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

March 2015

In This Issue

CoMSEF Elections

Elections for CoMSEF officers were held in the fall of 2014 for the positions of Vice Chair, Secretary-Treasurer, and 2 Liaison Directors. Jeff Errington (University at Buffalo) was elected Vice Chair, Joe Golab (Ineos) was elected Secretary-Treasurer, and Erik Santiso (NC State) and Michael Shirts (Virginia) were elected Liaison Directors.

After two years as Vice Chair, the Vice Chair serves a two-year term as Chair. Liaison Directors Facilitate programming with other organizations by identifying opportunities for co-sponsorship, communicate and advocate CoMSEF activities with other organizations, and as members of the Executive Committee, aid the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter.

Thanks to Jim Pfaendtner and Scott Shell (liaison directors) and David Sholl (chair) who completed their terms.

McCabe Winner of 2014 CoMSEF Impact Award

Professor Clare McCabe from Vanderbilt University is the winner of the 2014 CoMSEF Impact Award, which cites her "*...development of practical molecular equations of state for simulating thermophysical properties of fluids and novel coarse-grained simulation models for biomedical applications*."

Clare received her award during the CoMSEF Plenary Session at the 2014 AIChE Annual Meeting, where she also gave a talk titled “Understanding the Self-Assembly of Skin Lipids” describing her research.

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

Beckham Winner of 2014 CoMSEF Young Investigator Award

Dr. Gregg Beckham from the National Renewable Energy Laboratory's National Bioenergy Center is the winner of the 2014 CoMSEF Young Investigator Award. Gregg joined NREL in 2007... With this award, Gregg is cited “*...for elucidation of cellulose degradation mechanisms towards improved enzymes for biofuels and other renewable energy applications.*” Gregg received his award during the CoMSEF Plenary Session at the 2014 AIChE Annual Meeting, where he also gave a talk titled “How the Walls Come Crumbling Down: Elucidating Mechanisms of Cellulose-Active Enzymes Using Molecular Simulation” describing his 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.

2014 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were awarded for the 9th consecutive year at the annual AIChE Meeting in Atlanta. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Two awardees were selected based on the nomination letters received from each student’s advisor, their CV, and a poster presented at the CoMSEF poster session. The winners were announced at the CoMSEF/Area 1a annual General Meeting.

The 2014 student winners were:

- Heather Mayes (Northwestern, advisor: Linda Broadbelt)
- Yamil Colón (Northwestern, advisor: Randall Snurr)

From left: Prof. Jeff Errington (CoMSEF Vice Chair), Yamil Colón (Northwestern), Heather Mayes (Northwestern), and Prof. Coray Colina (CoMSEF Chair)

Research Highlight: You got your molecular dynamics in my Monte Carlo!

Lev Gelb, The University of Texas at Dallas

Allen and Quigley, in the recent special issue of Molecular Physics for Giovanni Ciccotti's 70th birthday, review techniques intermediate between MD and MC and point out some links and relationships between them which are, they feel, not well enough known [1]. The focus of the paper is on configurational sampling; dynamical phenomena are not considered.

Hybrid Monte Carlo (HMC) uses short microcanonical MD trajectories started with Boltzmann-sampled velocities to generate new trial states. This is shown to be a 'Metropolized' version of Andersen-type thermostatted molecular dynamics. A simple demonstration is given of the failure of the Andersen algorithm to recover the target configurational temperature for large time steps, while the Metropolized version does much better.

Likewise, it was recognized long ago that purely random displacements in MC might be improved upon by incorporating gradient (force) information, leading to Force-Bias Monte Carlo (FBMC) and Smart Monte Carlo (SMC) (and some debate as to how different they were, and which was better [2].) SMC is a 'Metropolized' form of Brownian Dynamics (BD), and Allen and Quigley argue that both can be thought of as variants of HMC.

