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

May 2013

In This Issue

New Officers

We welcome two new Liaison Directors, who were elected in the fall of 2012. Our new Liaison Directors, who will hold this office from 2012-2014 are Jim Pfaendtner (University of Washington) and Scott Shell (UCSB).

We greatly appreciate the work done by our outgoing Liaison Directors, Arthi Jayaraman and Monica Lamm.

2013 Young Investigator Award for Modeling and Simulation

We are pleased to announce a new award that will be given annually to honor a young investigator from the CoMSEF community. 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 in the year of nomination for the award. Nominees must be current members of CoMSEF. The CoMSEF Chair and Vice-Chair are ineligible for nomination while they hold these offices, but other CoMSEF officers may be nominated. The award will be presented at the AIChE Annual Meeting and the award recipient will be invited to give a talk in the CoMSEF Plenary Session.

A single nomination package consisting of the nominee's CV, a nomination letter (typically from the nominee's department head or immediate supervisor) and two supporting letters of recommendation should be submitted as a pdf file to the CoMSEF Past-Chair, Kristen Fichthorn (fichthorn@psu.edu). The nomination should provide a clear statement as to the impact of the nominee's work on the field, and include an award citation of 25 words or less beginning with the word "For". Self nominations are discouraged.

The deadline for nominations in 2013 will be May 20.

Graduate Student Awards in Computational Molecular Science and Engineering

We congratulate the winners of the 2012 CoMSEF Graduate Student Award winners, who were selected on the basis of a nomination letter from their advisor and their poster presentation at the Fall AIChE Meeting in Pittsburgh:

Chris Wilmer (Northwestern University, Advisor: Randy Snurr)
Andrew White (University of Washington, Advisor: Shaoyi Jiang)

To be eligible for the 2013 Graduate Student Award, the student should submit a poster to the CoMSEF Poster Session and have their advisor send a nomination letter to the CoMSEF Chair, David Sholl (david.sholl@chbe.gatech.edu).

Left to Right: Kristen Fichthorn, CoMSEF Chair; Andrew White; Chris Wilmer; and Dave Kofke, Chair of Grad Student Award Committee

Impact Award in Computational Molecular Science and Engineering

CoMSEF is soliciting nominations for the 2013 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), Bernhardt Trout (2011), and Fernando Escobedo (2012). Nominees for the 2013 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 1998 onwards are award eligible. Nominees must be current members of CoMSEF.

Kristen Fichthorn presents the 2012 award to Fernando Escobedo

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, David Sholl (david.sholl@chbe.gatech.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 20 for the 2013 award with the recipient being announced prior to the Fall AIChE meeting.

2013 GROMACS USA Workshop and Conference

A conference and workshop on molecular simulation using GROMACS will be held at the University of Virginia, Charlottesville, VA, on September 13th-15th. This event is officially sponsored by the GROMACS developer community.

The 2013 GROMACS USA workshop and conference is designed:

- to provide direct instruction to GROMACS users on best practices and advanced methodologies;
- to bring GROMACS developers to GROMACS users, allowing users to become better informed about GROMACS philosophies, visions, capabilities, and plan;
- to bring GROMACS users to GROMACS developers in order to improve understanding of use cases, problems, and potential improvement of the software;
- to share research success stories, helping inspire molecular simulation students to try more complicated but more effective simulation techniques, and;
- to create an integrated workshop-tutorial framework to be posted online which will continue to be useful after the conference

For more information, visit http://faculty.virginia.edu/gromacsworkshop

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Research Highlight: Enhanced Sampling for Everyone

By Jim Pfaendtner

The past decade has seen a proliferation in the publication of new methods to carry out so-called "enhanced sampling" calculations in molecular dynamics and Monte Carlo simulations. The central challenge these calculations try and address is the fact that free-energy barriers (both enthalpy and entropy dominated) frustrate exploration of phase space and frequently limit accurate calculation of quantitative thermodynamic observables. There now exists a huge menu of choices for a researcher using molecular simulation to speed convergence, use compute resources more efficiently, and generally add confidence to results. The merits of different methods will undoubtedly continue to be debated, and it is likely that proficiency in several methods will be a desirable skill for graduate students and postdocs with expertise in MD/MC.

In recognition of the challenges of learning and applying new methods as well as the need for at least a modest amount of standardization in our community, Prof. Michael Shirts at the University of Virginia has been a leading figure in the effort to develop a set of best practices for free energy calculations. In a recent publication [1], Profs Shirts and Mobley (UC Irvine) introduce the concept of best practices in enhanced sampling calculations and take first steps towards guiding the simulation community towards a consensus for how we implement, validate and use new methods. Last summer at the FOMMS meeting, Prof. Shirts lead a stimulating discussion on this subject and a workshop on a similar theme. As more and more users are introduced to enhanced sampling calculations these issues will continue to grow in importance, and the authors are applauded for their foresight

and efforts in this area.

