SciCADE 2019

International Conference on Scientific Computation and Differential Equations

Innsbruck, July 22nd - 26th, 2019

「350」
universität innsbruck
Wir bauen Brücken. Seit 1669

Contents

Welcome

On behalf of the Department of Mathematics of the University of Innsbruck, it is our very great pleasure to welcome you to SciCADE 2019 in this, the 350th anniversary year of the foundation of the university.

We are pleased that SciCADE 2019 has met with immense interest. More than 300 international participants are going to attend this year's meeting. The numerous contributions include plenary presentations, mini-symposia, contributed talks as well as posters. SciCADE 2019 offers a broad diversity of topics within the field of the various applications of scientific computing and differential equations. We are looking forward to a fruitful and stimulating meeting.

SciCADE 2019 has been made possible by the great commitment of many individuals, who have provided their tireless support und precious time, as well as by the generous support of sponsors, who are listed at the back of this booklet. A heartfelt thanks goes to all these people.

We very much hope that you will find SciCADE 2019 enjoyable, productive and rewarding. If you need assistance or information, please do not hesitate to ask.

We would like to inform you that SciCADE 2021 will take place in Reykjavík, Iceland.

The Local Organising Committee

- Lukas Einkemmer
- Alexander Ostermann (Chair)
- Chiara Piazzola
- Stefan Rainer
- Mirko Residori

Administrative Support

- Judith Courian
- Brigitte Eller

Technical support

- Gernot Baumgartner
- Markus Lechner

The scientific committee

- Weizhu Bao (Singapore)
- Chris Budd (Bath)
- Elena Celledoni (Trondheim)
- Charlie Elliott (Warwick)
- Erwan Faou (Rennes)
- Christian Lubich (Tübingen)
- Robert McLachlan (Massey)
- Alexander Ostermann (Innsbruck, Chair)
- Linda Petzold (UCSB)

Essential information

Venue

The conference will take place in the SoWi building of the University of Innsbruck (Universitätsstraße 15). The building is situated in the centre of the city within walking distance from most of the hotels.
Maps with all relevant information are included in this booklet on pages 12, 13, and 14.

Internet Access

Wi-Fi is available at the university via the "eduroam" network. If you do not have access to this network, please sign in to the "UIBK" network (user: c115135, password: SciCADE2019). If you need help, please contact the conference office.

Online Resources

All conference information can be found at
https://scicade2019.uibk.ac.at
In particular there is a downloadable PDF version of the book of abstracts.

Registration

Registration will take place in the conference office, which is situated between the main entrance and the canteen (SoWi-Lounge), on the right side of the entrance (see location on the map on page 14). Registration will be open on Sunday evening from 5pm to 8pm. On Monday registration will be open from 8am. During the rest of the week the conference office is always open from 8:30am.

Conference Queries

If you have any questions, please do not hesitate to ask

- the student guides on hand all week wearing orange shirts.
- the staff in the conference office in the SoWi building near the main entrance, who will be there every day from 8:30am.
- Alternately, please write an e-mail to:
  scicade2019@uibk.ac.at
  You will get an answer as soon as possible.

Working areas

One of the rooms in the SoWi building, namely room SR 1 (see map on page 14), is reserved as a possible meeting point and work place for everyone who is in need of a quiet space. In addition, there are several places in the foyer where you can work.

Plenary Presentations

9am Monday 22nd July

Hinke M. Osinga
University of Auckland, New Zealand

The art of computing global manifolds

Global manifolds are the backbone of a dynamical system and key to the characterisation of its behaviour. They arise in the classical sense of invariant manifolds associated with saddle-type equilibria or periodic orbits and, more recently, in the form of finite-time invariant manifolds in systems that evolve on multiple time scales. Dynamical systems theory relies heavily on the knowledge of such manifolds, because of the geometric insight that they can offer into how observed behaviour arises. In applications, global manifolds need to be computed and visualised so that quantitative information about the overall system dynamics can be obtained. This requires accurate numerical methods and a precise understanding of how the computations depend on various model parameters. The computation of global manifolds is a serious challenge, but an effort that pays off. This talk will focus on two case studies that represent the most recent developments in this area.

