Beckman Institute
Theoretical and Computational Biophysics Group

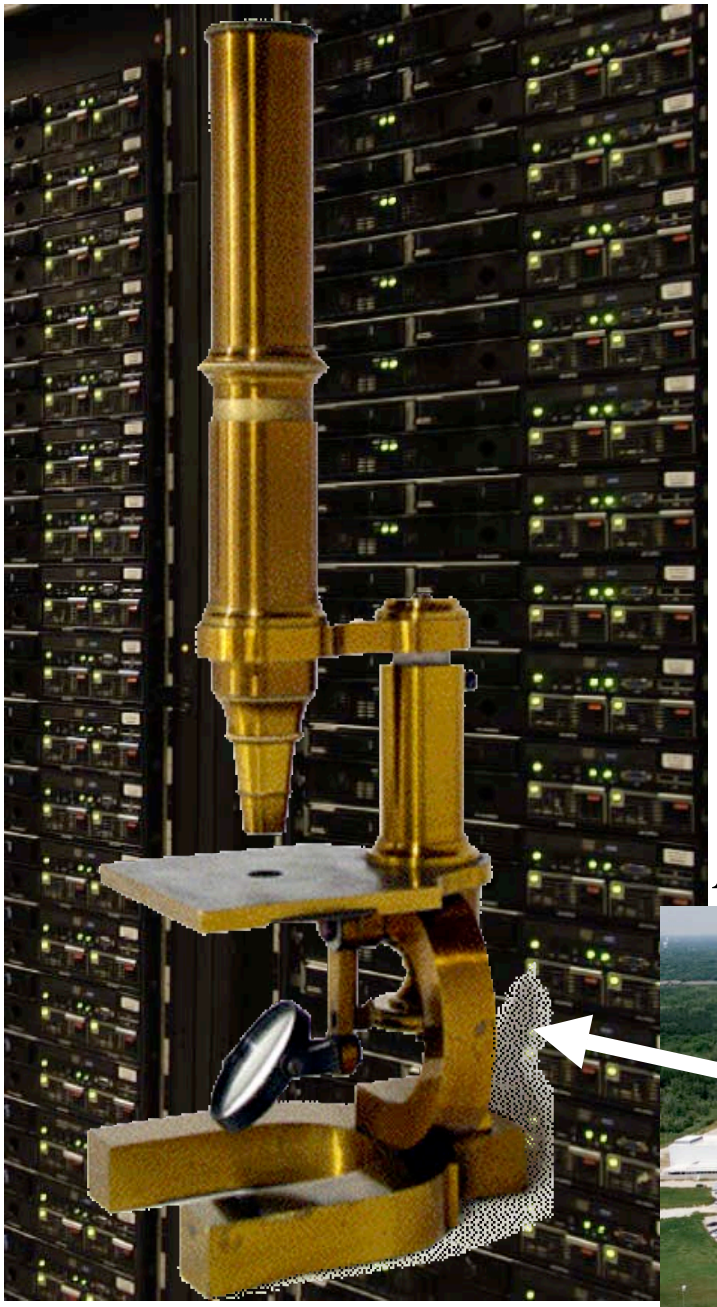
Ultimate Microscopy through Computer Visualization and Terascale-Petascale Computational Modeling

Started in 1989; 5 faculty (biochem., chem., comp. science, physics), 14 staff, 28 scientists; external funding of > $2 Mill. /year from NIH, NSF, DOE; National NIH Resource; 90,000 registered users; 350 publications with 10,000 citations; global training, web site 600,000 visits + 1.2 TByte/year

Mission: Microscopy

The Illinois Computational Microscope Views Living Systems

- 90,000 registered users
- guides bionanotechnology
- develops renewable energy
- supports biomedicine
- trains next generation

