

The Theoretical and Computational Biophysics Group presents:
Hands-on Workshop in Computational Biophysics
Beckman Institute, Urbana, Illinois
April 6-10, 2015



Urbana, Illinois



The Program

Hands-on Workshop in Computational Biology



Prof. Klaus Schulten



Prof. Emad Tajkhorshid



Prof. Zan Luthey-Schulten



Prof. Alek Aksimentiev



Prof. Chris Chipot

Locations:

Morning lectures:

Afternoon labs:

3269 Beckman

3269 Beckman

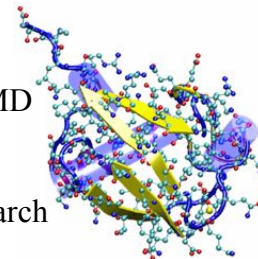
TCBG Innovation
Areas I & II



Mon, 04/06: *Introduction to Protein Structure and Dynamics*



08:00-08:30	<i>Registration & Coffee</i>
08:30-09:00	Welcome, Overview, and Opening Remarks
09:00-10:30	Introduction to Molecular Dynamics with NAMD
<i>Break</i>	
10:50-12:00	Applications of VMD/NAMD to Modern Research
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
16:15-18:00	VMD Tutorial - Using VMD; NAMD Tutorial; Movies & Images

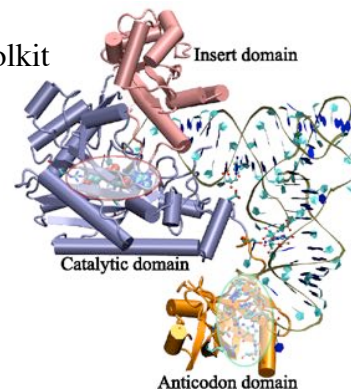


Ubiquitin

Tue, 04/07: *Force Field Parameterization*



08:30-09:00	<i>Coffee Break</i>
09:00-10:30	Introduction to Topology, Parameters, and Structure Files
<i>Break</i>	
10:50-12:00	Examples & Applications; Force Field Toolkit
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	Parameterizing a Novel Residue; ffTk
<i>Break</i>	
16:15-18:00	Topology File Tutorial



AspRS-tRNA

Wed, 04/08: *Introduction to Bioinformatics and Cell Simulations*

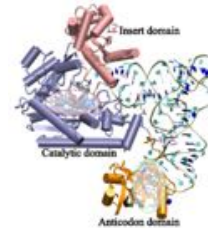


08:30-09:00

Coffee Break

09:00-10:30

Applications of Evolutionary Concepts and Network Analysis in VMD



AspRS-tRNA

Break

10:50-12:00

Introduction to Simulations of Whole Cells

12:00-12:30

Q & A; *Group Picture*

Lunch

14:00-16:00

Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis

Break

16:15-18:00

Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis; Lattice Microbe Simulations

Thu, 04/09: *Computational Nano-Bio*



08:30-09:00

Coffee Break

09:00-10:30

Introduction to Modeling and Simulations of Nucleic Acid Systems

Break

10:50-12:00

Modeling the Interface Between Biological and Synthetic Materials

12:00-12:20

Q & A

Lunch

14:00-16:00

Bionanotechnology Tutorial; User-Defined Forces in NAMD; Simulation of Water Permeation through Nanotube; Electrostatic Maps; Introduction to MD Simulation of DNA-protein Systems

Break

16:15-18:00

Bionanotechnology Tutorial; User-Defined Forces in NAMD; Simulation of Water Permeation through Nanotube; Electrostatic Maps; Introduction to MD Simulation of DNA-protein Systems



Bellflower pentamer

Fri, 04/10: *Free Energy Calculations*



08:30-09:00 *Coffee Break*

09:00-10:30 Introduction to Free Energy Calculations I

Break

10:50-12:00 Introduction to Free Energy Calculations II

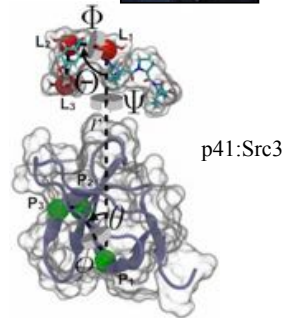
12:00-12:20 Q & A

Lunch

14:00-16:00 Adaptive Biasing Force Tutorial; In Silico Alchemy Tutorial; Protein-Ligand Binding Tutorial; Stretching Deca-Alanine

Break

16:15-18:00 Adaptive Biasing Force Tutorial; In Silico Alchemy Tutorial; Protein-Ligand Binding Tutorial; Stretching Deca-Alanine

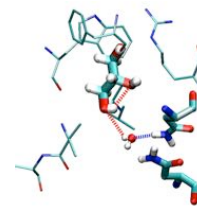
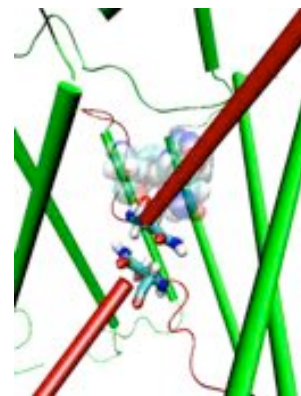


General

- 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

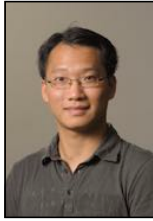


Acknowledgements

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Mike Hallock



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