The paper then turns to flat-histogram methods that use MD-like sampling, in particular those based on a modified hamiltonian which depends not on the potential energy but the density of states [3]. Once again, an Andersen stochastic thermostat is used; once again, if Metropolized, this becomes an HMC method. A simple demonstration is performed using Statistical Temperature MD (but now with Metropolization, which is not normally used), and excellent agreement with exact results is obtained. The paper closes with some final thoughts on non-iterative flat-histogram schemes and adaptive force-biasing.

I found this a very clean overview of the topic, and appreciated both the educational motivation of the paper and its emphasis on checking that one is sampling the correct ensemble, as recently highlighted by Shirts [4].

In another recent review [5], Neyts and Bogaerts discuss many of the same techniques, but with the objective of accessing longer time-scales ("You got your Monte Carlo in my molecular dynamics!"). Neyts and Bogaerts also discuss recent variants of FBMC that incorporate a statistical time-scale, and hybrid techniques which alternate between MD-like and MC-like methods; examples taken from the literature are used to illustrate some of these.

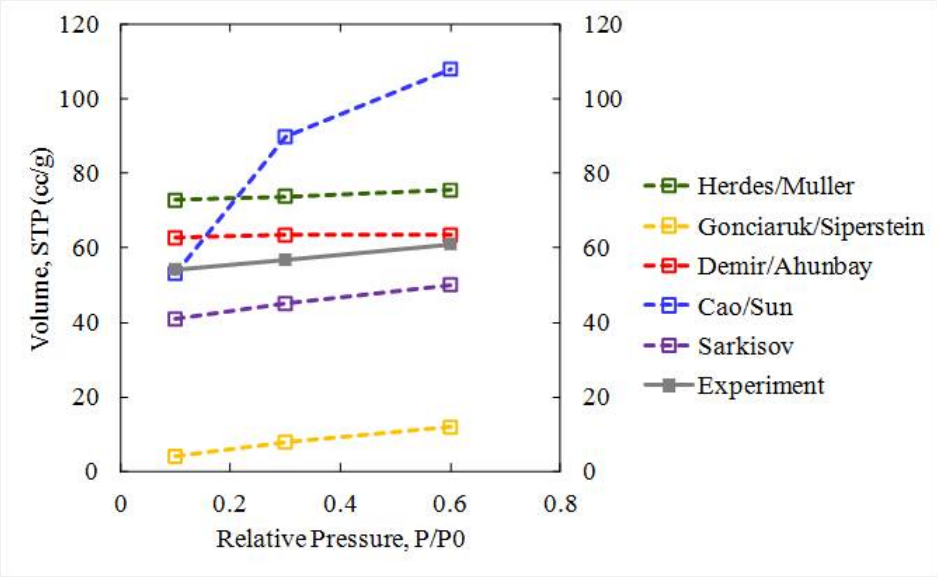
[1] M. P. Allen and D. Quigley, “Some comments on Monte Carlo and molecular dynamics methods,” *Mol. Phys.* **111** (2013) 3442-3447. http://dx.doi.org/10.1080/00268976.2013.817623
[2] M. Rao and B. J. Berne, “On the force bias Monte Carlo simulation of simple liquids,” *J. Chem. Phys.* **71** (1979) 129-132. http://dx.doi.org/10.1063/1.438111
[3] U. H. E. Hansmann., Y. Okamoto and F. Eisenmenger, “Molecular dynamics, Langevin and hybrid Monte Carlo simulations in a multicanonical ensemble,” *Chem. Phys. Letts.* **259** (1996) 321-330. http://dx.doi.org/10.1016/0009-2614(96)00761-0
[4] M. R. Shirts, “Simple Quantitative Tests to Validate Sampling from Thermodynamic Ensembles,” *J. Chem. Theor. Comput.* **9** (2013) 909-926. http://dx.doi.org/10.1021/ct300688p
[5] E. C. Neyts and A. Bogaerts, “Combining molecular dynamics with Monte Carlo simulations: implementations and applications,” *Theor. Chem. Acc.* **132** (2013) 1320. http://dx.doi.org/10.1007/s00214-012-1320-x

