

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



San Francisco, California



The Program

Hands-on Course in Computational Biology



Prof. Klaus Schulten



Prof. Zan Luthey-Schulten



Dr. Emad Tajkhorshid

Location: Apollo Room

Handouts: Hands-on Sessions
Unix Primer
Mac Primer

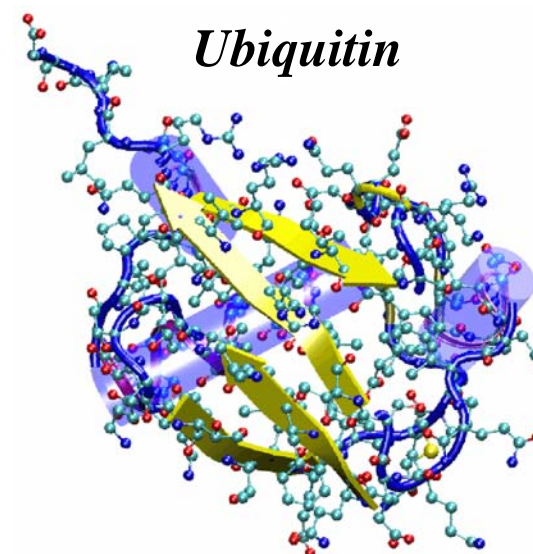


Sun, 6/26: *Introduction to Protein Structure and Dynamics*



Apollo Room

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



Mon, 6/27: *Statistical Mechanics of Proteins*



Apollo 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

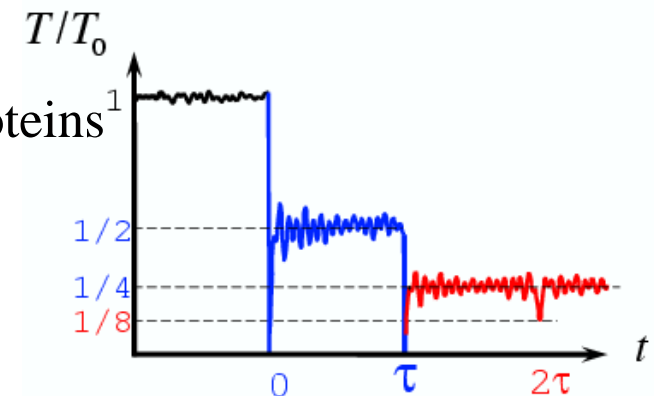
11:50-12:00 Daily Q & A
Group photo

Lunch

19:00-20:30 Molecular Dynamics Tutorial

Break

20:45-23:00 Molecular Dynamics Tutorial (continued)



Tue, 6/28: *Introduction to Bioinformatics*



Apollo 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

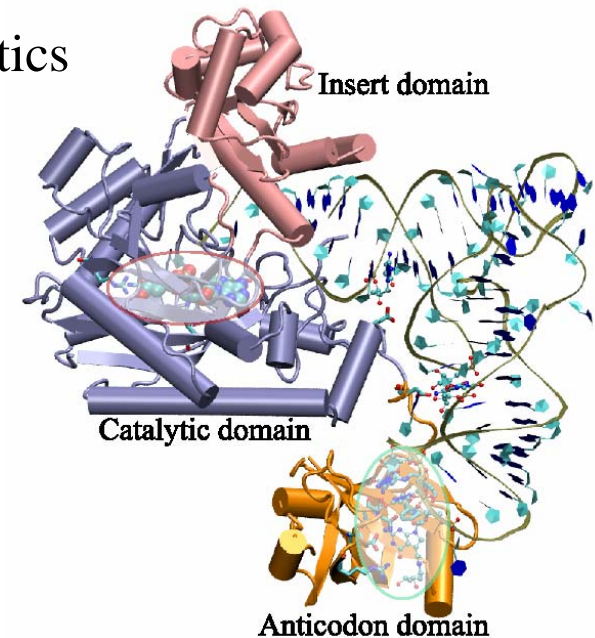
11:50-12:00 Daily Q & A

Lunch

14:00-16:00 Evolution of Protein Structure –
Aspartyl tRNA Synthetase

Break

16:15-18:00 Sequence Alignment Algorithms/
Bioinformatics of Aquaporins



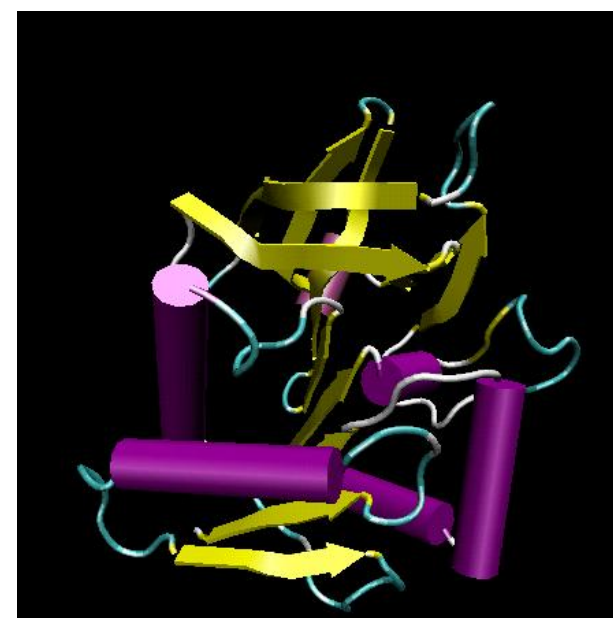
AspRS-tRNA

Wed, 6/29: *Parameters for Classical Force Fields*



Apollo Room

09:00-10:00	Introduction and Examples
10:00-10:40	Force Fields Parameterization
<i>Break</i>	
11:00-11:50	Applications
11:50-12:00	Daily Q&A
<i>Lunch</i>	
19:00-21:00	Parameterizing a Novel Residue
<i>Break</i>	
21:15-23:00	Topology File Tutorial

