Hands-on Workshop on Computational Biophysics

by

The Theoretical and Computational Biophysics Group (TCBG)
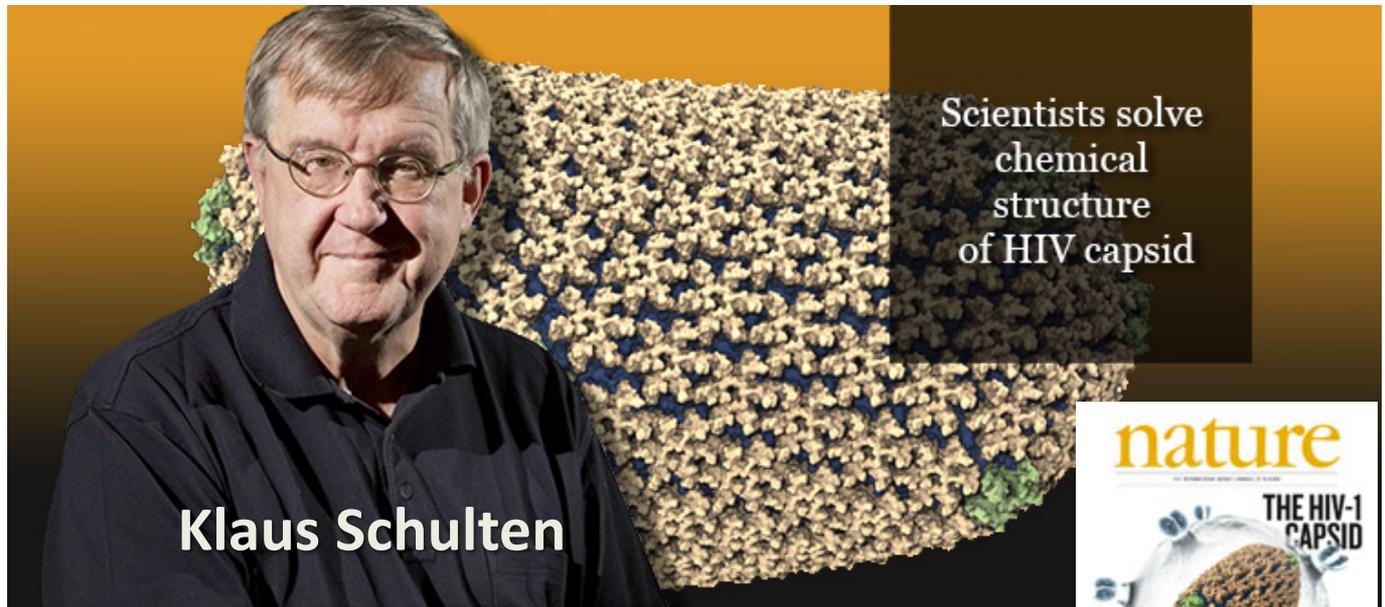
and

The National Center for Multiscale Modeling of Biological Systems (MMBioS)

TCBG Funded in 1989

NIH Biomedical

"Bringing Physics to Life"

Software - Citations
NAMD   5,000+
VMD   10,000+

Scientists solve chemical structure of HIV capsid

Klaus Schulten

nature

THE HIV-1 CAPSID

UNIVERSITY OF ILLINOIS
AT URBANA-CHAMPAIGN

NIH-funded Biomedical Technology & Research Centers

TCBG Funded in 1989

NIH Biomedical   "Bringing Physics to Life"

| Software - Citations	
NAMD	7,000+
VMD	18,000+

Professor Zaida (Zan) Luthey-Schulten

William and Janet Lycan Professor of Chemistry
Department of Chemistry, Department of Physics, Beckman Institute - NIH Resource for Macromolecular Modeling and Bioinformatics, Center for Biophysics and Computational Biology, Institute for Genomic Biology
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Lattice microbes
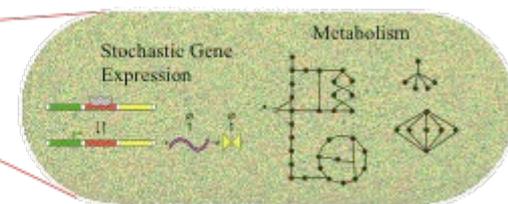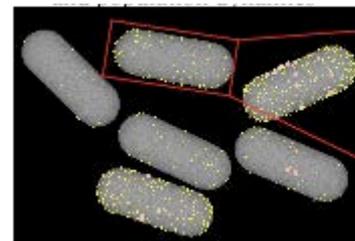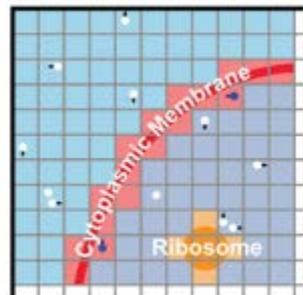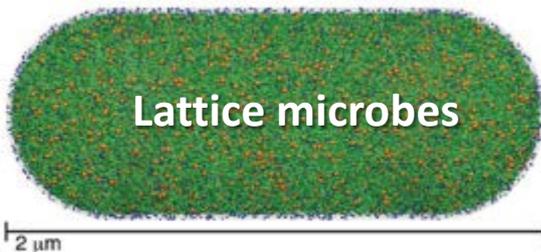
Bacterial Colonies

