Computational Molecular Science and Engineering Forum
for the combined community of engineers and scientists developing and applying molecularly based theories, modeling, and simulation
http://comsef.org/

CoMSEF Newsletter

AIChE

October 2007

In This Issue

CoMSEF General Meeting in Salt Lake City

CoMSEF will hold its annual General Meeting during the Fall 2007 AIChE Meeting in Salt Lake City. The meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties) on Wednesday November 7 from 6:15-7:15 p.m. Look for the room number in the material handed out at the meeting. All CoMSEF members are invited to attend.

2007 Graduate Student Awards in Computational Molecular Science and Engineering

The 2nd annual CoMSEF Graduate Student Awards will be awarded at this year's AIChE Meeting in Salt Lake City. The awards are meant to recognize excellence in research by graduate students in the field of computational molecular science and engineering. Two awardees will be selected based on a nomination letter and on poster presentations Tuesday evening November 6 in the CoMSEF poster session (session #334). The winners will be announced Wednesday morning at the start of session #377 "Recent Advances in Molecular Simulation Methods." Each winner received a certificate and a cash award.

A Tribute to Keith Gubbins

Kenneth R. Cox

At the 2007 Annual AIChE meeting CoMSEF is sponsoring two very special sessions in honor of Keith Gubbins in the year of his 70th birthday. Professor Gubbins pioneered the application of molecular theory and simulation in the field of chemical engineering. His contributions are far too extensive to do justice in the confines of a short newsletter, but perhaps the following gives a flavor for the impact Keith has made promoting the application of molecular principles in chemical engineering practice.

One of Keith's former students has likened him to the champion surfer whose keen eye always captures the very best wave. Indeed, he has ridden a number of very fine waves over the course of his very productive career. Early in his academic career, Keith became well known for the application of extended corresponding states models for transport properties. He demonstrated to us how to use molecular simulation techniques to find the free energy of molecules and how to leverage perturbation theory for better predictions for polar and polarizable molecules. Of course, many of us were inspired to participate in this field by his first book "Applied Statistical Mechanics" which distilled the seemingly esoteric concepts of molecular theory into a form that opened the door for application by engineers. He popularized the "three-front assault" approach that combines theory, computer simulation, and experiment in comprehensive studies of physical properties and phase behavior.

But then there have been so many more great waves to follow. He had the foresight to study phase equilibria and interfacial properties of confined fluids in pores long before the evolution of nanotechnology led others to appreciate the great importance of this knowledge. These studies were among the best demonstrations of their time that simulation could provide insight to a problem not easily addressed through experimental studies. Many breakthroughs studies seeded in his research group have become widely accepted standards in industry and academia alike. An example is the SAFT equation of state which was conceived as an innovative approach for modeling polar fluids and polymers. This flexible approach has since found application to the widest variety of fluid mixtures including surfactants and electrolytes.

Keith's most recent surfing adventures have led him to the nano-realm. His current research seeks molecular insight into the behavior of nanoscale solids and liquids, with special attention given to nano-porous materials. On the same scale he is studying properties and phase behavior of surfactant systems and also chemical reactions. Following the successful approach he

developed early in his career, he continues to combine theory, computer simulation, and experiments in his studies of these systems. And, he has continued to demonstrate to us all how these fundamental studies can be applied to real world problems by practicing engineers.

Keith's accomplishments have been recognized through the many awards he has received. He has been a member of the National Academy of Engineering since 1989 and is also a Fellow of the American Institute of Chemical Engineers. Recently he was awarded the ACS Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids. He is the recipient of the AIChE Alpha Chi Sigma Research Award and the AIChE William H. Walker Award.

Professor Gubbins currently serves as the W.H. Clark Distinguished University Professor at North Carolina State University. He also serves as Co-Director of the Center for High Performance Simulation (CHiPS) at NC State. Previously he was the Thomas R. Briggs Professor of Engineering at Cornell University and served as Director of the School of Chemical Engineering there for many years. He started his academic career at University of Florida after completing his college degrees (B.Sc. in chemistry and PhD in chemical engineering) at the University of London.

