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 2009

In This Issue

CoMSEF General Meeting in Nashville, TN

CoMSEF will hold its annual General Meeting on Wednesday November 11th from 6:15-7:15 p.m. during the Fall 2009 AIChE Meeting in Nashville. As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend. The winners of the CoMSEF Graduate student awards will be announced at the meeting.

CoMSEF Elections and Proposed Bylaw Changes

The annual CoMSEF election is currently underway. This year, we will elect two Liaison Directors. All CoMSEF members can vote in the election at the CoMSEF website through October 22rd 2009.

Included in the ballot of this years election will also be changes to the CoMSEF bylaws. These changes are being proposed by the CoMSEF Executive Committee to better define the role of Liaison Directors within CoMSEF, define the procedure to be followed in the event of an election tie, and clearly define the election timeline to be followed.

Vote (login required) at http://comsef.org/election/2009

Inaugural CoMSEF Early Career Award

The CoMSEF Executive Committee is pleased to announce that Professor Ed Maginn of the University of Notre Dame has been selected as the recipient of the inaugural CoMSEF Early Career Award. This new annual award recognizes outstanding research in our field and will be given to Ed at the start of session 113 - Recent Advances in Molecular Simulation Methods I - at 12:30 PM on Monday November 9 in room Tennessee C of the Gaylord Opryland Hotel during the Annual AIChE meeting.

Ed received his B. S. in Chemical Engineering from Iowa State University in 1987. He then worked for Procter and Gamble as an operations engineer for three years before entering the graduate program in Chemical Engineering at the University of California at Berkeley, where he received his PhD in 1995 under the direction of Doros Theodorou and Alex Bell. He joined the faculty of Notre Dame in 1995 and is presently Professor of Chemical and Biomolecular Engineering. Ed has over 90 refereed publications and two patents and is the recipient of the Dow Outstanding New Faculty Award from the American Society for Engineering Education as well as an CAREER Award from the National Science Foundation. He has also received several teaching awards, including the BP Outstanding Teacher award for the Notre Dame College of Engineering, two John A. Kaneb Awards from the University of Notre Dame and the AIChE Student Chapter Outstanding Teaching Award.

Ed is receiving the CoMSEF Early Career Award ***for his development of molecular simulation algorithms to study fundamental thermodynamics and transport behavior and his specific contributions to the understanding of nanoporous materials and ionic liquids***. CoMSEF Early Career Award recipients must be in the early stages of their professional careers (in academia, industry, or a national laboratory), defined as being within 15 years of completion of the highest degree and be current members of CoMSEF.

Membership Renewal

It's renewal time. To renew your membership for another year (including CoMSEF), go to:
http://www.aiche.org/MemberCenter/Renew.aspx

CoMSEF will sponsor and co-sponsor 21 technical sessions at the Fall AIChE Meeting

Session #	Session Name
18	Computational Catalysis I: Methodology
46	Opportunities for Chemical Engineering in Petascale Computing [Invited Talks]
85	Computational Catalysis II: Transition Metals
102	Molecular Modeling of Biophysical Processes I
113	Recent Advances in Molecular Simulation Methods I
156	Molecular Modeling of Biophysical Processes II
167	Recent Advances in Molecular Simulation Methods II
178	CoMSEF Poster Session
330	Thermodynamics of Energy Systems
358	First-Principles Simulations of Condensed Phases: Bulk Materials
399	Chemistry and Kinetics Integrated CFD Modeling
456	First-Principles Simulations of Condensed Phases: Surfaces
517	Industrial Applications of Computational Chemistry and Molecular Simulation I
525	Multiscale Modeling I
563	Industrial Applications of Computational Chemistry and Molecular Simulation II
574	Multiscale Modeling II
621	Multiscale Modeling and Characterization of Polymers
665	Molecular Simulation of Adsorption I
650	Computational Studies of Self-Assembly
692	Development of Intermolecular Potential Models
700	Molecular Simulaton of Adsorption II

Research Highlight: Massive Computing Power Delivers The Direct Calculation of Particle-Particle and Particle-Surface Interactions!