Juan R Perilla

Cassidy et al. (2015) CryoEM and computer simulations reveal a novel kinase conformational switch in bacterial chemotaxis signaling, *eLife* 4:e08419

Chemotactic Sensory Array - Keith Cassidy
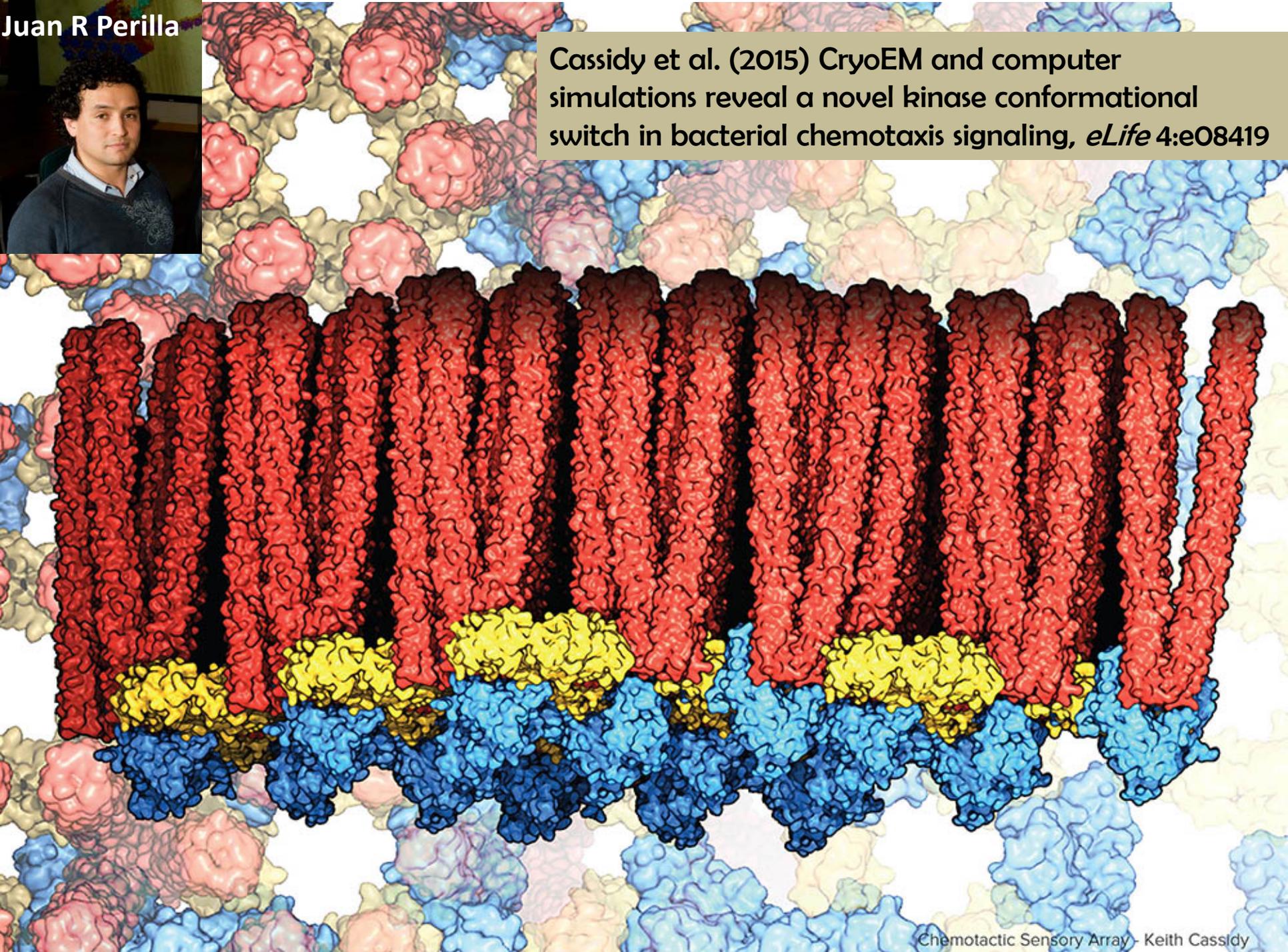
High Performance Computing
for
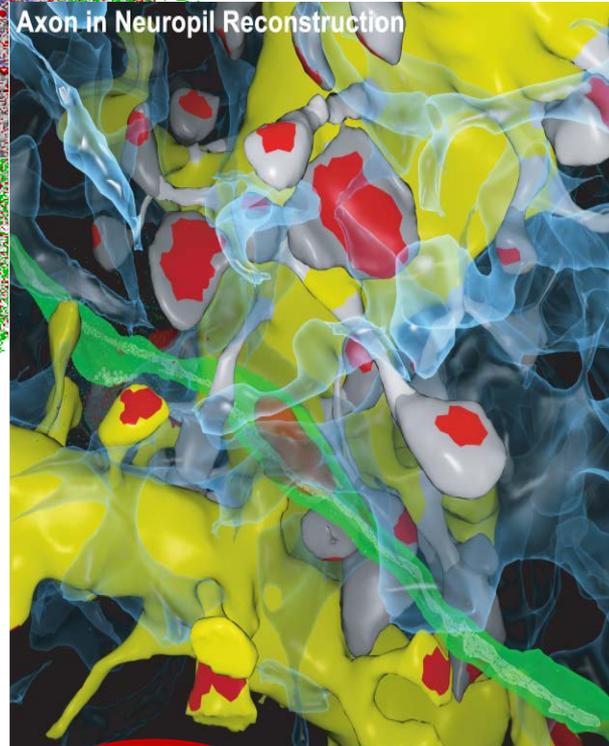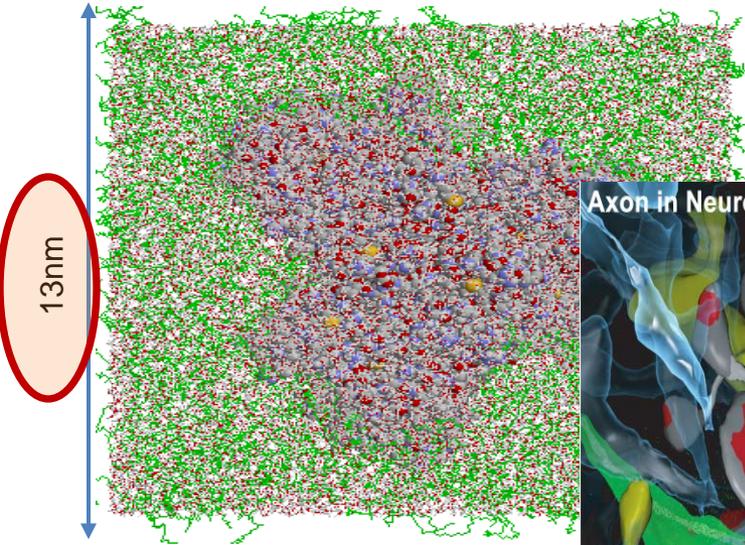# Multiscale Modeling of Biological Systems (MMBioS)