The 8th Industrial Fluid Properties Simulation Challenge

Activated carbons are among the most widely used industrial materials. Due to their low cost of production and high adsorption capacity, they have found use in applications including: gas and electrolyte storage; gas and fluid purification; and catalysts and catalyst supports. Activated carbons are typically synthesized from organic carbonaceous precursors such as woods, coconut shells and coals. By judicious choice of the precursor materials and synthesis conditions, they can be synthesized with a wide range of features such as pore size distribution, specific surface area and chemical composition

With increasing numbers of applications, the ability to predict the performance of activated carbon adsorbents for a wide range of sorbent compounds would be very valuable in pre-optimizing systems and reducing product development time. Molecular simulation techniques in principle could be ideal to predict the adsorption isotherms of activated carbon sorbents for sorbates of varied chemistry as well as for various chemically-modified activated carbon adsorbents.

The 8th Simulation Challenge continued the adsorption theme of the 7th Challenge in order 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 in order to benchmark the state-of-the-art capability in this important application area. In particular, the entrants were challenged to predict the adsorption isotherm of n-perfluorohexane (n-C6F14) on the Certified Reference Material BAM-P109 Carbon at a temperature of 273 K and at relative pressures of 0.1, 0.3, and 0.6. The relative pressure is defined as that relative to the bulk saturation pressure predicted by the model for the given temperature. At these relative pressures, the micropores of BAM-P109 are expected to be filled with adsorbate, and an accurate simulation model for adsorption in the carbon micropores would be necessary for successful predictions. Evaluating this capability is the primary goal for the 8th Simulation Challenge.



The Challenge was announced in January of 2014, and entries were due on September 26. Five entries were received from: a) Herdes, Forte, Jackson, and Muller (Imperial College); b) Gonciaruk, Runcieman, Avendano-Jimenez, and Siperstein (U. Manchester); c) Demir and Ahunbay (Istanbul Technical U.); d) Cao, Jing, and Sun (Shanghai Jiao Tong U.); and e) Sarkisov (U. Edinburgh). Their simulation results and the experimental data are summarized in the figure above.

The team of Demir and Ahunbay were named Champions of the 8th Challenge at a special session sponsored by CoMSEF at the AIChE annual meeting. In the photo below, Goktug Ahunbay is congratulated by Daniel Siderius of NIST at the IFPSC session.

Thank you to all who participated and to 3M and Quantachrome for providing the benchmark data for the Challenge. More details about the 8th Challenge and news about the upcoming 9th will be posted at http://fluidproperties.org and articles describing the benchmark data and entries for the 8th Challenge will be published in the journal Adsorption Science & Technology in 2015.

New CoMSEF Award: Conference Presentation Award

CoMSEF Conference Presentation Award recognizes excellence in research by undergraduate students, graduate students and/or postdoctoral researchers. The intent of the award is to reward significant contributions to research in computational molecular science and engineering by young researchers. The award consists of an announcement for the presentation (e.g. a ribbon to place on the poster) and a waived conference registration fee for the awardee.

Nominations should consist of a single nomination package (in PDF format) consisting of a **summary of nominee's presentation** at the meeting in extended abstract style along with a **clear statement** as to how the work impacts CoMSEF's mission. A **nominating letter** from the student's research advisor and the **curriculum vitae** of the nominee (Nominee's abbreviated/ highlighted CV (~ 1-2 pages)).

This year CoMSEF will be sponsoring a Conference Presentation Award to participate in FOMMS (fomms.org). A single nominations should be sent by the advisor via e-mail in pdf format to the CoMSEF co-Chair (co-chair@comsef.org) by March 12, 2015.

In addition, nominees must **present a poster** (or talk) at the Conference. The nominee must be an **undergraduate student**, **graduate student or postdoctoral researcher** at the time of the the presentation, and **the faculty nominator must be a member of CoMSEF**. The winners will be selected by a committee composed of CoMSEF officers and a conference representative (i.e. chair.)