9am Tuesday 23rd July

Alison Marsden
Stanford University, United States of America

Computatonal methods for blood flow simulation and personalized medicine in cardiovascular disease

Cardiovascular disease is the leading cause of death worldwide, with nearly 1 in 4 deaths caused by heart disease alone. In children, congenital heart disease affects 1 in 100 infants, and is the leading cause of infant mortality in the US. Patient-specific modeling based on medical image data increasingly enables personalized medicine and individualized treatment planning in cardiovascular disease patients, providing key links between the mechanical environment and subsequent disease progression. We will discuss recent methodological advances in cardiovascular simulations, including (1) optimization algorithms enabling customized treatments for individual patients, (2) uncertainty quantification tools to compute confidence in simulation predictions, and (3) novel methods for fluid structure interaction with incompressible tissues and wall mechanobiology. Clinical application of these methods will be demonstrated in two applications: 1) coronary bypass graft surgery and the biomechanics of vein graft failure, and 2) prediction of disease progression in pediatric patients with pulmonary hypertension. We will provide an overview of our open source SimVascular project, which makes our tools available to the scientific community (www.simvascular.org). Finally, we will provide an outlook on recent successes and challenges of translating modeling tools to the clinic.

Plenary Presentations

9am Wednesday 24th July

Carsten Gräser
Freie Universität Berlin, Germany

Multiscale modelling of particles in membranes

Due to their rich structure the mathematical modelling of cell membranes is a challenging task. Even the restriction to very few aspects leads to coupled multiscale problems. We discuss the mathematical modelling of membranes with embedded membrane-shaping particles by hybrid approaches. The resulting models combine continuum membrane descriptions with discrete particle descriptions. While hybrid membrane-particle models are well-established in physics, the mathematical and numerical analysis of such models is still in its infancy. The talk will give an overview of recent results on modelling, analysis, and numerical treatment of coupled membrane-particle systems and on current work combining such models with concepts from statistical mechanics and molecular dynamics.

9am Thursday 25th July

Yongyong Cai
Beijing Computational Science Research Center, China, People's Republic of China

Recent advance on numerical methods for oscillatory dispersive PDEs

Highly oscillatory dispersive PDEs, such as Klein-Gordon equation in the non-relativistic limit, Dirac equation in the non-relativistic limit, Schrödinger equation in the semi-classical limit, arise from many different areas, e.g. computational chemistry, plasma physics, quantum mechanics. These oscillatory PDEs usually exhibit solutions with high frequency waves in time and/or in space, and are generally computational expensive. In this talk, we report some recent advances on the numerical methods and analysis for some typical highly oscillatory dispersive PDEs.

Plenary Presentations

4:30pm Thursday 25th July

Katharina Schratz
Karlsruhe Institute of Technology, Germany

Nonlinear Fourier integrators for dispersive equations

A large toolbox of numerical schemes for nonlinear dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever *non-smooth* phenomena enter the scene since the underlying PDEs have very complicated solutions exhibiting high oscillations and loss of regularity. This leads to huge errors, massive computational costs and ultimately provokes the failure of classical schemes. Nevertheless, *non-smooth phenomena* play a fundamental role in modern physical modeling (e.g., blow-up phenomena, turbulences, high frequencies, low dispersion limits, etc.) which makes it an essential task to develop suitable numerical schemes.

In this talk I present a new class of Fourier integrators for the nonlinear Schrödinger and the Korteweg-de Vries equation at low-regularity. The key idea in the construction of the new schemes is to tackle and hardwire the underlying structure of resonances into the numerical discretization. This new approach offers strong geometric structure at low regularity and high oscillations - linking the finite dimensional discretization to powerful existence.

