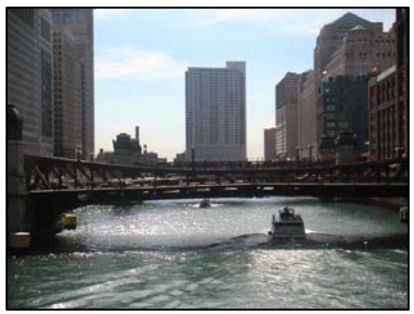
The TCBG and NIH Present: Hands-on Course in Computational Biology

Chicago, Illinois



The Program

Hands-on Course in Computational Biology


Prof. Klaus Schulten


Prof. Zan Luthey-Schulten


Dr. Emad Tajkhorshid

Location: Buckingham/Westminster Room

Handouts: Hands-on Sessions

Unix Primer

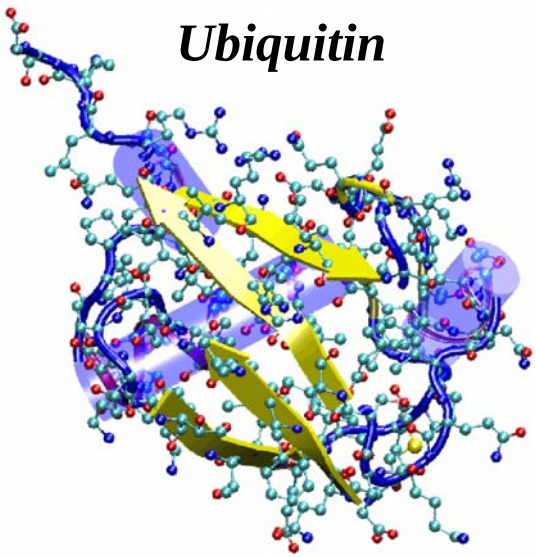
Mac Primer

Thu, 6/9: *Introduction to Protein Structure and Dynamics*

Buckingham/Westminster Room

09:00-09:30	Opening Remarks
09:30-10:40	Molecular Graphics Perspective of Protein Structure & Function
Break	
11:00-11:50	Molecular Dynamics Method
11:50-12:00	Daily Q & A
Lunch	
14:00-14:45	Overview of Hands-on Sessions
15:00-15:30	Molecular Graphics Tutorial
Break	
15:45-18:00	Molecular Graphics Tutorial

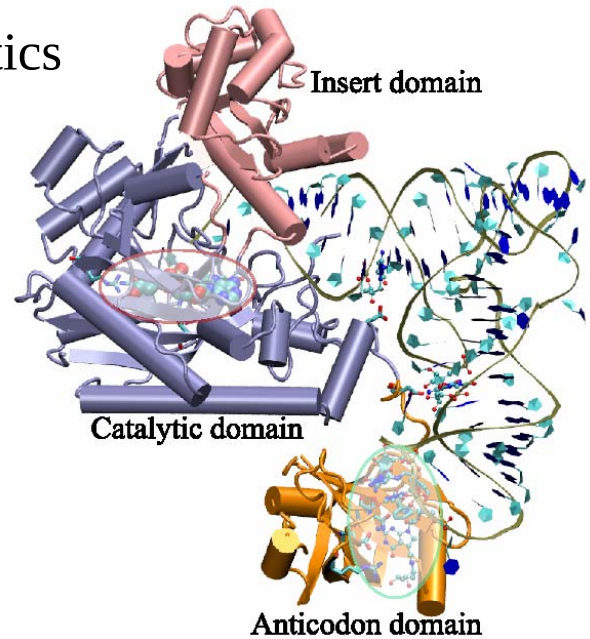
Ubiquitin



Fri, 6/10: *Introduction to Bioinformatics*

Buckingham/Westminster Room (lecture), Adams Room (lab)

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	
19:00-21:00	Evolution of Protein Structure – Aspartyl tRNA Synthetase
Break	
21:15-23:00	Sequence Alignment Algorithms/ Bioinformatics of Aquaporins

