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

April 2012

In This Issue

New Officers

During the fall of 2011, we elected two new Liaison Directors. Congratulations to the newly-elected officers and thanks to all who participated!

Liaison Directors (2011-2013):

- Cynthia Lo (University of Washington in St. Louis)
- Francisco Hung (Louisiana State University)

Thanks also to the two out-going Liaison Directors, Ilja Siepmann and Coray Colina, for their participation! A complete listing of the CoMSEF Executive Committee is available on the web:

http://comsef.org/executivecommittee

Become a CoMSEF Officer!

In 2012 we will be holding elections for several officer positions. These will be:

- Vice-Chair, which is a two-year position on the executive committee that leads to the position of Chair (a two-year term) and past Chair (also a two-year term). The Vice-Chair is in charge of programming within AIChE.
- Two Liaison Directors, which are two-year positions.
- Secretary-Treasurer, which is a two-year position.

If you would like to get involved in CoMSEF and run for one of these elected positions, please contact any of the CoMSEF officers who can discuss the details of these positions with you. You can also find out more information on the CoMSEF web page under the forum bylaws (http://comsef.org/bylaws). We are always looking for new people to get involved with new ideas to keep CoMSEF active and relevant so don't be shy and volunteer!

2011 Graduate Student Awards in Computational Molecular Science and Engineering

Congratulations to the 2011 CoMSEF Graduate Student Award winners:

Andrew Paluch (University of Notre Dame)
Advisor: Ed Maginn

Lauren Abbott (Penn State University)
Advisor: Coray Colina

The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees were selected on the basis on a nomination letter from the advisor (who must be a member of CoMSEF), their CV, and their poster presentation at the Fall AIChE Meeting in Minneapolis.

Left to Right: Andrew Paluch; Ilja Siepmann, Chair of Grad Student Award Committee; Lauren Abbott; Kristen Fichthorn, CoMSEF Chair

2012 Impact Award in Computational Molecular Science and Engineering

CoMSEF is soliciting nominations for the 2012 CoMSEF Impact Award, which recognizes outstanding research in computational molecular science and engineering by a member of CoMSEF. Previous award winners include Ed Maginn (2009), David Sholl (2010), and Bernhardt Trout (2011).

Kristen Fichthorn presents the 2011 award to Bernhardt Trout

Nominees for the 2012 award may hold positions in academia, industry, or a national laboratory, and must be within 15 years of completion of their highest degree. Candidates earning PhD degrees from 1997 onwards are award eligible. Nominees must be current members of CoMSEF.

A nomination package consisting of the nominee's CV, a nomination letter and two supporting letters of recommendation should be sent as a single file in pdf format to the CoMSEF Chair, Kristen Fichthorn (fichthorn@psu.edu). The nomination should provide a clear statement as to the impact of the nominees work on the field and an award citation of 25 words or less, beginning with the word 'For'. Self-nominations are discouraged. The deadline for receipt of nominations will be May 1st for the 2012 award with the recipient being announced prior to the Fall AIChE meeting.

Please note that renomination of candidates is encouraged. It is recommended but not required that the contents of the nomination package be updated each year; while supporting letters may be re-used, the nomination form must have current dates.

The Seventh Industrial Fluid Properties Simulation Challenge

Objective

The 7th Industrial Fluid Properties Simulation Challenge (IFPSC) will focus on predicting adsorption isotherms of n-perfluorohexane (n-C6F14) in BCR-704 Faujasite type zeolite.

Timeline

March, 2012 - Challenge problem announced
Friday, September 21, 2012 - Challenge final entries due

Background

Zeolite adsorbents are used in a variety of applications due to their high surface area and ability to adsorb or desorb sorbates depending upon the applied conditions. Applications include the removal of volatile organic compounds and toxic gases from air and storage of corrosive chemicals during shipping.

With increasing numbers of applications, the ability to predict the performance of zeolites for a wide range of adsorbents would be very valuable in pre-optimizing systems and reducing product development time. Molecular simulation techniques, in principle, could be ideal for predicting adsorption in zeolites with various chemistry.

