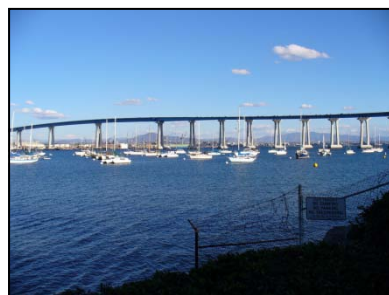


Resource for Macromolecular Modeling and Bioinformatics • National Resource for Automated Molecular Microscopy • National Biomedical Computation Resource present:

‘Hands-on’ Workshop on Computational Biophysics



San Diego, California





The training workshop is organized jointly with the Automated Molecular Imaging Center at The Scripps Research Institute.

We thank TSRI for its effort and hospitality. We thank in particular Professors Bridget Carragher and Clint Potter for their support and collegiality.

The Molecular Imaging Center is funded as a National Resource by NIH.

The Program

Hands-on Workshop in Computational Biology



Prof. Klaus Schulten



Prof. Zan Luthey-Schulten



Prof. Emad Tajkhorshid

Locations at Scripps:

Lectures and labs: Room CB107

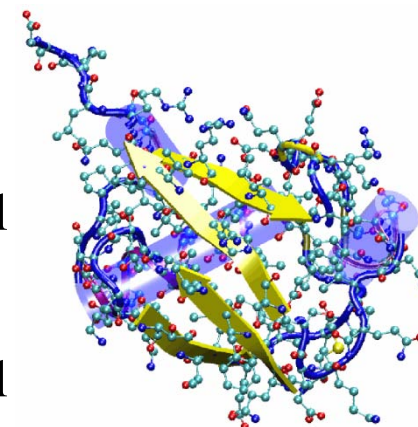
Breaks Room CB129



Mon, 7/12: *Introduction to Protein Structure and Dynamics*



08:30-09:00	Registration
09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
<i>Break</i>	
11:00-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
16:15-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



Ubiquitin

Tue, 7/13: *Statistical Mechanics of Proteins*



09:00-10:30 Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD

Break

10:50-12:00 Exemplary Applications of VMD / NAMD in Modern Research

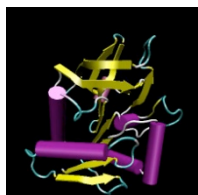
12:00-12:30 Q & A; Group picture

Lunch

14:00-16:00 Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials

Break

16:15-18:00 Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set Tutorials; Free Energy Set Tutorials



HisH

Wed, 7/14: *Introduction to Bioinformatics*



09:00-10:30 Introduction to Evolutionary Concepts in Bioinformatics:
MultiSeq in VMD

Break

10:50-12:00 Application of MultiSeq to Evolution of Translation
Machinery

12:00-12:20 Daily Q & A

Lunch

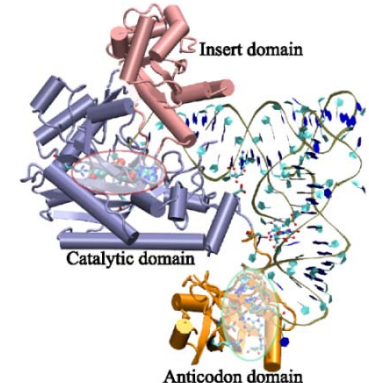
13:20-14:20 NBCR CADD Pipeline – Rommie Amaro

14:20-16:00 Tutorial options: Basic Sequence Analysis - Aquaporins with VMD;
Expert Sequence Analysis - Evolution of Translation – tRNA,
Ribosome, EF-Tu; Work on own projects

Break

16:15-18:00 Tutorial options: Basic Sequence Analysis - Aquaporins with VMD;
Expert Sequence Analysis - Evolution of Translation – tRNA,
Ribosome, EF-Tu; Work on own projects

