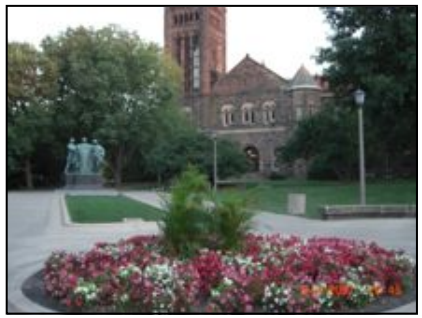
The Theoretical and Computational Biophysics Group

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


Prof. Chris Chipot

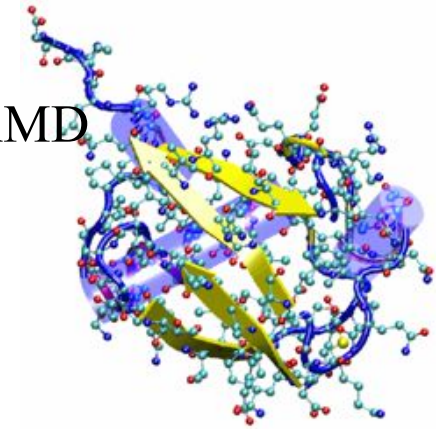
Locations:

Lectures and morning labs: 3269 Beckman

Afternoon labs: TCBG Innovation Areas, 3169 and 3151 Beckman

Mon, 11/1: *Introduction to Protein Structure and Dynamics*

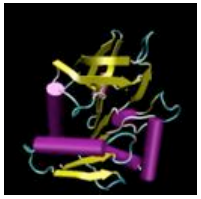
08:30-09:00	Registration
09:00-10:30	Using VMD; NAMD Tutorial
Break	
10:50-11:00	Opening Remarks
11:00-12:30	Structure and Sequence Analysis with VMD
Lunch	
13:30-14:30	Introduction to Molecular Dynamics with NAMD
14:30-14:50	Q & A
14:50-15:40	Using VMD; NAMD Tutorial
Break	
16:00-18:00	Using VMD; NAMD Tutorial



Ubiquitin

Tue, 11/2: *Statistical Mechanics of Proteins*


09:00-10:30	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD – K. Schulten
Break	
10:50-12:20	Good Practices in Free-Energy Calculations - C. Chipot
12:20-12:40	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



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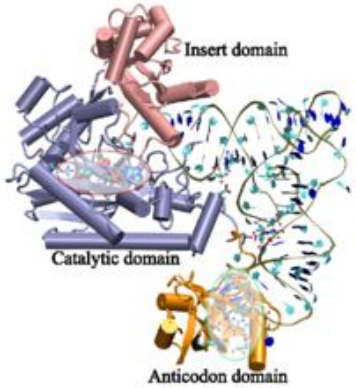
Wed, 11/3: *Introduction to Bioinformatics*

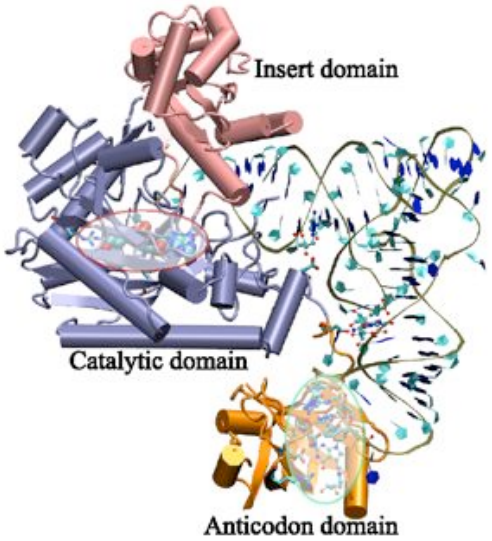
09:00-09:45	Introduction to Evolutionary Concepts in Bioinformatics: MultiSeq in VMD
09:45-11:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects
Break	
11:15-12:00	Introduction to Evolutionary 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, 11/4: *Parameters for Classical Force Fields*

