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. Emad Tajkhorshid

Prof. Zan Luthey-Schulten

Location in iHotel:

Lectures: Technology Room

Labs: Technology Room

Teaching Assistants


Jen Hsin


Danielle Chandler


Yanxin Liu


Yan Chan


J.C. Gumbart


Damien Mathew


Eduardo Cruz-Chu


Ramya Gemini


David Tanner

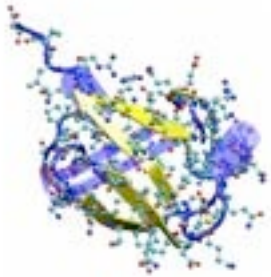

Fatemeh Khalili Araghi


John Eargle


Ke Chen

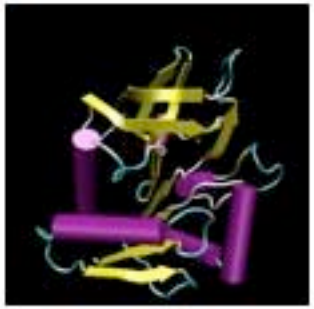
Mon, 7/06: *Introduction to Protein Structure and Dynamics*

09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
Break	
11:00-12:10	VMD for Structure Building and Dynamics Analysis
12:10-12:30	Q & A
Lunch	
14:00-15:30	VMD Tutorial I
Break	
16:00-18:00	VMD Tutorial II


Ubiquitin

Tue, 7/07: *Statistical Mechanics of Proteins*

09:00-10:30	Molecular Dynamics with NAMD I
Break	
10:50-12:10	Molecular Dynamics with NAMD II
12:10-12:30	Q&A Group photo
Lunch	
14:00-16:00	NAMD Tutorial I
Break	
16:15-18:00	NAMD Tutorial II



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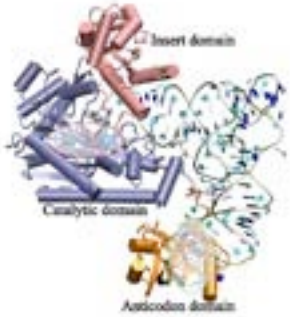
Wed, 7/08: *Parameters for Classical Force Fields*

09:00-10:30	Introduction to Topology, Parameters, and Structure Files
Break	
10:50-12:10	Examples and Applications
12:10-12:30	Q & A
Lunch	
14:00-16:30	Parameterizing a Novel Residue, Topology File Tutorials
Break	
16:45-18:00	Stretching Deca-alanine Tutorial

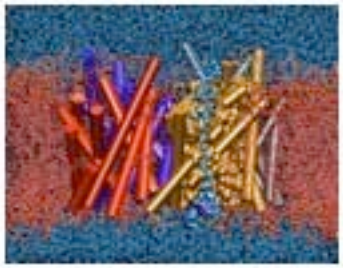


AspRS-tRNA

Thu, 7/09: *Simulating Membrane Channels*

09:00-10:30	Introduction and Examples
Break	
10:50-12:10	Transport in Aquaporins; Nanotubes
12:10-12:30	Daily Q&A
Lunch	
14:00-16:30	Membrane Proteins Tutorial
Break	
16:45-18:00	Nanotubes/IMD

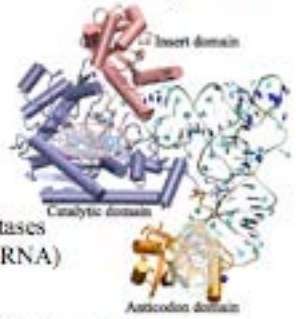
Water Permeation through Aquaporin



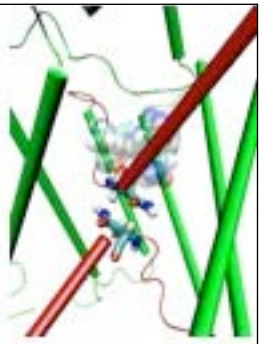
Fri, 7/10: *Introduction to Bioinformatics*

09:00-10:30	Introduction to Evolutionary Concepts in Bioinformatics: MultiSeq in VMD
Break	
10:50-12:10	Application of MultiSeq to Evolution of Translation Machinery
12:10-12:30	Daily Q & A
Lunch	
14:00-16:00	Evolution of Translation Tutorials I & II: Class I Aminoacyl-tRNA Synthetases and the Elongation Factor Tu (EF-Tu:tRNA)
Break	
16:45-18:00	Evolution of Translation Tutorial III: tRNA and the Ribosome, or Bioinformatics Study of Aquaporins

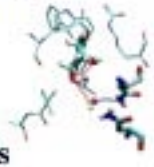
AspRS-tRNA



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