By Alberto Striolo

Lane et al. [J.M.D. Lane, A.E. Ismail, M. Chandross, C.D. Lorenz, G.S. Grest, *Forces between functionalized silica nanoparticles in solution,* Phys. Rev. E 79 (2009) 050501 http://link.aps.org/doi/10.1103/PhysRevE.79.050501] recently reported the results of massive molecular dynamics simulations [the largest system simulated contains more than 7 million atoms] to precisely calculate equilibrium and hydrodynamic forces acting when one nanoparticle approaches a surface, and when two nanoparticles approach each other in aqueous solutions. Specifically, the Authors considered silica nanoparticles functionalized by 3.1 PEO chains per nm2 of nanoparticle surface in water. The Authors showed that the grafted PEO chains induce a strong repulsion between approaching silica nanoparticles, and that they alter the interfacial solvent structure; the Authors also identified the length scale at which macroscopic theories (i.e., the Brenner's prediction for the increased drag experienced by a particle as it approaches a surface) work, and where they need to be augmented my molecular-scale details.

More importantly, in this reader's opinion, Lane et al. demonstrated that all-atom simulations can now be used to calculate precisely the effective forces acting between nanoparticles, surfaces, and, why not? small proteins. With these capabilities our community will be able to test theoretical predictions for the stabilization of nanoparticles in solution, to improve widely applied but deficient macroscopic theories, such as the DLVO, that describe protein-protein interactions, and eventually to predict entire phase diagrams for nanoparticles and/or proteins in complex, real media. Applications of these new capabilities will positively impact a number of industries, including pharmaceutical, materials, and many others.

Research Highlight: Turner group paves the way for nanoelectronic devices

By Jeff Errington

Wei An and C. Heath Turner, “Transition-Metal Strings Templated on Boron-Doped Carbon Nanotubes: A DFT Investigation”, J. Phys. Chem. C 113, 15346 (2009).
http://dx.doi.org/10.1021/jp9052715

Nanoelectronics represents an exciting research direction due to the numerous potential applications that may stem from it, including more powerful computer processors, more efficient solar cells, and novel sensors. One of the current obstacles for realizing such devices involves the lack of techniques for assembly of tiny nanowires into well-defined patterns. In a recent article, An and Turner showed that boron-doped carbon nanotubes provide effective materials for precisely organizing transition metals into desirable structures. The authors first demonstrate that pristine carbon nanotubes do not provide enough of a driving force to facilitate this assembly process. They then show the favorable adsorption characteristics of strings of transition metal atoms (tiny wires) onto (8,0) and (6,6) single-walled carbon nanotubes with two distinct boron dopant arrangements. Their calculations indicate that strings consisting of atoms such as Au, Pt, Ag, Ni, Cu, and Ti bind to the doped nanotubes with energies of 1 to 2 eV. In addition to potential use within the area of nanoelectronics, An and Turner suggest that these structures could prove useful as nanocatalysts as well as in the design of tunable materials.

2009 CoMSEF Graduate student awards

The CoMSEF Graduate student Awards in Computational Molecular Science and Engineering will be awarded for the 5th time at the annual AIChE Meeting in Nasvhille. 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 the nomination letters received from each students advisor and a poster presented at the CoMSEF poster session (session #178) to be held Monday evening from 6 - 8 pm. The winners will be announced at the CoMSEF annual General Meeting (Wednesday November 11th from 6:15-7:15 p.m).

Project to develop molecular simulation programming interface debuts at FOMMS 2009

By Dave Kofke

One of the challenges faced by practitioners and developers of molecular simulation is keeping up with the constant evolution of both molecular simulation methods and computing platforms on which they’re implemented. Simulation codes developed in-house cannot compete with finely tuned simulation engines such as LAMMPS, and with the advent of multicore processors and GPUs as platforms for computational science, this problem is likely to grow. At the same time, developers of such engines cannot hope to implement all methods of potential interest, not to mention incorporate all new techniques as they emerge.