9am Friday 26th July

Ernst Hairer
Université de Genève, Switzerland

Numerics of charged particle dynamics in a magnetic field

Combining the Lorentz force equations with Newton's law gives a second order differential equation in space for the motion of a charged particle in a magnetic field. The most natural and widely used numerical discretization is the Boris algorithm, which is explicit, symmetric, volumen-preserving, and of order 2.

In a first part we discuss geometric properties (long-time behaviour, and in particular near energy conservation) of the Boris algorithm. This is achieved by applying standard backward error analysis. Near energy conservation can be obtained also in situations, where the method is not symplectic.

In a second part we consider the motion of a charged particle in a strong magnetic field. Backward error analysis can no longer be applied, and the accuracy (order 2) breaks down. To improve accuracy we modify the Boris algorithm in the spirit of exponential integrators. Special attention is paid to the approximation of the gyrocenter (guiding center). Theoretical estimates are obtained with the help of the modulated Fourier expansion of the exact and numerical solutions.

This talk is based on joint work with Christian Lubich.

Related publications (2017-2019) can be downloaded from http://www.unige.ch/~hairer/preprints.html

Plenary Presentations

Special Session

12:45pm Friday 26th July

Jonathan Mattingly
Duke University, United States of America

Long time accuracy of some MCMC and Bayesian sampling schemes

I will give an overview of a number of methods used to control longtime averages in various computational algorithms. I will give a high level overview which tries to draw together some common themes as well as highlight the central difficulties. I will complement this by some specific examples from Bayesian sampling where approximations are made to improve computational efficiencies and Markov Chain Monte Carlo where some standard mathematical assumptions are violated by systems of physical interest. If time permits, I will talk about some recent work around sampling in political applications.

5:45pm Tuesday 23rd July

John C. Butcher
University of Auckland, New Zealand

45 years of B-series

In the paper [Hairer, E. and Wanner, G. *Computing* **13** (1974), 1–15], the term "B-series" was introduced. Although the motivation was the analysis of numerical methods for differential equations, the Hopf algebra on which B-series are based, now has wide-ranging applications to various fields, including geometry, quantum field theory and stochastic processes.

In this 45 year anniversary, some of the combinatoric and algebraic structures, on which B-series are built, will be reviewed; together with an introduction to some of the applications to the analysis of numerical methods.

6:15pm Tuesday 23rd July

Gerhard Wanner
Université de Genève, Switzerland

How numerical analysis emerged in Innsbruck

Some twelve years ago, a professor of the University of Graz (the second largest university city in Austria after Vienna) asked me:
"Mr. Wanner, you are from Innsbruck, right? How is it possible — Innsbruck is sooo small — how is it possible that such an important, widely visible, school of numerical analysis emerged there?"
This talk tries to explain, how this was possible.

Talks, Posters and Prizes

Talks

Each mini-symposium or contributed talk must not last longer than 30 minutes, including time for questions. Chairs will be asked to be very strict about timings.

All talks will take place in the SoWi building.

All rooms are equipped with full AV facilities, which are operated from a console on the front lectern. All rooms are also equipped with a Microsoft Windows 10 PC with a PDF reader suitable for beamer presentations, Microsoft Power Point and a media player for basic video playback as well as a web browser. Please bring your presentation on a USB stick and upload it before your session starts.

If you intend to present from your own laptop or Mac, please ensure that you bring adapters. In addition, please bring the files you require for your talk on a USB stick in case there should be any technical issues. Stewards and AV technicians will be available, if you have problems.

Posters

Posters will be on display on Tuesday and Wednesday in the foyer of the SoWi building. There will be a dedicated time for poster presentation on Tuesday from 6:45pm to 8pm. During the poster session assorted drinks will be served.

Prizes

The following prizes will be awarded during SciCADE 2019 in the aula of the SoWi building.

- **Germund Dahlquist Prize:** This prize, established in 1995, is awarded for original contributions to fields associated with Germund Dahlquist, especially the numerical solution of differential equations and numerical methods for scientific computing.
  This award will be announced, and a lecture presented by the winner, on Monday at 4:30pm.

