Hands-on Workshop on Computational Biophysics

Theoretical and Computational Biophysics Group (TCBG)

and

National Center for Multiscale Modeling of Biological Systems (MMBioS)

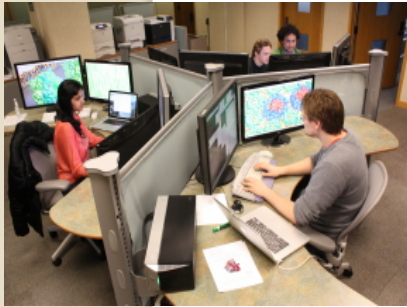# TCBG Funded in 1989

"Bringing Physics to Life"

Software - Citations
NAMD   9,000+
VMD   20,000+

Scientists solve chemical structure of HIV capsid

Klaus Schulten

UNIVERSITY OF ILLINOIS
AT URBANA-CHAMPAIGN

nature
THE HIV-1 CAPSID

NIH-funded Biomedical Technology & Research Centers

MMBioS

High Performance Computing BTRC
for
Multiscale Modeling of Biological Systems
(MMBioS)

Overarching biological theme:
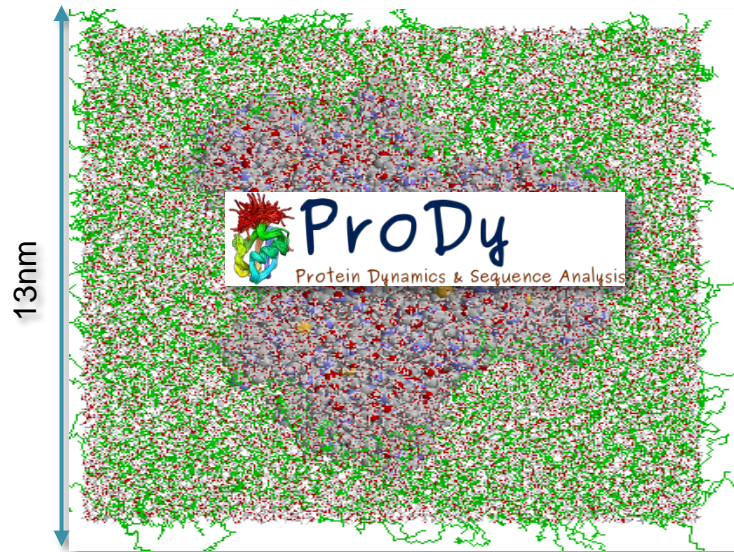
- Spatial organization
- Temporal evolution

of

Synaptic Signaling & Regulation

NIGMS

Salk

PSC

PITT

CMU

MMBioS

Software development at multiple scale

13nm
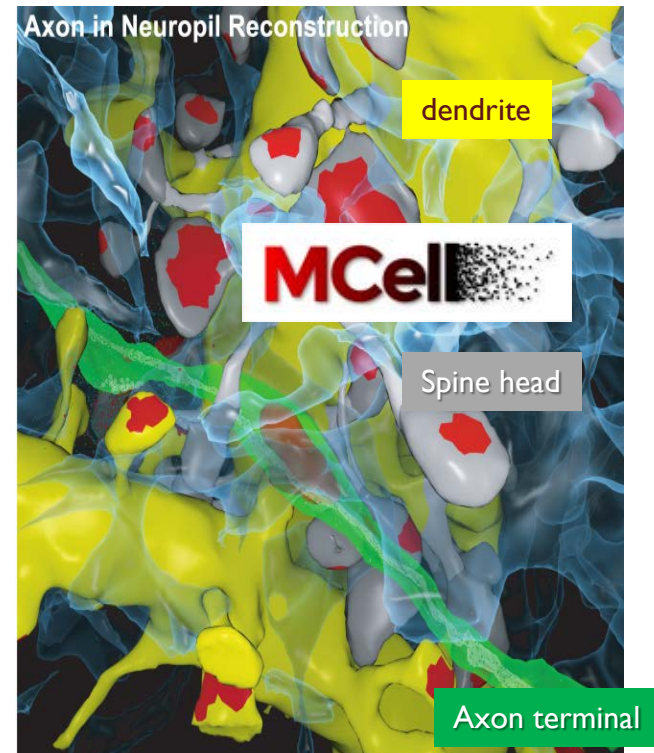
ProDy
Protein Dynamics & Sequence Analysis

Bakan & Bahar, *PNAS* 2009;
Bakan et al. *Bioinformatics* 2011 and 2014

May 30, 2017
Hands-on Workshop on
Computational Biophysics

June 26, 2017
Cell Modeling Workshop

to cellular architecture,

Axon in Neuropil Reconstruction

dendrite

MCell

Spine head

Axon terminal

T. Sejnowski

Tom Bartol

from 6 x 6 x 5 μm^3 sample of adult rat hippocampal stratum radiatum neuropil (by Kristen Harris). Visualization of *MCell* models is with *Blender*.