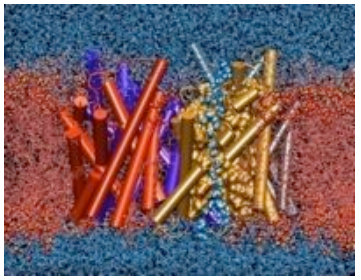
09:00-10:30	Introduction to Topology, Parameters, and Structure Files
Break	
10:50-12:00	Examples and Applications
12:00-12:20	Q & A
Lunch	
14:00-16:00	Parameterizing a Novel Residue
Break	
16:15-18:00	Topology File Tutorial



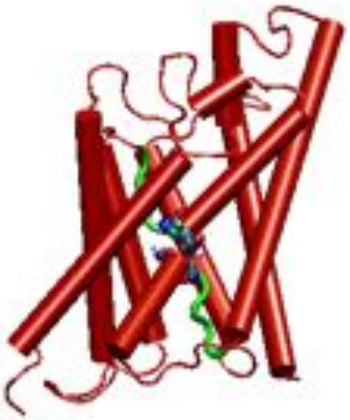
AspRS-tRNA

Fri, 11/5: *Simulating Membrane Channels*

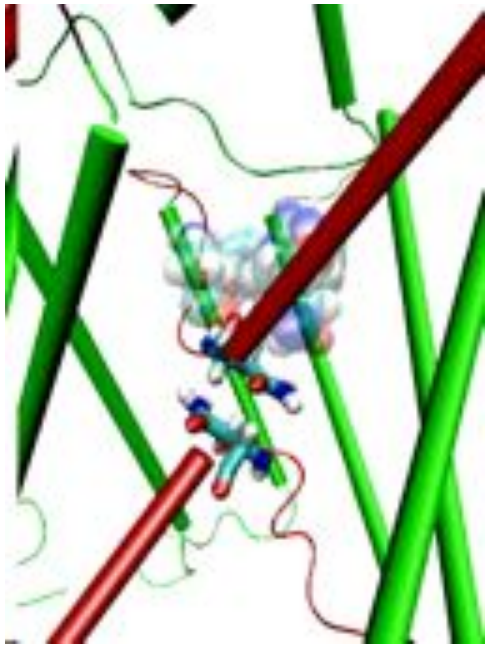
09:00-10:00	Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials
10:00-10:45	Introduction and Examples, Part I
Break	
11:00-12:00	Introduction and Examples, Part II
Lunch	
13:30-15:00	Transport in Aquaporins; Nanotubes
15:00-15:20	Q & A
Break	
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



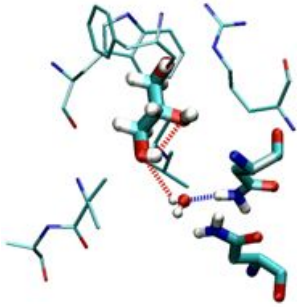
Water Permeation through Aquaporin



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



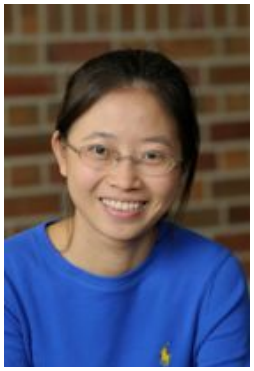
- Model your own system

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

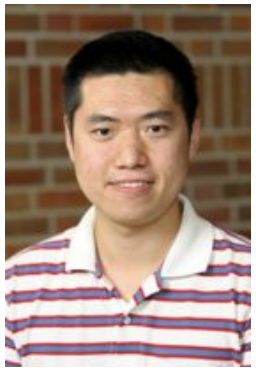
Acknowledgements

Teaching Assistants

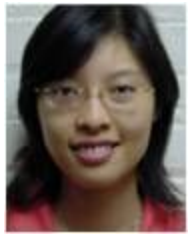
J.C. Gumbart



Xueqing Zou



Hang Yu



Ke Chen