Although adsorption in porous media has been an area of extensive activity in the field of molecular simulation (e.g. in zeolites [1,2], metal-organic frameworks [3,4], nanotubes [5], and other porous carbons [6,7]), it has not yet been the focus of the IFPSC. Organizing a simulation challenge to assess the capability of molecular simulation methods and force fields to accurately predict adsorption in porous media for practically relevant and moderately complex chemical systems is of interest in order to benchmark the state-of-the-art capability in this important application area.

Studies of adsorption equilibria by molecular simulation employing both Monte Carlo [8-10] and molecular dynamics [11,12] techniques have become relatively common. However, applying these methods to study adsorption equilibria using force fields (potential energy models) developed for bulk phase conditions remains an open issue. General, transferable force fields that are reasonably accurate over a wide range of state conditions in the bulk are not necessarily transferable to the adsorbed phase. Moreover, active sites on the surface of the adsorbent can dramatically affect the adsorption behavior.

The focus of the current challenge is to assess the potential of molecular simulation methods to predict organic sorbate adsorption isotherms. Specifically, the challenge will focus on predicting the adsorption isotherms of n-perfluorohexane in BCR-

704 Faujasite type zeolite.

The certified reference material BCR-704 Faujasite type zeolite will be used in the experimental benchmark studies. The BCR-704 zeolite material is supplied by the Institute of Reference Materials and Measurement (IRMM) and can be obtained from Sigma-Aldrich.

Argon and Nitrogen adsorption isotherm studies have been carried out to characterize the BCR-704 zeolite. The adsorption studies have been carried out by the industry-leading company Quantachrome Corporation. The results of the argon and nitrogen studies will be provided to Challenge entrants to aid in validating simulation models. The adsorption and isotherm data will be provided via a posting on the IFPSC web-site no-later then the end of March 2012.

Elemental analysis has also been carried out on BCR-704 Faujasite type zeolite and is reported in IRMM report EUR 21065 Certification of the Specific Micropore Volume and the Median Micropore Width of Two Microporous Reference Materials According to Draft-DIN 66135-4, BCR-704, BCR-705 (see section 3.2.2). Argon adsorption studies are also reported. Details of an FAU type framework can be found in database of zeolite stuctures from the Structure Commission of the International Zeolite Association (link). Elemental analysis studies are also in progress at 3M Company and will be reported on the IFPSC web-site when completed.

The experimental benchmark adsorption studies for n-perfluorohexane (n-C6F14) in BCR-704 zeolite will also be carried out by Quantachrome Corporation. n-perfluorohexane (n-C6F14) is a high performance material produced by 3M Company.

Challenge

For n-perfluorohexane (n-C6F14), compute adsorption isotherms in BCR-704 zeolite at a temperature of 293K and at relative pressures of 0.01, 0.05, 0.1, 0.2, 0.4, 0.6, and 0.8. The relative pressure is defined as that relative to the bulk saturation pressure predicted by the model for the given temperature (293K in this case).

More details are available at http://fluidproperties.org

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Research Highlight: Assessment of Convergence and Decorrelation Times in Biomolecular Simulations

By Monica H. Lamm

Romo TD and Grossfield A, J. Chem. Theory Comput., 2011, 7, 2464-2472
http://dx.doi.org/10.1021/ct2002754

The topics of structural convergence and statistically significant sampling are too often overlooked by practitioners of molecular simulation. However, as simulations for biological systems now routinely reach the microsecond timescale, assessment of the statistical quality of the trajectories that are generated becomes increasingly important. Romo and Grossfield have recently introduced a new method, the block covariance overlap method (BCOM), for examining the extent to which a simulation trajectory has converged. The authors illustrate the method for three different G protein-coupled receptors and compare decorrelation times estimated from the BCOM to other recent sample quality measures like the effective sample size (Lyman E and Zuckerman DM, J. Phys. Chem. B, 2007, 111, 12876-82). This article emphasizes the importance of using multiple methods of assessment, from simple analysis of the root mean-square deviation from average structure to more sophisticated methods like the BCOM and effective sample size, to completely characterize the quality of the simulation trajectory. All of the analysis tools used in the article are available in the Lightweight Object-Oriented Structure (LOOS) library available at http://loos.sourceforge.net.