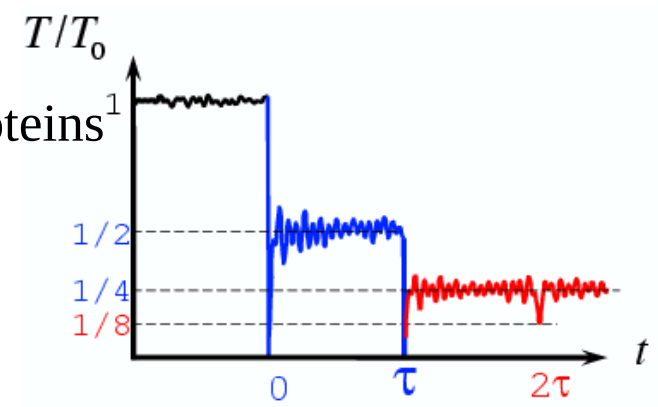


AspRS-tRNA

Sat, 6/11: *Statistical Mechanics of Proteins*

Buckingham/Westminster Room

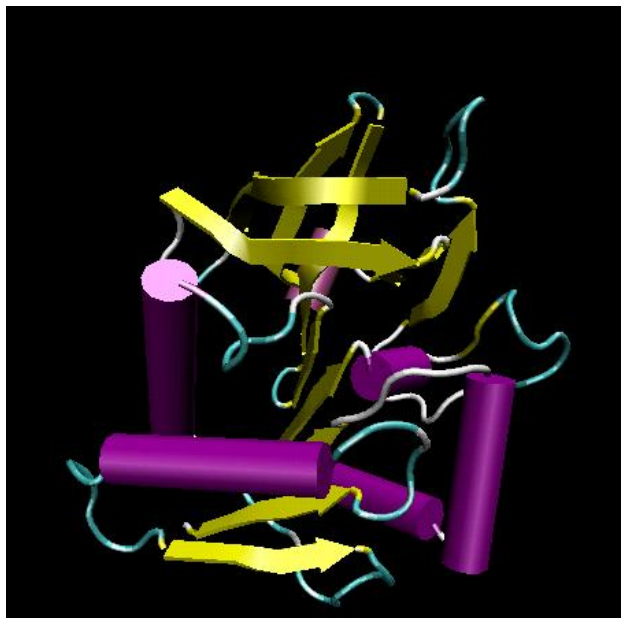
09:00-10:00	Molecular Dynamics with NAMD
10:00-10:40	Equilibrium Properties of Proteins
Break	
11:00-11:50	Nonequilibrium Properties of Proteins
11:50-12:00	Daily Q & A
Lunch	
19:00-20:30	Molecular Dynamics Tutorial
Break	
20:45-23:00	Molecular Dynamics Tutorial (continued)



Sun, 6/12: *Parameters for Classical Force Fields*

Buckingham/Westminster Room

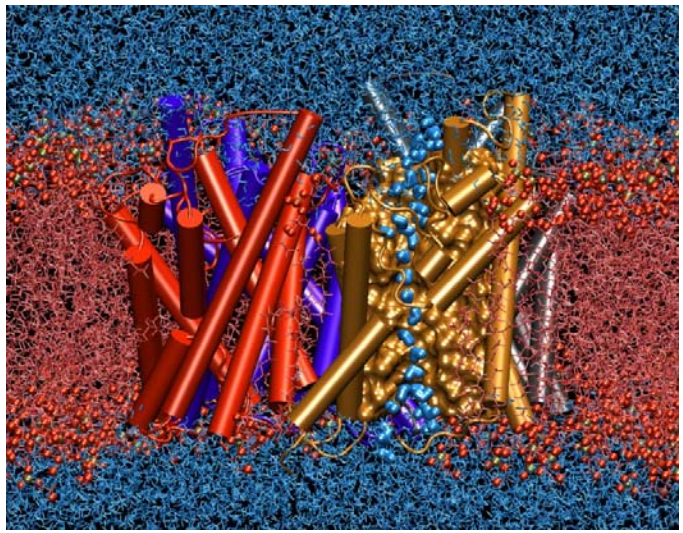
09:00-10:00	Introduction and Examples
10:00-10:40	Force Fields Parameterization
Break	
11:00-11:50	Applications
11:50-12:00	Daily Q&A
Lunch	
14:00-15:30	Parameterizing a Novel Residue
Break	
15:45-18:00	Topology File Tutorial



