational experiments are presented to demonstrate the efficiency of the proposed methods.

ID: 306 / MS20-1: 1

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

A Variational Approach to the Modelling of Evaporating Droplets

Tiezheng Qian

Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); maqian@ust.hk

Sessile liquid droplets on solid surfaces are ubiquitously found in nature and practical applications. Based on our earlier works on the modelling of contact line dynamics and thin film dynamics, we derive a continuum model for evaporating droplets by applying Onsager's variational principle. This approach ensures that the continuum model is thermodynamically consistent in describing the coupling of many physical processes, including viscous momentum transport in the liquid, diffusive transport in the liquid (for binary mixture), contact line motion, evaporation, and vapor diffusion.

ID: 312 / MS20-1: 3

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Hydrodynamics of a thin film of active nematic fluid

Yakun LI

HKUST, Hong Kong S.A.R. (China); ylinv@connect.ust.hk

The dynamics of self-propelled particle suspensions has been a subject of enduring interest. In this study, we delve into the hydrodynamics of a thin film of active nematic fluid which is placed on a solid substrate and contains oriented filaments with active stress. By applying the Onsager's variational principle, we derive the hydrodynamic equations governing the thin-film time evolution and stationary state. A characteristic length scale is introduced to measure the competition between active and capillary forces. It is demonstrated analytically and numerically that this length scale is in the control of droplet spreading, stationary shape, and droplet migration.

ID: 322 / MS20-2: 5

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Evolving finite element methods with an artificial tangential velocity for mean curvature flow and Willmore flow

Jiashun Hu, Buyang Li

The Hong Kong Polytechnic University, Hong Kong S.A.R. (China); jiashunhu0716@gmail.com

An artificial tangential velocity is introduced into the evolving finite element methods for mean curvature flow and Willmore flow to improve the mesh quality in the computation. The stability of the artificial tangential velocity is proved. The optimal-order convergence of the evolving finite element methods with artificial tangential velocity are proved for both mean curvature flow and Willmore flow. Extensive numerical

experiments are presented to illustrate the convergence of the method and the performance of the artificial tangential velocity in improving the mesh quality.

ID: 421 / MS20-2: 2

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Efficient methods for interface related optimization problems

Dong Wang

Shenzhen International Center on Industrial and Applied Mathematics, The Chinese University of Hong Kong, Shenzhen, China, People's Republic of; wangdong@cuhk.edu.cn

In this talk, we will talk efficient and stable numerical methods for interface related optimization problems, with applications ranging from image processing, topology optimization, to optimal partition. The deep learning methods for these problems involving multiphyiscs constraints will also be discussed.

ID: 450 / MS20-3: 2

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Structure-preserving parametric finite element method for some curvature flows with nonlocal terms

Lifang Pei

Zhengzhou University, China, People's Republic of; plf5801@zzu.edu.cn

Structure-preserving parametric finite element methods (SP-PFEMs) based on the BGN scheme are presented and analyzed to simulate the motion of closed curves/surfaces governed by some mean curvature flows with nonlocal terms. Structure-preserving properties of variational formulations and semi-discrete schemes as well as fully discrete schemes are rigorously discussed. In addition, numerical experiments are carried to test the performs of SP-PFEMs, including the accuracy, structure-preserving properties and mesh quality during evolution.

ID: 612 / MS20-3: 1

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Original Energy Dissipation Preserving Exponential Time Differencing Runge--Kutta methods for Phase-field Gradient Flows

Jiang Yang

Southern University of Science and Technology, China, People's Republic of; yangj7@sustech.edu.cn

We identify a set of conditions that ETDRK schemes need to satisfy in order to preserve the original energy dissipation for a class of phase-field gradient flows, show that the commonly used third-order and fourth-order ETDRK schemes do not satisfy these conditions, and construct, with proper stabilization, new third-order ETDRK schemes which satisfy the conditions and thus unconditionally decrease the energy. This is the first work to study the unconditionally energy stability of arbitrarily high-order ETDRK methods, and it is hopeful that our general framework will lead to constructions of higher than third-order unconditional energy stable ETDRK schemes.

ID: 705 / MS20-3: 3

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

A Structure-Preserving Parametric Finite Element Method of Anisotropic Geometric Flows

Yifei Li

National University of Singapore, Singapore; liyifei@nus.edu.sg

Designing a numerical scheme that can preserve the geometric structure for anisotropic geometric flows with an arbitrary anisotropic surface energy is a long-standing problem. In this talk, for anisotropic mean curvature flow and anisotroic surface diffusion, we propose and analyze a structure-preserving parametric finite element methods (SP-PFEM) for the evolution of a closed curve in 2D, which preserve two geometric structures – area conservation and energy dissipation – at the full-discretized level, Extensive numerical results demonstrate its efficiency, stability, and success in other geometric flows.

ID: 708 / MS20-2: 1

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Transformed Model Reduction for Partial Differential Equations with Sharp Inner Layers

Tianyou Tang, Xianmin Xu

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; xmxu@lsec.cc.ac.cn

Small parameters in partial differential equations can give rise to solutions with sharp inner layers that evolve over time. However, the standard model reduction method becomes inefficient when applied to these problems due to the slowly decaying Kolmogorov N-width of the solution manifold. In this talk, we will present some recent efforts to deal with the difficulties. In particular, we show a new approach to transform the equation in such a way that the transformed solution manifold exhibits a fast decaying Kolmogorov N-width. This enables us to develop efficient model reduction methods.

ID: 711 / MS20-3: 4

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

High order in time, BGN-based parametric finite element methods for solving geometric flows

Wei Jiang[1], Chunmei Su[2], Ganghui Zhang[2]

[1]Wuhan University, China, People's Republic of; [2]Tsinghua University, China, People's Republic of; jiangwei1007@whu.edu.cn

Geometric flows have recently attracted lots of attention from scientific computing communities. One of the most popular schemes for solving geometric flows is the so-called BGN scheme. However, the BGN scheme only can attain first-order accuracy in time, and how to design a temporal high-order numerical scheme is challenging. Recently, based on a novel approach, we have successfully proposed temporal high-order, BGN-based parametric finite element method for solving geometric flows of curves/surfaces.

ID: 713 / MS20-1: 4

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related

Geometric Flows

Capillary Folding of Thin Elastic Sheets

Zhixuan Li

National University of Singapore, Singapore; zhixuanli@u.nus.edu

Capillary folding is the process of folding planar objects into three-dimensional (3D) structures using capillary force. In this talk, we propose a 3D model for the capillary folding of thin elastic sheets with pinned contact lines. We derive the governing equations for the static system using a variational approach. We then discuss the numerical method to find equilibrium solutions via a relaxation dynamics. Finally, we present simulation results which qualitatively agree well with physical experiments and exhibit rich and fully 3D behaviors not captured by previous 2D models.

ID: 715 / MS20-1: 2

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Mechanics at Nano-Bio interface: Cellular Packing of Flexible Nanomaterials and Membrane Targeting Antimicrobials

Guijin Zou[1], Xin Yi[2], Huajian Gao[3]

[1]School of Mechanical and Aerospace Engineering, College of Engineering, Nanyang Technological University, Singapore 639798, Singapore; [2]Department of Mechanics and Engineering Science, College of Engineering, Peking University, Beijing 100871, China; [3]Mechano-X Institute, Applied Mechanics Laboratory, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China.; guijin.zou@ntu.edu.sg

At the nano-bio interface, mechanics significantly influence the development of health-related technologies. In this talk, we will explore two examples. First, we examine how the mechanical properties of flexible nanomaterials impact their encapsulation in lipid vesicles, with potential applications in the design of artificial cells and biohybrid microrobots. Next, we introduce the field of membrane targeting nanomedicine (MTN), demonstrating how atomistic modeling and simulation identify membrane targeting antimicrobials (MTAs) that selectively penetrate and disrupt bacterial lipid membranes, highlighting the potential of simulation-assisted platforms to advance nanomedicine.

ID: 716 / MS20-2: 4

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Numerical investigations on solving surface interface problems

Xufeng Xiao

Xinjiang University, China, People's Republic of China; xiaoxufeng111@sina.com

Surface interface problems are examples of partial differential equations with discontinuous coefficients on manifolds. In this talk, I will show three types of numerical method for solving the surface interface problems. The first one is the local tangential lifting based immersed boundary method for the discrete delta function. The second part is a meshless method including the generalized finite difference (GFD) and the RBF methods. The third one is the extension of the immersed interface finite element method. Finally, some conclusions and future works will be show.

ID: 721 / MS20-1: 5

MS20 Mathematical Modeling, Analysis and Numerical Methods for Interface Problems and Related Geometric Flows

Modeling inertial migration of particles in curved duct flow

Brendan Harding

Victoria University of Wellington, New Zealand; brendan.harding@vuw.ac.nz

For a particle suspended in steady laminar flow in a confined duct geometry, inertial migration causes the particle to migrate across the fluid streamlines. This phenomena has a number of applications in inertial microfluidics which has motivated many studies. Much is known in the case of straight ducts but detailed studies of curved ducts, where migration is further complicated by the presence of Dean flow, are uncommon. We devised a method for efficient and detailed calculation in curved duct flows. I'll describe our approach and how it has led to valuable insights into the complicated dynamics of particle migration.

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems

Organizers: Yingda Cheng (yingda@vt.edu)

ID: 337 / MS21-1: 3

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems

Finite Expression Method: A Symbolic Approach for Scientific Machine Learning

Haizhao Yang

University of Maryland College Park, United States of America; hzyang@umd.edu

In this talk, we introduce a new method for a symbolic approach to solving scientific machine learning problems. This method seeks interpretable learning outcomes via combinatorial optimization in the space of functions with finitely many analytic expressions and, hence, this methodology is named the finite expression method (FEX). It is proved in approximation theory that FEX can avoid the curse of dimensionality in discovering high-dimensional complex systems. As a proof of concept, a deep reinforcement learning method is proposed to implement FEX for learning the solution of high-dimensional PDEs and learning the governing equations of raw data.

ID: 358 / MS21-1: 4

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems

A Reduced Order Model Enhanced Iterative Solver for Parametric Radiative Transfer Equation

Zhichao Peng

The Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); pengzhic@ust.hk

Radiative transfer equation (RTE) models particles propagating through and interacting with a background medium. Applications, such as uncertainty quantification, medical imaging, and shape optimization, require solving RTE many times for various parameters.

Source Iteration (SI) with Diffusion Synthetic Acceleration (DSA) for solving RTE does not exploit low-rank structures of the solution manifold concerning parameters of parametric problems. It may also become less efficient without a strong enough scattering effect.

To address these issues, we utilize data-driven reduced order models, which leverage low-rank structures concerning parameters, to enhance SI by providing better initial guesses and more efficient Synthetic Acceleration strategies.

ID: 382 / MS21-1: 2

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems

Hyperbolic machine learning moment closure models for the radiative transfer equation

Juntao Huang

Texas Tech University, United States of America; juntao.huang@ttu.edu

In this talk, we take a data-driven approach and apply machine learning to the moment closure problem for the radiative transfer equation. Instead of learning the unclosed high order moment, we propose to directly learn the gradient of the high order moment using neural networks, called the gradient-based moment closure. Moreover, we introduce two approaches to enforce the hyperbolicity of our gradient-based machine learning moment closures. A variety of benchmark tests, including the variable scattering problem, the Gaussian source problem, and the two material problem, show both good accuracy and generalizability of our machine learning closure model.

ID: 459 / MS21-1: 1

MS21 Recent Progress on Data Driven Reduced Order Models for Kinetic Transport Problems

A symplectic deep autoencoder for Hamiltonian systems

Wei Guo

Texas Tech University; weimath.guo@ttu.edu

We introduce a novel symplectic deep autoencoder for model order reduction (MOR) of simulating parametric Hamiltonian systems. The existing MOR techniques for parametric Hamiltonian systems suffer two limitations. First, the inherent symplectic structure of Hamiltonian systems is not necessarily inherited by the reduced order model. Second, due to non-dissipative nature of Hamiltonian systems, the popular global linear subspace solution representation becomes less effective. To overcome the difficulties, we propose a deep autoencoder using HenonNets that can preserve the symplectic structure. Hence, the reduced system is still Hamiltonian, and the system energy and long-term stability is preserved.

MS22 Stochastic Numerics with Applications to Sampling

Organizers: Peter Archibald Whalley (s2110992@ed.ac.uk), Akash Sharma (akashs@chalmers.se)

ID: 192 / MS22-1: 2

MS22 Stochastic Numerics with Applications to Sampling

Enhanced Gradient Flows of Parameters and Probability Measures for Statistical Inference

Sam Power[1], Rocco Caprio[2], Adam Johansen[2], Jen Ning Lim[2], Juan Kuntz[3]

[1]University of Bristol, United Kingdom; [2]University of Warwick, United Kingdom; [3]Polygeist;

sam.power@bristol.ac.uk

In the context of optimisation, gradient flows offer a compelling paradigm for the design and analysis of algorithms. Recent developments have emphasised that this paradigm remains valuable for studying the sampling problem, and even for various 'hybrid' probabilistic tasks which involve a combination of optimisation of model parameters and sampling of model states.

This talk will discuss some recent developments in this area, connecting i) formalisation of diverse statistical and computational tasks as optimisation problems, ii) construction of suitable dynamical systems which solve these problems, iii) numerical discretisation and iv) convergence analysis of the resulting algorithms.

ID: 314 / MS22-1: 3

MS22 Stochastic Numerics with Applications to Sampling

Application of the Hopf algebra structures of exotic aromatic series to stochastic numerical analysis

Adrien Laurent[1], **Eugen Bronasco**[2]

[1]INRIA Rennes, France; [2]University of Geneva, Switzerland; adrien.laurent@inria.fr

The exotic aromatic formalism of Butcher series is a strong tool for the high-order sampling of the invariant measure of ergodic SDEs. In this talk, we uncover the Hopf algebra structures related to the composition and substitution laws of exotic aromatic series, and use them to provide an explicit expression for the modified vector field. In particular, we show that the modified vector field writes naturally and at any order as an exotic aromatic B-series.

ID: 477 / MS22-1: 1

MS22 Stochastic Numerics with Applications to Sampling

Unbiased Kinetic Langevin Monte Carlo Methods

Neil Kumar Chada[1], **Benedict Leimkuhler**[2], **Daniel Paulin**[3], **Peter Whalley**[4]

[1]City University of Hong Kong, Hong Kong; [2]University of Edinburgh; [3]University of Edinburgh; [4]University of Edinburgh; neilchada123@gmail.com

We present an unbiased method for Bayesian posterior means based on kinetic Langevin dynamics that combines advanced splitting methods with enhanced gradient approximations. Our approach avoids Metropolis correction by coupling Markov chains at different discretization levels in a multilevel Monte Carlo approach. Theoretical analysis demonstrates that our proposed estimator is unbiased, attains finite variance, and satisfies a central limit theorem. Various numerical experiments are proposed on a range of problems such as MNIST regression, a Gaussian toy example and a Poisson soccer model. Our method desmontrates clear efficiency over gold standard methods like randomized Hamiltonian Monte Carlo.

ID: 732 / MS22-1: 4

MS22 Stochastic Numerics with Applications to Sampling

Collective Behavior in Interacting Particle Systems

Benedict Leimkuhler[1], **René Lohmann**[1], **Greg Pavliotis**[2], **Peter Whalley**[1]

[1]University of Edinburgh, United Kingdom; [2]Imperial College London; r.lohmann@ed.ac.uk

Interacting particle systems are used to model the behavior of plasmas, stellar objects, biological agents, and even the evolution of opinions. The interactions between particles at the microscale often lead to the emergence of collective behavior at the macroscale, such as cluster formation (stellar dynamics), emergence of consensus (opinion dynamics), or swarming of animal populations. In this talk, we will look at cluster formation in terms of both theory and simulation. We will describe the microscopic model based on Langevin

dynamics, present corresponding numerical experiments, and compare their outcomes with predictions made by macroscopic theory obtained via a mean-field limit.

MS23 Modeling and Simulations for Multiphase Interface Problem

Organizers: Xinpeng Xu (xu.xinpeng@gtiit.edu.cn), Zhenlin Guo (zguo@csrc.ac.cn), Meng Zhao (mzhao9@hust.edu.cn)

ID: 230 / MS23-1: 4

MS23 Modeling and Simulations for Multiphase Interface Problem

Structure preserving primal dual methods for free interface dynamics as gradient flows with respect to transport distances

Chaozhen Wei

University of Electronic Science and Technology of China, China, People's Republic of; cwei4@uestc.edu.cn

I will present a novel structure-preserving numerical method for gradient flows with respect to Wasserstein-like transport distances induced by concentration-dependent mobilities, which arise widely in materials science and biology. Based upon the minimizing movement scheme and modern operator-splitting schemes, our method has built-in positivity or boundedness preserving, mass conservation, and energy-dissipative structures. I will show the flexibility and performance of our methods through simulation examples including porous medium equations, nonlocal aggregation diffusion equations and Cahn-Hilliard equations with degenerate mobility and wetting boundary conditions.

ID: 295 / MS23-1: 1

MS23 Modeling and Simulations for Multiphase Interface Problem

Multiscale topology optimization method for lattice materials

Yibao Li[1], **Binhu Xia**[2]

[1]Xi'an Jiaotong University, China, People's Republic of; [2]Xijing University, China, People's Republic of; yibaoli@xjtu.edu.cn

In this talk, we will introduce an efficient multiscale topology optimization method for lattice materials. In macro-scale, we will present a second-order unconditionally energy stable schemes for the topology optimization problem. We will prove that our scheme is unconditionally energy stable. In macro-scale, we will propose a simple volume merging method for triply periodic minimal structure.The mean curvature on the surface will be constant everywhere at the equilibrium state. Computational experiments are presented to demonstrate the efficiency of the method.

ID: 424 / MS23-1: 2

MS23 Modeling and Simulations for Multiphase Interface Problem

A novel steepness-adjustable harmonic volume-of-fluid method for interface capturing

Weidan Ni[1], **Qinghong Zeng**[1], **Yucang Ruan**[2], **Zhiwei He**[1,3]

[1]Institute of Applied Physics and Computational Mathematics, Fenghaodong Road, Haidian District, Beijing 100094, China; [2]State Key Laboratory for Turbulence and Complex Systems, College of Engineering, Peking University, Beijing 100871, China; [3]National Key Laboratory of Computational Physics, Beijing 100088, China; 15001214829@163.com

A novel algebraic volume-of-fluid (VOF) method, without the operations of switching back and forth adopted by the previous algebraic VOF methods, is constructed within a unified framework of the steepness-adjustable harmonic scheme. A thorough validation of the present method is conducted, examining the pure advection of the interface indicator function. The results indicate that the present method can resolve the interface capturing with substantially low numerical diffusion and low numerical oscillations.

ID: 445 / MS23-1: 3

MS23 Modeling and Simulations for Multiphase Interface Problem

Decoupled multiscale finite element methods for the Stokes-Darcy model

Haibiao Zheng

East China Normal University, Shanghai; hbzheng@math.ecnu.edu.cn

In this talk, we employ the multiscale finite element method and propose an decoupled algorithm for solving the non-stationary Stokes Darcy model with multiscale characteristics in the permeability coefficient of the Darcy region. Our algorithm involves two steps: First, conducting the parallel computation of multiscale basis functions in the Darcy region. Second, utilizing these multiscale basis functions, we employ a partitioned time-tepping scheme to solve the Stokes-Darcy equations. A significant characteristic of the algorithm is solving problems on relatively coarse grids, thus significantly reducing computational costs. The rationality and effectiveness of the algorithm are verified through some numerical experiments

ID: 479 / MS23-2: 1

MS23 Modeling and Simulations for Multiphase Interface Problem

A fourth-order kernel-free boundary integral method for variable coefficients elliptic PDEs

Yaning Xie

Zhejiang university of technology, China, People's Republic of; xieyaning@zjut.edu.cn

We propose a fourth-order generalized boundary integral method for variable coefficients elliptic PDEs, including both boundary value and interface problems. The method is kernel-free in the sense that there is no need to know analytical expressions for kernels of the boundary and volume integrals in the solution of boundary integral equations. Evaluation of a boundary or volume integral is replaced with interpolation of a fourth-order Cartesian grid-based solution, which satisfies an equivalent discrete interface problem, while the interface problem is solved by a fast solver in the Cartesian grid. Numerical results are presented.

ID: 541 / MS23-2: 2

MS23 Modeling and Simulations for Multiphase Interface Problem

Three-layer Hele-Shaw problem driven by a sink

Meng Zhao

Huazhong Univeristy of Science and Technology, China, People's Republic of; mzhao9@hust.edu.cn

We investigate a sink-driven three-layer flow in a radial Hele-Shaw cell performing numerical simulations. The three fluids are of different viscosities with one fluid occupying an annulus-like domain, forming two interfaces with the other two fluids. The interaction between the two interfaces introduces novel dynamics leading to rich pattern formation phenomena, manifested by two typical events: cusp-like morphology or interface merging. In particular, the inner interface can be wrapped by the other to have both scenarios. We

find that multiple parameters contribute to the dynamics including the width of annular region, the location of the sink, and the mobilities of the fluids.

ID: 712 / MS23-2: 3

MS23 Modeling and Simulations for Multiphase Interface Problem

Exploring Cancer Mechanisms: Mechanical and Chemical Interactions in Tumor Growth

Min-Jhe Lu

University of California, Irvine, United States of America; minjhel@uci.edu

The building of the mechano-chemical tumor model aims to understand how the mechanical interaction and the biochemical reactions can influence the dynamics of tumor growth. In essence, the mechanical interactions within cellular structures generate stress responses, while the concomitant biochemical reactions involve various chemical species that, for example, supply nutrients to the tumor. In this talk, I will illustrate the construction of these tumor models incorporating elasticity. I will also present numerical simulations using both sharp and diffuse interface formulations. Additionally, I will discuss the application of these models to brain and breast cancer studies.

ID: 733 / MS23-2: 4

MS23 Modeling and Simulations for Multiphase Interface Problem

A Cartesian grid method for nonhomogeneous elliptic interface problems on unbounded domains

Wenjun Ying

Shanghai Jiao Tong University, China, People's Republic of; wying@sjtu.edu.cn

We will present a Cartesian grid based fast and accurate method for evaluating boundary and volume integrals in an indirect boundary-volume integral method for nonhomogeneous elliptic interface problems on unbounded domains. The indirect calculation is done by solving equivalent but simple interface problems. We accelerate the calculation by introducing an intermediate, transitional circle or sphere and taking advantages of super-convergent numerical quadrature on circles/spheres. We first map the boundary or volume integral on the irregular boundary or domain to the intermediate circle/sphere; then evaluate the boundary integral on the intermediate circle/sphere to get boundary conditions for the simple interface problem.

ID: 734 / MS23-2: 5

MS23 Modeling and Simulations for Multiphase Interface Problem

A parameter-free staggered-grid Lagrangian scheme for two-dimensional compressible flow problems

Xihua Xu

Beijing Institute of Applied Physics and Computational Mathematics, China, People's Republic of; xu_xihua@iapcm.ac.cn

The present study aims to develop a parameter-free staggered-grid Lagrangian scheme that avoids the empirical parameters needed for artificial viscosity and anti-hourglass force. The artificial viscosity is equal to the pressure jump. The anti-hourglass force is established using pressure compensation. The scheme maintains the conservation of total mass, momentum, and energy. Numerical experiments show that the scheme is highly robust for extreme flow problems with different fine meshes such as Sedov, Noh, Saltzmann triple point and Rayleigh-Taylor instability.

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems

Organizers: Bin Dong (dongbin@math.pku.edu.cn), Hui Ji (matjh@nus.edu.sg), Xiaoqun Zhang (zhangxq@sjtu.edu.cn)

ID: 447 / MS24-1: 1

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems

Sampling Strategies in Sparse Bayesian Inference

Yiqiu Dong

Technical University of Denmark, Denmark; yido@dtu.dk

Regularization is a common tool in variational inverse problems to impose assumptions on the parameters of the problem. One such assumption is sparsity, which is commonly promoted using lasso and total variation-like regularization. Although the solutions can often be considered as MAP point estimates, samples from these distributions are generally not sparse. In this talk, we present a sampling strategy for an implicitly defined probability distribution that combines the effects of sparsity imposing regularization with Gaussian distributions. We study the properties of these regularized distributions, and show its potential to be extended to broader regularisers.

ID: 622 / MS24-1: 2

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems

Neural Expectation Maximization for Self-supervised Blind Image Deblurring

JI HUI

National University of Singapore, Singapore; matjh@nus.edu.sg

Camera shake during photo capture often leads to blurred images, posing a significant challenge in image restoration. Traditional methods typically train a deep neural network (DNN) using datasets of blurred and sharp image pairs. This talk introduces an innovative dataset-free approach, utilizing DNN-based re-parametrization of latent images and blur kernels. We employ a Monte Carlo Expectation Maximization (MCEM) technique with Langevin dynamics to train the DNN without sharp reference images. Our experiments demonstrate this method's superior effectiveness in eliminating motion blur from static scenes compared to existing techniques.

ID: 696 / MS24-1: 3

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems

PDEformer: Towards a Foundation Model for Solving Parametric PDEs and Beyond

Bin Dong

Peking University, China, People's Republic of; dongbin@math.pku.edu.cn

In this presentation, I will outline our work on the design and training of a foundation model, named PDEformer, which aims to serve as a flexible and efficient solver across a spectrum of parametric PDEs. PDEformer is specifically engineered to facilitate a range of downstream tasks, including but not limited to

parameter estimation and system identification. Its design is tailored to accommodate applications necessitating repetitive solving of PDEs, where a balance between efficiency and accuracy is sought.

ID: 741 / MS24-1: 4

MS24 Mathematical and Machine Learning Methods in Imaging and Inverse Problems

Bi-modality Images Transfer with a Discrete Process Matching Method

Zhe Xiong, Qiaoqiao Ding, Xiaoqun Zhang

Shanghai Jiao Tong University, China, People's Republic of; xqzhang@sjtu.edu.cn

Generative models achieve tremendous success for natural image processing and generation. It also provides new solution for medical image synthesis. We propose to utilize both forward and backward ODE flow and enhance the consistency on the intermediate images of few discrete time steps, resulting in a transfer process with much less iteration steps while maintaining high-quality generations for both modalities. Our experiments on three datasets of MRI T1/T2 and CT/MRI demonstrate that DPM outperforms other state-of-the-art flow-based methods for bi-modality image synthesis, achieving higher image quality with less computation time cost.

MS25 Analysis and Numerical Computations for Kinetic Models

Organizers: Liu Liu (lliu@math.cuhk.edu.hk), Yanli Wang (ylwang@csrc.ac.cn)

ID: 340 / MS25-1: 3

MS25 Analysis and Numerical Computations for Kinetic Models

Efficient asymptotic preserving SL-DG methods for multiscale kinetic transport equations

Tao Xiong

University of Science and Technology of China, China, People's Republic of; taoxiong@ustc.edu.cn

In this work, we have formulated a class of asymptotic-preserving (AP) semi-Lagrangian discontinuous Galerkin methods, for kinetic transport equations under a diffusive scaling. We reformulate the model with characteristic tracking, so that the low dimensional density can be updated first without time step restrictions. Then the high dimensional distribution function can be solved efficiently in a parallel way with decoupled discrete velocities by using a discrete velocity method. Numerical results from 1D to 3D problems have verified the effectiveness, efficiency and AP property of our proposed approach.

ID: 407 / MS25-2: 2

MS25 Analysis and Numerical Computations for Kinetic Models

Reduced Variance Random Batch Methods for nonlocal meanfield equations

Mattia Zanella

University of Pavia, Italy; mattia.zanella@unipv.it

Random Batch Methods (RBM) for mean-field interacting particle systems enable the reduction of the quadratic computational cost associated with particle interactions to a linear cost. We propose a variance reduction technique for RBM applied to nonlocal PDEs of Fokker-Planck type based on a control variate strategy. The core idea is to construct a surrogate model that can be computed on the full set of particles at a linear cost while maintaining enough correlations with the original particle dynamics. Examples from

models of collective behavior in opinion and swarming dynamics demonstrate the great potential of the present approach.

ID: 420 / MS25-1: 4

MS25 Analysis and Numerical Computations for Kinetic Models

Neural PDE Solvers toward Digital Twin: Theory and Applications

Hyung Ju Hwang, **Hwi Jae Son, Jaeyong Lee, Hyuntae Jo**

Pohang University of Science and Technology, Korea, Republic of (South Korea); hjhwang@postech.ac.kr

A digital twin is a virtual representation of real-world physical objects. In this talk, I will briefly introduce how Physics can be encoded into Neural Networks such as PINN and Operator Learning. Then we will explore real-world applications of AI-based partial differential equation (PDE) solvers in various fields.

ID: 428 / MS25-1: 2

MS25 Analysis and Numerical Computations for Kinetic Models

Kinetic modeling of infectious viral dynamics based on mutual utility functions

Giulia Bertaglia[1], **Lorenzo Pareschi**[2,3], **Giuseppe Toscani**[4,5]

[1]Department of Environmental and Prevention Sciences, University of Ferrara; [2]Maxwell Institute and Department of Mathematics, Heriot-Watt University; [3]Department of Mathematics and Computer Science, University of Ferrara; [4]Department of Mathematics, University of Pavia; [5]IMATI, Institute for Applied Mathematics and Information Technologies "Enrico Magenes"; giulia.bertaglia@unife.it

In this talk, we present a model for describing the temporal evolution of a viral disease through the use of Boltzmann-type kinetic equations for a multi-agent system consisting of different population classes with individuals interacting pairwise. These interactions involve the agents and the virus in them, if any, and are defined on the basis of an agent-virus mutual utility target by drawing on the principles of price theory, particularly the Cobb-Douglas utility functions and the Edgeworth box. Several numerical experiments will emphasize the central role of this mechanism in driving the phenomenon toward endemicity.

ID: 442 / MS25-2: 4

MS25 Analysis and Numerical Computations for Kinetic Models

Stochastic Galerkin Particle Methods for Kinetic Equations of Plasmas with Uncertainties

Andrea Medaglia

University of Pavia, Italy; andrea.medaglia02@universitadipavia.it

The study of plasma models with uncertainties is receiving a great deal of attention because of its applications to nuclear fusion reactors. At the kinetic scale, the time evolution of the distribution function is described by the Landau equation. In addition, the importance of considering uncertainties has been recognised.

In this talk, we present a class of numerical methods that combine a particle-based approximation of the distribution function together with a stochastic Galerkin expansion of the particles in the random space. These methods are spectrally accurate in the space of random parameters and preserve the structural properties of the equation.

ID: 592 / MS25-2: 3

MS25 Analysis and Numerical Computations for Kinetic Models

On a kinetic Elo rating model for players with dynamical strength

Bertram Düring

University of Warwick, United Kingdom; bertram.during@warwick.ac.uk

We discuss a new kinetic rating model for a large number of players, which is motivated by the well-known Elo rating system. Each player is characterised by an intrinsic strength and a rating, which are both updated after each game. We state and analyse the respective Boltzmann-type equation and derive the corresponding nonlinear, nonlocal Fokker-Planck equation. We investigate the existence of solutions to the Fokker-Planck equation and discuss their behaviour in the long time limit. Furthermore, we illustrate the dynamics of the Boltzmann and Fokker-Planck equation with various numerical experiments.

ID: 620 / MS25-2: 1

MS25 Analysis and Numerical Computations for Kinetic Models

A fast iteration for the moment model of the Boltzmann-BGK equation in near-continuum regimes

Zhicheng HU

Nanjing University of Aeronautics and Astronautics, China, People's Republic of; huzhicheng@nuaa.edu.cn

In recent years, the efficient simulation of the Boltzmann equation has attracted a great deal of attention in fields such as the rarefied gas dynamics. We concentrate on efficient solution strategies for the high-order moment model derived from the Boltzmann-BGK equation by the moment method. A novel fast alternating iteration using correction from the classical hydrodynamic equations will be introduced. It can not only significantly improve the efficiency in near-continuum regimes, but also be effectively combined with other acceleration techniques, such as fast sweeping iteration and multigrid method. Several numerical examples will be presented to show the performance of the resulting solver.

ID: 638 / MS25-1: 1

MS25 Analysis and Numerical Computations for Kinetic Models

Discontinuous Galerkin Finite Element Methods for Port-Hamiltonian Dynamical Systems

Yan Xu

University of Science and Technology of China, China, People's Republic of; yxu@ustc.edu.cn

In this paper, we present discontinuous Galerkin (DG) finite element discretizations of a class of hyperbolic port-Hamiltonian dynamical systems. The key point in constructing a port-Hamiltonian system is the definition of a Stokes-Dirac structure. Departing from the traditional approach of defining the strong form of the Dirac structure, we instead consider the weak form of the Dirac structure for linear dynamical systems in broken Sobolev spaces on a tessellation with polyhedral elements.The accuracy and capability of the methods developed in this paper will be demonstrated by presenting several numerical experiments.

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Organizers: Benjamin Carrel (benjamin.carrel@unige.ch), Thomas Trigo Trindade (thomas.trigotrindade@epfl.ch)

ID: 200 / MS26-1: 1

MS26 Dynamical Low Rank Approximation: From Theory to Applications

An overview of dynamical low-rank techniques for hyperbolic problems

Lukas Einkemmer

University of Innsbruck, Austria; lukas.einkemmer@uibk.ac.at

Dynamical low-rank methods are complexity reduction techniques that for high-dimensional PDEs can significantly reduce the computational and memory cost. For parabolic problems, regularity can often be used to justify that an approximation with a small rank can be used to faithfully reproduce the dynamics of the system. However, for hyperbolic problems, this is usually not the case as the solution can exhibit small-scale structures and even discontinuities. In this talk, we will consider some of the techniques that have been developed to specifically treat hyperbolic (mostly kinetic) problems in the context of dynamical low-rank approximation.

ID: 328 / MS26-2: 4

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Multi-level dynamical low-rank approximations for stochastic problems in radiation therapy

Pia Katharina Stammer[1,4], Jonas Kusch[2], Danny Lathouwers[3], Chinmay Patwardhan[1], Niklas Wahl[4]

[1]Karlsruhe Institute of Technology (KIT), Germany; [2]Norwegian University of Life Sciences (NMBU); [3]Delft University of Technology; [4]German Cancer Research Center - DKFZ, Germany; pia.stammer@kit.edu

Transport problems in applications such as radiotherapy are often stochastic due to both physical effects and uncertainties. This increases run-time and memory, making standard numerical solution methods infeasible.

We tackle the problem using the rank-adaptive dynamical low-rank approximation (DLRA) with multi-level hierarchies. First, a collided-uncollided split facilitates the inclusion of boundary conditions and stochastic energy loss. A second layer is then added to the multi-level formulation for uncertainty quantification. Here, the error tolerance in DLRA is used to define levels for a multi-level Monte Carlo approach. We discuss the relations between the rank/tolerance, error and computational costs.

