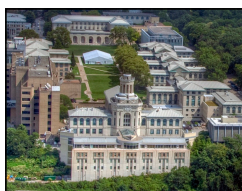


The Theoretical and Computational Biophysics Group and
 The National Center for Multiscale Modeling of Biological Systems presents:
Hands-on Workshop on Computational Biophysics
 Pittsburgh Supercomputing Center, Pittsburgh, Pennsylvania, June 1-5, 2015



Pittsburgh, PA



The Program

Hands-on Workshop on Computational Biophysics



Prof. Klaus Schulten



Prof. Zan Luthey-Schulten



Prof. Ivett Bahar



Prof. Timothy Lezon



Prof. Chakra Chennubhotla



Dr. Indira Shrivastava

Locations:

Morning lectures:

Room #103

Afternoon labs:

Room #110

Meals:

Room #102

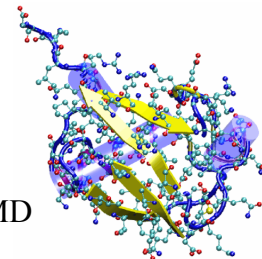
(MWF only)



Mon, 06/01: *Introduction to Protein Structure and Dynamics*



08:00-08:30	<i>Registration & Coffee</i>
08:30-09:00	Welcome, Overview, and Opening Remarks
09:00-10:30	Structure and Sequence Analysis with VMD
<i>Break</i>	
10:50-12:00	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

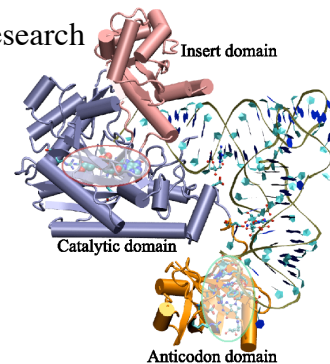


Ubiquitin

Tue, 06/02: *Statistical Mechanics of Proteins*



08:30-09:00	<i>Coffee Break</i>
09:00-10:30	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
<i>Break</i>	
10:50-12:00	Applications of VMD/NAMD in Modern Research
12:00-12:20	Q & A; Group Picture
<i>Lunch</i>	
14:00-16:00	NAMD Tutorial; Stretching Deca-alanine
<i>Break</i>	
16:15-18:00	GPU-accelerated Molecular Dynamics; Shape-based Coarse Graining



AspRS-tRNA

Wed, 06/03: *Introduction to Bioinformatics and Cell Simulations*



08:30-09:00

Coffee Break

09:00-10:30

Applications of Evolutionary Concepts and Network Analysis in VMD

Break

10:50-12:00

Introduction to Simulations of Whole Cells

12:00-12:30

Q & A

Lunch

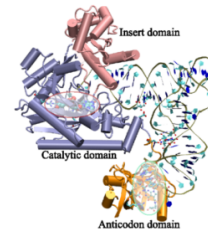
14:00-16:00

Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis

Break

16:15-18:00

Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis; Lattice Microbe Simulations



AspRS-tRNA

Thu, 06/04: *Collective Dynamics of Proteins Using Elastic Network Models*



08:30-09:00

Coffee Break

09:00-10:30

Elastic Network Models (ENMs) and Collective Motions using ANM Server and ProDy API

Break

10:50-12:00

Prody Overview and Applications

12:00-12:20

Q & A

Lunch

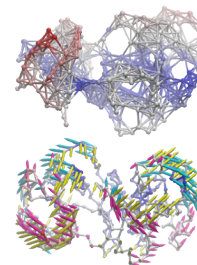
14:00-16:00

ProDy Tutorial; NMWiz Tutorial

Break

16:15-18:00

Option from: ENM Analysis; Ensemble Analysis; Structure Analysis; Trajectory Analysis; Conformational Sampling



Fri, 06/05: *Druggability Simulations and Sequence Evolution Patterns*



08:30-09:00 *Coffee Break*

09:00-10:30 Druggability: Methods and Applications using ProDy

Break

10:50-12:00 EVOL: Comparative Analysis of Sequence Evolution Patterns, Structure and Dynamics

12:00-12:20 Q & A

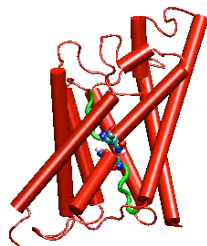
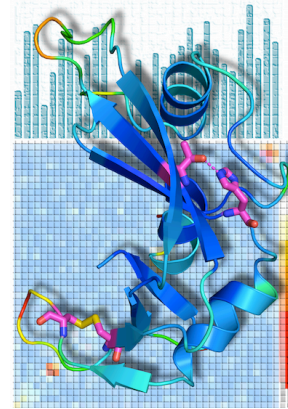
Lunch

14:00-15:30 Evol Tutorials in ProDy

15:30-16:00 Discussion and Closure

Break

16:15-18:00 Additional tutorials (optional)

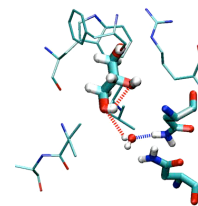
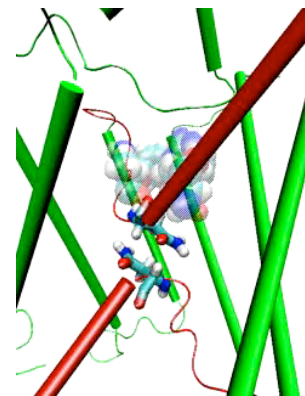


General

- **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

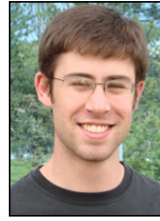
Teaching Assistants



Juan Perilla



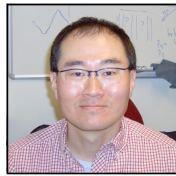
Keith Cassidy



Joseph Peterson



Mike Hallock



JiYoung Lee



She Zhang



Cihan Kaya