Hünfeld Workshop "Computer Simulation and Theory of Biomolecules"

Preliminary Program

Wednesday, May 23th, 2001

12.00 - 13.30 Arrival, registration, and lunch

13.30 - 15.00 Welcome and sketch of own field of research by group leaders:

13:30 – 13:40 **Volkhard Helms** (MPI für Biophysik, Frankfurt)
Computer Simulation Meets Membrane Biology

13:40 – 13:50 **Jürgen Sühnel** (Institut für Molekulare Biotechnologie, Jena)
Computational analysis of unusal interactions in proteins and nucleic acids-Combining quantum chemistry, molecular dynamics, and structural bioinformatics

13:50 – 14:00 **Rebecca Wade** (European Media Laboratory, Heidelberg)
Exploring protein interactions by modeling and simulation

14:00 – 14:10 **Jeremy C. Smith** (IWR, Universität Heidelberg)
Biomolecular Simulation at the Interdisciplinary Centre for Scientific Computing (IWR), Heidelberg University.

14:10 – 14:20 **Stefan Fischer** (IWR, Universität Heidelberg)
Molecular kinematics

14:20 – 14:30 **Milan Hodoscek** (Freie Universität Berlin)
Overview of the computational methods for proton transfer in biological macromolecular studies.

14:30 – 14:40 **Jörg Langowski** (Division Biophysics of Macromolecules, Heidelberg)
Structure and dynamics of the genome: from superhelical DNA to chromosome territories

14:40 – 14:50 **Jürgen Schlitter** (Ruhr-Universität Bochum)
Conformational changes of macromolecules: a challenge for computer simulation

14:50 – 15:00 **Helmut Grubmüller** (MPI für biophysikalische Chemie, Göttingen)
Moleculardynamics force probe simulations

15:00 – 15:30 Coffee break

15:30 – 15:45 **Peter Winn** (EMBL Heidelberg)
Predicting The Substrate Access Channels and Mechanisms of Four Cytochromes P450

15:45 – 16:00 **Bert de Groot** (MPI für biophysikalische Chemie, Göttingen)
Essential dynamics of reversible peptide folding

16:00 – 16:15 **Rainer Böckmann** (MPI für biophysikalische Chemie, Göttingen)
Energy Transfer in F_1-ATPsynthase and Stability of Secondary Structure Elements

16:15 – 16:30 **Alexander Tournier** (IWR, Universität Heidelberg)
Multiple heatbath methods

16:30 – 17:00 Coffee break

17:00 – 17:15 **Benno Portmann** (Ruhr-Universität Bochum)
First applications of XTMD, a new method for simulating conformational transitions

17:15 – 17:30 **Markus Lill** (MPI für Biophysik, Frankfurt)
QIP-MD, a New Method to Simulate Proton Transport

17:30 – 17:45 **Matthias Müller** (MPI für biophysikalische Chemie, Göttingen)
Predicting Unimolecular Chemical Reactions: Chemical Flooding

18:00 – 19:00 Dinner

19:00 – Discussions and beer: Common interests
Situation of the field in Germany
Future

Thursday, May 24th, 2001

8:00 – 9:00 Breakfast

9:00 – 9:15 **Heinz Sklenar** (Max-Delbrück-Centrum, Berlin)
Conformational Dynamics of Nucleic Acids: Monte Carlo Sampling in the Space of Rigid Body and Sugar Pucker

9:15 – 9:30 **Martin Zacharias** (Institut für Molekulare Biotechnologie, Jena)
Continuum solvent modelling of nucleic acid conformation and ligand binding

9:30 – 9:45 **Bernhard Egwolf** (Universität München)
Continuum Description of Solvents for Molecular Dynamics Simulations

9:45 – 10:00 **Sonja Schwarzl** (IWR, Universität Heidelberg)
Fast and accurate calculation of absolute binding free energies: affinity of benzamidine analogs for trypsin

10:00 – 10:15 Coffee break

10:15 – 10:30 **Volker Knecht** (MPI für biophysikalische Chemie, Göttingen)
Juxtamembrane Region of the t-SNARE Syntaxin-1A: Hinge or Transducer of Mechanical Energy?

10:30 – 10:45 **Dagmar Floeck** (MPI für Biophysik, Frankfurt)
Protein-Protein Docking of Electron Transfer Complexes - Cytochrome c Oxidase and Cytochrome c

10:45 – 11:00 **Christian Kandt** (Ruhr-Universität Bochum)
Long-time simulation of the bR trimer in POPC bilayer/water environment

11:00 – 11:15 **Thomas Renger** (Freie Universität Berlin)
On the Role of Bridge Dynamics in Electron Transfer Reactions: Application to Electron Transfer through the PI-stack of DNA

11:15 – 12:00 Concluding remarks and discussions

12:00 Lunch

13:00 Departure or attend the Biophysical Society meeting