ID: 329 / MS26-1: 3

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Semi-Implicit Dynamical Low Rank Approximation: Convergence to Equilibrium

Stefan Schnake[1], Eirik Endeve[1], Cory Hauck[1], Peiming Yin[2]

[1]Oak Ridge National Laboratory, United States of America; [2]The University of Texas El Paso; schnakesr@ornl.gov

In this presentation, I will summarize recent work on low-rank methods for a kinetic model of neutrino-matter interactions. The model itself is a simple linear ODE, but it highlights the need to simulate dynamics over long time scales. In particular, recovery of the equilibrium limit is a critical requirement of any numerical method. We investigate a discontinuous Galerkin approximation combined with the basis update and Galerkin (BUG) integrator with implicit integration in each substep. We provide conditions on the method to ensure that the solution converges to the correct equilibrium, and we demonstrate the theory with a few numerical results.

ID: 332 / MS26-1: 2

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Dynamical Low-Rank Approximation of SDEs

Yoshihito Kazashi[1], **Fabio Nobile**[2], **Fabio Zoccolan**[2]

[1]University of Strathclyde, Glasgow, United Kingdom; [2]EPFL, Switzerland; fabio.zoccolan@epfl.ch

We illustrate a rigorous mathematical setting of Dynamical Low Rank Approximation (DLRA) for SDEs using the so-called Dynamically Orthogonal (DO) framework. Also in this context, the DO system of equations is coupled and depends on the inverse of a Gramian. Therefore, both the existence of solutions and their numerical discretization are not trivial. We will also provide different first-order schemes of DO for SDEs, showing results of accuracy and pointing out practical advantages and drawbacks in applications. Our theoretical estimates will be supported by numerical simulations.

ID: 345 / MS26-2: 3

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Neural Network Training with Dynamical Low-Rank Inspired Optimizers

Steffen Schotthoefer[1], **Jonas Kusch**[2], **Gianluca Ceruti**[3], **Emanuele Zangrando**[4], **Francesco Tudisco**[5]

[1]Oak Ridge National Laboratory, United States of America; [2]Norwegian University of Life Sciences; [3]University of Innsbruck; [4]GSSI; [5]University of Edinburgh; schotthofers@ornl.gov

Memory footprint and computational demand are the grand challenges of large scale neural network training.

We propose a dynamical low-rank inspired optimization scheme to train neural networks efficiently on a low-rank manifold. Using methods from dynamical model order reduction allows us to provide approximation, stability, and descent guarantees. Moreover, our method

automatically and dynamically adapts the ranks of the network weight matrices during training to achieve the desired approximation accuracy. Further, a Tensor-valued formulation of the scheme allows us to compress more complex neural network structures.

ID: 397 / MS26-1: 4

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Dynamical low-rank tensor methods for quantum simulations

Dominik Sulz[1], **Christian Lubich**[1], **Gianluca Ceruti**[2], **Jonas Kusch**[3]

[1]University of Tübingen, Germany; [2]University of Innsbruck, Austria; [3]Norwegian University of Life Sciences, As, Norwa; dominik.sulz@uni-tuebingen.de

Dynamical low-rank approximation has proven to be an efficient tool for solving problems such as the many-body Schrödinger equation from quantum physics. In recent years, several time integration schemes have been derived for tree tensor networks, a data-sparse format for approximating tensors. All nodes in the tree are updated by solving only small matrix-/tensor differential equations, which makes the computation efficient. All methods are shown to have robust error bounds that are independent of small singular values. Numerical experiments validate the theoretical results and show several applications from quantum physics.

ID: 452

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Parametric PDEs and low-rank approximation of function-valued matrices

Stanislav Budzinskiy

University of Vienna, Austria; stanislav.budzinskiy@univie.ac.at

Parameter tuning for mathematical models relies on massive high-fidelity simulations and becomes more expensive with the growing complexity of the models. The idea of data-driven modeling is to build a surrogate model based on the results of high-fidelity simulations for a small number of parameter values. In this talk, we present a novel framework of data-driven modeling for bi-parametric PDEs. We propose to (i) treat them, after the discretization of the parameter space, as matrices whose entries are the solutions of the PDE for the corresponding parameter values; (ii) seek low-rank approximations of such function-valued matrices.

ID: 628 / MS26-2: 1

MS26 Dynamical Low Rank Approximation: From Theory to Applications

Dynamical low-rank approximation accelerated by the discrete empirical interpolation method

Benjamin Carrel, Bart Vandereycken

University of Geneva, Switzerland; benjamin.carrel@unige.ch

The dynamical low-rank approximation (DLRA) has shown good performance on a wide range of problems, but the intrusiveness of the integrators remains an issue for a large adoption of the methods. In this talk, we propose to perform DLRA with oblique projections using the discrete empirical method. The resulting integrators preserve the order of convergence, are quasi-optimal with the originals, and are much less intrusive (and often more efficient) than the usual DLRA.

MS27 SDE Methods and Data Science Applications

Organizers: Benedict Leimkuhler (b.leimkuhler@ed.ac.uk), Jianfeng Lu (jianfeng@math.duke.edu), Daniel Paulin (daniel.paulin@ed.ac.uk)

ID: 272 / MS27-1: 1

MS27 SDE Methods and Data Science Applications

Wasserstein convergence and bias estimates for kinetic Langevin integrators

Peter Archibald Whalley

University of Edinburgh, United Kingdom; s2110992@ed.ac.uk

We provide a framework to prove convergence rates for discretizations of kinetic Langevin dynamics for gradient-Lipschitz and strongly-convex potentials. Our approach gives convergence rates with explicit stepsize restrictions, which are of the same order as the stability threshold for Gaussian targets and are valid for a large interval of the friction parameter. We further provide second-order asymptotic bias estimates for the BAOAB scheme, which remain accurate in the high-friction limit by comparing it to modified stochastic dynamics which preserves the invariant measure.

ID: 398 / MS27-1: 4

MS27 SDE Methods and Data Science Applications

Wasserstein Convergence Guarantees for a General Class of Score-Based Generative Models

Xuefeng Gao

Chinese University of Hong Kong, Hong Kong S.A.R. (China); xfgao@se.cuhk.edu.hk

In this paper, we establish convergence guarantees for a general class of Score-based generative models (SGMs) in 2-Wasserstein distance, assuming accurate score estimates and log-concave data distribution. We specialize our result to several concrete SGMs, and obtain an upper bound on the iteration complexity for each model. Numerically, we experiment SGMs with different forward processes, some of which are newly proposed in this paper, for unconditional image generation on CIFAR-10. We find that the experimental results are in good agreement with our theoretical predictions on the iteration complexity. Joint work with Hoang M. Nguyen and Lingjiong Zhu.

ID: 432 / MS27-1: 3

MS27 SDE Methods and Data Science Applications

On the ergodicity and sharp error estimates of the stochastic gradient Langevin dynamics

Lei Li[1], Jian-Guo Liu[2], Yuliang Wang[1]

[1]Shanghai Jiao Tong University, China, People's Republic of; [2]Duke University; leili2010@sjtu.edu.cn

I will introduce some new results for the analysis of SGLD. First, the ergodicity of SGLD is proved by assuming only the confining property of the expected potential without global convexity. Second, the law of the iteration of SGLD is compared to the law of the exact Langevin diffusion. The Fisher information and the effect of random batch are carefully analyzed using the Girsanov transform. A uniform-in-time second order error estimate is proved for the KL-divergence.

ID: 471 / MS27-1: 2

MS27 SDE Methods and Data Science Applications

Sampling on manifolds via SDEs

Karthik Bharath[2], Alexander Lewis[3], Akash Sharma[1], Michael Tretyakov[2]

[1]University of Gothenburg and Chalmers University of Technology; [2]University of Nottingham; [3]University of Gottingen; akashs@chalmers.se

We derive error bounds for sampling and estimation using a discretization of an intrinsically defined Langevin diffusion on Riemannian manifold. Imposing no restrictions beyond a nominal level of smoothness on potential function, first-order error bounds, in discretization step size, on the bias and variances of estimators are derived. We will also discuss conditions for extending analysis to the case of non-compact manifolds and different variants of the algorithm. We will present numerical illustrations with distributions on the manifolds which verify the derived bounds.

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning

Organizers: Ana Djurdjevac (adjurdjevac@zedat.fu-berlin.de), Joscha Diehl (joscha.diehl@uni-greifswald.de)

ID: 184 / MS28-1: 2

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning

Optimal rate of convergence for approximations of nonlinear SPDEs with additive space-time white noise

Helena Katharina Kremp

Technische Universität Wien, Austria; helena.kremp@asc.tuwien.ac.at

We consider exponential Euler approximations of nonlinear stochastic reaction-diffusion equations driven by a 1+1-dimensional white noise and prove a strong rate of convergence of 1/2 in space and, crucially, 1 in time. This generalizes the results by Jentzen/Kloeden '08 to truly nonlinear coefficients and thus overcomes the previous order barrier. Joint work with Ana Djurdjevac and Máté Gerencsér.

ID: 342 / MS28-1: 4

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning

A multiplicative surface signature through its Magnus expansion

Joscha Diehl[1], Ilya Chevyrev[2], Kurusch Ebrahimi-Fard[3], Nikolas Tapia[4]

[1]University of Greifswald, Germany; [2]University of Edinburgh, UK; [3]NTNU Trondheim, Norway; [4]Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, Germany; joscha.diehl@uni-greifswald.de

We present a two-parameter analog to Chen's iterated-integrals signature, which can be applied to image data. It is based on 'surface development' from higher catagory and Kapranov's construction of the analog of the free Lie algebra. Its crucial property is a two-parameter Chen's identity. This enables efficient, and parallelizable, computation of the signature. Our approach is based on the Magnus expansion, which allows us to compute, up to a certain order, explicit expressions for the integrals appearing. On the analytic side, we provide a sewing lemma for surface development, which allows to go beyond the smooth case.

ID: 351 / MS28-1: 1

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning

Numerics on regualarization by noise

Chengcheng Ling

University of Augsburg, Germany; chengcheng.ling@uni-a.de

Regularization By Noise in the context of stochastic differential equations (SDEs) with coefficients of low regularity, known as singular SDEs, refers to the beneficial effect produced by noise so that the singularity from the coefficients is smoothed out yielding well-behaved equations. This field, initiated by works of Zvonkin and Veretennikov from 70's, has been extensively explored among different concepts from stochastic calculus. In this talk we will introduce the ideas from classical Itô calculus involving the theory from PDEs and modern tools from rough path theory and Malliavin calculus for tackling the problems on numerics.

ID: 474 / MS28-1: 3

MS28 Rough Analysis Methods in Numerical Schemes and Machine Learning

Primal and dual optimal stopping with signatures

Christian Bayer, Luca Pelizzari, John Schoenmakers

Weierstrass Institute, Germany; christian.bayer@wias-berlin.de

We propose two signature-based methods to solve the optimal stopping problem in non-Markovian frameworks. Both methods rely on a global approximation result for Lp−functionals on rough path-spaces,

using linear functionals of robust, rough path signatures. In the primal formulation, we present a non-Markovian generalization of the famous Longstaff-Schwartz algorithm, using linear functionals of the signature as regression basis. For the dual formulation, we parametrize the space of square-integrable martingales using linear functionals of the signature, and apply a sample average approximation. We prove convergence for both methods and present first numerical examples in non-Markovian and non-semimartingale regimes.

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations

Organizers: Anastasia Istratuca (a.istratuca@sms.ed.ac.uk), Aretha Teckentrup (a.teckentrup@ed.ac.uk)

ID: 216 / MS29-1: 1

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations

Kernel methods for solving rough nonlinear partial differential equations

Ricardo Baptista, Edoardo Calvello, Matthieu Darcy, Houman Owhadi, Andrew Stuart, Xianjin Yang

California Institute of Technology, United States of America; mdarcy@caltech.edu

Following the promising success of kernel methods in solving non-linear partial differential equations (PDEs), we investigate the application of Gaussian process methods to solve PDEs with rough forcing terms. We introduce an optimal recovery scheme defined by a Reproducing Kernel Hilbert Space (RKHS) of functions of greater regularity than that of the PDE's solution. We present the theoretical framework and prove convergence guarantees for the recovery of solutions to the PDE. We illustrate its application numerically to problems arising in nonlinear smoothing from stochastic partial differential equation models.

ID: 346 / MS29-1: 3

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations

A Budgeted Multi-Level Monte Carlo Method for Estimates on the Full Spatial Domain

Niklas Baumgarten

Universität Heidelberg, Germany; niklas.baumgarten@uni-heidelberg.de

We present a parallel high-performance budgeted multi-level Monte Carlo method to estimate statistical moments on the entire spatial domain. The method is designed to operate optimally within a memory and CPU-time constraint. To achieve this, we build on a budgeted multi-level Monte Carlo framework and enhance it with a novel parallel multi-index update algorithm. By using this update algorithm, we demonstrate that computing full spatial domain estimates is asymptotically equal in CPU-time to computing just a single quantity of interest, and that the maximal memory usage is similar to approximating the deterministic formulation of the problem.

ID: 426 / MS29-1: 4

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations

Multilevel Monte Carlo Methods with Smoothing

Anastasia Istratuca[1,2], Aretha Teckentrup[1]

[1]University of Edinburgh, United Kingdom; [2]Heriot-Watt University, United Kingdom; a.istratuca@sms.ed.ac.uk

We consider the computational efficiency of Monte Carlo (MC) and Multilevel Monte Carlo

(MLMC) methods applied to elliptic partial differential equations with random coefficients. We make use of the circulant embedding procedure to sample from the aforementioned coefficient. Then, to further improve the computational complexity of the MLMC estimator, we devise and implement the smoothing technique integrated into the circulant embedding method. This allows to choose the coarsest mesh on the first level of MLMC independently of the correlation length of the covariance function of the random field, leading to considerable savings in computational cost.

ID: 567 / MS29-1: 2

MS29 Efficient Methods for Uncertainty Quantification in Differential Equations

"The Mean-Field Ensemble Kalman Filter: From Analysis to Algorithms"

Edoardo Calvello

California Institute of Technology, United States of America; e.calvello@caltech.edu

The ensemble Kalman methodology is an innovative and flexible set of tools which can be used for both state estimation in dynamical systems and parameter estimation for generic inverse problems. Despite its widespread adoption in fields of application, firm theoretical foundations are only now starting to emerge. We consider a unifying approach to algorithms that rests on transport of measures and mean-field stochastic dynamical systems. With the goal of developing theoretical guarantees for ensemble Kalman methods applied to non-linear problems, we discuss the error analysis of the stochastic dynamical systems arising in ensemble Kalman filtering and the associated probability measures.

MS30 Advanced Numerical Methods for CFD with Applications

Organizers: Tiegang Liu (liutg@buaa.edu.cn), Kun Wang (wangkun@buaa.edu.cn), Xing Ji (xjiad@connect.ust.hk), Liang Pan (panliang@bnu.edu.cn)

ID: 197 / MS30-3: 2

MS30 Advanced Numerical Methods for CFD with Applications

Advanced computing process in HODG framework

Kun Wang, Tiegang Liu

Beihang University, China, People's Republic of; wangkun@buaa.edu.cn

In this work, we present HODG, a component-based development framework based on high order Discontinuous Galerkin (DG) methods for solving compressible Euler and Navier-Stokes equations. Built on the top-level design of components, HODG is a flexible yet pragmatic development framework that works right out of the box and is easy to use for starters and developers. In this presentation, we will focus on new advances in advanced computing such as high-order methods, massively parallel computing, GPU parallelism, and aerodynamic optimization in HODG software.

ID: 247 / MS30-2: 4

MS30 Advanced Numerical Methods for CFD with Applications

Multi-scale finite element method (MsFEM) for incompressible flows

Loïc Balazi[1,2], Grégoire Allaire[1], Pascal Omnes[2]

[1]Ecole Polytechnique, France; [2]CEA Saclay; loic.balazi@polytechnique.edu

Simulating the flow in a multi-scale medium with many obstacles is very challenging. We develop an enriched non-conforming Multi-scale Finite Element Method (MsFEM) in the vein of the Crouzeix-Raviart method to solve viscous incompressible flows (the Stokes and the Oseen problems) in heterogeneous media. We perform a rigorous theoretical study of the developed MsFEM in two and three dimensions at both continuous and discrete levels. We derive a new error estimate for the MsFEM applied to the Stokes problem. The perspective of this work is to solve the Navier-Stokes equations with MsFEM basis functions.

ID: 365 / MS30-2: 2

MS30 Advanced Numerical Methods for CFD with Applications

Physical-constraint-preserving high-order DG method for compressible multi-medium flows

Fan Zhang

University of Science and Technology Beijing, China, People's Republic of; zhangfan0128@ustb.edu.cn

This work develops a physical-constraint-preserving direct arbitrary Lagrangian-Eulerian discontinuous Galerkin method for compressible two-medium flows by solving the five-equation transport model. It satisfies the discrete geometric conservation law (D-GCL) which indicates that uniform flow is precisely preserved during the simulation. Moreover, based on the D-GCL condition, we present a theoretical analysis on designing an efficient physical-constraint-preserving limiting strategy for maintaining the boundedness of the volume fraction and the positivity of the partial density and internal energy. A series of benchmark cases are tested in order to demonstrate the accuracy and robustness of the proposed method.

ID: 387 / MS30-1: 2

MS30 Advanced Numerical Methods for CFD with Applications

A mechanism-informed reinforcement learning framework for shape optimization of airfoils

Jingfeng Wang, Guanghui Hu

Department of Mathematics, University of Macau, Macao S.A.R. (China); garyhu@um.edu.mo

In this paper, we propose a mechanism-informed reinforcement learning framework for airfoil shape optimization using the twin delayed deep deterministic policy gradient algorithm. Our approach leverages a PDEs-based solver with a geometry module using hundreds of sample points, ensuring robustness even with significant configuration changes. We integrate Laplacian smoothing, adaptive refinement, and Bézier fitting to streamline the deformation process, and our neural network architecture employs Bézier curves for efficient dimensionality reduction. Additionally, we customize reward and penalty mechanisms to ensure an efficient strategy for optimizing airfoil shapes within a high dimensionality.

ID: 400 / MS30-3: 1

MS30 Advanced Numerical Methods for CFD with Applications

High-fidelity simulation based on multi-moment finite volume method on hybrid unstructured grids

Bin Xie[1], Feng Xiao[2]

[1]Shanghai JiaoTong University, China, People's Republic of; [2]Tokyo Institute of Technology, Japan; xie.b.aa@sjtu.edu.cn

Unstructured grid has been the main solution to solve fluid engineering problems in computational fluid dynamics. In order to overcome the limitations of conventional unstructured methods, we have proposed VPM schemes for the accurate and robust numerical simulation. Some high-fidelity numerical models are

also developed for compressible and incompressible flows with free surfaces. Compared with the conventional method, the new model significantly improves the solution quality and convergence behavior of numerical results. This talk will also report some progresses for their applications to numerical simulation of complex flows in the field of ocean engineering.

ID: 405 / MS30-1: 5

MS30 Advanced Numerical Methods for CFD with Applications

Numerical Simulation of High Enthalpy Flows using Gas-Kinetic Scheme with Multi-Temperature Model

Hualin Liu[1], **Xing Ji**[2]

[1]China Jiliang University, People's Republic of China; [2]State Key Laboratory for Strength and Vibration of Mechanical Structures, Shaanxi Key Laboratory of Environment and Control for Flight Vehicle, School of Aerospace Engineering, Xi'an Jiaotong University, Xi'an, People's Republic of China; hualinliu@cjlu.edu.cn, jixing@xjtu.edu.cn

Numerical simulations for hypersonic and high enthalpy flows are carried out using Gas-Kinetic Scheme with multi-temperature model for nitrogen with double cone configuration. Molecular reaction dynamics including orientation effect and centrifugal barrier are considered to accurately calculate the chemical reaction rates. Transport Properties in current thermochemical non-equilibrium model are calculated using existing shock-tube experimental data. To overcome the serious numerical stiffness problems, a fully implicit LU-SGS algorithm is used for acceleration. The multi-temperature model together with Gas-Kinetic Scheme approximately reproduce the measured physical quantities on the surface.

ID: 411 / MS30-1: 4

MS30 Advanced Numerical Methods for CFD with Applications

A discontinutiy feedback factor for compressible flow simulation

Xing Ji

xi'an jiaotong university, China, People's Republic of; jixing@xjtu.edu.cn

The traditional limiters, such as van Leer and Venkatakrishnan, are widely used in finite volume methods for compressible flow. The purpose of limiters is to suppress Gibbs errors caused by numerical discontinuities and improve the robustness of numerical methods. However, traditional limiters (mainly priori limiters) cannot always detect discontinuties properly, making them difficult to achieve both robustness and accuracy. This talk will introduce the construction of discontinuity feedback factor (DF) which removes the continuity assumption within a finite volume cell, and the numerical results show that DF can be good alternative to the limiter.

ID: 469 / MS30-2: 3

MS30 Advanced Numerical Methods for CFD with Applications

Multiple-GPU accelerated high-order gas-kinetic scheme for direct numerical simulation of compressible turbulence

Liang Pan

Beijing Normal University, China, People's Republic of; panliang@bnu.edu.cn

High-order gas-kinetic scheme (HGKS) has become a workable tool for the direct numerical simulation (DNS) of turbulence. In this paper, to accelerate the computation, HGKS is implemented with the graphical processing unit (GPU) using the compute unified device architecture (CUDA). For large-scale DNS of turbulence, we develop a multi-GPU HGKS simulation using message passing interface (MPI) and CUDA. For multiple-GPU computation, multiple-GPU accelerated HGKS code scales properly with the increasing number of GPU.

ID: 659 / MS30-1: 1

MS30 Advanced Numerical Methods for CFD with Applications

Robust and Efficient Unstructured Finite Volume Method for Compressible Flow Simulations

Xiaoquan Yang, Jia Yan, Jue Ding

Shanghai University, China, People's Republic of; quanshui@shu.edu.cn

This paper proposes a robust and efficient method for simulating compressible flow, based on unstructured finite volume method. Key components of this method include the utilization of a compact Least-Squares reconstruction method for calculating gradients of flow field variables and an exact Jacobian matrix solving method for implicit temporal discretization. Numerical assessments conducted on several benchmark cases illustrate the superior stability and convergence of the proposed methods. Notably, these methods exhibit the capability for stable and rapid convergence even with large time steps (large CFL numbers), showcasing promising potential for applications in turbulent flow simulations within intricate configurations.

ID: 677 / MS30-1: 3

MS30 Advanced Numerical Methods for CFD with Applications

A compact fully-discrete high-order schemes for complex flow simulation

Shucheng Pan, Tong Zhou

Northwestern Polytechnical University, China, People's Republic of; shucheng.pan@nwpu.edu.cn

By constructing and discretizing the (quasi) exact solution of the Hamilton-Jacobi equation corresponding to the conservation law equation, we propose a compact fully discrete scheme which can achieve up to a 7th-order stencil with only 3 points, without significant computaion increase. In addition, combined with WENO reconstruction, the compact fully-discrete WENO scheme was constructed and extended to the Euler equation. Numerical experiments show that the this scheme has lower dissipation and higher resolution and computational efficiency than Runge-Kutta-WENO, which is especially significant for problems that require long-term computational evolution.

ID: 717 / MS30-2: 1

MS30 Advanced Numerical Methods for CFD with Applications

A staggered Lagrangian MHD method based on subcell Riemann solver

Zhijun Shen

Institute of Applied Physics and Computational Mathematics, China, People's Republic of; shen_zhijun@iapcm.ac.cn

This paper uses a general formalism to derive staggered Lagrangian method for 2D compressible magnetohydrodynamics (MHD) flows. A subcell method is introduced to discrete the system and Riemann problems over subcells are solved at the cell center and grid node respectively. In order to meet the

thermodynamic Gibbs relation in isentropic flows, an adaptive Riemann solver is implemented at the cell center, in which a criterion is proposed to reduce overheating errors in the rarefying problems and maintain the excellent shock-capturing ability simultaneously.

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Organizers: Tao Zhou (tzhou@lsec.cc.ac.cn), Liang Yan (yanliang@seu.edu.cn), Li Zeng (li.zeng@epfl.ch)

ID: 229 / MS31-1: 4

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Deep adaptive density approximation for Fokker-Planck type equations

Li Zeng

École Polytechnique Fédérale de Lausanne, Switzerland and Fuzhou University, Fujian, China;
li.zeng@epfl.ch

In recent years, deep learning algorithms based on deep neural networks have been widely applied to solving high-dimensional partial differential equations, which include physics-informed neural networks (PINNs), Deep Ritz method, and so on. In this talk, we start from Fokker-Planck equations and propose flow-based adaptive sampling strategies to improve the efficiency and accuracy of PINNs for solving partial differential equations whose solutions are probability density functions.

ID: 232 / MS31-1: 1

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Learning prediction function of prior measures for statistical inverse problems

Junxiong Jia

Xi'an Jiaotong University, United Kingdom; jjx323@xjtu.edu.cn

The statistical inverse problems of PDEs can be seen as the PDE-constrained regression problem. From this perspective, we propose general generalization bounds for learning infinite-dimensionally defined prior measures in the style of the probability approximately correct Bayesian learning theory. The theoretical framework is rigorously defined on infinite-dimensional function space, which makes the theories intimately connected to the usual infinite-dimensional Bayesian inverse approach. Based on the obtained bounds, infinite-dimensionally well-defined practical algorithms are formulated.

ID: 275 / MS31-1: 3

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Deep adaptive sampling for surrogate modeling without labeled data

Kejun Tang

PKU-Changsha Institute for Computing and Digital Economy, China, People's Republic of;
tangkejun@icode.pku.edu.cn

In this talk, we present a deep adaptive sampling method for surrogate modeling (DAS^2), where we generalize the deep adaptive sampling (DAS) method [Tang, Wan and Yang, JCP, 2023] to build surrogate models for low-regularity parametric differential equations. We demonstrate the effectiveness of DAS^2 with a series of numerical experiments, including the parametric lid-driven 2D cavity flow problem with a continuous range of Reynolds numbers from 100 to 1000. The numerical results show that DAS^2 outperforms non-adaptive algorithms and significantly improves the accuracy of all-at-once solutions regardless of neural network structures of the surrogate model.

ID: 532 / MS31-2: 2

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Resolution invariant deep operator network for PDEs with complex geometries

Yue Qiu

Chongqing University, China, People's Republic of; qiuyue@cqu.edu.cn

We propose a novel framework called resolution-invariant deep operator (RDO) that decouples the spatial domain of the input and output. RDO is motivated by the Deep operator network (DeepONet) and it does not require retraining the network when the input/output is changed compared with DeepONet. RDO takes functional input and its output is also functional so that it keeps the resolution invariant property of neural operators. It can also resolve PDEs with complex geometries whereas the Fourier neural operator (FNO) fails. Various numerical experiments demonstrate the advantage of our method over DeepONet and FNO.

ID: 553 / MS31-2: 1

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

Phase Field Smoothing-PINN: a neural network solver for partial differential equations with discontinuous coefficients

Zihao Yang[1], Rui He[1], Jizu Huang[2], Xiaofei Guan[3]

[1]Northwestern Polytechnical University, People's Republic of China; [2]Chinese Academy of Sciences, People's Republic of China; [3]Tongji University, People's Republic of China; yangzihao@nwpu.edu.cn

In this talk, we propose a phase field smoothing-physics informed neural network (PFSPINN) approach to efficiently solve partial differential equations (PDEs) with discontinuous coefficients. This method combines the phase field model and the PINN model to overcome the difficulty of low regularity solutions and eliminate the limitations of interface constraints in existing neural network solvers for PDEs with discontinuous coefficients. The proposed PFS-PINN approach includes two key parts, a neural network solver for phase field models is presented for constructing approximate PDEs with smooth coefficients, and the mixed PINN model is introduced to solve the approximate PDEs.

ID: 591 / MS31-1: 2

MS31 Advances in Scientific Machine Learning with Applications to Uncertainty Quantification

On theoretical understanding of generative distribution learning through the lens of infinite-dimensional statistics

Lin Liu[1], Ling Guo[2], Lei Ma[2], Sihui Zhao[1]

[1]Shanghai Jiao Tong University, China; [2]Shanghai normal university, China; 1000494866@smail.shnu.edu.cn

In this talk, we study the convergence rates of generative learning via the lens of infinite-dimensional statistics, using the celebrated generative adversarial networks as a running example. In contrast to previous works, we tackle this problem from the point of view of learning the transportation map to Holder densities from simple random input such as isotropic Gaussians. Additionally, we also consider the case where the

input and output dimensions differ and show the benefit of using random noise with larger dimensions. Finally, we demonstrate the utility of our theoretical results via large-scale numerical experiments.

MS32 Advances on Numerical Methods for Singular Perturbation Problems

Organizers: Natesan Srinivasan (natesan@iitg.ac.in)

ID: 262 / MS32-1: 3

MS32 Advances on Numerical Methods for Singular Perturbation Problems

On simple numerical scheme for interface problem

Shuo Zhang[1,2]

[1]Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; [2]University of Chinese Academy Sciences, China, People's Republic of; szhang@lsec.cc.ac.cn

This talk is devoted to the simple solution process of interface problem. With a simple process, we are concerned not only on the general features including stability and accuracy, but also on the ease and convenience for practical designers and users in constructing an implementable scheme. We will introduce a simple finite element scheme for fourth order interface problem, and, if time permits, a simple scheme by neural networks.

ID: 534 / MS32-1: 1

MS32 Advances on Numerical Methods for Singular Perturbation Problems

Error Analysis of Weak Galerkin FEM for Singularly Perturbed Fourth–order Parabolic PDEs

Natesan Srinivasan, Aayushman Raina

Indian Institute of Technology Guwahati, India; natesan@iitg.ac.in

Here, we propose an efficient numerical scheme to solve fourth–order singularly perturbed parabolic initial-boundary-value problem. The numerical scheme consists of Crank-Nicolson method for the time-derivative and weak Galerkin finite element method (WG-FEM) for the spatial derivatives. In order to overcome the boundary layer effects, here, we use the layer-adapted Shishkin meshes for the spatial discretization. Stability estimates for semi-discrete and fully-discrete WG-FEM scheme have been derived. Anisotropic error estimates in H^2 equivalent norm has also been obtained and uniform convergence of the proposed method has also been proved. Numerical examples are presented corroborating our theoretical findings.

ID: 575 / MS32-1: 2

MS32 Advances on Numerical Methods for Singular Perturbation Problems

Numerical solution for singularly perturbed time-delayed parabolic problems involving two small parameters

JUGAL MOHAPATRA[1]**, SUSHREE PRIYADASHANA**[2]

[1]National Institute of Technology Rourkela, India; [2]Institute of Technical Education and Research, Bhubaneswar, India; jugal@nitrkl.ac.in

Here, we propose an upwind-based numerical technique for time-delayed parabolic convection-reaction-diffusion problems with two small parameters. Different layer-rectifying meshes are used in the spatial direction to handle the abrupt change in the solution due to the presence of perturbation parameters. For the 1D case, the Richardson extrapolation technique is used to elevate the accuracy of the upwind scheme.

whereas in the case of 2D problems, the ADI-based operator-splitting algorithm is used which is computationally more robust.

ID: 577 / MS32-1: 4

MS32 Advances on Numerical Methods for Singular Perturbation Problems

Fractal cubic spline method for nonself-adjoint singularly perturbed boundary-value problems

Guru Prem Prasad Mahalingam[1], **Balasubramani N**[2], **Natesan S**[1]

[1]INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI, India; [2]NATIONAL INSTITUTE OF TECHNOLOGY TIRUCHIRAPPALLI, India; mgpp@iitg.ac.in

In this article, fractal cubic spline is used to get the numerical solutions of nonself-adjoint singularly perturbed boundary-value problems. Convergence analysis of the proposed method is carried out and it tells that the developed method has second order convergence. Numerical examples are provided to validate the theoretical results.

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Organizers: Steven Byram Roberts (roberts115@llnl.gov), Abhijit Biswas (abhijit.biswas@kaust.edu.sa), David George Shirokoff (david.shirokoff@njit.edu)

ID: 273 / MS33-1: 1

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Explicit Runge-Kutta Methods that Avoid Order Reduction with an Optimal Number of Stages

David George Shirokoff[1], **Abhijit Biswas**[2], **David Isaac Ketcheson**[2], **Steven Byram Roberts**[3], **Benjamin Seibold**[4]

[1]New Jersey Institute of Technology, United States of America; [2]King Abdullah University of Science and Technology (KAUST), Saudi Arabia; [3]Lawrence Livermore National Laboratory, United States of America; [4]Temple University, United States of America; shirokof@njit.edu

This talk discusses the general theory, and construction, of explicit Runge-Kutta (RK) methods that avoid order reduction on linear problems via "stiff" order conditions -- referred to as weak stage order (WSO). We develop general order barrier bounds that relate WSO, classical order and number of stages, thus characterizing the fundamental accuracy of ERK methods on stiff problems. We also devise WSO schemes that have a positive (linear) SSP coefficient, and an optimal number of stages, and demonstrate their efficacy on a suite of test cases. The mathematical ideas use RK irreducibility, orthogonal invariant subspaces and a Sylvester equation.

ID: 323 / MS33-2: 2

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Accurate Solution of the NLS Equation via Conservative Multiple-Relaxation ImEx Methods

Abhijit Biswas, **David I. Ketcheson**

King Abdullah University of Science and Technology, Saudi Arabia; abhijit.biswas@kaust.edu.sa

The nonlinear Schr\"{o}dinger equation possesses an infinite hierarchy of conserved densities, making the numerical preservation of some of these quantities critical for accurate long-time simulations, particularly for multi-soliton solutions. In this talk, I will present an essentially explicit discretization in time by combining

higher-order Implicit-Explicit (ImEx) time integrators with multiple relaxation and adaptive step size control, ensuring the conservation of the first two quantities using a conservative finite element spatial discretization. I will demonstrate the effectiveness of our proposed method via some numerical results.

ID: 362 / MS33-1: 3

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Accelerating non-equilibrium Green's function computation through dynamic mode decomposition and recurrent neural networks

Jia Yin[1], **Yang-hao Chan**[2], **Felipe Jornada**[3], **Diana Qiu**[4], **Steven Louie**[1,5], **Chao Yang**[1]

[1]Lawrence Berkeley National Laboratory; [2]Academia Sinica; [3]Stanford University; [4]Yale University; [5]University of California, Berkeley; cordelia_jia@outlook.com

Computing the numerical solution of the Kadanoff-Baym equations (KBE) satisfied by the two-time Green's functions for a quantum many-body system away from equilibrium is a challenging task. We have applied dynamic mode decomposition (DMD) to construct a data-driven reduced order model that can be used to extrapolate both the time-diagonal and off-diagonal elements of the Green's function from numerical solution of the KBE within a small time window.

Recently, we have also been working on using recurrent neural networks (RNNs) to learn and represent nonlinear integral operators, which we believe is applicable to solving the Green's function.

