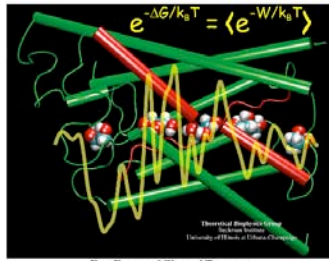


Announcement

An NCSA-sponsored Workshop on Theoretical and Computational Biophysics 2004

"Hands-On" Workshop on Computational Biophysics



Free Energy of Glycerol Transport

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.

University of Illinois, Urbana Champaign

TCBG Computational Biophysics Workshops

Dates: November 8 - 12, 2004

Theoretical & Computational Biophysics Group University of Illinois Urbana-Champaign 405 N Mathews Ave Urbana, IL 61802 237/244-2212 workshop@urbana@ks.uiuc.edu

Program

Instructors:

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

APPLICATIONS NO LONGER BEING ACCEPTED FOR THIS WORKSHOP

Contacts:

General Questions: workshop@urbana@ks.uiuc.edu

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

FAQ

Welcome



Theoretical and Computational Biophysics Group

Klaus Schulten
Zan Luthey-Schulten

Emad Tajkhorshid
together with students and postdocs of their group

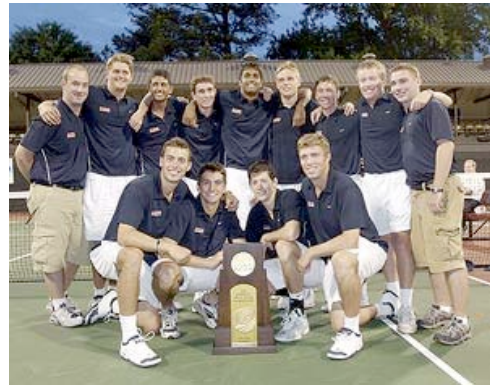
Organization: David Brandon and group staff



Rosemary Braun (primate at left)



Mu Gau



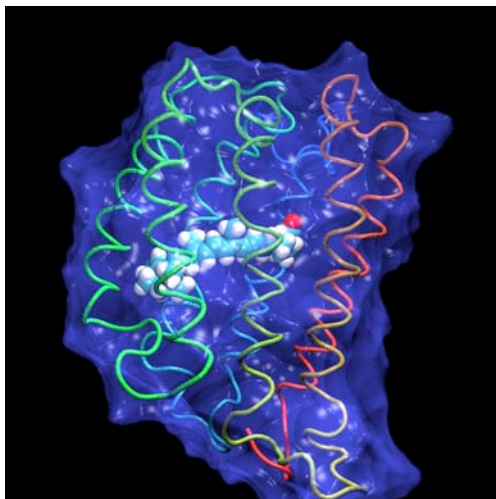
Our University

The Theoretical and Computational Biophysics Group



Half of us are physical and life science students and postdocs, half are research programmers, developers and system administrators. We have a 1:1 ratio researcher - support staff. We run a world-leading computational biology laboratory with many visitors a year.

Our Key Research Tool: VMD



<http://www.ks.uiuc.edu/Research/vmd/>

Humphrey *et al.*, 'VMD – Visual Molecular Dynamics', *J. Molec. Graphics* 1996, 14.1, 33-38.

VMD
Visual Molecular Dynamics

Molecular Analysis

Display and animation of macromolecules, volumetric data, sequence data

Multiple sequence and structure analysis

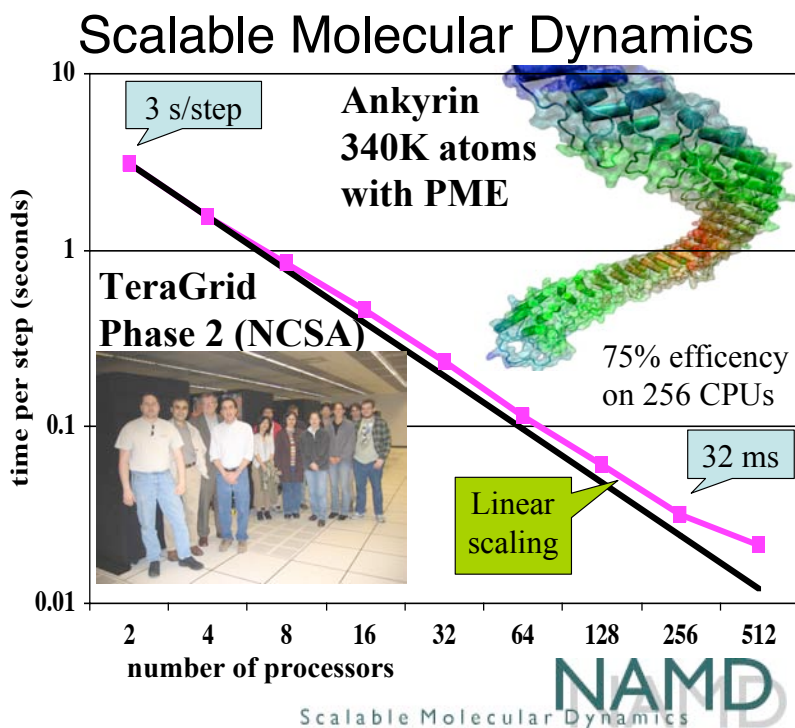
Project oriented plugin extensions aid researchers in performing modeling and analysis tasks

Supports MacOS X, Windows, and a wide variety of Unix platforms

Hardware accelerated 3-D rendering and stereoscopic display

Collaboration interfaces via BioCoRE

Our Key Research Tool: NAMD



Simulation of large biomolecular systems on parallel computers.

