NAMD Workshop on Computational Biophysics

The Theoretical and Computational Biophysics Group

presents

‘Hands-on’ Workshop on Computational Biophysics at Atlanta

Atlanta, Georgia

The Program

Hands-on Workshop in Computational Biology

Prof. Klaus Schulten

Prof. Zan Luthey-Schulten

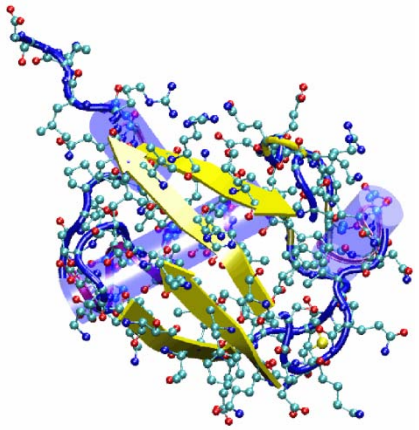
Prof. Emad Tajkhorshid

Locations:

Lectures and labs: Conference Room 102
Pettit Building

Mon, 3/21: *Introduction to Protein Structure and Dynamics*

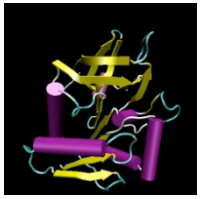
08:00-08:30	Registration
08:30-08:40	Opening Remarks, S. Harvey, K. Schulten
08:40-10:10	Introduction to Molecular Dynamics with VMD & NAMD, K. Schulten
Break	
10:30-12:00	From Molecules to Cells – Whole Cell Simulations, J. Skolnick
12:00-12:20	Q & A
Lunch	
13:20-15:00	VMD Tutorial - Using VMD; NAMD Tutorial
Break	
15:20-17:00	Using VMD; NAMD Tutorial



Ubiquitin

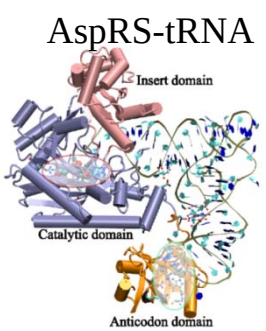
Tue, 3/22: *Statistical Mechanics of Proteins*

08:30-10:00	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
Break	
10:20-11:50	Exemplary Applications of VMD / NAMD in Modern Research
11:50-12:10	Q & A; Group picture
Lunch	
13:10-15:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials
Break	
15:20-17:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials



HisH

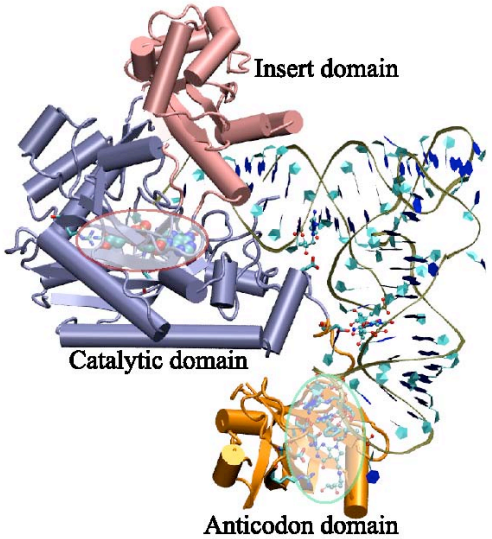
Wed, 3/23: *Introduction to Bioinformatics*



08:30-10:00	Introduction to Evolutionary Concepts in Bioinformatics: MultiSeq in VMD
Break	
10:20-11:40	Application of MultiSeq to Evolution of Translation Machinery
11:40-12:00	Q & A
Lunch	
13:00-15:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects
Break	
15:20-17:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Expert Sequence Analysis - Evolution of Translation – tRNA, Ribosome, EF-Tu; Work on own projects