ID: 572 / MS33-1: 2

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Adaptive methods for the two-time Kadanoff-Baym equations

David Gardner[1], **Thomas Blommel**[2], **Emanuel Gull**[2], **Carol Woodward**[1]

[1]Lawrence Livermore National Laboratory; [2]University of Michigan; gardner48@llnl.gov

A versatile approach to simulating non-equilibrium many-body quantum systems requires solving the Kadanoff Baym equations (KBE), a system of coupled, nonlinear integro-differential equations that describe the dynamics of the matrix valued, two-time Green's functions. The computational cost of solving the KBE scales cubically with the final time and many systems involve fast excitation and slow equilibration dynamics making long-time simulations with uniform temporal grids challenging. In this talk we present the application of adaptive integration methods from the SUNDIALS library to solve the KBE and show results demonstrating increased efficiency on models of diatomic hydrogen and interacting electrons.

ID: 617 / MS33-1: 4

MS33 Challenges and Innovations for the Time-Stepping of PDEs

On the rate of error growth in time for numerical solutions for chosen PDE problems

Sebastian Bleecke

Universität Mainz, Germany; s.bleecke@uni-mainz.de

Many time-dependent differential equations are equipped with invariants. Preserving such invariants under discretization can be important, e.g., to improve the qualitative and quantitative properties of numerical solutions. Recently, relaxation methods have been proposed as small modifications of standard time integration schemes guaranteeing the correct evolution of functionals of the solution. We apply these techniques to different nonlinear dispersve wave equations.

ID: 619 / MS33-1: 5

MS33 Challenges and Innovations for the Time-Stepping of PDEs

Leveraging Unconditional Stability Theory to Advance Index-1 Differential-Algebraic Equations Without Inverting Constraints

Kiera Eloise Harmatz-Kean[1], **Benjamin Seibold**[1], **Rujeko Chinomona**[1], **David Shirokoff**[2]

[1]Temple University, United States of America; [2]NJIT, United States of America; kiera.kean@temple.edu

We apply unconditional stability theory for ImEx multistep methods to the constraint equation of Hessenberg Index-1 differential algebraic equations. This enables us to avoid inverting the constraint, which may potentially be extremely costly. These methods are also shown to be effective for the solution of singularly perturbed problems.

ID: 655 / MS33-2: 1

MS33 Challenges and Innovations for the Time-Stepping of PDEs

On the order of Runge-Kutta methods applied to stiff, semilinear ODEs

Steven Byram Roberts[1], **David George Shirokoff**[2], **Abhijit Biswas**[3], **David Isaac Ketcheson**[3], **Benjamin Seibold**[4]

[1]Lawrence Livermore National Laboratory, United States of America; [2]New Jersey Institute of Technology; [3]King Abdullah University of Science and Technology; [4]Temple University; roberts115@llnl.gov

Classical error analysis for Runge-Kutta methods relies on assumptions that rarely hold for stiff ODEs: an asymptotically small timestep and a right-hand side function with a moderate Lipschitz constant. Without idyllic assumptions, Runge-Kutta methods can experience a problematic degradation in accuracy known as order reduction. While high stage order remedies order reduction, it is only viable for expensive, fully implicit Runge-Kutta methods. In this talk, I will discuss recent advancements in deriving computationally practical Runge-Kutta methods that truly attain high order for semilinear ODEs. Our new, stiff analysis leads to rich and interesting connections with the set of rooted trees.

MS34 Computational Techniques for Bayesian Data Assimilation

Organizers: Jeremie Houssineau (jeremie.houssineau@ntu.edu.sg), Jana De Wiljes (jana@dewiljes.de)

ID: 300 / MS34-1: 1

MS34 Computational Techniques for Bayesian Data Assimilation

Ensemble Kalman Inversion in high dimension

Xin Tong

National University of Singapore, Singapore; xin.t.tong@nus.edu.sg

Ensemble Kalman inversion (EKI) is an ensemble-based method to solve inverse problems. Its gradient-free formulation makes it an attractive tool for problems with involved formulation. However, EKI suffers from the ``subspace property''.To address this issue, we propose a novel approach using localization and dropout regularization to mitigate the subspace problem. We prove that these methods converge in the small ensemble settings, and the computational cost of the algorithm scales linearly with dimension. We also show that they reach the optimal query complexity, up to a constant factor. Numerical examples demonstrate the effectiveness of our approach.

ID: 355 / MS34-1: 2

MS34 Computational Techniques for Bayesian Data Assimilation

Tensor-Train Methods for Sequential State and Parameter Estimation in State-Space Models

Tiangang Cui[1], **Yiran Zhao**[2]

[1]University of Sydney, Australia; [2]Monash University, Australia; tiangang.cui@sydney.edu.au

Numerous real-world applications require the estimation, forecasting, and control of dynamic systems using incomplete and indirect observations. These problems can be formulated as state-space models, where the challenge lies in learning the model states and parameters from observed data. We present new tensor-based sequential Bayesian learning methods that jointly estimate parameters and states. Our methods provide manageable error analysis and potentially mitigate the particle degeneracy encountered in many particle-based approaches. Besides offering new insights into algorithmic design, our methods naturally incorporate conditional transports, enabling filtering, smoothing, and parameter estimation within a unified framework.

ID: 433 / MS34-1: 3

MS34 Computational Techniques for Bayesian Data Assimilation

Ensemble Kalman Filtering Meets Gaussian Process State-Space Models

Zhidi Lin

The Chinese University of Hong Kong, Shenzhen, China, People's Republic of; zhidilin@link.cuhk.edu.cn

The Gaussian process state-space models (GPSSMs) represent a versatile class of data-driven nonlinear dynamical system models. However, the presence of numerous latent variables in GPSSM incurs unresolved issues for existing variational inference approaches, particularly under the more realistic non-mean-field (NMF) assumption, including extensive training effort, compromised inference accuracy, and infeasibility for online applications, among others. In this talk, I will delve into how the ensemble Kalman filter (EnKF) provides a promising solution to these challenges. I will also offer analysis and insights into integrating EnKF into GPSSM, showcasing its potential to enhance data-driven nonlinear dynamical system modeling.

ID: 551

MS34 Computational Techniques for Bayesian Data Assimilation

Convergence rates of non-stationary and deep Gaussian process regression

Conor Moriarty-Osborne, **Aretha Teckentrup**

University of Edinburgh, United Kingdom; conor.osborne@ed.ac.uk

Gaussian processes are a versatile tool for reconstructing functions from known training points, used in machine learning, optimisation, and data assimilation. However, they can struggle with non-stationary or anisotropic functions. Deep Gaussian processes offer a more flexible approach by nesting Gaussian processes within each other. We examine the convergence rates of deep Gaussian processes concerning the number of training points and demonstrate their superior performance over standard Gaussian processes for reconstructing non-stationary and anisotropic functions.

MS35 Discretization Methods Involving Multiple Levels and Scales

Organizers: Moritz Hauck (hauck@chalmers.se), Roland Maier (roland.maier@kit.edu), Andreas Rupp (andreas.rupp@lut.fi)

ID: 213 / MS35-1: 5

MS35 Discretization Methods Involving Multiple Levels and Scales

Numerical homogenization of nondivergence-form PDEs in a Cordes framework

Timo Sprekeler

National University of Singapore; timo.sprekeler@nus.edu.sg

We study the homogenization of the PDE $-A(x/\varepsilon):D^2 u_{\varepsilon} = f$ posed in a bounded convex domain subject to a Dirichlet boundary condition and the numerical approximation of the corresponding homogenized problem, where the measurable, uniformly elliptic, periodic and symmetric diffusion matrix A is merely assumed to be essentially bounded and (if the dimension is greater than two) to satisfy the Cordes condition.

ID: 267 / MS35-1: 3

MS35 Discretization Methods Involving Multiple Levels and Scales

Hierarchical Super-Localized Orthogonal Decomposition Methods for Multiscale Elliptic Problems

José Carlos Garay, Hannah Mohr, Daniel Peterseim

University of Augsburg, Germany; jose.garay.fernandez@uni-a.de

We present the construction of a sparse-compressed operator that approximates the solution operator of elliptic PDEs with rough coefficients. To derive the compressed operator, we construct a hierarchical basis of an approximate solution space, with super-localized basis functions that are orthogonal across hierarchy levels with respect to the inner product induced by the energy norm. The super localization is obtained through a novel variant of the Super-Localized Orthogonal Decomposition method. We present an accuracy study of the compressed solution operator as well as numerical results illustrating our theoretical findings.

ID: 269 / MS35-1: 1

MS35 Discretization Methods Involving Multiple Levels and Scales

Error bounds for discrete minimizers of the Ginzburg-Landau energy in the high-κ regime

Benjamin Dörich[1], Patrick Henning[2]

[1]Karlsruhe Institute of Technology (KIT), Germany; [2]Ruhr-University Bochum, Germany; benjamin.doerich@kit.edu

In this talk, we present our results on discrete minimizers of the Ginzburg--Landau energy in finite element spaces. Special focus is given to the influence of the Ginzburg--Landau parameter. This parameter is of physical interest as large values can trigger the appearance of vortex lattices. Since the vortices have to be resolved on sufficiently fine computational meshes, it is important to translate the size of the parameter into a mesh resolution condition, which can be done through error estimates that are explicit with respect to the Ginzburg--Landau parameter and the spatial mesh width.

ID: 297 / MS35-1: 4

MS35 Discretization Methods Involving Multiple Levels and Scales

Information Geometric Regularization of the Barotropic Euler Equation

Ruijia Cao, Florian Schaefer

Georgia Institute of Technology, United States of America; fts@gatech.edu

This talk presents an inviscid regularization for mitigating shock formation in the barotropic Euler equations. Solutions of Euler's equations are paths on the manifold of diffeomorphisms. Shocks form when the deformation map reaches the boundary of this manifold. In this work, we regularize the barotropic Euler equation by modifying the geometry of the diffeomorphism manifold. This modified geometry is motivated by semidefinite programming and the information geometry of the fluid density. In the modified geometry, geodesics do not cross the boundary of the manifold but instead approximate it asymptotically, preventing shock formation while preserving the long-time behavior of the solutions.

ID: 422 / MS35-1: 2

MS35 Discretization Methods Involving Multiple Levels and Scales

A multicale generalized FEM based on locally optimal spectral approximations for high-frequency wave problems

Chupeng Ma[1], Christian Alber[2], Robert Scheichl[2]

[1]Great Bay University, China, People's Republic of; [2]Heidelberg University; chupeng.ma@gbu.edu.cn

In this talk, I will present a generalized finite element method (GFEM) with optimal local approximation spaces for solving high-frequency heterogeneous Helmholtz problems. The local spaces are built from selected eigenvectors of carefully designed local eigenvalue problems defined on generalized harmonic spaces. The method is developed at the continuous level as a multiscale discretization scheme, and also at the discrete level as a model order reduction technique for discrete Helmholtz problems resulting from standard FE discretizations. At both continuous and discrete levels, wavenumber explicit and nearly exponential decay rates for local and global approximation errors are established.

ID: 688 / MS35-2: 1

MS35 Discretization Methods Involving Multiple Levels and Scales

Solving Jump-Coefficient Problems with High Accuracy Using Immersed Three-Field Formulation

Michał Wichrowski

Heidelberg University, Germany; wichrowski@uni-heidelberg.de

We propose a method for solving the discontinuous coefficient Poisson problem by coupling two overlapping grids. This approach involves formulating two Poisson problems: one over the entire domain (background) and the other specifically over the inclusion (foreground). These are coupled at the boundary of the foreground mesh using Lagrange multipliers. Additionally, the formulation requires incorporating an auxiliary equation on the foreground to ensure consistency. Finally, we demonstrate the convergence rate through numerical experiments and discuss potential extensions to the Stokes problem.

ID: 727 / MS35-2: 2

MS35 Discretization Methods Involving Multiple Levels and Scales

Homogeneous multigrid for hybrid discretizations: application to HHO methods

Daniele A. Di Pietro[1], Zhaonan Dong[2], Guido Kanschat[3], Peipei Lu[4], Pierre Matalon[5], Andreas Rupp[6]

[1]University of Montpellier, France; [2]Inria, France; [3]Heidelberg University, Germany; [4]Soochow University, China; [5]École Polytechnique, France; [6]LUT University, Finland; andreas.rupp@lut.fi

We prove the uniform convergence of the geometric multigrid V-cycle for hybrid high-order (HHO) and other discontinuous skeletal methods. Our results generalize previously established results for HDG methods, and our multigrid method uses standard smoothers and local solvers that are bounded, convergent, and consistent. We use a weak version of elliptic regularity in our proofs. Numerical experiments confirm our theoretical results.

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Organizers: Gilles Vilmart (gilles.vilmart@unige.ch), Konstantinos C. Zygalakis (kzygalak@ed.ac.uk)

ID: 193 / MS36-1: 4

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Advanced Time-Adaptive PIROCK Method with Error Control for Magnetic Reconnection Simulations in Chromospheric Environments

Q. M. Wargnier[1,2], **G. Vilmart**[5], **J. Martinez-Sykora**[1,2,3], **V. H. Hansteen**[1,2,3,4], **B. De Pontieu**[1,3,4]

[1]Lockheed Martin Solar and Astrophysics Laboratory, United States of America; [2]Bay Area Environmental Research Institute; [3]Rosseland Centre for Solar Physics, University of Oslo; [4]Institute of Theoretical Astrophysics, University of Oslo; [5]Mathematics Section, University of Geneva; conferences.baer@gmail.com

Understanding the Sun's chromosphere heating mechanism is crucial in solar physics, with magnetic reconnection (MR) playing a key role. Recent observations highlight ion-neutral interactions' importance, yet current models struggle to fully integrate them. We introduce a numerical simulation using a Multi-Fluid Multi-Species (MFMS) model to explore MR in upper chromospheric environments, considering interactions among multiple species. Integrating the MFMS model is challenging due to its multi-scale nature, causing stability and efficiency issues for classical methods. Hence, we employ the second-order Partitioned Implicit-Explicit Runge-Kutta (PIROCK) method, renowned for handling such systems. Our findings underscore particle decoupling's vital role in facilitating efficient chromospheric heating mechanisms.

ID: 279 / MS36-1: 2

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Splitting methods with modified potentials for certain classes of nonlinear evolution equations

Fernando Casas

Universitat Jaume I, Spain; fernando.casas@mat.uji.es

Splitting methods constitute a powerful tool for the numerical integration of differential equations. The existence of negative coefficients restricts, however, their application to only order 2 in PDEs of parabolic type. To overcome this order barrier for linear problems, an alternative consists in incorporating double commutators into the scheme. In this talk we show how this technique can be generalized to certain classes of nonlinear equations. The resulting fourth-order methods are illustrated for the time-dependent Gross--Pitaevskii equation in three space dimension and for its parabolic counterpart for computations of the ground state and excited states.

ID: 280 / MS36-1: 3

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Overcoming the order barrier two in splitting methods when applied to semilinear parabolic problems with non-periodic boundary conditions

Ramona Häberli

Université de Genève, Switzerland; ramona.haeberli@unige.ch

In general, high order splitting methods suffer from an order reduction when integrating in time partial differential equations with non-periodic boundary conditions. In this talk, inspired by the recent corrector techniques for the Strang splitting scheme, we introduce a splitting method of order three for semilinear parabolic problems that avoids order reduction. We give the outline of a proof for the third order convergence of the method in a linear setting and confirm the result by numerical experiments. Moreover, we show numerically that the high order convergence persists for a nonlinear source term, and for an order four splitting method.

ID: 377 / MS36-1: 1

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Unbiased Kinetic Langevin Monte Carlo with Inexact Gradients

Neil Chada[2], Benedict Leimkuhler[1], Daniel Paulin[1], Peter Whalley[1]

[1]University of Edinburgh, United Kingdom; [2]Heriot-Watt University, Edinburgh, United Kingdom; dpaulin@ed.ac.uk

We present an unbiased method for Bayesian posterior means based on kinetic Langevin dynamics that combines advanced splitting methods with enhanced gradient approximations. Our approach avoids Metropolis correction by coupling Markov chains at different discretization levels in a multilevel Monte Carlo approach. Theoretical analysis demonstrates that our proposed estimator is unbiased, attains finite variance, and satisfies a central limit theorem. We prove similar results using both approximate and stochastic gradients and show that our method's computational cost scales independently of the size of the dataset. Our numerical experiments demonstrate that our unbiased algorithm outperforms the ``gold-standard'' randomized Hamiltonian Monte Carlo.

ID: 394 / MS36-2: 1

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Numerical methods for stochastic collisional dynamics

Benedict Leimkuhler[1], Akash Sharma[2], Michael Tretyakov[3]

[1]University of Edinburgh, United Kingdom; [2]Chalmers University, Sweden; [3]Nottingham University, United Kingdom; b.leimkuhler@ed.ac.uk

I will discuss numerical algorithms for overdamped and underdamped Langevin dynamics in which bodies undergo occasional collisions or interactions with a hard domain boundary. These types of models arise in various settings in physics, chemistry, biology, engineering, and statistics. I will discuss various approaches to the problem and describe a stochastic collisional integrator with a "superconvergence property." I will illustrate the use of the methods with a regularization scheme for machine learning applications.

ID: 402 / MS36-2: 2

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Exotic aromatic forests for high-order sampling of the invariant measure

Eugen Bronasco

University of Geneva, Switzerland; Eugen.Bronasco@unige.ch

Exotic aromatic forests, an extension of aromatic forests into the stochastic context, serve pivotal roles in generating order conditions for invariant measure sampling and studying the algebraic properties of stochastic integrators. This talk unveils practical benefits through a new method, a generalization of the Leimkuhler-Matthews method, while also briefly exploring the favorable algebraic properties of exotic aromatic forests.

Based on joint works with A. Laurent, B. Leimkuhler, D. Phillips, G. Vilmart.

ID: 425 / MS36-2: 3

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

Uniform in time numerical approximations of (multiscale) SDEs

Michela Ottobre

Heriot Watt university, United Kingdom; m.ottobre@hw.ac.uk

We consider approximation methods for (multiscale) SDEs and present a flexible framework for analysis which produces simple criteria to check when the approximation at hand is a uniform-in-time approximation of the given SDE – property which is key in virtually all statistical applications. We demonstrate how such a method is very general, and can be used when the approximation is produced by numerical schemes, particle methods or multiscale methods, to mention just a few. For illustration, we focus on multiscale approaches to Maximum Marginal Likelihood Estimation.

ID: 738 / MS36-2: 4

MS36 Geometric and Multiscale Methods for High-Dimensional Dynamics

State-Space Systems as Dynamic Generative Models

Florian Rossmannek

Nanyang Technological University, Singapore; florian.rossmannek@ntu.edu.sg

Reservoir computing is a powerful tool in learning temporal dynamics and forecasting time series. Although applications often have a stochastic flavour, the existing theory mainly deals with deterministic problems. This poses a significant gap between theory and practice, which we fill in this talk. We do so by establishing a stochastic version of the so-called echo state property, which is the key property needed for successful implementation. We will see that this equates to studying the behaviour of state-space systems as generative models and that the stochastic theory is much richer and much more intricate than its deterministic counterpart.

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Organizers: Li-Lian Wang (lilian@ntu.edu.sg), Bo Wang (bowang@hunnu.edu.cn), Zhiguo Yang (yangzhiguo@sjtu.edu.cn)

ID: 210 / MS37-1: 4

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

A perfectly matched layer method for signal-propagation problems in axon

Xue Jiang

Beijing University of Technology, China; jiangx@bjut.edu.cn

This talk considers the modelling of signal propagations in myelinated axons. The well-posedness of model is established. Using the perfectly matched layer (PML) method, we truncate the unbounded background medium and propose an approximate problem on the truncated domain. The well-posedness of the PML problem and the exponential convergence of the approximate solution to the exact solution are established. Numerical experiments are presented to demonstrate the theoretical results and the efficiency of our methods to simulate the signal propagation in axons.

ID: 545 / MS37-1: 3

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Structure-preserving spectral and spectral-element methods for Vlasov-Maxwell equations

Zhiguo Yang

Shanghai Jiao Tong University, China, People's Republic of; yangzhiguo@sjtu.edu.cn

In this talk, I will present our recent progress on structure-preserving spectral and spectral-element methods for Vlasov-Maxwell equations, which are crucial for achieving long-time accurate, stable, consistent and physically meaningful plasma simulations. We first present H(div)-conforming spectral bases with exact preservation of the magnetic Gauss's law constraint. Next, we extend these ideas to a mixed divergence-free spectral-element method. We then present some numerical examples for high-dimensional Vlasov-Maxwell system to illustrate both the accuracy and efficiency of the proposed method.

ID: 561 / MS37-1: 1

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Cavity scattering problems for the biharmonic wave equation

Peijun Li

Chinese Academy of Sciences, China, People's Republic of; lipeijun@lsec.cc.ac.cn

The talk is concerned with the cavity scattering problems associated with biharmonic waves in an infinite thin plate. Based on the operator splitting, the scattering problem is recast into a coupled boundary value problem for the Helmholtz and modified Helmholtz equations. A novel boundary integral formulation is proposed for the coupled problem. The convergence is analyzed for the semi- and full-discrete schemes of the boundary integral system. The inverse problem is to determine the domain of the cavity, for which two uniqueness results will be presented, utilizing far-field patterns and phaseless near-field data.

ID: 580 / MS37-2: 4

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

A general tetrahedral spectral element method and its implementation to Kohn-Sham equation

Hongfei Zhan[1], **Guanghui Hu**[2]

[1]Peking University, China, People's Republic of; [2]University of Macau, Macao SAR, China;
zhanhf@math.pku.edu.cn

In this work, we firstly design a tetrahedral spectral element method for partial differential equations tailored for general tetrahedral meshes, utilizing generalized Koornwinder polynomials. A transformation is devised between degree of freedoms on local elements and ones on global geometries to ensure the global C^0 property of the approximations. Then features of the proposed tetrahedral spectral element method are demonstrated through solving the all-electron Kohn-Sham equation, in which the proposed method is employed for spatial discretization. Results from a benchmark harmonic oscillator problem clearly deliver the desired spectral convergence.

ID: 594 / MS37-2: 3

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Numerical simulation of nonlocal effects in metallic nanostructures using generalized HD model

Maohui Lyu

Beijing University of Posts and Telecommunications, China, People's Republic of; mlyu@bupt.edu.cn

The classical hydrodynamical Drude model provides fairly accurate description for the nonlocal optical interactions in metallic nanostructures. However, for small nano-particles of size down to subwavelength, the HD model is not able to capture the electron distribution within a thin transition layer around the material surfaces. In this talk, by revisting the hamiltonian of the electron system, we first derive a generalized HD model with self-consistent electron distribution to take account the electron spill-out and tunnelling effects. We further develop and analyze DG method for this generalized model to simulate nonlocal effects in single nanowire and dimers.

ID: 596 / MS37-1: 2

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Low regularity estimates of the Lie-Trotter time-splitting Fourier spectral method for the logarithmic Schrödinger equation

Xiaolong Zhang, Li-Lian Wang

Nanyang Technological University, Singapore; xlzhang@hunnu.edu.cn

The logarithmic Schrödinger equation exists rich dynamics and possesses some unique properties when compared to usual Schrödinger equation with cubic nonlinearity. However, the presence of the logarithmic nonlinear term f(u) = u ln (|u|^2) poses significant challenge in both numerical solution and error analysis, largely due to the low regularity and singularity. In this talk, we shall characterize such a low regularity in suitable fractional Sobolev space and derive an error estimates for the time-splitting Fourier spectral methods with initial value of fractional order regularity.

ID: 645 / MS37-2: 2

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Fast boundary element method for scattering problem in layered media

Bo Wang

Hunan Normal University, China, People's Republic of; bowang@hunnu.edu.cn

In this talk, a fast algorithm is proposed for solving scattering problem in layered media. Boundary integral equation is derived for the exterior problem by using the layered Green's function. Collocation method is employed to discretize the boundary integral equation and the GMRES iterative method with fast multipole algorithm for layered Green's function is used to provide a fast solver for the dense linear system.

ID: 684 / MS37-2: 1

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Structure-preserving particle-in-cell method for plasma simulations

Zhenli Xu

Shanghai Jiao Tong University, China, People's Republic of; xuzl@sjtu.edu.cn

We introduce structure-preserving numerical methods for models in plasma simulations. We construct curl-free basis functions for the Vlasov-Ampère equations which is equivalent to the Vlasov-Poisson equations. The scheme with energy conservation is designed, together with an asymptotic-preserving preconditioner such that the scheme can simulate systems with small Debye length. We also present an energy-stable asymptotic preserving PIC for the Vlasov-Maxwell system, which can simulate systems at the quasi-neutral limit. Classical benchmarks including the Landau damping, two-streaming instability and bump-on-tail instability are present to show the necessity of structure preserving and the attractive performance of the new algorithms.

ID: 699 / MS37-2: 5

MS37 High-Order Methods for Linear and Nonlinear Wave Propagation

Numerical methods for the biharmonic nonlinear Schrödinger equation

Zhang Teng

Guangxi University, China, People's Republic of; zhangteng@gxu.edu.cn

The biharmonic nonlinear Schrödinger equation (BNLS) is a foundational model in nonlinear optics, as the biharmonic operator provides additional stability for soliton solutions, offering a refined description of light propagation in nonlinear media. The high dispersion term from the biharmonic operator imposes numerical burdens that requires either large computational domain or high-accuracy method. In this talk, I will discuss several numerical methods for solving the BNLS and present the corresponding error estimates, including two finite difference methods and time-splitting sine spectral method. Additionally, numerical examples illustrating the dispersion relation and simulations of soliton collisions, and 2D problems will be provided.

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

Organizers: Xu Yang (xuyang@math.ucsb.edu), Hailong Guo (hailong.guo@unimelb.edu.au), Lihui Chai (chailihui@mail.sysu.edu.cn), Ping Tong (tongping@ntu.edu.sg)

ID: 260 / MS38-1: 3

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

Seismic tomography with random batch gradient reconstruction

Yixiao Hu, Lihui Chai, Xu Yang, Zhongyi Huang

Sun Yat-sen University, China, People's Republic of; chailihui@mail.sysu.edu.cn

We propose to use random batch methods to construct the gradient used for iterations in seismic tomography. Specifically, we use the frozen GAussian approximation to compute seismic wave propagation, and then construct stochastic gradients by random batch method. The method inherits the spirit of stochastic gradient descent methods for solving high-dimensional optimization problems. We prove the convergence of the random batch method in the mean-square sense, and show the numerical performance of the proposed method by two-dimensional and three-dimensional examples of wave-equation-based travel-time inversion and full-waveform inversion.

ID: 261 / MS38-1: 4

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

Scalable Iterative Data-Adaptive RKHS Regularization

Haibo Li[1], **Jinchao Feng**[2], **Fei Lu**[3]

[1]The University of Melbourne, Australia; [2]Great Bay University, China; [3]Johns Hopkins University, USA; haibo.li@unimelb.edu.au

We present iDARR, a scalable iterative Data-Adaptive RKHS Regularization method, for solving ill-posed linear inverse problems. The method searches for solutions in subspaces where the true solution can be identified, with the data-adaptive RKHS penalizing the spaces of small singular values. At the core of the method is a new generalized Golub-Kahan bidiagonalization procedure that recursively constructs orthonormal bases for a sequence of RKHS-restricted Krylov subspaces. The method is scalable with a complexity of O(kmn) for m-by-n matrices with k denoting the iteration numbers. Numerical tests demostrate its good performance for Fredholm integral equations and 2D image deblurring.

ID: 265 / MS38-1: 2

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

A class of second-order dissipative hyperbolic PDEs and their applications in variational problems

Guozhi Dong

Central South University, China, People's Republic of; guozhi.dong@csu.edu.cn

The exploration of accelerated gradient flows is an emerging field in scientific computing and applied mathematics. We introduce some novel dissipative hyperbolic partial differential equations, which provide versatile tools for solving variational problems, particularly for nonconvex problems. We present an overview on some of the recent progress, with applications from different fields.

ID: 499 / MS38-1: 1

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

Machine Learning and Seismic Tomography

Xu Yang

University of California, Santa Barbara, United States of America; xuyang@math.ucsb.edu

Deep neural networks (DNNs) are a major workhorse in machine learning. In this talk, we present some preliminary results on connecting DNNs to applications in seismic tomography. We utilize deep neural networks to construct a reliable PmP database from massive seismic data and investigate a case study in Southern California. The main challenge lies in the rarity of identifiable PmP waves, making the task of identifying them from a massive seismic database inherently unbalanced.

ID: 581 / MS38-1: 5

MS38 High-Performance Computational Methods for Wave Phenomena and Related Applications

Adjoint method for elliptically anisotropic wave equations with application in medical and seismic imaging

Ping Tong

Nanyang Technological University, Singapore; tongping@ntu.edu.sg

We present an innovative approach utilizing the adjoint method for elliptically anisotropic wave equations, focusing on its application in medical and seismic imaging. The spectral-element method is employed to solve the forward and adjoint problems. In medical imaging, this technique enhances the reconstruction of high-resolution images of biological tissues, improving diagnostic capabilities and treatment planning. In seismic imaging, the adjoint method enables precise characterization of subsurface structures, aiding in resource exploration and hazard assessment. The effectiveness and versatility of the proposed approach are demonstrated through theoretical analysis and numerical simulations, highlighting its potential impact across various domains of imaging science.

MS40 Iterative Numerical Methods for Optimization and Control

Organizers: Bernhard Heinzelreiter (S2167334@ed.ac.uk), Andrés Miniguano-Trujillo (andres.miniguano-trujillo@ed.ac.uk)

ID: 271 / MS40-2: 2

MS40 Iterative Numerical Methods for Optimization and Control

Multi-level Optimal Control with Neural Surrogate Models

Estefania Loayza Romero[1], Dante Kalise[1], Kirsten A. Morris[2], Zhengang Zhong[3]

[1]Department of Mathematics, Imperial College London; [2]Department of Applied Mathematics, University of Waterloo; [3]Centre for Process Systems Engineering, Imperial College London; k.loayza-romero@imperial.ac.uk

In this talk, we study the optimal actuator and control design as a multi-level optimisation problem. The actuator design is evaluated based on the performance of the associated optimal closed loop. However, the evaluation of the optimal closed loop for a given actuator realisation is a computationally demanding task, for this reason, we propose the use of a neural network surrogate. The use of neural network surrogates to replace the lower level of the optimisation hierarchy enables the use of fast gradient-based and gradient-free consensus-based optimisation methods to determine the optimal actuator design.

ID: 277 / MS40-1: 1

MS40 Iterative Numerical Methods for Optimization and Control

Saddle Point Preconditioners for PDE-constrained optimisation: a case study from Data assimilation

Jemima M. Tabeart[1], John W. Pearson[2]

[1]TU Eindhoven, Netherlands, The; [2]The University of Edinburgh, Scotland; j.m.tabeart@tue.nl

In numerical weather prediction PDEs are used to model the evolution of the atmosphere and ocean. Variational data assimilation (VDA) methods, which are used to combine information from prior forecasts and measurement data, are a particular type of PDE-constrained optimisation problem. Solving the VDA

problem using iterative methods is still costly due to multiple evaluations of the expensive model operator. In this talk I will present new structure-exploiting preconditioners for a saddle point formulation, which improve convergence of MINRES and GMRES and reduce the total number of model evaluations.

ID: 468 / MS40-1: 3

MS40 Iterative Numerical Methods for Optimization and Control

Parallel-in-time Preconditioner for Parabolic Optimal Control Problems

Po Yin Fung, Sean Hon

Hong Kong Baptist University; seanyshon@hkbu.edu.hk

In this work, we introduce a novel preconditioned Krylov subspace method for solving an optimal control problem involving parabolic equations. Specifically, we develop an efficient block α-circulant-based preconditioner for the all-at-once linear system that arises from the optimal control problem of interest. The proposed preconditioner can be efficiently diagonalized using fast Fourier transforms in a parallel-in-time fashion. Its effectiveness is theoretically supported, which leads to rapid convergence when the generalized minimal residual method is employed. Numerical results are provided to demonstrate the effectiveness of our proposed solver.

ID: 473 / MS40-1: 2

MS40 Iterative Numerical Methods for Optimization and Control

Solving tree-coupled linear systems

Christoph Hansknecht

TU Clausthal, Germany; christoph.hansknecht@tu-clausthal.de

An increasing demand for the solution of numerical problems of ever increasing size in the realm of nonlinear programming necessitate the continuous improvement of solution codes. The algorithmic backbone of most codes consists of the solution of large systems of linear equations. The key to increasing the performance therefore lies in accelerating the required linear algebra by exploiting the well-structuredness of real-world problems. An interesting and highly relevant structure appears in problems given by a collection of subproblems coupled together based on equations linking subsets of variables. We examine the linear algebra of these systems, developing algorithmic approaches greatly accelerating their solution.

ID: 521 / MS40-2: 1

MS40 Iterative Numerical Methods for Optimization and Control

Non-smooth shape optimization with applications for fluid-mechanical problems under uncertainty

Tim Suchan[1], Caroline Geiersbach[2], Volker Schulz[3], Kathrin Welker[4]

[1]Helmut Schmidt University/University of the Federal Armed Forces Hamburg, Germany; [2]Weierstrass Institute Berlin, Germany; [3]Trier University, Germany; [4]TU Bergakademie Freiberg, Germany; suchan@hsu-hh.de

The realm of shape optimization continues to captivate both theoreticians and practitioners. From a theoretical point of view, the utilization of differential-geometric methodologies on infinite-dimensional Riemannian manifolds has emerged as a crucial approach, particularly when striving for mesh-independent outcomes. The existence of non-smoothness or uncertainties in the problem formulation further complicates the optimization.

In this presentation, we provide the theoretical background and show numerical results of constrained optimization within Riemannian shape spaces, illuminating key concepts and methodologies along the way. We show how to include uncertainties and describe some intricacies of nonsmoothness in numerical optimization.

ID: 627 / MS40-2: 4

MS40 Iterative Numerical Methods for Optimization and Control

Self isolation or social distancing: a nonlocal PDE-constrained optimisation approach for disease containment

Andrés Miniguano-Trujillo

Maxwell Institute for Mathematical Sciences, United Kingdom; Andres.Miniguano-Trujillo@ed.ac.uk

In this work, we study an optimal control approach for parameter selection applied to a dynamical density functional theory model. This is applied in particular to a spatially-dependent SIRD model where social distancing and isolation of infected persons are explicitly taken into account. Special attention is paid when the strength of these measures is considered as a function of time and their effect on the overall infected compartment. A first order optimality system is presented, and numerical simulations are presented using a pseudo spectral quasi-Newton method. This work could potentially provide some mathematical insights into the management of disease outbreaks.

ID: 630 / MS40-1: 4

MS40 Iterative Numerical Methods for Optimization and Control

A Diagonalization-Based Parallel-in-Time Preconditioner for Instationary Flow Control Problems

Bernhard Heinzelreiter, John Pearson

University of Edinburgh, United Kingdom; S2167334@ed.ac.uk

PDE-constrained optimization problems arise in various applications including the optimal control of flows. In recent years, preconditioned iterative methods have been successfully applied to these problems. In this work, we explore a diagonalization-based approach to create effective preconditioners for a range of problems, including unsteady Stokes and Oseen control. Our methodology involves approximating the original problem by a time-periodic equivalent, allowing us to perform a temporal diagonalization. This results in a parallel-in-time preconditioner tailored for solving complex flow control problems. Our approach demonstrates robustness with respect to model parameters and the discretization.

