

June 6-10, 2016

Hands-on Workshop on Computational Biophysics

by

**The Theoretical and Computational Biophysics
Group (TCBG)**

and

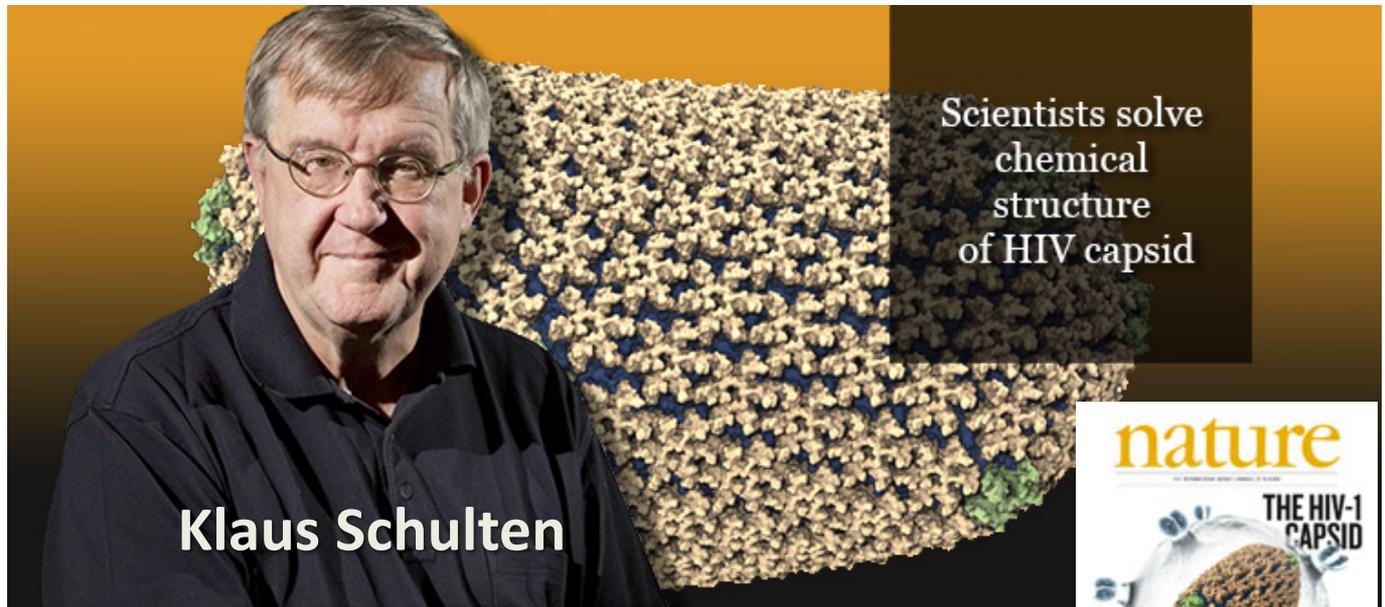
**The National Center for Multiscale Modeling of
Biological Systems (MMBioS)**

TCBG Funded in 1989

NIH Biomedical “Bringing Physics to Life”

Software - Citations

NAMD	5,000+
VMD	10,000+



Klaus Schulten

Scientists solve
chemical
structure
of HIV capsid



NIH-funded Biomedical Technology & Research Centers

TCBG Funded in 1989

NIH Biomedical “Bringing Physics to Life”

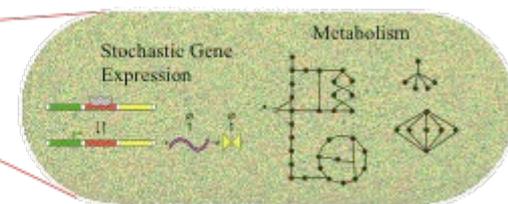
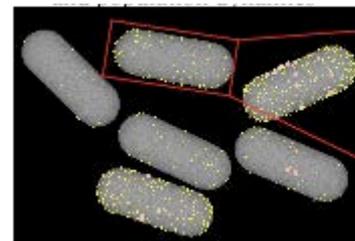
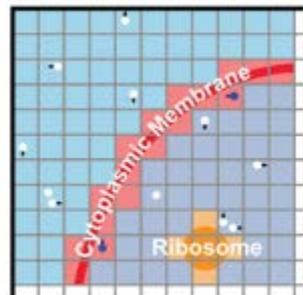
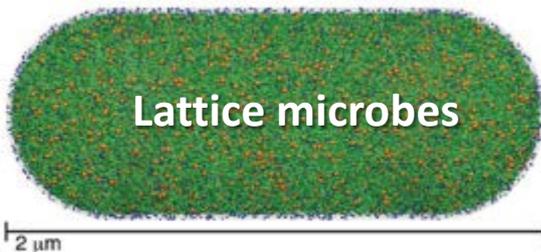
Professor Zaida (Zan) Luthey-Schulten