Overarching biological theme:

- Spatial organization
- Temporal evolution

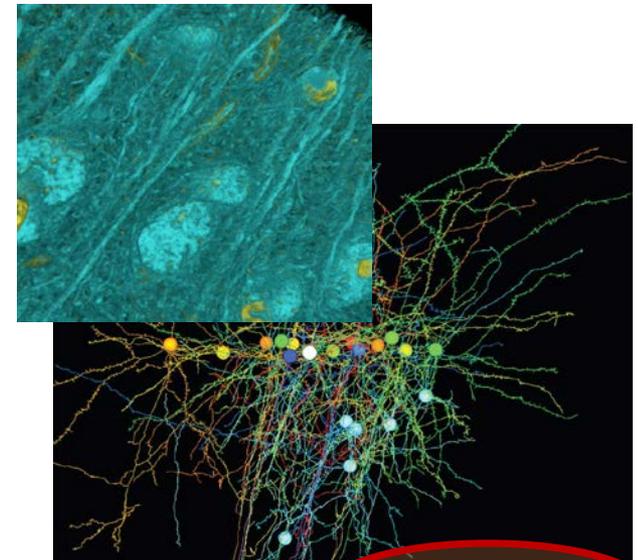of (neuro)signaling systems/events

Salk

PSC

PITT

CMU

From small molecules, to multimeric assemblies,

to cellular architecture,

13nm

Axon in Neuropil Reconstruction

from $6 \times 6 \times 5 \ \mu m^3$ sample of adult rat hippocampal stratum radiatum neuropil

