

The Theoretical and Computational Biophysics Group *presents* 'Hands-on' Workshop on Computational Biophysics at Urbana



Urbana, Illinois



The Program

Hands-on Workshop in Computational Biology



Prof. Klaus Schulten



Prof. Zan Luthey-Schulten



Prof. Emad Tajkhorshid

Locations:

Lectures and morning labs:

3269 Beckman

Afternoon labs:

TCBG Innovation
Areas, 3169 and

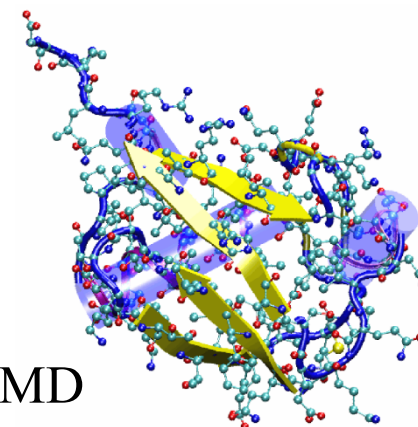
3151 Beckman



Mon, 11/29: *Introduction to Protein Structure and Dynamics*



08:30-09:00	Registration
09:00-10:30	Using VMD; NAMD Tutorial
<i>Break</i>	
10:50-11:00	Opening Remarks
11:00-12:30	Structure and Sequence Analysis with VMD
<i>Lunch</i>	
14:00-15:00	Introduction to Molecular Dynamics with NAMD
15:00-15:20	Q & A
<i>Break</i>	
15:40-18:00	Using VMD; NAMD Tutorial



Ubiquitin

Tue, 11/30: *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

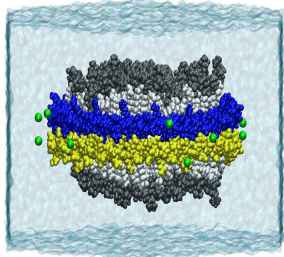
12:00-12:30 Q & A; Group picture

Lunch

14:00-16:00 Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials

Break

16:15-18:00 Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials



HDL

Wed, 12/1: *Introduction to Bioinformatics*



09:00-09:45 Introduction to Evolutionary Concepts in Bioinformatics:
MultiSeq in VMD

09:45-11:00 Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects

Break

11:15-12:00 Introduction to Evolutionary Concepts in Bioinformatics:
MultiSeq in VMD

Lunch

13:30-14:40 Application of MultiSeq to Evolution of Translation Machinery

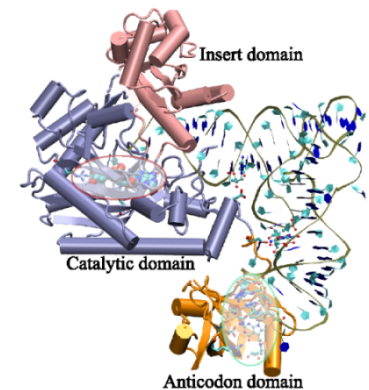
14:40-15:00 Q & A

15:00-16:00 Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects

Break

16:15-18:00 Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects

AspRS-tRNA



Thu, 12/2: *Parameters for Classical Force Fields*



09:00-10:30 Introduction to Topology, Parameters, and Structure Files

Break

10:50-12:00 Examples and Applications

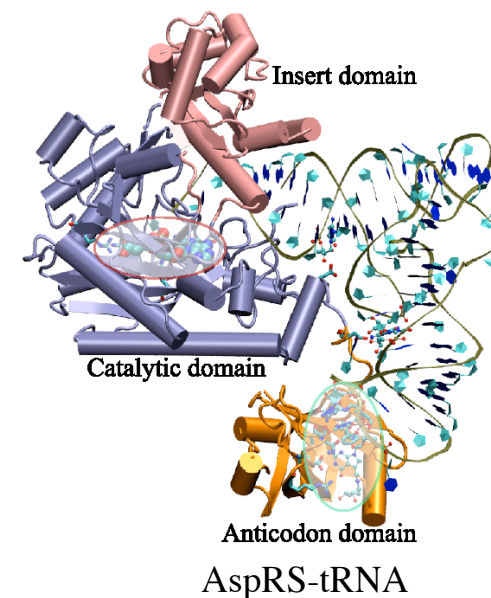
12:00-12:20 Q & A

Lunch

14:00-16:00 Parameterizing a Novel Residue

Break

16:15-18:00 Topology File Tutorial



Fri, 12/3: *Simulating Membrane Channels*



09:00-10:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials

10:00-10:45 Introduction and Examples, Part I

Break

11:00-12:00 Introduction and Examples, Part II

Lunch

13:30-15:00 Transport in Aquaporins; Nanotubes

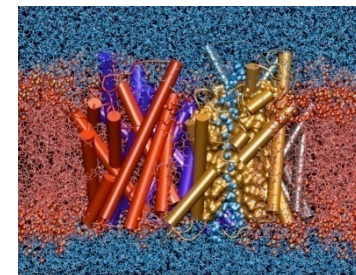
15:00-15:20 Q & A

Break

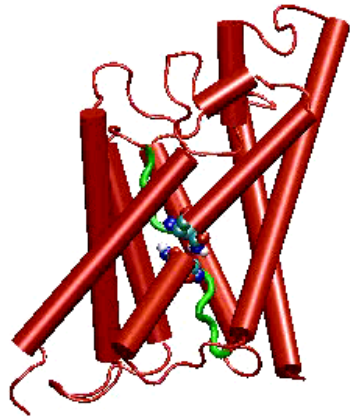
15:40-16:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials

Break

16:15-18:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials

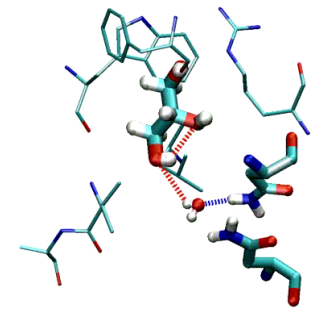
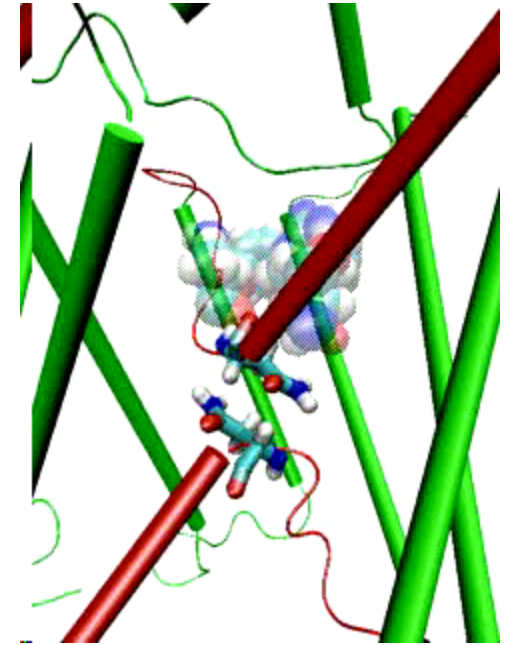


*Water Permeation
through Aquaporin*



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**
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- **Model your own system**
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- **Please give us feedback to improve lectures and tutorials**
 - **Please give us feedback to encourage future courses**



Acknowledgements

Teaching Assistants



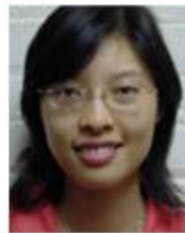
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