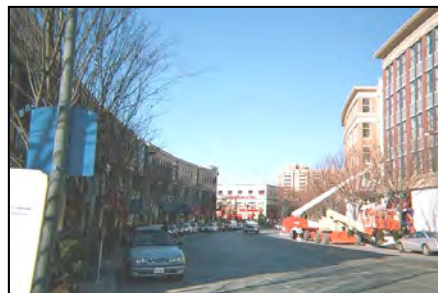


Helix Systems, Center for Information Technology & The Resource for Macromolecular Modeling & Bioinformatics *present:* Hands-on Workshop in Computational Biology



Bethesda, Maryland



The Program

Hands-on Workshop in Computational Biology



Prof. Klaus Schulten



Prof. Emad Tajkhorshid

Locations in Building 12A:

Lectures: Room B51

Labs: Room B51



Mon, 11/5: *Introduction to Protein Structure and Dynamics*



09:00-09:10 Opening Remarks

09:10-10:40 Structure and Sequence Analysis with VMD

Break

11:00-12:10 VMD for Structure Building and Dynamics Analysis

12:10-12:30 Q & A

Lunch

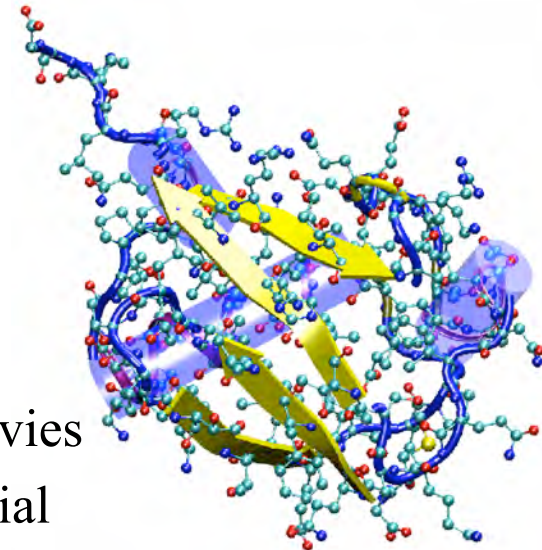
14:00-15:30 VMD Tutorial I

Break

16:00-17:30 VMD Tutorial II

Optional: VMD Images & Movies

Begin NAMD Tutorial



Ubiquitin

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



09:00-10:30 Molecular Dynamics with NAMD I

Break

10:50-12:10 Molecular Dynamics with NAMD II

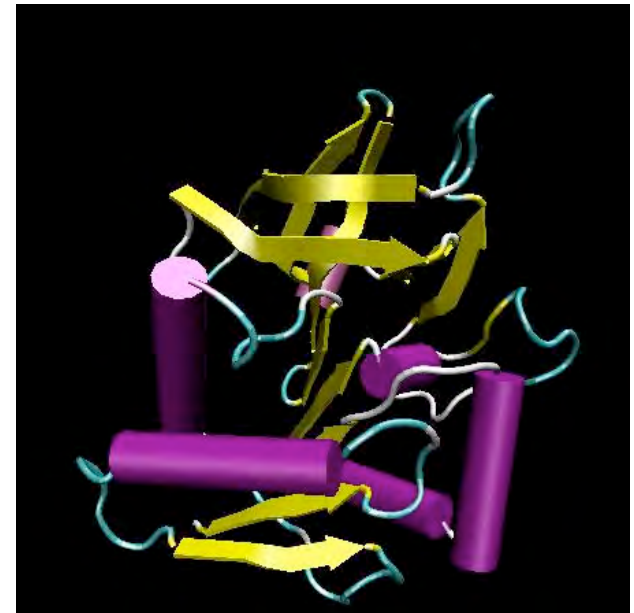
12:10-12:30 Q&A
Group photo

Lunch

14:00-16:00 NAMD Tutorial I

Break

16:15-18:00 NAMD Tutorial II



HisH

Wed, 11/7: *Parameters for Classical Force Fields*



09:00-10:30

Molecular Dynamics of Cellular Processes I – E. Tajkhorshid

Break

10:50-12:10

Molecular Dynamics of Cellular Processes II – K. Schulten

12:10-12:30

Q & A

Lunch

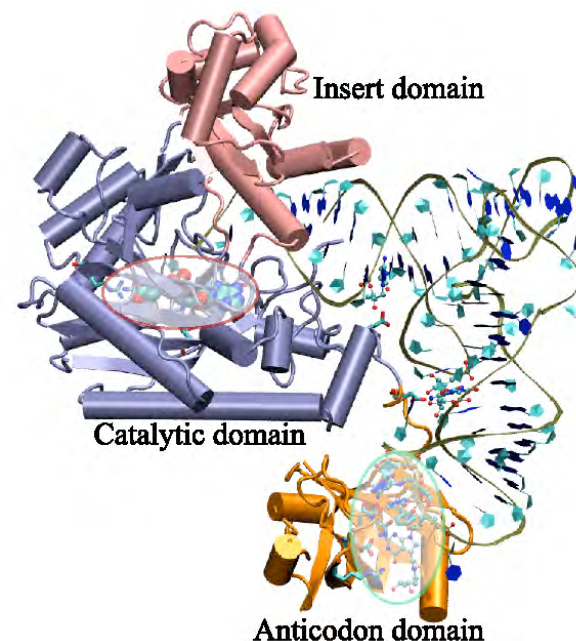
14:00-16:30

Parameterizing a Novel Residue,
Topology File Tutorials

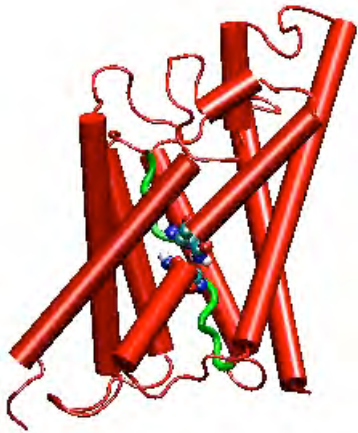
Break

16:45-18:00

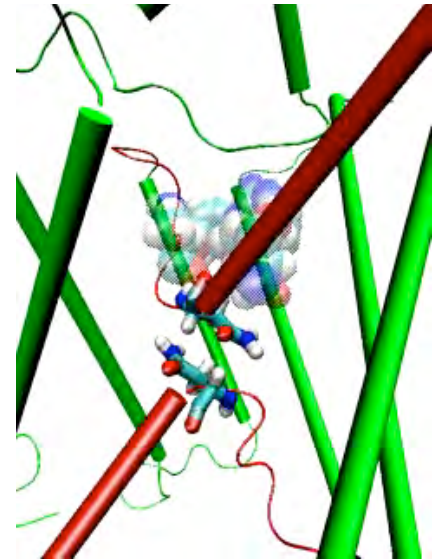
Nanotubes, Stretching Deca-alanine
Tutorials



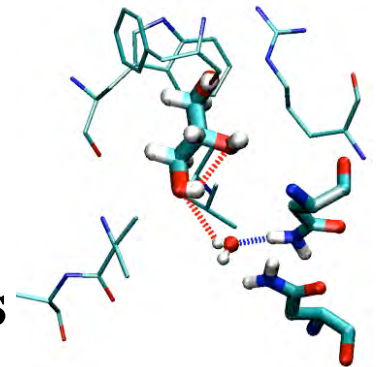
AspRS-tRNA



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

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J.C. Gumbart

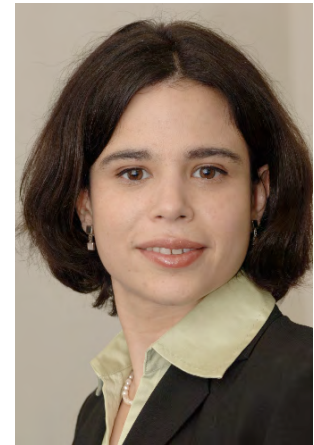


Marcos Sotomayor



Jen Hsin

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Dr. Rosemary Braun

<http://www.ks.uiuc.edu/Training/>

THEORETICAL *and* COMPUTATIONAL BIOPHYSICS GROUP

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

