CRC 1114

funded by DFG

**IRTG of the CRC 1114**

# 3rd PhD workshop

**30 May – 2 June 2016**

Venue: Kurhaus am Inselsee, Güstrow, www.kurhaus-guestrow.de

# Program

## Day 1 – Monday 30th May 2016

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| 08.30 | Meeting at Berlin Hauptbahnhof at the platform of departure (current information: platform 5) |
| 08.45 | Departure to Güstrow (train RE 4354, destination Rostock) |
| 11.00 | Arrival at Güstrow train station, group taxis to venue |
| 12.00-13.00 | Lunch |
| 13.00-13.45 | Check-in |
| 13.45-14.00 | Opening of the workshop |
| 14.00-15.00 | Guest talk by Dr. Walter Acevedo, SFB 1114 / University of Potsdam<br>*Data assimilation applications for state and parameter estimation* |
| 15.00-15.30 | Coffee break |
| 15.30-17.00 | Guest talk by Dr. Guillermo Pérez-Hernández, FU Berlin<br>*Introduction to Molecular Dynamics and its analysis with Markov state models* |
| 17.00-17.45 | Coffee break |
| 17.45-18.45 | Guest talk by Prof. Dr. Alexander Mielke, SFB 1114 / WIAS<br>*Multiscale modeling via evolutionary Gamma convergence* |
| 19.00-20.00 | Dinner |
| 20.00-20.30 | Information on the IRTG program by Dr. Nina Fabjančič |

## Day 2 – Tuesday 31st May 2016

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| 08.00-09.00 | Breakfast |
| 09.00-09.30 | Jannes Quer<br>*Estimating exit rates in rare event dynamical systems via extrapolation* |
| 09.30-10.00 | Katarzyna Ziółkowska<br>*A PhD student's guide to running MD simulations for exploring protein's conformational changes and binding events with Markov State Modeling* |
| 10.00-10.30 | Lara Neureither<br>*Towards understanding timescales in MD* |
| 10.30-11.00 | Coffee break |
| 11.00-11.30 | Irtaza Hassan<br>*Vibrational spectra for probing peptide structure and dynamics* |
| 11.30-12.00 | Hossein Batebi<br>*Theoretical IR Spectroscopy Based on QM/MM Calculations Provides Changes in protonation state, dihedral angles and charge distribution induced by Ala-Leu* |
| 12.00-12.30 | Sandra Döpking<br>*Error-aware analysis of multi-scale reactivity models for photochemical surface reactions* |
| 12.30-14.00 | Lunch |

14.00-15.00 Robert Schulz and Feliks Nüske
*Introduction to Markov state modeling*
15.00-15.30 Luca Donati
*Markov state models with reweighting*
15.30-16.00 Coffee break
16.00-16.30 Robert Schulz
*Markov state modeling for bulk water dynamics*
16.30-17.00 Julian Kappler
*Investigating chain molecules in water using Markov state models*
17.00-17.30 Coffee break
17.30-18.00 Feliks Nüske
*(Variational-) Tensor approaches*
18.00-18.30 Markus Mittnenzweig
*Gradient structures for Lindblad equations satisfying detailed balance*
19.00-20.00 Dinner

## Day 3 – Wednesday 1st June 2016

08.00-09.00 Breakfast
09.00-10.00 Christoph Ritschel and Julian Kappler
*Introduction to fluid dynamics*
10.00-10.30 Christoph Ritschel
*Coupling a stochastic rainfall generator to large scale dynamics*
10.30-11.00 Coffee break
11.00-11.30 Gottfried Hastermann
*Towards an asymptotic preserving integrator for the rotational shallow water equations*
11.30-12.00 Maria Reinhardt
*A balance preserving interpolation scheme for the LETKF*
12.00-13.30 Lunch
13.30-14.00 Joscha Podlesny
*Numerical homogenization of elliptic multiscale problems*
14.00-14.30 Tobias Kies
*Analysis and simulation of a hybrid model for particles in lipid bilayers*
14.30-15.00 Coffee break
15.00-19.30 Outdoor activity
19.30-20.30 Dinner

## Day 4 – Thursday 2nd June 2016

08.00-09.00 Breakfast
09.00-10.00 Guest talk by Prof. Yannis Kevrekidis, Princeton University
*The science of crystal balls*
10.00-10.30 Coffee break
10.30-11.30 Open forum and check-out
11.30-12.30 Lunch
12.30 Departure from the venue by a charter bus, arrival approx. 15.30 at Arnimallee 6, Berlin
16.00-18.00 CRC Colloquium at Arnimallee 6, Room 032
18.00 Get-together at Arnimallee 6, Foyer