The Centre Européen de Calcul Atomique et Moléculaire and the Theoretical and Computational Biophysics Group present:

Hands-on Workshop in Computational Biophysics

Bremen, Germany

The Program

Hands-on Workshop in Computational Biophysics

Prof. Klaus Schulten

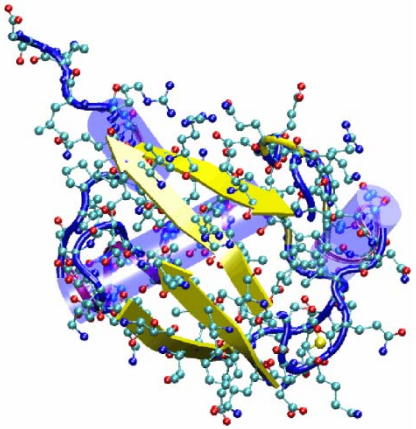
Prof. Emad Tajkhorshid

Location at Jacobs University:

Conference Hall, Campus Center

Mon, 10/17: *Introduction to Protein Structure and Dynamics*

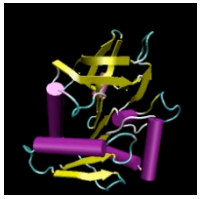
08:00-08:45	Registration
08:45-09:00	Welcome and Brief Overview - Ulrich Kleinekathoefer
09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
Break	
11:00-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
Lunch	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
Break	
16:00-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



Ubiquitin

Tue, 10/18: *Statistical Mechanics of Proteins*

09:00-10:30	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
Break	
10:50-12:00	Exemplary Applications of VMD / NAMD in Modern Research
12:00-12:30	Q & A; Group photo
Lunch	
14:00-16:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials
Break	
16:00-18:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials



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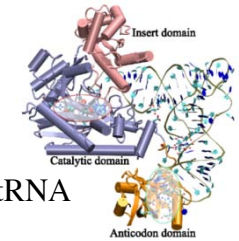
Wed, 10/19: *Introduction to Bioinformatics & Forcefields*

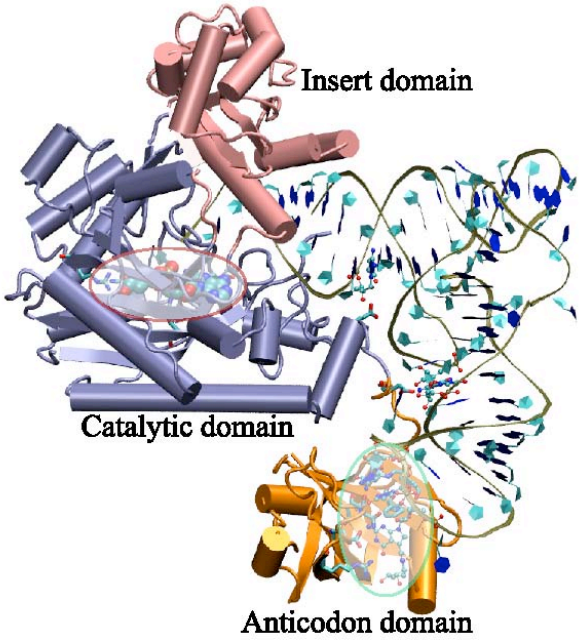
09:00-10:30	Introduction to Structure and Sequence Alignment (K. Schulten)
Break	
10:50-12:00	Introduction to Topology, Parameters, and Structure Files, Part I (E. Tajkhorshid)
12:00-12:20	Daily Q & A
Lunch	
14:00-16:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials; work on own projects
Break	
16:45-18:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials; work on own projects



AspRS-tRNA

Thu, 10/20: *Parameters for Classical Force Fields*

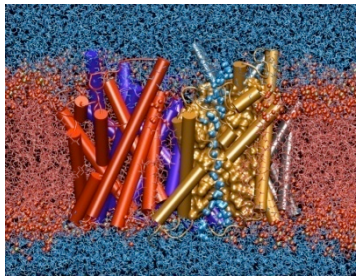
09:00-10:30	Introduction to Topology, Parameters, and Structure Files, Part II
Break	
10:50-12:00	Examples and Applications
12:00-12:20	Q & A
Lunch	
14:00-16:30	Parameterizing a Novel Residue
Break	
16:45-18:00	Topology File Tutorial



