
Funded by DFG

# CRC 1114 Spring School 2017
# Methods for Particle Systems with Multiple Scales

Date: 29 May – 2 June 2017

Venue: WIAS, Mohrenstr. 39, 10117 Berlin

The Spring School 2017 is organized by the CRC 1114 and hosted by WIAS

External support by BMS


## Mini Courses

Joep Evers, Dalhousie University Halifax
Ben Leimkuhler, University of Edinburgh
Tiejun Li, Peking University

## Contributed Talks

Bettina Keller, CRC 1114 / Freie Universität Berlin
Robert Patterson, CRC 1114 / Weierstrass Institute
Sebastian Reich, CRC 1114 / University of Potsdam

## PhD Students' Talks

Luca Donati, CRC 1114 / Freie Universität Berlin
Franziska Erlekam, Zuse Institute Berlin
Thomas Frenzel, Weierstrass Institute
Patrick Gelß, CRC 1114 / Freie Universität Berlin
Gottfried Hastermann, CRC 1114 / Freie Universität Berlin
Markus Mittnenzweig, CRC 1114 / Weierstrass Institute
Jannes Quer, CRC 1114 / Zuse Institute Berlin
Katarzyna Ziółkowska, CRC 1114 / Max Planck Institute of Colloids and Interfaces / Freie Universität Berlin
Wei Zhang, CRC 1114 / Freie Universität Berlin
Johannes Zonker, BMS / Zuse Institute Berlin

## Program Committee and Organisation Team

Alexander Mielke, CRC 1114 / Weierstrass Institute
Michiel Renger, CRC 1114 / Weierstrass Institute
Nina Fabjančič, CRC 1114 / Freie Universität Berlin
Silvia Hoemke, CRC 1114 / Freie Universität Berlin
Lisa Schürmann, CRC 1114 / Freie Universität Berlin

# Mini Courses

Joep Evers, Dalhousie University Halifax

## Evolution Equations for Systems Driven by Social or Biological Interactions

**First Lecture, Tuesday 9.30**

This mini-course consists of three parts. The first part is an introduction to particle- and PDE-based models common in mathematical physics, here applied to social and biological systems; examples are cells, animals, people and vehicles. I will give an overview of several modelling perspectives (microscopic/macroscopic, first-order/second-order) and I will show associated numerics to connect with the aforementioned applications. The subsequent parts build on this introductory lecture.

**Second Lecture, Wednesday 11.30**

In the second part we will consider a one-dimensional, measure-valued transport equation on a bounded domain. The problem setting is inspired by two scenarios: hormone transport inside oblong plant cells, and pedestrian dynamics inside a corridor with an exit of limited capacity at one end. This part is analysis-oriented, aiming at deriving well-defined boundary conditions. Along the way we will get more insight in measure-valued transport equations per se.

**Third Lecture, Friday 9.30**

In the third part we explore spatial pattern formation of two interacting species (inspired by self-organization of cell colonies). We mimic the biology by a simple model seen in the introductory part, which has a natural extension to two species. We investigate the existence and stability of certain steady states, that are compactly supported and have constant density. The stability analysis is based on perturbations of the boundaries of the support. We exploit the connection between particle- and PDE-based models: the analysis is done at the level of the PDE, while we perform numerics using a system of ODEs.

Ben Leimkuhler, University of Edinburgh

## Molecular Dynamics

**First Lecture, Monday 11.30**

I will discuss the goals and purposes of molecular dynamics. I will introduce the Hamiltonian and stochastic dynamics frameworks and discuss the use of splitting methods to integrate the equations of motion. I will show that it is possible to analyze the errors in the invariant distribution of numerical methods.

**Second Lecture, Wednesday 9.30**

I will talk about the design of efficient stochastic algorithms based on changing the formulation of the equations, e.g. holonomic constraints, isokinetic methods, and ensemble preconditioners. In the first part, I will focus on applications in biomolecular modelling, but the last part will be more relevant for statistical computation.

**Third Lecture, Thursday 9.30**

I will show that we can use thermostats to solve a variety of problems including canonical sampling with gentle perturbation of the underlying system and schemes for adaptive Brownian dynamics which also have application in nonequilibrium simulation. I will discuss an application in data science.

**Exercise (together with Matthias Sachs), Tuesday 14.15: From classical molecular dynamics to Markov chain Monte Carlo**

In this practical session participants will work through example programs which demonstrate key concepts from the lectures, such as ergodicity of various thermostat methods and different types of error sources in estimates obtained via sampling using sampling algorithms based on direct discretisation of ergodic stochastic differential equations. We will also discuss the efficiency of these methods in comparison to asymptotically exact Markov chain Monte Carlo methods.

