

Workshop Program

Monday 19.05.2008

- 07:40 Pick up at Hotels in Jülich
08:00-09:00 Registration
09:00-09:05 Welcome by Prof. Dr. A. Bachem (CEO, FZ Jülich)
09:05-09:15 Introductory Remarks (Ulrich H.E. Hansmann, NIC-CBB)

Morning Session (Chair: Ulrich H.E. Hansmann)

- 09:15-09:45 Christoph Pospiech (IBM, Dresden, Germany):
Scalable Systems for Computational Biology
09:45-10:30 Volkhard Helms (Saarland University, Saarbrücken, Germany):
Computer Simulations of Protein-Protein Association in Water and at
Membranes
10:30-11:00 Coffee break
11:00-11:45 Ruben Abagyan (The Scripps Research Institute, La Jolla, USA):
Induced Fit in Molecular Docking
11:45-12:30 John Rice (IBM T.J. Watson Research Center, Yorktown Heights, NY,
USA):
High Performance Computing in Multiscale Modeling Cardiac Contraction:
Bridging Proteins to Cells to Whole Heart
12:30-14:00 Lunch

Afternoon Session (Chair: Jan Meinke)

- 14:00-14:45 Henri Orland (Commissariat à l'Energie Atomique, Gif-sur-Yvette,
France):
Dominant Pathways in Protein Folding
14:45-15:05 Alexander Schug (University of California San Diego, San Diego,
USA):
Mutations as Trapdoors: The Rop-dimer with two Competing Native
Conformations
15:05-15:25 Nikolay Dokholyan (University of North Carolina at Chapel Hill,
Chapel Hill, USA):
Simplified Approaches to Complex Biological Systems
15:25-15:45 Mai Suan Li (Polish Academy of Sciences, Warsaw, Poland):
New Force Replica Exchange Method and Mechanical Unfolding of
Proteins
15:45-16:15 Coffee break

- 16:15-17:00 Wei Yang (Florida State University, Tallahassee, FL, USA):
Advancing Drug and Protein Binding Affinity Predications via Generalized Ensemble Based Methods
- 17:00-17:20 Iris Antes (Max-Planck-Institut für Informatik, Saarbrücken, Germany):
Protein-ligand Docking Including Protein Flexibility – An Hierarchical Approach
- 17:20-17:40 Slawomir Orłowski (Nicolaus Copernicus University, Torun, Poland):
Computer Modeling of Small Ligands Diffusion in Drosophila Melanogaster Hemoglobin
- 17:40-18:00 Bogdan Lesyng (University of Warsaw, Faculty of Physics, Warsaw, Poland):
Protein-ligand Docking with a Two-scale Receptor Dynamics and a QM/MM Interaction Potential
- 18:00 Welcome Reception and Poster Session
- 20:30 Bus to Hotels in Jülich

Tuesday 20.05.2008

- 08:10 Pickup at Hotels in Jülich

Morning Session (Chair: Olav Zimmermann)

- 09:00-09:45 Andrzej Kolinski (University of Warsaw, Warsaw, Poland):
Multiscale Modeling of Protein and Protein Assemblies
- 09:45-10:05 Shura Hayryan (Academis Sinica, Taipei, Taiwan (ROC)):
Some Aspects of RNA Folding Studied by Lattice Simulations
- 10:05-10:25 Kay Hamacher (TU Darmstadt, Darmstadt, Germany):
Coarse-Grained Molecular Models for High-Throughput and Multi-Scale Functional Investigations
- 10:25-11:00 Coffee break
- 11:00-11:45 Ron Elber (University of Texas at Austin, Austin, USA):
Atomically Detailed Simulations of Kinetics in Molecular Biophysics by Milestoning
- 11:45-12:05 Anton Feenstra (Free University Amsterdam, Amsterdam, The Netherlands):
Predicting Protein Interactions from Functional Specificity using Multi-Relief and Multi-Harmony
- 12:05-12:25 Sebastian Kmiecik (Selvita, Krakow, Poland):
Designing an Automatic Pipeline for Protein Structure Prediction
- 12:25-12:40 Group-Photo
- 12:40-14:00 Lunch