- **New Talent Award:** This prize is awarded to the best paper submitted to the panel, on a topic in a field covered by the SciCADE conference. The recipient must be a graduate student or should have obtained a PhD or equivalent degree within the four calendar years prior to the year of the award.
  This award will be announced, and a lecture presented by the winner, on Tuesday at 4:30pm.

- **Butcher Prize:** The prize, in honour of Prof. John Butcher, is for the best student presentation at SciCADE.
  It will be awarded on Friday before the final plenary presentation of Prof. Jonathan Mattingly at 12:40pm.

Refreshments and Dining

Morning and Afternoon Breaks

Tea, coffee and snacks will be served in the foyer of the SoWi building during morning and afternoon breaks throughout the week.

Monday Evening Welcome Drink at the SoWi Building and Guided Tour

On Monday evening from 5:30pm to 6pm a welcome drink will be served in the foyer of the SoWi building.

At 6pm, following the welcome drink there will be a guided tour through the centre of Innsbruck to give you the opportunity to get to know the city and learn interesting facts. Meeting point will be in front of the SoWi building.

Tuesday Evening Wine Reception and Poster Session

On Tuesday evening at 6:45pm there will be a wine reception and a poster presentation in the foyer of the SoWi building, following the talks given by Prof. Butcher and Prof. Wanner.

Wednesday Evening Conference Dinner

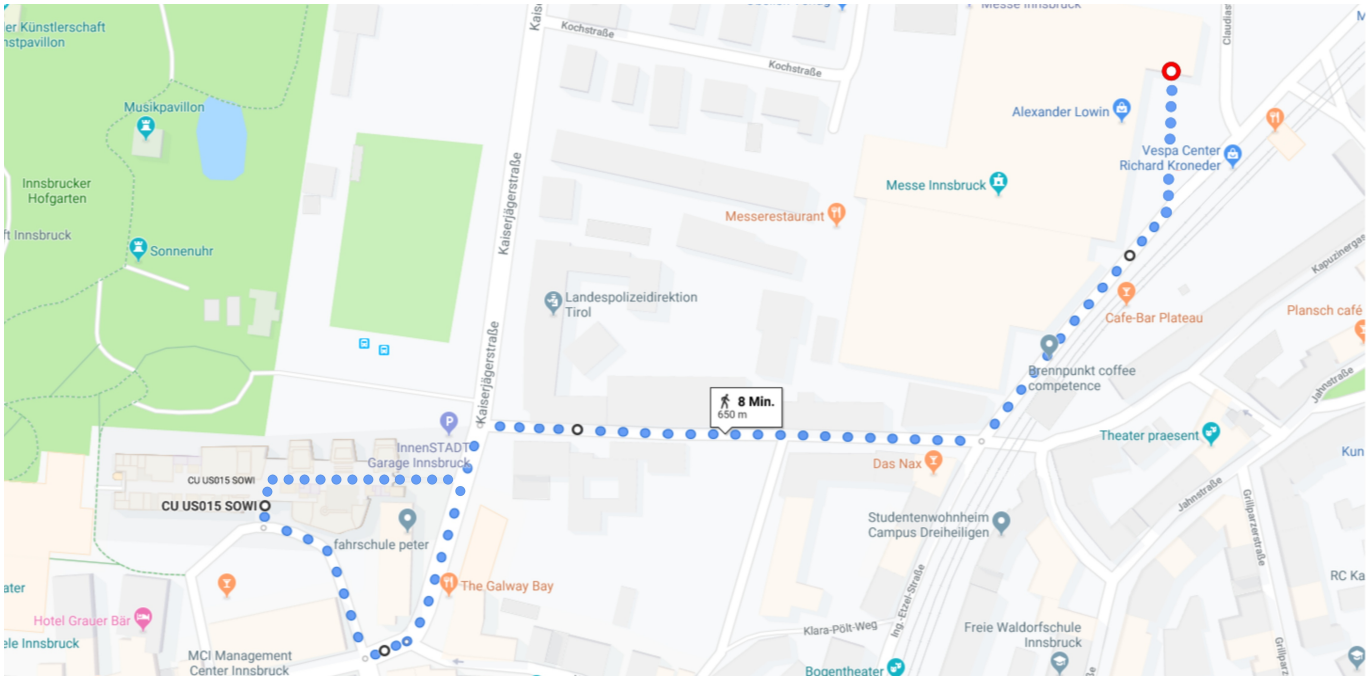
On Wednesday evening at 7pm the conference dinner will take place at the "Messe Innsbruck" (https://www.cmi.at/de/messe-innsbruck.html), Ing.-Etzel-Straße (see map).
Drinks will be served from 7pm with dinner served from 8pm.

