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

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
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
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
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

08.00-09.00 Breakfast
09.00-09.30 Jannes Quer
Estimating exit rates in rare event dynamical systems via extrapolation
09.30-10.00 Katarzyna Ziolkowska
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
Towards understanding timescales in MD
10.30-11.00 Coffee break
11.00-11.30 Irtaza Hassan
Vibrational spectra for probing peptide structure and dynamics
11.30-12.00 Hossein Batebi
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
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