Software - Citations

NAMD	7,000+
VMD	18,000+



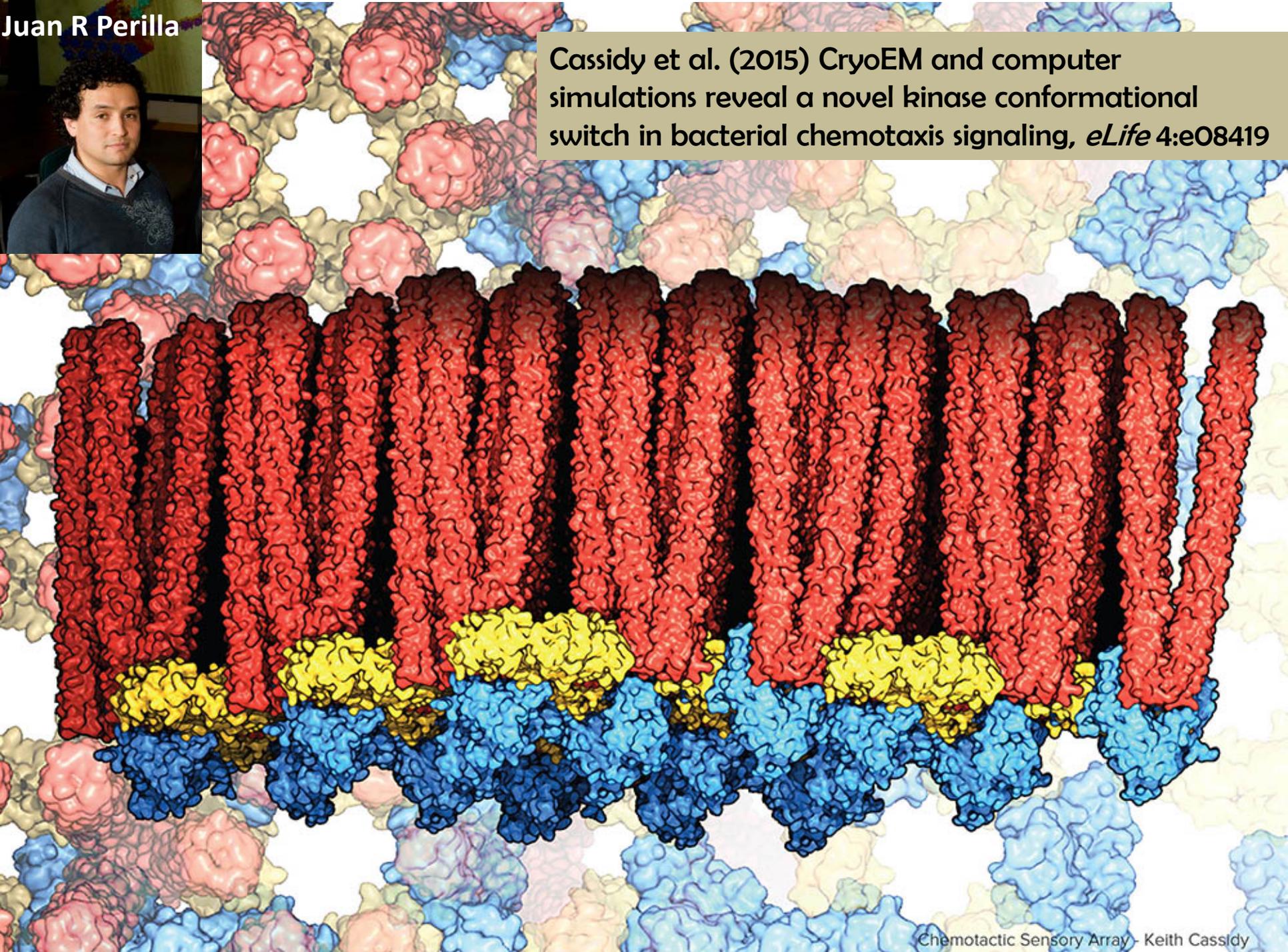
William and Janet Lycan Professor of Chemistry
[Department of Chemistry, Department of Physics, Beckman Institute - NIH Resource for Macromolecular Modeling and Bioinformatics, Center for Biophysics and Computational Biology, Institute for Genomic Biology](#)
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Bacterial Colonies



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



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

Overarching biological theme:

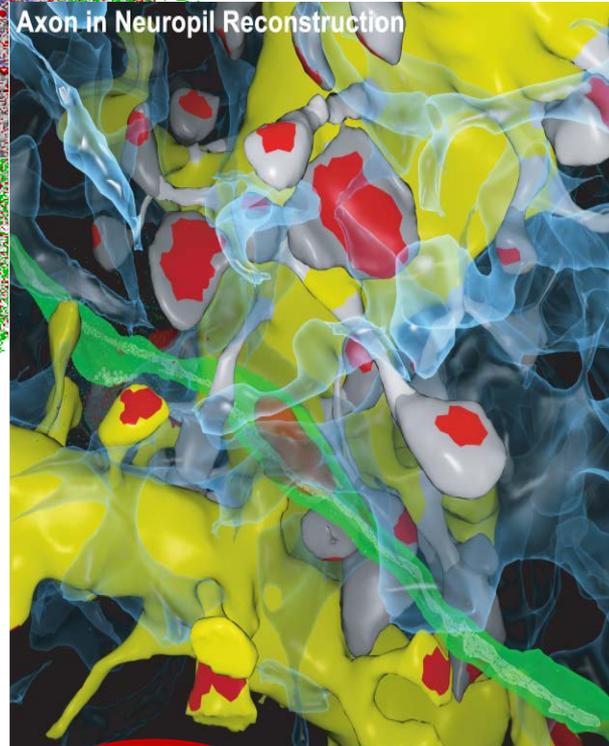
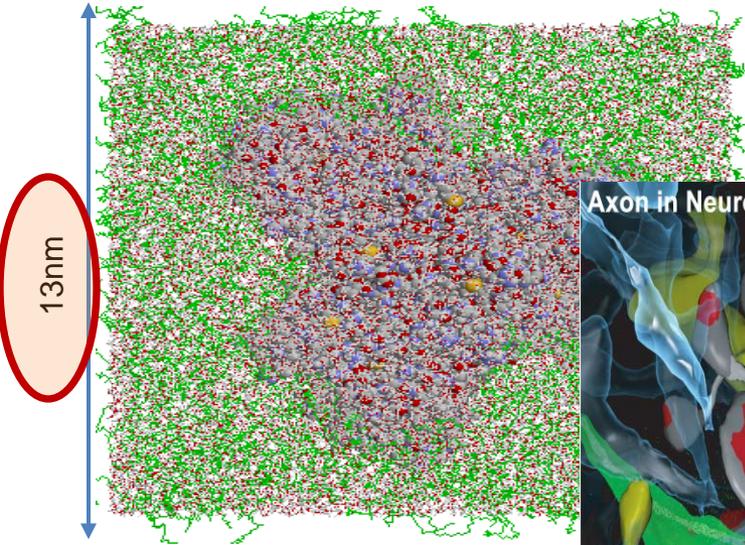
- Spatial organization
 - Temporal evolution
- of (neuro)signaling systems/events



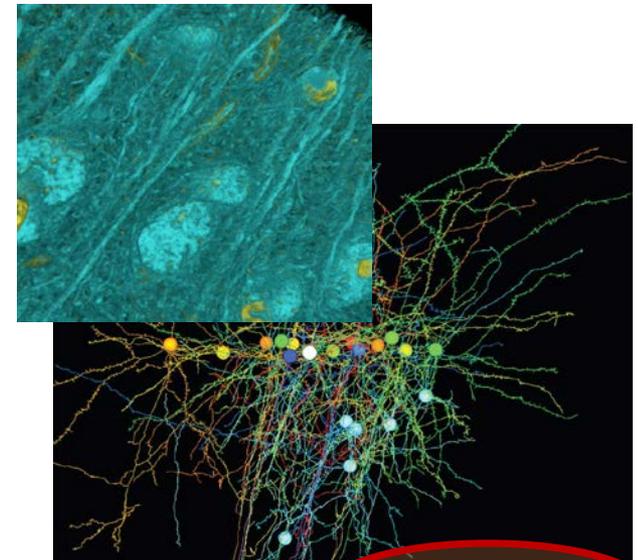
From small molecules, to multimeric assemblies,

to cellular architecture,

to neural circuits



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



From ssEM images, $400 \times 400 \times 50 \mu\text{m}^3$

Training and Dissemination

Co-Leaders



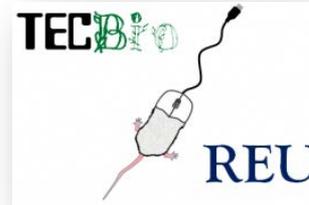
Alex Ropelewski

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

← → ↻ anm.csb.pitt.edu/cgi-bin/anm2/anm2.cgi ☆

Anisotropic Network Model Web Server 2.0 (2014)

What's new in this version? Having Java problems?

