

June 10-14, 2013

# Hands-on Workshop on Computational Biophysics

by

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

and

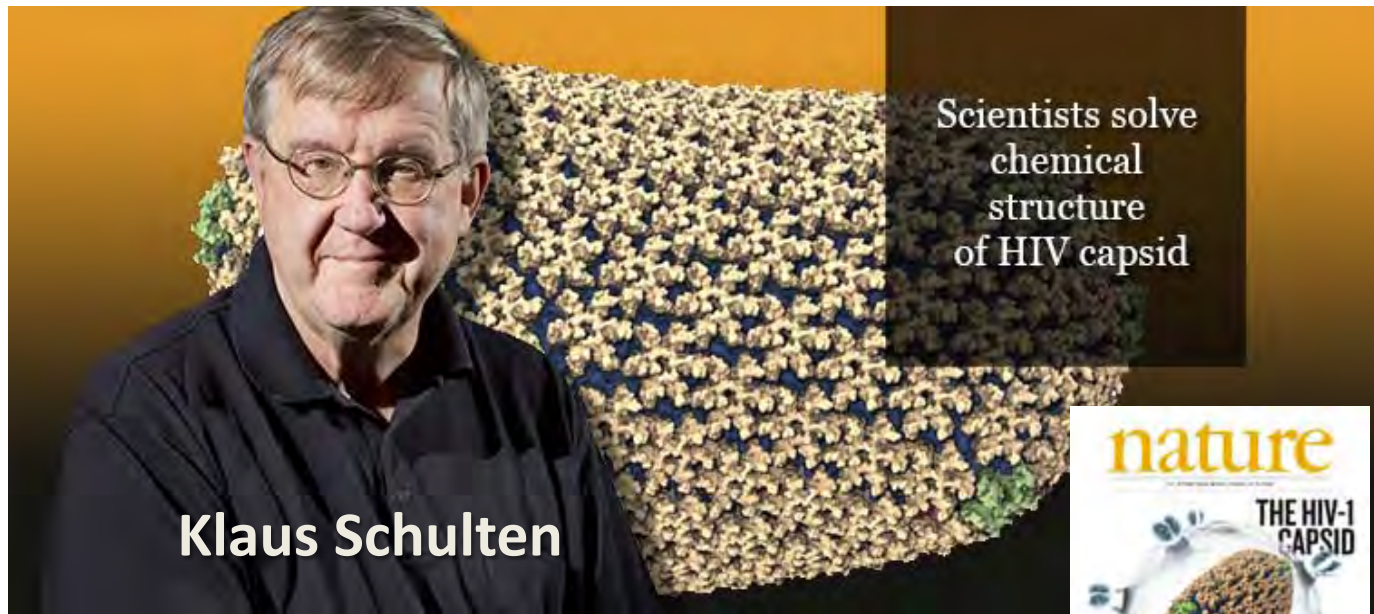
**The National Center for Multiscale Modeling of  
Biological Systems (MMBioS)**