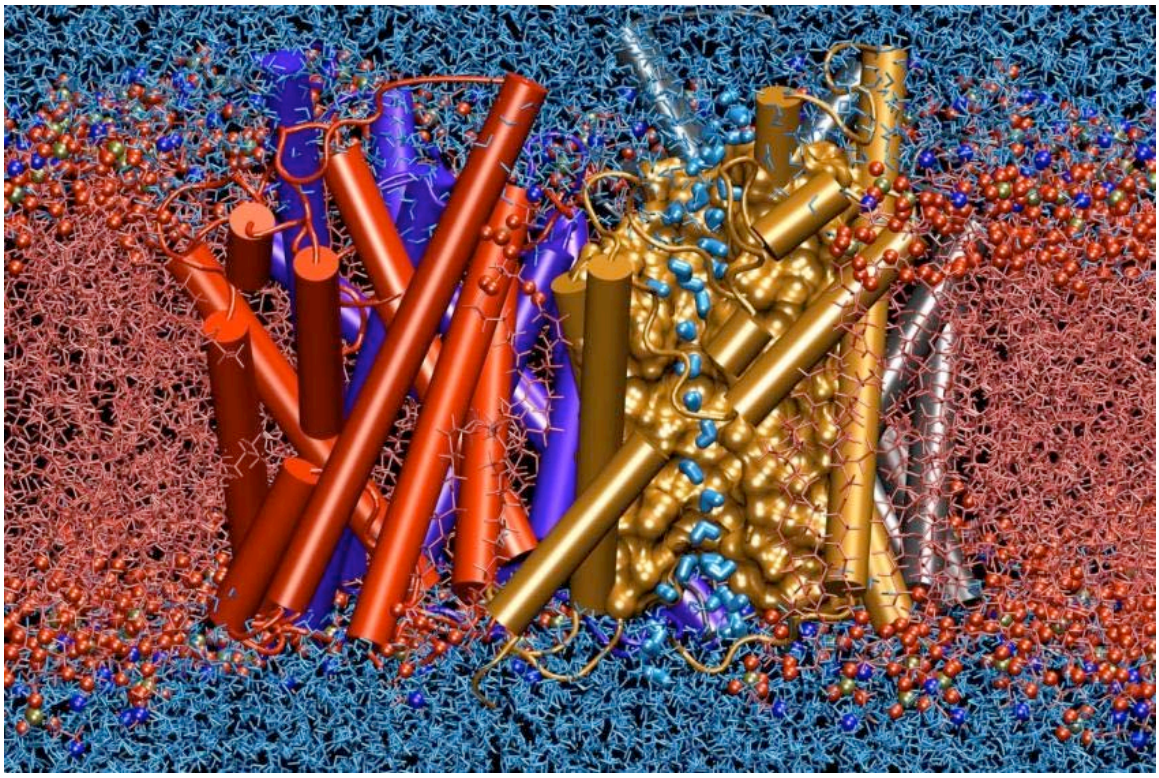


Visualization Through Petascale Computing

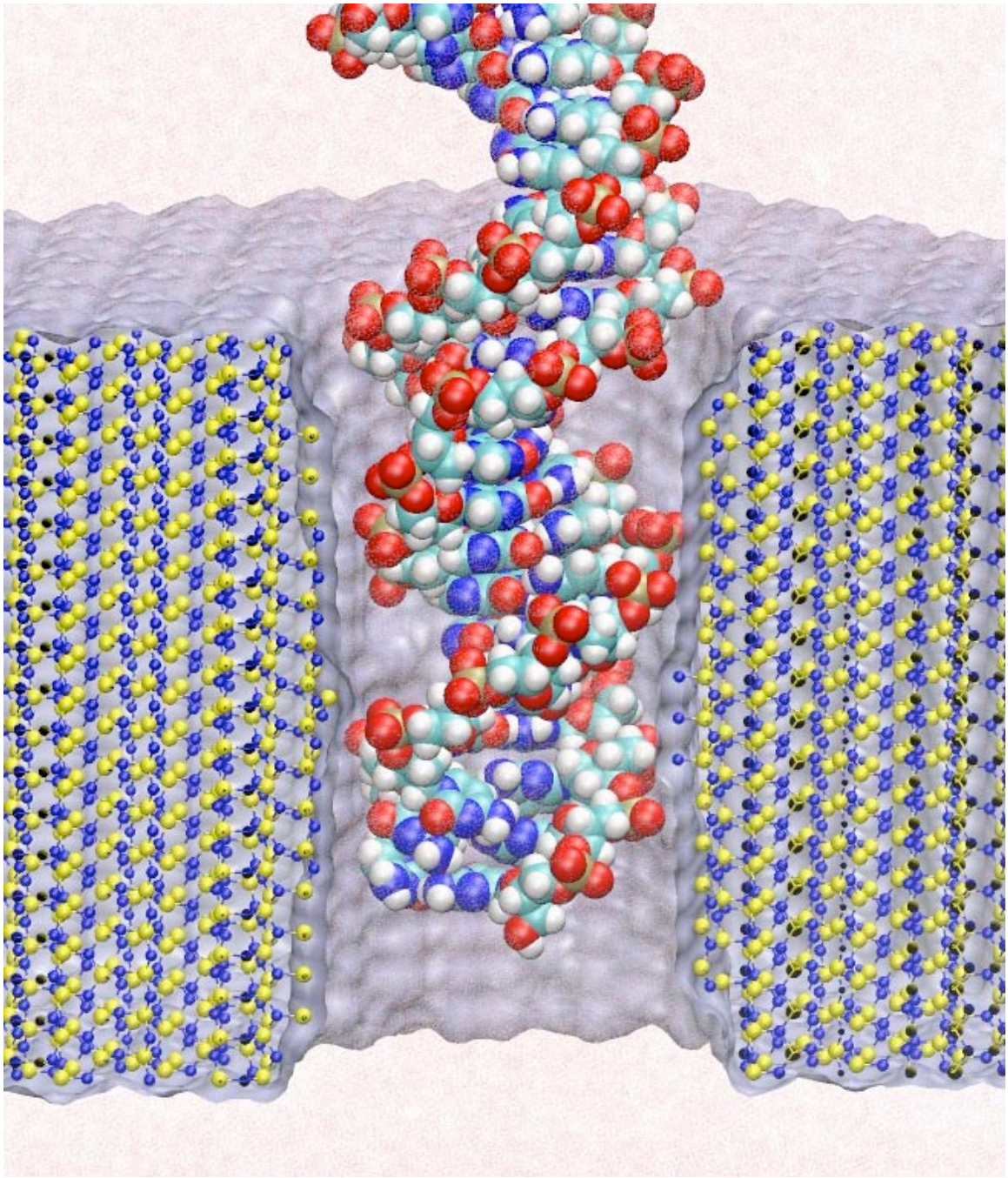
Light Microscope