Part of this problem can be remedied by decoupling the simulation engine from the application. An “application” would be something such as free-energy perturbation, or transition path sampling, which can be largely abstracted from the details of how the simulation is implemented on a particular platform. The application and the engine can interact through a well defined application programming interface (API) that encapsulates the basic operations of a molecular simulation into a large, well-defined set of generic commands. In this manner, developers of new applications can write them to the interface, and expect that they will function correctly with any simulation engine that implements the API. Likewise, engine developers can expect that their advances can be exploited in a wide variety of applications, if only they take care to implement the interface (or if someone provides an adapter that does). In addition to leveraging programming efforts this way, such an infrastructure can further aid in benchmarking for performance and correctness.

At the FOMMS 2009 Conference, an initiative to develop such a molecular simulation API was discussed in a workshop led by David Kofke and Andrew Schultz of the University at Buffalo. The project is funded by an NSF Chemistry Cyberinfrastructure grant to Kofke and co-investigators Lev Gelb (Washington-St. Louis), Sharon Glotzer (Michigan), Peter Cummings (Vanderbilt) and David Chandler (UC Berkeley). The aim of the workshop was to inform the simulation community of this ongoing effort, and to invite participation by others in the development of the API. Persons interested in getting involved can join a discussion mailing list that is working toward a consensus draft API. Additional information is available at http://etomica.org/wiki/API

Job Postings on the CoMSEF web site

In the Forum section of the CoMSEF web site is a place for job postings. Recently 2 post-doc positions and a faculty position were posted. Check it out if you’re interested in posting a position or finding out about positions that are open: http://comsef.org/forum

Upcoming Conferences of Interest to CoMSEF Members

12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)
May 16th - 21st 2010
http://www.ppeppd2010.cn/

The PPEPPD conference series endeavors to provide an effective forum for academic and industrial researchers to meet and communicate on the status and future trends in properties and phase equilibria important to the design of products or processes. The unifying thread of the meeting is the language of thermodynamics and an interest in the measurement, calculation, and prediction of properties. Distinctive characteristics of PPEPPD include a well-balanced participation of both academia and industry, an emphasis on both product and process design, following the shifting paradigms in the chemical engineering profession worldwide, and an emphasis on interaction; there are no parallel sessions and the size of the conference is limited to 250 participants. The scientific themes of PPEPPD 2010 are:

- Biological and Pharmaceutical Systems
- Energy, Environment and Sustainability
- Materials (Metals, inorganic solids, polymers and liquid crystals)
- Molecular Simulation and Multiscale Simulation
- Nanoscience and Nanotechnology
- Phase Equilibria (Theory and Experiments)
- Product and Process Engineering
- Quantum Computation and Force Fields
- Surfaces, Interfaces and Confinement Effects

Invited speakers that have already confirmed their participation include:

Frank Caruso *University of Melbourne*	*Lynn Orr* *Stanford University*
Mauricio Futran *Bristol-Myer-Squibb*	*Richard Smith* *Tohoku University*
Amparo Galindo *Imperial College London*	*Kathleen J. Stebe* *University of Pennsylvania*
Keith Gubbins *North Carolina State University*	*Thomas M. Truskett* *University of Texas at Austin*
Hans Hasse, *Kaiserslautern University*	*Philippe Ungerer* *IFP, France*
Martin P. Head-Gordon *University of California, Berkeley*	*Yuliang Yang* *Fudan University, China*
Huen Lee *KAIST, South Korea*	*Jackie Ying* *National University of Singapore*
Clare McCabe *Vanderbilt University*	*Suojiang Zhang,* *Chinese Academy of Science*

8th Liblice Conference on the Statistical Mechanics of Liquids
June 13th - 18th 2010
http://liblice.icpf.cas.cz/2010/2010.php

The 8th Liblice Conference will be held in Brno in the Czech Republic and will follow the spirit of the previous meetings, with emphasis on informal discussions rather than on formal presentations to highlight current achievements and challenges in both theoretical and applied aspects of the discipline. In addition to the traditional conference focus on the fundamentals of liquid-state theories and molecular simulation methodology and novel applications the program of the 8th Liblice meeting will include recent specific developments in the fields of:

- Fluid interfaces and fluids in confinement
- Aqueous systems
- Soft matter
- Supercooled/glassy states

Keynote speakers that have already confirmed their participation include:

