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 2013

In This Issue

CoMSEF General Meeting in San Francisco

CoMSEF will hold its annual General Meeting on Wednesday November 6 from 6:15-7:15 pm in Union Square 16 (Hilton) during the Fall 2013 AIChE Annual Meeting. 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 and the new Liaison Directors will be announced and programming for future AIChE meetings will be discussed.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year we will elect two Liaison Directors. Information about the candidates and the duties of each office can be found at http://comsef.org/election-2013. You should have received voting instructions by email. If you didn't receive the email or lost it, contact admin@comsef.org for help. The deadline for casting your vote is October 24th.

Errington Winner of 2013 CoMSEF Impact Award

Professor Jeffrey Errington from the University of Buffalo is the winner of the 2013 CoMSEF Impact Award, which cites his "*advancement of transition-matrix Monte Carlo methods, and their application to interfacial phenomena and to probing the link between thermodynamics and transport properties*." Professor Errington has been on the faculty at the University of Buffalo since 2001 after completing a postdoctoral appointment at Princeton and his PhD at Cornell.

Jeff will receive his award during the CoMSEF Plenary Session at the 2013 AIChE Annual Meeting, where he will also give a talk describing his research.

The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Jayaraman Winner of Inaugural CoMSEF Young Investigator Award

Professor Arthi Jayaraman from the Department of Chemical and Biological Engineering at the University of Colorado is the inaugural winner of the CoMSEF Young Investigator Award. Arthi joined the University of Colorado, where she is currently the Patten Assistant Professor, in 2008 after performing postdoctoral research at the University of Illinois and a PhD at North Carolina State University. With this award, Arthi is cited "*for insightful theory and simulation studies of polymers, linking molecular interactions to morphology for optimal design of materials for energy and biomedical applications*." Arthi will receive her award during the CoMSEF Plenary Session at the 2013 AIChE Annual Meeting, where she will also give a talk describing her research.

The CoMSEF Young Investigator Award for Modeling and Simulation is awarded annually to a member of CoMSEF who is within 7 years of completion of their highest degree in the year of the award.

2013 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded for the 8th consecutive year at the annual AIChE Meeting in San Francisco. 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, their CV, and a poster presented at the CoMSEF poster session (session #214) to be held Monday evening from 6 - 8 pm in the Hilton Grand Ballroom B. The winners will be announced at the CoMSEF/Area 1a annual General Meeting (Wednesday, from 6:15-7:15 pm).

The 8th Industrial Fluid Properties Simulation Challenge

Building on the 7th challenge (adsorption in zeolites), the 8th challenge will focus on adsorption in activated carbons. At session #455 (Thursday, November 6, 2013: 8:30 AM, Franciscan A - Hilton) the details of the 8th challenge will be announced and several adsorption modeling experts will present their perspectives. Please join us!

Here is the agenda:
08:30 Introduction and Announcement of the 8th Challenge - Richard B. Ross
08:45 QSDFT Model for Simulation of Adsorption Isotherms and Characterization of Adsorbents - Alexander V. Neimark
09:10 Predictive Adsorption Models for High Surface Area Activated Carbons - Lev Sarkisov
09:35 Amorphous Microporous Materials: Virtual Design and Characterization - Coray M. Colina
10:00 Development of Accurate Coarse Grained Surface-Particle Force Fields - Erich A. Müller
10:25 Physical Adsorption, ESCA, and XRD Benchmark Studies of Activated Carbons for the 8th Industrial Fluid Properties Simulation Challenge - Matthias Thommes and Riaz Ahmad

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Annual Meeting Sessions

CoMSEF has an exciting range of programming at the upcoming 2013 AIChE Annual Meeting in San Francisco, with 27 sponsored and co-sponsored sessions, running from Monday (AM) to Thursday (PM). Of special note are the Computational Molecular Science and Engineering Plenary Session at 12:30 on Wednesday and the CoMSEF Poster Session on Monday from 6:00-8:00 pm. Full details on all of the CoMSEF sessions are available on pages T33 and T34 of the CEP magazine September issue and are available on the web at:

https://aiche.confex.com/aiche/2013/webprogram/Symposium3081.html

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Upcoming Conferences of Interest to CoMSEF Members

Technical Meeting on High-Throughput Molecular Dynamics 2013
November 7-8, 2013
Barcelona, Spain
http://htmdworkshop.wordpress.com/programme/

Gordon Conference: Protein Folding Dynamics
January 5-10, 2014
Galveston, TX, USA
http://www.grc.org/programs.aspx?year=2014&program=protfold

