



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”



Klaus Schulten



NIH-funded Biomedical Technology & Research Centers

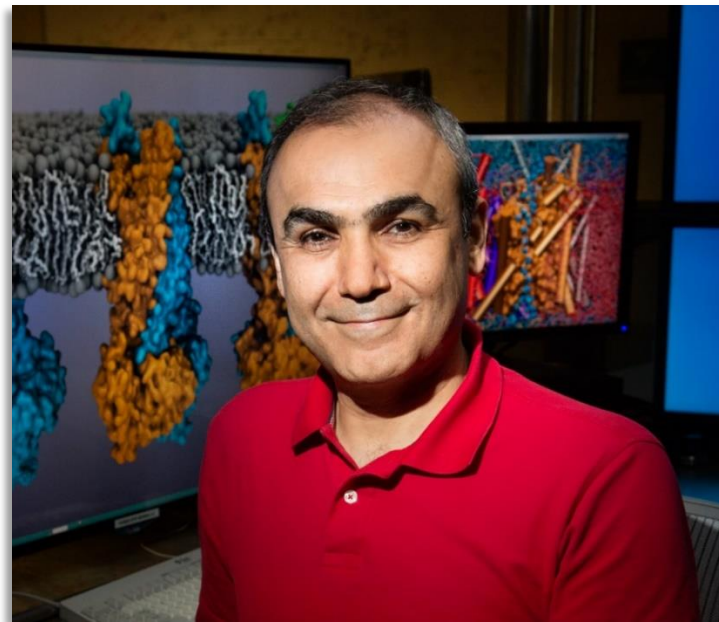
TCBG Funded in 1989

“Bringing Physics to Life”

Software - Citations

NAMD 11,800+

VMD ~28,600



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



Dr. João Ribeiro



Dr. Mariano Spivak

NIH-funded Biomedical Technology & Research Centers

MMBioS Funded in 2012

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

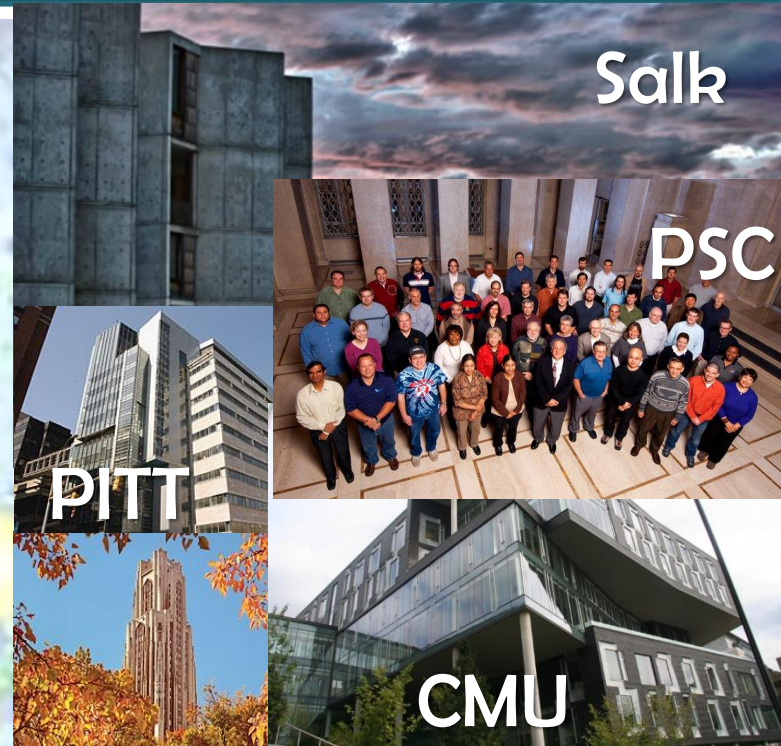
Overarching biological theme:

