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 2008

In This Issue

CoMSEF General Meeting in Philadelphia

CoMSEF will hold its annual General Meeting during the Fall 2008 AIChE Meeting in Philadelphia. The meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties) on Wednesday November 19 from 6:15-7:15 p.m. in the Pennsylvania Convention Center, Meeting Room 102-A (Street Level). All CoMSEF members are invited to attend.

2008 Graduate Student Awards in Computational Molecular Science and Engineering

The 3rd annual CoMSEF Graduate Student Awards will be awarded at this year's AIChE Meeting in Philadelphia. The awards 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 (due Oct 1) and on poster presentations Monday evening November 17 in the CoMSEF poster session (session #185). The winners will be announced Wednesday 12:30 p.m. at the start of session #506 "Recent Advances in Molecular Simulation Methods I." Each winner will receive a certificate and a cash award.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year, we are electing a Vice Chair, a Secretary/Treasurer, and 2 Liaison Directors. All CoMSEF members can vote at the CoMSEF website http://comsef.org until October 23.

CoMSEF announces new award for outstanding research achievement

This academic year will mark the first time that CoMSEF has offered an award to recognize an individual who has published outstanding research in computational molecular science and engineering, broadly defined to include advances in modeling, computation, and simulation techniques. This award will be given annually to a computational specialist holding a professional position in academia, industry, or in a government lab. We are targeting the award to someone in the early stages of their professional careers, which we have defined as being within 15 years of completion of highest degree (e.g., for the 2009 award, anyone receiving the PhD degree within the calendar year 1994 or afterward is eligible).

We feel that the existence of this new award is timely as it fills an unmet need to recognize the research achievements of younger computational professionals. The two major existing awards in areas pertinent to CoMSEF are the European CECAM Berni Alder prize and the PPEPPD Prausnitz award, both of which are typically awarded to more senior faculty and neither of which is awarded every year. We hope that the existence of this award will raise the visibility of the winner's achievements and make him or her more competitive for other professional awards, both within AIChE and in other professional societies. Ultimately, we hope that the existence of this award will play a contributory role towards the facilitating in increase in computational specialists who gain membership in the National Academies of Sciences and Engineering.

The first call for nominees will take place in spring 2009 coincident with the AIChE Annual Meeting's call for papers. Details of the nomination process will be available on the web at http://comsef.org.

Research Highlight: Coarse-Graining of Condensed Phase and Biomolecular Systems

Roland Faller

Coarse Graining has gained increasing importance as a research area in molecular modeling. And now a brand new book entirely dedicated to this area has just appeared: Coarse-Graining of Condensed Phase and Biomolecular Systems by CRC Press. It is edited by Greg Voth from the University of Utah, one of the most eminent leaders in coarse-graining, especially for biomolecular systems. The book deals with both technical and practical details of the field as well as a variety of applications mainly in the area of soft matter. Proteins, polymers and biological membranes are all addressed and their similarities and differences pertaining to coarse graining are discussed in 27 chapters written by different authors. The biggest group of chapters addresses various aspects of protein modeling. The group of authors has been drawn from a wide range of experts in coarse-graining. The book is a helpful new tool both for the novice modeler as well as expert coarse-grainer as most chapters first discuss the concepts of a specific technique in the area of coarse-graining and then go on to deal with the latest state of the art. As always with books containing chapters of different authors it is non-homogeneous.
Disclosure: R. Faller's group contributed a chapter to the book.

Research Highlight: Comparing the Use of Gibbs Ensemble and Grand-Canonical Transition Matrix Monte Carlo Methods to Determine Phase Equilibria

Ed Maginn

Andrew S. Paluch, Vincent K. Shen and Jeffrey R. Errington, Ind. Eng. Chem. Res., 47, 4533-4541 (2008)
Accurate simulation of phase equilibrium is one of the most important (and difficult) tasks of a simulator. Although there are several techniques that can be used for these simulations, the Gibbs ensemble method developed twenty years ago by Panagiotopoulos has been the workhorse among chemists and engineers because of its conceptual elegance and simplicity. In a recent paper by Paluch, Shen and Errington, it is shown that the use of grand canonical Monte Carlo with transition matrix methods can yield significantly more accurate results for the vapor-liquid coexistence properties of complex systems than is attainable with Gibbs ensemble methods. This paper provides a practical "how to" guide to transition matrix methods, which have been used by Errington and co-workers for the past several years to compute properties as diverse as surface tension, Henry's constants and protein solution behavior. Vapor-liquid equilibria calculations are performed for ethane, n-octane, cyclohexane, 2,5 dimethylhexane, 1-propanol and water. It is shown that while Gibbs ensemble methods typically provide suitable "order of magnitude" estimates of equilibria over short simulation times, significantly more precise results are obtained (in most cases) with the transition matrix method and longer simulations. This paper provides a compelling reason for more groups to begin utilizing this powerful new concept.