CCPBioSim/CCP5 Multiscale Modelling Conference 2014
January 7-9, 2014
Manchester, UK
http://www.ccpbiosim.ac.uk/?q=multiscale2014

Active Fluids: Bridging Complex Fluids and Biofluids
Jan 27-Feb 2, 2014
Aspen, CO
http://www.math.vt.edu/people/renardyy/Aspen2014/website.html

10th International Conference of Computational Methods in Sciences and Engineering
Apr 4-7, 2014
Athens, Greece
http://www.iccmse.org/

NINTH LIBLICE CONFERENCE on the Statistical Mechanics of Liquids
Jun 15-20, 2014
Czech Republic
http://liblice.icpf.cas.cz/2014/2014.php

27th European Symposium on Applied Thermodynamics: Experiments meet Theory and Simulation
July 6-9, 2014
Eindhoven, The Netherlands
http://www.esat2014.org/

Gordon Conference: Polymer Physics
July 13-18, 2014
Mount Holyoke College, South Hadley, MA, USA
http://www.grc.org/programs.aspx?year=2014&program=polyphys

Gordon Conference: Quantum Science
July 27 - August 1, 2014
Stonehill College, Easton, MA, USA
http://www.grc.org/programs.aspx?year=2014&program=quantsci

Gordon Conference: Water & Aqueous Solutions
July 27 - August 1, 2014
Holderness School, Holderness, NH, USA
http://www.grc.org/programs.aspx?year=2014&program=water

Nineteenth Symposium on Thermophysical Properties
June 21-26, 2015
Boulder, CO, USA
http://thermosymposium.boulder.nist.gov/

Foundations of Molecular Modeling and Simulation (FOMMS) 2015
Summer 2015
TBD
http://fomms.org/

Properties and Phase Equilibria for Product and Process Design (PPEPPD)
2016, Portugal

Research Highlight: Coarse-Graining Coming of Age

M. Scott Shell, Department of Chemical Engineering, UC Santa Barbara

Simple coarse-grained (CG) or toy molecular models have long provided insights into the molecular-thermodynamic behavior of a broad range of chemical systems. However, the past decade has seen rapidly-growing interest in new techniques and formalisms for their systematic rather than reasoned development, in order to enable "bottom-up" simulations of complex systems at dramatically larger scales. Many exciting new ideas are emerging. At the heart of this problem is how to develop a low-resolution model when a higher-resolution reference system is available, such as one described by an all-atom semi-empirical force field. Of course, now well-established are techniques that solve this problem by parameterizing CG force fields in order to match low-dimensional structural correlation functions or forces of the reference systems, yet many fundamental questions remain despite the established utility and prevalence of these algorithms.

In an excellent and detailed *Perspective* in the Journal of Chemical Physics [1], Noid provides a timely critical assessment and outlook for systematic coarse-graining techniques. Although specifically addressing CG techniques in the context of biomolecular models, he identifies several quite broad challenges that are at the heart of recent activity in the field. Some particularly prominent issues include: (1) Are there theoretically robust and intuitive ways to automatically determine the "mapping" of CG models, that is, how CG sites or pseudoatoms are placed and how many coarse degrees of freedom are required for a given accuracy? Moreover, should the design of CG models consider dynamics? (2) How can one assess the need for and incorporate many-body effects into CG models in a manner that retains computational efficiency? (3) Is it possible to develop a consistent thermodynamic treatment of CG models when the interactions are inevitably free-energetic in nature? In particular, what is the right way to create and use models that are *transferable* from, say, one state point to another?

Indeed many of these challenges illustrate that a more basic conceptual tug-of-war has existed between needs for practically efficient models and algorithms and the needs for new fundamental approaches to CG thermodynamics and dynamics. Recent progress suggests that we may be moving towards a more satisfying resolution. To mention a few works of note—Rudzinsky and Noid uncovered a close connection between structure-matching and force-matching techniques for coarse-graining, highlighting the key role played by higher-order structural correlations when simple CG models are parameterized [2,3]. Moreover, Voth and coworkers recently introduced an "ultra-coarse-graining" framework that combines very low-resolution pseudoatom models with discrete-state representations, in effect hybridizing conventional CG bead-spring type systems with techniques similar to Markov state decompositions [4].

Kremer and coworkers [5] have also made important developments in "adaptive resolution" simulations in which molecules become coarse-grained in particular spatial domains. Namely, they argue that such transformations naturally incur thermodynamic forces emerging from the coarse-graining process itself, a novel idea that may lead to generalizations. Finally, Katsoulakis and Plecháč [6] proposed a path-integral, information-theoretic approach to developing accurate models of CG dynamics; their theory gives a particularly telling closed-form procedure for estimating Markovian dynamics of CG models. In all, current efforts in coarse-graining suggest an exciting time for creative approaches in terms of both practicality and fundamentals with many interesting developments likely forthcoming.