Argonne Advanced Photon Source

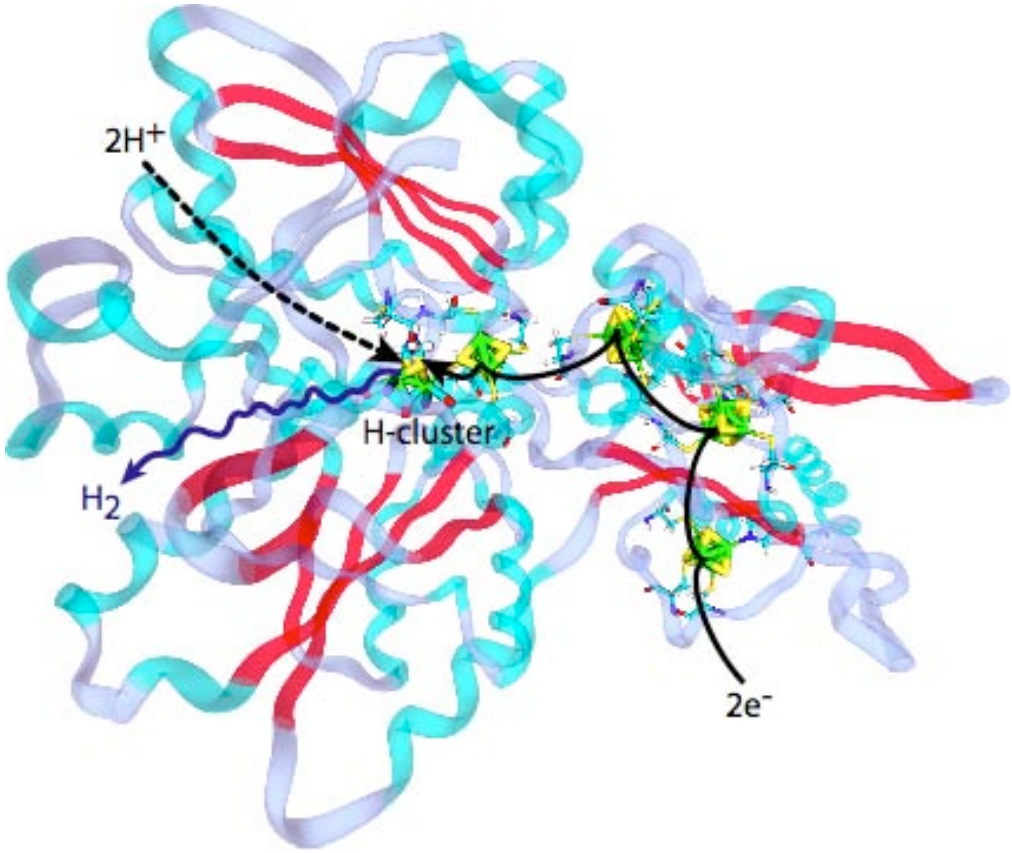
Computational Microscopy of Biological Water Channels



