NIH-funded Biomedical Technology & Research Centers

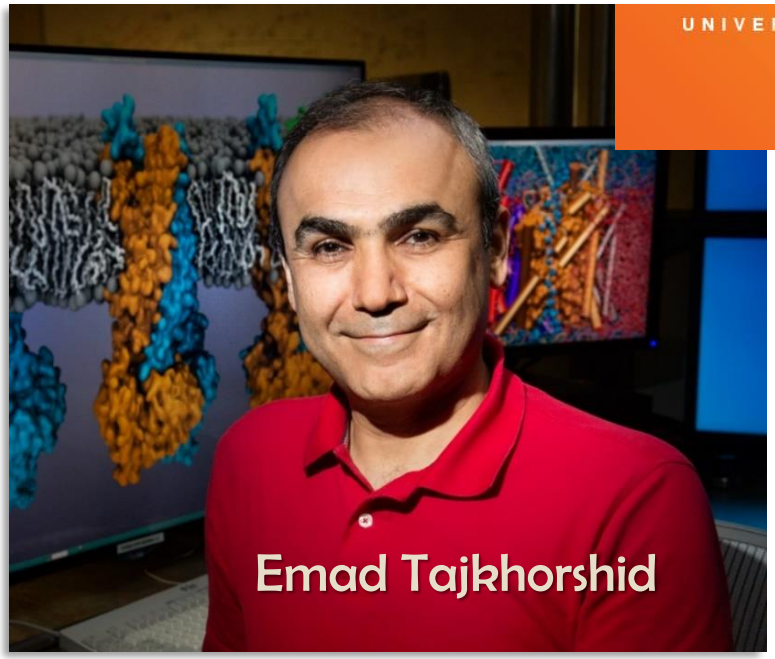
Hands-on Workshop on Computational Biophysics

Theoretical and Computational Biophysics Group (TCBG) and
National Center for Multiscale Modeling of Biological Systems (MMBioS)

June 28 -July 1, 2021

TCBG - Funded in 1989

"Bringing Physics to Life"



UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Professor of Biochemistry and Pharmacology, Biophysics and Computational Biology, Beckman Institute, U of Illinois, Urbana-Champaign

Software	Citations
NAMD	15,000+
VMD	38,000+

NIH-funded Biomedical Technology & Research Centers

MMBioS Funded in 2012

High Performance Computing BTRC *for* Multiscale Modeling of Biological Systems

Overarching biological theme:

- Spatial organization
- Temporal evolution

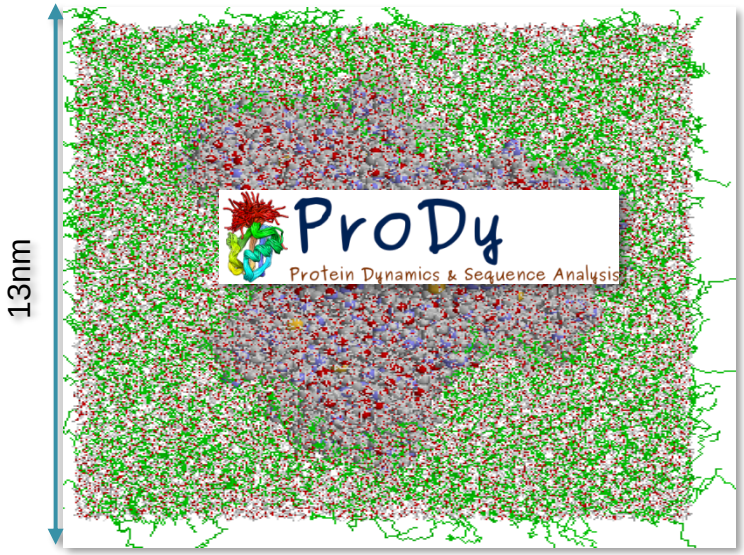
of

NIGMS

Synaptic Signaling & Regulation

MMBioS

Software development at multiple scale



to cellular architecture,

Ivet Bahar

Pemra Doruker

Burak Kaynak

Organization

Rozita Laghaei

Research Scientist, Pittsburgh Supercomputing Center rlagha@psc.edu

Ivan Cao-Berg
Research Software Specialist, PSC

Anna Reinhard
Dept Comp & Sys Biol, Pitt
ANR189@pitt.edu

Administrators

Gengkon Lum, BS
Senior System Administrator
gengkon@pitt.edu

Afshin E Nasrabad, PhD
System Administrator
afe9@pitt.edu

Adam Kohlhaas
Dept Comp & Sys Biol, Pitt
KohlhaasA@pitt.edu

Welcome!

Agenda

Day 1: Collective Dynamics of Proteins Using Elastic Network Models	
9:30-10:00	Welcome and Brief Overview by Ivet Bahar
10:00-11:20	Elastic Network Models (ENMs) and Collective Motions. Basic Theory and Methods, *Ivet Bahar*
11:20-11:40	Break / Social
11:40-1:00	Ensemble Analysis of Structures for Inferring Functional Mechanisms, DynOmics Server, *Pemra Doruker*
1:00-1:20	Q & A and Lunch / Dinner break
2:00-3:30	ProDy API Basics, *Burak Kaynak* GNM Analysis of Equilibrium Dynamics, *Burak Kaynak*
3:30-3:50	Break / Social
3:50-5:45	ANM Analysis of Collective Motions and Visualization by NMWiz, *Burak Kaynak* Ensemble Analysis by ProDy, *Bentley Wingert*

Agenda

Day 2: Bridging Sequence, Structure and Function, Allostery, Druggability	
10:00-11:20	Evol: Bridging Sequence and Structure,; Signature Dynamics of Protein Families, ENM for Membrane Proteins *Pemra Doruker*
11:20-11:40	Break / Social
11:40-1:00	Allostery and Druggability Simulations, *Burak Kaynak* and *Pemra Doruker,*
1:00-1:20	Q & A and Lunch / Dinner break
2:00-3:30	Evol and SignDy, *Daniel Penaherrera* and *Bentley Wingert* Membrane ANM, *Daniel Penaherrera*
3:30-3:50	Break / Social
3:50-5:45	ESSA, *Burak Kaynak* Druggability Suite, *Jiyoung Lee*