Equally important to best practices is the ease with which new methods can be incorporated into existing codes. Many groups make use of highly parallelized codes like GROMACS, NAMD and LAMMPS. While these codes offer fantastic scalability and a wide range of features, adding new methods to the core force/energy routines is not trivial and can be fraught with major difficulties. To address this challenge, a team of volunteer developers have produced a near-universal plugin called PLUMED [2]. Originally developed to incorporate the metadynamics method, the PLUMED code has been extended to a huge range of enhanced sampling methods and portable to 8 popular MD engines. The plugin is freely available at http://www.plumed-code.org and is supported by excellent documentation and an active mailing list. In a special effort to lower the barrier to using these methods, several tutorials and hands-on workshops have proliferated a huge number of specific examples (provided on the above website).

[1] M. R. Shirts and D. L. Mobley, An introduction to best practices in free energy calculations, *Methods Mol. Biol.,* 2013, 924, 271-311.

[2] M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R.A. Broglia and M. Parrinello, PLUMED: a portable plugin for free energy calculations with molecular dynamics, *Comp. Phys. Comm.*, 2009, 180, 1961-1972.

Research Highlight: Ions and organic molecules in atmospheric water droplets

By Francisco Hung

Atmospheric aerosols are a portion of particulate matter that play an important role in climate, air quality and fate of pollutants in the atmosphere, although significant uncertainties remain due to limited knowledge on the sources, composition and path of formation of these aerosols.[1-4] In the well-known smog-fog-smog cycle,[5] fog forms by condensation of water on sub-micron particles, which then uptakes organics from different sources (automobile emissions, plants, etc.). These organics can react with atmospheric oxidants [e.g., ozone and radicals such as hydroxyl (•OH) and nitrate ($\bullet NO_3$)] in the fog droplets to yield more organics and aerosols as fog dissipates, leading to the formation of more particulate matter where water can condense in the next fog episode.[1,5] Furthermore, processes at the sea surface such as waves and bubble-bursting can eject sea water droplets carrying halide anions (Cl^-, Br^-). These airborne sea water droplets provide a favorable environment for these anions to react with •OH or O_3, which can have direct implications in the ozone cycle. Therefore, understanding the properties of organic molecules and ions in water droplets is relevant to the chemical processing of these species in the atmosphere.

In a couple of recent studies,[6,7] the group of David van der Spoel used potential of mean force (PMF) calculations to analyze the solvation of ions and organic molecules in water droplets. Constrained molecular dynamics simulations were used to determine the PMF as a function of the position of the solute (i.e., within the water droplet, at the air/water interface, or in gas phase). Interestingly, the PMF was decomposed into its enthalpic and entropic components, and the enthalpy was then further separated into water-water and solute-water interactions. For the case of ions,[6] van der Spoel *et al.* found that Cl^-, Br^- and I^- have a thermodynamic preference to remain at the air/water interface, mainly because water-water interactions are dominant and drive these anions to be partially desolvated at the interface. In contrast, cations such as Li^+, Na^+ K^+, Rb^+ and Cs^+, and the F^- anion prefer to stay inside the bulk of water droplets, but the causes of this behavior are different; entropic effects dominate in the case of the small F^- anion, whereas the solute-water interaction energies are predominant in the case of the cations. For the case of organic molecules (i.e., methanol, ethanol, propanoic acid, *n*-butylamine, diethyl ether and neopentane),[7] the authors found that all of these molecules have a PMF minimum at the air/water interface. These PMF minima are mainly caused by enthalpic effects, although the entropic contribution at the interface becomes larger for solutes with larger nonpolar groups such as neopentane. In these studies, the decomposition of the PMF into entropic and enthalpic components, and the latter into water-water and water-solute contributions, allowed the group of David van der Spoel to shed light into the factors governing the solvation of ion and organic solutes in water droplets.