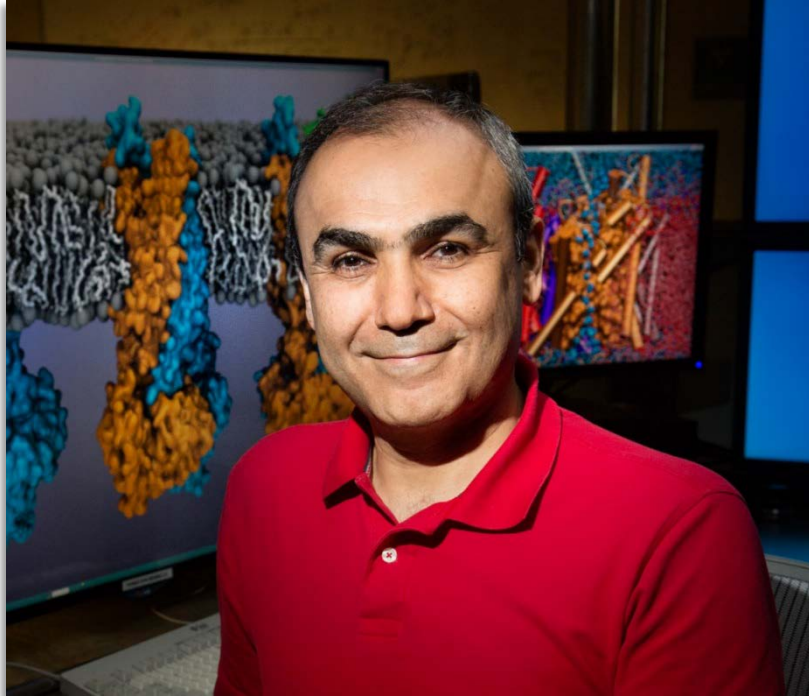http://www.mmbios.org/

Instructors/PIs

Ivet Bahar *Distinguished Professor*
JK Vries Chair, Computational & Systems Biology
U of Pittsburgh, School of Medicine

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

Training and Dissemination

Joao Ribeiro

Co-Leaders
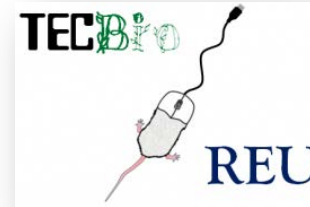
TECBio
REU

Alex Ropelewski
Senior Bioinformatics Specialist
Co-Director of MARC Initiative
Pittsburgh Supercomputing Center,
Carnegie Mellon University

Joseph Ayoob
Associate Professor, Computational and
Systems Biology Department, Pitt
Director, TecBio and DiscoBio Programs

MARC, training scientists/educators in
minority-serving institutions

Assistant Instructors

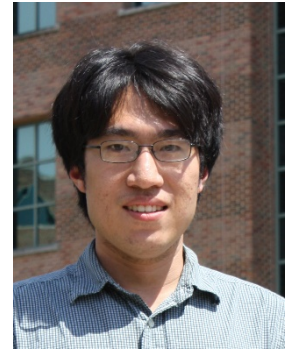**Dr. Hongchun Li**
Postdoctoral fellow, Pitt

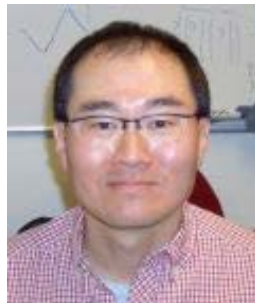**Cihan Kaya**
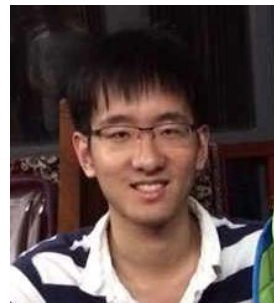PhD student Pitt/CMU

Dr. Karolina Mikulska-Ruminska
Postdoctoral fellow, Pitt

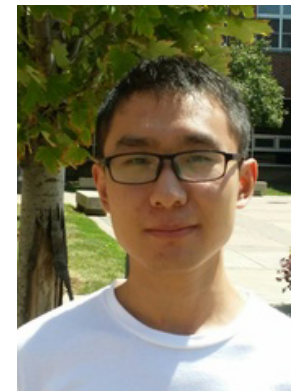**Dr. Paween Mahinthichaicha**
Postdoctoral fellow UIUC

Dr. JiYoung Lee
Res Assoc, Pitt

She (John)Zhang
PhD student, Pitt/CMU

Dr. James Krieger
Postdoctoral fellow, Pitt

Zhiyu Zhao
PhD student (UIUC)

Program

Tuesday, May 30

Collective Dynamics of Proteins Using Elastic Network Models. From single molecules to biological assemblies
Ivet Bahar

Wednesday May 31

Bridging Sequence, Structure and Function, and Experiments and Computations. Druggability Simulations
Ivet Bahar

Thursday June 1

Principles and Applications of Molecular Dynamics Simulations with NAMD, VMD & QwikMD
Emad Tajkhorshid

Friday June 2

Parameterization for Classical Force Fields with FFTK
Emad Tajkhorshid

Logistics

- [Downloads](#) if you will use your own la[ptop]
- Dinner on Thursday night
- Breakfast & lunch will be served
- Restaurants/cafes nearby (Porch, Red Oaks, Piada Italian Street Food)
- Photo on Thursday lunch break