FOMMS 2012 update

The Foundations of Molecular Modeling and Simulation (FOMMS) meeting will be held July 22-26, 2012 at The Resort near Mount Hood, Oregon. The theme of the meeting is “Foundations for Data and Discovery”. The meeting will feature sixteen invited talks by leading experts clustered around the following themes

- Complex fluids
- Multi-resolution simulations
- Product and process design
- Energy and environment
- Life Sciences
- Cyberinfrastructure

In addition, there will be an opening plenary lecture given by Prof. Matthias Scheffler of the Fritz Haber Institute, Germany and the meeting will conclude with the traditional FOMMS medal winner, Prof. Keith Gubbins of North Carolina State, giving a closing lecture. In addition, there will be two poster sessions for contributed papers and two hands-on workshops. One will deal with software suites and application interfaces, and the second will focus on validation methods. An optional outing can be taken by participants to enjoy the surroundings one afternoon.

We wish to thank the sponsors of FOMMS 2012: The National Science Foundation, Procter and Gamble, Accelrys, Culgi and Materials Design.

The deadline for early registration is May 31, 2012. More information may be found at the conference website fomms.org.

CoMSEF Sessions at the AIChE 2012 Annual Meeting

CoMSEF is sponsoring or co-sponsoring 31 sessions at the AIChE Annual Meeting in Pittsburgh. Abstracts for any of these sessions can be submitted via AIChE’s online system until May 2, 2012. Although all of these sessions are excellent opportunities to interact with the CoMSEF community, two deserve special mention. Peter Cummings and Seung-Soon Jang are chairing a session on “GPUs, cloud computing, and crowdsourcing”, which seeks work in the rapidly growing area of non-traditional architectures and venues for computing. The CoMSEF poster session is an ideal venue for graduate students to interact with a broader cross section of the community than in a traditional oral presentation. We are endeavoring to draw a range of excellent presentations into the poster session to continue the tradition of this poster session being a vital part of the overall technical programming. Graduate-student participants in the poster session can be considered for a CoMSEF Graduate Student Award (see the Call for Nominations below). We encourage graduate students to present their best work at the poster session, as well as orally.

Happy Birthday, Professor Gubbins!
Please join us in celebrating the remarkable achievements of Keith Gubbins as we note his 75th birthday with a series of talks sponsored by Area 1A and co-sponsored by CoMSEF.

A highlight of the CoMSEF programming will be the CoMSEF Plenary Session. Presentations for this session are selected by the CoMSEF executive committee and represent some of the best work from the CoMSEF community. Please consider submitting your best work here! This session will also feature an invited presentation by the CoMSEF Impact Award winner.

Upcoming Conferences

Midwest Thermodynamics and Statistical Mechanics Conference
May 20-22, 2012
University of Minnesota, Minneapolis, MN
https://gemini.cems.umn.edu/orgs/MTSM_12/

Vanderbilt/Columbia Molecular Modeling Cybercamp
May 28-31, 2012
Nashville, TN
https://huggins.vuse.vanderbilt.edu/cybercamp/?q=node/12

Midwest Theoretical Chemistry Conference
June 7-9, 2012
University of Wisconsin, Madison, WI

http://www.mwtcc.org

Searching for Reaction Coordinates and Order Parameters
June 17-21, 2012
Telluride Science Research Center, Telluride, CO
http://www.telluridescience.org/reg/workshop_details.php?wid=309

18th Symposium on Thermophysical Properties
June 24-29, 2012
Boulder, CO
http://thermosymposium.boulder.nist.gov/
This triennial symposium is organized by the ASME/AIChE Joint Committee on Thermophysical Properties, provides ample opportunities for oral and poster presentations and informal discussions and takes place on the beautiful CU Boulder campus.

FOMMS 2012
July 22-26, 2012
The Resort at the Mountain, Welches, Oregon
http://fomms.org/

International Conference on Chemical Thermodynamics (ICCT 2012) / CALCON 2012
August 5 - 10, 2012
Búzios, Brazil
http://www.icct2012.org/
The International Conference on Chemical Thermodynamics (ICCT) is held every two years, organized by the International Association for Chemical Thermodynamics (IACT – link – http://iactweb.org) under the auspices of IUPAC.