G. Ciccotti, Rome	*P. Monson, Amherst*
A. Garcia, Troy (NY)	*P. Rossky, Austin*
L. Gelb, St. Louis	*F. Sciortino, Rome*
S. C. Glotzer, Ann Arbor	*S. Shell, Santa Barbara*
J. P. Hansen, Cambridge	*G. A. Voth, Salt Lake City*
A. Luzar, Richmond	N. B. Wilding, Bath

STATPHYS 24, the XXIV International Conference on Statistical Physics of the International Union for Pure and Applied Physics (IUPAP)
July 19-23 2010
http://www.statphys.org.au/

STATPHYS 24 will be held in the Convention Centre, Cairns, Queensland, Australia, 19-23 July, 2010**.** The STATPHYS Conference series takes place every three years in a different continent to enhance the international relevance and visibility of the leading world event in the broad field of Statistical Physics and all its interdisciplinary developments. Recent meetings have been held in GENOVA (Italy), BANGALORE (India), CANCUN (Mexico) and PARIS (France). STATPHYS 24 will be the first time this event is held in Australia and only the second time in the southern hemisphere. According to tradition, the highest international recognition in the field of Statistical Physics, the Boltzmann Medal, will be awarded at this meeting. In addition several satellite meetings will be held along with the main event, adding to the scientific value of the meeting. A broad range of topics will be covered at the meeting including:

- General aspects of statistical physics: phase transitions, critical phenomena, thermodynamics, networks and graphs, etc.
- Nonequilibrium processes: driven systems, transport theory, relaxation phenomena, random processes, fluctuations, large deviations etc.
- Fluids and soft matter: molecular and ionic fluids, metastable liquids, polymers, gels, liquid crystals, microemulsions, foams, membranes, colloids, granular materials, etc.
- Surfaces and Interfacial phenomena: growth processes, wetting, surface effects, films, confined systems, etc.
- Biological physics: molecular motors, dynamics at the scale of the cell, spatio-temporal organization in biological systems, biological membranes, biopolymer folding, etc.

Confirmed Plenary speakers (partial list):

Rodney Baxter (Canberra)	*Wolfgang Ketterle (MIT)*
Mike Cates (Edinburgh)	*Hidetoshi Nishimori (Tokyo)*
Sergio Ciliberto (Lyon)	*Subir Sachdev (Harvard)*
Bertrand Eynard (Saclay)	*Michelle Wang (Cornell)*
Daniel Fisher (Stanford)	

FOMMS 2009

By Sharon Glotzer

Foundations of Molecular Modeling and Simulation (FOMMS) is an 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 leads 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.

FOMMS 2009 is the 4th international conference, held every three years, in a distinguished series that focuses on the theory and practice of molecular modeling and simulation. The overall goal of the FOMMS conference series is to evaluate current progress in the molecular modeling and simulation field and to identify new intellectual challenges that may have a funda-

mental impact on future practice. The theme of the FOMMS 2009 conference, Foundations for Innovation, reflects recent advances and innovation in the fundamentals of molecular modeling and simulation and its application.

An important aim of FOMMS 2009 was to bring together and foster interactions among world-renowned experts from academia, government and industry, graduate students, and postdoctoral associates. Invited speakers discussed a broad range of theoretical and applied topics with applications in the chemical, petrochemical, pharmaceutical, materials, and energy related industries. Contributed posters allowed the presentation of recent research results and provided a forum for informal discussions. The first FOMMS medal was awarded to Professor Michele Parrinello for his contributions to the field of molecular simulation. A tutorial on graphics processors for scientific simulation and workshops on the development of open-source molecular simulation software and the use of simulation modules in education were held. Our hope is that the scientific contributions presented at FOMMS 2009 and included in these proceedings will stimulate new advances and innovations in molecular modeling and simulation.

FOMMS 2009 was organized under the auspices of the CACHE Corporation and was co-sponsored by CACHE and the CoMSEF Division of AIChE. We would like to acknowledge the financial and other support of the National Science Foundation, AIChE, IFP, the University of Michigan, the National Center for Supercomputing Applications, and the Virtual School of Computational Science and Engineering. Additional information on the FOMMS 2009 conference can be found at: http://fomms.org.