

The Theoretical and Computational Biophysics Group presents:  
*Hands-on Workshop in Computational Biophysics*

Beckman Institute, Urbana, Illinois  
February 11-15, 2012



*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:

3269 Beckman

3169 Beckman

TCBG Innovation

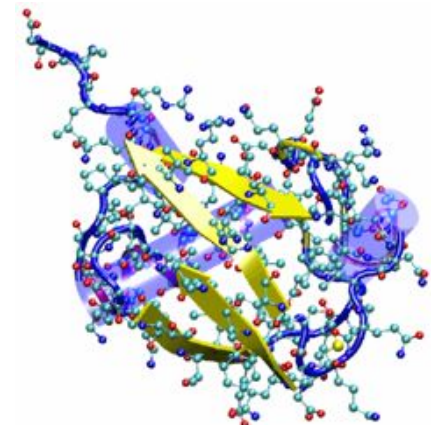
Areas I & II



# Sat, 2/11: *Introduction to Protein Structure and Dynamics*



08:30-09:00	<i>Registration &amp; Continental breakfast</i>
09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
<i>Break</i>	
11:00-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
16:00-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



*Ubiquitin*

# Sun, 2/12: *Statistical Mechanics of Proteins*



08:30-09:00 *Continental breakfast*

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

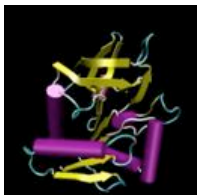
12:00-12:30 Q & A; Group photo

*Lunch*

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

*Break*

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



**HisH**

# Mon, 2/13: *Parameters for Classical Force Fields*



08:30-09:00

*Continental breakfast*

09:00-10:30

Introduction to Topology, Parameters, and Structure Files

*Break*

10:50-12:00

Examples and Applications

12:00-12:20

Daily Q&A

*Lunch*

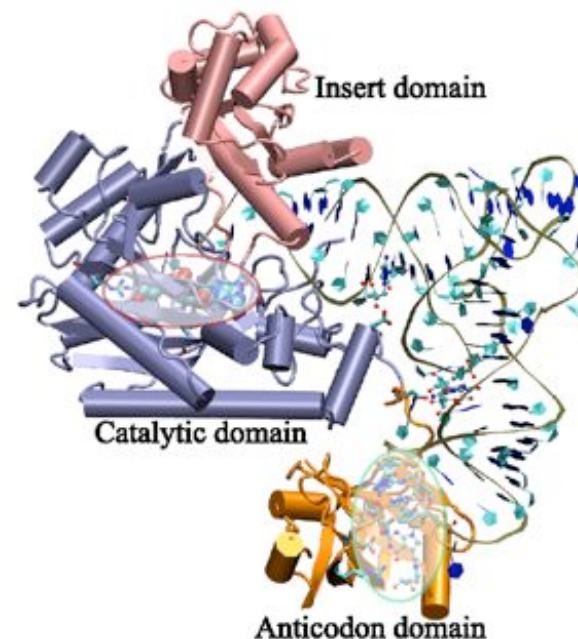
14:00-16:00

Parameterizing a Novel Residue

*Break*

16:15-18:00

Topology File Tutorial



AspRS-tRNA

# Tue, 2/14: *Simulating Membrane Channels*



08:30-09:00

*Continental breakfast*

09:00-10:30

Introduction and Examples

*Break*

10:50-12:00

Transport in Aquaporins; Nanotubes

12:00-12:20

Daily Q&A

*Lunch*

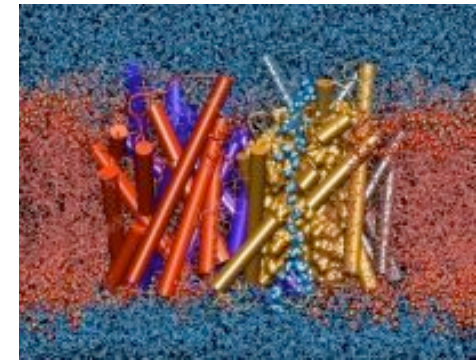
14:00-16:00

Tutorial options: Membrane Proteins & Nanotubes Tutorials;  
Expert NAMD Set Tutorials; Free Energy Set Tutorials

*Break*

16:15-18:00

Tutorial options: Membrane Proteins & Nanotubes Tutorials;  
Expert NAMD Set Tutorials; Free Energy Set Tutorials



*Water Permeation  
through Aquaporin*

# Wed, 2/15: *Introduction to Bioinformatics*



08:30-09:00

*Continental breakfast*

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

12:00-12:20

Daily Q & A

*Lunch*

14:00-16:00

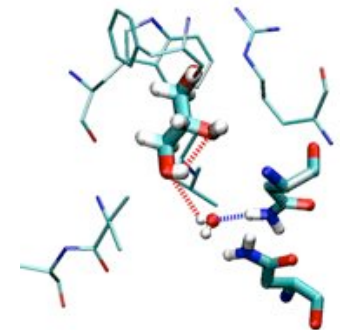
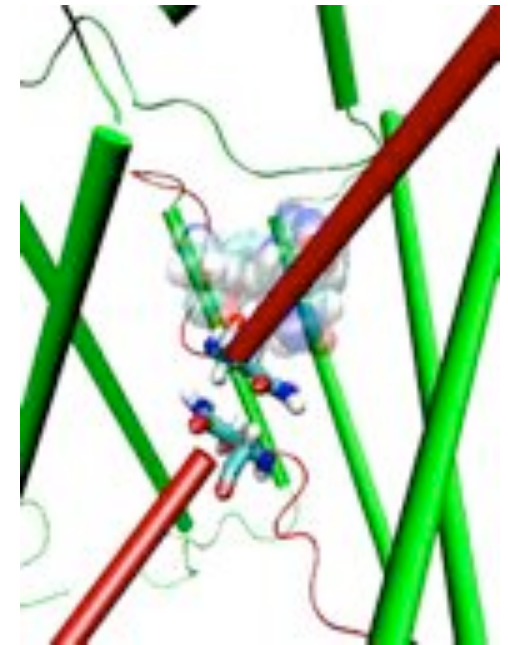
Tutorial options: Basic Sequence Analysis - Aquaporins with VMD;  
NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set  
Tutorials; Free Energy Set Tutorials; work on own projects

*Break*

16:15-18:00

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

# 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*



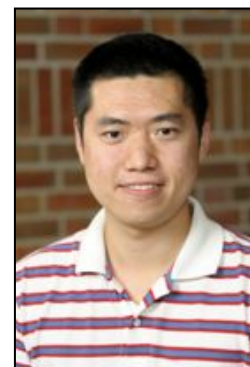
Yanxin Liu



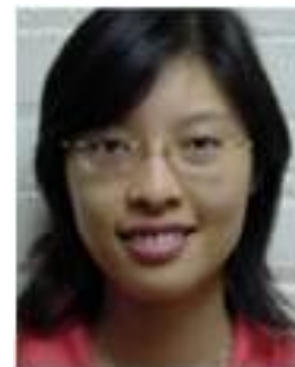
Ross Bodnar



Juan Perilla



Hang Yu



Ke Chen