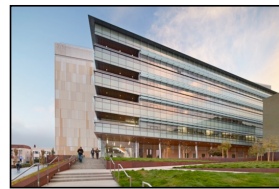
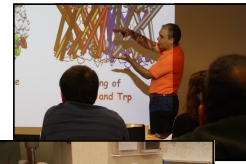


The Theoretical and Computational Biophysics Group presents:
Hands-on Workshop on Computational Biophysics
Energy Biosciences Institute, Berkeley, California, Aug 3-7, 2015



Berkeley, CA



The Program

Hands-on Workshop on Computational Biophysics



Prof. Klaus Schulten



Prof. Emad Tajkhorshid



Mr. Ryan McGreevy



Prof. Zan Luthey-Schulten

Locations:

Morning lectures:

Room #115

Afternoon labs:

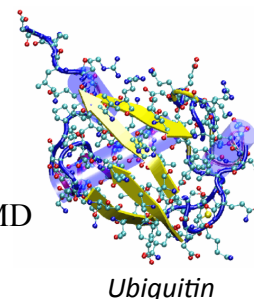
Room #115



Mon, 08/03: *Introduction to Protein Structure and Dynamics*



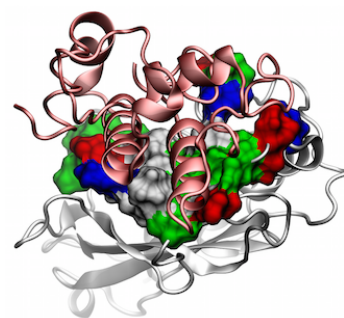
08:00-08:30	<i>Registration & Coffee</i>
08:30-09:00	Welcome, Overview, and Opening Remarks
09:00-10:30	Structure and Sequence Analysis with VMD
<i>Break</i>	
10:50-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
<i>Lunch</i>	
13:30-15:30	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
15:50-17:00	VMD Tutorial - Using VMD; NAMD Tutorial



Tue, 08/04: *Statistical Mechanics of Proteins*



08:00-08:30	<i>Coffee Break</i>
08:30-10:00	Analysis of Equilibrium and Non-equilibrium Properties of Proteins with NAMD
<i>Break</i>	
10:20-11:30	Applications of VMD/NAMD in Modern Research
11:30-11:50	Q & A; Group Picture
<i>Lunch</i>	
13:00-15:00	NAMD Tutorial; Stretching Deca-alanine
<i>Break</i>	
15:20-17:00	Stretching Deca-alanine; User-defined Forces in NAMD

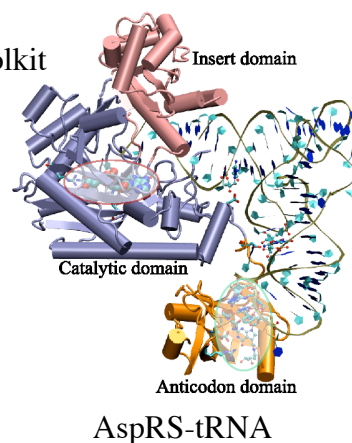


Cohesin-Dockerin

Wed, 08/05: *Force Field Parameterization*



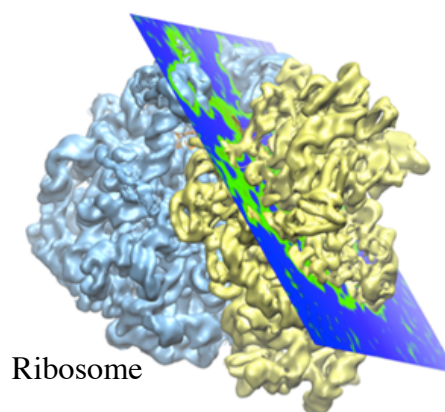
- 08:00-08:30 *Coffee Break*
- 08:30-10:00 Introduction to Topology, Parameters, and Structure Files
- Break*
- 10:20-11:30 Examples & Applications; Force Field Toolkit
- 11:30-11:50 Q & A
- Lunch*
- 13:00-15:00 Parameterizing a Novel Residue
- Break*
- 15:20-17:00 Topology File Tutorial



Thu, 08/06: *Molecular Dynamics Flexible Fitting*



- 08:00-08:30 *Coffee Break*
- 08:30-10:00 Molecular Dynamics Flexible Fitting Method I
- Break*
- 10:20-11:30 Molecular Dynamics Flexible Fitting Method II
- 11:30-11:50 Q & A
- Lunch*
- 13:00-15:00 MDFF; Structure Check
- Break*
- 15:20-17:00 MDFF; Structure Check



Fri, 08/07: *Introduction to Bioinformatics and Cell Simulations*



08:00-08:30

Coffee Break

08:30-10:00

Applications of Evolutionary Concepts and
Network Analysis in VMD

Break

10:20-11:30

Introduction to Simulations of Whole Cells

11:30-11:50

Q & A

Lunch

13:00-15:00

Lattice Microbe Simulations

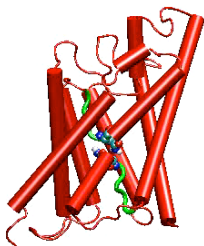
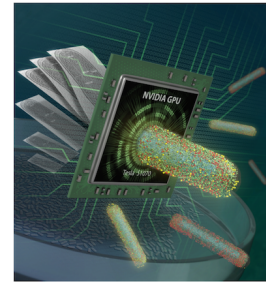
Optional: Evolution of Translation; Dynamical Network Analysis

Break

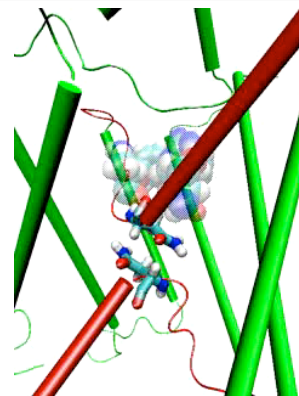
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Lattice Microbe Simulations

Optional: Evolution of Translation; Dynamical Network Analysis



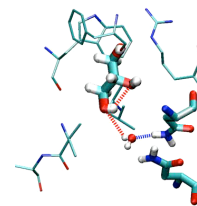
General



- 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

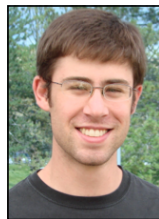
Teaching Assistants



Noah Trebesch



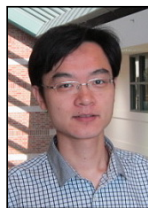
Keith Cassidy



Joseph Peterson



Mike Hallock



Wen Ma



Yi Zhang