Call for Nominations: CoMSEF Awards

In addition to the new Conference Presentation Award, nominations for the other CoMSEF awards are being accepted in the coming weeks and months.

****2015 Impact Award in Computational Molecular Science and Engineering****

Purpose: This award recognizes outstanding research in computational molecular science and engineering, encompassing both methods and applications. Nominees may hold positions in academia, industry, or a government lab, and must be ***within 15 years of completion*** of their highest degree (e.g., someone receiving a PhD degree in 2000 is eligible for the award through 2015).

Requirement: Nominees must be current members of CoMSEF. The CoMSEF Chair and Vice-Chair are ineligible for nomination while they hold these offices. Other CoMSEF officers are eligible for nomination.

Nomination process: A single nomination package consisting of the nominee's CV, a nomination letter (typically from the nominee's department chair or supervisor) and two supporting letters of recommendation should be submitted as a single pdf file to the CoMSEF chair (chair@comsef.org). 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. Call for nominations will coincide with the announcement of the AIChE Annual Meeting's call for papers. **Deadline for receipt of nominations will be May 1st, 2015.**

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.

Selection process: An ad hoc selection committee consisting of the current CoMSEF chair, the CoMSEF vice-chair and two representatives drawn from related organizations (e.g., area 1a committee, CACHE trustees) will choose the winner based on the overall strength of the research accomplishments of the candidate. A decision regarding the winner of the award will be made by July 1st in order to allow for the award winner to appear in promotional material for the annual meeting.

The award will be presented at the Annual Meeting and the awardee is expected to give a invited talk in the CoMSEF plenary session at the annual meeting.

Frequency: Awarded annually

Prize: A plaque and a cash award

****2015 Young Investigator Award for Modeling and Simulation****

Purpose: This award recognizes outstanding research in computational molecular science and engineering, encompassing both methods and applications. Nominees may hold positions in academia, industry, or a government lab, and must be within 7 years of completion of their highest degree (e.g., someone receiving a PhD degree in 2010 is eligible for the award through 2017).

Requirement: Nominees must be current members of the Computational Molecular Science and Engineering Forum (CoMSEF). The CoMSEF Chair and Vice-Chair are ineligible for nomination while they hold these offices. Other CoMSEF officers are eligible for nomination.

Nomination process: A single nomination package consisting of the nominee's CV, a nomination letter (typically from the nominee's department chair or immediate supervisor) and two supporting letters of recommendation should be submitted as a single portable document format (pdf) file to the CoMSEF chair (chair@comsef.org). The nomination should provide a clear statement of the impact of the nominee's work on the field and include an award citation of 25 words or fewer beginning with the word 'For'. Self- nominations are discouraged. The deadline for receipt of nominations is May 1st 2015.

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.

Selection process: An ad hoc selection committee consisting of current CoMSEF officers and two representatives drawn from related organizations (e.g., Area 1a committee, CACHE trustees) will choose the winner based on the overall strength of the research accomplishments of the candidate. A decision regarding the winner of the award will be made by July 1st in order to allow for the award winner to appear in promotional material for the annual AIChE meeting. The award will be presented at the annual AIChE meeting and the awardee shall give an invited talk in the CoMSEF plenary session.

Frequency: Awarded annually

Prize: A plaque and a cash award

****Graduate Student Awards in Computational Molecular Science and Engineering****

AIChE's Computational Molecular Science and Engineering Forum (CoMSEF) graduate student awards recognize 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.

Nominations should consist of a **nominating letter** from the student's research advisor and the **curriculum vitae** of the nominee. These should be sent by the advisor via e-mail in pdf format to the CoMSEF co-Chair (co-chair@comsef.org) by **October 1.**

In addition, nominees must **present a poster** at the CoMSEF Poster session at the AIChE annual meeting. 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 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.

FOMMS 2015

We are pleased to announce that the 6th conference on Foundations of Molecular Modeling and Simulation (FOMMS) will be held July 12-16, 2015 near Mt. Hood in Oregon (USA).