Keith has played a major pioneering role in the application of molecular theory and simulation to the solution of problems encountered in chemical engineering practice. He has inspired many students, postdocs, and collaborators, who have followed his footsteps to also become leaders in this field.

I hope all of you will join us in celebrating Keith's many accomplishments by attending the CoMSEF sessions in his honor at the AIChE Annual meeting. Be sure to wish him a happy 70th birthday!

CoMSEF will co-sponsor 22 technical sessions at the Fall AIChE Meeting in Salt Lake City

Session #	Session Name	Primary Sponsor	Co-Sponsor
334	CoMSEF Poster Session	21	
472	First-principles Simulations of Condensed Phases	21	
179	Keith Gubbins 70th Birthday Celebration I	21	1a
302	Keith Gubbins 70th Birthday Celebration II	21	1a
561	The Fourth Industrial Fluid Properties Simulation Challenge	21	1a
592	Industrial Applications of Computational Chemistry and Molecular Simulation I	21	1a
632	Industrial Applications of Computational Chemistry and Molecular Simulation II	21	1a
377	Recent Advances in Molecular Simulation Methods	21	1a
432	Multiple Time-scale Modeling in Molecular Simulation	21	10d, 20
437	Numerical Methods and Simulation of Multiscale Systems I	10d	21, 20
?	Numerical Methods and Simulation of Multiscale Systems II	20	21, 10d
492	Numerical Methods for Molecular and Mesoscopic Systems	10d	21
19	Computational Catalysis I	20	21, 1g
76	Computational Catalysis II	20	21, 1g
62	20 Years of the Gibbs Ensemble	1a	21
469	Development of Intermolecular Potential Models	1a	21
371	Nucleation and Growth	1a	21
408	Computational Studies of Self-Assembly	1a	21
132	Molecular Modeling of Biophysical Processes	15c	21
250	Molecular Modeling of Adsorption	2e	21
113	Theories of Adsorption	2e	21
543	Multiscale Modeling & Characterization of Polymers	8a	21

Spring 2008 AIChE and ACS Meetings

The 2008 Spring AIChE and ACS meetings will be held concurrently April 6-10, 2008, at the New Orleans Convention Center. Registrants for either meeting will be able to attend sessions in both. CoMSEF will be taking advantage of this opportunity to program at the Spring meeting by co-sponsoring sessions with the Computers in Chemistry Division of the ACS. This should be a great opportunity to have a presence at the Spring meeting and to expand the visibility of CoMSEF within AIChE and ACS. Three symposia are scheduled, including Computational Catalysis (organized by Suljo Linic, Michigan, and Andy Rappe, Penn), Computational Evaluation of Rate Constants (Herbert DaCosta, Caterpillar, and Thanh Truong, Utah), and Computational Phase Equilibria (Ilja Siepmann, UMinn, and Karl Johnson, Pitt). Further information on these sessions and instructions for submitting abstracts are available at http://aiche.confex.com/aiche/s08/computation.htm. The deadline for submission is October 28, 2007. Please check out the sessions and consider submitting an abstract.