File compatible with original community codes CHARMM & AMBER.

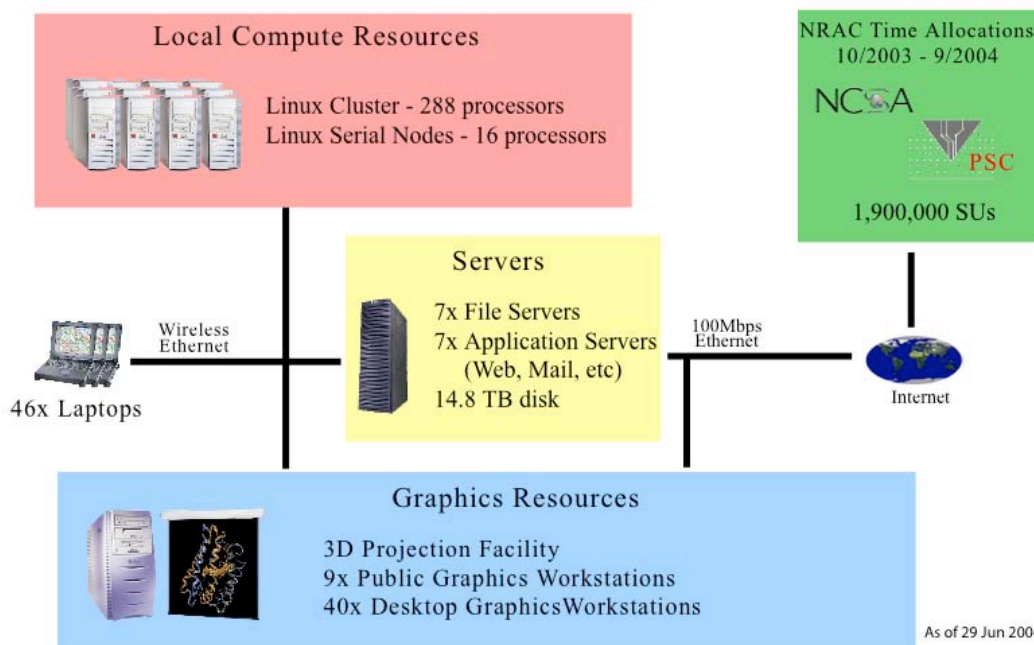
Ten-year collaboration with UIUC Parallel Programming Lab.

2002 Gordon Bell Award for parallel scalability.

Runs at NSF centers, on clusters, and on desktop.

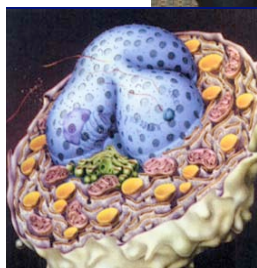
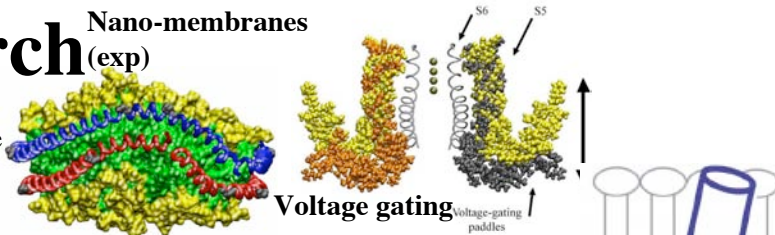
Available for free as precompiled binaries; includes source code; 10,000 registered users.

Our Computing Facility

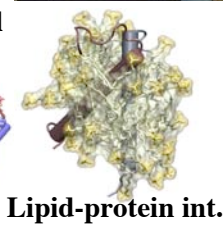
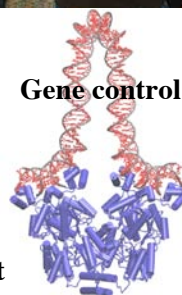


Our Research

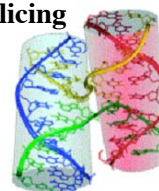
Yi Amy Fatemeh Sharlene
Elizabeth Jin
Rosemary



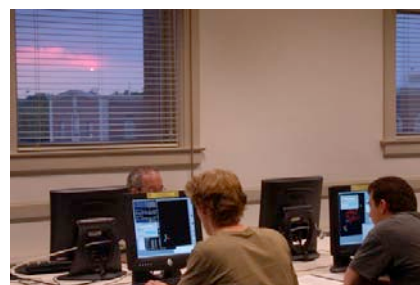
Nuclear pore transport



DNA splicing



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

Thank you

University of Illinois at Urbana-Champaign

NCSA



Special thanks to:

David Brandon

Brijeet Dhaliwal



**Let's enjoy a week
of scholarship**



**and
collegiality**

