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CRC 1114 Spring School: Methods for Particle Systems with Multiple Scales

Date: 29 May – 2 June 2017

Venue: WIAS, Mohrenstr. 39, 10117 Berlin

Speakers

Mini courses

Dr. Joep Evers, Dalhousie University Halifax, <http://www.mathstat.dal.ca/~jevers/index.html>

Prof. Dr. Ben Leimkuhler, University of Edinburgh, <https://tinyurl.com/hrq3vgn>

Prof. Dr. Tiejun Li, Peking University, <http://dsec.pku.edu.cn/~tieli/>

Matthias Sachs, University of Edinburgh, <https://tinyurl.com/ztvka3w>

Contributed talks

Prof. Dr. Bettina Keller, CRC 1114, Freie Universität Berlin, <https://tinyurl.com/htsszda>

Dr. Robert Patterson, CRC 1114, WIAS, <https://www.wias-berlin.de/people/patterso/>

Prof. Dr. Sebastian Reich, CRC 1114, University of Potsdam, <http://www.math.uni-potsdam.de/~sreich/>

Program committee

Prof. Dr. Alexander Mielke, CRC 1114, WIAS, <https://www.wias-berlin.de/people/mielke/?lang=0>

Dr. Michiel Renger, CRC 1114, WIAS, <https://www.wias-berlin.de/~renger/>

Preliminary Schedule

Monday 29 May 2017

08.45-09.15	Arrival & registration
09.15-09.30	Welcome and organizational information
09.30-11.00	Lecture Tiejun Li Averaging of the multiscale systems Abstract: In this lecture, I will mainly talk about the averaging of the multiscale systems in time. The averaging idea and the methods for deterministic or stochastic dynamical systems will be introduced, and its application in chemical reaction kinetics will be emphasized.
11.00-11.30	Coffee break
11.30-13.00	Lecture Ben Leimkuhler Molecular dynamics I: motivation, models and numerical methods
13.00-14.15	Lunch break
14.15-15.45	Lecture Tiejun Li Energy landscape and large deviations Abstract: In this lecture, I will talk about the energy landscape concepts for the dynamical systems, which is a hot topic in biophysics in recent years. I will mention its connection with the large deviation theory.
15.45-16.15	Coffee break
16.15-17.45	6 short talks by the PhD students

Tuesday 30 May 2017

- 09.30-11.00 Lecture Joep Evers
Evolution equations for systems driven by social or biological interactions I
- 11.00-11.30 [Coffee break](#)
- 11.30-13.00 Lecture Tiejun Li
Two-scale large deviations for chemical reaction kinetics
Abstract: In this lecture, I will introduce the two-scale large deviations for chemical reaction kinetics. The motivation, results and basic ideas will be mentioned.
- 13.00-14.15 [Lunch break](#)
- 14.15-15.30 Ben Leimkuhler and Matthias Sachs: Exercise ***
- 15.30-19.00 [Outdoor activity](#)

Wednesday 31 May 2017

- 09.30-11.00 Lecture Ben Leimkuhler
Molecular dynamics II: stabilized Langevin integrators for dynamics and sampling
- 11.00-11.30 [Coffee break](#)
- 11.30-13.00 Lecture Joep Evers
Evolution equations for systems driven by social or biological interactions II
- 13.00-14.15 [Lunch break](#)
- 14.15-15.30 Tiejun Li: Exercise ***
- 15.30-16.00 [Coffee break](#)
- 16.00-17.30 6 short talks by the PhD students
- 17.30-19.30 [Get-together with fingerfood and drinks](#)

Thursday 1 June 2017

- 09.30-11.00 Lecture Ben Leimkuhler
Molecular dynamics III: from Brownian dynamics to the generalized Langevin equation
- 11.00-11.30 [Coffee break](#)
- 11.30-13.00 Joep Evers: Exercise ***
- 13.00-14.15 [Lunch break](#)
- 14.15-15.30 Lecture Bettina Keller
Analyzing molecular dynamics simulations - Markov state models and the variational approach to molecular dynamics
- 15.30-16.00 [Coffee break](#)
- 16.00-18.00 CRC 1114 Colloquium at WIAS
Robert Patterson: Stochastic Soot Simulation
Abstract: One major challenge in soot simulations is that the chemical reactivity and measurement response of the soot particles is influenced by structure both on the level of interatomic bonds and on the level of aggregate shape. I will describe a two-part stochastic method, where individual molecules within soot are simulated with the Gillespie SSA and the aggregate structures are simulated separately. Time permitting I will also discuss two strategies for coupling soot simulations to reacting flow calculations. This is joint work with Edward Yapp and Markus Kraft.

Friday 2 June 2017

- 09.30-11.00 Lecture Joep Evers
Evolution equations for systems driven by social or biological interactions III
- 11.00-11.30 [Coffee break](#)
- 11.30-13.00 Lecture Sebastian Reich
Playing games with data: Interacting particle approximations for assimilation of data into dynamical systems
Abstract: I will review recent results on interacting particle systems for estimating the state of a dynamical system using partial and noisy observations. I will start from the ensemble Kalman filter (EnKF) and discuss its generalisation to the continuous-time filtering problems. It will be revealed that the general filtering problem still allows for an interacting particle approximation in the form of a generalised Kalman gain formulation. I will also review recent results on the stability and accuracy of the EnKF and links to optimal transportation.

The lectures and talks take place in the lecture hall on the ground floor (Erhard-Schmidt-Hörsaal).

The exercises (marked with ***) take place in the lecture hall on the 4th floor.

The coffee breaks and the get-together take place in the foyer on the ground floor.