Afternoon Session (Chair: Walter Nadler)

- 14:00-14:45 Wilfred F. van Gunsteren (ETH Zürich, Zürich, Switzerland):
Computer Simulation of Biomolecular Systems: Where Do We Stand?
- 14:45-15:05 Karine Voltz (German Cancer Research Center, Heidelberg, Germany):
A Coarse-grained Model for the Nucleosome
- 15:05-15:25 Maciej Długosz (University of Warsaw, Warsaw, Poland):
Interactions of Aminoglycosidic Antibiotics with the 30S Subunit -
Brownian Dynamics Study
- 15:25-15:45 Junalyn Navarra-Madsen (TWU, Denton, USA):
Coloring the Mu Transpososome
- 15:45-16:15 Coffee break
- 16:15-17:00 Roland Netz (Technical University Munich, München, Germany):
Peptide Adhesion and Friction: Theoretical Approaches
- 17:00-17:20 Rainer Böckmann (Saarland University, Saarbrücken, Germany):
Kinetics, Statistics, and Energetics of Lipid Membrane Electroporation
Studied by Molecular Dynamics Simulations
- 17:20-17:40 Borries Demeler (The University of Texas, Health Science Center at
San Antonio, San Antonio, Texas, USA):
Modeling Conformational and Molecular Weight Heterogeneity with
Analytical Ultracentrifugation Experiments (AUC)
- 17:40-18:00 Wolfgang Fischer (National Yang-Ming University, Taipei, Taiwan):
Short Membrane Proteins from Viruses: Channel-pore Dualism?
- 18:15 Bus to Castle Obbendorf (Hambach) for Dinner
- 18:30 Dinner (Sponsored by IBM Germany)
Greetings by Dr. Sebastian Schmidt, Divisional Director of Research
Centre Jülich
- 22:00 Bus to Hotels in Jülich

Wednesday 21.05.2008

- 8:10 Pickup at Hotels in Jülich

Morning Session (Chair: Sandipan Mohanty)

- 09:00-09:45 Michael Feig (Michigan State University, East Lansing, USA):
Simulating Biomolecules in Cellular Environments
- 09:45-10:05 Giovanni La Penna (National Research Council, Sesto Fiorentino,
Italy):
Modelling the Free Energy of Polypeptides in Different Environments
- 10:05-10:25 Joachim Dzubiella (Technical University Munich, Garching, Germany):
Insights from Atomistic Computer Simulations of Halophilic Proteins
- 10:25-11:00 Coffee break

- 11:00-11:45 Philippe Derreumaux (CNRS and University of Paris 7, Paris, France):
Simulating the Early Steps of Amyloid Fibril Formation and Disassembly
- 11:45-12:05 Alfonso De Simone (University of Cambridge, Cambridge, UK):
Probing the Prion Hydration by Molecular Dynamics Simulations:
From Native via Misfolded to Amyloid Conformations
- 12:05-12:25 Volker Knecht (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany):
Folding and Aggregation of Model Amyloid Peptides in Explicit Solvent and at an Interface
- 12:25-14:00 Lunch

Afternoon Session (Chair: Ulrich H. E. Hansmann)

- 14:00-14:20 Horacio Sanchez (Forschungszentrum Karlsruhe, Eggenstein-Leopoldshafen, Germany):
High Throughput in-silico Screening against Flexible Protein
- 14:20-14:40 Michal Wojciechowski (Polish Academy of Sciences, Warsaw, Poland):
Effects of Confinement on Protein Folding
- 14:40-15:25 Dietmar Schomburg (Technische Universität Braunschweig, Braunschweig, Germany):
Bioinformatics, Metabolomics, and Systems Biology
- 15:25-15:30 Concluding Remarks (Ulrich H. E. Hansmann, NIC-CBB)
- afterwards Bus to Cologne
Social Event: Visit of a Traditional Brewhouse (drinks and food on one's own expense)
- 21:00 Bus to Jülich