Thu, 3/24: *Parameters for Classical Force Fields*

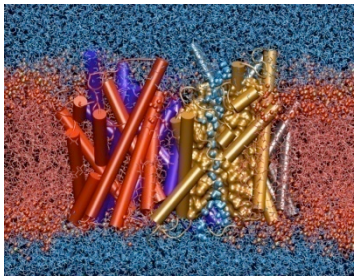
08:30-10:00	Introduction to Topology, Parameters, and Structure Files
Break	
10:20-11:40	Examples and Applications
11:40-12:00	Q & A
Lunch	
13:00-15:00	Parameterizing a Novel Residue
Break	
15:20-17:00	Topology File Tutorial



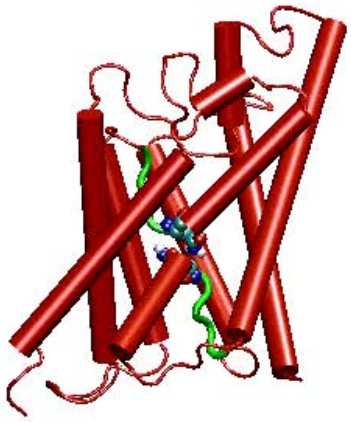
AspRS-tRNA

Fri, 3/25: *Simulating Membrane Channels*

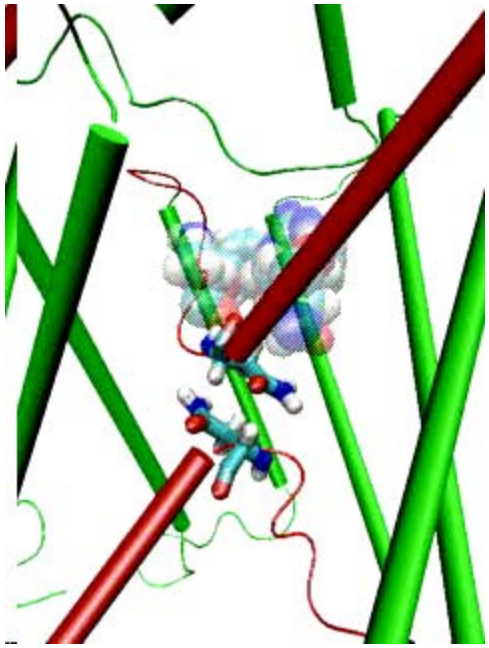
08:30-10:00	Modeling and Molecular Dynamics of Cellular Processes
Break	
10:20-11:40	Nanotubes
11:40-12:00	Q & A
Lunch	
13:00-15:00	Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials
Break	
15:20-17:00	Tutorial options: Membrane Proteins & Nanotubes Tutorials; Expert NAMD Set Tutorials; Free Energy Set Tutorials



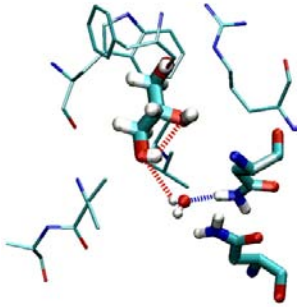
Water Permeation through Aquaporin



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**

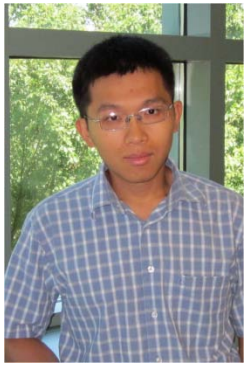
- **Please give us feedback to improve lectures and tutorials**
- **Please give us feedback to encourage future courses**

Acknowledgements

Guest Lecturer

Jeffrey Skolnick

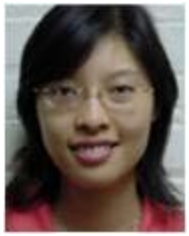
Teaching Assistants



Ivan Teo

Mark Arcario

Ramya Gamini



Ke Chen

Special Thanks

Steve Harvey

Sponsoring Groups

Integrative BioSystems Institute at Georgia Tech
Institute for Data and High Performance Computing at Georgia Tech
Parker H. Petit Institute for Bioengineering and Bioscience at Georgia Tech
National Institutes of Health – National Center for Research Resources
(NIH P41-RR005969 Resource for Macromolecular Modeling and Bioinformatics)