Tiejun Li, Peking University

### Averaging of the Multiscale Systems, Energy Landscape and Large Deviations, Two-Scale Large Deviations for Chemical Reaction Kinetics

**First Lecture, Monday 9.30**

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.

**Second Lecture, Monday 14.15**

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.

**Third Lecture, Tuesday 11.30**

In this lecture, I will introduce the two-scale large deviations for chemical reaction kinetics. The motivation, results and basic ideas will be mentioned.

# Contributed Talks

Bettina Keller, CRC 1114 / Freie Universität Berlin

### Analyzing Molecular Dynamics Simulations – Markov State Models and the Variational Approach to Molecular Dynamics

Abstract tba

Robert Patterson, CRC 1114 / Weierstrass Institute

### Stochastic Soot Simulation

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.

Sebastian Reich, CRC 1114 / University of Potsdam

### Playing Games with Data – Interacting Particle Approximations for Assimilation of Data into Dynamical Systems

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.

# PhD Students' Talks

**Luca Donati, CRC 1114 / Freie Universität Berlin**

## Metadynamics on Path Space

Markov State Models (MSM) is a powerful tool to study the dynamics of a molecular systems. However, the quality of a MSM depends on the sampling of the trajectory. We now propose a new strategy that exploits Metadynamics to explore the energy surface of a system and the Girsanov theorem, to reweigh the MSM built on the trajectory generated by the biased potential.

**Franziska Erlekam, Zuse Institute Berlin**

## Beyond ITC: Measuring Multivalent Ligand-Receptor Binding with kinITC

In contrast to conventional Isothermal Titration Calorimetry (ITC) kinetic ITC (kinITC) not only gains thermodynamic, but also kinetic information from biochemical binding processes. Moreover, kinITC gives insights of reactions consisting of two separate kinetic separate steps such as sequential binding processes. Experimental kinITC measurement data has been compared to the predictions of a mathematical model for bivalent bindings.

**Thomas Frenzel, Weierstrass Institute**

## EDP-convergence for a wiggly energy model

Gradient systems are strongly related to the LDP of many particle systems. EDP-convergence is a notion of convergence for gradient systems inducing a flow. We focus on the analysis and perform the limit passage via EDP-convergence for a wiggly energy model and emphasize the occurrence of a non-quadratic dissipation potential.

**Patrick Gelß, CRC 1114 / Freie Universität Berlin**

## The Tensor-Train Format and its Applications – Modeling and Analysis of Chemical Reaction Networks, Catalytic Processes, Fluid Flows, and Brownian Dynamics

The simulation and analysis of high-dimensional problems is often infeasible due to the curse of dimensionality. In this talk, we demonstrate the potential of tensor decompositions for mitigating this curse when considering highly diverse systems from several application areas. The results show that the tensor-train format enables us to reduce the memory consumption and the computational costs compared to classical approaches significantly.

**Gottfried Hastermann, CRC 1114 / Freie Universität Berlin**

## Motion under Strong Constraining Force, a Short Review

We will review important results concerning the Hamiltonian motion of particles under a strong constraining potential. Furthermore we will illustrate the connection to the „slow manifold" of such systems. Our motivation will be the use of Bayesian, sequential data assimilation methods, which violate the balances (invariants) of such a multi scale motion.

**Markus Mittnenzweig, CRC 1114 / Weierstrass Institute**

## An entropic gradient structure for quantum master equations

The so called Lindblad equations are a special type of quantum master equations and are frequently used to model open quantum systems. We will show that, in the case of detailed balance, all Lindblad equations on a finite-dimensional Hilbert space possess a gradient flow structure with respect to the relative von Neumann entropy. The corresponding Riemannian metric for the density matrices can be viewed as a non-commutative analog of the 2-Wasserstein metric for probability distributions. This is joint work with Alexander Mielke.

**Jannes Quer, CRC 1114 / Zuse Institute Berlin**

## Accelerated Molecular Dynamics: A Convolution Approach

In this talk we are going to present a new idea of enhanced sampling a so called convolution approach. In the convolution approach a family of potentials is create each of them is less metastable. We then sample the quantity of interest is sample in each of those potentials and we reweight or extrapolate to get the original quantity of interest with less computational power.

**Wei Zhang, CRC 1114 / Freie Universität Berlin**

## Statistical Analysis of the First Passage Path Ensemble of Jump Process

The transition mechanism of jump process between two different subsets in state space reveals important dynamical information of the process. In this talk, we study the first passage path ensemble of both discrete-time and continuous-time jump processes on a finite state space. The connections with the transition path theory (TPT) will be discussed. Finally, we also consider some concrete examples in order to illustrate the analysis.