ID: 724 / MS40-2: 3

MS40 Iterative Numerical Methods for Optimization and Control

Transformers Meet Image Denoising: Mitigating Over-smoothing in Transformers via Regularized Nonlocal Functionals

Tam Nguyen[1], Tan Minh Nguyen[2], Richard Baraniuk[1]

[1]Rice University; [2]National University of Singapore; tanmn@nus.edu.sg

We show that self-attention layers in transformers minimize a functional which promotes smoothness, thereby causing token uniformity. We then propose a novel regularizer that penalizes the norm of the difference between the smooth output tokens from self-attention and the input tokens to preserve the fidelity of the tokens. Minimizing the resulting regularized energy functional, we derive the Neural

Transformer with a Regularized Nonlocal Functional (NeuTRENO), a novel class of transformer models that can mitigate the over-smoothing issue. We empirically demonstrate the advantages of NeuTRENO over the baseline transformers and state-of-the-art methods in reducing the over-smoothing on various practical tasks.

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Organizers: Haijun Yu (hyu@lsec.cc.ac.cn), Xiang Zhou (xizhou@cityu.edu.hk)

ID: 235 / MS41-1: 3

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Gaussian process for parameter estimation in dynamic systems

Hongqiao Wang

Central South University, China, People's Republic of; hongqiao.wang@csu.edu.cn

Differential equations are customarily used to describe dynamic systems (DS). Kernel method is a quick and one-step technique, but it can't obtain the estimation of solution and its derivatives which absolutely fulfills physical law. We propose a brief and simple Bayesian framework to infer the unknown parameters and the hyper-parameters in one-step by maximizing the marginal likelihood, with use of the explicit gradient information. We derive estimates and confidence intervals, and show that these have low bias and good coverage properties respectively for simulated model and real data.

ID: 236 / MS41-1: 1

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Theoretical Insights into the Structure of SGD Noise

Lei Wu

Peking University, China, People's Republic of; leiwu@math.pku.edu.cn

In this talk, we present a theoretical study of noise geometry for minibatch stochastic gradient descent (SGD), a phenomenon where noise aligns favorably with the geometry of local landscape. We propose two metrics, derived from analyzing how noise influences the loss and subspace projection dynamics, to quantify the alignment strength. Both theoretical evidence on simplified models and numerical experiments on realistic models are provided. To showcase the utility of our noise geometry characterizations, we present a refined analysis of the mechanism by which SGD escapes from sharp minima.

ID: 455 / MS41-2: 2

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Thermodynamically Consistent Model Reduction of Polymeric Fluid Dynamics using OnsagerNet

Haijun Yu

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; hyu@lsec.cc.ac.cn

Polymeric fluid dynamical models based on molecular theory, such as the Doi-Smoluchowski equation for rigid-rod polymers, are physically sound but computationally expensive due to their high dimensions. Handcrafted closure models are cheap but inaccurate for systems with large external perturbations. In this talk, we introduce a data-driven approach to develop closure models capable of reproducing both

qualitative properties and quantitative accuracy of the original high-dimensional models. Specifically, mass conservation and energy dissipation are maintained in the learned models, which are parameterized by deep neural networks with the embedded structure of a generalized Onsager principle. Numerical results will be provided.

ID: 462 / MS41-2: 3

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

A hybrid adaptive sampling for solving Fokker-Planck equations

Jiayu Zhai

ShanghaiTech University, China, People's Republic of; zhaijy@shanghaitech.edu.cn

In this work, we propose a hybrid framework for sampling collocation points that are used in solving Fokker-Planck equations. The method uses both solution value and residual distributions as the sampling distributions.The residual distribution is used adversarially as in the adversarial adaptive sampling (AAS) method. The solution value distribution provides another sampling guidance that can make the adaptive sampling more efficient.

ID: 495 / MS41-1: 2

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

SAV-based optimization methods for the training in deep learning

Zhiping Mao

Eastern Institute of Technology, Ningbo, China, People's Republic of; zpmao@xmu.edu.cn

The optimization algorithm plays an important role in deep learning and significantly affects the stability and efficiency of the training process, and consequently the accuracy of the neural network approximation. We develop in this work efficient and energy stable SAV-based optimization methods for the training in deep learning by considering the gradient flows arising from deep learning. We also combine the adaptive strategy used in Adam algorithm to improve the accuracy. We present a number of numerical tests to demonstrate that the SAV-based schemes significantly improve the efficiency and stability of the training as well as the accuracy of the neural network approximation.

ID: 498 / MS41-1: 4

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

A Minimal Control Family of Dynamical Syetem for Universal Approximation

Yifei Duan, Yongqiang Cai

School of Mathematical Sciences, Laboratory of Mathematics and Complex Systems, MOE, Beijing Normal University, 100875 Beijing, China.; 202331130036@mail.bnu.edu.cn

We demonstrate the applicability of the universal approximation property (UAP) of neural networks to dynamical systems. We find that a control family F_1 containing linear maps and only one nonlinear function, ReLU, can uniformly approximate orientation-preserving diffeomorphisms on any compact domain. We establish mild conditions, such as affine invariance, on the control family, revealing a connection between neural network approximation and control systems. These results offer theoretical insights for designing control systems in engineering applications.

ID: 543

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Weak Generative Sampler to Efficiently Sample Invariant Distribution of Stochastic Differential Equation

Zhiqiang CAI[1], **Yu CAO**[2], **Yuanfei HUANG**[1], **Xiang ZHOU**[1,3]

[1]School of Data Science, City University of Hong Kong; [2]Institute of Natural Sciences and School of Mathematical Sciences, Shanghai Jiao Tong University; [3]Department of Mathematics, City University of Hong Kong; zqcai3-c@my.cityu.edu.hk

In this talk, we introduce a weak generative sampler (WGS) framework to directly generate independent and identically distributed (iid) samples from a transport map derived from the stationary Fokker-Planck equation. Our proposed loss function, rooted in the weak form of the Fokker--Planck equation, seamlessly integrates the use of normalizing flows to characterize the invariant distribution and to facilitate sample generation from the base distribution. Unlike conventional generative models, this method does not require the invertibility of the transport map or mini-max optimization and Jacobian determinant computation. Experiments demonstrate the method's efficiency and ability to explore multiple metastable states.

ID: 547 / MS41-2: 1

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Bridging data and dynamics in single-cell transcriptomics analysis through machine learning

Peijie Zhou

Peking University, China, People's Republic of; pjzhou@pku.edu.cn

In this talk, I will discuss how machine learning has enabled us to use dynamical systems techniques to analyze the emerging scRNA-seq data in biology. I will introduce the low-dimensional dynamical manifold to identify attractor basins and transition probabilities in snapshot data. I will also present the usage of non-equilibrium theory to analyze attractor stability and identify transition-driving genes in gene expression and splicing processes. Finally, I will discuss our efforts to interpolate non-stationary time-series scRNA-seq data using Wasserstein-Fisher-Rao metric, unbalanced optimal transport, and its neural network-based partial differential equation implementations.

ID: 674 / MS41-2: 4

MS41 Machine Learning and Novel Numerical Methods for Dynamical Systems

Functional Tipping Indicators via Schrödinger Bridge

Jin Guo, **Ting Gao**

Huazhong University of Science and Technology, China, People's Republic of; jinguo0805@hust.edu.cn, tgao0716@hust.edu.cn

Action functionals between two meta-stable states in stochastic dynamical systems are good tools to study the critical transitions and tipping. We will present our recent findings on tipping indicators based on the Onsager-Machlup action functional and Schrödinger bridge. The latter also extends the transition paths to be pathway measures between two given invariant manifolds. To validate our framework, we apply our methodology to some neural models as well as real brain data, such as EEG and fMRI from epilepsy and Alzheimer's disease.

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems

Organizers: Hao Wang (wangh@scu.edu.cn)

ID: 427 / MS42-1: 1

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems

Moving Sampling Physics-informed Neural Networks induced by Moving Mesh PDE

Qiaolin He

Sichuan University, People's Republic of China; qlhejenny@scu.edu.cn

In this work, we propose an end-to-end adaptive sampling framework based on deep neural networks and the moving mesh method (MMPDE-Net), which can adaptively generate new sampling points by solving the moving mesh PDE. This model focuses on improving the quality of sampling points generation. Moreover, we develop an iterative algorithm based on MMPDE-Net, which makes sampling points distribute more precisely and controllably. Since MMPDE-Net is independent of the deep learning solver, we combine it with physics-informed neural networks (PINN) to propose moving sampling PINN (MS-PINN) and show the error estimate of our method under some assumptions.

ID: 435 / MS42-1: 2

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems

High order asymptotic computations for the Dirichlet eigenvalue problem in perforated domain with multiscale cavities.

Qiang Ma

School of Mathematics, Sichuan University, People's Republic of China; maqiang809@scu.edu.cn

A top–down strategy based on the second-order asymptotic method is presented for solving the Dirichlet eigenvalue problems on composite perforated materials with three-scale and two-periodic structures. Firstly, the second-order two-scale asymptotic expansion is performed between the macroscopic and the mesoscopic scale. Then, the second-order two-scale analysis is further developed on the mesoscopic cell functions at the microscopic level. The three-scale asymptotic expansions of the eigenvalues are derived based on the "corrector equations" in a uniform manner and calculated in the integration form. The multi-scale finite element procedures are established and the two-dimensional asymptotic computations are carried out.

ID: 556 / MS42-1: 3

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems

A Framework for Generalization Analysis of Machine-Learned Interatomic Potentials: A Case Study on Crystalline Defects

Yangshuai Wang

University of British Columbia, Canada; yswang2021@math.ubc.ca

Machine-learned interatomic potentials (MLIPs) are typically trained on datasets that cover only a subset of potential input structures, posing challenges for their generalization to a wider range of systems beyond the training set. In this talk, our goal is to explain the good generalization properties observed in MLIPs. We undertake a thorough theoretical and numerical exploration of MLIP generalization in the realm of crystalline

defect simulations. We precisely quantify how simulation accuracy is directly influenced by key factors such as the size of training structures, the selection of training observations and the level of accuracy achieved during training.

ID: 740 / MS42-1: 4

MS42 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems

Automated discovery of fundamental variables hidden in experimental data

Kuang Huang

The Chinese University of Hong Kong, Hong Kong S.A.R. (China); kuanghuang@cuhk.edu.hk

Physical laws can be described as relationships between state variables that give a complete and non-redundant description of the relevant dynamical systems. We propose a framework for determining how many state variables an observed system is likely to have, and what these variables might be, directly from video streams. We also demonstrate the effectiveness of this approach using video recordings of a variety of dynamical systems, ranging from elastic double pendulum to fire flames.

MS43 Mathematical Methods for Scientific Machine Learning

Organizers: Tiangang Cui (tiangang.cui@sydney.edu.au)

ID: 263 / MS43-2: 2

MS43 Mathematical Methods for Scientific Machine Learning

Interplay between Machine Learning and Optimisation via Algorithmic Stability

Yiming Ying

University of Sydney, Australia; yiming.ying@sydney.edu.au

Stochastic gradient methods (SGMs) have become the workhorse of machine learning (ML) due to their incremental nature with a computationally cheap update. In this talk, I will mainly discuss the close interaction between computational optimisation and statistical generalisation in machine learning, for SGMs in the framework of statistical learning theory (SLT). The core concept for this study is algorithmic stability which characterises how the output of an ML algorithm changes upon a small perturbation of the training data.

ID: 335 / MS43-2: 1

MS43 Mathematical Methods for Scientific Machine Learning

Adaptive Finite Element Interpolated Neural Networks

Santiago Badia[1], Wei Li[1], Alberto F. Martin[2]

[1]Monash University, Australia; [2]Australian National University, Australia; santiago.badia@monash.edu

In this work, we introduce h-adaptive finite element interpolated neural networks. The method relies on the interpolation of a neural network onto a finite element space that is gradually adapted to the solution during the training process to equidistribute a posteriori error indicator. The use of adaptive interpolation is essential in preserving the non-linear approximation capabilities of the neural networks to effectively tackle problems with localised features. The training relies on a gradient-based optimisation of a loss function based on the (dual) norm of the finite element residual of the interpolated neural network.

ID: 354 / MS43-1: 1

MS43 Mathematical Methods for Scientific Machine Learning

Convergence of the Randomized Kaczmarz Algorithm in Hilbert Spaces

Xin Guo[1], **Junhong Lin**[2], **Dingxuan Zhou**[3]

[1]The University of Queensland, Australia; [2]Zhejiang University, China; [3]The University of Sydney, Australia; xin.guo@uq.edu.au

Existing works on the convergence analysis of the randomized Kaczmarz algorithm typically provide exponential rates of convergence, with the base tending to one as the condition number of the system increases. Results of this kind do not work well for large systems of linear equations, and do not apply to the online algorithms on Hilbert spaces for machine learning. In this talk, we provide a condition number-free analysis, which leads to polynomial rates of weak convergence for the randomized Kaczmarz algorithm. We also show the applications to kernel-based machine learning.

ID: 380 / MS43-2: 4

MS43 Mathematical Methods for Scientific Machine Learning

Nonparametric Distribution Learning via Neural ODEs

Jakob Zech

Universität Heidelberg, Germany; jakob.zech@uni-heidelberg.de

In this talk, we explore approximation properties and statistical aspects of Neural Ordinary Differential Equations (Neural ODEs). Neural ODEs are a recently established technique in computational statistics and machine learning, that can be used to characterize complex distributions. We investigate the regularity properties of the velocity fields used to push forward a reference distribution to the target, and derive a concentration inequality for the maximum likelihood estimator of general ODE-parametrized transport maps. Our discussion will particularly focus on C^k densities on the d-dimensional unit cube $[0,1]^d$.

ID: 415 / MS43-1: 3

MS43 Mathematical Methods for Scientific Machine Learning

Ensemble Kalman filtering for epistemic uncertainty

Chatchuea Kimchaiwong[2], **Jeremie Houssineau**[1], **Adam Johansen**[2]

[1]Nanyang Technological University, Singapore; [2]University of Warwick, UK; jeremie.houssineau@ntu.edu.sg

It is widely acknowledged that there are two types of uncertainty, random/aleatory and deterministic/epistemic. Yet, Bayesian inference conflates these and use probability theory throughout. In this talk, I will argue that there are cases where possibility theory can be successfully used instead of, or in conjunction with, probabilistic Bayesian inference to yield intuitive yet principled solutions to data assimilation via an analogue of the ensemble Kalman filter.

ID: 624 / MS43-1: 4

MS43 Mathematical Methods for Scientific Machine Learning

Deterministic Sampling Algorithms

Colin Fox[1], **Li-Jen Hsiao**[1], **Jeong-Eun {Kate} Lee**[2]

[1]University of Otago, New Zealand; [2]The University of Auckland, New Zealand; colin.fox@otago.ac.nz

We address the multivariate inverse Frobenius–-Perron problem: given a prescribed target probability distribution, find a deterministic map such that iterations of the map tend to the target distribution. We give a novel factorization that combines the forward and inverse Rosenblatt transformations with a uniform map, to show that there are infinitely many solutions and provide practical computing in moderate dimensions.

ID: 632 / MS43-1: 2

MS43 Mathematical Methods for Scientific Machine Learning

Classification with Deep Neural Networks

Lei Shi

Fudan University, China, People's Republic of; leishi@fudan.edu.cn

In this talk, I will report our recent progress in the generalization analysis of classification with deep neural networks. This is a joint work with Zihan Zhang and Prof. Ding-Xuan Zhou.

ID: 704 / MS43-2: 3

MS43 Mathematical Methods for Scientific Machine Learning

Global Well-posedness and Convergence Analysis of Score-based Generative Models via Sharp Lipschitz Estimates

Zhongjian Wang

Nanyang Technological University, Singapore; zhongjian.wang@ntu.edu.sg

We establish global well-posedness and convergence of the score-based generative models (SGM) under minimal general assumptions of initial data for score estimation. For the smooth case, we start from a Lipschitz bound of the score function with optimal time length. The optimality is validated by an example whose Lipschitz constant of scores is bounded at initial but blows up in finite time. This necessitates the separation of time scales in conventional bounds for non-log-concave distributions. In contrast, our follow up analysis only relies on a local Lipschitz condition and is valid globally in time.

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

Organizers: Jan ten Thije Boonkkamp (j.h.m.tenthijeboonkkamp@tue.nl), BV Rathish Kumar (drbvrk11@gmail.com)

ID: 276 / MS44-1: 4

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

Finite volume Complete Flux Scheme for the Incompressible Navier-Stokes Equations

Chitranjan Pandey[1], J.H.M ten Thije Boonkkamp[2], B.V. Rathish Kumar[1]

[1]Indian Institute of Technology, Kanpur, India; [2]Eindhoven University of Technology, Eindhoven, The Netherlands; chitranjanp4@gmail.com

We construct a novel finite-volume discretization of the incompressible Navier-Stokes equations on a 2-D staggered rectangular mesh. The calculation of fluxes have been done by solving appropriate local non-linear boundary value problems (BVP) using the cross-flux gradient and pressure gradient as source terms. We derive three flux approximation schemes to realize the impact of the source terms on the complete flux(collective contribution of convective and viscous-friction fluxes). The numerical validation of the scheme is done for benchmark problems of fluid flow.

ID: 371 / MS44-1: 3

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

A complete flux scheme for anisotropic advection-diffusion equations

Hanz Martin Cheng, Jan ten Thije Boonkkamp

Lappeenranta University of Technology, Finland; hanz.cheng@lut.fi

In this talk, we explore the usage of the hybrid mimetic mixed - Scharfetter Gummel (HMM-SG) method as a homogeneous flux in the context of the complete flux (CF) scheme. The HMM-SG allows the homogeneous flux to handle anisotropic diffusion tensors on generic polygonal (polytopal) grids. We then discuss how to combine the HMM-SG with an inhomogeneous flux in order to obtain a CF scheme which is uniformly second order, even when the problem is advection dominated.

ID: 457 / MS44-1: 5

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

A Novel Finite Volume Complete-Flux Scheme for Boussinesq Model

B.V. Rathish Kumar[1], Chitranjan Pandey[2], Thije Boonkkamp, . Jan ten[3]

[1]IIT Kanpur, India; [2]IIT Kanpur, India; [3]TU Eindhoven, Netherlands; bvrk@iitk.ac.in

A new complete-flux based finite-volume scheme for the tightly coupled combined mass, momentum and energy conserving nonlinear PDE system constituting the Boussinesq Model has been proposed which has applications in free-convection problem on a staggered grid. The numerical fluxes are approximated by solving appropriate local non-linear boundary value problems (BVP). The numerical scheme is first successfully validated on a benchmark problem prior to the detailed analysis of Boussinesq model. Interesting, multi-cellular cat-eyed circulation pattern and centrally located sharp thermal plumes are seen in the flow and thermal fields of the Boussinesq model respectively.

ID: 481 / MS44-1: 1

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

Mathematical and numerical modelling of multi-component diffusion

Jan ten Thije Boonkkamp, Jan van Dijk

Eindhoven University of Technology, Netherlands, The Netherlands; j.h.m.tenthijeboonkkamp@tue.nl

To compute numerical solutions of the coupled system of conservation laws describing multi-component diffusion in mixtures, we employ the vectorial version of the complete flux scheme. The basic idea is to compute the numerical flux vector from a local system BVP, thus including the coupling between the constituent equations in the discretization. The scheme has favorable properties, such as conservation of total mass. We will demonstrate the performance of the scheme for some examples.

ID: 517 / MS44-1: 2

MS44 Novel Flux Approximation Schemes for Convection-Diffusion-Reaction Models

Complete Flux Scheme for time Fractional ADR Equation

Rinki Rawat[1], Chitranjan Pandey[1], B.V. Rathish Kumar[1], J.H.M ten Thije Boonkkamp[2]
[1]Indian Institute of Technology,Kanpur, India; [2]Eindhoven University of Technology, The Netherlands; rinkir21@iitk.ac.in

A novel finite-volume complete flux scheme for the Caputo time fractional ADR equation will be proposed. The proposed numerical scheme will be first validated against benchmark cases with exact solution. The ability of the scheme in evaluating the influence of the important parameters like Peclet Number will be assessed. The time evolution of the solution with different fractional order derivatives will be traced and the physics behind the obtained results will be analysed and discussed.

MS45 Numerical Methods for Quantum Many-Body Problems

Organizers: Yuehaw Khoo (ykhoo@uchicago.edu), Michael Lindsey (lindsey@math.berkeley.edu)

ID: 393 / MS45-1: 3

MS45 Numerical Methods for Quantum Many-Body Problems

Parallel Coordinate Descent Full Configuration Interaction

Weiguo Gao, Yingzhou Li, Yuejia Zhang
Fudan University, China, People's Republic of; yingzhouli@fudan.edu.cn

We develop a mutli-threaded parallel coordinate descent full configuration interaction algorithm, for the electronic structure ground-state calculation in the configuration interaction framework. The algorithm solves an unconstrained nonconvex optimization problem, via a modified block coordinate descent method with a deterministic compression strategy. CDFCI captures and updates appreciative determinants with different frequencies proportional to their importance. We demonstrate the efficiency of the algorithm on practical systems.

ID: 441 / MS45-1: 2

MS45 Numerical Methods for Quantum Many-Body Problems

Density Estimation via Sketching and its Applications in Solving Fokker-Planck Equation

Siyao Yang
University of Chicago, United States of America; siyaoyang@uchicago.edu

We propose a sketching algorithm for estimating high-dimensional probability densities. Our method constructs a tensor train (TT) representation for the target density from samples by solving a sequence of small linear systems to obtain the TT cores. The proposed density estimation method is then applied to solve high-dimensional Fokker-Planck equation combining with particle method. In specific, we add a proximal regularization term to the free energy and derive a biased Langevin dynamics. We apply our sketching algorithm to re-estimate the solution from samples and use it as a new reference TT for biasing while evolving the dynamics.

ID: 583 / MS45-1: 1

MS45 Numerical Methods for Quantum Many-Body Problems

Adaptive diagonal basis sets for electronic structure theory

Michael Lindsey
UC Berkeley, United States of America; lindsey@berkeley.edu

Electronic structure calculations usually begin with the choice of a truncated basis set for functions of a single space variable.The four-index tensor of electron repulsion integrals (ERI) induced by this basis set can be difficult to manage computationally. Diagonal basis sets---smooth, orthogonal basis sets that behave like delta functions---can be constructed to yield ERI that are highly structured in a way that simplifies many downstream calculations. However, these constructions are typically grid-based and can require a large basis set to yield acceptable accuracy. We describe new approaches for constructing adaptive diagonal basis sets that conform to individual problem geometries.

ID: 611 / MS45-1: 4

MS45 Numerical Methods for Quantum Many-Body Problems

Augmented Lagrangian method for coupled-cluster

Fabian Maximilian Faulstich

Rensselaer Polytechnic Institute, United States of America; faulsf@rpi.edu

We propose to improve the convergence properties of the single-reference coupled cluster (CC) method through an augmented Lagrangian formalism. The CC method changes a linear high-dimensional eigenvalue into a problem of determining the roots of a nonlinear system of equations that has a manageable size. However, current numerical procedures for solving this system of equations to get the lowest eigenvalue suffer from practical issues. We show these issues can be dealt with when a suitably defined energy is minimized in addition to solving the original CC equations. We propose an augmented Lagrangian method for coupled cluster to solve the resulting constrained optimization problem.

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

Organizers: Yongyong Cai (yongyong.cai@bnu.edu.cn)

ID: 414 / MS46-1: 1

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

An unconditionally stable IMEX scheme for Allen-Cahn/Cahn-Hilliard equation perturbed by multiplicative noise

Can Huang

Xiamen University, China, People's Republic of; canhuang@xmu.edu.cn

We develop fully discrete implicit-explicit schemes for stochastic Allen-Cahn and Cahn-Hilliard equations driven by multiplicative noise respectively. The spatial discretization is a polynomial based spectral method and the temporal discretization is a tamed semi-implicit scheme which treats the nonlinear term explicitly. We show that the scheme is unconditionally stable under various norms for both cases, and establish optimal strong convergence rates. We also present numerical experiments to validate our theoretical results.

ID: 465 / MS46-1: 3

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

Spectral Methods for Partial Differential Equations on Complex Geometries

Sheng CHEN

Beijing Normal University, China, People's Republic of; shengchen@bnu.edu.cn

The spectral method is indispensable in solving partial differential equations (PDEs), given its critical role in various applications. However, extending spectral methods to complex geometries while effectively handling singularities presents a significant challenge. In this study, we introduce a spectral-element Galerkin method designed to address these challenges. We rigorously analyze and provide convergence proofs for two types of problems: the exterior problem and the interior problem. Additionally, for singular problems, we propose the use of Log orthogonal functions, which demonstrate satisfactory results, particularly at hinge points.

ID: 542 / MS46-1: 4

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

Stability of the Minimal Energy Path

Huajie Chen

Beijing Normal University, China; chen.huajie@bnu.edu.cn

The minimum energy path (MEP) is the most probable transition path that connects two equilibrium states of a potential energy landscape. It has been widely used to study transition mechanisms as well as transition rates in the fields of chemistry, physics, and materials science. In this talk, we show a novel result establishing the stability of MEPs under perturbations of the energy landscape. The result also represents a crucial step towards studying the convergence of numerical discretisations of MEPs. This is a joint work with Xuanyu Liu (BNU) and Christoph Ortner (UBC).

ID: 568 / MS46-1: 5

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

The sticky particle system with alignment interactions

Changhui Tan

University of South Carolina, United States of America; tan@math.sc.edu

In this talk, we present the Euler-alignment system, which describes collective behaviors in animal flocks. We establish a global well-posedness theory for the weak entropic solution to the system in one spatial dimension. Specifically, we demonstrate that the solution can be constructed and approximated through the dynamics of sticky particles with Cucker-Smale type alignment interactions. We present an analytical convergence result and examine the formation of clusters over both finite and infinite time frames. This is joint work with Trevor Leslie.

ID: 718 / MS46-1: 2

MS46 Recent Advance on Numerical Methods and Analysis for Complex Problems

Analysis for a high accuracy nonlinear scheme for strong nonlinear diffusion problem

Xia Cui[1], Yu-Jie Gong[2], Guang-Wei Yuan[1]

[1]Institute of Applied Physics and Computational Mathematics, Beijing, People's Republic of China;

[2]University of Macau, Macau, People's Republic of China; cuixia09@163.com

A fully implicit BDF2 finite difference scheme for a conservative strong nonlinear diffusion problem is analyzed. By developing discrete functional analysis method and applying novel argument techniques to overcome the difficulties coming from the high nonlinearity of the conservative diffusion operator, under a coercive condition according with the nature of the problem, we prove the scheme is unconditionally stable,

uniquely solvable and convergent with second-order space-time accuracy. Numerical examples confirm its high precision and efficiency.

MS47 Recent Advances in Numerical Homogenization

Organizers: Viet Ha Hoang (vhhoang@ntu.edu.sg), Timo Sprekeler (timo.sprekeler@nus.edu.sg)

ID: 215 / MS47-1: 4

MS47 Recent Advances in Numerical Homogenization

Numerical Methods for Multiscale Equations with Discontinuous Coefficients

Chen Hui Pang, **Viet Ha Hoang**

Nanyang Technological University, Singapore; chenhui.pang@ntu.edu.sg

We consider a two-scale diffusion problem in a composite material embedded with a periodic array of inclusions with conductivity different from the host material. Solving such multiscale problems using microscopic mesh is prohibitively expensive. We instead solve the high dimensional two-scale homogenized problem which provides all the microscopic and macroscopic information, using sparse tensor product finite elements. The method is essentially optimal in the error versus the total number of degrees of freedom.

ID: 353 / MS47-1: 2

MS47 Recent Advances in Numerical Homogenization

Reliable coarse-scale approximation of spatial network models

Moritz Hauck[1], **Axel Målqvist**[1], **Roland Maier**[2]

[1]Chalmers University of Technology and University of Gothenburg, Sweden; [2]Karlsruhe Institute of Technology, Germany; hauck@chalmers.se

In this talk, we present a multiscale approach for the reliable coarse-scale approximation of spatial network models represented by a linear system of equations with respect to the nodes of a graph. The method generalizes the ideas of the localized orthogonal decomposition (LOD) to a fully algebraic setting. This allows the method to be applied to geometrically challenging objects such as corrugated cardboard. We present a rigorous a priori error analysis of the proposed method under suitable assumptions on the considered network. Numerical experiments illustrate the theoretical results.

ID: 566 / MS47-1: 3

MS47 Recent Advances in Numerical Homogenization

Wavelet-based Edge Multiscale Parareal Algorithm for subdiffusion equations with heterogeneous coefficients in a large time domain

Guanglian Li

The University of Hong Kong, Hong Kong S.A.R. (China); lotusli0707@gmail.com

We present the Wavelet-based Edge Multiscale Parareal (WEMP) Algorithm, recently proposed in [Li and Hu, J. Comput. Phys., 2021], for efficiently solving subdiffusion equations with heterogeneous coefficients in long time. This algorithm combines the benefits of multiscale methods, which can handle heterogeneity in the spatial domain, and the strength of parareal algorithms for speeding up time evolution problems when sufficient processors are available. Our algorithm overcomes the challenge posed by the nonlocality of the

fractional derivative in previous parabolic problem work by constructing an auxiliary problem on each coarse temporal subdomain to completely uncouple the temporal variable.

ID: 686 / MS47-1: 1

MS47 Recent Advances in Numerical Homogenization

An efficient exponential integrator for generalized multiscale finite element methods

Eric Chung

The Chinese University of Hong Kong, Hong Kong S.A.R. (China); eric.t.chung@cuhk.edu.hk

In this talk, we present an efficient exponential integrator generalized multiscale finite element method for solving a class of time-evolving partial differential equations in bounded domains. The exponential integration strategy for the time variable allows us to take full advantage of the multiscale method as it enables larger time steps due to its stability properties. The research is partially supported by Hong Kong RGC General Research Fund (Projects: 14304021 and 14302620).

MS48 Recent Advances on Spectral and High-Order Methods

Organizers: Haiyong Wang (haiyongwang@hust.edu.cn), Shuhuang Xiang (xiangsh@csu.edu.cn), Jing Gao (jgao@xjtu.edu.cn)

ID: 196 / MS48-1: 1

MS48 Recent Advances on Spectral and High-Order Methods

A framework for stable spectral methods in d-dimensional unit balls

Jing GAO

Xi'an Jiaotong University, China, People's Republic of; jgao@xjtu.edu.cn

The subject of this talk is the design of efficient and stable spectral methods for time-dependent partial differential equations in unit balls. We construct the W-function basis in the d dimensional ball keeping skew symmetry of the differentiation matrix. The method is stable. We resolve it by representing the underlying space as an affine space and splitting the underlying functions for its behaviour at the origin. Numerical examples illustrate how our choice of basis attains the best outcome out of a number of alternatives. This is a joint work with Prof. Arieh Iserles.

ID: 239 / MS48-1: 3

MS48 Recent Advances on Spectral and High-Order Methods

A convolution quadrature using derivatives and its application

Junjie Ma

Guizhou Unversity, China, People's Republic of; jjma@gzu.edu.cn

In this talk, we discuss the convolution quadrature based on a class of two-point Hermite collocation methods. Incorporating derivatives into the numerical scheme enhances the accuracy while preserving stability, which is confirmed by the onvergence analysis for discretization of the initial value problem. Moreover, we employ the resulting quadrature to evaluate a class of highly oscillatory integrals. The frequency-explicit convergence analysis demonstrates that the proposed quadrature surpasses its conventional counterparts, achieving the highest convergence rate with respect to the oscillation among them. Numerical experiments involving convolution integrals with various kernels illustrate the reliability and efficiency of the proposed convolution quadrature.

ID: 375 / MS48-1: 4

MS48 Recent Advances on Spectral and High-Order Methods

A unified superconvergent postprocessing technique for Galerkin time-stepping methods

Lijun Yi

Shanghai Normal University, China; ylj5152@shnu.edu.cn

In this presentation, we introduce a unified postprocessing technique for Galerkin methods (including CG and DG) employed in solving initial value problems for first and second-order ODEs. The essence of this approach lies in enhancing the existing Galerkin approximation of degree k with an additional term involving a generalized Jacobi polynomial of degree $k+1$. Theoretical findings suggest a one-order improvement in convergence rate. We further apply this postprocessing technique to Galerkin time discretization of nonlinear parabolic and hyperbolic equations, showcasing its effectiveness and higher order accuracy through comprehensive numerical experiements.

ID: 503 / MS48-1: 2

MS48 Recent Advances on Spectral and High-Order Methods

Finite-difference method on the surface of the helical pipes

Yujian Jiao

Shanghai Normal University, China, People's Republic of; yj-jiao@shnu.edu.cn

Owing to the remarkable characteristics, helical pipe have been used in many theory and application scenarios. In this talk, we introduce finite difference methods on the surface of helical pipe geometries for steady-state model, Gray-Scott model and Cahn-Hilliard equations. We prove their stability and convergence by a rigorous error analysis, respectively. Finally, we design numerical experiment to verify the convergence order and give pattern formation.

ID: 504 / MS48-2: 1

MS48 Recent Advances on Spectral and High-Order Methods

Spectral collocation method for numerical solution to the fully nonlinear Monge-Amp\`{e}re equation

Zhaoxiang LI

Shanghai Normal University, China, People's Republic of; zxli@shnu.edu.cn

In this talk, the Legendre-Gauss-Labatto spectral collocation method is proposed to solve the fully nonlinear Monge-Ampere equation in both two and three dimensional settings with the Dirichlet boundary conditions. We propose a novel approach for approximating the initial value, which significantly reduces the number of Newton iteration steps, thus simplifying the computations compared to existing methods. The convergence analysis of the proposed scheme is discussed. Numerical examples are presented to validate the theoretical estimates.

ID: 600 / MS48-2: 2

MS48 Recent Advances on Spectral and High-Order Methods

Novel spectral methods for maxwell eigenvalue problem using divergence free curl-orthogonal polynomials

Jing Zhang

Central China Normal University, China; zjing@ccnu.edu.cn

We propose and analyze an efficient spectral method for the Maxwell eigenvalue problem. To handle it, we design an effective algorithm using divergence free curl -orthogonal basis functions. Finally, we provide some numerical experiments to validate our theoretical results and demonstrate the efficiency of the algorithms.

