The TCBG & the University of Pittsburgh Department of Structural Biology present: Hands-on Workshop in Computational Biology

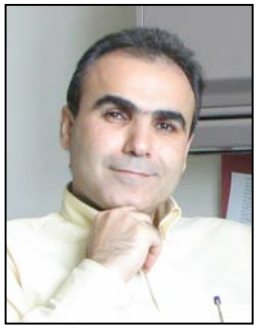
Pittsburgh, Pennsylvania

The Program

Hands-on Course in Computational Biology

Prof. Klaus Schulten

Prof. Zan Luthey-Schulten



Prof. Emad Tajkhorshid

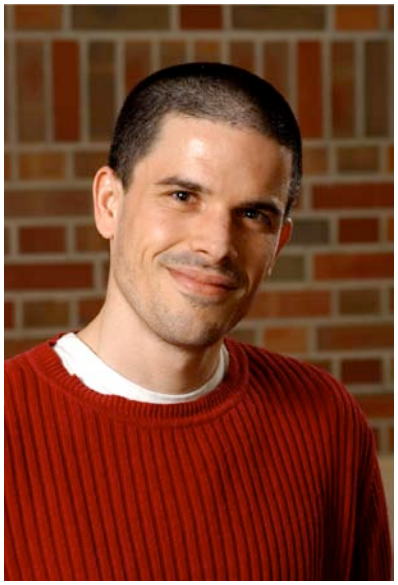
Locations in Biomedical Science Tower 3:

Lectures: Room 1018

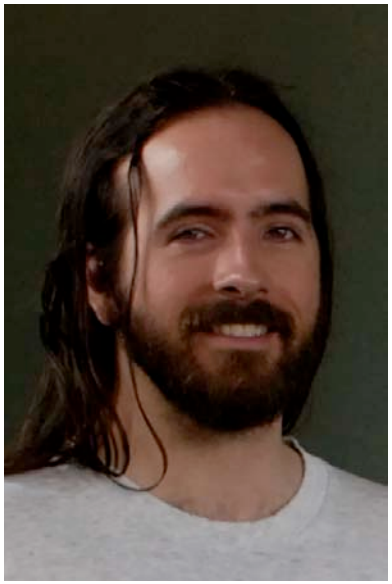
Labs: Suite 1047 (Rooms 1048, 1949)

Breaks: Outside Room 1018

Teaching Assistants



Markus Dittrich



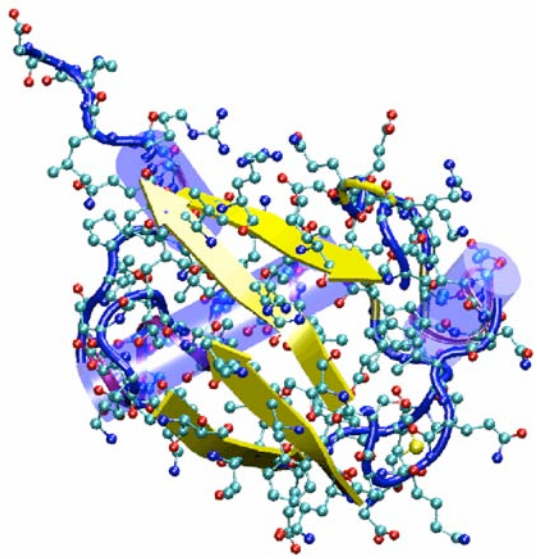
John Eargle

J.C. Gumbart

at PSC!

