

The Theoretical and Computational Biophysics Group presents:
Hands-on Workshop in Computational Biophysics
Beckman Institute, Urbana, Illinois
October 22-26, 2012



Urbana, Illinois



The Program

Hands-on Workshop in Computational Biology



Prof. Klaus Schulten



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Locations:

Morning lectures:

Afternoon labs:

Evening lectures:

3269 Beckman

3269 Beckman
TCBG Innovation
Areas I & II

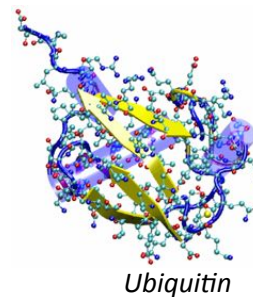
3269 Beckman



Mon, 10/22: *Introduction to Protein Structure and Dynamics*



08:30-09:00	<i>Registration & 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
<i>Dinner</i>	
19:30-21:00	Evening Lectures

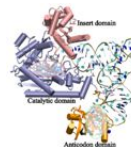


Tue, 10/23: *Introduction to Bioinformatics*



09:00-10:30	Introduction to Evolutionary Concepts in Bioinformatics: MultiSeq in VMD
<i>Break</i>	
10:50-12:00	Application of MultiSeq to Evolution of Translation Machinery
12:00-12:20	Daily Q & A
<i>Lunch</i>	
14:00-16:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis; Dynamical Network Analysis; work on own projects
<i>Break</i>	
16:15-18:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis; Dynamical Network Analysis; work on own projects
<i>Dinner</i>	
19:30-21:30	Evening Lectures

AspRS-tRNA



Wed, 10/24: *Statistical Mechanics of Proteins*

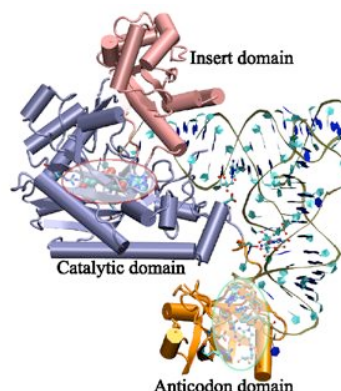


09:00-10:00	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
10:00-10:45	Applications of VMD/NAMD in Modern Research
<i>Break</i>	
11:00-12:00	Introduction to GPU Accelerated NAMD Simulation - K. Schulten, R. McGreevy
12:00-12:30	Q & A; Group photo
<i>Lunch</i>	
14:00-16:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials; GPU Tutorial
<i>Break</i>	
16:15-18:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials; GPU Tutorial
<i>Dinner</i>	
19:30-21:00	Evening Lectures

Thu, 10/25: *Parameters for Classical Force Fields*



09:00-10:30	Introduction to Topology, Parameters, and Structure Files
<i>Break</i>	
10:50-12:00	Examples and Applications
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	Parameterizing a Novel Residue
<i>Break</i>	
16:15-18:00	Topology File Tutorial
<i>Dinner</i>	
19:30-21:00	Evening Lectures



AspRS-tRNA

Fri, 10/26: *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

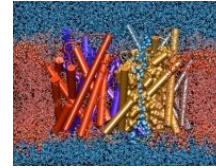
14:00-16:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials

Break

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

Dinner

19:30-21:00 Evening Lectures



Water Permeation through Aquaporin

10/22-26: *Evening Lectures*

Monday, 10/22

PL = Participant Lecture

- VMD from the Developer's Perspective – John Stone
- Computational Investigation of DNA Detection Using Graphene Nanopores - Chaitanya Sathe
- PL: Atomistic Molecular Dynamics Simulation of Poliovirus - Jason Roberts

Tuesday, 10/23

- NAMD from the Developer's Perspective - Jim Phillips
- Molecular Dynamics Simulation of Protein Folding - Yanxin Liu
- PL: Construction, Validation and Testing of a Novel Comprehensive Pharmacophore Model for Anthrax Toxin Lethal Factor Inhibitors - Ting-Lan Chiu
- PL: Modelling Osmotic Stress Effects on Macromolecules - Ajith Rajapaksha

Wednesday, 10/24

- VMD Timeline for Molecular Dynamics Trajectories - Barry Isralewitz
- Membrane Sculpting by F-BAR Domains Studied by Molecular Dynamics Simulations - Hang Yu
- PL: Structural Basis for the Cooperativity between Heterogenous Subunits of Group II Chaperonin - Kai Zhang

10/22-26: *Evening Lectures, continued*

PL = Participant Lecture

Thursday, 10/25

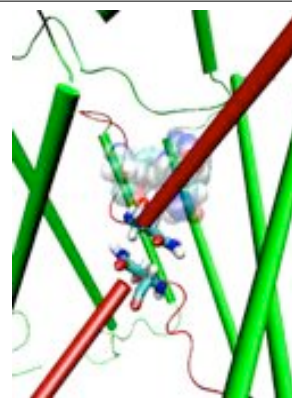
- Molecular Dynamics Flexible Fitting - Ryan McGreevy
- Structural Analyses of the Ribosome by Hybrid Approach - Yan Chan
- PL: Deprotonation of D96 in Bacteriorhodopsin Opens the Proton Uptake Pathway - Ting Wang

Friday, 10/26

- PL: Applying the Stochastic Liouville Equation to Light-Harvesting Complexes - Albrecht Goez
- PL: The Effect of Hydroxyl Groups on Thermodynamics of Ligand-Protein Binding for the Phenyl based Ligands - Oleg Starovoytov
- PL: Computational Studies of Sodium Dodecyl Sulfate - Anne Laustsen
- PL: Nanoparticle Transport in Confining Environments - Thiruvillamalai S. Mahadevan



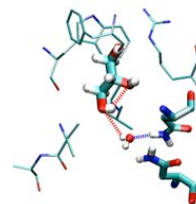
General



- **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



Rafael Bernardi



Rezvan Shahoei



Hang Yu



Ivan Teo



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Giray Enkavi



Joshua Vermaas



Zhijuan Huang



Jing Li



Mohamad Kalani



Jonathan Lai