The theme of the meeting is "Molecular Modeling and the Materials Genome." We have an outstanding line-up of invited speakers. Highlights include:
-- Opening Keynote Lecture by Prof. Frank Stillinger
-- FOMMS Medal Lecture by Prof. Carol Hall
-- Three hands-on workshops
-- Two poster sessions
More details, including the full list of speakers and session titles, are available at fomms.org.

Registration is now open, and information about abstract submission for poster presentations is available on the website (fomms.org). Abstracts must be submitted by March 16, 2015.

We hope to see you in Oregon this summer!

Best regards,

Randy Snurr	Claire Adjiman	Dave Kofke
FOMMS Chair	Co-chair	Co-chair

Upcoming Conferences of Interest to CoMSEF Members

29th Molecular Modeling Workshop 2015
March 9-11, 2015
University Erlangen-Nuremberg
http://mmws2015.mgms-ds.de/

Workshop: Computing Free Energy Across Disciplines: From Method Development to Applications
March 9-11, 2015
Munster, GER
http://www.uni-muenster.de/FEW2015/

Computational Molecular Science 2015
March 15-18, 2015
Coventry, UK
http://www2.warwick.ac.uk/fac/sci/chemistry/news/events/cms2015

11th International Conference of Computational Methods in Sciences and Engineering
March 20-23, 2015
Athens, Greece
http://www.iccmse.org/

249th ACS National Meeting
March 22-26, 2015
Denver, CO
http://www.acs.org

MRS Spring Meeting
April 6-10, 2015
San Francisco, CA
http://www.mrs.org/spring2015/

AMBER Workshop
April 26-30, 2015
Haifa, Israel
http://biology.technion.ac.il/~amber_workshop_technion_israel/

AIChE Spring Meeting
April 26-30, 2015
Austin, TX
http://www.aiche.org/conferences/aiche-spring-meeting-and-global-congress-on-process-safety/2015

ICCCE 2015 : XIII International Conference on Chemistry and Chemical Engineering
May 14-15, 2015
Amsterdam, The Netherlands
https://www.waset.org/conference/2015/05/amsterdam/ICCCE

15th International Congress of Quantum Chemistry
June 8-13, 2015
Beijing, China
http://www.icqc2015.org/

Nanotech 2015
June 14-17, 2015
Washington, DC
http://www.techconnectworld.com/Nanotech2015/

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
July 12-16, 2015
Mt. Hood, Oregon
http://fomms.org/

Gordon Conference: New Frontiers in Computer-Aided Drug Design
July 19-24, 2015
West Dover, VT
http://www.grc.org/programs.aspx?id=12080

Gordon Conference: Nano-Mechanical Interfaces—Theory, Computations and Experiments
July 19-24, 2015
Hong Kong, China
http://www.grc.org/programs.aspx?id=15890

250th ACS National Meeting
August 16-20, 2015
Boston, MA
http://www.acs.org

ICCEAC 2015 : XIII International Conference on Chemical Engineering and Applied Chemistry
September 17-18, 2015
Rome, Italy
https://www.waset.org/conference/2015/09/rome/ICCEAC

AIChE Annual Meeting
November 8-13, 2015
Salt Lake City, UT
http://www.aiche.org/conferences/aiche-annual-meeting/2015

ICMMN 2015 : XIII International Conference on Molecular Materials and Nanosystems
November 12-13, 2015
Kyoto, Japan
https://www.waset.org/conference/2015/11/kyoto/ICMMN/

MRS Fall Meeting
November 29-December 4, 2015
Boston, MA
http://www.mrs.org/fall2015/

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

STATPHYS26
July 18-22, 2016
Lyon, France
http://statphys26.sciencesconf.org/

11th Asian Thermophysical Properties Conference
October 2- 6, 2016
Yokohama, Japan
http://atpc2016.org/

Why CoMSEF?

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!