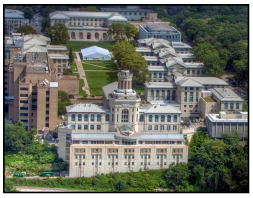
The Theoretical and Computational Biophysics Group and
The National Center for Multiscale Modeling of Biological Systems presents:
Hands-on Workshop on Computational Biophysics
Pittsburgh Supercomputing Center, Pittsburgh, Pennsylvania, June 1-5, 2015

Pittsburgh, PA



The Program

Hands-on Workshop on Computational Biophysics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Prof. Chakra Chennubhotla

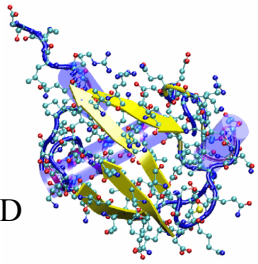

Dr. Indira Shrivashasta

Locations:

Morning lectures:	Room #103
Afternoon labs:	Room #110
Meals:	Room #102 (MWF only)

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

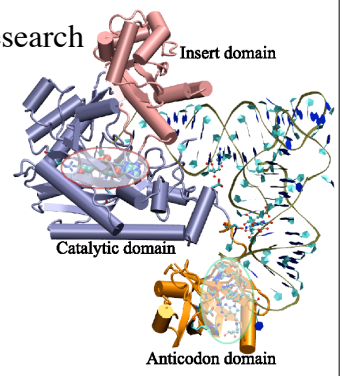
08:00-08:30	*Registration & Coffee*
08:30-09:00	Welcome, Overview, and Opening Remarks
09:00-10:30	Structure and Sequence Analysis with VMD
Break	
10:50-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
Lunch	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
Break	
16:15-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



Ubiquitin

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

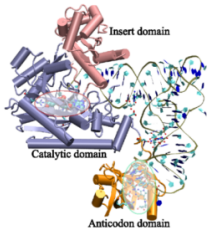
08:30-09:00	*Coffee Break*
09:00-10:30	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
Break	
10:50-12:00	Applications of VMD/NAMD in Modern Research
12:00-12:20	Q & A; Group Picture
Lunch	
14:00-16:00	NAMD Tutorial; Stretching Deca-alanine
Break	
16:15-18:00	GPU-accelerated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



AspRS-tRNA

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

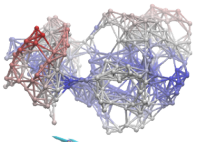
08:30-09:00	*Coffee Break*
09:00-10:30	Applications of Evolutionary Concepts and Network Analysis in VMD
Break	
10:50-12:00	Introduction to Simulations of Whole Cells
12:00-12:30	Q & A
Lunch	
14:00-16:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis
Break	
16:15-18:00	Tutorial options: Basic Sequence Analysis - Aquaporins with VMD; Evolution of Translation; Dynamical Network Analysis; Lattice Microbe Simulations

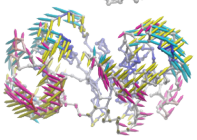


AspRS-tRNA

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

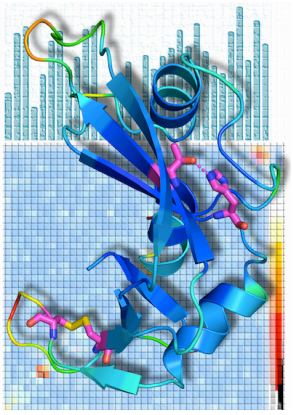
08:30-09:00	*Coffee Break*
09:00-10:30	Elastic Network Models (ENMs) and Collective Motions using ANM Server and ProDy API
Break	
10:50-12:00	Prody Overview and Applications
12:00-12:20	Q & A
Lunch	
14:00-16:00	ProDy Tutorial; NMWiz Tutorial
Break	
16:15-18:00	Option from: ENM Analysis; Ensemble Analysis; Structure Analysis; Trajectory Analysis; Conformational Sampling

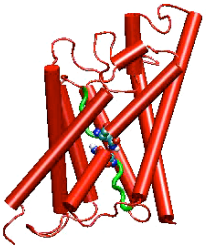




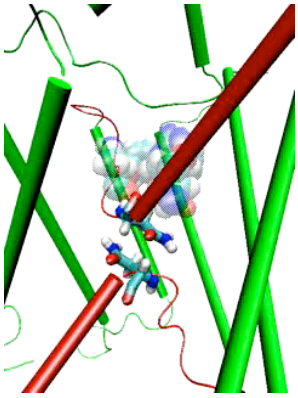
Fri, 06/05: *Druggability Simulations and Sequence Evolution Patterns*


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)

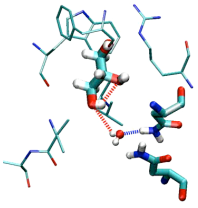




General



- **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

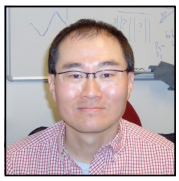
Teaching Assistants


Juan Perilla


Keith Cassidy


Joseph Peterson


Mike Hallock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