# 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

UNIVERSITY OF

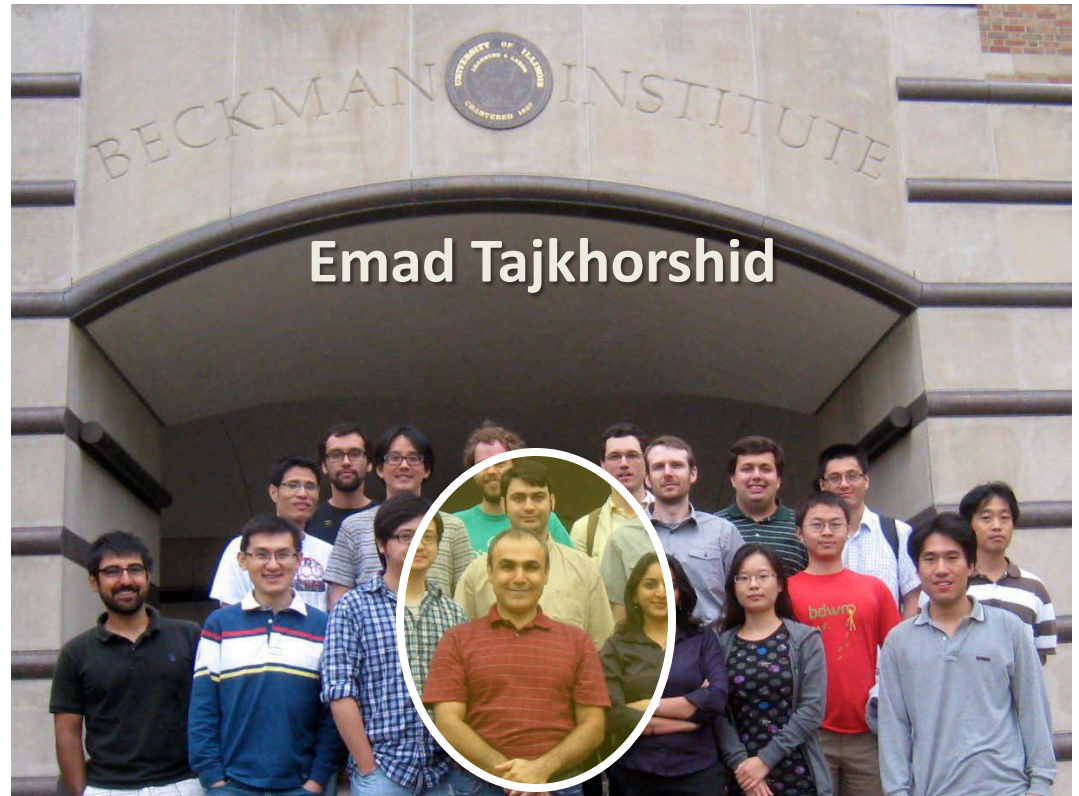
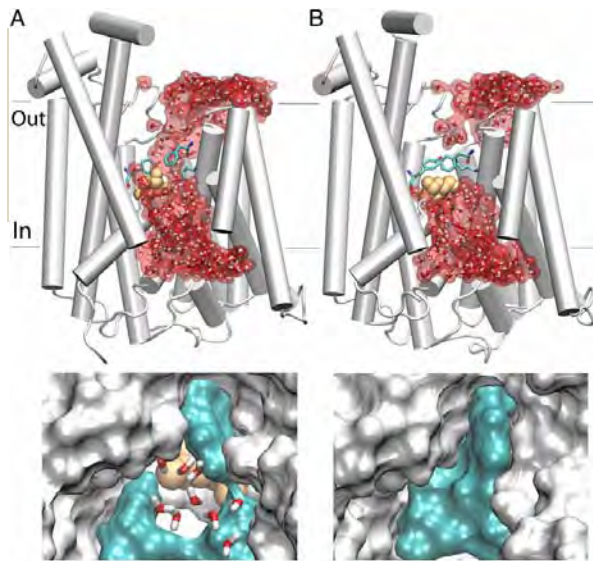
Distinguished Service Award, Biophysical Society (2013)

AT URBANA-CHAMPAIGN

NIH-funded Biomedical Technology & Research Centers

# TCBG Funded in 1989

NIH Biomedical “Bringing Physics to Life”



Li et al. *Proc Natl Acad Sci USA* 2013 **110**: 7696–701

**Associate Professor of Biochemistry, Biophysics, and Pharmacology**

Dept of Biochem, School of Mol and Cell Biol; Pharmacol, Coll of Medicine  
Center for Biophys & Comp Biol, Beckman Inst for Advanced Sci & Technol



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



John K. Vries Chair and Founder of the Dept of  
Computational & Systems Biology (CSB), School of Medicine  
(SOM), U of Pittsburgh (Pitt); Director of MMBioS Center