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

Organizers: Qiumei Huang (qmhuang@bjut.edu.cn), Hui Liang (lianghui@hit.edu.cn), Yin Yang (yangyinxtu@xtu.edu.cn), Jiwei Zhang (jiweizhang@whu.edu.cn)

ID: 325 / MS49-2: 2

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

A general collocation analysis for weakly singular Volterra integral equations with variable exponent

Hui Liang[1], Martin Stynes[2]

[1]Harbin Institute of Technology, Shenzhen, China, People's Republic of; [2]Beijing Computational Science Research Center, Beijing, China, People's Republic of; lianghui@hit.edu.cn

In the present paper the general theory (existence, uniqueness, regularity of solutions) of variable-exponent weakly singular VIEs is developed, then used to underpin an analysis of collocation methods where piecewise polynomials of any degree can be used. The sharpness of the theoretical error bounds obtained for the collocation methods is demonstrated by numerical examples.

ID: 336 / MS49-2: 1

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

Solving fractional differential equations in unbounded domains via rational approximation

Huifang Yuan

Harbin Institute of Technology, Shenzhen, China, People's Republic of; yuanhuifang@hit.edu.cn

Many PDEs involving fractional Laplacian are naturally set in unbounded domains with underlying solutions decay very slowly, subject to certain power laws. Using AAA algorithm, we develop a specific rational approximation of the involved Fourier kernel, which then leads to an approximation of the original fractional differential equation by a series of second-order differential equations. Numerical results are provided to show the effectiveness of this approach.

ID: 341 / MS49-1: 4

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

Multiscale Model Reduction for Heterogeneous Perforated Domains based on CEM-GMsFEM

Yin Yang[1], Wei Xie[1], Yunqing Huang[1], Eric Chung[2]

[1]xiangtan university, China, People's Republic of; [2]The Chinese university of HongKong, Hong Kong SAR; yangyinxtu@xtu.edu.cn

In this presentation, we unveil a robust framework for addressing multiscale complexities in diverse perforated domains, employing the Constraint Energy Minimizing - Generalized Multiscale Finite Element Method (CEM-GMsFEM). Simulating within such domains is computationally intensive due to varying perforation and domain scales. Our method addresses both the Poisson equation and linear elastic problems within these domains. Our approach comprises two main steps: firstly, solving an eigenvalue problem within a coarse block, and secondly, resolving a minimization problem within an oversampled domain. Furthermore, we demonstrate the variability of oversampling layers in controlling exponential decay.

ID: 378 / MS49-1: 5

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

An efficient second-order discontinuous finite volume element scheme for the three-dimensional neutron transport equations

Yanni Gao[1], Xueding Hang[2], Guangwei Yuan[3]

[1]Institute of Applied Physics and Computational Mathematics, China, People's Republic of; [2]Institute of Applied Physics and Computational Mathematics, China, People's Republic of; [3]Institute of Applied Physics and Computational Mathematics, China, People's Republic of; gaoyn10@163.com

We propose an efficient second-order discontinuous finite volume element (DFVE) scheme for the discrete ordinates neutron transport equations on general hexahedral meshes. The iso-parametric trilinear element and the piecewise constant space are taken as the trial and test spaces, respectively. The face integrals on the non-planar cell faces are well discretized by the effective face method, by which not only the reentrance problems are successfully handled, but also the computational cost is reduced remarkably. Compared with the discontinuous finite element (DFE) scheme, the proposed DFVE scheme spares the volume integral of the transport term and avoids the complicated calculation of the face integrals.

ID: 418 / MS49-1: 3

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

Implicitly linear Jacobi spectral-collocation methods for two-dimensional weakly singular Volterra-Hammerstein integral equations

Qiumei Huang, Huiting Yang

Beijing University of Technology, China, People's Republic of China; yanghuiting2021@emails.bjut.edu.cn

Weakly singular Volterra integral equations of the second kind typically have nonsmooth solutions near the initial point of the interval of integration, which seriously affects the accuracy of spectral methods. We present Jacobi spectral-collocation method to solve two-dimensional weakly singular Volterra-Hammerstein integral equations based on smoothing transformation and implicitly linear method. weight function and eliminate the influence of the weakly singular kernel on the method.

Convergence analysis in the $L\infty$-norm is carried out and the exponential convergence rate is obtained and the efficiency of the proposed method is demonstrated by numerical examples.

ID: 506 / MS49-1: 1

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

Numerical solution of fractional integro-differential equations with singularities

Kaido Latt, Arvet Pedas

Institute of Mathematics and Statistics, University of Tartu, Estonia; kaido.latt@ut.ee

We consider a class of fractional integro-differential equations with certain type of singularities at the origin. We study the regularity of the exact solution and construct a collocation based numerical method for finding the approximate solution of the problem under consideration. We also present results of some numerical experiments.

ID: 510 / MS49-1: 2

MS49 Recent Advances on the Theory and Computation of Integral and Integro-differential Equations

A collocation method based on central part interpolation for fractional integro-differential equations

Mikk Vikerpuur

University of Tartu, Estonia; mikk.vikerpuur@ut.ee

In the present contribution we introduce a collocation method based on central part interpolation for finding a numerical solution to a class of fractional integro-differential equations involving Caputo fractional derivatives. The central part interpolation approach was first formulated for solving Fredholm integral equations of the second kind, and it has shown accuracy and numerical stability advantages compared to standard piecewise polynomial collocation methods, including collocation at Chebyshev knots. We adapt their approach for weakly singular Volterra integral equations, derive the optimal convergence estimates of the proposed method and test the theoretical results with several numerical experiments.

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Organizers: Zhongjian Wang (zhongjian.wang@ntu.edu.sg), Zhiwen Zhang (zhangzw@hku.hk)

ID: 320 / MS50-1: 1

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Generalization of DeepONets for Learning Operators Arising from a Class of Singularly Perturbed Problems

Zhongyi Huang

Tsinghua University, China, People's Republic of; zhongyih@mail.tsinghua.edu.cn

Singularly perturbed problems present inherent difficulty due to the presence of boundary/interior layers in its solution. To overcome this difficulty, we propose using deep operator networks (DeepONets). In this talk, we demonstrate for the first time the application of DeepONets to onedimensional singularly perturbed problems. We consider the convergence rate of the approximation error incurred by the operator networks in approximating the solution operator, and examine the generalization gap and empirical risk, all of which are shown to converge uniformly with respect to the perturbation parameter.

ID: 384 / MS50-1: 3

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Structure-preserving generative models and their statistical guarantees

Wei Zhu

Georgia Institute of Technology, United States of America; mrzw731@gmail.com

In this presentation, I will detail how intrinsic structures, such as group symmetries, of underlying distributions can be seamlessly integrated into generative models to enhance data efficiency. Crucially, I will explore the precise reduction in sample complexity—namely, the requisite number of samples to effectively "learn" the target distribution—achieved by preserving such structural characteristics within the model. Intriguingly, the findings reveal that the outcomes are not as intuitive as one might expect and, in certain instances, prove to be counterintuitive.

ID: 505 / MS50-1: 2

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Exploring the Optimal Choice for Generative Processes in Diffusion Models

Yu Cao, Jingrun Chen, Yixin Luo, Xiang Zhou

City University of Hong Kong, Hong Kong S.A.R. (China); xizhou@cityu.edu.hk

The diffusion model has shown remarkable success in computer vision, but it remains unclear whether the ODE-based probability flow or the SDE-based diffusion model is more superior and under what circumstances. We study the problem for two limiting scenarios: the zero diffusion (ODE) case and the large diffusion case. Our findings indicate that when the perturbation occurs at the end of the generative process, the ODE model outperforms the SDE model with a large diffusion coefficient. However, when the perturbation occurs earlier, the SDE model outperforms the ODE model.

ID: 507 / MS50-1: 4

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

A convergent interacting particle method for computing KPP front speeds in random flows

Tan Zhang[1], Zhongjian Wang[2], Jack Xin[3], Zhiwen Zhang[1]

[1]Department of Mathematics, The University of Hong Kong, Hong Kong S.A.R. (China); [2]Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371; [3]Department of Mathematics, University of California at Irvine, Irvine, CA 92697, USA; thta@connect.hku.hk

Front propagation and diffusion enhancement in fluid flows are two fundamental problems to analyze and characterize the front speeds. We aim to efficiently compute the spreading speeds of reaction-diffusion-advection fronts in random flows under the KPP nonlinearity, We study a stochastic interacting particle method for the reduced principal eigenvalue(Lyapunov exponent) problem of an associated linear advection-diffusion operator with spatial randomness. The particles undergo advection-diffusion, and mutation/selection through a function originated in the FK semigroup, We analyze the algorithm's convergence and present numerical results on representative flows such as 2D cellular flow and 3D ABC flow under random perturbations

ID: 586 / MS50-2: 2

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

On Asymptotic-Preserving Neural Networks for the Semiconductor Boltzmann Equation

Liu Liu

The Chinese University of Hong Kong, Hong Kong S.A.R. (China); lliu@math.cuhk.edu.hk

In this talk, we will propose the asymptotic-preserving neural networks (APNNs) for solving the semiconductor Boltzmann equation under the diffusive scaling. We will incorporate the micro-macro decomposition method to design the loss function, which has shown to be efficient and accurate in capturing the limiting macroscopic behavior when the Knudsen number goes to zero. Then we will study its corresponding uncertainty quantification problem in the stochastic Galerkin framework, as well as the inverse problem on inferring parameter of interests in the model. This is a joint work with Zhenyi Zhu, Yating Wang and Xueyu Zhu.

ID: 629 / MS50-2: 3

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Probabilistic Forecasting with Stochastic Interplants and Follmer Processes

Yifan Chen

NYU, United States of America; yifanc96@gmail.com

In this work, we address probabilistic forecasting via generative modeling. To do so, we construct novel SDEs that map a point mass of the current state to a conditional distribution of future states, based on the framework of stochastic interplants. The SDEs can be learned from data via simulation-free training, and the drifts can be tuned a posteriori to optimize the estimation accuracy in KL divergence of path measures. We show that the optimal drift corresponds to Follmer processes. Experiments on stochastic Navier Stokes equations and video forecasting demonstrate the effectiveness and scope of this work.

ID: 634 / MS50-2: 1

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Convex Relaxation for Fokker-Planck

Yian Chen, Yuehaw Khoo, Lek-Heng Lim

The University of Chicago, United States of America; ykhoo@uchicago.edu

We propose an approach to directly estimate the moments or marginals for a high-dimensional equilibrium distribution in statistical mechanics, via solving the high-dimensional Fokker-Planck equation in terms of low-order cluster moments or marginals. With this approach, we bypass the exponential complexity of estimating the full high-dimensional distribution and directly solve the simplified partial differential equations for low-order moments/marginals. Moreover, the proposed moment/marginal relaxation is fully convex and can be solved via off-the-shelf solvers. We show the proposed method can recover the meanfield approximation of an equilibrium density. Numerical results are provided to demonstrate the performance of the proposed algorithm for high-dimensional systems.

ID: 652 / MS50-2: 4

MS50 Recent Development of Generative Models in Computational Mathematics and Data Sciences

Randomized methods for computing optimal transport without regularization and their convergence analysis

Yue Xie[1], Zhongjian Wang[2], Zhiwen Zhang[1]

[1]The University of Hong Kong; [2]Nanyang Technological University; yxie21@hku.hk

We introduced the random block coordinate descent (RBCD) methods to directly solve the linear programming (LP) problem motivated by optimal transport (OT). Our approach restricts the potentially large-scale LP to small LP subproblems constructed via randomly chosen working sets. We equip the vanilla version of RBCD with almost sure convergence and a linear convergence rate. To further improve the efficiency, we explore the special structure of constraints in OT and refine the random working set selection. Preliminary numerical experiments demonstrate that the accelerated RBCD compares well with other solvers and offers the advantage of saving memory.

MS51 Recent Trends in Stabilized FE Methods for Fluid Flows

Organizers: Rathish Kumar BV (bvrk@iitk.ac.in)

ID: 527 / MS51-1: 1

MS51 Recent Trends in Stabilized FE Methods for Fluid Flows

Variational Multiscale FEM for Cahn-Hillard-Navier-Stokes Model

Anil Rathi, **B. V. Rathish Kumar**

Indian Institute of Technology Kanpur, India; anilr20@iitk.ac.in

In this paper, we derive the Variational Multiscale Finite Element (VMSFE) scheme for Cahn-Hillard-Navier-Stokes equations. The method is based on the subgrid-scale approach and approximation of the subscales. The subscales are time-dependent, and the VMSFE formulation is generated by eliminating fine scales in terms of coarse scales. A priori error estimates have been derived to establish the theoretical convergence of the VMSFE scheme.

ID: 698 / MS51-1: 2

MS51 Recent Trends in Stabilized FE Methods for Fluid Flows

Variational multiscale Stabilized FEM for unified FSI model

DIPAK KUMAR SAHOO, **B V RATHISH KUMAR**

Indian Institute of Technology Kanpur, India; dipakhcu@gmail.com

In this article, we present a fluid–structure interaction problem involving a linear elastic solid and an in-compressible Newtonian fluid and solved using stabilized finite element method. The key stabilization parameters are derived using Fourier analysis. The level set method combined and a displacement field extension procedure was employed to capture the moving interfaces. This method is capable of simulating the dynamic interactions of fluid and structure also computes the stress fields in both phases. Few bench marks problems have been solved to demonstrate the efficiency of the scheme. The results obtained are in good agreement with the published data.

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning

Organizers: Michael Kraus (michael.kraus@ipp.mpg.de), Benedikt Brantner (benedikt.brantner@ipp.mpg.de)

ID: 487 / MS52-1: 2

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning

Time Series-Aware Structure-Preserving Neural Networks

Benedikt Brantner

Max Planck Institute for Plasma Physics, Germany; benedikt.brantner@ipp.mpg.de

Neural networks are finding increasing application in the field of reduced complexity modeling in both the offline and the online phase. If neural networks are used in the online phase, then these are mostly recurrent neural networks (especially LSTMs). In the past few years LSTMs have however (almost) completely been replaced by transformer neural networks in other fields. The advantage of the transformer neural network not only lies in its enormous speed ups during training but also its straightforward interpretability. This interpretability makes it possible to further imbue transformers with structure-preserving properties, making them a good choice for many applications.

ID: 512 / MS52-1: 3

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning

Generalized Hamiltonian Neural Networks for Parameter-dependent Hamiltonian Systems

Philipp Horn, Barry Koren

Eindhoven University of Technology, Netherlands, The; p.horn@tue.nl

When solving Hamiltonian systems numerically, it is essential to preserve the symplectic structure of the flow map. However, for parameter-dependent Hamiltonian systems, no symplectic neural networks have been developed so far. We propose a neural network architecture based on the Generalized Hamiltonian Neural Networks that can learn a parameter-dependent flow map while preserving the symplectic structure. In numerical experiments, Parameterized Generalized Hamiltonian Neural Networks (PGHNNs) are able to extrapolate to areas of the phase space without training data, while physics-unaware multilayer perceptrons are not. PGHNNs achieve this with the same prediction speed as multilayer perceptrons.

ID: 524 / MS52-1: 1

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning

Learning of Lagrangian odes and pdes from data with UQ

Christian Offen

Paderborn University, Germany; christian.offen@uni-paderborn.de

I will show how to use Gaussian Process regression to learn variational dynamical systems from data in a structure preserving manner. The method allows for uncertainty quantification of any linear observable. It is applied to discrete and continuous variational odes and pdes.

ID: 644 / MS52-1: 4

MS52 Structure-Preserving Reduced Complexity Modelling and Machine Learning

Autoencoders for structure-preserving model reduction of stochastic Hamiltonian systems

Tomasz Michal Tyranowski

University of Twente, Netherlands, The; t.m.tyranowski@utwente.nl

Recently, Tyranowski (2024) showed that SVD-based model reduction techniques, like proper orthogonal decomposition, extend to stochastic differential equations, reducing computational costs arising from both the high dimension of the considered system and the large number of independent Monte Carlo runs. They improve efficiency when the Kolmogorov n-width of the solution manifold decays quickly with reduced space dimension. In this study, we adapt recently proposed symplectic autoencoders (Brantner&Kraus, 2023; Buchfink,Glas&Haasdonk, 2023) to the stochastic setting, applying them to stochastic Hamiltonian systems

characterized by slowly decaying Kolmogorov n-widths. We test and compare their performance against the linear proper symplectic decomposition (PSD) method.

MS53 Surface Evolution and Harmonic Maps

Organizers: Buyang Li (buyang.li@polyu.edu.hk), Balázs Kovács (balazs.kovacs@math.uni-paderborn.de)

ID: 188 / MS53-1: 2

MS53 Surface Evolution and Harmonic Maps

Numerical analysis for fourth order geometric curve evolutions based on the DeTurck trick

Robert Nürnberg[1], **Klaus Deckelnick**[2]

[1]University of Trento, Italy; [2]Otto-von-Guericke-Universität Magdeburg, Germany;

robert.nurnberg@unitn.it

We introduce novel weak formulations for curve diffusion and elastic flow that generalize the so-called DeTurck trick known from curve shortening flow. The solutions of the obtained variational formulations admit a nontrivial tangential motion that drives solutions towards an arclength parameterization. We then derive optimal H^1--error bounds for continuous-in-time semidiscrete finite element approximations that use piecewise linear elements. In addition, we consider fully discrete schemes and, in the case of curve diffusion, prove unconditional stability. Numerical simulations confirm the derived error bound. Moreover, the presented simulations suggest that the tangential motion leads to equidistribution in practice.

ID: 286 / MS53-1: 3

MS53 Surface Evolution and Harmonic Maps

Accelerated gradient flows for large bending deformations of nonlinear plates

Guozhi Dong[1], **Hailong Guo**[2], **Shuo Yang**[3]

[1]School of Mathematics and Statistics, HNP-LAMA, Central South University, Changsha, China, People's Republic of; [2]School of Mathematics and Statistics, The University of Melbourne, Parkville, VIC, Australia; [3]Beijing Institute of Mathematical Sciences and Applications, China, People's Republic of;

shuoyang@bimsa.cn

In this work, we propose and analyze a series of novel algorithms based on projection- free accelerated gradient flows to minimize bending energies for nonlinear plates with non-convex metric constraints. We discuss the stability and constraint consistency in a semi-discrete setting for both bilayer and prestrained plates. Our proposed algorithms demonstrate substantial improvements, in both efficiency and accuracy, over current state-of-the-art methods based on gradient flows.

ID: 403 / MS53-1: 1

MS53 Surface Evolution and Harmonic Maps

Error estimates for inextensible elastic curves

Soeren Bartels

University of Freiburg, Germany; bartels@mathematik.uni-freiburg.de

We present new error estimates for the numerical approximation of stationary configurations and flows of inextensible elastic curves. The underlying energy functional is the bending energy of an elastic curve that

inextensible. The pointwise constraint implies that curves are parametrized by arclength and introduces a Lagrange multiplier in the equations that depends nonlinearly on the parametrization. For energy-stable minimizers we derive an error estimate via the inverse function theorem while for evolutions we use suitably constructed test functions. The estimates and numerical experiments show that the constraint has to be imposed in a non-canonical way to obtain optimal error bounds.

ID: 429 / MS53-1: 4

MS53 Surface Evolution and Harmonic Maps

Convergence of an evolving finite element method for surface evolution with tangential motion by harmonic map heat flow

Guangwei Gao, Buyang Li, Rong Tang

The Hong Kong Polytechnic University; claire.tang@polyu.edu.hk

The finite element approximation of surface evolution under an external velocity field is studied. A tangential motion is designed, by using harmonic map heat flow from the initial surface onto the evolving surface, to improve the mesh quality. By exploiting the intrinsic cancellation structure in the weak formulation and carefully characterizing error in the normal vector, the convergence of evolving finite element approximations is proved for finite elements of degree {$k\geq 4$}. Extensive numerical experiments are presented to demonstrate both the convergence of the algorithm and the performance of the artificial tangential velocity in improving mesh quality.

ID: 668 / MS53-2: 1

MS53 Surface Evolution and Harmonic Maps

Numerics of the stochastic Landau-Lifshitz-Gilbert equation

Michael Feischl

TU Wien, Austria; michael.feischl@tuwien.ac.at

We demonstrate that adaptive mesh refinement and adaptive time-stepping can stabilize blow-up scenarios of the Landau-Lifshitz-Gilbert (LLG) equation and give better convergence rates. We also show a possible way to prove optimal convergence rates of adaptive time-stepping for non-linear equations in the future.

For the stochastic version of LLG, we show convergence rates for a sparse grid approximation of the distribution of solutions. Beyond being a frequently studied equation in engineering and physics, the stochastic Landau-Lifshitz-Gilbert equation poses many interesting challenges such as constraints, non-linearity, and low regularity.

ID: 742

MS53 Surface Evolution and Harmonic Maps

Stability and Volume Conservation in the Multi-Phase Mullins-Sekerka Problem: A Finite Element Perspective

Tokuhiro Eto

The University of Tokyo, Japan; tokuhiro.eto@gmail.com

In this talk, we present a structure-preserving finite element method for addressing the multi-phase Mullins-Sekerka problem with triple junctions. This sharp interface formulation is designed to handle networks of evolving curves, driven by the reduction of total surface energy while preserving the areas of the enclosed

phases. Our scheme guarantees unconditional stability and exact volume conservation. We demonstrate the efficacy of our method through several numerical examples, including a convergence experiment for the three-phase Mullins-Sekerka flow.

MS54 Theoretical and Numerical Aspects of Integrable Systems

Organizers: Baofeng Feng (baofeng@gmail.com), Zuonong Zhu (znzhu@sjtu.edu.cn)

ID: 324 / MS54-1: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

Nondegenerate N-soliton solutions for coupling PDEs

Ji Lin

Zhejiang Normal University, China, People's Republic of; linji@zjnu.edu.cn

We apply for the bilinear method and the KP reduction method to study the non-degenerate multi-bright soliton and bright-dark soliton solutions of higher-order coupled Schrodinger equation, Manakov equation, multi-component Schrodinger equation. Furthermore, we discuss the propagation properties of these non-degenerate solitons.

ID: 366 / MS54-1: 3

MS54 Theoretical and Numerical Aspects of Integrable Systems

Symmetry study of a novel integrable supersymmetric dispersionless system

Man JIA

Ningbo University, China, People's Republic of; jiaman@nbu.edu.cn

A novel integrable supersymmetric dispersionless fermion system is proposed and studied by means of symmetry approach and the bosonization method, which is integrable under the meaning of possessing infinitely many higher order symmetries. By using the bosonization approach, the system can be bosonized to some special dark integrable systems which can be exactly solved in general.

ID: 374 / MS54-1: 4

MS54 Theoretical and Numerical Aspects of Integrable Systems

The general rogue wave patterns of nonlinear Schrödinger equation

Liming Ling

South China University of Technology, China, People's Republic of; linglm@scut.edu.cn

The rogue wave patterns show different types of temporal-spatial distributions, which are related to the Adler-Moser polynomials by the recent work of Yang et.al. In a general case, we consider the case of mutiple roots of Adler-Moser polynomials. The new patterns, such as claw-like and double column structures, are found in this background. Compared with the previous patterns in the literature, the general patterns admit a certain free manipulation of distribution.

ID: 376 / MS54-1: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Some New Results on Integrable Integro-differential Equations

XingBiao Hu
Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; hxb@lsec.cc.ac.cn

Some nonlinear integro-differential equations have gained great attention since the last century. Among them, the Benjamin–Ono (BO) equation and the Intermediate Long Wave (ILW) equation are two typical equations, which are completely integrable.In the talk, I will report some new results on the BO and sine-Hilbert-type equations. This is joint work with Yajie Liu, Lingjuan Yan and Yingnan Zhang.

ID: 448 / MS54-2: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

Localized waves solutions of the massive Thirring model via bilinear KP-hierarchy reduction and PINN deep learning

Junchao Chen
Lishui University, China, People's Republic of; junchaochen@aliyun.com

In this talk, we will talk about localized waves solutions of the massive Thirring model. These solutions including bright/dark soliton, breather and rogue waves are derived by using the bilinear KP hierarchy reduction method and presented explicitly in terms of determinants. Rogue wave patterns are discussed when one of the internal parameters is large. The patterns are shown to be associated with the root structures of the Yablonskii-Vorob'ev polynomial hierarchy. Data-driven localized waves and parameter discovery of this coupled model are studied via extended physics-informed neural networks with interface zones. This work is joint with Bo Yang, Bao-Feng Feng and Zhenya Yan.

ID: 461 / MS54-2: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Lax pairs informed neural networks solving integrable systems.

Yong Chen
East China Normal University, China, People's Republic of; ychen@sei.ecnu.edu.cn

In this talk, we propose the Lax pairs informed neural networks (LPINNs) tailored for integrable systems with Lax pairs by designing novel network architectures and loss functions, comprising LPINN-v1 and LPINN-v2. On the basis of LPINN-v1, we additionally incorporate the compatibility condition/zero curvature equation of Lax pairs in LPINN-v2, its major advantage is the ability to solve and explore high-accuracy data-driven localized wave solutions and associated spectral problems for all integrable systems with Lax pairs. The numerical experiments in this work involve several important and classic low-dimensional and high-dimensional integrable systems, abundant localized wave solutions and their Lax pairs.

ID: 464 / MS54-2: 3

MS54 Theoretical and Numerical Aspects of Integrable Systems

The spatial structure, discrete solitons and stability analysis of the non-integrable discrete Hirota equation

LiYuan Ma
Zhejiang Universtiy of Technology, China, People's Republic of; mly2016@zjut.edu.cn

We focus on the properties of the non-integrable discrete focusing Hirota equation. Through a nonlinear dynamical map method, we construct the spatially periodic solutions of the non-integrable discrete stationary Hirota equation under special conditions. The types of fixed points are classified based on the defined residue. We numerically analyse the influence of the distinct parameters and the initial points on general orbits of the map.The stationary solitons and traveling wave solutions of the non-integrable discrete Hirota equation are constructed using the modified Neumann iteration scheme. we elaborate the linear stability of the stationary solitary waves under small perturbation.

ID: 530 / MS54-2: 4

MS54 Theoretical and Numerical Aspects of Integrable Systems

Large genus asymptotics for a class of enumerative invariants

Di Yang

University of Science and Technology of China, China, People's Republic of; diyang@ustc.edu.cn

We give uniform large genus asymptotics for a class of enumerative invariants, including psi-class intersection numbers, BGW numbers and etc. We also provide new proofs of the polynomiality conjectures in large genera. Applications to differential equations are considered.

ID: 536 / MS54-3: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

Applications of non-intersecting paths to integrable systems

Shi-Hao Li

Sichuan University, China, People's Republic of; shihao.li@scu.edu.cn

In recent years, there have been numerous applications about the theory of non-intersecting paths in combinatorics. In this talk, I'll discuss some non-intersecting path models and their connections with block determinant and Pfaffian tau functions. Some multi-component KP and DKP systems will be considered with these tau functions.

ID: 537 / MS54-3: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Some properties of spatially discrete Boussinesq hierarchy and their continuous counterparts

Haiqiong Zhao

Shanghai University of International Business and Economics, People's Republic of China;
hqzhao@163.com

In this talk, a spatially discrete integrable Boussinesq hierarchy is investigated. The integrability of the hierarchy is confirmed by showing the existence of Lax hierarchy and infinite number of conservation laws. Further, by combining the Darboux transformations and the solution classification for corresponding eigenfunction, we provide a comprehensive approach to construct diverse kinds of exact solutions to the hierarchy. Lastly, we prove that the theory of spatially discrete Boussinesq hierarchy including the Lax pair, the conservation laws, the Darboux transformations and the exact solutions wholly converge to the corresponding theory of the Boussinesq hierarchy in the continuous limit.

ID: 546 / MS54-3: 3

MS54 Theoretical and Numerical Aspects of Integrable Systems

On the Coupled Modified Complex Short Pulse Equation

Hongqian Sun[1], **Shoufeng Shen**[1], **Zuonong Zhu**[2]

[1]Zhejiang university of Technology, China, People's Republic of; [2]Shanghai jiao tong university,China, People's Republic of; Fuyao Institute of Technology, China, People's Republic of; znzhu@sjtu.edu.cn

The short pulse equation is an important integrable equation in nonlinear optics. This talk focuses on a coupled modified complex short pulse (cm-CSP) equation. We will construct the Darboux transformation for the focusing-focusing and focusing-defocusing cm-CSP equation. Through the Darboux transformation, we derived bright-dark soliton solutions, periodic-like solutions, rational solution and mixed solution (rational-soliton) for the cm-CSP equation with vanishing and non-vanishing backgrounds. These solutions can be divided into smooth, cuspon, and loop cases. Asymptotic behavior of soliton solutions to the cm-CSP equation are analyzed.

ID: 554 / MS54-3: 4

MS54 Theoretical and Numerical Aspects of Integrable Systems

Solutions to semi-discrete integrable equations on theta-function periodic backgrounds

Ruomeng Li

Zhengzhou University, China, People's Republic of; liruomeng@zzu.edu.cn

A new method to construct localized-wave solutions of the semi-discrete and continuous NLS equation on theta-function backgrounds is developed. By rewriting the difference-quotient equation in the form of Hiorta bilinear equations, a theta-function seed solution for the difference-quotient NLS equation is derived. Using the Baker-Akhiezer functions on algebraic curves, a systematic method for solving continuous and semi-discrete spectral problems with theta-function potentials is given, from which rogue-wave and breather solutions of the semi-discrete NLS equation on theta-function backgrounds are constructed with the aid of the derived Darboux transformations. It is found that the semi-discrete NLS equation has extremely high rogue waves.

ID: 555 / MS54-4: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

Application of tetragonal curves to coupled Boussinesq equations

Xianguo Geng

Zhengzhou University, China, People's Republic of; xggeng@zzu.edu.cn

The hierarchy of coupled Boussinesq equations related to a 4×4 matrix spectral problem is derived by using the zero-curvature equation and Lenard recursion equations. The characteristic polynomial of the Lax matrix is employed to introduce the associated tetragonal curve and Riemann theta functions.The detailed theory of resulting tetragonal curves is established by exploring the properties of Baker–Akhiezer functions and a class of meromorphic functions. The Abel map and Abelian differentials are used to precisely determine the linearization of various flows. Finally, algebro-geometric solutions for the entire hierarchy of coupled Boussinesq equations are obtained.

ID: 560 / MS54-4: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Dynamics of higher-order peaked and smooth solitary waves

Xiaochuan Liu

Xi'an Jiaotong University, China, People's Republic of; liuxiaochuan@mail.xjtu.edu.cn

In this talk, I will report our recent results on the issue of stability of higher-order peaked and smooth solitary wave solutions for a Hamiltonian generalized Camassa-Holm equation introduced by Hakkaev-Kirchev and Anco.

ID: 562 / MS54-5: 4

MS54 Theoretical and Numerical Aspects of Integrable Systems

Solitons in the integrable and nearly-integrable fractional nonlinear wave equations

Zhenya Yan

Academy of Mathematics and Systems Science, Chinese Academy of Sciences China, People's Republic of; zyyan@mmrc.iss.ac.cn

In this talk, we will discuss some developments about solitons in some integrable and nearly-integrable fractional nonlinear wave equations.

ID: 565 / MS54-4: 3

MS54 Theoretical and Numerical Aspects of Integrable Systems

New revival phenomena for the Kadomtsev-Petviashvili equation

Jing Kang

Northwest University, China, People's Republic of; jingkang@nwu.edu.cn

In this talk, we report our recent results on the dispersive revival and fractalization phenomena for two-dimensional linear dispersive equations over a bounded domain on the plane subject to periodic boundary conditions. In particular, we study the periodic initial-boundary value problem for the linear Kadomtsev-Petviashvili equation subject to step-function initial data on a square, and analyze the manifestation of the revival phenomenon for the corresponding solution at rational times. We show that the solution will take on different qualitative behavior in x-direction and y-direction.

ID: 573 / MS54-4: 4

MS54 Theoretical and Numerical Aspects of Integrable Systems

Analytic and numerical aspects of Novikov-type equations and their multipeakons

Xiang-Ke Chang

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China, People's Republic of; changxk@lsec.cc.ac.cn

A family of integrable PDEs admit the so-called peakon solutions, the dynamics of which may be characterized by implementing the related forward/inverse spectral analysis. The spectral problems often involve non-self-adjoint operators, while the inverse spectral analysis usually involve Hermite-Padé approximation problems, which have motivated new (bi)orthogonality and random matrix models, etc. This talk will focus on analytic and numerical aspects for the peakon flows of Novikov-type equations.

ID: 579 / MS54-5: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

On the coupled Sasa-Satsuma equation

Bao-Feng Feng[1], **Chengfa Wu**[2]

[1]The University of Texas Rio Grande Valley, USA; [2]Shenzhen University, People's Republic of China; cfwu@szu.edu.cn

In this talk, we bilinearize a coupled Sasa-Satsuma equation under nonzero boundary condition and link it to KP-Toda hierarchy via a set of 33 bilinear equations. Two alternative determinant formulas are derived for dark and breather solutions. Resonant dark and breather solutions are found and analyzed.

ID: 607 / MS54-5: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Darboux transformation of generalized Camassa-Holm equation

LIN LUO

Shanghai Polytechnic University, China, People's Republic of; luolin@sspu.edu.cn

In this talk, we study an integrable generalization of Camassa-Holm equation. The generalized equation is shown to be integrable in the sense of Lax pair. The Darboux transformation for the equation is derived with the help of the gauge transformation between two Lax pairs. As an application, soliton solutions and periodic wave solutions are given through the Darboux transformation.

ID: 609 / MS54-5: 3

MS54 Theoretical and Numerical Aspects of Integrable Systems

Darboux transformations for the nonlinear Schrodinger and derivative nonlinear Schrodinger type systems

Zhiwei Wu

Sun Yat-sen University, China, People's Republic of; wuzhiwei3@mail.sysu.edu.cn

In this tali, we will discuss the algebraic structure of the nonlinear Schrodinger and derivative nonlinear Schrodinger type systems associated to irreducible compact Hermitian symmetric spaces. We construct the Darboux transformations from the corresponding loop group factorization. Furthermore, permutability formula is derived and explicit solutions are obtained. This talk is based on the joint work with Liu, Hsiao-Fan.

ID: 641 / MS54-6: 1

MS54 Theoretical and Numerical Aspects of Integrable Systems

Asymptotics of the integrable equations with WKI-type spectral problem

Jian Xu

University of Shanghai for Science and Technology, China, People's Republic of; jianxu@usst.edu.cn

We report some asymptotic behaviors of the completely integrable equations with WKI spectral problem,such as short pulse equation, complex short pulse equation, modified Camassa-Holm equation by using the nonliear steepest descent method, based on the Riemann-Hilbert problem formulation of the associated equations.

ID: 676 / MS54-6: 2

MS54 Theoretical and Numerical Aspects of Integrable Systems

Dubrovin-Frobenius manifolds and the extended Weyl group of type B

Dafeng Zuo

University of Science and Technology of China; dfzuo@ustc.edu.cn

We present an extension of Weyl group of type B and obtain an analogue of Chevalley-type theorem for their invariants. We further show the existence of several different Dubrovin-Frobenius manifold structures on the corresponding orbit space and also construct Landau--Ginzburg superpotentials for these Dubrovin-Frobenius manifold structures.