Bars and Restaurants

As Innsbruck is a tourist and student city there is a great variety of restaurants available in the city, especially in the near vicinity of the SoWi building.

Please find enclosed a map of various restaurants and bars near the SoWi building, where you can take your lunch.

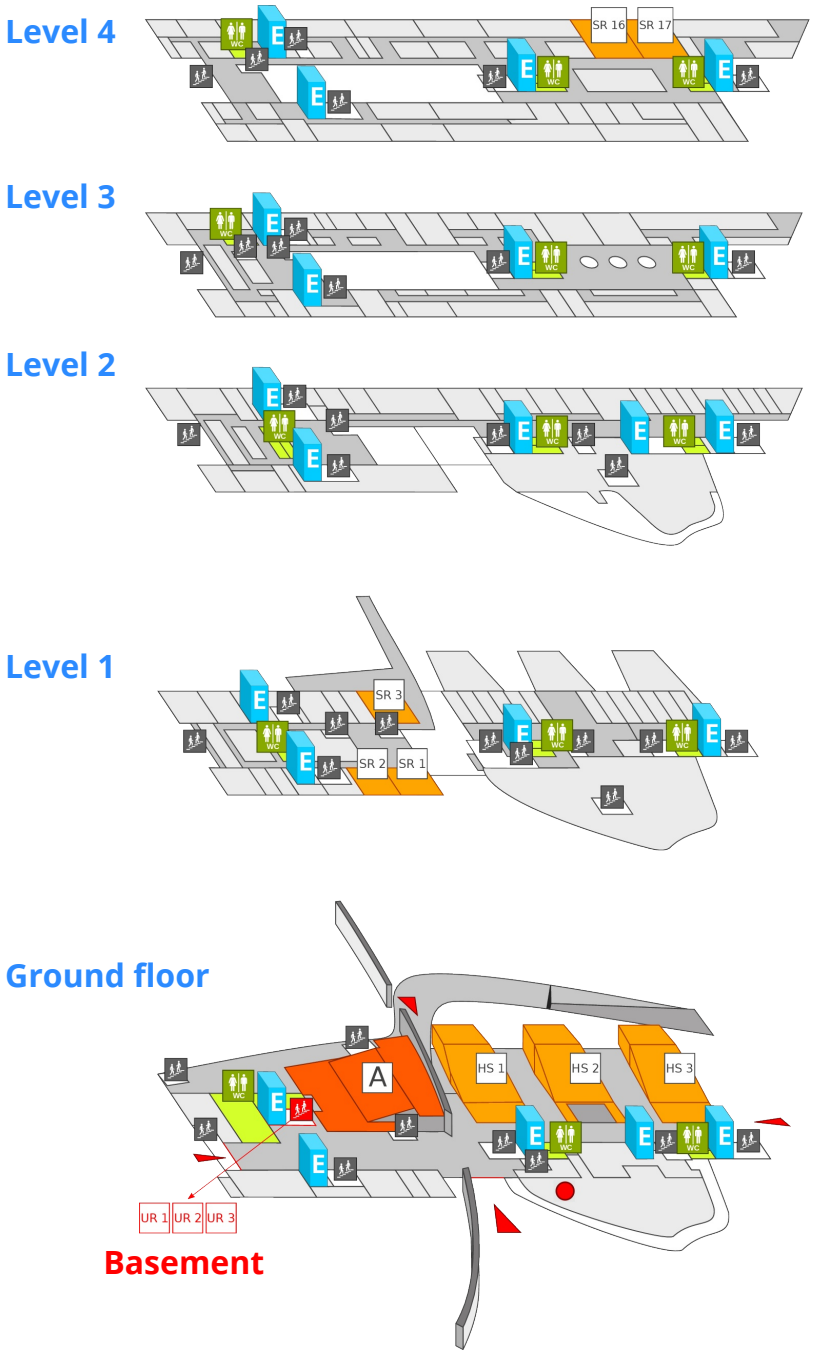
For a comprehensive list of restaurants and places to eat in Innsbruck, please see https://www.innsbruck.info/en/see-and-experience/food-and-drink/restaurant-search.html as well as the city guide included in your conference map.



