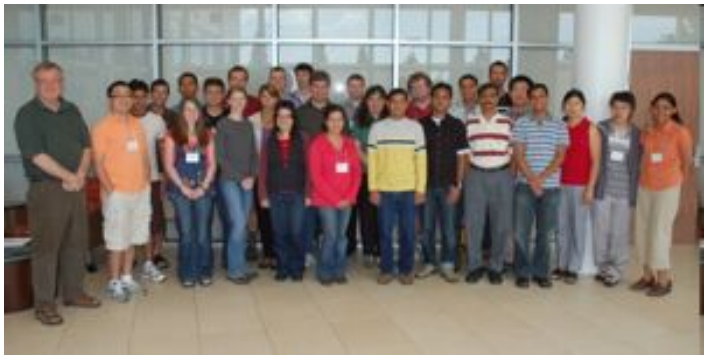
The Theoretical & Computational Biophysics Group

presents

"Hands-on" Workshop on Computational Biophysics



Champaign, Illinois

The Program

Hands-on Workshop in Computational Biology

Prof. Klaus Schulten

Prof. Zan Luthey-Schulten

Prof. Emad Tajkhorshid

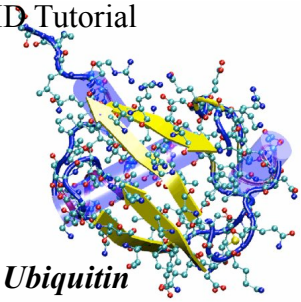
Locations:

Lectures: Technology Room

Labs: Technology Room & Beckman Institute

Mon, 8/10: *Introduction to Protein Structure and Dynamics*

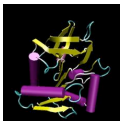
09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
Break	
11:00-12:10	Introduction to Molecular Dynamics with NAMD
12:10-12:30	VMD 1.8.7 - Key features of recent release; John Stone
Lunch	
14:00-15:30	VMD Tutorial - Using VMD; NAMD Tutorial
Break	
16:00-18:00	NAMD Tutorial
Dinner	
20:00-23:00	Open lab time at Beckman Institute



Ubiquitin

Tue, 8/11: *Statistical Mechanics of Proteins*

09:00-10:30	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
Break	
10:50-12:10	Exemplary Applications of VMD / NAMD in Modern Research
12:10-12:30	NAMD 2.7 - Key features of upcoming release; Chris Harrison
Lunch	
14:00-15:00	Research demonstrations at Beckman Institute
15:00-16:00	Tutorial options: NAMD Tutorial; Expert NAMD; Free Energy
Break	
16:15-18:00	Tutorial options: NAMD Tutorial, Expert NAMD, Free Energy
Dinner	
20:00-23:00	Open lab time at Beckman Institute



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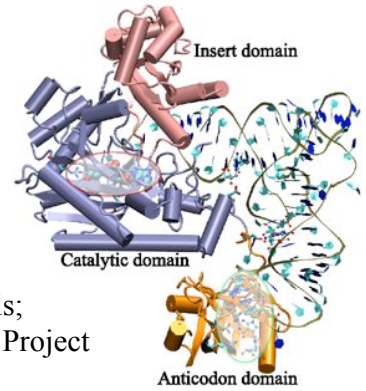
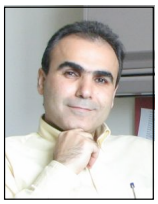
Wed, 8/12: *Introduction to Bioinformatics*

09:00-10:30	Introduction to Evolutionary Concepts in Bioinformatics: MultiSeq in VMD
Break	
10:50-12:00	Application of MultiSeq to Evolution of Translation Machinery
12:00-12:30	Sequence analysis in VMD 1.8.7 - Key features; Kirby Vandivort
Lunch	
14:00-16:00	Tutorial Options: Basic Sequence Analysis; Expert Sequence Analysis; Work on your Project
Break	
16:45-18:00	Tutorial Options: Basic Sequence Analysis; Expert Sequence Analysis; Work on your Project
Dinner	
20:00-23:00	Open lab time at Beckman Institute

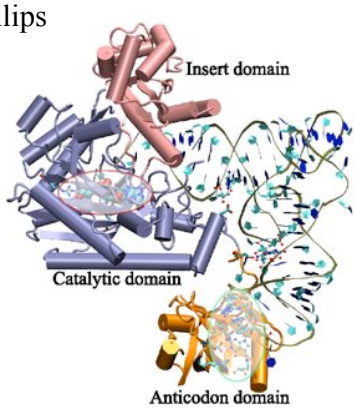


AspRS-tRNA

Thu, 8/13: *Parameters for Classical Force Fields*



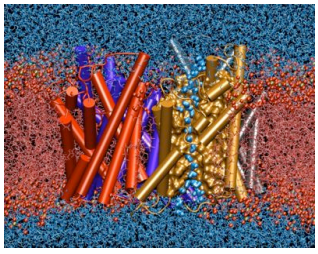
09:00-10:30	Introduction to Topology, Parameters, and Structure Files
Break	
10:50-12:00	Examples and Applications
12:00-12:30	GPU accelerated NAMD 2.7; Jim Phillips
Lunch	
14:00-16:30	Parameterizing a Novel Residue, Topology File Tutorials
Break	
16:45-18:00	Simulation of Water Permeation through Nanotubes
Dinner	
20:00-23:00	Open lab time at Beckman Institute



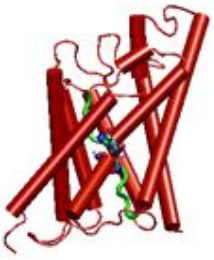
AspRS-tRNA

Fri, 8/14: *Simulating Membrane Channels*

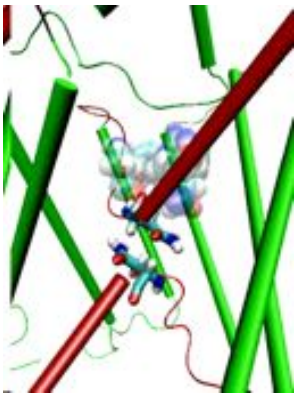
09:00-10:30	Introduction and Examples
Break	
10:50-12:00	Transport in Aquaporins; Nanotubes
12:00-12:30	Highlights of VMD plugins; Robert Brunner
Lunch	
14:00-16:30	Tutorial Options: Membrane Proteins Tutorial; Expert NAMD Set; Free Energy Set
Break	
16:45-18:00	Tutorial Options: Membrane Proteins Tutorial; Expert NAMD Set; Free Energy Set
Dinner	
20:00-23:00	Farewell reception and "Protein Beauty Contest"



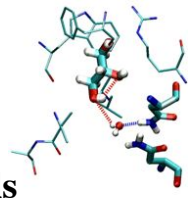
Water Permeation through Aquaporin



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

Staff Lecturers

John Stone
Senior Research
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Chris Harrison
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Jim Phillips
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Programmer

Kirby Vandivort
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