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Organizers: Elena Celledoni (elena.celledoni@ntnu.no), James Jackaman (james.jackaman@ntnu.no), Davide Murari (davide.murari@ntnu.no), Brynjulf Owren (brynjulf.owren@ntnu.no), Carola-Bibiane Schönlieb (cbs31@cam.ac.uk), Ferdia Sherry (fs436@cam.ac.uk)

ID: 223 / MS55-2: 1

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Designing Stable Neural Networks using Convex Analysis and ODEs

Ferdia John Sherry[1], Elena Celledoni[2], Matthias Joachim Ehrhardt[3], Davide Murari[2], Brynjulf Owren[2], Carola-Bibiane Schönlieb[1]

[1]University of Cambridge, United Kingdom; [2]NTNU, Norway; [3]University of Bath, United Kingdom; fs436@cam.ac.uk

Motivated by work on numerical integration of ODEs we present a ResNet-styled neural network architecture that encodes non-expansive operators, assuming certain constraints on the weights are satisfied. Analysis of the proposed architecture shows that the weights can also be constrained to ensure that the network is an averaged operator, making it a natural candidate for a denoiser in Plug-and-Play image reconstruction. Using an adaptive way of enforcing the constraints, we show that it is possible to train performant networks. The proposed networks are applied to adversarially robust image classification, to image denoising, and finally to the inverse problem of deblurring.

ID: 311 / MS55-4: 1

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Almost sure convergence of stochastic Hamiltonian descent methods

Måns Williamson

Lund University, Sweden; mans.williamson@math.lth.se

Gradient normalization and soft clipping are two popular techniques for tackling instability issues and improving convergence of stochastic optimization algorithms .

In this talk, we study these types of methods through the lens of dissipative Hamiltonian systems. Gradient normalization and certain types of soft clipping algorithms can be seen as (stochastic) implicit-explicit Euler discretizations of dissipative Hamiltonian systems, where the kinetic energy function determines the type of clipping that is applied.

We make use of unified theory from dynamical systems to show that all of these schemes converge almost surely to stationary points of the objective function.

ID: 334 / MS55-1: 2

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Neural network aided simulation of ordinary differential equations

Marta Betcke[4], Priscilla Canizares[3], Lisa Kreusser[2], Davide Murari[1], Ferdia Sherry[3], Zak Shumaylov[3]

[1]Norwegian University of Science and Technology, Norway; [2]University of Bath, United Kingdom; [3]University of Cambridge, United Kingdom; [4]University College London, United Kingdom; davide.murari@ntnu.no

Approximating solutions of ordinary differential equations has been a long-standing challenge in numerical analysis. Since the first attempts in the '90s to use neural networks to propose a solution for such a challenge, the field has seen fast developments in the last few years. Still, there is much to theoretically understand about neural networks in this setting and how they interface with more classical numerical methods. In this talk, we present some results connecting (geometric) numerical methods for ODEs with neural network-based solvers.

ID: 389 / MS55-4: 4

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Stochastic interpolation, score matching and generative models

Eldad Haber

UBC, Canada; eldadHaber@gmail.com

In this talk we review and explore the dynamical systems that govern stochastic interpolation and score matching techniques. We discuss how such a flow can be regularized and learned efficiently.

ID: 409 / MS55-4: 3

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Convolving dynamics between scales

James Jackaman

NTNU, Norway; james.jackaman@ntnu.no

In this talk we utilise neural networks to resolve sub-grid scale dynamics for the shallow water equation as a methodology for coupling models between scales. In particular, we exploit convolutional neural networks and discuss connections between established techniques in image super-resolution and learning (error) dynamics.

ID: 413 / MS55-5: 4

MS55 Dynamical Systems, Structure Preservation and Deep Learning

An attempt to apply particle method for the Cahn-Hilliard equation to preserve some invariant properties

Daisuke Furihata

Osaka University, Japan; daisuke.furihata.cmc@osaka-u.ac.jp

We want to perform appropriate and fast numerical calculations using machine learning of the time-evolving operator of some conservation partial differential equations, such as the Cahn-Hilliard equation. Still, in the context of FDM and FEM, the amount of machine learning becomes enormous. Therefore, we consider applying a particle method based on the Voronoi decomposition and calculating particle behavior using machine learning.

ID: 437 / MS55-2: 2

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Stability of numerical methods on Riemannian manifolds with applications to neural networks.

Brynjulf Owren, Elena Celledoni

NTNU, Norway; Brynjulf.Owren@ntnu.no

The importance of neural networks set on Riemannian manifolds seems to be increasing and there is a need to develop the theory of non-expansive layer maps in such a setting.

We present some ideas from Arnold et al. (2024) where some simple numerical methods for Riemannian manifolds are studied. We consider whether these methods can be non-expansive when applied to non-expansive vector fields. For the geodesic implicit Euler method, which also feature in the proximal gradient method for optimisation, we find that its behaviour is strongly dependent on the sectional curvature of the manifold.

ID: 451 / MS55-3: 3

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Multi-Resolution Learning of Partial Differential Equations with Deep Operators and Long Short-Term Memory Networks

Katarzyna Michalowska

SINTEF Digital, Norway; katarzyna.michalowska@sintef.no

DeepONets offer an advantage over traditional neural networks in their ability to be trained on multi-resolution data. While this becomes especially relevant when high-resolution measurements are difficult to obtain compared to low-resolution data, DeepONets alone struggle in modeling long sequences. We propose a novel framework that leverages multi-resolution data and provides precise models with limited high-resolution data. We achieve this through extending the DeepONet with an LSTM and training it in a three-step procedure with data of varying resolution. The proposed multi-resolution DON-LSTM achieves significantly lower error and requires fewer high-resolution samples on multiple non-linear PDEs compared to vanilla models.

ID: 486 / MS55-5: 3

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Surrogate Simulations of Charged Particle Dynamics Using Structure-Preserving Neural Networks

Jian Liu

Shandong University, China, People's Republic of; liu_jian@sdu.edu.cn

Surrogate simulations based on data and machine learning have become an emerging direction in plasma simulation research. However, surrogate models depending purely on data usually have poor generalization capabilities. It is necessary to integrate physical information into machine learning models. One way to achieve this is to construct structure-preserving neural networks, such as symplectic networks and volume-preserving networks, which can provide structure-preserving mapps exactly. The application and performance of structure-preserving networks on charged particle dynamics in plasmas are investigated. The potential of surrogate dynamical simulation are also discussed via some key physical problems in fusion devices.

ID: 488 / MS55-5: 1

MS55 Dynamical Systems, Structure Preservation and Deep Learning

PiLocNet: Physics-informed neural network on 3D localization with rotating point spread function

Mingda Lu[1], Zitian Ao[2], Chao Wang[2], Sudhakar Prasad[3], Raymond Chan[1]

[1]City University of Hong Kong, Hong Kong SAR, China; [2]Southern University of Science and Technology, China, People's Republic of; [3]University of Minnesota, USA; wangc6@sustech.edu.cn

We consider the 3D localization problem of the point spread function (PSF) engineering and propose a novel framework based on the physics-informed neural network (PINN), namely PiLocNet, to solve this problem. Our PiLocNet combines deep learning and variational methods, which enhances the black box neural networks by employing the known physics information of the forward process into the framework as the data fitting term. In the meantime, it incorporates the regularization terms from the variational method that best fits the noise model. This work focuses on the single-lope PSF, while it is widely applicable to other PSFs or other imaging problems.

ID: 513 / MS55-2: 4

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Reversible numerical methods in deep learning

Sofya Maslovskaya[1], Sina Ober-Blöbaum[1], Christian Offen[1], Pranav Singh[2], Boris Wembe[1]

[1]Paderborn University, Germany; [2]University of Bath, United Kingdom; sofyam@math.uni-paderborn.de

Deep learning proved to be efficient in different learning tasks, but in many applications, the use of deep networks is limited due to the high memory costs. This problem can be solved by considering networks based on reversible numerical methods. However, there is a lack of higher order reversible methods allowing adaptivity. Such methods are especially important for learning dynamical systems. In this work, we present a construction method for higher order reversible methods. Our numerical tests show the advantages of the networks based on higher order methods.

ID: 523 / MS55-4: 2

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Geometric Learning with Group Convolutions: PDE-Based Equivariant Neural Networks and Optimal Transport.

Gautam Pai

Eindhoven University of Technology, Netherlands, The; g.pai@tue.nl

The roto-translation group SE(2) has been of active interest in image analysis due to methods that lift the image data to multi-orientation representations. In this talk, I will overview some recent advances on SE(2) group convolutions: (1.) Equivariant Neural Networks that use linear and morphological convolutions that are the solutions to specific interpretable PDE's leading to competitive architectures with fewer parameters

and less training data. (2.) Entropic Optimal Transport. Convolutions with an-isotropic kernels on SE(2) are equivariant and exhibit a contour propagation behavior that is beneficial for processing images like meaningful barycenters of 2D shapes and expressive neural networks.

ID: 563 / MS55-3: 1

MS55 Dynamical Systems, Structure Preservation and Deep Learning

A Structure-Preserving Kernel Method for Learning Hamiltonian Systems

Jianyu Hu, Juan-Pablo Ortega, Daiying Yin

Nanyang Technological University, Singapore; juan-pablo.ortega@ntu.edu.sg

A structure-preserving kernel ridge regression method is presented that allows the recovery of potentially high-dimensional and nonlinear Hamiltonian functions out of datasets made of noisy observations of Hamiltonian vector fields. The method proposes a closed-form solution that yields excellent numerical performances that surpass other techniques proposed in the literature in this setup. A full error analysis is conducted that provides convergence rates using fixed and adaptive regularization parameters. The good performance of the proposed estimator is illustrated with various numerical experiments. This is joint work with Jianyu Hu and Daiying Yin.

ID: 564 / MS55-3: 2

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Kernel-based techniques for the learning of Poisson systems

Jianyu Hu, Juan-Pablo Ortega, Daiying Yin

Nanyang Technological University, Singapore; jianyu.hu@ntu.edu.sg

In this talk, we present a structure-preserving kernel method for learning Poisson systems, which is a significant generalization of previous work done by the authors for symplectic vector spaces. The proposed method guarantees that the learned vector field comes from a Hamiltonian function. We shall start by establishing differential reproducing properties on Riemannian manifolds. We then study the learning problem over Poisson manifolds using a kernel ridge regression and provide an operator-theoretic framework to represent estimators. Furthermore, we establish the differential kernel representation and an error analysis is conducted that provides convergence rates using fixed and adaptive regularization parameters.

ID: 582 / MS55-3: 4

MS55 Dynamical Systems, Structure Preservation and Deep Learning

On The Temporal Domain of Differential Equation Inspired Graph Neural Networks

Moshe Eliasof

University of Cambridge, United Kingdom; me532@cam.ac.uk

Graph Neural Networks (GNNs) excel in modeling complex relationships within graph-structured data. A recent advancement is Differential Equation-Inspired GNNs (DE-GNNs), leveraging continuous dynamical systems to model graph information flow with features like smoothing. However, DE-GNNs typically rely on first or second-order temporal dependencies. This paper introduces TDE-GNN, a neural extension that surpasses conventional temporal methods by capturing a broader range of dynamics. TDE-GNN

demonstrates superior performance over predefined temporal models across various graph benchmarks, emphasizing the value of learned temporal dependencies.

ID: 610 / MS55-5: 2

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Compositional Physics Informed Neural Network

Pratham Lalwani, Andy Wan

University of California, Merced, United States of America; andywan@ucmerced.edu

Physics Informed Neural Networks (PINN) have recently been applied to solve many forward and inverse problems. Traditionally, solving time-dependent problems using PINN involves sampling from a residual loss function on a fixed space-time domain, which can result in poor generalizability beyond its training time domain.

We introduce Compositional Physics Informed Neural Network (CPINN) where forward flow maps are learned by a variant of PINN while preserving compositional structure of flow maps. We show the error of CPINN beyond the training time can be bounded by the training error on a fixed training time interval and sampling error of the residual.

ID: 618 / MS55-1: 3

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Greedy algorithm with randomized dictionaries in application to ReLU^k shallow neural network approximation

Jongho Park, Xiaofeng Xu, Jinchao Xu

King Abdullah University of Science and Technology, Saudi Arabia; xiaofeng.xu@kaust.edu.sa

Greedy algorithms have been successfully analyzed and applied in training neural networks for solving variational problems with guaranteed convergence orders.

However, their practical applicability in high-dimensional problems is limited due to the subproblems, which involve an exhaustive search over a discrete dictionary and incur significant computational costs.

We propose a more practical approach of randomly discretizing the dictionary. We prove that the proposed algorithm realizes a weak greedy algorithm, achieving optimal convergence orders.

Through numerical experiments, we demonstrate the advantage of using randomly discretized dictionaries by showing order of magnitude reductions in the discrete dictionary size, particularly in higher dimensions.

ID: 621 / MS55-2: 3

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Deep learning and oscillatory dynamical systems

Richard Tsai

University of Texas at Austin, United States of America; ytsai@math.utexas.edu

In this presentation, we explore several crucial challenges associated with developing robust deep learning models for computing large-step flow maps for oscillatory dynamical systems. Key topics of discussion include the selection of an optimal training data distribution, strategies for effective sampling from this distribution, the creation of balanced loss functions, the identification of suitable network architectures, and

the development of specialized optimization algorithms tailored for this application. We will demonstrate our methodologies and discuss the practical implications and potential solutions for these challenges.

ID: 637 / MS55-1: 4

MS55 Dynamical Systems, Structure Preservation and Deep Learning

An error bound of PINNs for solving differential equations

Takashi Matsubara[1], **Takaharu Yaguchi**[2]

[1]Hokkaido University, Japan; [2]Kobe University, Japan; yaguchi@pearl.kobe-u.ac.jp

In recent years, applications of neural networks to physics have attracted much attention. In this talk, we show an error estimate of physics-informed neural networks for solving partial differential equations. In particular, the approximation rates of neural networks are taken into account in the error analysis. Based on the derived error bound, we reconsider the cases where PINNs are effective.

ID: 722 / MS55-1: 1

MS55 Dynamical Systems, Structure Preservation and Deep Learning

Nearest Neighbors GParareal: Improving Scalability of Gaussian Processes for Parallel-in-Time Solvers

Lyudmila Grigoryeva[1], **Guglielmo Gattiglio**[2], **Massimiliano Tamborrino**[2]

[1]University of St. Gallen; [2]University of Warwick; lyudmila.grigoryeva@unisg.ch

With the advent of supercomputers, multi-processor environments and parallel-in-time (PinT) algorithms offer ways to solve initial value problems for ordinary and partial differential equations (ODEs and PDEs) over long time intervals, a task often unfeasible with sequential solvers within realistic time frames. A recent approach, GParareal, combines Gaussian Processes with traditional PinT methodology (Parareal) to achieve faster parallel speed-ups. The method is known to outperform Parareal for low-dimensional ODEs and a limited number of computer cores. Here, we present Nearest Neighbors GParareal (NN-GParareal), a novel data-enriched PinT integration algorithm.

Part IV Contributed Talks

ID: 131

Contributed Talks

Keywords: vortex filament equation, Schrödinger map equation, finite difference methods, hyperbolic space

Recent progress on the Schrödinger map equation

Sandeep Kumar

CUNEF University, Spain; sandeep.kumar@cunef.edu

In this talk, we will explore the richness of the Schrödinger map equation whose equivalent form, the vortex filament equation, describes the motion of a vortex filament in a real fluid. When solving numerically, the dynamics of these equations for polygonal initial data exhibit qualitative features of real fluids, e.g., the axis-switching phenomenon. The corresponding algebraic solution not only supports the numerical evolution but also indicates randomness. I will discuss some recent results on helical-shaped vortices and curves in the hyperbolic space and show that this unusual behaviour (randomness) resulting from a differential equation indeed appears as a generic phenomenon.

ID: 169

Contributed Talks

Keywords: multi-scale simulations, dynamical low-rank approximation, energy stability, macro-micro decomposition, parallel computations

A multi-scale low-rank integrator for Marshak waves

Chinmay Patwardhan[1], **Jonas Kusch**[2], **Martin Frank**[1]

[1]Karlsruhe Institute of Technology, Germany; [2]Norwegian University of Life Sciences, Norway; chinmay.patwardhan@kit.edu

Phenomena like supernova explosions, star formations, or radiation emitted from a hohlraum striking a fusion target, involve the formation and propagation of thermal radiation fronts in a cold medium called Marshak waves. Multiple time scales must be resolved to efficiently simulate these thermal radiation fronts while keeping a low memory footprint. We propose an energy-stable and asymptotic-preserving numerical algorithm based on macro-micro decomposition and, the model-order reduction technique, dynamical low-rank approximation for simulating Marshak waves.

ID: 170

Contributed Talks

Keywords: Mirror descent-ascent, mean-field optimization, min-max problems, convergence rate analysis, Bregman divergence

Mirror Descent-Ascent for mean-field min-max problems

Razvan-Andrei Lascu

Heriot-Watt University, United Kingdom; rl2029@hw.ac.uk

We study two variants of the mirror descent-ascent algorithm for solving min-max problems on the space

of measures: simultaneous and sequential. We show how these schemes arise naturally as discretizations of Fisher-Rao flows. We assume convexity-concavity and relative smoothness of the objective function with respect to a suitable Bregman divergence, defined on the space of measures via flat derivatives. We prove that the convergence rates to mixed Nash equilibria, measured in the Nikaidò-Isoda error, are of order $\mathcal{O}\left(N^{-1/2}\right)$ and $\mathcal{O}\left(N^{-2/3}\right)$ for the simultaneous and sequential schemes, respectively.

ID: 172

Contributed Talks

Keywords: Elastic wave equation, Full-waveform inversion, Recurrent neural network, Automatic differentiation, Stochastic optimization

Elastic full-waveform inversion as training a neural network

Wensheng Zhang

Academy of Mathematics and System Sciences, Chinese Academy of Sciences, China, People's Republic of; zws@lsec.cc.ac.cn

In this talk, I will introduce the full-waveform inversion (FWI) for the elastic wave equation as training a neural network. The FWI problem is equivalent to neural network training of recurrent neural network. A variety of stochastic optimization methods including Adgrad, RMSprop, Adam, Nadam and Admax are applied in the training process. The gradient of the objective function with the model parameters is computed by the technique of automatic differentiation instead of the traditional adjoint method. Numerical computations show that the algorithms except Adgrad can yield good inversion results.

ID: 173

Contributed Talks

Keywords: Fast algorithm; Active Droplets; Brownian Dynamics; Integral equation method; Immersed boundary method

Modeling and Fast Algorithms for the Dynamics of Auto-Chemotactic Chiral Active Droplets

Zecheng Gan

Hong Kong University of Science and Technology (Guangzhou), China, People's Republic of; zechenggan@ust.hk

we develop a Brownian dynamics model coupled with a diffusion equation to examine the self-propulsion dynamics of auto-chemotactic chiral active droplets in 2D and 3D systems. A fast algorithm framework is developed based on an efficient and accurate quadrature scheme for the integral-equation based formulation for chemical diffusion, and an immersed-boundary method for particle motion. Our simulations well reproduce the curling and helical trajectories of nematic droplets in expriments. This is a joint work with Prof. Rui Zhang (HKUST, physics), students Kyle Chan and Johnson Yang.

ID: 187

Contributed Talks

Keywords: Machine-learning augmented hybrid simulation

Mitigating distribution shift in machine learning-augmented hybrid simulation

Jiaxi Zhao, **Qianxiao Li**

National University of Singapore, Singapore; jiaxi.zhao@u.nus.edu

We study the problem of distribution shift commonly arising in machine-learning augmented hybrid simulation, where parts of simulation algorithms are replaced by data-driven surrogates. We develop a mathematical framework to understand this phenomenon as a new type of instability, akin to those in classical numerical simulation. This motivates a class of tangent-space regularization algorithms that effectively combat instabiliy. We demonstrate our method on the reaction-diffusion equation and the incompressible Navier-Stokes equations, showcasing marked improvements. Additionally, we establish theoretical guarantees for its performance over linear dynamics.

ID: 201

Contributed Talks

Keywords: Quasi-2D geometry, long range interaction, Sum-of-Exponentials, random batch sampling

Fast Algorithm for Quasi-2D Coulomb Systems

Xuanzhao Gao[1,2], **Zecheng Gan**[1,2], **Jiuyang Liang**[3], **Zhenli Xu**[3]

[1]Thrust of Advanced Materials, The Hong Kong University of Science and Technology (Guangzhou), Guangdong, China; [2]Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR; [3]School of Mathematical Sciences, MOE-LSC and CMA-Shanghai, Shanghai Jiao Tong University, Shanghai, China; xz.gao@connect.ust.hk

Quasi-2D Coulomb systems are of fundamental importance and have attracted much attention in many areas nowadays. Their reduced symmetry and the long-range nature of Coulomb interaction gives rise to interesting collective behaviors but also brings great challenges for particle-based simulations. In our work, we employ an efficient Sum-of-Exponentials (SOE) approximation for the long-range kernel associated with Ewald splitting, reducing the complexity to $O(N^{1.4})$. Furthermore, we combine our method with the random batch sampling technique, resulting in a stochastic approximation with linear complexity.

ID: 206

Contributed Talks

Keywords: Electronic structure calculations, Self-consistent field iteration, Acceleration

Acceleration of self-consistent field iteration for electronic structure calculations

Fei Xu

Beijing University of Technology, China, People's Republic of; fxu@bjut.edu.cn

lectronic structure calculations involve complicated nonlinear models that require iterative algorithms to obtain approximate solutions. However, for complex molecular systems, the classical self-consistent field iteration does not converge or converges slowly. In order to improve the efficiency of self-consistent field iteration, we proposes a new accelerating algorithm. The main idea is to fit out a polynomial based on the error of the derived approximate solution, and then extrapolate the error into zero to obtain a new approximation. The developed scheme can not only be applied to electronic structure calculation but also to accelerate the nonlinear iterations of other nonlinear equations.

ID: 207

Contributed Talks

Keywords: Stochastic Control, Energy Storage, Optimisation

A Model Independent Approach for Empirically Identifying the Optimal Control Strategy of a Power Storage Facility

Fraser John Wilkinson O'Brien

The Maxwell Institute for Mathematical Sciences, Heriot-Watt University, United Kingdom; s2119422@ed.ac.uk

Finding the optimal control strategy of a power storage facility involves the consideration of a double sided boundary problem, because the optimal points for discharging and charging the facility needs identifying. The complexity is increased when considering facilities' variable efficiency levels. Developing classical theoretical approaches to the problem of optimal control of stochastic processes, we present a model independent empirical approach suitable for application on real-world data, alongside an expression for the relationship between the optimal control points and efficiency. Combining the theoretical and empirical results allows for a complete optimal control strategy to be identified directly from price data.

ID: 212

Contributed Talks

Keywords: Boundary Layer, Singularly Perturbed Problems, Orthogonal Spline Collocation Methods, Reaction-Diffusion Problems, Parameter Uniform Convergence, Time Delay

Parameter Uniform Numerical Methods Based on OSCM for The Singularly Perturbed Differential Equations with Delay in Time

Jewel Howlader[1], pankaj Mishra[2], Kapil K. Sharma[1]

[1]South Asian University, New Delhi-110068, India; [2]Deshbandhu College, University of Delhi, New Delhi-110019, India; jewelmth34@gmail.com

This paper develops and analyses a parameter uniform numerical method for singularly perturbed time delay parabolic reaction-diffusion problems with Dirichlet boundary condition. The problem exhibits parabolic boundary layers particularly for small values of perturbation parameter ε. To handle such boundary layer behaviour of the solution a Shishkin mesh is utilised and an orthogonal spline collocation approach with C1-cubic spline basis functions is applied in the spatial direction. The Crank-Nicolson technique is applied to an equidistant mesh in the temporal direction. Numerical experiments confirming the theoretical results have been provided.

ID: 219

Contributed Talks

Keywords: Tooth detection, Deep learning, Active contour, Oral CBCT images, Level set

WITS: Weakly-supervised individual tooth segmentation model trained on box-level labels

Ruicheng Xie, Yunyun Yang, Zhaoyang Chen

Harbin Institute of Technology (Shenzhen), China, People's Republic of China; yangyunyun@hit.edu.cn

Accurately and automatically segmenting teeth from cone-beam computed tomography (CBCT) images plays an essential role in dental disease diagnosis and treatment. This paper presents an automatic tooth segmentation model that combines deep learning methods and level-set approaches. By quantitative evaluation, we show that the proposed model can accurately segment teeth. The performance is more

accurate and stable than those of classical level-set models and deep-learning models.

ID: 222

Contributed Talks

Keywords: MHD, Sisko Fluid, Exponential stretching sheet, Chemical reaction, Soret effect.

Study of Soret Effect in Magnetized Dissipative Chemically Reactive Sisko Nanofluid Flow: A Numerical Insight

Reema Jain, **Yogesh Dadhich**

Manipal University Jaipur, India; reemajain197@gmail.com

The current study deals with the continuous, two-dimensional flow of chemically reactive Sisko fluid over a sheet which is stretched exponentially and is subjected to the simultaneous impacts produced by the magnetic field and Soret effect. The mathematical modelling gives rise to a complex set of PDEs, which are highly nonlinear. Consequently, similarity transformations are used to convert them to ODEs. The thorough discussion of similarity solutions in comparison with the established findings not only verifies the precision of the numerical outcomes but also highlights the reliability and robustness of the methodology applied in this study.

ID: 226

Contributed Talks

Keywords: the Wong-Zakai approximation, exponential Euler scheme, exponential trapezoidal scheme, strong convergence, space-time white noise

Exponential integrator for stochastic strongly damped wave equation based on the Wong-Zakai approximation

Yibo Wang

Southeast University, China, People's Republic of; wangyb@seu.edu.cn

We consider strong convergence of numerical approximations for a stochastic strongly damped wave equation. Through the Wong-Zakai approximation to the noise, we obtain an approximate equation. Based on the consistency and high regularity of the approximate equation, we develop two exponential integrators for time-stepping discretization and use the spectral Galerkin method in space to develop full-discrete schemes.

We show that the optimal strong order of the proposed WZ-approximation-based exponential Euler scheme is $|\beta|/2$ order higher than the existing works, and the proposed WZ-approximation-based exponential trapezoidal schemeit can break the first order barrier and obtain a higher accurate numerical solution.

ID: 231

Contributed Talks

Keywords: mixed finite element method, thin plate spline, adaptive refinement, error indicator

Data-based adaptive mesh refinement of finite element thin plate spline

Lishan Fang

Huaqiao University, China, People's Republic of; Lishan.Fang@outlook.com

The finite element thin plate spline is a data fitting and smoothing technique that was developed to efficiently

interpolate large data sets. In this talk, we will talk about its iterative adaptive mesh refinement process and error indicators, which were adapted from adaptive mesh refinement developed for PDEs. We will give some convergence results and demonstrate its performance using real-world data sets.

ID: 234

Contributed Talks

Keywords: Magnetohydrodynamic equation, second-order decoupling projection method, optimal error estimates

Optimal Error Estimates of a Crank-Nicolson Finite Element Projection Method for Magnetohydrodynamic Equations

Zeyu Xia

Harbin Institute of Technology, Shenzhen, China, People's Republic of; xiazeyu@hit.edu.cn

Magnetohydrodynamic (MHD) equations are widely applied in engineering and industrial production. In this talk we will introduce a modified Crank-Nicolson finite element scheme to solve the MHD equation, and present the energy stability analysis and optimal error estimates. We particularly utilize a second-order decoupling projection method of the Van Kan type in the Stokes solver, which computes the intermediate velocity field based on the gradient of the pressure from the previous time level, and enforces the incompressibility constraint via the Helmholtz decomposition of the intermediate velocity field. A error estimate measured in $L^{\infty}(0,T;L^2)$ norm has been proven.

ID: 242

Contributed Talks

Keywords:

Optimal convergence of the arbitrary Lagrangian–Eulerian interface tracking method for two-phase Navier–Stokes flow

Buyang Li[1], Shu Ma[2], Weifeng Qiu[3]

[1]The Hong Kong Polytechnic University; [2]National University of Singapore; [3]City University of Hong Kong; shuma@nus.edu.sg

Optimal-order convergence in the H^1 norm is proved for an ALE interface tracking finite element method for the sharp interface model of two-phase Navier-Stokes flow using high-order curved evolving mesh. In this method, the interfacial mesh points move with the fluid's velocity to track the sharp interface between two phases of the fluid, and the interior mesh points move according to a harmonic extension of the interface velocity. The error of the semidiscrete arbitrary Lagrangian-Eulerian interface tracking finite element method is shown to be $O(h^k)$ in the H^1 norm for the Taylor- Hood finite elements of degree $k \ge 2$.

ID: 256

Contributed Talks

Keywords: WG method, recovery type a posteriori error estimator, SAV, Allen-Cahn equation

Recovery-based a posteriori error estimate for the weak Galerkin finite element method

Ying Liu[1], Yufeng Nie[2]

[1]Xi'an University of Technology; [2]Northwestern Polytechnical University; liuyinglixueyuan@xaut.edu.cn

The practice of engineering calculation shows that the adaptive finite element method is quite an efficient

numerical method for solving PDEs, where the reliable and effective a posteriori error estimator plays a crucial role. In this work, we design a weak gradient recovery type a posteriori error estimator of the WG method for the elliptic equation. Then, the estimator is exploited for the adaptive computation of the SAV-WG scheme for the Allen-Cahn equation. Some benchmark numerical examples simulate the dynamic interface evolution of the Allen-Cahn equation.

ID: 258

Contributed Talks

Keywords: x

Implicit Peer Triplets in Gradient-Based Solution Algorithms for ODE Constrained Optimal Control

Jens Lang[1], Bernhard A. Schmitt[2]

[1]Technische Universität Darmstadt, Germany; [2]Philipps-Universität Marburg, Germany;

lang@mathematik.tu-darmstadt.de

Recently, we have developed and analyzed implicit two-step Peer triplets for nonlinear ODE constrained optimal control problems. We combine some standard Peer methods for inner grid points with carefully designed starting and end methods to achieve order four for the state variables and order three for the adjoint variables in a first-discretize-then-optimize approach. These methods do not suffer from order reduction – a phenomenon that is usually observed for one-step methods as e.g. symplectic Runge-Kutta methods. In this talk, we will present novel implicit two-step Peer triplets, which can be applied together with a projected gradient method. We will present several numerical examples.

ID: 288

Contributed Talks

Keywords: crack problem, variational inequality, finite element method, error estimate, elastic problem

Numerical method for the crack problem with a Signorini-type contact condition on a linear combination of displacement and velocity

Guanyu Zhou

University of Electronic Science and Technology of China, China, People's Republic of;

wind_geno@live.com

We consider the finite element approximation to the dynamic of a linear elastic body with a crack. The tangential velocity on the crack is subject to the Tresca-friction law. At the same time, in the normal direction, we enforce a Signorini-type condition involving a linear combination of displacement and velocity. We study the well-posedness and error estimates of both semi- and fully-discrete schemes. And we propose the Uzawa algorithm to solve the variational inequality. Several numerical experiments are carried out to test the accuracy of the discrete scheme and the efficiency of the Uzawa algorithm.

ID: 293

Contributed Talks

Keywords: Mesh size function, local mesh generation, error estimator, discontinuous coefficients

Node-based adaptive local mesh generation method and its application

Weiwei Zhang, Yuqing Zhou

Northwestern Polytechnical University, People's Republic of China; wwzhang@nwpu.edu.cn

In this talk, we develop a mesh adaptive algorithm that combines a posteriori error estimation with bubble-type local mesh generation (BLMG) strategy for elliptic differential equations. The advantages of the BLMG-based AFEM, compared with other known methods, are given as follows: the refining and coarsening are obtained fluently in the same framework; the local a posteriori error estimation is easy to implement through the adjacency list of the BLMG method; at all levels of refinement, the updated triangles remain very well shaped, even if the mesh size at any particular refinement level varies by several orders of magnitude.

ID: 298

Contributed Talks

Keywords: Optimal trade execution, self-attention neural network, HJB equation, computational finance

Self-Attention Network for Solving HJB Equation arising from Optimal Trade Execution

Andrew Na, Justin Wan

David R. Cheriton School of Computer Science, University of Waterloo, Canada; justin.wan@uwaterloo.ca

In this talk, we propose a novel machine learning approach for solving the high dimensional PDEs associated with the optimal trade execution problem in finance. Combining an HJB/BSDE formulation and a residual U-net with self-attention, our model numerically approximates the value function which can be used to determine the time consistent optimal trading strategies. With our framework, we can show how agents with different price impacts interact with one another. Furthermore, we will present results of the performance of multiple sellers and buyers and how they compare to a holding strategy under different economic conditions.

ID: 304

Contributed Talks

Keywords: Aggregation, dimension reduction method, Kuramoto model, synchronization

Asymptotic convergence of heterogeneous first-order aggregation models: from the sphere to the unitary group

Dohyun Kim[1], Hansol Park[2]

[1]Sungkyunkwan University, Korea, Republic of (South Korea); [2]Department of Mathematics, Simon Fraser University, 8888 University Dr., Burnaby, BC V5A 1S6, Canada; dohyunkim@skku.edu

In this talk, we provide the detailed asymptotic behavior for first-order aggregation models of heterogeneous oscillators on the unit sphere and the unitary group. In order to establish the convergence result, we introduce a novel method, called dimension reduction method that can be applied to a specific situation when the degree of freedom of the heterogenity is one. To this end, although a small perturbation is allowed, convergence toward an equilibrium of the perturbed gradient flow is still guaranteed.

ID: 310

Contributed Talks

Keywords: Volterra Integral Equation, Galerkin Methods, Iterated Galerkin Methods

Superconvergent Jacobi Spectral Methods for System of Nonlinear Volterra- Integro-Differential Equations

Rakesh Kumar, BV Rathish Kumar

Indian Institute of Technology Kanpur, India; rakeshh20@iitk.ac.in

In this paper, the Jacobi Spectral Galerkin (JSG) and iterated Jacobi Spectral Galerkin (IJSG) methods for a nonlinear integro-differential equations in Volterra type have been proposed. Jacobi polynomial-based Galerkin and iterated Galerkin techniques have been used to tackle these integral equations. The convergence analysis is carried out for the proposed method, and error estimates are derived. The IJSG method improves the JSG method in terms of convergence rates. The theoretical outcomes are verified numerically.