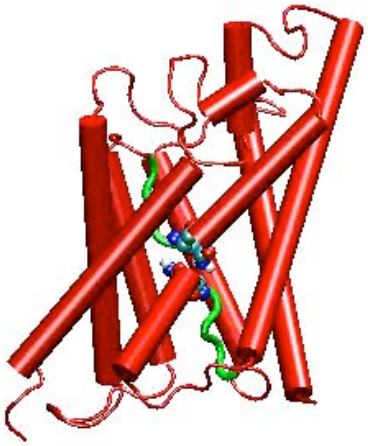
AspRS-tRNA

Fri, 10/21: *Simulating Membrane Channels*

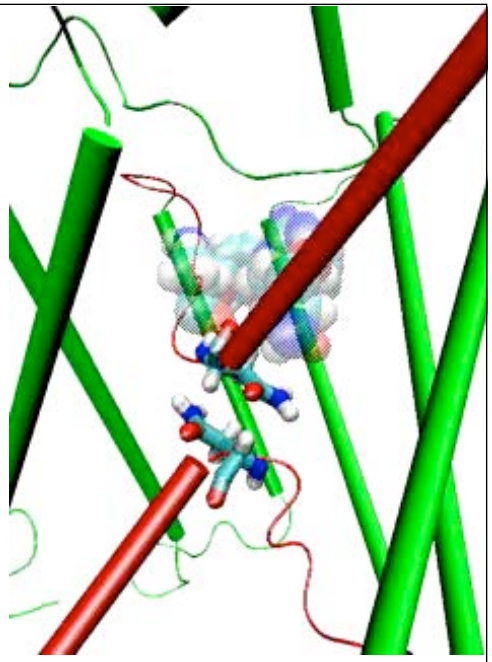
09:00-10:30	Introduction and Examples
Break	
10:50-12:00	Transport in Aquaporins; Nanotubes
12:00-12:20	Daily Q&A
Lunch	
14:00-16:00	Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials
Break	
16:45-18:00	Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials



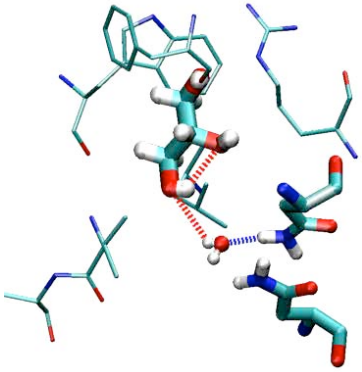
Water Permeation through Aquaporin



General



- The course is a volunteer effort
- The main focus are the hands-on sessions
- The aim is to get you to do computational biology
- The lecturers / teaching assistants provide tutorials for you
- The optimal course is that you help each other



- Model your own system

- Please give us feedback to improve lectures and tutorials
- Please give us feedback to encourage future courses

Work shop Evaluations 2006-2011

Date	Location	No. of Participants	Percentage of Workshop Participants Agreeing with Evaluation Statements: Improved Understanding of Concepts	Improved Ability to Research	Workshop Met My Research Needs
Computational Biophysics Workshops					
October 2011	Bremen	-	-	-	-
May 2011	Pittsburgh	25	100%	100%	94%
March 2011	Atlanta	51	97%	81%	81%
Nov.-Dec. 2010	Urbana	31	91%	74%	91%
November 2010	Urbana	28	100%	96%	100%
July 2010	San Diego	33	100%	78%	88%
May 2010	Pittsburgh	30	100%	100%	n/a
July 2009	Champaign	23	90%	82%	90%
August 2009	Champaign	21	93%	87%	87%
2007-2008 unfunded period[a]					
November 2007	Bethesda	30	93%	93%	93%
November 2006	Talca, Chile	39	83%	92%	96%
November 2006	Pittsburgh	20	n/a	n/a	n/a
In-residence Workshop					
August 2011	Urbana	4	100%	100%	100%
GPU Programming for Molecular Modeling Workshop (Specialty)					
August 2010	Urbana	19	100%	75%	76%
Cluster Building Workshop (Specialty)					
Nov.-Dec. 2006	Urbana	21	94%	94%	76%
Online Workshops on Membranes					
August 2011	Urbana	21	90%	80%	90%
February 2007	Urbana	26	100%	81%	90%

[a]During 2007-2008 the Center did not have workshop funds available.

New Workshop Tutorials, 2006-2011

New Tutorial	Pages	File Size[a]
User-Defined Forces in NAMD	49	4 MB
Alchemical Free Energy Perturbation Calculations in NAMD	39	2 MB
Adaptive Biasing Force Calculations in NAMD	31	38 MB
Evolution of Translation: Class-I aminoacyl-tRNA Synthetases	56	6 MB
Evolution of Translation: EF-Tu	34	284 MB
Evolution of Translation: Ribosome	22	41 MB
Membrane Proteins Tutorial	42	508 MB
Shape-Based Coarse Graining	35	7 MB
Molecular Dynamics Flexible Fitting	31	1 MB
Structure Check	16	720 KB
Residue-Based Coarse Graining using MARTINI Force Field in NAMD	25	125 MB

[a]File size includes material aside from tutorial text, (*e.g.*, pdb files, scripts, trajectory files)

Planned Workshop Tutorials

- *Quantum Mechanical/Molecular Mechanical Simulations using NAMD*
- *Parallel Trajectory Analysis using VMD*
- *Advanced Timeline Tutorial*
- *Hybrid MD-Go Simulation*

Acknowledgements

Teaching Assistants

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