Exploring Innsbruck

On Wednesday afternoon, there will be the opportunity to explore Innsbruck and its surroundings. Please find detailed information in the two booklets *Walks to explore* and *Innsbruck Card* which you find in your blue conference bag. Relevant information can also be found at https://www.innsbruck.info/
If you have any questions, please feel free to contact the conference office.

Map of the SoWi Building



WC Toilet

Stairway

E Elevator

A Aula

HS Lecture hall

SR Seminar room

UR Classroom

Conference office

Programme

Monday 22nd July 2019

8:00am	**Registration** SoWi building							
8:45am	**Welcome Opening** Alexander Ostermann							
9:00am	**Plenary P1 - Hinke M. Osinga** The art of computing global manifolds							
10:00am	**Coffee Break**							
10:30am	**MS 07: Part 1** Geometry and structure preservation in numerical differential equations	**MS 03: Part 1** Asymptotic preserving schemes for kinetic problems	**MS 14: Part 1** Numerical methods for rare events and applications	**MS 22: Part 1** Optimal control problems with ODEs and DAEs	**MS 27: Part 1** Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers	**MS 28: Part 1** Selected topics in computation and dynamics: machine learning and multiscale methods	**CS 09** Schrödinger equations	**CS 10** Dynamical systems
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
12:30pm	**Lunch**							
2:00pm	**MS 07: Part 2** Geometry and structure preservation in numerical differential equations	**MS 03: Part 2** Asymptotic preserving schemes for kinetic problems	**MS 14: Part 2** Numerical methods for rare events and applications	**MS 22: Part 2** Optimal control problems with ODEs and DAEs	**MS 27: Part 2** Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers	**MS 28: Part 2** Selected topics in computation and dynamics: machine learning and multiscale methods	**CS 02** Plasma physics	**CS 07** Time integration
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
4:00pm	**Coffee Break**							
4:30pm	**Plenary P2** Germund Dahlquist Prize							
5:30pm	**Welcome Drink**							
6:00pm	**Guided Tour**							