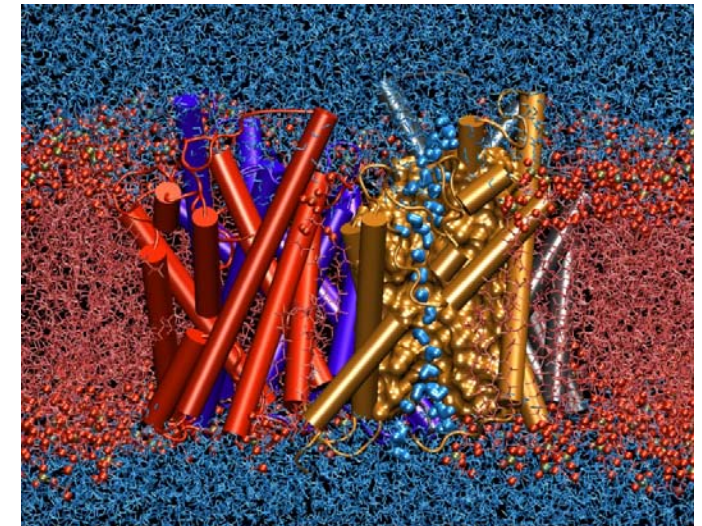


HisH

Thu, 6/30: *Simulating Membrane Channels*



Water Permeation through Aquaporin



Apollo Room

09:00-10:00 Introduction and Examples

10:00-10:40 Transport in Aquaporins

Break

11:00-11:50 Nanotubes

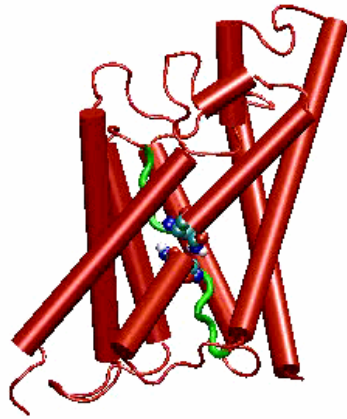
11:50-12:00 Daily Q&A

Lunch

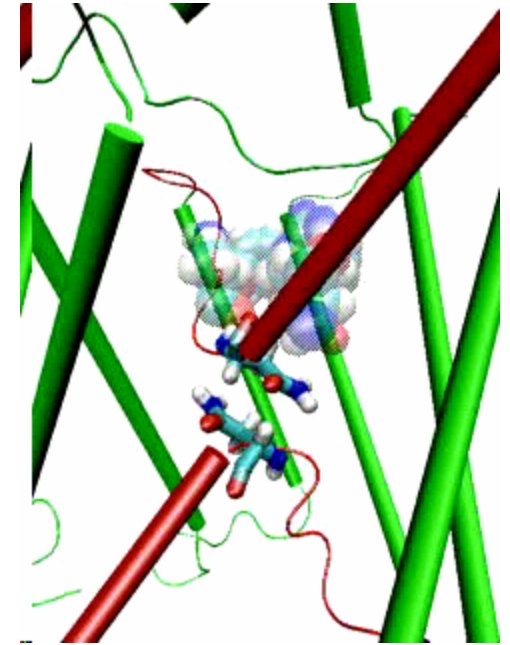
14:00-15:30 Nanotubes/IMD

Break

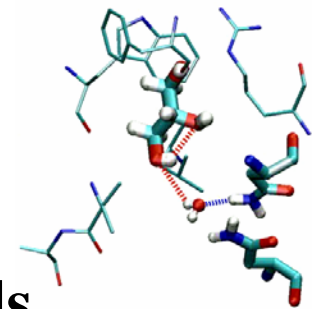
15:45-18:00 Deca-alanine/Open tutorial work time



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

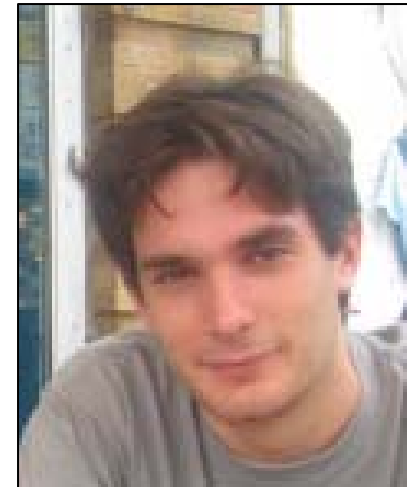
**A
s
s
i
s
t
a
n
t
s**



Elizabeth Villa



Rommie Amaro



Jordi Cohen

Laptop Preparation:



M. Bach