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Nobel News

In early October The Royal Swedish Academy of Sciences announced its decision to award the Nobel Prize in Chemistry for 2013 to Martin Karplus (Université de Strasbourg, France and Harvard University, Cambridge, MA, USA), Michael Levitt (Stanford University School of Medicine, Stanford, CA, USA), and Arieh Warshel (University of Southern California, Los Angeles, CA, USA) "*for the development of multiscale models for complex chemical systems*." From the press release:

> *The work of Karplus, Levitt and Warshel is ground-breaking in that they managed to make Newton's classical physics work side-by-side with the fundamentally different quantum physics. Previously, chemists had to choose to use either or. The strength of classical physics was that calculations were simple and could be used to model really large molecules. Its weakness, it offered no way to simulate chemical reactions. For that purpose, chemists instead had to use quantum physics. But such calculations required enormous computing power and could therefore only be carried out for small molecules.*

Podcast Interview with Michael Levitt (starting at 12:08): http://goo.gl/8SRUOk
More info: http://goo.gl/2foDWO http://goo.gl/LofkB8 http://goo.gl/LQW82r

Research Highlight: Resolving the structure of liquid water

Cynthia Lo, Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis

The structure of liquid water has been the subject of intense academic research for the past decade ever since researchers analyzing the X-ray absorption spectra (XAS) of liquid water interpreted the presence of a pronounced pre-edge peak as evidence for the "rings and chains" structure [1]. At the time, this statement sparked much controversy, as the notion that water preferentially forms two strong hydrogen bonds and two weak hydrogen bonds contrasted with the conventional view that water is locally tetrahedral. Subsequently, an analysis of the Raman spectra seemed to confirm the tetrahedral coordination of liquid water [2]. Second-generation Car-Parrinello molecular dynamics simulations [3] were used to compute the oxygen-oxygen radial distribution function (RDF) of liquid water at ambient conditions, and integration of the RDF up to the first minimum peak indicated that water is tetrahedrally coordinated [4].

In the recent work by Kühne and Khaliullin [5], they show that a quantum treatment of the nuclei, rather than the classical treatment employed in [4], is necessary to capture the asymmetrical bonding in liquid water. The intermolecular interactions are described in terms of physically meaningful components, including weak dispersive forces, electrostatic effects (e.g. charge-charge, charge-dipole and charge-induced dipole interactions) and donor-acceptor type orbital (i.e. covalent) interactions. Thus, intermediate (bonding) states can be defined to include both intermolecular charge transfer and intramolecular charge reorganization, simply by constructing the wavefunction from variationally optimized absolutely localized molecular orbitals (ALMOs) [6]. The main advantage to this approach is a fully self-consistent treatment of polarization effects, which is necessary to study the charge transfer effects in liquid water. By incorporating ALMOs and an energy decomposition analysis with the second generation Car-Parrinello approach, Kühne and Khaliullin simulated the XAS spectra of liquid water and confirmed that the pre-edge peak is attributed to the water molecules in asymmetric environments; however, this apparent asymmetry is created by instantaneous distortions in a fluctuating hydrogen bonding network. Since XAS probes timescales of less than a femtosecond, it captures this asymmetry. On average, however, these fluctuations are averaged out over timescales of a few hundred femtoseconds so that water appears to be tetrahedrally coordinated when probed by other techniques that more closely follow nuclear motions. This paper represents an important step in resolving the controversy over the structure of liquid water and, more generally, reminds us that chemical bonds are truly dynamic at atomic scales.

References

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Member Spotlights

Mark A. Plummer (MP*r&d*, LLC)

My basic training is in chemical engineering at the Colorado School of Mines where I received B.S., M.S. and Ph.D. degrees. Most of my career was with Marathon Oil Company doing process development. One such development concerned the removal of sulfate ions from seawater using membrane technology. This technology is currently processing over 6 million bbl/day of seawater worldwide. For this development, Marathon received the Hart E&P 2003 Award for Engineering Innovation.

Then, I set up my own company MP*r&d,* LLC (http://mprdllc.com) to do applied and fundamental work in computational chemistry. This was due to my interest in understanding how molecules affect human life and the role they play in industrial processing. In this effort, I have published eight computational chemistry papers dealing with

- protein folding to optimize hydrogen production from water,
- sulfur removal from gasoline using liquid extraction,
- xylene and naphol separation using adsorption,
- hydrogen recovery from hydrogen sulfide,
- hydrocarbon adsorption on tetrachloroaluminates.