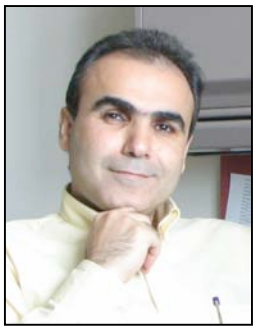
Mon, 11/6: *Introduction to Protein Structure and Dynamics*

09:00-09:15	Opening Remarks
09:15-10:00	Molecular Dynamics Method
10:00-10:45	Molecular Dynamics with NAMD
Break	
11:00-11:50	Equilibrium Properties of Proteins
11:50-12:00	Daily Q & A
Lunch	
14:00-14:15	Overview of Hands-on Sessions
14:15-15:30	Molecular Dynamics/NAMD Tutorial
Break	
15:45-18:00	Molecular Dynamics/NAMD Tutorial (continued)

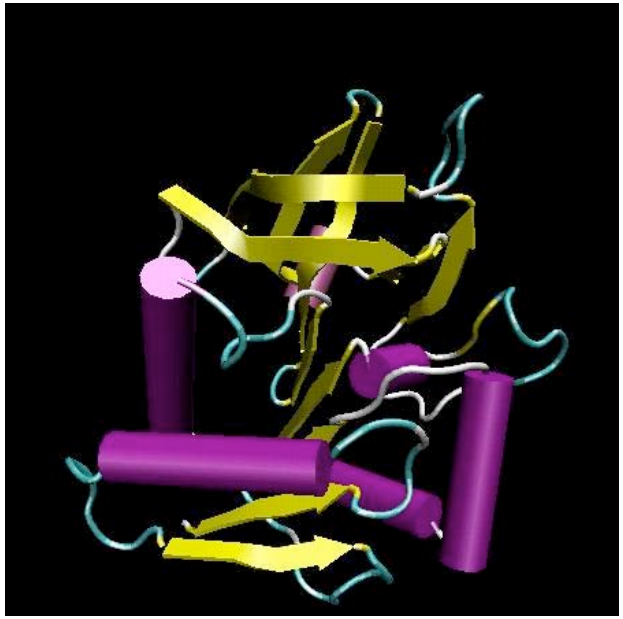


Ubiquitin

Tue, 11/7: *Parameters for Classical Force Fields*



09:00-10:00	Nonequilibrium Properties of Proteins
10:00-10:40	Classical Force Fields
Break	
11:00-11:50	Force Fields Parameterization
11:50-12:00	Daily Q&A Group photo
Lunch	
14:00-15:30	Molecular Dynamics/ NAMD Tutorial (continued)
Break	
15:45-18:00	Topology File & Parameterization Tutorials

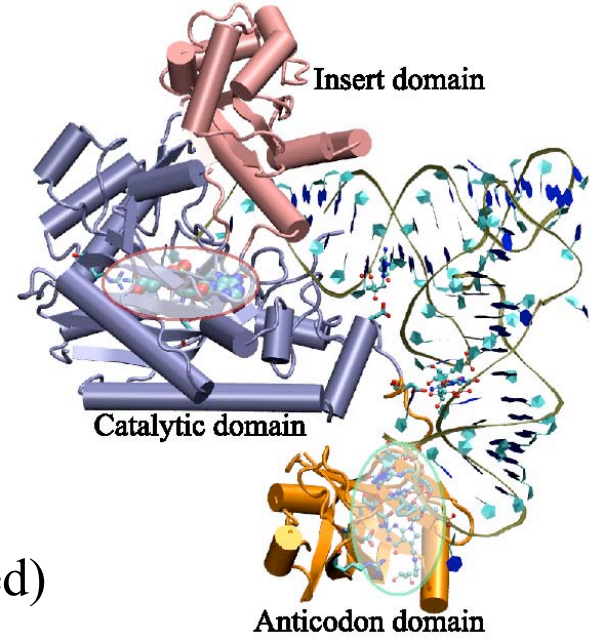


HisH

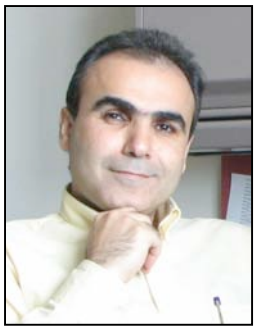
Wed, 11/8: *Introduction to Bioinformatics*

09:00-10:00	Intro to Bioinformatics: Sequence, Structure, and Alignment
10:00-10:40	Evolutionary Concepts in Bioinformatics
Break	
11:00-11:50	Application of Bioinformatics
11:50-12:00	Daily Q & A
Lunch	
14:00-16:30	Evolution of Protein Structure – Aspartyl tRNA Synthetase
Break	
16:45-18:00	Evolution of Protein Structure – Aspartyl tRNA Synthetase (continued)