## *Overarching biological theme:*

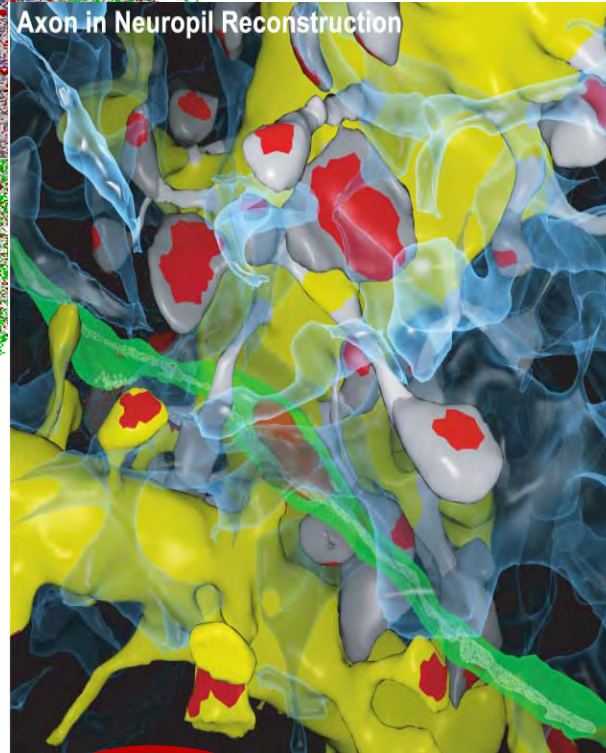
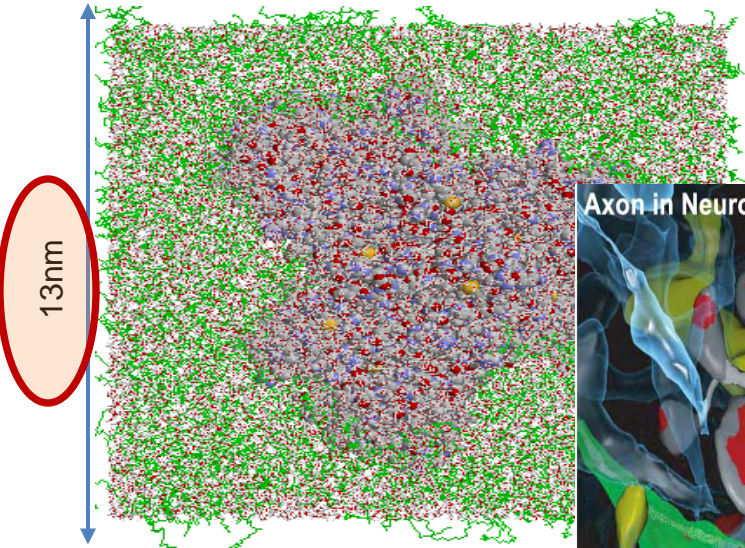
- Spatial organization
  - Temporal evolution
- of (neuro)signaling systems/events



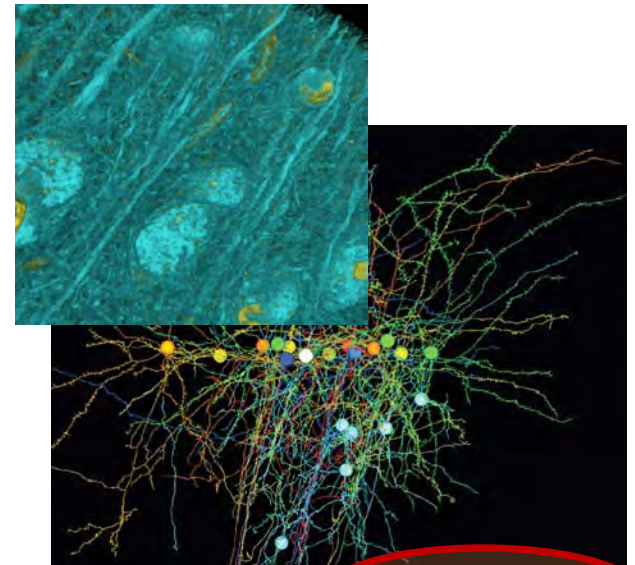
From small molecules, to multimeric assemblies,