AspRS-tRNA



Thu, 7/15: *Parameters for Classical Force Fields*



09:00-10:30 Introduction to Topology, Parameters, and Structure Files

Break

10:50-12:00 Examples and Applications

12:00-12:20 Q & A

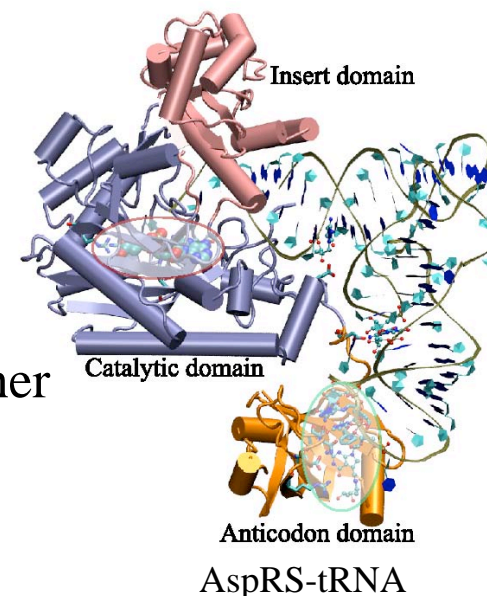
Lunch

14:00-14:30 Overview of NRAMM – Bridget Carragher

14:30-16:30 Parameterizing a Novel Residue

Break

16:45-18:00 Topology File Tutorial



Fri, 7/16: *Simulating Membrane Channels*



09:00-10:30 Introduction and Examples

Break

10:50-12:00 Transport in Aquaporins; Nanotubes

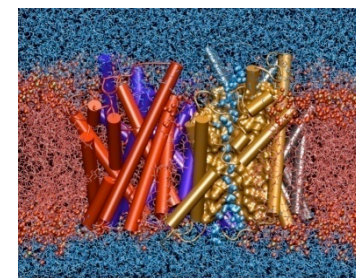
12:00-12:20 Daily Q&A

Lunch

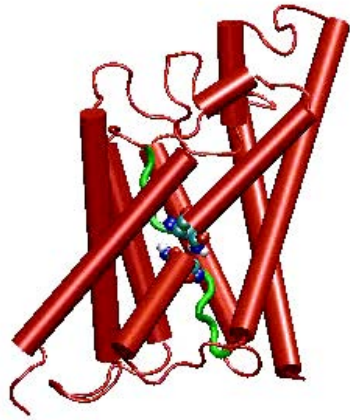
14:00-16:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials

Break

16:15-18:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials

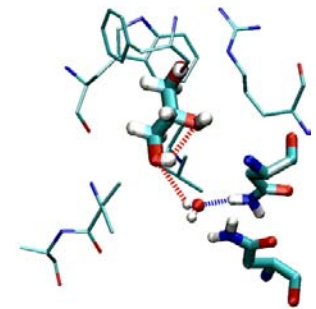
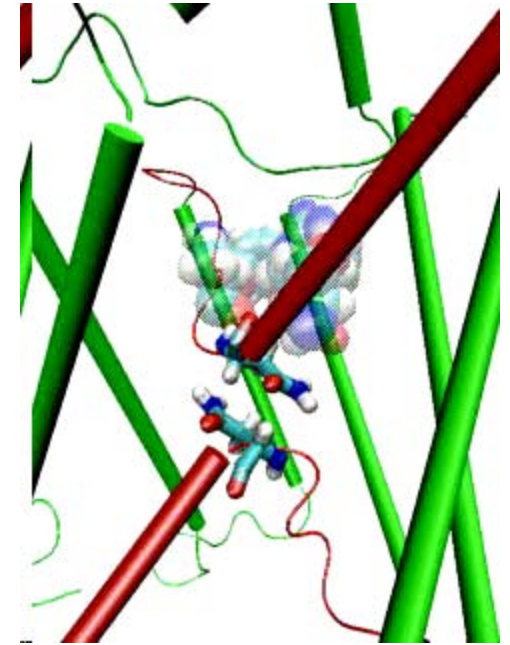


*Water Permeation
through Aquaporin*



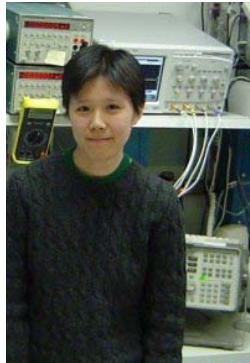
General

- **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

Teaching Assistants



Jen Hsin



J.C. Gumbart



John Eargle

National Institutes of Health,
National Center for Research Resources:

National Biomedical Computation Resource
Peter Arzberger, Director

National Resource for Automated Molecular Microscopy
Dr. Bridget Carragher, Director