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Training

The Resource recognizes the vital importance of training for the education and professional growth of scientists. With so many techniques and technologies, researchers must continue to learn new and better ways of completing research, and should always be on the lookout for new tools to use, and new ways to use existing tools. In the sections below, we strive to provide a collection of tutorials and training methods to help scientists better utilize their talents, so that they may continue to advance their research. This section offers demos and tutorials on tools created by Resource members, and on techniques to assist the use of those tools. The links on this page lead to local as well as third-party training resources.

Spotlight

Hands-on Workshop in Urbana, Illinois. The Theoretical and Computational Biophysics Group offered a workshop, attempting to teach both the craft and art of modeling through learning by doing. During the week of November 8-12, 2004, 21 participants attended the **workshop** at the University of Illinois, in the Beckman Institute for Advanced Science and Technology. Participants learned how to stretch proteins, pull water through molecular channels, mine genomic data, and study biomolecules.

Other Spotlights



Announcements

- **New tutorial: Bionanotechnology Tutorial**

Brochures and Media Coverage

- **Training for the New Discipline** brochure ([pdf](#))
- 2004 Urbana Workshop brochure ([pdf](#))
- 2003 Summer School brochure ([pdf](#))
- Bringing Physics to Life ([html](#)) ([pdf](#))
- Media coverage ([story1](#), [story2](#)) of the Talca workshop (in Spanish)

Tutorials

- **Overview of Tutorials**
- **Main tutorials page**
- **Aquaporins with the VMD MultiSeq Tool**
- **Bionanotechnology Tutorial** NEW
- **Evolution of Biomolecular Structure: Class II tRNA-Synthetases and tRNA**
- **User-Defined Forces in NAMD**
- **NAMD Tutorial**
- **Parameterizing a Novel Residue**
- **Sequence Alignment Algorithms**