Programme

Tuesday 23rd July 2019

9:00am	**Plenary P3 - Alison Marsden** Computational methods for blood flow simulation and personalized medicine in cardiovascular disease								
10:00am	**Coffee Break**								
10:30am	**MS 04: Part 1** Computational methods for quantum dynamic problems	**MS 06: Part 1** Wave problems	**MS 02: Part 1** Energy stable methods for gradient flows and applications	**MS 08: Part 1** Discrete integrable systems and numerical methods	**MS 12: Part 1** Numerical methods for plasma physics	**MS 39: Part 1** Recent developments in multirate and related numerical methods for multiscale problems	**MS 26: Part 1** Numerical approximation of stochastic systems	**CS 11** Boundaries and boundary layers	**CS 15** Partial differential equations
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 2	SR 3	SR 16	SR 17
12:30pm	**Lunch**								
2:00pm	**MS 04: Part 2** Computational methods for quantum dynamic problems	**MS 06: Part 2** Wave problems	**MS 02: Part 2** Energy stable methods for gradient flows and applications	**MS 08: Part 2** Discrete integrable systems and numerical methods	**MS 12: Part 2** Numerical methods for plasma physics	**MS 39: Part 2** Recent developments in multirate and related numerical methods for multiscale problems	**MS 26: Part 2** Numerical approximation of stochastic systems	**CS 08** Exponential integrators	**CS 13** Runge-Kutta methods
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 2	SR 3	SR 16	SR 17
4:00pm	**Coffee Break**								
4:30pm	**Plenary P4** New Talent Award								
5:45pm	**Special Session** **John C. Butcher** 45 years of B-series **Gerhard Wanner** How numerical analysis emerged in Innsbruck								
6:45pm	**Poster Session and Wine Reception**								

Programme

Wednesday 24th July 2019

9:00am	**Plenary P5 - Carsten Gräser** Multiscale modelling of particles in membranes							
10:00am	**Coffee Break**							
10:30am	**MS 10** Surface and geometric PDEs	**MS 13** Algebraic structures for numerical differential equations	**MS 23** Optimality conditions given by differential equations	**MS 34** Models and simulations of cellular systems: from single-cells to population dynamics	**MS 36** Low-rank methods for matrix- and operator-valued differential equations	**MS 37** Simulation and sensitivity analysis of nonsmooth dynamical systems	**CS 03** Wave equations	**CS 05** Monte Carlo, SDEs
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
12:30pm	**Free Afternoon**							
7:00pm	**Conference Dinner**							

Programme

Thursday 25th July 2019

9:00am	**Plenary P6 - Yongyong Cai** Recent advance on numerical methods for oscillatory dispersive PDEs							
10:00am	**Coffee Break**							
10:30am	**MS 01: Part 1** Multiscale methods and analysis for oscillatory PDEs	**MS 21: Part 1** Numerical methods for stochastic (partial) differential equations	**MS 24: Part 1** Theory and computation of nonlinear waves	**MS 29: Part 1** Implicit-explicit methods for differential systems	**MS 30: Part 1** Spectral deferred correction methods for time integration	**MS 32** Numerical methods for pattern formation in PDEs and applications	**CS 04** Maxwell - electro-magnetism	
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	
12:30pm	**Lunch**							
2:00pm	**MS 01: Part 2** Multiscale methods and analysis for oscillatory PDEs	**MS 21: Part 2** Numerical methods for stochastic (partial) differential equations	**MS 24: Part 2** Theory and computation of nonlinear waves	**MS 29: Part 2** Implicit-explicit methods for differential systems	**MS 30: Part 2** Spectral deferred correction methods for time integration		**CS 14** Space dis-cretization	**CS 12** Model order reduction
room	HS 1	HS 2	HS 3	UR 1	UR 3		SR 16	SR 17
4:00pm	**Coffee Break**							
4:30pm	**Plenary P7 - Katharina Schratz** Nonlinear Fourier integrators for dispersive equations							

Programme

Friday 26th July 2019

9:00am	**Plenary P8 - Ernst Hairer** Numerics of charged particle dynamics in a magnetic field							
10:00am	**Coffee Break**							
10:30am	**MS 09** Computational PDEs in cell biology	**MS 25** Rosenbrock-Wanner-type methods: theory and applications	**MS 31** Structural approaches for differential-algebraic systems	**MS 33** Probabilistic numerics for differential equations	**MS 35** Time-integration of partial differential equations	**MS 38** Spatially-adapted time discretizations for PDEs	**CS 01** Monte Carlo methods SDEs	**CS 06** Highly oscillatory problems, symplectic-ity
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
12:40pm	**Butcher Prize**							
12:45pm	**Plenary P9 - Jonathan Mattingly** Long time accuracy of some MCMC and Bayesian sampling schemes							
1:45pm	**Closing**							

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