AspRS-tRNA

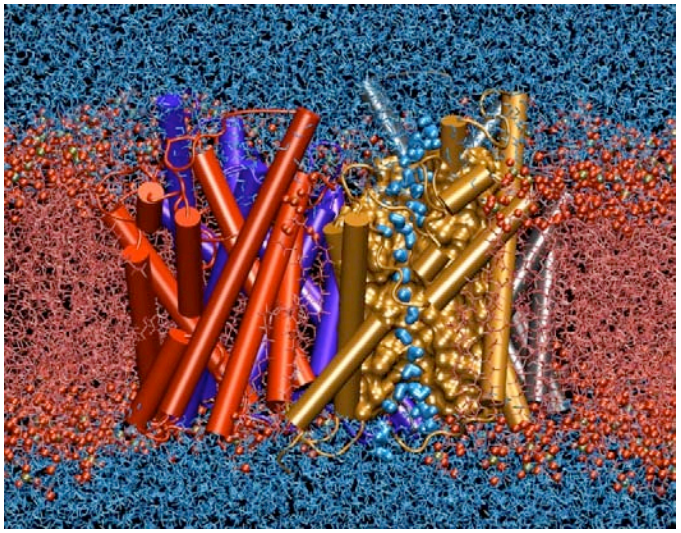


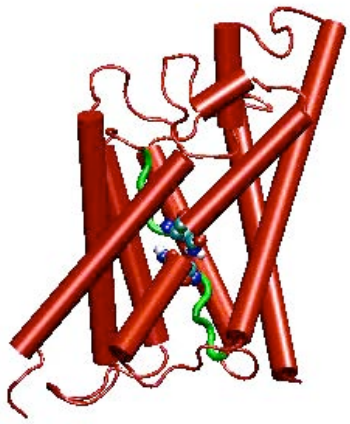
Thu, 3/23: *Simulating Membrane Channels*



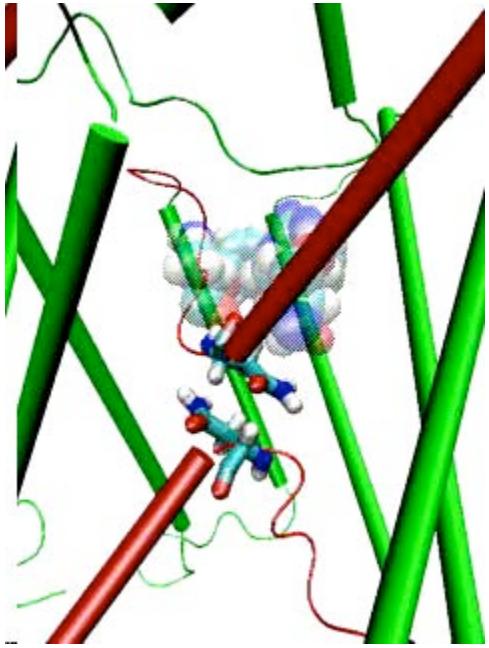
08:30-09:00	Introduction and Examples
09:00-10:00	Transport in Aquaporins
Break	
10:10-10:50	Nanotubes
10:50-11:00	Daily Q&A
Lunch	
14:00-15:30	Nanotubes/IMD
Break	
15:45-18:00	Stretching Deca-alanine/Open tutorial work time

Water Permeation through Aquaporin

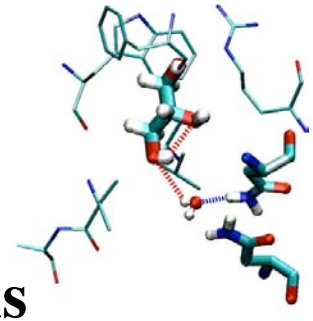




General



- The course is a volunteer effort
- The main focus are the hands-on sessions
- The aim is to get you to do computational biology
- We provide self-study(with assistance!) 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