Research Highlight

By Roland Faller

It is not everyday that we find the results of a "pure" molecular simulation featured on the on the cover of Nature (*Aggregation and vesiculation of membrane proteins by curvature-mediated interactions* Benedict J. Reynwar, Gregoria Illya, Vagelis A. Harmandaris, Martin M. Müller, Kurt Kremer, and Markus Deserno Nature *447*, 461-464, 2007)). The Deserno group from the MPI for Polymer Research, Germany (now Carneggie-Mellon) got this rare honor for their simulations of protein interactions mediated through a lipid bilayer. These interactions can e.g. help describe how organelles in a cell with highly curved surfaces like mitochondria develop. The group developed a coarse-grained water free model of a bilayer which they first tested for reproducing the generic behavior of biomembranes. Then they showed that large-scale interactions by undulations in the membrane are the reason for the proteins to be able to induce curvature in a collective fashion. Only the highly intertwined long range interactions between proteins and the membrane lead to this important effect. Here no specific direct protein-protein or protein-lipid binding is a play. This work is a prime example of the potency of coarse-grained molecular models which break into the realm of microseconds a feat not achievable by any computational means only a few years ago. It also shows that simulations can shed the light of understanding on a problem where experiments are at best indirect and analytical theory is not yet possible.

Postdoc and PhD positions available

Looking for a postdoc or PhD position? Check about the jobs section of the CoMSEF forums (http://comsef.org/forum/3) (login required). You'll find listings from the Stockholm Center for Biomembrane Research, the University of South Carolina, Vanderbilt University, and the University of Tennessee-Knoxville.

News Briefs

IBM creates world's most powerful computer
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Meeting the Ethanol Challenge
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'Grand Challenge' Science Taps Supercomputers at LLNL
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Fast Computation of Many-Particle Hydrodynamic and Electrostatic Interactions in a Confined Geometry, Juan P. Hernández-Ortiz, Juan J. de Pablo, and Michael D. Graham, Phys. Rev. Lett
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Heterogeneous Diffusion in a Reversible Gel, Pablo I. Hurtado, Ludovic Berthier, and Walter Kob, Phys. Rev. Lett.
Link

Exploring the Mechanism of Flexible Biomolecular Recognition with Single Molecule Dynamics, Qiang Lu, H. Peter Lu, and Jin Wang, Phys. Rev. Lett.
Link

Conformational Temperature Characterizing the Folding of a Protein, Naoko Nakagawa, Phys. Rev. Lett.
Link

Formation of Gold Nanowires with Impurities: A First-Principles Molecular Dynamics Simulation, Eduardo Anglada, José A. Torres, Félix Yndurain, and José M. Soler, Phys. Rev. Lett.
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Swollen-to-Globular Transition of a Self-Avoiding Polymer Confined in a Soft Tube, Jeff Z. Y. Chen, Phys. Rev. Lett.
Link

Static and Dynamic Heterogeneities in a Model for Irreversible Gelation, T. Abete, A. de Candia, E. Del Gado, A. Fierro, and A. Coniglio, Phys. Rev. Lett.
Link

First-Principles Simulations on the Nature of the Melting Line of Sodium, Eduardo R. Hernández and Jorge Íñiguez, Phys. Rev. Lett.
Link

How Complex Is the Dynamics of Peptide Folding?, Rainer Hegger, Alexandros Altis, Phuong H. Nguyen, and Gerhard Stock, Phys. Rev. Lett.
Link

Mechanism of Thermal Transport in Dilute Nanocolloids, Jacob Eapen, Ju Li, and Sidney Yip, Phys. Rev. Lett.
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Atomistic Simulations of a Thermotropic Biaxial Liquid Crystal, Jorge Peláez and Mark R. Wilson, Phys. Rev. Lett.
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Quantum Molecular Dynamics Simulations for the Non-metal-to-Metal Transition in Fluid Helium, André Kietzmann, Bastian Holst, Ronald Redmer, Michael P. Desjarlais and Thomas R. Mattsson, Phys. Rev. Lett.
Link

Inter-DNA Electrostatics from Explicit Solvent Molecular Dynamics Simulations, Alexey Savelyev and Garegin A. Papoian, J. Am. Chem. Soc.
Link

Structure and Dynamics of the Homologous Series of Alanine Peptides: A Joint Molecular Dynamics/NMR Study, Jürgen Graf, Phuong H. Nguyen, Gerhard Stock, and Harald Schwalbe, J. Am. Chem. Soc.
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UT-ORNL Team Explores Mystery of Protein Folding
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