to neural circuits

From ssEM images, $400 \times 400 \times 50 \ \mu m^3$
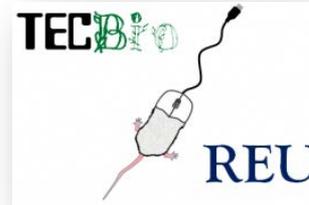
Training and Dissemination

Co-Leaders

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

MMBioS Resources

Eyal et al., *Bioinformatics* 2015

Li et al., *Nucleic Acids Res* 2016

MMBioS Resources

Bakan et al., Bioinformatics 2011; 2014

Zwier et al., *J Chem Theo Comp* 2015

Workshop Program

Mon, June 6: Introduction to Protein Structure and Dynamics - *Juan Perilla*

Tue, June 7: Statistical Mechanics of Proteins; Force Field Parameterization- *Juan Perilla*

Wed, June 8: Introduction to Evolutionary Concepts, Network Analysis and Cell Simulations- *Zaida Luthey-Schulten*

Thu, June 9: Collective Dynamics of Proteins Using Elastic Network Models - *Ivet Bahar*

Fri, June 10: Statistical Mechanics of Trajectories, Weighted Ensemble method – *Dan Zuckerman*
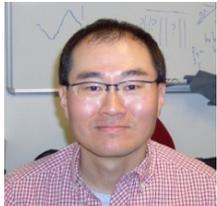
Assistant Instructors

Cihan Kaya
PhD student
Computational Biology
Carnegie Mellon University/University of Pittsburgh

Indira Shrivastava, PhD
Research Assistant Professor
Computational & Systems Biology, Pitt

JiYoung Lee, PhD
Research Associate
Department of Computational & Systems Biology
University of Pittsburgh

She Zhang
PhD student
Computational Biology
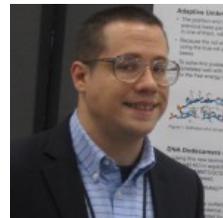Carnegie Mellon University/University of Pittsburgh

Karolina Mikulska-Ruminska, PhD
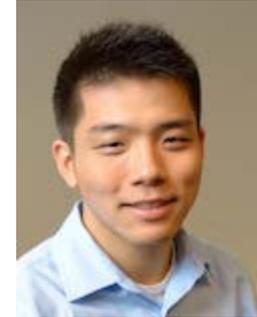Computational & Systems Biology, Pitt

Ernesto Suarez, PhD
Computational & Systems Biology, Pitt

Justin Spiriti, PhD
Computational & Systems Biology, Pitt

Yi Zhang
UIUC

Muyun Lihan
UIUC

Administration

Jessalynn M Oliver (Pitt)
jmo39@pitt.edu

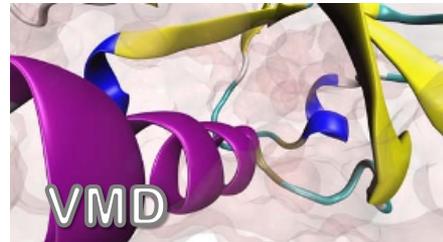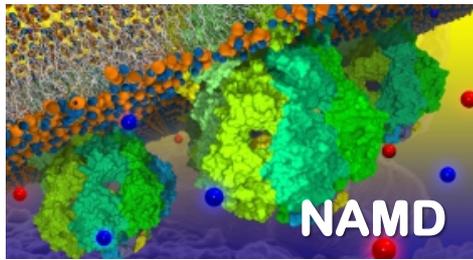**Patricia Sudac (PSC)**
sudac@psc.edu

NIH National Institutes of Health
Turning Discovery Into Health

Tutorials

Days 1-3

http://www.ks.uiuc.edu/Training/Tutorials/

NAMD

VMD

Day 4

http://www.csb.pitt.edu/prody/#tutorials

ProDy

NMWiz