Modeling and Design of Molecular Materials 2012
September 10-14, 2012
Wrocław, Poland
http://mdmm.pl/2012/

DPG-School on Physics
Efficient Algorithms in Computational Physics
Physics Center Bad Honnef, Germany, 10. - 14. September 2012
http://www.dpg-physik.de/dpg/pbh/aktuelles/S112.html?lang=en

6th International Symposium on Molecular Thermodynamics and Molecular Simulation
September 25-28, 2012
Higashi-Hiroshima Campus of Hiroshima University, Hiroshima, Japan
http://www2.scej.org/pp/MTMS12/

Properties and Phase Equilibria for Product and Process Design 2013
May 26-30, 2013
Iguazu Falls, Argentina, Brazil
http://www.ppeppd2013.plapiqui.edu.ar/openconf.php

RESEARCH HIGHLIGHT: Complex capacitance scaling in ionic liquids-filled nanopores

By: Francisco R. Hung

Wu, P.; Huang, J.; Meunier, V.; Sumpter, B. G.; Qiao, R. ACS Nano 2011, 5, 9044-9051
DOI: http://dx.doi.org/10.1021/nn203260w

Electrochemical double-layer capacitors (EDLCs), or supercapacitors, are devices that have a structure similar to a battery, but differ from those in that electrical energy is stored physically at the interface between a nanoporous electrode and an electrolyte in EDLCs. These devices exhibit fast charge/discharge times and can provide bursts of energy very quickly, but cannot store as much energy as fuel cells and batteries. These limitations have hampered a more extensive use of EDLCs. However, recent experimental results suggest that carefully controlling the properties of the nanoporous electrodes and the electrolytes can lead to significant improvements in the energy storage in EDLCs. In particular, some experiments involving nanopores filled with organic electrolytes or ionic liquids (ILs) suggest that a reduction in pore size can lead to anomalous increases in the capacitance of these systems (see, e.g., Largeot et al., J. Am. Chem. Soc. 2008, 130, 2730-2731; Chmiola et al., Science 2006, 313, 1760-1763). The reasons behind this behavior are not fully understood; furthermore, a recent experimental study (Centeno et al.,

Phys. Chem. Chem. Phys. 2011, 13, 12403-12406) have reported that the capacitance of similar systems remain relatively constant upon variation of the pore size.

Very recently, Wu et al. (ACS Nano 2011, 5, 9044-9051) reported molecular dynamics (MD) simulations of systems of charged slit-shaped nanopores of different sizes in contact with an IL electrolyte. Their results show that the capacitance of these IL-filled nanopores has a U-shaped behavior with pore size, with a minimum around 0.9 nm. Further reductions in pore size leads to increases in the capacitance, in agreement with the experiments of Chmiola et al. and Largeot et al. Wu et al. also found that pore sizes larger than 0.9 nm also lead to increases in the capacitance; a couple of recent studies suggest that the specific capacitance has a decaying oscillatory behavior as the pore size increases (Feng and Cummings, J. Phys. Chem. Lett. 2011, 2859-2864; Jiang et al., Nano Lett. 2011, 11, 5373-5377). Finally, Wu et al. rationalized how changes in the molecular-level structure of the ions in the pores, as induced by variations in pore size and voltage, translate into changes in the capacitance. These computational results suggest that one can optimize the capacitance in EDLCs not only by varying the pore size of the nanoporous electrodes, but also by carefully choosing the ion pairs of an IL-based electrolyte based on size, shape and chemical details of the ions.

Call for Nominations: 2012 CoMSEF Graduate Student Awards

CoMSEF is soliciting nominations for the 2012 graduate student awards recognizing excellence in research by graduate students. The intent of the awards is to reward significant contributions to research in computational molecular science and engineering by students. The award consists of a certificate and an honorarium. Two awards are to be given annually. The 2012 awards will be presented at the Annual Meeting in Philadelphia.

Nominations should consist of a nominating letter from the student's research advisor and the CV of the nominee. We encourage advisors to note that these documents form an important part of the decision process; this is not just a poster competition. The nominee must be a graduate student at the time of the poster presentation and the faculty nominator must be a member of CoMSEF. The nomination should be sent as a single pdf file via e-mail from the advisor to the CoMSEF Chair, Kristen Fichthorn (fichthorn@psu.edu), by October 1, 2012.