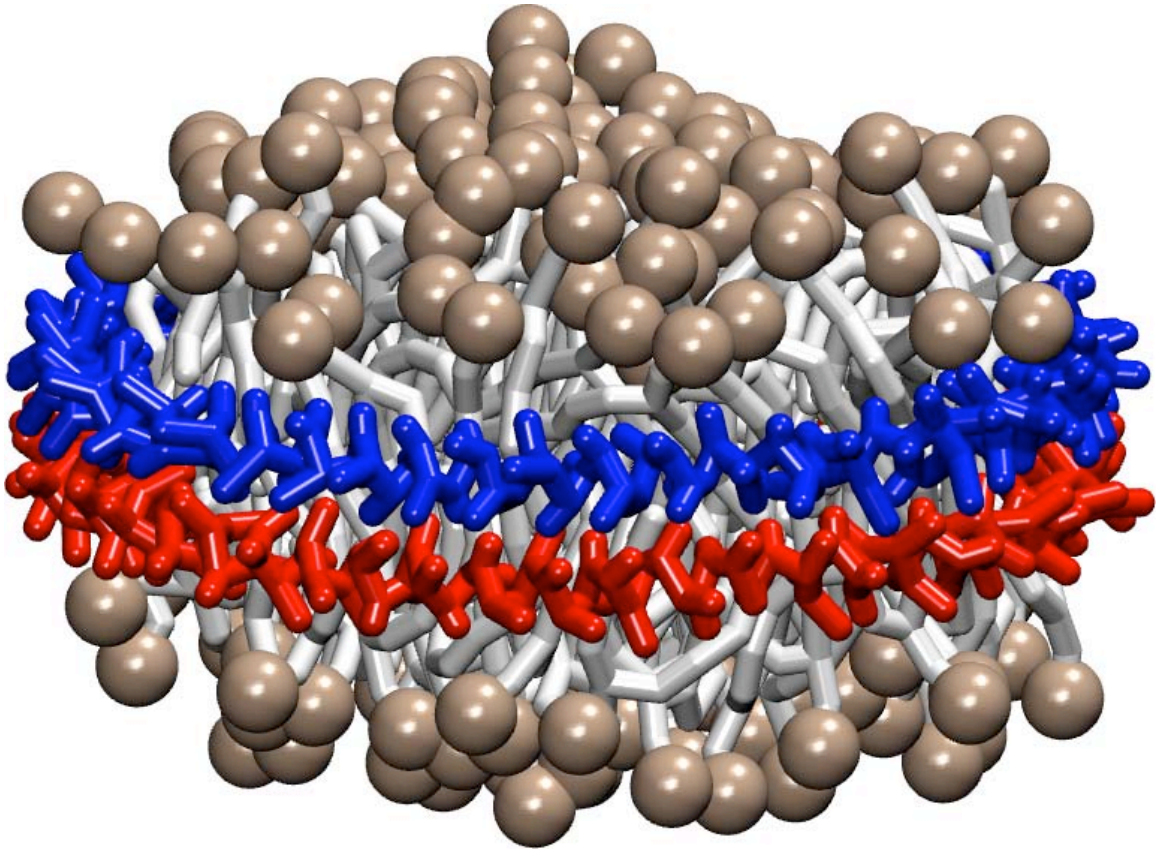
Computational Microscopy of Bio-Nanodevices