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

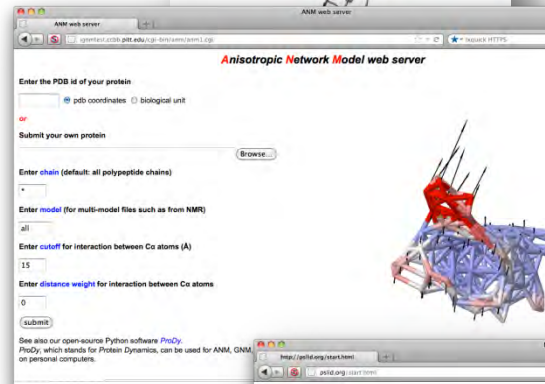


# Training and Dissemination

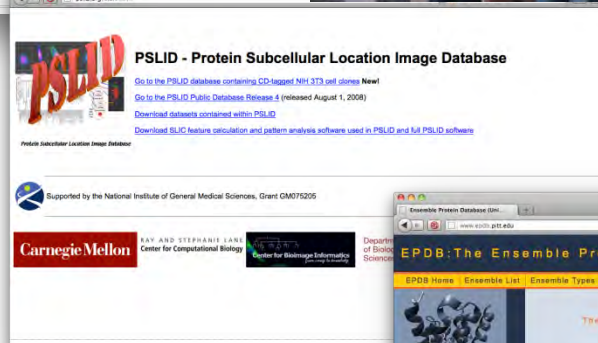
Leader



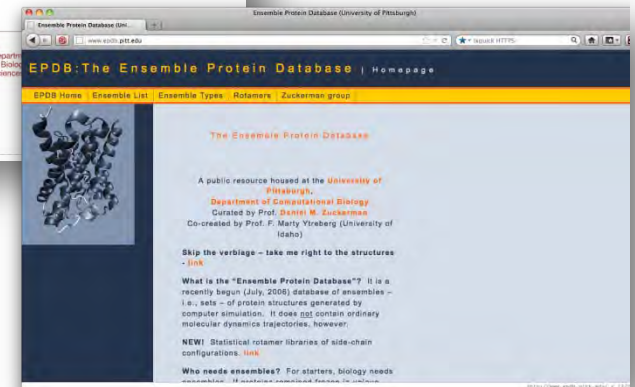
**Markus Dittrich, PhD**  
MMBioS and NRBC Group Leader,  
Pittsburgh Supercomputing Center,  
Carnegie Mellon University



