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




Lake Tahoe & The Granlibakken Resort




The Program

Hands-on Course in Computational Biology


Prof. Klaus Schulten


Prof. Zan Luthey-Schulten


Dr. Emad Tajkhorshid

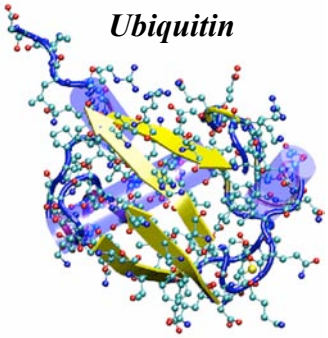
Location: Mountain Room

Handouts: Hands-on Sessions
Unix Primer
Mac Primer

Mon, 5/23: *Introduction to Protein Structure and Dynamics*

Mountain 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	
19:00-19:45	Overview of Hands-on Sessions
20:00-20:30	Molecular Graphics Tutorial
Break	
20:45-23:00	Molecular Graphics Tutorial

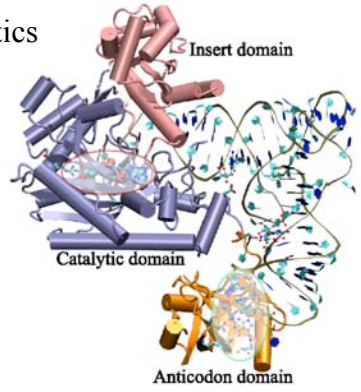


Ubiquitin

Tue, 5/24: *Introduction to Bioinformatics*

Mountain Room

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 Algorhithms/ Bioinformatics of Aquaporins

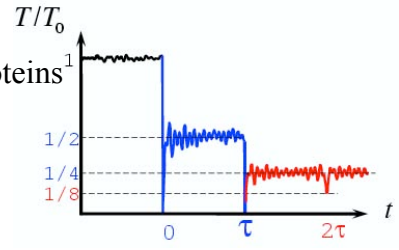


AspRS-tRNA

Wed, 5/25: *Statistical Mechanics of Proteins*

Mountain Room

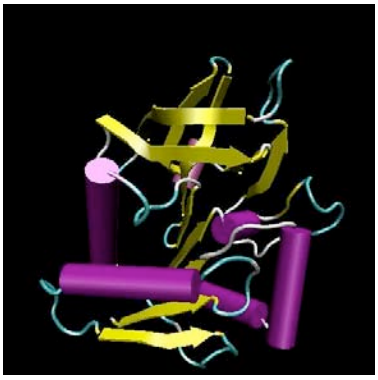
09:00-10:00	Molecular Dynamics with NAMD
10:00-10:40	Equilibrium Properties of Proteins
Break	
11:00-11:50	Nonequilibrium Properties of Proteins
11:50-12:00	Daily Q & A
Lunch	
19:00-20:30	Molecular Dynamics Tutorial
Break	
20:45-23:00	Molecular Dynamics Tutorial (continued)



Thu, 5/26: *Parameters for Classical Force Fields*

Mountain Room

09:00-10:00	Introduction and Examples
10:00-10:40	Force Field Parameterization
Break	
11:00-11:50	Applications
11:50-12:00	Daily Q&A
Lunch	
19:00-20:30	Parameterizing a Novel Residue
Break	
20:45-23:00	Topology File Tutorial



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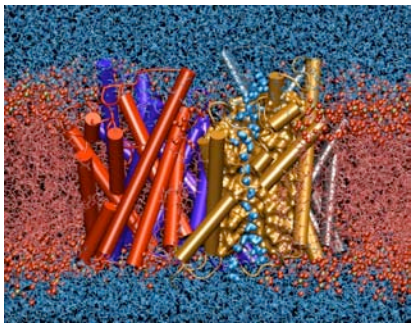
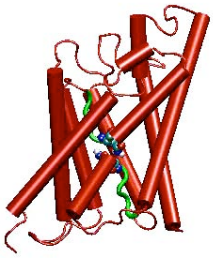
Fri, 5/27: *Simulating Membrane Channels*

Water Permeation through Aquaporin

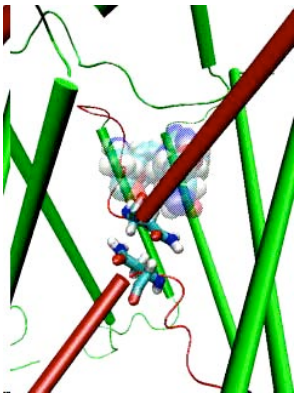


Mountain Room

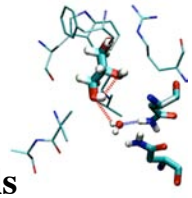
09:00-10:00	Introduction and Examples
10:00-10:40	Transport in Aquaporins
Break	
11:00-11:50	Nanotubes
11:50-12:00	Daily Q&A
Lunch	
19:00-20:00	Nanotubes
20:00-20:30	Steered Molecular Dynamics Tutorial
Break	
20:45-23:00	Steered Molecular Dynamics Tutorial (continued)



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

J.C. Gumbart

Anton Arkhipov

Laptop Preparation:

M. Bach