

Workshop Program

Wednesday 02.05.2007

- 07:40 Pick up at Hotels in Jülich
08:00-09:00 Registration
09:00-09:20 Welcome by Prof. Dr. A. Bachem (CEO, FZ Jülich)
09:20-09:30 Introductory Remarks (Prof. U. H. E. Hansmann, NIC-CBB)

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

- 09:30-10:15 Harold Scheraga (Cornell University, Ithaca, USA):
Evolution of Protein Simulation
10:15-11:00 Robert B. Russell (EMBL, Heidelberg, Germany):
Pushing Details into the Interactome
11:00-11:30 Coffee break
11:30-12:15 Koichi Takahashi (tMSI, Berkeley, USA):
The E-Cell Project and Challenges in Computational Systems Biology
12:30-14:00 Lunch

Afternoon Session (Chair: Jan H. Meinke)

- 14:00-14:45 Adrian Roitberg (University of Florida, Gainesville, USA):
Mixed Quantum Mechanics/Classical Mechanics Methods for the Study
of Enzymatic Reactions
14:45-15:30 Marek Cieplak (Polish Academy of Sciences, Warsaw, Poland):
Stretching to Understand Proteins
15:30-16:00 Coffee break
16:00-16:30 Bernd Berg (FSU, Tallahassee, USA):
Residual Entropy of Ice I from Multicanonical Simulations
16:30-17:00 Abhinav Verma (FZK, Karlsruhe, Germany):
All-Atom Protein Folding and Structure Prediction in a Transferable
Universal Free-Energy Force-Field
17:00-17:30 Walter Nadler (MTU, Houghton, USA):
Channel Transport and Molecular Motors without Brownian Ratchets
17:30-18:00 Inta Liepina (Latvian Institute of Organic Synthesis, Riga, Latvia):
Multiple Beta-Sheet Molecular Dynamics of Two Abl-SH3 Domain
Peptides
18:00 Welcome Reception and Poster Session
20:00 Open Discussion: Supercomputing and the Physics of Cells
20:00/21:30 Bus to Hotels in Jülich

Thursday 03.05.2007

08:10 Pickup at Hotels in Jülich

Morning Session (Chair: Olav Zimmermann)

- 09:00-09:45 Jeffrey Skolnick (Georgia Institute of Technology, Atlanta, USA):
Prediction of Protein Structure, Function and Druggability on a Proteomic Scale
- 09:45-10:30 Christodoulos Floudas (Princeton University, Princeton, USA):
Advances In De Novo Protein Design
- 10:30-11:00 Coffee break
- 11:00-11:30 Mai Suan Li (Polish Academy of Sciences, Warsaw, Poland):
Mechanism of Fibril Formation of Short Peptides
- 11:30-12:00 Velia Minicozzi (University of Rome "Tor Vergata", Rome, Italy):
The Role of Metals in Misfolding and Aggregation Processes X-ray Spectroscopy and Numerical Simulations
- 12:00-12:30 Wolfhard Janke (University of Leipzig, Leipzig, Germany):
Microcanonical Analyses of Peptide Aggregation Processes
- 12:30-14:00 Lunch

Afternoon Session (Chair: Tatjana Eitrich)

- 14:00-14:45 Rebecca Wade (EML, Heidelberg, Germany):
Bridging from Molecular Simulation to Biochemical Networks
- 14:45-15:30 Adam Liwo (University of Gdansk, Gdansk, Poland):
Mesoscopic Dynamics with the UNRES Force Field – a Tool for Studying the Kinetics and Thermodynamics of Protein Folding
- 15:30-16:00 Coffee break
- 16:00-16:30 Peter Virnau (Johannes Gutenberg-Universität, Mainz, Germany):
Knots in Proteins, DNA and Polymers: Statistics, Function and Evolution
- 16:30-17:00 Siegfried Höfinger (MTU, Houghton, USA):
Comparing Semi-Empirical versus Classic Charge Assignments in BioMolecules and their Effect on Electrostatic Potentials
- 17:00-17:30 Klaas Hellingwerf (University of Amsterdam, Amsterdam, NL):
Photosensory Proteins as Vehicles to Bridge Computational Biophysics and Systems Biology to Initiate the Field of Synthetic Biology
- 17:30-18:00 Léo Degrève (Universidade de São Paulo, Ribeirao Preto, Brazil):
A Molecular Dynamics Study of the Basic Fibroblast Growth Factor – Fibroblast Growth Factor Receptor Complex
- 18:15 Bus to Castle Obbendorf (Hambach) for Dinner
- 18:30 Dinner in Celebration of 20 Years of NIC (sponsored by IBM)
Commemorative Speech by Prof. Dr. Dr. Thomas Lippert, Director of NIC and ZAM
- 22:00 Bus to Hotels in Jülich

Friday 04.05.2007

8:10 Pickup at Hotels in Jülich

Morning Session (Chair: Sandipan Mohanty)

- 09:00-09:45 Dave Thirumalai (University of Maryland, College Park, USA):
Measuring Energy Landscape Parameters of Biomolecules and their
Complexes
- 09:45-10:30 Bogdan Lesyng (Warsaw University, Warsaw, Poland):
Causality and Correlation Analyses of Molecular Dynamics Simulation
Data
- 10:30-11:00 Coffee break
- 11:00-11:30 Nikolay Korolev (Nanyang Technological University, Singapore):
DNA Packaging and Electrostatic Interactions
- 11:30-12:00 Georgios Papadopoulos (University of Thessaly, Larisa, Hellas):
The Zinc-Finger Motif of T.thermophilus Ribosomal Protein S14 and
the Functionality of E.coli Ribosome
- 12:00-12:30 Giovanni La Penna (National Research Council, Florence, Italy):
Anisotropic Internucleosome Interactions and Geometrical Constraints
Favour the Two-Start Helical Structure of Chromatin
- 12:30-13:30 Lunch

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

- 13:30-14:15 José Onuchic (UCSD, La Jolla, USA):
Mechanisms of Protein Assembly and Folding: Lessons from Minimal-
ist Models
- 14:15-15:00 Jörg Langowski (Deutsches Krebsforschungszentrum, Heidelberg, Ger-
many):
Chromatin Dynamics in Silicio
- 15:00-15:05 Concluding Remarks (Prof. Ulrich H. E. Hansmann, NIC-CBB)
- afterwards Bus to Cologne
Social Event: Guided Tour Cologne Cathedral and Treasure Chamber,
Visit of a Traditional Brewhouse
- 21:30 Bus to Jülich