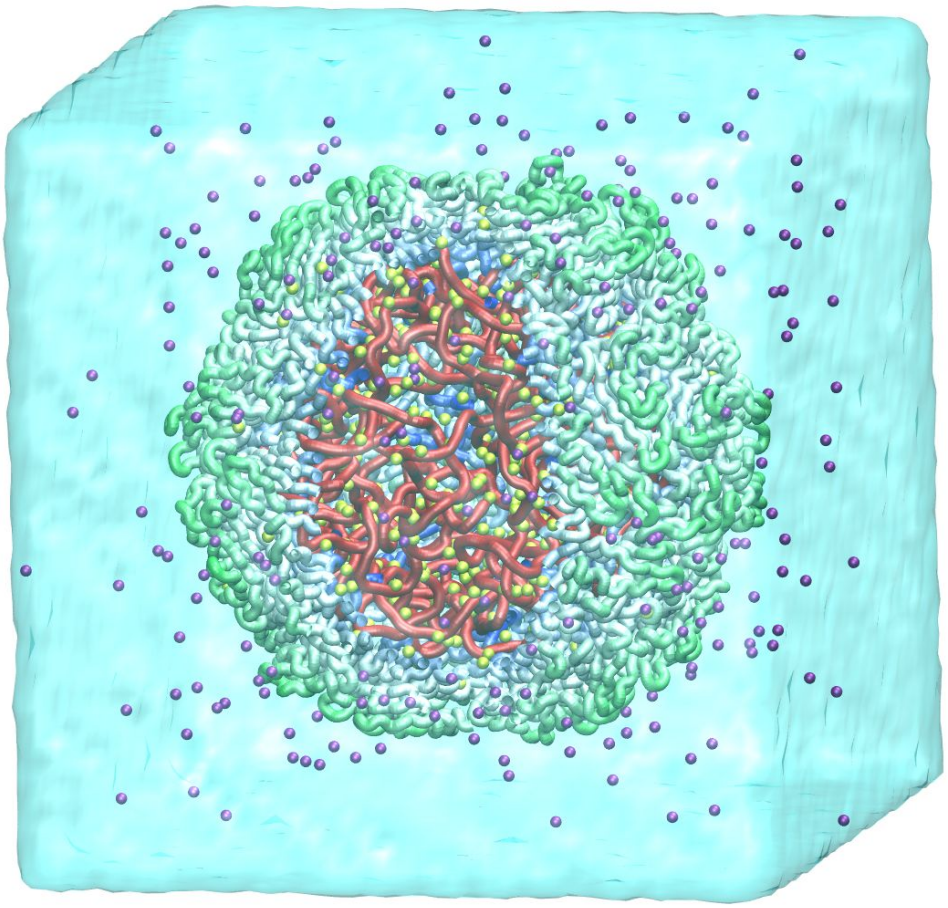
Computational Microscopy of Hydrogenase



Computational Microscopy of "Good Cholesterol"



Computational Microscopy of Viruses



Hands-on Training in Computational Biology

UIUC lab (Jun. 2003) → Resource laptops (Jun. 2004) → Off-site lab (Nov. 2005) → Anywhere! (Mar. 2006)

Urbana

Perth, Australia

Pittsburgh

Frankfurt, Germany

$$ NSF, NIH

Global Campus (all material on web site)

Urbana, 2003

Perth, 2004

Urbana, 2004

Boston, 2004

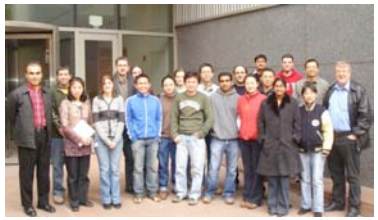
Lake Tahoe, 2005

Chicago, 2005

San Francisco, 2005

Pittsburgh, 2005

Frankfurt, 2006



Pittsburgh, 2006

THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP

NIH RESOURCE FOR MACROMOLECULAR MODELING AND BIOINFORMATICS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Global training and service