I have also worked in sudden infant death syndrome chemistry and potassium transport through human cell walls. Currently, I am doing fundamental computational work in protein folding and applied work in maximizing oxygen tolerance of hydrogen producing proteins.

Yiannis N. Kaznessis (University of Minnesota)

I am Professor in the Department of Chemical Engineering and Materials Science at the University of Minnesota. I received degrees in Chemical Engineering from the Aristotle University in Thessaloniki (Diploma, 1994) and the University of Notre Dame (Ph.D., 1999). I worked at Pfizer Global Research and Development and at the University of Michigan as a Postdoctoral Fellow.

I enjoy teaching “Statistical Thermodynamics” to graduate students at Minnesota. Two thirds of the course is devoted to the fundamentals of ensemble theory and one third is devoted to elements of Monte Carlo and molecular dynamics simulations. After trying various textbooks for a decade I decided it was time to offer my own “Statistical Thermodynamics and Stochastic Kinetics: An Introduction for Engineers”.

Fascination with biological complexity is what drives my research. My group is using computational methods to understand this complexity in terms of molecular interactions governed by laws of statistical thermodynamics.

With models we guide experimental efforts to engineer antibiotic cellbots. These are modified lactic acid bacteria that can be delivered in the gastrointestinal tract of mammals. Inside GI tracts, the lactic acid bacteria detect pathogens, such as antibiotic-resistant enterococcus, and then release antimicrobial peptides that kill the pathogenic microbes.

Aravind Asthagiri (The Ohio State University)

I obtained my B.S. in Chemical Engineering (1998) from The Ohio State University, and a Ph.D. in Chemical Engineering from Carnegie Mellon (2003) with Prof. David Sholl. From 2005-2010, I was an assistant professor at the University of Florida before moving in 2010 to Ohio State as an associate professor. Our group uses atomistic simulations to understand structure-property relationships in materials with a focus on energy-related applications.

I came to my career in computational modeling by accident. In graduate school, I was told to talk to a new faculty member in computational modeling. I knew nothing about this area but once I started the research I felt this was an ideal fit for me. Besides not having to do any experiments, I loved the opportunity to work on problems at a fundamental level. When we solve (or think we have) a problem using computational modeling there is the satisfaction of being able to know exactly why the behavior is the way it is. I enjoy the process of working with experimental collaborators and students in trying to sift out the fundamental mechanisms underlying the phenomena. That this insight can have an impact on applications that are important to society is an added bonus.

Why CoMSEF?

CoMSEF has well over 200 members, and occasionally it is worthwhile to remind everyone what CoMSEF does for our community and why your membership support is important. CoMSEF was founded in 2000, and since that time it has worked to advance molecular science and engineering in diverse ways:

* We provide a forum for communication and networking within the community. The document you're reading now is a prime example, but there is more. The annual membership meeting provides a venue for communication and interaction among members. The CoMSEF web site http://comsef.org is another useful resource for this purpose. It often hosts notices about upcoming workshops, available post-doc positions, etc.

* We provide a vehicle for communication and advocacy for molecular science and engineering in relation to other research communities. For example, our four Liaison Directors identify opportunities for co-sponsorship of sessions at the AIChE Annual Meeting, facilitate programming with other organizations, and communicate and advocate CoMSEF activities with other organizations.

* We help to recognize and promote outstanding researchers and promising graduate students by funding and administering several awards. Most recently we initiated the Young Investigator Award for Modeling and Simulation. This and our other awards help the contributions of some of our best researchers to be recognized by a broad audience, extending into the larger chemical engineering community. Your dues make these awards possible.

* We provide technical programming support, ensuring we have sessions of interest to you at the AIChE meeting. These include the many sessions we sponsor or co-sponsor, as well as the CoMSEF plenary, CoMSEF poster, and Industrial Fluid Properties Simulation Challenge sessions. We also work externally to AIChE, providing technical sponsorship to conferences in our discipline (e.g., FOMMS), where we help to ensure that these events have molecular science and engineering content of the highest quality.

Your support of CoMSEF through your membership is very important in enabling us to fulfill our mission. The financial element is valuable of course, but we also gain strength in demonstrating the size of the community we represent. So please make sure to check the box to include renewal of your CoMSEF membership whenever you pay your annual dues to AIChE. When the opportunity arises, encourage your non-member colleagues in the molecular science and engineering community to join too!