In addition, nominees must submit an abstract to the CoMSEF Poster session. The deadline for submission of poster abstracts is May 2, 2012.

The winners will be selected by a committee composed of CoMSEF officers based on the student's CV, the nomination letter from the advisor (who must be a member of CoMSEF), and the quality of the poster presentation.

Please contact Kristen Fichthorn (fichthorn@psu.edu) if you have questions about the award.

Vanderbilt/Columbia Molecular Modeling Cybercamp

Vanderbilt University, Columbia University and CAChE Molecular Modeling Task Force, are holding the second annual Cybercamp at Vanderbilt for anyone interested in learning about molecular modeling techniques used in computational materials science, chemistry and biology.

What: A 4-day hands-on intensive course on molecular modeling methods (molecular dynamics, Monte Carlo, quantum chemistry, visualization) taught by leading simulators.
Who: Suitable for undergraduates, new graduate students, and talented high school students who want to learn how to perform molecular simulation.
Why: Learn how to do simulation while enjoying a social program in Music City USA.
When: May 28-31, 2012.

Please encourage your students and postdocs to participate again this year.

The link for the cybercamp is https://huggins.vuse.vanderbilt.edu/cybercamp/?q=node/12. There is a pre-registration form for people to express interest. We have reserved 20 on-campus dorm rooms for participants. We expect to be able to cover the local expenses of students staying in the dorm rooms (including the cost of the dorm rooms); however, we are unable to cover travel costs to Vanderbilt, nor the local accommodation costs of participants staying hotels. >

Due to limited classroom space, attendance will be limited to 35 participants.

Member Spotlights

The "member spotlight" is a new newsletter feature intended to introduce CoMSEF members (selected at random) to the rest of the CoMSEF membership.

John Brennan (U.S. Army Research Laboratory)

I am a research chemical engineer in the Weapons and Materials Research Directorate at the U.S. Army Research Laboratory (ARL) in Maryland. I'm responsible for performing computational and theoretical research investigations to determine the physical and chemical processes of materials of interest to the Army at both the atomistic and coarse-grain levels. My duties include leading ARL's coarse-grain modeling efforts to study the multiscale response of energetic materials. I earned a Ph.D. in chemical engineering from Wayne State University in 1999. I have held post-doc positions at the Institut de Recherché sur la Catalyse (CNRS) in Lyon, France with Wei Dong, and then with Keith Gubbins at North Carolina State University.

Computational science and engineering sits at the crossroads of my two scientific loves, mathematics and chemistry. I still remember the thrill of successfully writing a Monte Carlo code during graduate school and thinking this was perfect work for a clumsy-handed and impatient-minded student looking to avoid actual laboratory work. At the time, I didn't appreciate the role that computational science and engineering would play in guiding advancements in many areas of science, but I'm eternally grateful to my graduate advisor, William Madden for introducing me to this fascinating realm of science.

C. Heath Turner (The University of Alabama)

Identifying a good career match can be a challenge for many students. However, during a graduate recruiting weekend at NC State, I was fortunate enough to talk with Carol Hall, and later with Keith Gubbins, about their research. I felt like the computational approach to modeling molecular-level behavior was fascinating, plus I had been writing computer programs since elementary school. I was immediately sold! Now, as a professor, I find it very motivating to work along with experimentalists, as even very simple modeling studies can provide a great deal of value and insight.

Biographical Sketch: Prof. Turner completed his B.S. in Chemical Engineering from Auburn University and his Ph.D. in Chemical Engineering from NC State University with Prof. Keith Gubbins. He spent several years in industry with Monsanto, Birmingham Steel, and Trinity Consultants. He joined the University of Alabama in 2003, later appointed as the Reichhold-Shumaker assistant professor, and he is now an associate professor. Over the past few years, he has been a visiting fellow at NASA in Langley, VA and at the Naval Research Lab in Washington, D.C. *His research deals with the computer simulation of chemical reactions and adsorption on surfaces and at interfaces.*