Consider the following system of nonlinear Volterra integro-differential equation $$ u_i^{'}(x) = g(x,u_i(x))+ \int_0^x(\delta(x)-\delta(t))^{-\mu} {k}\left(x, t, {u_1}(t), {u_2}(t),{u_1}^{\prime}(t), {u_2}^{\prime}(t)\right) d t, \quad 0 \leq x \leq 1,$$ $$u_i(0)=\beta_i, $$

ID: 317

Contributed Talks

Keywords: Weak Galerkin mixed finite element method, parabolic interface problems, Crank-Nicolon scheme, a priori error analysis

Weak Galerkin Mixed FEM for the Crank-Nicolson Scheme of Parabolic Interface Problems

Amit Kumar Pal, Jhuma Sen Gupta

BITS Pilani Hyderabad, India; p20210064@hyderabad.bits-pilani.ac.in

The main aim of this talk is to present a priori error analysis for the weak Galerkin (WG) mixed finite element method for the fully discrete Crank-Nicolon approximation for parabolic interface problems. More precisely, the method allows one to use the discontinuous mixed WG finite element spaces for the spatial discretizations and for the time, the implicit Crank-Nicolon approximation has been used. An almost optimal order a priori error bound has been derived for both the solution and the flux variable in the $L^\infty(L^2)$ norm.

ID: 331

Contributed Talks

Keywords: High-frequency wave propagation, nonlinear Friedrichs system, diffractive geometric optics, slowly varying envelope approximation, error bounds

On error bounds for approximations to high-frequency wave propagation in nonlinear dispersive media

Julian Baumstark, Tobias Jahnke

Karlsruhe Institute of Technology, Germany; tobias.jahnke@kit.edu

We consider systems of semilinear PDEs where both the differential equations and the initial data contain the inverse of a small parameter ε. The solution oscillates in time and space with wavelength of $O(\varepsilon)$ and has to be computed on long time intervals with length of $O(1/\varepsilon)$. Solving such problems numerically with a standard method is prohibitively inefficient or even infeasible, because this requires a very fine discretization in time and space. We discuss an approach to approximate the original problem by a numerically more suitable system of PDEs, and we present new error bounds which improve previous results significantly.

ID: 343

Contributed Talks

Keywords: Reaction-diffusion system, Basic reproduction number, Numerical Simulation.

Study on dynamical behaviour of reaction-diffusion epidemic model

Hariharan Soundararajan, Shangerganesh Lingeshwaran

National Institute of Technology Goa, India; hariharan@nitgoa.ac.in

The study of infectious diseases is vital for public health. This work introduces a reaction-diffusion PDE epidemic model with quarantine compartment to analyse infection spread. Spatial diffusion is incorporated to capture geographical disease spread. Basic reproduction number is estimated and numerical simulations using the finite difference method are performed to examine solution characteristics. This research offers insights into disease dynamics and enhances understanding of the disease management by considering both temporal and spatial components.

ID: 347

Contributed Talks

Keywords: Bifurcation diagram, Exact multiplicity, Positive solution, ⊂-shaped bifurcation curve, Generalized logistic problem

Evolutionary bifurcation diagrams of a multiparameter generalized logistic problem

KUO-CHIH HUNG[1], SHIN-HWA WANG[2]

[1]National Chin-Yi University of Technology, Taiwan; [2]National Tsing Hua University, Taiwan; shwang@math.nthu.edu.tw

We study the one-dimensional generalized logistic problem with constant yield harvesting: \begin{equation*} \left \{ \begin{array}{l} u^{\prime \prime }(x)+\lambda g(u)-\mu =0,\;-1<x<1\text{,} \\ u(-1)=u(1)=0,% \end{array}% \right. \end{equation*} where g satisfies $g(0)=g(1)=0$, $g(u)>0$ on $(0,1)$, and g is either convex-concave or convex-concave-convex on $(0,1)$ and satisfies certain conditions. We prove that, for any fixed harvesting parameter $\mu >0,$ on the $(\lambda ,\left \Vert u\right \Vert _{\infty })$-plane, the bifurcation diagram consists of a $\subset $-shaped curve and then we study the structures and evolution of bifurcation diagrams for varying $\mu >0.$

ID: 352

Contributed Talks

Keywords: Weak Galerkin mixed finite element method, weak divergence operator, a priori error analysis

On the weak Galerkin mixed FEM for parabolic interface problems

Jhuma Sen Gupta[1], Amit Kumar Pal[1], Rajen Kumar Sinha[2]

[1]BITS Pilani Hyderabad, India; [2]Indian Institute of Technology Guwahati; jhuma@hyderabad.bits-pilani.ac.in

This talk aims to present a priori error analysis for the fully discrete backward Euler weak Galerkin (WG) mixed finite element method for linear parabolic interface problems. The WG method allows one to use the classical divergence operator in its weak form which makes the method more flexible in term of less restrictions on the underlying finite element spaces. A nearly optimal order a priori error bounds for both the solution and the flux variables are derived in the $L^{\infty}(L^2)$ norm. Numerical experiments are performed to underline the theoretical analysis.

ID: 359

Contributed Talks

Keywords: Convolution quadrature, fractional derivatives, fractional dissipative systems, fractional differential equations, variational principles, variational integrators

Fractional variational integrators based on convolution quadrature

Khaled Hariz[1], **Fernando Jimenez**[2], **Sina Ober-Blöbaum**[1]

[1]Paderborn university, Germany; [2]Universidad Nacional de Educación a Distancia, Spain; hariz@math.uni-paderborn.de

Fractional dissipation is a powerful tool to study non-local physical phenomena such as damping models. Based on the doubling of variables and their fractional derivatives, one can derive dissipative systems using purely variational way. Our aim is to derive higher-order fractional variational integrators by means of convolution quadrature (CQ) based on backward difference formulas. We then provide numerical methods that are of order 2 improving a previous result. The convergence properties of the fractional variational integrators and saturation effects due to the approximation of the fractional derivatives by CQ are studied numerically.

ID: 369

Contributed Talks

Keywords: Partial Migration, Synchronous cycles, Ideal Free Distribution, Evolutionary Game Theory, Evolutionary Stable Strategy

Synchronous cycles in migrating population dynamics

Ram Surendra Singh, **Yogesh Trivedi, Anushaya Mohapatra**

Birla Institute of Technology and Science, Pilani , K K Birla Goa Campus,India.; p20190013@goa.bits-pilani.ac.in

Migration is a diverse phenomenon and can be categorized into many forms. The most common type of migration is partial migration. Using a discrete stage structure matrix model, we investigate which kind of density dependence mechanisms would cause a stable cyclic behavior with alternating and separated generations of juveniles, migrant, and non-migrant adults. Using an adaptive dynamics approach, we showed the existence of an evolutionary stable strategy and examined how the ideal free distribution (IFD) arises in the context of a temporally separated population. We also show that the ideal free distributions for synchronous 2-cycles are evolutionary stable strategies.

ID: 370

Contributed Talks

Keywords: Fluid-Structure Interactions, Direct Numerical Simulation, Diffuse Interface Method, Phase Field Method, Multiscale Modeling and Simulations

Simulation Method of Microscale Fluid-Structure Interactions: Diffuse-Resistance-Domain Approach

Xinpeng Xu

Guangdong Technion - Israel Institute Of Technology, China; xu.xinpeng@gtiit.edu.cn

We consider the microscale fluid-structure interactions from different fields such as particle focusing in microchannels from microfluidics, deformable objects suspending in microswimmer suspensions from

microbiology, and two-phase flows on solid surfaces from various contexts, e.g., microscale manufacturing, and geophysics, etc. For this purpose, we developed a diffuse interface approach -- Diffuse Resistance Domain (DRD) approach by following the general framework of Onsager's linear irreversible thermodynamics and two fluid model. Here, some preliminary results using DRD approach are presented.

ID: 372

Contributed Talks

Keywords: convex optimization, continuous dynamics, accelerated methods, Runge-Kutta methods, numerical stability

Explicit Runge-Kutta methods for quadratic optimization with optimal rates

Tuo Liu, David Ketcheson

King Abdullah University of Science and Technology, Saudi Arabia; tuo.liu@kaust.edu.sa

This paper focuses on analyzing and developing accelerated optimization methods for the class of smooth and strongly convex functions. We derive a family of optimal gradient-based methods for quadratic programming (OERKD) by building a mapping between continuous dynamics and discrete updates of optimization algorithms. Optimality is justified by analysis of explicit Runge-Kutta methods on linear gradient flow equation with stability conditions. Experiments demonstrate the effectiveness of the proposed algorithm even on classical nonlinear problems. A noteworthy byproduct is proving the asymptotic equivalence between OERKD and Polyak's heavy ball method, which subtly bridges two primary integration schemes.

ID: 395

Contributed Talks

Keywords: Modified method of characteristics; Isogeometric analysis; Transport problems; NURBS functions; Activator and inhibitor; Developmental biology

An L^2-projection isogeometric analysis based on Strang splitting for nonlinear systems of convection-diffusion-reaction

Ilham Asmouh, Alexander Ostermann

University of Innsbruck, Austria; ilham.asmouh@uibk.ac.at

In this study, we present a new algorithm for the numerical solution of convection-diffusion-reaction equations arising from developmental biology. The semi-Lagrangian method is combined with isogeometric analysis (IGA) to construct a stable and highly accurate method. At the interpolation stage, non-uniform rational B-splines are used to update the solution in an L^2-projection framework. The proposed method maintains the advantages of the semi-Lagrangian method in reducing the truncation errors and allowing for large CFL numbers in the simulations. The performance of the new isogeometric semi-Lagrangian analysis is demonstrated for a class of advection-diffusion-reaction systems.

ID: 396

Contributed Talks

Keywords: Navier–Stokes equations, Locally refined time stepsizes, Nonsmooth initial data, Error estimate

Optimal-order convergence of the linearly extrapolated Crank–Nicolson method and the two-step BDF method for the Navier–Stokes equations with H^1 initial data

Na Wang

Harbin Institute of Technology, Shenzhen, China, People's Republic of; wangna@hit.edu.cn

In this talk, we focus on the convergence analysis of the fully discrete linearly extrapolated Crank–Nicolson time-stepping scheme and the linearly extrapolated two-step backward difference time-stepping scheme, combined with the finite element method in space, for the two-dimensional Navier–Stokes equations with H^1 initial data (without any additional compatibility conditions), i.e., $u^0\in[H_0^1(\Omega)]^2$, and $\nabla\cdot u^0=0$. By utilizing properly designed variable time stepsizes locally refined towards $t=0$, we prove the second-order convergence of both methods in both time and space without any CFL conditions. Numerical examples are provided to illustrate the convergence of the two methods.

ID: 410

Contributed Talks

Keywords: fractional integral, fractional differential equations, generalized convolution quadrature, variable steps, graded meshes

Generalized Convolution Quadrature for non smooth sectorial problems

Jing Guo[1], **Maria Lopez-Fernandez**[2]

[1]The Chinese University of Hong Kong, Shenzhen Research Institute of Big Data; [2]University of Malaga, Spain; maria.lopezf@uma.es

We consider the application of the generalized Convolution Quadrature (gCQ), with variable steps, to approximate an important class of sectorial problems arising in fractional calculus. Typically the solution to these problems is not very smooth and Lubich’s Convolution Quadrature, with uniform steps, presents an order reduction. We show how the full order of the method can be achieved by choosing an appropriate time grid, which is graded around the singularities of the data. An important advantage of the gCQ method is that it allows for a fast and memory reduced implementation.

ID: 446

Contributed Talks

Keywords: bulk-surface splitting, dynamic boundary conditions

Bulk-surface splitting for parabolic problems with dynamic boundary conditions

Robert Altmann

OvGU Magdeburg, Germany; robert.altmann@ovgu.de

We introduce bulk-surface splitting schemes for semilinear parabolic PDEs with dynamic boundary conditions of first and second order. In contrast to previously proposed splitting approaches, these schemes do not suffer from order reduction or dependencies on the spatial discretization. The results are illustrated by a number of numerical examples.

ID: 466

Contributed Talks

Keywords: Multilevel Richardson-Romberg, Mutilevel Monte Carlo, Derivative Pricing, Importance Sampling

Efficient Multilevel Importance Sampling in Derivative Pricing

Devang Sinha, **Siddhartha Pratim Chakrabarty**

Indian Institute of Technology Guwahati, India; dsinha@iitg.ac.in

This research proposes a novel integration of Multilevel Richardson-Romberg extrapolation with parametric importance sampling to develop a sophisticated multilevel estimator for computing $E[P(X_T)]$. Here, $P(x)$ denotes a payoff functional and $\{X_t\}_{0\leq t\leq T}$ denotes a stochastic process driven by an underlying stochastic differential equation (SDE). The crux of our investigation lies in assessing the impact of employing higher-order discretization schemes within the importance sampling paradigm, primarily to achieve substantial variance reduction. Through a series of numerical experiments, our research underscores the efficiency and computational superiority of our proposed integrative approach over the conventional multilevel algorithm in estimating $\mathbf{E}[P(X_T)]$.

ID: 470

Contributed Talks

Keywords: Kolmogorov PDE, Gaussian Process Regression, Feynman-Kac Formula

An Uncertainty-aware Mesh-free Numerical Method for Kolmogorov PDEs

Daisuke Inoue[1], Yuji Ito[1], Takahito Kashiwabara[2], Norikazu Saito[2], Hiroaki Yoshida[1]

[1]Toyota Central R&D Labs. Inc.; [2]The Graduate School of Mathematical Sciences, The University of Tokyo; daisuke-inoue@mosk.tytlabs.co.jp

This study introduces an uncertainty-aware, mesh-free numerical method for solving Kolmogorov PDEs. We use Gaussian process regression (GPR) to smoothly interpolate pointwise solutions that are obtained by Monte Carlo methods based on the Feynman-Kac formula. The proposed method has two main advantages: 1. uncertainty assessment, which is facilitated by the probabilistic nature of GPR, and 2. mesh-free computation, which allows efficient handling of high-dimensional PDEs. To analyze the performance of the method, we derive a lower bound on the posterior variance. Extensive tests on three representative PDEs demonstrate the high accuracy and robustness of the method compared to existing methods.

ID: 490

Contributed Talks

Keywords: CIP method, semi-Lagrangian method, Hermite interpolation, advection equation

Error estimates of the CIP scheme for one-dimensional advection equations

Haruki Takemura, Takahito Kashiwabara

The University of Tokyo, Japan; takemura@ms.u-tokyo.ac.jp

Cubic interpolated pseudo-particle (CIP) scheme is a numerical method for advection equations with low numerical diffusion and high accuracy, and is a semi-Lagrangian method with the cubic Hermite interpolation. It is observed by numerical experiments that the CIP scheme has third-order accuracy in time and space. We present an error estimate of order $O(\Delta t^3+h^4/\Delta t)$ in L^2 norm, where the spatial and temporal mesh sizes are denoted by h and Δt respectively.

ID: 502

Contributed Talks

Keywords: random batch, molecular dynamics, heterogeneous, high-performance computing, cross-scale simulations

RBMD: Random Batch Molecular Dynamics on Heterogeneous Computing Architectures

Weihang Gao

Shanghai Jiao Tong University, China, People's Republic of; gaowh2019@sjtu.edu.cn

We develop a high-performance MD software utilizing random batch algorithms to realize collaborative acceleration of long and short-range force computations. It is found that RBMD exhibits an average speed-up of 10 times (maximum 60 times) over LAMMPS on three different NVIDIA architectures. Furthermore, RBMD can scale the system up to 10 times larger than LAMMPS, which proves crucial for performing cross-scale simulations in fields such as materials science, energy research and chemistry.

ID: 509

Contributed Talks

Keywords: Hamiltonian systems, Deep learning for physics, Classification

Enhancing Modeling Accuracy via Discriminating Hamiltonian Systems

Yuhan Chen, Takaharu Yaguchi

Kobe University, Japan; yuhanchen@lion.kobe-u.ac.jp

Improving the accuracy of deep learning for physics is a great concern in various scientific and engineering fields. Classifying unknown datasets based on their underlying dynamical properties can significantly improve the accuracy of simulation models. In this talk, we propose a new strategy for distinguishing Hamiltonian systems from non-Hamiltonian systems prior to modeling, which adjusts the learning process according to the intrinsic dynamics of the dataset and thus improves the prediction performance.

ID: 515

Contributed Talks

Keywords: time-evolution equations, operator learning, Newton's method, unsupervised learning, generalization error

Fast implicit hybrid solvers for stiff time-evolution equations

Tianyu Jin[1], Georg Maierhofer[2], Katharina Schratz[3]

[1]Department of Mathematics, Hong Kong University of Science and Technology; [2]Mathematical Institute, University of Oxford; [3]LJLL, Sorbonne University; tjinac@connect.ust.hk

In this work, we propose a novel operator learning based hybrid Newton's method to solve implicit schemes of stiff time-evolution equations. Unlike most existing neural operators, our neural time stepper with extremely simple structure, once trained by an implicit scheme based unsupervised learning strategy, can give us a better initial guess in iteration and accelerate iteration consistently until equilibrium. Theoretical analysis is provided on the generalization error of our unsupervised learning strategy and how much Newton's method can be accelerated by initialization. Numerical experiments, demonstrating the efficiency of our proposed method, are also presented.

ID: 516

Contributed Talks

Keywords: rBergomi model, neural SDE, initial forward variance, Wasserstein 1-distance, summation of exponentials

Neural Option Pricing for Rough Bergomi Model

Changqing TENG, Guanglian LI

The University of Hong Kong, Hong Kong S.A.R. (China); u3553440@connect.hku.hk

The rBergomi model could effectively capture several stylized facts of financial markets from option pricing

point of view, but its calibration is still an open problem. This work investigates the potential of learning the forward variance curve in the rBergomi model using a neural SDE. We propose an efficient solver of it which simulates the volatility process by modified summation of exponentials. Using the Wasserstein 1-distance as the loss function, the learned forward variance curve is capable of calibrating price of underlying asset and price of European options simultaneously. Several numerical tests are provided to demonstrate its performance.

ID: 531

Contributed Talks

Keywords: M-product, Moore-Penrose inverse, group inverse, multilinear systems

Two-Step iterative method for solving singular tensor equations $\mathcal{A}*_M\mathcal{X}=\mathcal{B}$ under M-product

Jajati Keshari Sahoo

BITS Pilani K K Birla Goa Campus, Goa, India; jksahoo@goa.bits-pilani.ac.in

Consider the following singular system of linear equations $\mathcal{A}*_M\mathcal{X}=\mathcal{B}$, $\mathcal{A}\in \mathbb{R}^{m\times n\times p}, ~~\mathcal{B}\in \mathbb{R}^{m\times 1\times p}$. The singular multilinear systems arise in various branches of Science and Engineering, such as statistical models, forecast modeling, and partial differential equations, which are generalizations of matrix-structured computations. Several iterative methods have been studied recently for linear systems but not explored much in the case of multilinear systems, specifically under the M-product. To deal with such a multilinear system, in this talk, we will discuss a matrix splitting-based three-step iterative scheme for solving the above singular system.

ID: 533

Contributed Talks

Keywords: Supersymmetric dispersionless system; Dimensional analysis; Covariant derivative operator; Higher order super-symmetries.

Supersymmerties with Arbitrary Functions of a New Supersymmetric Dispersionless System and the classifications

Ruoxia Yao

Shaanxi Normal University, China, People's Republic of; rxyao2@hotmail.com

Infinitely many higher order super-symmetries with arbitrary functions of a new integrable supersymmetric dispersionless system proposed recently by us are constructed via the symmetry analysis and bosonization methods along with a dimensional analysis method based on the operation of covariant derivative operator under the scheme of fermion field, whic shows that the system is integrable. Several super-symmetries are obtained respectively in some cases with the same {\it ranks/dimensions} of the quantities consisted in the general super-symmetric form. Some of the classifications of such models are introduced.

ID: 559

Contributed Talks

Keywords: Nonlocal nonlinear Schrodinger equation, Nonlocal Yajima–Oikawa system, Binary Darboux transformation, Exact solutions

Nonlocal Yajima–Oikawa system: binary Darboux transformation, exact solutions and dynamic properties

Caiqin Song[1], **Hai-qiong Zhao**[2], **Zuo-nong Zhu**[3]

[1]University of Shanghai for Science and Technology, China, People's Republic of; [2]School of Statistics and Information, Shanghai University of International Business and Economics, Wenxiang Road, Shanghai, People's Republic of China; [3]School of Mathematical Sciences, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai People's Republic of China; caiqinsong@usst.edu.cn

In this paper, we propose a new type integrable nonlocal Yajima–Oikawa (YO) system, which can be derived from the special reduction in the two-component YO system. We show that the binary Darboux transformation is an effective method to construct not only multi-soliton solutions, but also other types of solutions for this type nonlocal integrable systems. Additionally, some novel solutions of the nonlocal YO system are obtained, and further are analyzed in detail to reveal several interesting dynamic features, such as the moving bright soliton with sudden position shift, the collision of two-breather waves

ID: 574

Contributed Talks

Keywords: Nonclassical symmetry analysis, Conservation laws, Porous media flow, Cross-flow.

Nonclassical Symmetry Analysis to Find out Analytical Solution of a Porous Media Flow Model

Sougata Mandal, **Sukhendu Ghosh**

Indian Institute of Technology Jodhpur, India; mandal.5@iitj.ac.in, sukhendu.math@iitj.ac.in

This investigation focuses on the invariance principle-based nonclassical symmetry analysis approach to find out an analytical solution for a viscous and incompressible flow in a channel filled with isotropic porous material. The channel features a uniform cross-flow through its upper and lower porous walls which generates a flow inside the porous media channel. Using the nonclassical symmetry, a single non-linear ordinary differential equation is obtained and it is solved analytically. Moreover, a set of conservation laws for the governing system is also investigated in this work.

ID: 584

Contributed Talks

Keywords: DWR-based adaptation, multi-target functional, multi-mesh calculation, Newton-GMG solver

Towards the calculation generalized target functional with multi-mesh approach

Jingfeng Wang, **Guanghui Hu**

University of Macau, Macau S.A.R. (China); shankswang953@gmail.com

The calculation of target functionals plays a pivotal role in optimization design. Adjoint-based techniques are commonly employed to estimate errors in these functionals or to provide local indicators for adaptive refinement. However, the frameworks developed in recent decades often struggle to generalize to more complex functionals. In this work, we analyze multi-target functionals and develop algorithm with multi-mesh technique. Focusing on aerodynamic design, our experiments demonstrate that our approach robustly solves the lift-drag ratio and multiple airfoils' target functional, thereby enhancing the reliability of target functional computation in complex scenarios.

ID: 608

Contributed Talks

Keywords: linear relaxation; energy quadratization; phase field models; energy stable; phase-field crystal model

Linear Relaxation Method with Regularized Energy Quadratization for Phase Field Model

Maosheng Jiang

Qingdao University, China, People's Republic of; msjiang@qdu.edu.cn

In this talk, we establish a novel linear relaxation method with regularized energy quadratization for phase field models, which we name the RREQ method. We employ the Allen–Cahn equation, the Cahn–Hilliard equation, the molecular beam epitaxy model and the phase-field crystal model as test beds to illustrate the concept. Rigorous theoretical analysis demonstrates that these resulting schemes from the RREQ method satisfy the modified discrete energy dissipation laws and preserve the discrete mass conservation for the PFC and MBE models. Furthermore, we present numerical results to confirm our theoretical results and demonstrate our method's effectiveness in solving phase field models.

ID: 643

Contributed Talks

Keywords: Finite difference, Weighted essentially non-oscillatory, Neural network

A THIRD-ORDER FINITE DIFFERENCE WENO SCHEME WITH SHALLOW NEURAL NETWORK

Kwanghyuk Park[1], Xinjuan Chen[2], Dongjin Lee[1], Jiaxi Gu[3], Jae-Hun Jung[3]

[1]Graduate school of AI, Pohang University of Science and Technology, Korea, Republic of (South Korea);
[2]Department of Mathematics, College of Science, Jimei University, Xiamen, Fujian 361021, China;
[3]Department of Mathematics, Pohang University of Science and Technology, Korea, Republic of (South Korea); pkh0219@postech.ac.kr

Neural networks are increasingly used in computational fluid dynamics, particularly in weighted essentially non-oscillatory schemes (WENO). This work addresses challenges in achieving maximum-order convergence and the ENO property by incorporating a neural network into the WENO scheme. By utilizing a neural network as a weighting function and introducing additional loss on reconstruction weights, the our model WENO3-SNN scheme achieves enhanced convergence compared to WENO-Z. Demonstrations on one- and two-dimensional test cases, including strong shocks and shock-density wave interactions, exhibit the scheme's excellent generalization across various resolutions, with performance comparable to or better than the classical WENO5-JS scheme.

ID: 670

Contributed Talks

Keywords: DeepONet, operator learning, error estimate, deep learnimg

Improved estimate of the number of input points of DeepONet

Dehami Kiryu, Baige Xu, Takaharu Yaguchi

Kobe University, Japan; 245s002s@stu.kobe-u.ac.jp

DeepONet is an operator learning method mainly used to estimate solutions to differential equations. In this talk, we first revisit the estimate of the number of input points required to predict the solutions shown by Lu et al. We then show an improved estimate under almost the same assumptions. This improved estimate can

be applied to a simple network model with the same structure as DeepONet.

ID: 672

Contributed Talks

Keywords: HIV Model, Multi-strain Model, Treatment, Drug Adherence

HIV Community Transmission under Treatment: A Two-strain Modelling Approach

Ashish Poonia, Siddhartha Pratim Chakrabarty

Inidan Institute of Technology Guwahati, India; pooniaa75@gmail.com

In this study, we introduced a two-strain model involving drug-sensitive and drug-resistant strains to analyze the dynamics of Human Immunodeficiency Virus (HIV) transmission within a community. We incorporated a treatment compartment into the modelling framework by considering drug adherence. Both the treatment-free, as well as the treatment model are analyzed. A comprehensive stability and bifurcation analysis reveals the impact of treatment availability and drug adherence on the spread of different strains of HIV.

ID: 673

Contributed Talks

Keywords: Nonlinear Wave, Operator Learning, Hamiltonian PDE

Operator Learning of Hamiltonian Density for Modeling Nonlinear Waves

Baige Xu[1], Yusuke Tanaka[2], Takashi Matsubara[3], Takaharu Yaguchi[1]

[1]Kobe University, Japan; [2]NTT Corporation, Japan; [3]Hokkaido University, Japan; baigexu@stu.kobe-u.ac.jp

For learning Hamiltonian dynamics, existing methods based on deep neural networks such as Hamiltonian Neural Networks and their variants have achieved progress. However, these works depend on the discretization of data, and the determination of required differential variables is often necessary. Instead, we propose an operator learning approach for modeling nonlinear waves, which is able to learn the operator of Hamiltonian density from data with unspecific discretization, without any differential variable determination.

ID: 675

Contributed Talks

Keywords: Finite difference, Wave propagation, Staggered grid, Summation by parts operators, Shear Alfvén waves

Energy-preserving discretizations of anisotropic waves applied to plasma physics

Micol Bassanini[1,2], Simone Deparis[1], Paolo Ricci[2]

[1]École polytechnique fédérale de Lausanne (EPFL), MATH-SB, Switzerland; [2]École polytechnique fédérale de Lausanne (EPFL), Swiss Plasma Center (SPC), Switzerland; micol.bassanini@epfl.ch

We develop a finite difference method on staggered grids for wave-like problems, which is energy-preserving and accurate. This method retains key properties of the summation-by-parts operators framework, in particular, it preserves the divergence theorem at the discrete level. The method is applied to a reduced two-fluid plasma model describing plasma dynamics in the boundary region of fusion devices. The model includes the shear Alfvén waves, a highly anisotropic fast wave present in many plasma systems.

ID: 679

Contributed Talks

Keywords: Loan Portfolio; Liquidity Risk; Limited Liability; Haircut

Impact of Liquidity Risk and Limited Liability in Loan Portfolio Management

DEB NARAYAN BARIK, S IDDHARTHA P. C HAKRABARTY

Indian Institute of Technology Guwahati, India; d.narayan@iitg.ac.in

This study discusses a bank loan portfolio with liquidity risk and limited liability. We have constructed a novel three-step model with a threshold level of liquidity. Initially, the bank chooses its portfolio, and finally, it either makes a profit or faces bankruptcy, and at the intermediate time step, it liquidates some of its assets to meet the depositors' claims. We have proved that the inclusion of liquidity increases stability, and introducing the risk threshold of the liquidated portfolio improves stability.

ID: 685

Contributed Talks

Keywords: Absolute value equations; Linear complementarity problem; Unique solution

Unique Solvability conditions for the absolute value equations and absolute value matrix equations

Shubham Kumar, Deepmala --

PDPM Indian Institute of Information Technology, Design & Manufacturing, Jabalpur, India; shub.srma@gmail.com

This research paper explores the conditions that guarantee the unique solvability and unsolvability of absolute value equations. Further, we give the possible revised version of the unique solvability conditions for the two incorrect results that appeared in the published paper by Wu et al. (76:195-200, 2018). We also gave the two counter-examples for two unique solvability conditions that appeared in the published paper by Wu et al. (169:705-712, 2016) and provided alternative results.

ID: 695

Contributed Talks

Keywords: PDE-constrained optimization, optimal control theory, mathematical biology, chemotaxis, flux-corrected transport

PDE-constrained optimization with flux-correction in mathematical biology

Karolina Benkova[1,2], John Pearson[2], Mariya Ptashnyk[1]

[1]Heriot Watt University, UK; [2]University of Edinburgh, UK; k.benkova@ed.ac.uk

Modelling pattern formation and cell migration by PDE systems poses challenges due to unmeasurable parameters. We pose an inverse problem from PDE-constrained optimization (PDECO) to estimate these parameters, however, when solving systems that include chemotaxis, we encounter numerical issues like blow-up and unphysical oscillations. We present a numerical solver, utilizing the flux-corrected transport technique within the PDECO problem, which addresses these challenges, promising more accurate parameter identification and deeper insights into biological mechanisms.

ID: 703

Contributed Talks

Keywords: Hyperbolic equations, Finite difference, Time filter

A Time Filtered Scheme for Non-linear Hyperbolic Equations Motivated by Modeling DNA Transcription Process

Faranak Pahlevani[1], **Kevin Courtney**[2], **Lisa Davis**[3]

[1]Penn State University-Abington, United States of America; [2]Penn State University-Lehigh Valley, United States of America; [3]Montana State University, United States of America; fxp10@psu.edu

The focus of this presentation is the development and analysis of a time filtering process for a non-linear hyperbolic equation inspired by the modeling of the transcription of ribosomal RNA in bacteria. Recently the time filter has been combined with fully implicit schemes for nonlinear problems in order to increase accuracy with minimal modifications to existing code. In this talk, we demonstrate the numerical study of adding a time filter to first and second order finite difference schemes for non-linear hyperbolic problems. A new explicit implementation is presented, and accuracy analysis of the filtered scheme is presented for test problems.

ID: 742

Contributed Talks

Keywords: Two-dimensional three-component model, Nonconforming FEM, VEM

Stable and efficient methods for 2D-3C clamped plate and shallow shell models

Xiaoqin Shen

Xi'an University of Technology, China, People's Republic of; xqshen@xaut.edu.cn

In this talk, we share our work on the numerical methods for the two-dimensional three-component (2D-3C) clamped plate and shallow shell problems. We introduce discretization schemes of conforming, nonconforming FEM and VEM. Moreover, the new contributions include well-posedness and stability for the approximate problem and analysis of the convergence of the numerical solution. Finally, numerical results show that the stability and convergence of the numerical schemes are verified.

Part V Posters

ID: 205

Poster Session

Keywords: Electronic structure calculations, Self-consistent field iteration, Acceleration

Acceleration of self-consistent field iteration for electronic structure calculations

Fei Xu

Beijing University of Technology, China, People's Republic of; fxu@bjut.edu.cn

Electronic structure calculations involve complicated nonlinear models that require iterative algorithms to obtain approximate solutions. However, for complex molecular systems, the classical self-consistent field (SCF) iteration does not converge. To improve the efficiency of SCF iteration, we proposes a new accelerating algorithm. The main idea is to fit out a polynomial based on the error of the derived approximate solution, and then extrapolate the error into zero to obtain a new approximation. The developed scheme can not only be applied to electronic structure calculation but also to accelerate the nonlinear iterations of other nonlinear equations.

ID: 217

Poster Session

Keywords: Anisotropic diffusion, exponential methods, cosmic rays

Exponential Methods for Anisotropic Diffusion

Pranab J Deka[1], Lukas Einkemmer[2], Ralf Kissmann[3]

[1]Centre for Mathematical Plasma-Astrophysics, KU Leuven, Belgium; [2]Department of Mathematics, University of Innsbruck, Austria; [3]Institute for Astro- and Particle Physics, University of Innsbruck, Austria; pranab.deka@kuleuven.be

Anisotropic diffusion is imperative in understanding cosmic ray diffusion across the Galaxy. In order to conduct numerical simulations of time-dependent anisotropic cosmic ray transport, the implicit Crank-Nicolson integrator has been traditionally favoured over the CFL-bound explicit integrators to be able to take large time-step sizes. We propose exponential methods that directly compute the exponential of the underlying matrix to treat the linear anisotropic diffusion equation. The boost in the performance offered by the exponential methods without compromising the accuracy of the solutions makes them an excellent alternative to the traditional methods for treating the time-dependent cosmic ray transport equation.

ID: 350

Poster Session

Keywords: Nehari manifold optimization, 1-saddle, Nehari retraction, global convergence, semilinear elliptic PDE

Nehari manifold optimization and its application for finding unstable solutions of semilinear elliptic PDEs

Zhaoxing Chem[1], Wei Liu[2], Ziqing Xie[1], Wenfan Yi[3]

[1]Hunan Normal University, China; [2]National University of Singapore, Singapore; [3]Hunan University, China; wliu.hunnu@foxmail.com, wfyi@hnu.edu.cn

A Nehari manifold optimization method (NMOM) is introduced for finding 1-saddles, i.e., saddle points with Morse index 1, of a generic nonlinear functional in Hilbert spaces. It is based on the variational characterization on the Nehari manifold for 1-saddles. The global convergence is rigorously established in the infinite-dimensional setting. By combining with an easy-to-implement Nehari retraction and the negative Riemannian gradient direction, the NMOM is successfully applied to compute the unstable ground-state solutions of a class of semilinear elliptic PDEs. In particular, the symmetry-breaking phenomenon of the ground states of H\'enon equation is explored numerically with interesting numerical findings reported.

ID: 388

Poster Session

Keywords: causal inference, conditional local independence, nonparametric test

Testing conditional local independence for diffusion processes: Nonparametric rates

Sihui Zhao[1], **Ting Gao**[2], **Lin Liu**[1]

[1]Shanghai Jiao Tong University, China, People's Republic of; [2]Huazhong University of Science and Technology; shzhao0115@sjtu.edu.cn, tgao0716@hust.edu.cn, linliu@sjtu.edu.cn

Continuous event dynamics can be modeled using diffusion processes, enabling causal inference through testing conditional local independence among corresponding processes. We present a nonparametric framework for testing conditional local independence between diffusion processes. We introduce a functional parameter to quantify deviations from the hypothesis, providing estimators for drift functions and functional parameter using functional approximation theory and cross-fitting method. Our findings demonstrate bounded bias and variance for the nonparametric estimators, validating test efficacy under complex drift functions.

