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

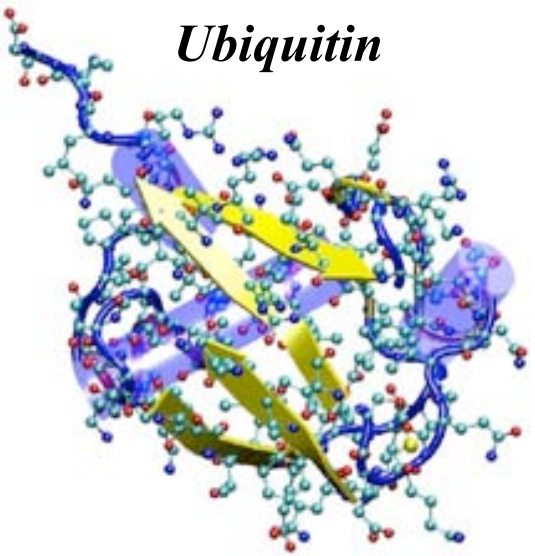
Handouts: Hands-on Sessions
Unix Primer
Mac Primer

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

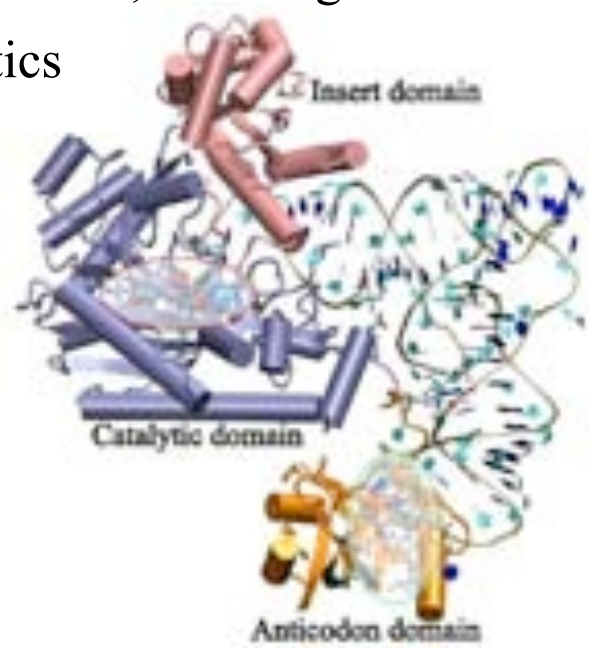
Ubiquitin



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

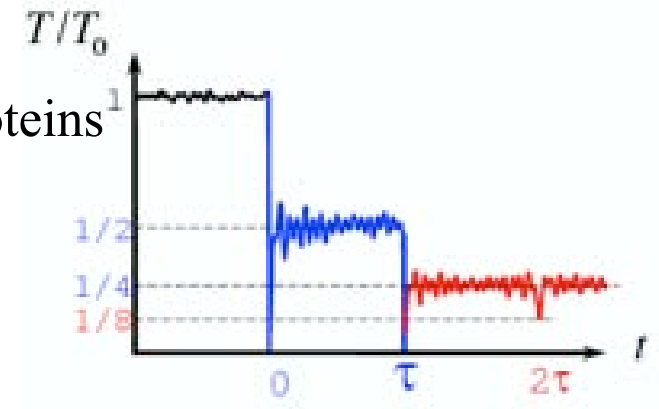


AspRS-tRNA

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

Buckingham/Westminster Room

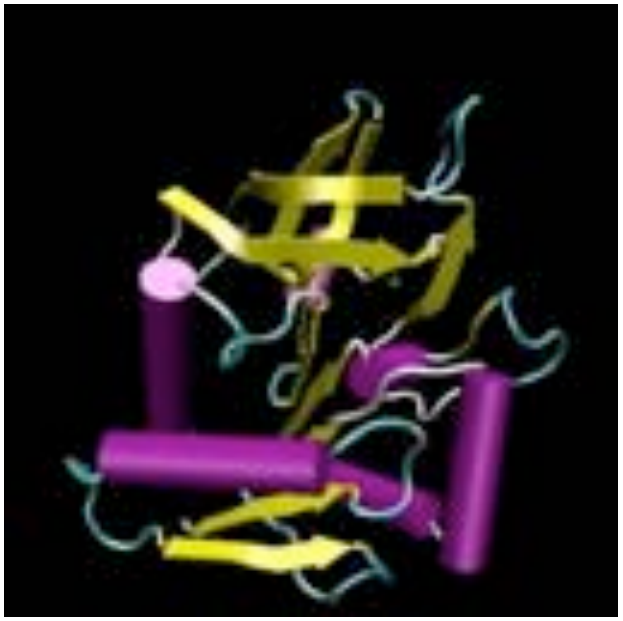
09:00-10:00	Molecular Dynamics with NAMD
10:00-10:40	Equilibrium Properties of Proteins
Break	
11:00-11:50	Nonequilibrium Properties of Proteins
11:50-12:00	Daily Q & A
Lunch	
19:00-20:30	Molecular Dynamics Tutorial
Break	
20:45-23:00	Molecular Dynamics Tutorial (continued)