**Johannes Zonker, BMS / Zuse Institute Berlin**

## Agent-based Modeling of Innovation Spreading

I will present a model with interacting agents that move in an energy landscape. This is an example for the application of particle dynamics in the humanities.

# Organizational Information

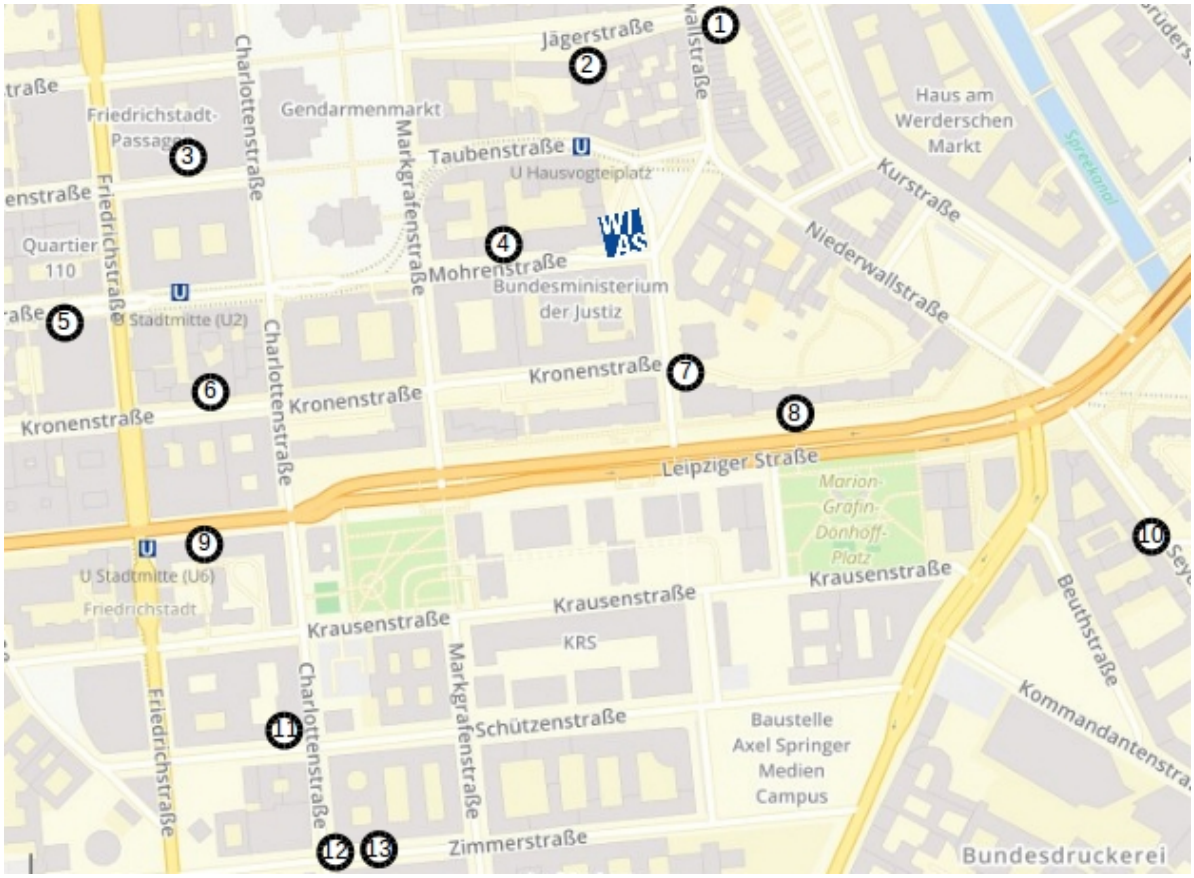
The Spring School takes place at **WIAS, Mohrenstr. 39, 10117 Berlin** (U2 Hausvogteiplatz or U6/U2 Stadtmitte).

The lectures and talks take place in the lecture hall on the ground floor (Erhard-Schmidt-Hörsaal).
The exercises take place in the seminar room 406 on the 4th floor.
The coffee breaks and the get-together take place in the foyer on the ground floor.

Access to the internet through Eduroam WLAN.

In urgent cases during the Spring School you can contact Michiel Renger at 01575-2931814.

