

The Theoretical and Computational Biophysics Group and the National Resource for Biomedical Supercomputing present: Hands-on Workshop in Computational Biology



Pittsburgh, Pennsylvania



The Program

Hands-on Workshop in Computational



Prof. Klaus Schulten

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Prof. Zan Luthey-Schulten



Prof. Emad Tajkhorshid

Locations at PSC:

Lectures: Room 103

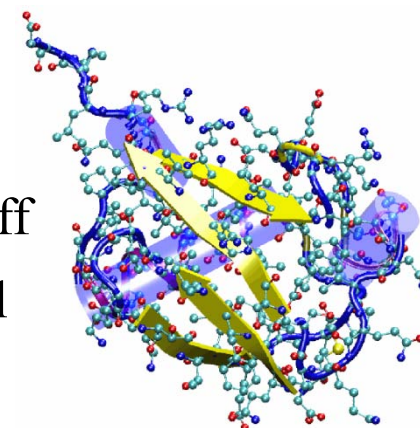
Labs: Room 110



Mon, 5/16: *Introduction to Protein Structure and Dynamics*



08:00-08:30	Registration and Continental Breakfast
08:30-09:00	Welcome and Brief Overview of the NRBSC - Markus Dittrich
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>	
13:30-14:00	Brief Overview of PSC - PSC Allocations Staff
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
16:00-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



Ubiquitin

Tue, 5/17: *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

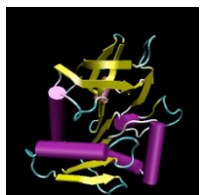
12:00-12:30 Q & A; Group picture

Lunch

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

Break

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



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Wed, 5/18: *Parameters for Classical Force Fields*



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

Break

10:50-12:00 Examples and Applications

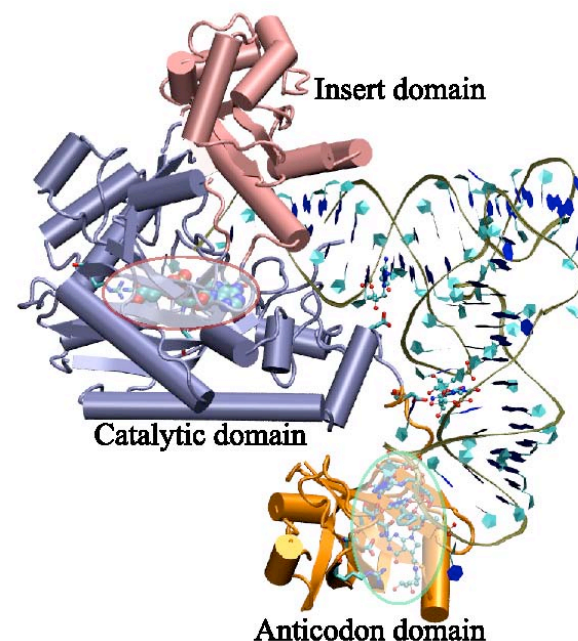
12:00-12:20 Q & A

Lunch

14:00-16:30 Parameterizing a Novel Residue

Break

16:45-18:00 Topology File Tutorial



AspRS-tRNA

Thu, 5/19: *Simulating Membrane Channels*



09:00-10:30 Introduction and Examples

Break

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

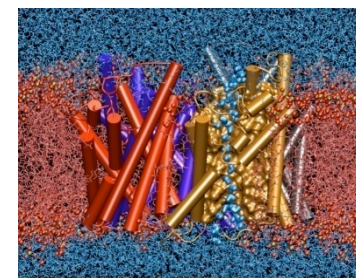
12:00-12:20 Daily Q&A

Lunch

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

Break

16:45-18:00 Tutorial options: Membrane Proteins & Nanotubes Tutorials;
Expert NAMD Set Tutorials; Free Energy Set Tutorials



Water Permeation
through
Aquaporin

Fri, 5/20: *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

14:00-16:00

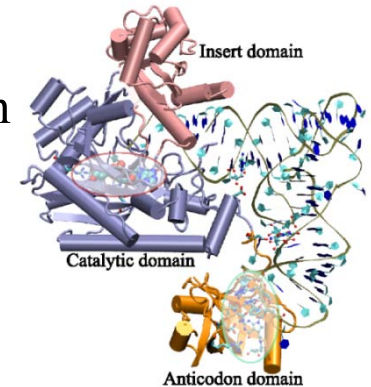
Tutorial options: Basic Sequence Analysis - Aquaporins with
VMD; Expert Sequence Analysis - Evolution of Translation –
tRNA, Ribosome, EF-Tu; Work on own projects

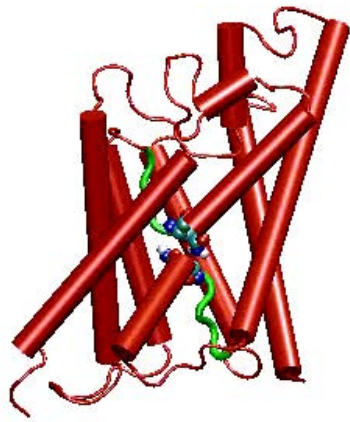
Break

16:45-18:00

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

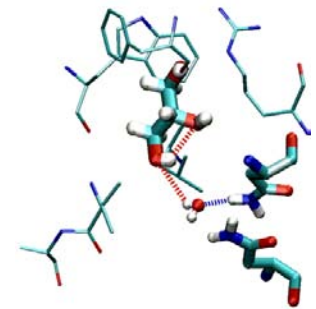
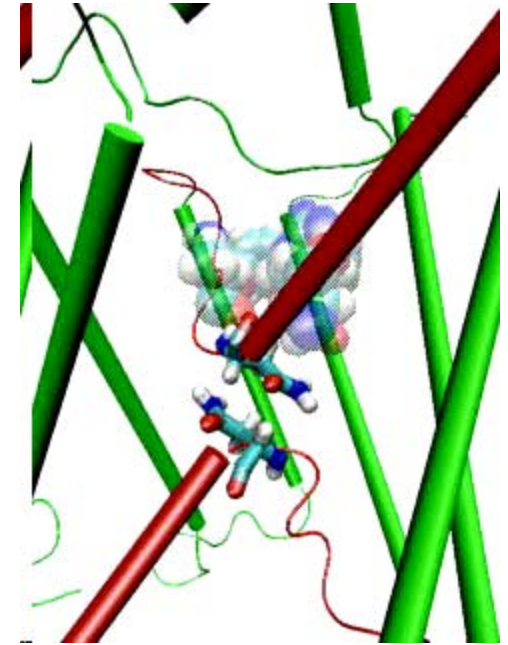
AspRS-tRNA





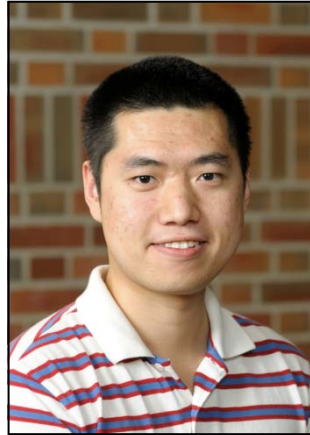
General

- 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
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- Model your own system
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- Please give us feedback to improve lectures and tutorials
 - Please give us feedback to encourage future courses



Acknowledgements

Teaching Assistants



Hang Yu



Yanxin Liu



John Eargle

Special
Thanks



Dr. Markus Dittrich
NRBS/PSC