Enter the PDB id of your protein

pdb coordinates biological unit

or

Submit your own protein

No file chosen

ences Jmol site Related links Contact us S

iGNM 2.0 - Gaussian Network Model Database

[Home](#) | [Tutorial](#) | [Theory](#) | [References](#) | [oGNM 2.0](#) | [ANM 2.0](#) | [Computational & Systems Biology](#) | [NTHU site](#)

What is the GNM DB? Which questions can be answered?

Several studies in the last decade have drawn attention to the significance of intrinsic dynamics as a major determinant of the mechanism of action of proteins and their complexes (1-5). Intrinsic dynamics refers to conformational changes intrinsically favored by 3D structure, which often underlie the adaptation of biomolecules to functional interactions (6). As a consequence, an important question is to assess which structural elements (e.g. residues, secondary structures, domains, or entire subunits) undergo large fluctuations away from their mean positions (i.e. those enjoying high *mobility*), or which ones provide adequate *flexibility* to enable conformational changes (e.g. hinge-bending sites) that may be relevant to function. Furthermore, it is often of interest to determine which structural elements are subject to strongly correlated (or anticorrelated) motions, toward gaining insights into allosterically coupled regions. The GNM (7, 8) addresses these questions. It further allows to dissect these properties into the contributions of individual modes, thus elucidating the cooperative (*global*) couplings (cross-correlations) underlied by low frequency modes. For more information see [Theory](#) and [Tutorial](#).

Note: Query the GNM DB (iGNM 2.0) with a single PDB code (e.g., 1O1M and 4NIH, etc.); or, search the database with customized condition(s) using the "Advanced search".

PDB ID:

Biological assembly: Yes No

Molecular viewer: JsMol Jmol (fast response for big structures)

Advanced search:

Eyal et al., *Bioinformatics* 2015

MMBioS Resources

The image shows two overlapping browser windows. The foreground window displays the ProDy website (prody.csb.pitt.edu), which features a navigation menu with options like 'Evol', 'NIMWiz', 'membrANM', 'MechStiff', 'DruGUI', 'coMD', 'Downloads', 'Tutorials', and 'Statistics'. The main content area is titled 'ProDy Project' and describes it as a free and open-source Python package for protein structural dynamics analysis. It lists various analysis capabilities such as 'Structure analysis' (PDB and DCD file parsers, contact identification) and 'Dynamics analysis' (Principal component analysis, Normal mode analysis). A reference is cited: Bakan A, Meireles LH, Bahar I. ProDy: Protein Dynamics Inferred from Theory and Experiments 2011 *Bioinformatics* 27(11):1575-1577. The website also includes sections for 'People', 'Community', 'Source Code', and 'Problems?'. The background window shows the 'Anisotropic Network Model Web Server 2.0 (2014)' and the WESTPA GitHub repository page (https://westpa.github.io/westpa/), which includes a 'What is WESTPA?' section and a list of key features like 'Highly scalable' and 'Interoperable'.

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



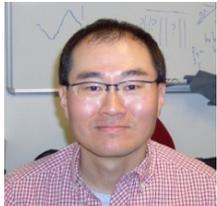
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Karolina

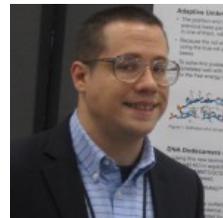
Mikulska-Ruminska, PhD

Computational & Systems Biology, Pitt



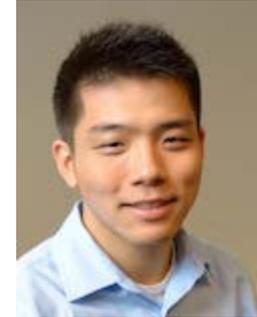
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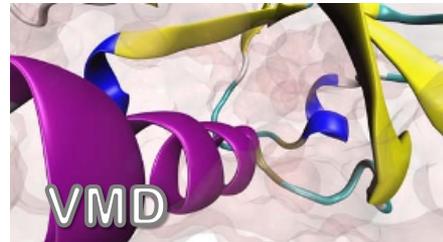
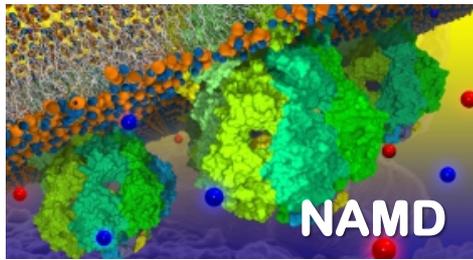


National Institutes of Health
Turning Discovery Into Health

Tutorials

Days 1-3

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



Day 4

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