ID: 401

Poster Session

Keywords: stochastic differential equations, invariant measure, order conditions, exotic aromatic forests

Exotic aromatic forests for high-order sampling of the invariant measure

Eugen Bronasco

University of Geneva, Switzerland; Eugen.Bronasco@unige.ch

Exotic aromatic forests, an extension of aromatic forests into the stochastic context, serve pivotal roles in generating order conditions for invariant measure sampling and studying the algebraic properties of stochastic integrators. Our study unveils practical benefits through a new method, a generalization of the Leimkuhler-Matthews method, while also briefly exploring the favorable algebraic properties of exotic aromatic forests. Based on joint works with A. Laurent, B. Leimkuhler, D. Phillips, G. Vilmart.

ID: 416

Poster Session

Keywords: approximation theory, composite functions, numerical analysis

Deep Univariate Polynomial and Conformal Approximation

Zhen Wei {Kingsley} Yeon[1], **Jonathan Goodman**[2]

[1]University of Chicago, United States of America; [2]Courant Institute of Mathematical Sciences, New York University, United States of America; yeon@uchicago.edu

A deep approximation is an approximating function defined by composing more than one layer of simple functions. We study deep approximations of functions of one variable using layers consisting of low-degree polynomials or simple conformal transformations. Computational experiments show a composite of two and three polynomial layers can give more accurate approximations than a single polynomial with the same number of coefficients. We study the related problem of reducing the Runge phenomenon by composing polynomials with conformal transformations.

ID: 518

Poster Session

Keywords: deep learning, neural operator, partial differential equation, energy-based theory, Hamiltonian mechanics

Neural Operators for Hamiltonian and Dissipative PDEs

Yusuke Tanaka[1], Takaharu Yaguchi[2], Tomoharu Iwata[1], Naonori Ueda[3]

[1]NTT, Japan; [2]Kobe University, Japan; [3]RIKEN Center for AIP, Japan; ysk.tanaka@ntt.com

There is a great interest in operator learning to obtain solution operators of PDEs via neural networks. This study presents a framework that can utilize the laws of physics as inductive biases for training neural operators. Our key idea is introducing a novel penalty function inspired by the energy-based theory. Experiments on several PDEs show that our framework can accurately predict solutions than baselines while adhering to the energy conservation or dissipation law from data.

ID: 520

Poster Session

Keywords: Stokes flow; Dynamics; Synchronization; Droplet

Dynamics and hydrodynamic interactions of droplets ladened by active agents

Zheng Yang[1,2], Chun Wing Chan[1], Zecheng Gan[1,2], Rui Zhang[1]

[1]The Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); [2]The Hong Kong University of Science and Technology (Guangzhou), China; zyangcc@connect.ust.hk

Active droplets which can autonomously locomote are of both fundamental interest and practical importance. Due to the action of the active agents in the droplets, surface active flow will arise, which can drive the droplets to propel. We investigate the dynamics of droplets above a no-slip bottom wall, driven by neutral swimmers on their surfaces. For a single droplet, its trajectories exhibit petal-like circular motions. Synchronization phenomena are observed in the presence of multiple droplets, due to translation-rotation hydrodynamic coupling. Our work sheds light on understanding the surface flow mediated autonomous motion of active droplets.

ID: 550

Poster Session

Keywords: Reduced Order Modeling (ROM); Proper Orthogonal Decomposition (POD); Limited Data; parametric PDE

A reduced-order spectral Galerkin (ROSG) approach for solving parametric PDEs with limited data

Tianhao HU, Zecheng Gan

Hong Kong University of Science and Technology(Guang Zhou), China, People's Republic of; thu176@connect.hkust-gz.edu.cn

We propose a novel framework, reduced order spectral Garlerkin (ROSG) method, which guarantees spectral

convergence and promises efficiency as Reduced Order Modeling (ROM), particularly in the case of limited data, where conventional ROM fails to achieve high accuracy .
ROSG creates a hierarchy of subspace in a data-driven way. Proper Orthogonal Decomposition (POD) is applied to find representative basis from the data projected inside each subspace.
Test results on solving a prototypical reaction-diffusion equation shows given tolerance 1e-9 ROSG outperforms spectral method by 14% with 2 samples and 54% with 4 samples in terms of the number of basis functions required.

ID: 578

Poster Session

Keywords: Partial differential equations, Eikonal equations, Ray tracing, Algorithm

An Adaptive Ray Tracing Method for Eikonal Equation on Spheres

Wai Ming Chau, Shingyu Leung

The Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); wmchau@connect.ust.hk

We propose an efficient and accurate numerical algorithm for obtaining the ray tracing solution of the surface eikonal equation on $\mathbb{S}^2$. We estimate a new wavefront from the previous one by solving the equation's characteristic system. At each time step, we interpolate new rays or remove existing ones from the wavefront when the difference in several parameters between adjacent rays exceeds a predefined maximum or minimum threshold. This ensures an even sampling of the wavefront. By utilizing our adaptive ray tracing algorithm, which incorporates high-order and stable interpolation scheme integrators on $\mathbb{S}^2$, we can accurately capture high-order multivalued solutions.

ID: 616

Poster Session

Keywords: Inverse problem, level set optimization, gravimetry, low-rank approximation, total variation L1 regularization

A Fast Level Set Based Optimization for Inverse Gravimetry

Nishan Gurung

The Hong Kong University of Science and Technology, Hong Kong S.A.R. (China); ngurung@connect.ust.hk

We propose a fast algorithm for level set based optimization to solve the inverse problem $A\mathbf{x}=\mathbf{b}$, where $\mathbf{x}$ represents an unknown domain to be recovered. Our algorithm is a two-step procedure: (i) flipping points from inside the level set to outside and vice-versa to decrease the energy and (ii) minimizing TV-L1 denoising model for regularization. To speed up our algorithm, we also introduce an efficient low-rank approximation to our energy update. Numerical experiments for the inverse gravimetric problem demonstrate the effectiveness of our approach.

ID: 678

Poster Session

Keywords: operator learning, dynamical systems, recurrent neural networks, long-time intergration

Multi-Resolution Learning of Partial Differential Equations with Deep Operators and Long Short-Term Memory Networks

Katarzyna Michalowska

SINTEF Digital, Norway; katarzyna.michalowska@sintef.no

DeepONets offer an advantage over traditional neural networks in their ability to be trained on multi-resolution data. While this becomes especially relevant when high-resolution measurements are difficult to obtain compared to low-resolution data, DeepONets alone struggle in modeling long sequences. We propose a novel framework that leverages multi-resolution data and provides precise models with limited high-resolution data. We achieve this through extending the DeepONet with an LSTM and training it in a three-step procedure with data of varying resolution. The proposed multi-resolution DON-LSTM achieves significantly lower error and requires fewer high-resolution samples on multiple non-linear PDEs compared to vanilla models.

ID: 680

Poster Session

Keywords: Tooth detection, Deep learning, Active contour, Oral CBCT images, Level set

WITS: Weakly-Supervised Individual Tooth Segmentation Model Trained on Box-Level Labels

Yunyun Yang, Ruicheng Xie, Zhaoyang Chen

Harbin Institute of Technology (Shenzhen), China, People's Republic of China; yangyunyun@hit.edu.cn

Accurately and automatically segmenting teeth from cone-beam computed tomography (CBCT) images plays an essential role in dental disease diagnosis and treatment. This paper presents an automatic tooth segmentation model that combines deep learning methods and level-set approaches. By quantitative evaluation, we show that the proposed model can accurately segment teeth. The performance is more accurate and stable than those of classical level-set models and deep-learning models.

ID: 707

Poster Session

Keywords: Traffic Flow Model, Lighthill-Whitham-Richards, Time-FIlter, Hyperbolic Equation.

Time Filtering Method for a Traffic Flow Model Inspired by DNA Transcription Modeling

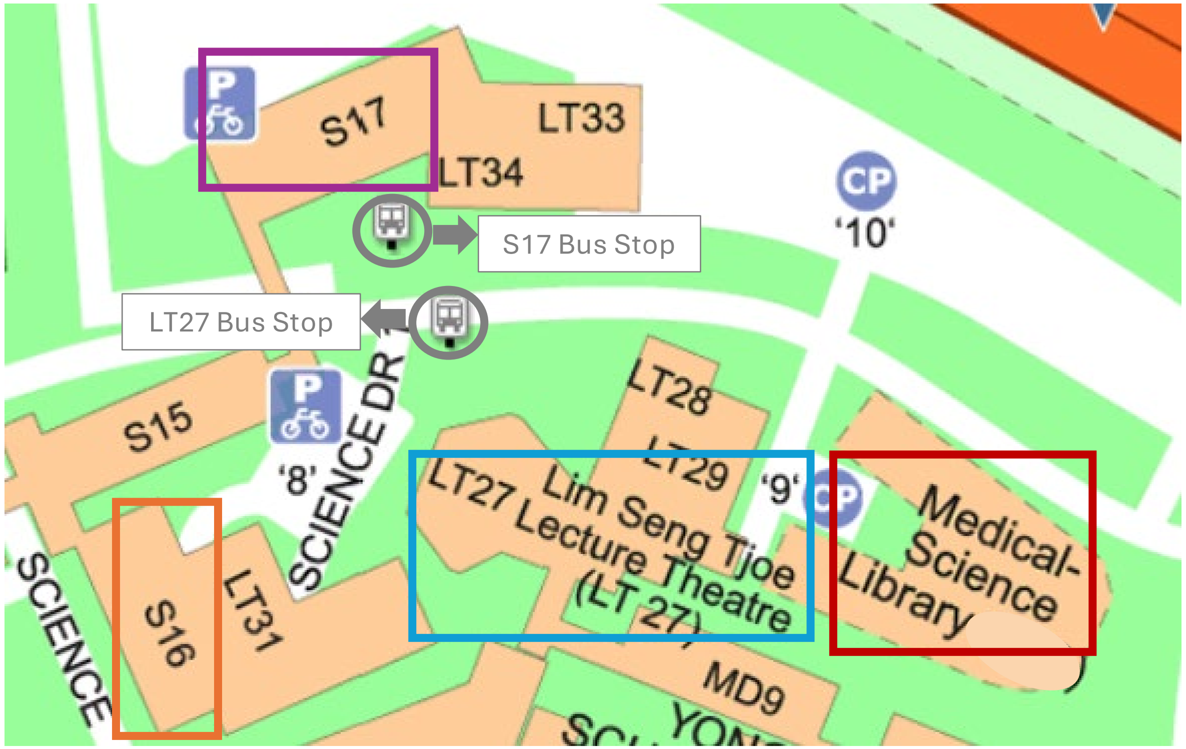
Kevin Brian Courtney[1], Lisa Davis[2], Faranak Pahlevani[3]

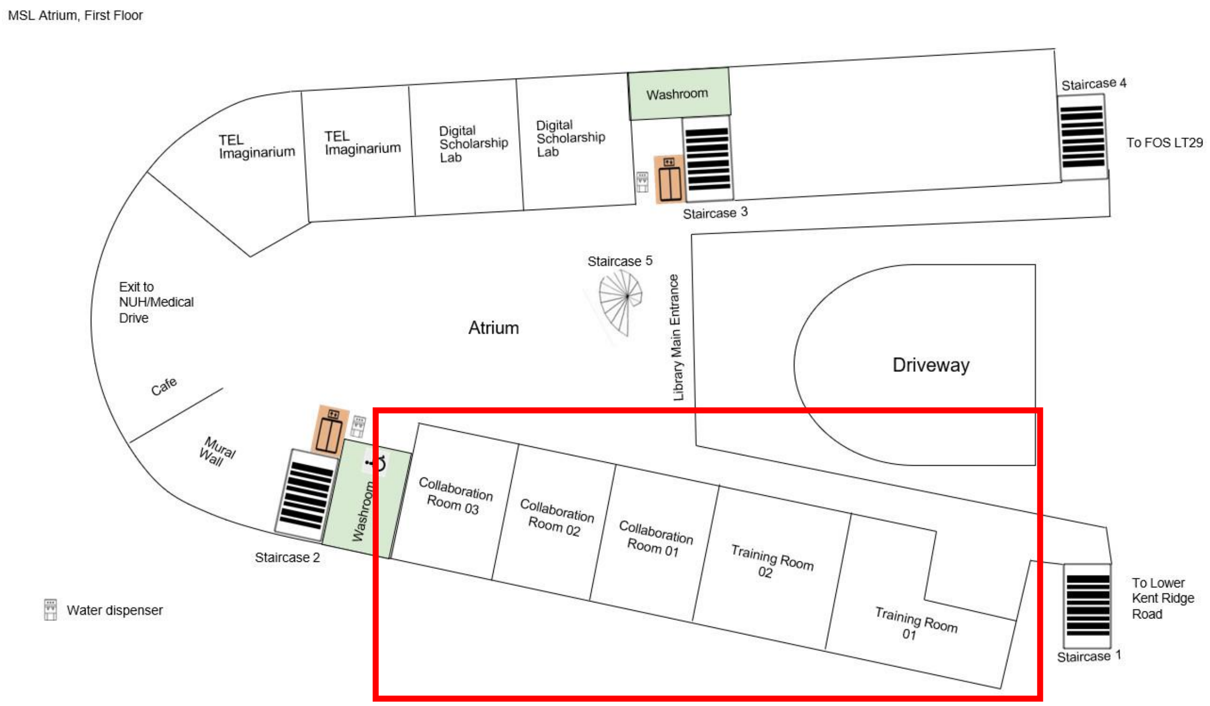
[1]Penn State University - Lehigh Valley, United States of America; [2]Montana State University, United States of America; [3]Penn State University - Abington, United States of America; kbc5720@psu.edu

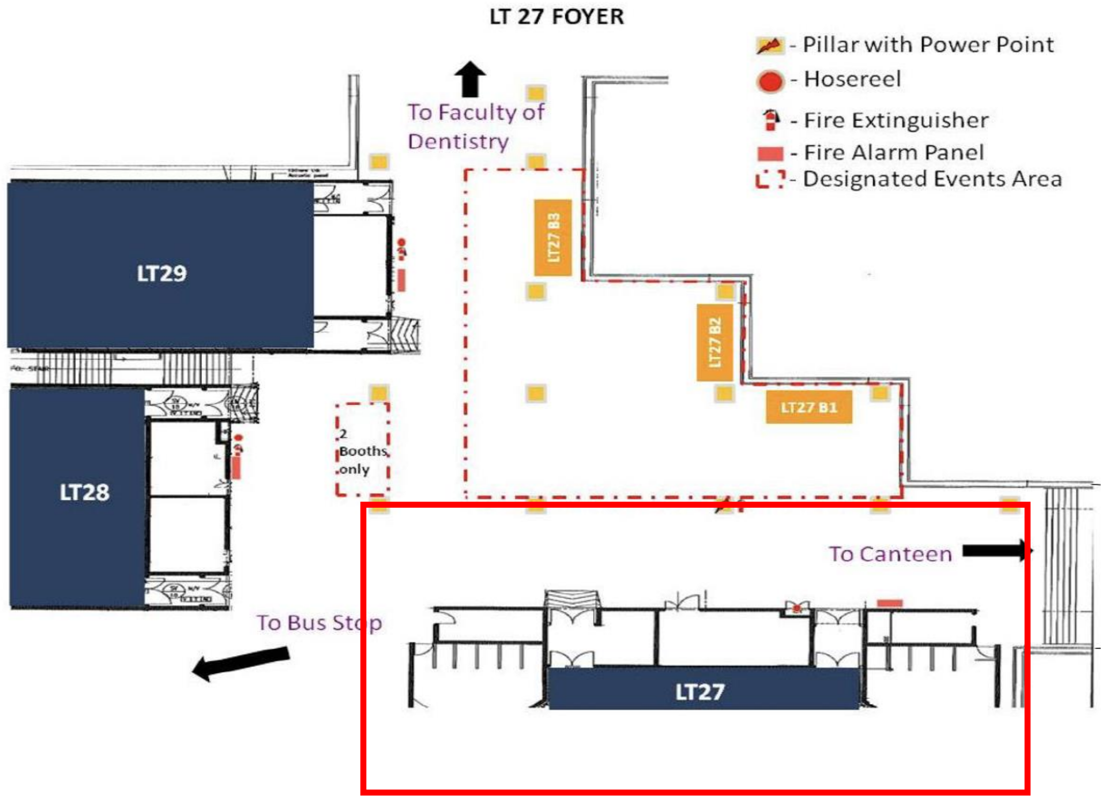
The focus of this presentation is the development, numerical simulation and parameter analysis of a model of the transcription of ribosomal RNA in highly transcribed genes. Inspired by the well-known classic traffic flow model Lighthill-Whitham-Richards (LWR), a non-linear advection continuum model is used to describe the DNA transcription process. The numerical treatment for model simulations includes introducing a low complexity and time accurate method by adding a simple linear time filter to explicit and implicit finite difference schemes. This improved new method is modular and requires a minimal modification of adding only one line code resulting in increased accuracy without increased computational expense.

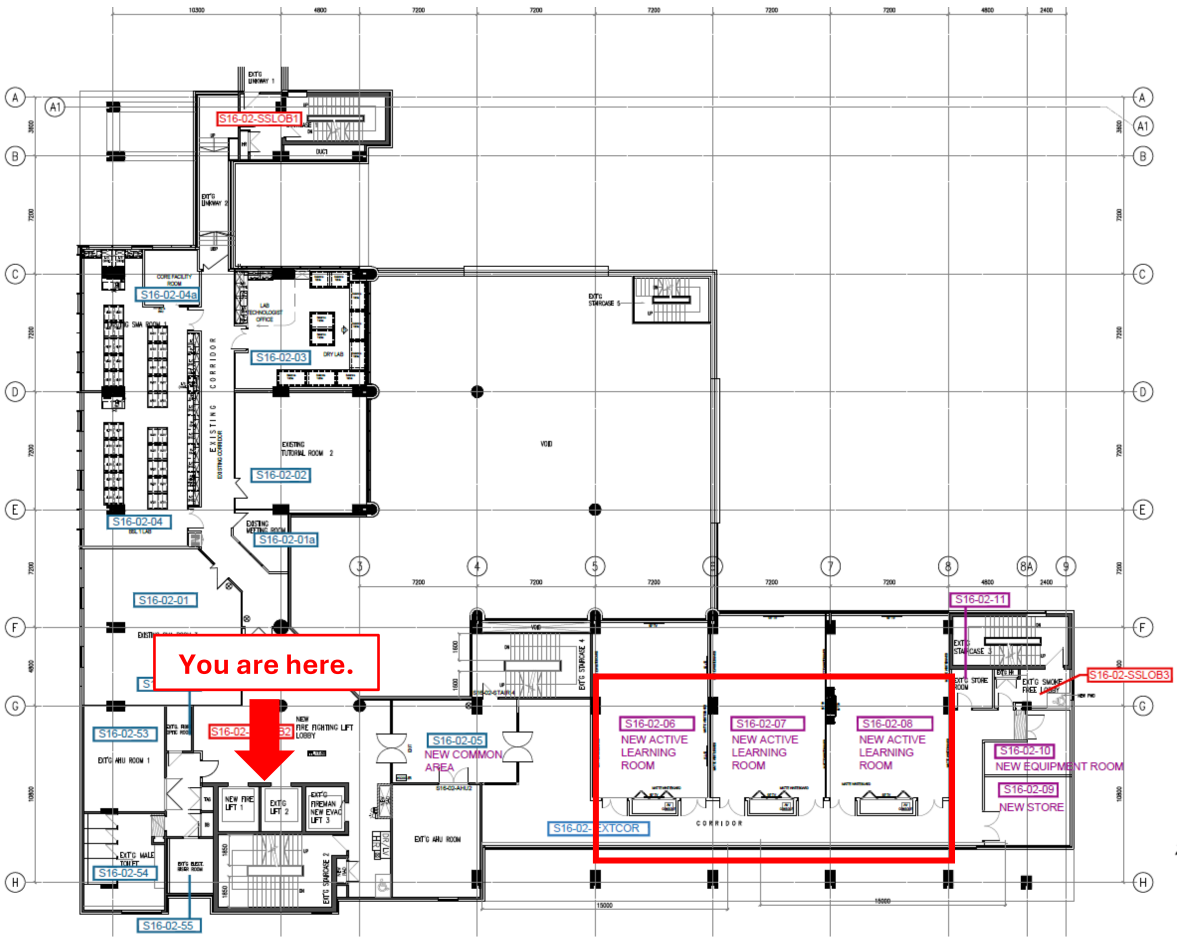
Overview of SciCADE 2024 Venues and Rooms

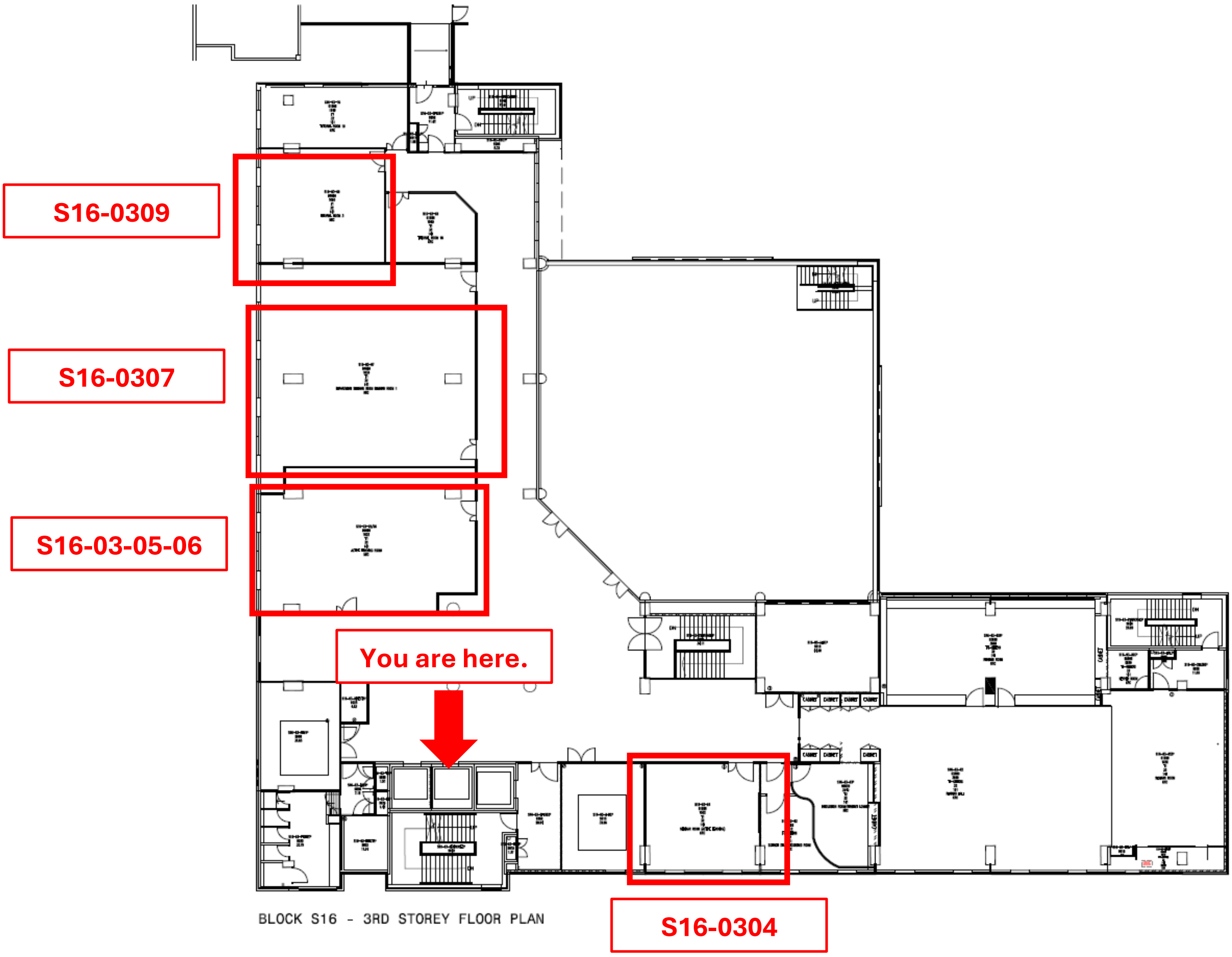
LT27	S17	S16	Medical Science Library
Plenary Lectures 1 to 8	S17-04-01 Conference Room	S16-02-06 New Active Learning Room	Registration Desk
Dahlquist Prize Lecture	S17-04-04 Seminar Room 3	S16-02-07 New Active Learning Room	MSL Training Room 1
New Talent Award Lecture	S17-04-05 Seminar Room 2	S16-02-08 New Active Learning Room	MSL Training Room 2
	S17-05-11 Seminar Room 5	S16-0304	MSL Collaboration Room 01
	S17-05-12 Seminar Room 4	S16-03-0506	MSL Collaboration Room 02
	S17-06-11 Seminar Room 6	S16-0307	MSL Collaboration Room 03
		S16-0309	

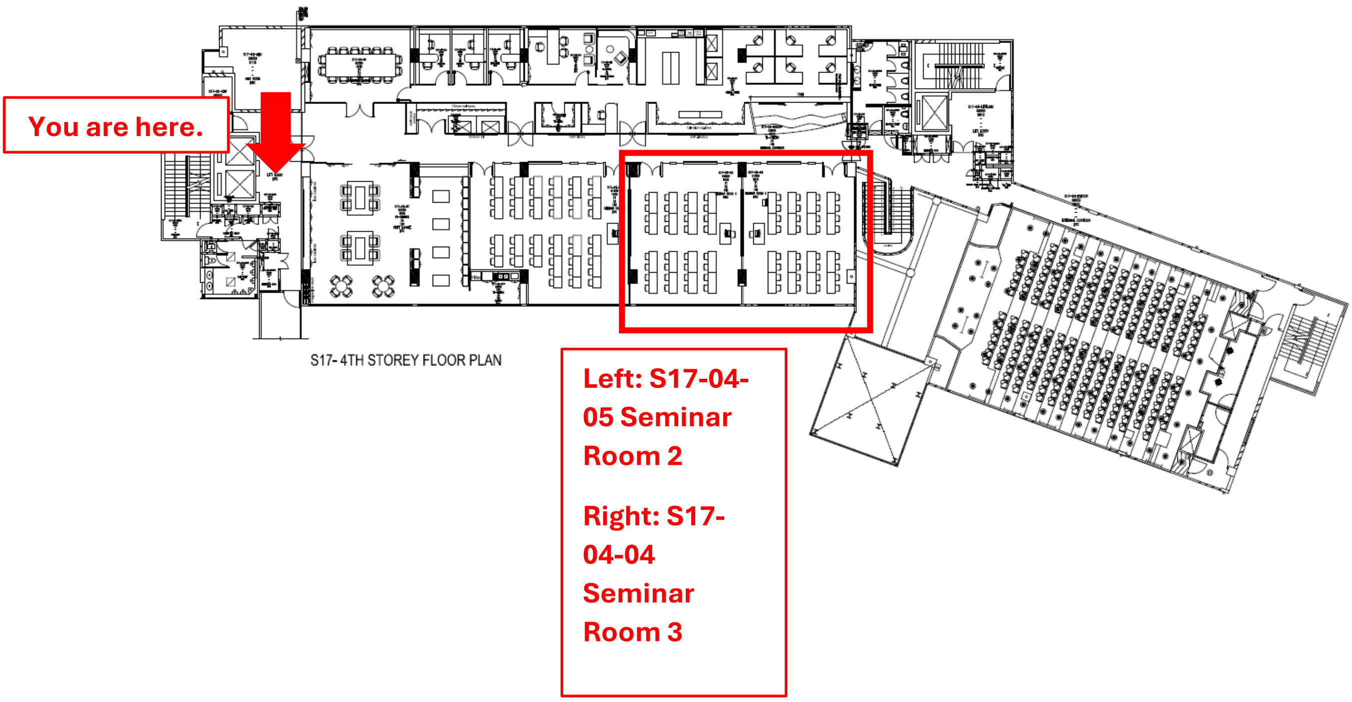


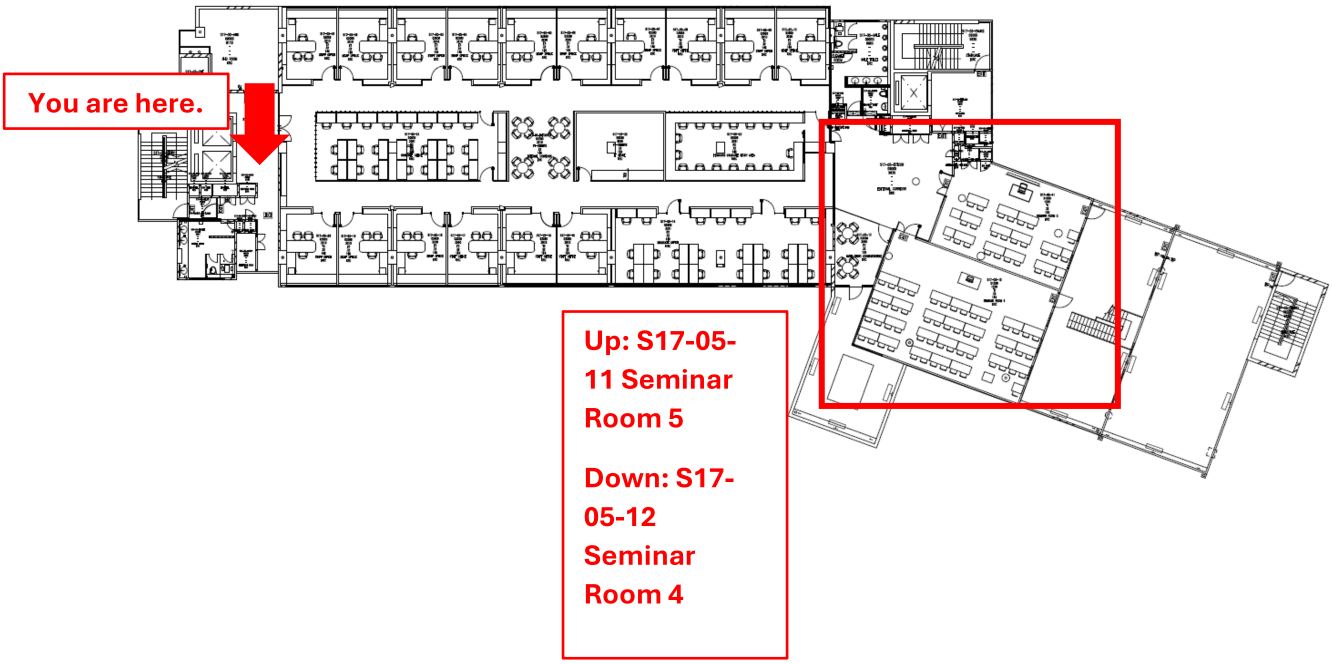

MSL Atrium, First Floor
TEL Imaginarium
TEL Imaginarium
Digital Scholarship Lab
Digital Scholarship Lab
Washroom
Staircase 4
To FOS LT29
Staircase 3
Staircase 5
Exit to NUH/Medical Drive
Atrium
Library Main Entrance
Driveway
Cafe
Mural Wall
Washroom
Collaboration Room 03
Collaboration Room 02
Collaboration Room 01
Training Room 02
Training Room 01
Staircase 2
To Lower Kent Ridge Road
Staircase 1
Water dispenser

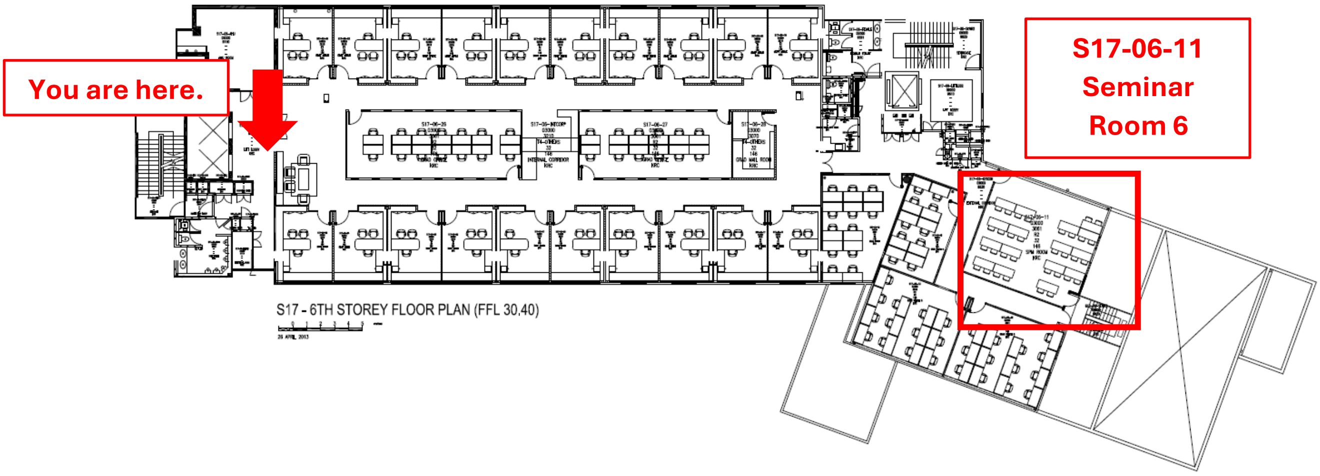

LT 27 FOYER
To Faculty of Dentistry
- Pillar with Power Point
- Hosereel
- Fire Extinguisher
- Fire Alarm Panel
- Designated Events Area
LT29
LT27 B3
LT27 B2
LT27 B1
LT28
2 Booths only
To Canteen
To Bus Stop
LT27


You are here.
S16-02-SSLOB1
S16-02-04a
S16-02-03
S16-02-02
S16-02-04
S16-02-01a
S16-02-01
S16-02-53
S16-02-54
S16-02-55
S16-02-05
NEW COMMON AREA
S16-02-EXTCOR
S16-02-06
NEW ACTIVE LEARNING ROOM
S16-02-07
NEW ACTIVE LEARNING ROOM
S16-02-08
NEW ACTIVE LEARNING ROOM
S16-02-11
S16-02-SSLOB3
S16-02-10
NEW EQUIPMENT ROOM
S16-02-09
NEW STORE
VOID
CORRIDOR
EXT'G AHU ROOM 1
EXT'G AHU ROOM
NEW FIRE FIGHTING LIFT LOBBY


S16-0309
S16-0307
S16-03-05-06
You are here.
S16-0304
BLOCK S16 - 3RD STOREY FLOOR PLAN


You are here.
S17- 4TH STOREY FLOOR PLAN
Left: S17-04-05 Seminar Room 2
Right: S17-04-04 Seminar Room 3


You are here.
Up: S17-05-11 Seminar Room 5
Down: S17-05-12 Seminar Room 4


You are here.
S17-06-11 Seminar Room 6
S17 - 6TH STOREY FLOOR PLAN (FFL 30.40)

Sponsors

NUS National University of Singapore | Department of Mathematics, Faculty of Science

NUS National University of Singapore | IMS Institute for Mathematical Sciences

Nanyang Technological University Singapore | School of Physical and Mathematical Sciences, College of Science