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Highlights of our Work

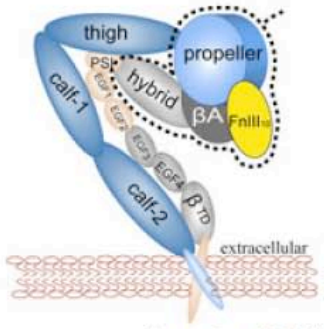

image size: 468.6KB

Mammalian cells adhere to each other forming tissues. The adhesion is due to a network of proteins, so-called extracellular matrix proteins, "gluing" the cells together. The cell membranes are too soft to provide anchoring points for the extracellular matrix proteins; rather, the cells furnish on their outer surface specialized hooks for anchoring the extracellular matrix proteins. The hooks, in the form of surface proteins, are linked directly through the membranes to the intracellular cytoskeleton that stabilizes and shapes cells. Integrins are an important family of such surface proteins that form hooks specific for certain types of extracellular matrix proteins. The hooks are flexible, they can be open for contacts or closed, the switch being induced by signals from inside or outside the cell through interactions with other proteins. The interactions between integrins and extracellular matrix proteins are rather complex, as the proteins are composed of many subunits; fortunately, their overall structures are presently being solved through crystallography. In a **recent report** a major component of an integrin and an extracellular matrix protein have been investigated through molecular modeling using **NAMD**, including steered molecular dynamics. The study described in detail how the extracellular matrix protein induces a transition in integrin, potentially strengthening its adhesion property. See also **previous highlights**: the May 2006 "Killer's Entry Route", Dec 2004 "Snap Fastener on Biological Cells", Dec 2003 "Body's Glue", and Mar 2002 "Cells Sense Push and Pull". More on modeling of extracellular matrix proteins and integrins can be found **here**.

Quick Links

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Review Bionanotechnology
Bringing Physics to Life
Bringing Computing to Life
Training for the New Discipline
NIH Center for Research Resources
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Recent Publications

Assembly of lipoprotein particles revealed by coarse-grained molecular dynamics simulations. *Journal of Structural Biology*, 2006. In press.

All Publications

Software

VMD - Molecular Graphics Viewer
NAMD - Molecular Dynamics Simulator
BioCoRE - Collaboratory Environment
MD Service Suite
Structural Biology Software Database

Announcements

14 Nov 2006 - Prospective Graduate Students
07 Nov 2006 - Gateway to the Nucleus
21 Sep 2006 - One Protein, Two Channels
18 Sep 2006 - VMD Adds Evolutionary View
12 Sep 2006 - Aksimentiev in Synergy magazine
11 Sep 2006 - Postdoctoral Position
31 Aug 2006 - NAMD 2.6 released
25 Aug 2006 - VMD 1.8.5 released
25 Aug 2006 - VMD MultiSeq in BMC Bioinformatics

In the News - Archive

Research

Membrane Biophysics
Mechanobiology
Nanoengineering
Bioenergetics
Steered/Interactive Molecular Dynamics
Quantum Biology
Neurobiology
Other Topics
Collaborations

Outreach

TCB Group Overview
Group Members - Recent Photos
Computational Environment
Tutorials
Case Studies
Training and Workshops
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How To Acknowledge Us

Upcoming Seminars

11 Dec 2006 - Dr. Kakoli Mitra - Understanding the Mechanisms of Translation by the Ribosome and Protein Translocation at Membranes

Recent Seminars

600,000 visitors downloaded 1.2 TBytes in 2005

How the Theoretical and Computational Biophysics Group Is Important for UIUC

- is well funded, single NIH Biotechnology Resource at UIUC
- has nearly 100,000 users of its software
- is highly productive (publications) and visible (citations)
- supports biomedicine in treating diseases
- guides bioengineering for renewable energy
- assists engineers in developing biomedical nanodevices
- supports and collaborates with many other UIUC groups
- offers innovative intramural and extramural training
- realizes through its popular web site the global campus