HisH

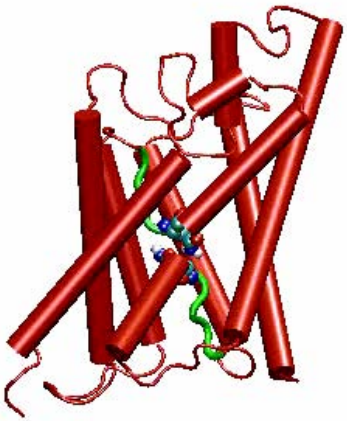
Mon, 6/13: *Simulating Membrane Channels*

Water Permeation through Aquaporin

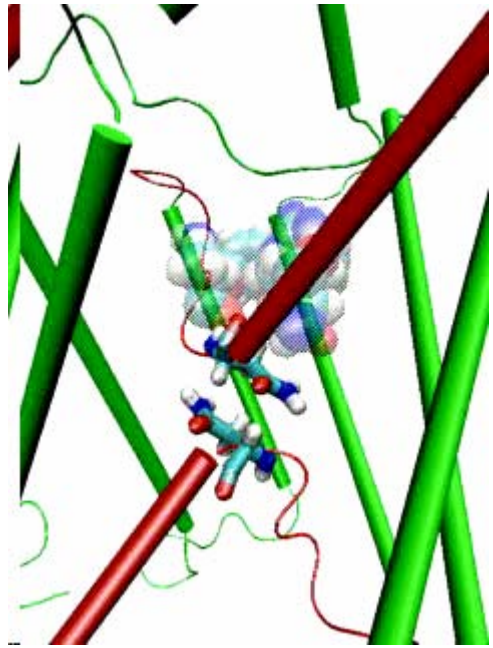


Buckingham/Westminster Room

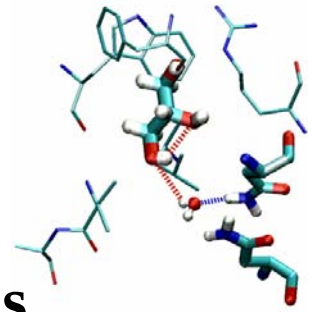
09:00-10:00	Introduction and Examples
10:00-10:40	Transport in Aquaporins
Break	
11:00-11:50	Nanotubes
11:50-12:00	Daily Q&A
Lunch	
14:00-15:30	Nanotubes/IMD
Break	
15:45-18:00	Deca-alanine/Open tutorial work time



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**

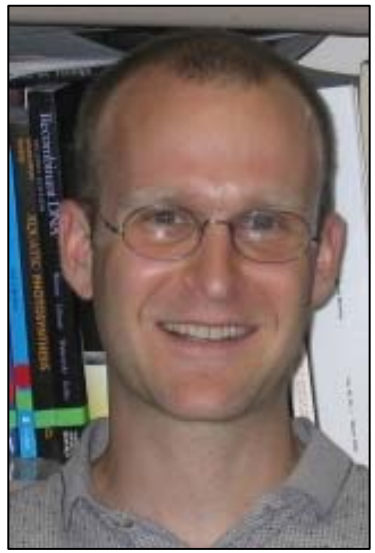
- **Please give us feedback to improve lectures and tutorials**
- **Please give us feedback to encourage future courses**

Acknowledgements

Assistants

Marcos Sotomayor

Eduardo Cruz-Chu



Elijah Roberts

Laptop Preparation:

M. Bach