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

Scientists solve chemical structure of HIV capsid

NIH-funded Biomedical Technology & Research Centers
TCBG Funded in 1989

“Bringing Physics to Life”

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

Software - Citations
NAMD 11,800+
VMD ~28,600

Dr. João Ribeiro

Dr. Mariano Spivak

NIH-funded Biomedical Technology & Research Centers
Overarching biological theme:

- Spatial organization
- Temporal evolution

Synaptic Signaling & Regulation

Funded in 2012
Software development at multiple scale

from 6 x 6 x 5 μm³ sample of adult rat hippocampal stratum radiatum neuropil (by Kristen Harris). Visualization of MCell models is with Blender.

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

http://www.mmbios.org/
Training & Dissemination

Co-Leaders

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Comp & Systems Biology
School of Medicine, Pitt

Phillip Compeau, PhD
Assistant Professor
Computational Biology
Carnegie Mellon University

Alexander Ropelewski
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<table>
<thead>
<tr>
<th>Day</th>
<th>Topic</th>
<th>Speaker(s)</th>
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<tbody>
<tr>
<td>Monday, May 21</td>
<td>Collective Dynamics of Proteins Using Elastic Network Models. From Single Molecules to Biological Assemblies</td>
<td>Bahar</td>
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<tr>
<td>Tuesday, May 22</td>
<td>Bridging Sequence, Structure and Function, and Experiments and Computations. Signature Dynamics and Allosteric Signaling</td>
<td>Doruker</td>
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<td>Wednesday, May 23</td>
<td>Modeling &amp; Simulations of Membrane Proteins and Druggability</td>
<td>Bahar</td>
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<td>Comput Studies of Biomol Systems with MD simulations</td>
<td>Tajkhorshid</td>
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<td>Thursday, May 24</td>
<td>Introduction to QwikMD &amp; Parameterization for Classical Force Fields with FFTK</td>
<td>Ribero, Mariano/Soumyo</td>
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<td>Friday, May 25</td>
<td>Investigating Biological Membranes and Membrane Proteins in Action Using Advanced Simulation Techniques</td>
<td>Tajkhorshid &amp; Ribero</td>
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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
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TECBio REU Internship

**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: Ayoob

> 2 undergraduate students each summer to work w/ MMBioS Investigators
  - 17 trainees over 6 summers
TECBio REU Internship
Welcome!