

EMERSON CENTER LECTURESHIP AWARD SYMPOSIUM

Computational and Mathematical Modeling in Large Systems: From Proteins to Cells

Cherry L. Emerson Center for Scientific Computation, Emory University



Dr. Cherry L. Emerson

Monday, April 3, 2006

Location: Room 207 White Hall, Emory University

AWARD WINNER & KEYNOTE SPEAKER:



Martin Karplus

Professor Emeritus, Department of Chemistry & Chemical Biology, Harvard University & Laboratoire de Chimie Biophysique, ISIS Université Louis Pasteur, 67000 Strasbourg France

Living cells are a collection of molecular machines, which carry out many of the functions essential for the cells' existence, differentiation and reproduction. Most, though not all, of these machines are made up of proteins. Because of their complexity, an understanding of how they work requires a synergistic combination of experimental and theoretical studies. The use of simulations to analyze some fundamental physical characteristics of proteins will be described. Applications to understand how proteins function will then be presented with specific focus on the molecular motors GroEL and F₁-ATPase.

INVITED SPEAKERS:

SCHEDULE OF EVENTS:



Stephen C. Harvey
*School of Biology
Georgia Tech., Atlanta*



Dieter Jaeger
*Department of Biology
Emory University, Atlanta*



David G. Lynn
*Dept. of Chemistry & Biology
Emory University, Atlanta*



Kurt Warncke
*Department of Physics
Emory University, Atlanta*



Ying Xu
*Dept. of Biochem. & Mol. Biology
University of Georgia, Athens*

9:00 - 9:20	OPENING CEREMONY & AWARD PRESENTATION
9:20 - 10:30	Prof. M. Karplus (ISIS Université Louis Pasteur, France, & Harvard University, USA): <i>How Proteins Work: Insights from Simulations</i>
10:30 - 11:25	Prof. D. Lynn (Emory University): <i>Protein Self-Assembly: Predicting Form and Function</i>
11:25 - 1:00	POSTER PRESENTATIONS
1:00 - 2:00	LUNCH
2:00 - 2:55	Prof. S. Harvey (Georgia Tech.): <i>The Challenges of Modeling Very Large Systems: Applications to Viruses</i>
2:55 - 3:50	Prof. Y. Xu (Univ. of Georgia.): <i>Computational Prediction of Biological Networks in Microbes</i>
3:50 - 4:10	COFFEE BREAK
4:10 - 5:05	Prof. K. Warncke (Emory University): <i>Combining Computation and Experiment to Reveal the Molecular Mechanism of Radical Catalysis in B₁₂ Enzymes</i>
5:05 - 6:00	Prof. D. Jaeger (Emory University): <i>Simulating Single Neurons Faithfully: How to Find Valid Solutions in a Very Large Parameter Space</i>
6:30 - 8:30	DINNER (by invitation)

REGISTRATION AND CONTACT INFORMATION:

Email: clec@euch4e.chem.emory.edu
<http://www.emerson.emory.edu/conferences/index.html>
*Abstracts of invited talks are available at the website.
 Registration is free, but you must register to attend.*

The Emerson Center Lectureship Award was established in the fall of 2003 to recognize distinguished achievements by scientists in computational sciences and to facilitate collaboration among different disciplines of computational sciences. On the board of the Emerson Center Lectureship Award Selection Committee are Professors Kurt Warncke (Physics, chair), Rustom Antia (Biology), Michele Benzi (Math & Computer Science), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), and Keith Wilkinson (Biochemistry) of Emory University. Dr. Jamal Musaev (Emerson Center) is the Lectureship Coordinator.



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