- Spatial organization
- Temporal evolution

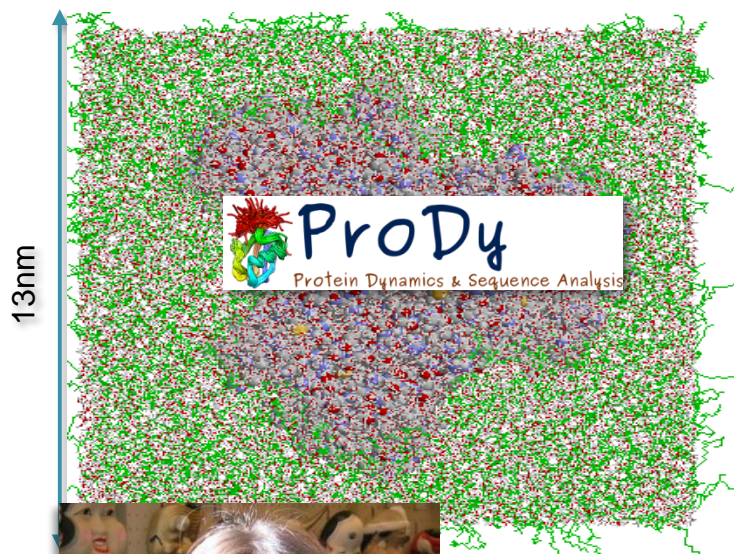
of

Synaptic Signaling & Regulation

NIGMS



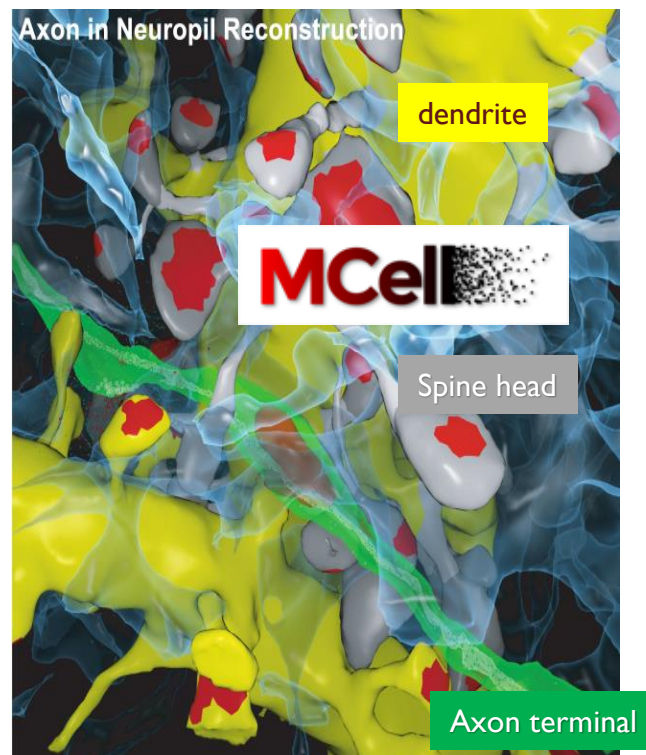
Software development at multiple scale



09;
2011 and 2014

Ivet Bahar Distinguished Professor
Computational & Systems Biology
U of Pittsburgh, School of Medicine

to cellular architecture,



from $6 \times 6 \times 5 \mu\text{m}^3$ sample of adult rat hippocampal stratum radiatum neuropil (by Kristen Harris). Visualization of *MCell* models is with *Blender*.

Training & Dissemination

Co-Leaders



Joseph C Ayoob, PhD
Associate Professor
Comp & Systems Biology
School of Medicine, Pitt



Phillip Compeau, PhD
Assistant Professor
Computational Biology
Carnegie Mellon University



Alexander Ropelewski
Director, Biomedical Applications
Pittsburgh Supercomputing Center



University of
Pittsburgh

Carnegie Mellon



Organization

Leader



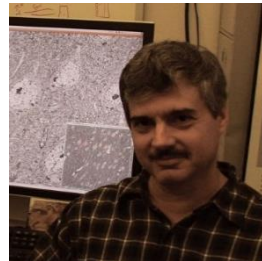
Alex Ropelewski

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Rozita Laghaei

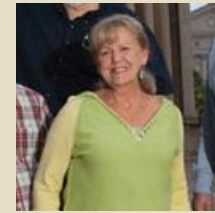
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Program

Monday, May 21

Collective Dynamics of Proteins Using Elastic Network Models. From Single Molecules to Biological Assemblies (Bahar)

Tuesday May 22

Bridging Sequence, Structure and Function, and Experiments and Computations. Signature Dynamics and Allosteric Signaling (Doruker)

Wednesday May 23

Modeling & Simulations of Membrane Proteins and Druggability (Bahar)
Comput Studies of Biomol Systems with MD simulations (Tajkhorshid)

Thursday May 24

Introduction to QwikMD & Parameterization for Classical Force Fields with FFTK (Ribero, Mariano/Soumyo)

Friday May 25

Investigating Biological Membranes and Membrane Proteins in Action Using Advanced Simulation Techniques (Tajkhorshid & Ribero)

Logistics

- [Downloads](#) if you will use your own laptop
- Dinner on Thursday night (Legume on S Craig Street)
- Breakfast & lunch will be served
- [Restaurants/cafes nearby](#) (Lulu's, Ali Baba, Porch, Piada, Five Guys, etc)
- Photo on Thursday lunch break



2015

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TECBio REU Internship



TECBIO REU
UNIVERSITY OF PITTSBURGH

Training and Experimentation in Computational Biology Research Experiences for Undergraduates

- 10 weeks; 12 students
- 320 applications/year
- Diverse – racially/ethnically and academically
- NSF (DBI-1659611) + Pitt funded (2 spots)
- PI: Ayooob

≥2 undergraduate students each summer to work w/MMBioS Investigators

- 17 trainees over 6 summers

TECBio REU Internship



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Welcome!