## Restaurants and cafeterias near the venue




1. Lunch Time(v) – Pasta
2. Little Green Rabbit(v) – Soups & Salats
3. 2nd floor: Mensa Studentenwerk Musikhochschule(lv) (vegan as well, no mensacard needed)
   3rd floor: Kantine Konzerthaus (no mensacard needed)
4. Chupenga(lv) – Burrito
5. Café 4You(v) – Russian
6. Pasta Deli(lv) – Pasta
7. Bistro Vital(v) – Russian
8. Fontana di Trevi(lv) – Pizza and other Italian dishes (a bit more expensive)
9. Otito(v) – Vietnamese (a bit more expensive)
10. Yesda – Turkish home-made (10m further from the coffee shop with the same name)
11. Rice & Roll(lv) – Asian (vegan as well)
12. Ishin(v) – Japanese (mostly fish, one nice vegetarian dish which is not on the menu)
13. Viet Bowl(v) – Vietnamese (a bit more expensive)

(v) Vegetarian options
(l) Suitable for larger groups

## Outdoor activity

The outdoor activity on Tuesday afternoon – beach volleyball – takes place at **Beach Mitte, Caroline-Michaelis-Str. 8, 10115 Berlin** (about 20 minutes door to door from WIAS, taking the underground line U6 from U-Stadtmitte to U-Naturkundemuseum).

Please bring some sports clothes and flipflops. Sports shoes are not needed, as volleyball is played barefoot on the sand.
There are changing rooms and showers at Beach Mitte, as well as a possibility to buy drinks and snacks.

Afterwards you will be kindly invited to join for dinner and drinks at **Weinerei Forum, Fehrbelliner Str. 57, 10119 Berlin** (U8-Rosenthaler Platz).

Please note that the costs at Beach Mitte and Weinerei are at your own expense.

## Monday 29 May 2017

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|---|---|
| 08.45-09.15 | Arrival & Registration |
| **09.15-09.30** | **Welcome by Alexander Mielke and Organizational Information by Nina Fabjančič** |
| **09.30-11.00** | **Tiejun Li: Averaging of the Multiscale Systems** |
| 11.00-11.30 | Coffee Break |
| **11.30-13.00** | **Ben Leimkuhler: Molecular Dynamics I** |
| 13.00-14.15 | Lunch Break |
| **14.15-15.45** | **Tiejun Li: Energy Landscape and Large Deviations** |
| 15.45-16.15 | Coffee Break |
| **16.15-17.30** | **PhD Students' Talks: Gottfried Hastermann, Wei Zhang, Thomas Frenzel, Markus Mittnenzweig, Jannes Quer** |

## Tuesday 30 May 2017

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|---|---|
| **09.30-11.00** | **Joep Evers: Evolution Equations for Systems Driven by Social or Biological Interactions I** |
| 11.00-11.30 | Coffee Break |
| **11.30-13.00** | **Tiejun Li: Two-Scale Large Deviations for Chemical Reaction Kinetics** |
| 13.00-14.15 | Lunch Break |
| **14.15-15.30** | **Ben Leimkuhler and Matthias Sachs: Exercise (seminar room 406, 4th floor)** |
| **16.30-18.00** | **Outdoor Activity: Beach Volleyball at Beach Mitte, Caroline-Michaelis-Straße 8, 10115 Berlin** |
| **Afterwards** | **Weinerei Forum, Fehrbelliner Straße 57, 10119 Berlin** |

## Wednesday 31 May 2017

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|---|---|
| **09.30-11.00** | **Ben Leimkuhler: Molecular dynamics II** |
| 11.00-11.30 | Coffee Break |
| **11.30-13.00** | **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 (seminar room 406, 4th floor)** |
| 15.30-16.00 | Coffee Break |
| **16.00-17.15** | **PhD Students' Talks: Luca Donati, Franziska Erlekam, Johannes Zonker, Patrick Gelß, Katarzyna Ziółkowska** |
| **17.15-19.00** | **Get-together with finger food and drinks (WIAS foyer)** |

## Thursday 1 June 2017

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|---|---|
| **09.30-11.00** | **Ben Leimkuhler: Molecular Dynamics III** |
| 11.00-11.30 | Coffee Break |
| **11.30-13.00** | **Joep Evers: Exercise (seminar room 406, 4th floor)** |
| 13.00-14.15 | Lunch Break |
| **14.15-15.30** | **Bettina Keller: Analyzing Molecular Dynamics Simulations – Markov State Models and the Variational Approach to Molecular Dynamics** |
| 15.30-16.00 | Coffee Break |
| **16.00-17.30** | **Robert Patterson: Stochastic Soot Simulation (this lecture is part of the CRC 1114 Colloquium)** |

## Friday 2 June 2017

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|---|---|
| **09.30-11.00** | **Joep Evers: Evolution Equations for Systems Driven by Social or Biological Interactions III** |
| 11.00-11.30 | Coffee Break |
| **11.30-13.00** | **Sebastian Reich: Playing Games with Data – Interacting Particle Approximations for Assimilation of Data into Dynamical Systems** |