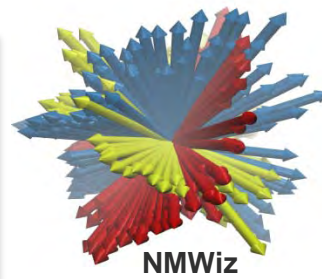
ANM



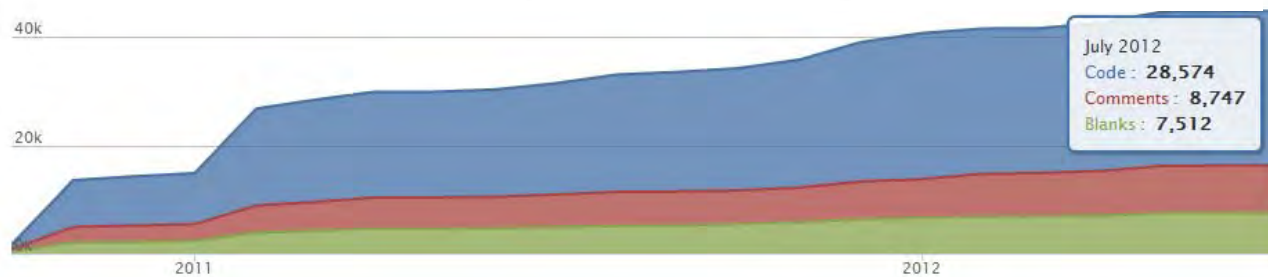
PSLID



EPDB



## Code Analysis & Usage Statistics

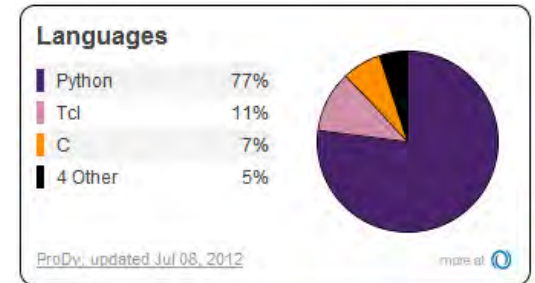
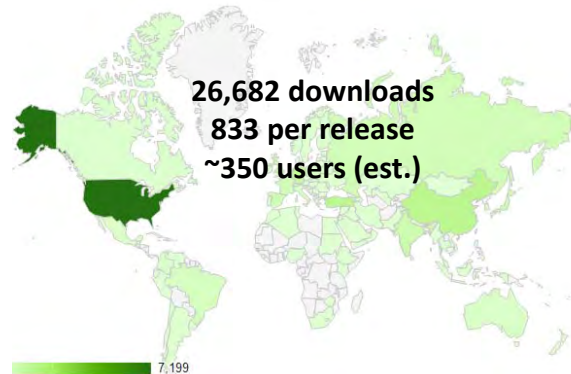


**Dr. Ahmet Bakan**  
Res Assoc, Dept Comp  
and Sys Biol (DCSB), Pitt



**Dr. Timothy R Lezon**  
Assistant Prof, DCSB, Pitt

[i/ProDy](#)



**Pages / Visit: 4.10**

**Avg. Visit Duration: 00:05:27**

Source <http://www.google.com/analytics/>

### Reference:

Bakan A, Meireles LM, **Bahar I.** (2011) ProDy: Protein dynamics inferred from theory and experiments *Bioinformatics* **27**:1575-7

# Workshop Program

**Mon, June 10: Introduction to Protein Structure and Dynamics -**

*Klaus Schulten*

**Tue, June 11: Statistical Mechanics of Proteins; Force Field**

**Parameterization- *Klaus Schulten and Emad Tajkhorshid***

**Wed, June 12: Simulating Membrane Proteins - *Emad Tajkhorshid***

**Thu, June 13: Collective Dynamics of Proteins Using Elastic Network**

**Models - *Ivet Bahar, Tim Lezon and Ahmet Bakan***

**Fri, June 14: Druggability Simulations, and Analyzing Sequence**

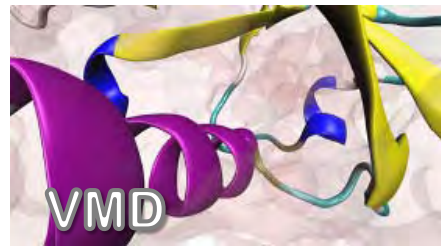
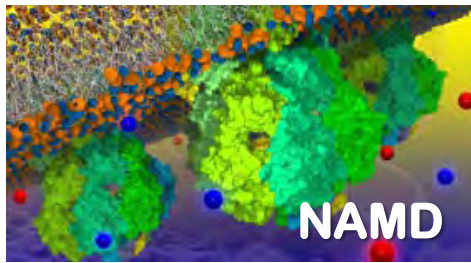
**Patterns and Structural Dynamics - *Ivet Bahar and Ahmet Bakan***



# Tutorials

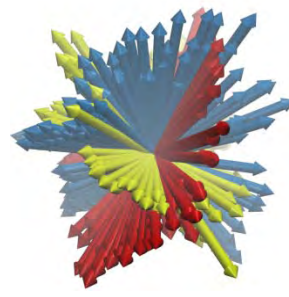
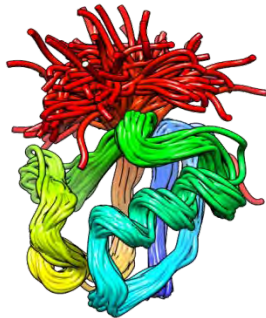
## Days 1-3

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



## Days 4-5

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



# Acknowledgments

## Teaching Assistants



[Juan Perilla](#)



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