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

Buckingham/Westminster Room

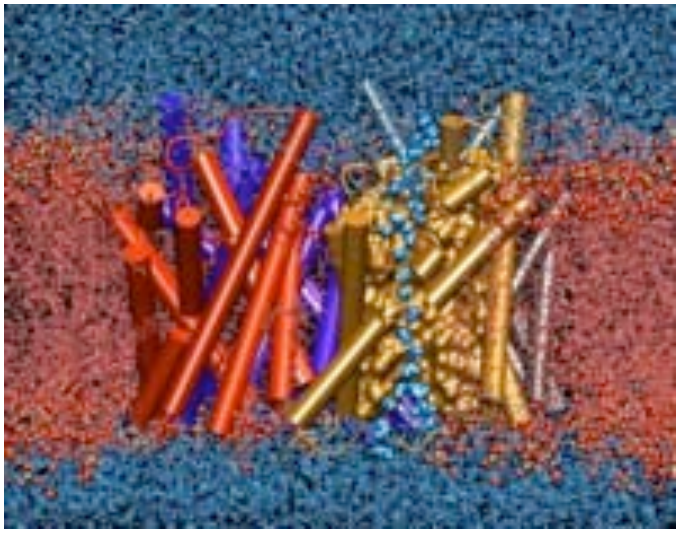
09:00-10:00	Introduction and Examples
10:00-10:40	Force Fields Parameterization
Break	
11:00-11:50	Applications
11:50-12:00	Daily Q&A
Lunch	
14:00-15:30	Parameterizing a Novel Residue
Break	
15:45-18:00	Topology File Tutorial



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

Welcome from our Group

"Hands-On" Workshop on Computational Biophysics

Water Permeating Through Aquaporin

The workshop will explore physical models and computational approaches used for the simulation of biological systems and the investigation of their function at an atomic level. The course will be based on case studies including the properties of membranes and membrane proteins, mechanisms of molecular motors, trafficking in the living cell through water and ion channels, and signaling pathways. Relevant physical concepts, mathematical techniques, and computational methods will be introduced, including force fields and algorithms used in molecular modeling, molecular dynamics simulations on parallel computers and steered molecular dynamics simulations.
The workshop is designed for graduate students and postdoctoral researchers in computational and/or biophysical fields who seek to extend their research skills to include computational and theoretical expertise, as well as other researchers interested in theoretical and computational biophysics. Theory sessions in the morning will be followed by hands-on computer labs in the afternoon in which students will be able to set up and run simulations. Enrollment limited to 20 participants.

TCBG Computational Biophysics Workshops

Dates:
December 3 - 8, 2004

Theoretical & Computational Biophysics Group
Beckman Institute
University of Illinois
Urbana-Champaign
405 N. Mathews Ave.
Urbana, IL 61801
(217) 265-4313
workshop-tcbg@ks.uiuc.edu

Program

Instructors:

K. Schulten (UIUC)
Z. Luthey-Schulten (UIUC)
E. Tajkhorshid (UIUC)

CLICK HERE TO APPLY TO WORKSHOP

Contacts:

General Questions:
workshop+tcbg@ks.uiuc.edu

Application, Registration, Housing & Local Resources:
Diane Wolff
wolff@ks.uiuc.edu

FAQ

Theoretical and Computational Biophysics Group

Klaus Schulten
Zan Luthey-Schulten
Emad Tajkhorshid
together with students and postdocs of their group
Organization: David Brandon and group staff

Rosemary Braun (primate at left)

Mu Gau

Thank you

University of Illinois at Urbana-Champaign

NCSA

Special thanks to:

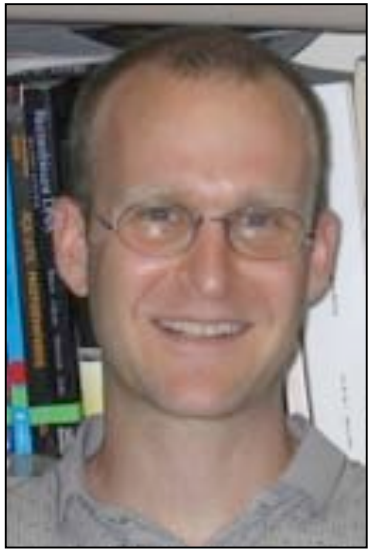
David Brandon

Acknowledgements

Assistants

Marcos Sotomayor

Eduardo Cruz-Chu

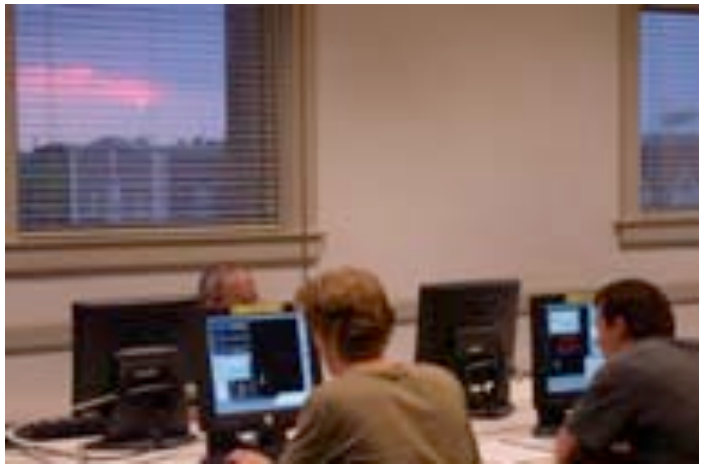


Elijah Roberts

Laptop Preparation:

M. Bach

Please note



- **The workshop 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 (Friday opportunity for presentation)**

- **Please give us feedback to improve lectures and tutorials**
- **Please give us feedback to encourage more schools**

Let's enjoy a week of scholarship and collegiality