CoMSEF will sponsor or co-sponsor 27 technical sessions at the Fall AIChE Meeting in Philadelphia

Session #	Session Name	Primary Sponsor	Co-Sponsor
185	CoMSEF Poster Session	21	
451	Symposium Honoring H. Ted Davis I	21	1a, 1c
564	Symposium Honoring H. Ted Davis II	21	1a, 1c
506	Recent Advances In Molecular Simulation Methods I	21	1a, 7p
669	Recent Advances In Molecular Simulation Methods II	21	1a
596	First-Principles Simulations I	21	
646	First-Principles Simulations II	21	
709	Overview of An International Assessment of Research and Development in Simulation-Based Engineering and Science	21	
734	Industrial Applications of Computational Chemistry and Molecular Simulation	21	1a
771	The Fifth Industrial Fluid Properties Simulation Challenge	21	
762	Integrated Multiscale Molecular Simulation	21	
533	Development of Intermolecular Potential Models	1a	21
404	Computational Studies of Self-Assembly I	1a	21
470	Computational Studies of Self-Assembly II	1a	21
530	Computational Studies of Self-Assembly III	1a	21
426	Molecular Simulation of Adsorption I	2e	21
490	Molecular Simulation of Adsorption II	2e	21
367	Numerical Methods for Molecular and Mesoscopic Systems	10d	21
717	Molecular Modeling for Product Design	12g	21
425	Molecular Modeling of Biophysical Processes I	15c	21
489	Molecular Modeling of Biophysical Processes II	15c	21
403	Computational Catalysis I	20	21, 1g
469	Computational Catalysis II	20	21, 1g
529	Computational Catalysis III	20	21, 1g
585	Computational Catalysis IV	20	21, 1g
319	The Evolution of Molecular Modeling into a Chemical Engineering Tool I	TH024	21
383	The Evolution of Molecular Modeling into a Chemical Engineering Tool II	TH025	21

FOMMS 2009

FOMMS 2009 (July 12-16, 2009 at the beautiful and relaxing Semiahmoo Resort in Blaine, WA) is the fourth international conference showcasing the applications and theory of computational quantum chemistry, molecular science, and engineering simulation. The motivation for this conference is the continual need for precise control of product properties, the accurate prediction of physical properties, and the development of a fundamental understanding of the chemical processes that allow the efficient creation of new products that meet specific marketplace demands. Theoretical and algorithmic advances along with modern computing technology routinely leads companies to capture the cash value of truly sustainable, far-reaching competitive advantage. A molecular-level understanding of these chemical processes lead to model mechanisms that are robust, pertinent, scalable, and most importantly, integratable across statistical, chemical, and engineering technologies. The future for these methods is extremely bright as they continue to prove their value to the chemical and chemical-related industries in the coming decade.

Topics of special interest (along with the speakers that have been confirmed) include the following:

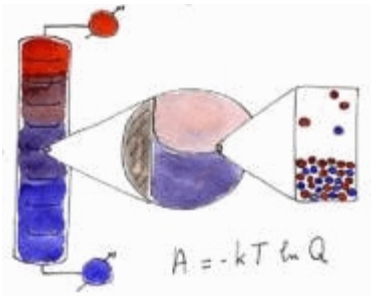
- New perspectives in molecular simulation: Daan Frenkel (Cambridge)
- From proteins to systems biology: Charlie Brooks (UM)
- Linking process scale simulation and molecular modeling: Linda Broadbelt (NWU) and Dion Vlachos (U Delaware)
- Rare events: acceleration algorithms and transition path sampling: Baron Peters (UCSB)
- Open source modeling & simulation software
- Soft materials and complex fluids: Ilja Siepmann (U Minn), Clare McCabe (Vanderbilt) and Lev Gelb (Wash U)
- Simulation-based engineering & science - Novel materials and industrial applications: Caroline Mellot (UCL, UK), Shinichiro Nakamura (Mitsubishi, Japan), Herve' Toulhoat (IFP, France) and roundtable
- Petascale computing and emerging architectures for modeling and simulation: David Shaw (D.E. Shaw/ Columbia), Klaus Schulten (UIUC), and George Karniadakis (Brown)

In addition to outstanding invited lectures and discussion on a range of topics in molecular modeling and simulation, the conference will include a mini-workshop on open source code development for molecular simulation, tutorial sessions on massively multicore chip architectures and GPUs for scientific simulation, and a special, inaugural FOMMS Award banquet. In addition, the schedule provides large blocks of time for informal discussions, relaxation, or leisure as well as several receptions to facilitate interaction between conference participants.

Thermodynamics 2009

September 23-25, 2009 @ Imperial College London, U.K.

On behalf of the organizing committee, I am pleased to announce the "Thermodynamics 2009" conference. The 21st meeting of this series will be held at Imperial College London from Wednesday 23rd to Friday 25th September 2009. Thermodynamics 2009 will focus on innovative approaches for better understanding the relationship between the atomic structure of materials and their macroscopic properties. For this purpose, molecular simulation, classical thermodynamic approaches (equations of state) and experimental tools will be considered with equal balance.



The conference will feature the 2009 Lennard-Jones Lecture and Prize awarded this year to Prof. Dr. Kurt Binder by the Statistical Mechanics and Thermodynamics Group of the Royal Society of Chemistry, UK. Other confirmed lectures include:

- Peter Bolhius
- Norman Carnahan
- Michael Cates
- Charles Knobler
- Lev Gelb
- Keith Gubbins
- Laurent Pitre
- Doros Theodorou
- Carsten Tschierske
- Alfons von Blaaderen.

In addition, the Christopher Wormald Prize will be awarded to a research student nominated by members of the community. The winner will receive a cash prize and be given the opportunity to present an oral contribution at the conference.

We encourage you to refer to the conference web page : www.thermodynamics2009.org which is regularly updated and to an consider oral or poster presentation in line with one of the topics proposed:

- Statistical thermodynamics
- Molecular simulation of soft matter and complex fluids
- Thermodynamic modelling and equations of state
- Phase diagrams and supercritical fluids
- Experimental thermodynamics

Should you have any question, or if you wish to be added/ removed from the mailing list, please feel free to contact me.

Kindest regards,
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