(1) Donaldson, D. J., Valsaraj, K. T.: Adsorption and Reaction of Trace Gas-Phase Organic Compounds on Atmospheric Water Film Surfaces: A Critical Review. *Environ. Sci. Technol.* **2010**, *44*, 865-873.
(2) George, I. J.; Abbatt, J. P. D.: Heterogeneous oxidation of atmospheric aerosol particles by gas-phase radicals. *Nat. Chem.* **2010**, *2*, 713-722.
(3) Hallquist, M.; Wenger, J. C.; Baltensperger, U.; Rudich, Y.; Simpson, D.; Claeys, M.; Dommen, J.; Donahue, N. M.; George, C.; Goldstein, A. H.; Hamilton, J. F.; Herrmann, H.; Hoffmann, T.; Iinuma, Y.; Jang, M.; Jenkin, M. E.; Jimenez, J. L.; Kiendler-Scharr, A.; Maenhaut, W.; McFiggans, G.; Mentel, T. F.; Monod, A.; Prevot, A. S. H.; Seinfeld, J. H.; Surratt, J. D.; Szmigielski, R.; Wildt, J.: The formation, properties and impact of secondary organic aerosol: current and emerging issues. *Atmospheric Chemistry and Physics* **2009**, *9*, 5155-5236.
(4) Donahue, N. M.; Robinson, A. L.; Pandis, S. N.: Atmospheric organic particulate matter: From smoke to secondary organic aerosol. *Atmospheric Environment* **2009**, *43*, 94-106.
(5) Munger, J. W.; Jacob, D. J.; Waldman, J. M.; Hoffmann, M. R.: Fogwater chemistry in an urban atmosphere. *J. Geophys. Res. - Oc. Atm.* **1983**, *88*, 5109-5121.
(6) Caleman, C.; Hub, J. S.; van Maaren, P. J.; van der Spoel, D.: Atomistic simulation of ion solvation in water explains surface preference of halides. *Proc. Natl. Acad. Sci. U. S. A.* **2011**, *108*, 6838-6842.
(7) Hub, J. S.; Caleman, C.; van der Spoel, D.: Organic molecules on the surface of water droplets - an energetic perspective. *Physical Chemistry Chemical Physics* **2012**, *14*, 9537-9545.

CoMSEF Sessions at the 2013 Annual Meeting

CoMSEF will sponsor or co-sponsor 28 sessions at the 2013 AIChE Annual Meeting. Abstracts for presentations at the meeting will be accepted via AIChE's online system. The call for papers will close on May 13, 2013 at 11:59pm EDT. Many sessions that have been popular in the past will be continued at this meeting.

A highlight of the CoMSEF programming will be the CoMSEF Plenary Session. Presentations for this session are selected by the CoMSEF executive committee, so submitting your best work to this session is a great opportunity to highlight your accomplishments. This session will also feature an invited presentation by the CoMSEF Impact Award winner.

Students and Advisors: Don't Forget the Monday Evening Poster Session!

A yearly highlight is the CoMSEF Poster Session, where the CoMSEF Graduate Student Award winners are selected. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering.

Awardees are selected on the basis of a nomination letter from their advisor (who must be a member of CoMSEF), their CV, and their poster presentation.

Upcoming Conferences

11th International Conference on the Fundamentals of Adsorption
May 19-24, 2013
Baltimore, MD
http://foa11.org/index.html

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

MAPPER Summer School on Distributed Multiscale Computing
June 3-4, 2013
Barcelona, Spain
http://www.mapper-project.eu/web/guest/second-seasonal-school

Workshop on Modeling and Computing Multiscale Systems (MCMS)
June 5-7, 2013
Barcelona, Spain
http://www.computationalscience.nl/MCMS2013/

Gordon Conference: Polymers
June 9-14, 2013
South Hadley, MA
http://www.grc.org/programs.aspx?year=2013&program=polymers

European Polymer Congress
June 16-21, 2013
Pisa, Italy
http://www.epf2013.org/

Gordon Conference: Proteins
June 16-21, 2013
Holderness, NH
http://www.grc.org/programs.aspx?year=2013&program=proteins

NanoFormulation2013
June 18-21, 2013
Manchester
http://www.formulation.org.uk/mnf13home.html:

11th International Conference on Materials Chemistry (MC11)
University of Warwick, UK
July 8-11, 2013
http://www.rsc.org/ConferencesAndEvents/RSCConferences/MC11/

27th Annual Symposium of the Protein Society
July 20-23, 2013
Boston, MA
http://www.proteinsociety.org/symposium/

CCP5 summer school
July 21-30, 2013
Manchester
http://www.ccp5.ac.uk/events/summer_school_2013/

Gordon Conference: Biological Molecules in the Gas Phase & in Solution
July 21-26, 2013
Holderness, NH
http://www.grc.org/programs.aspx?year=2013&program=gasphase

STATPHYS 25
July 22-26, 2013
Seoul, Korea
http://www.statphys25.org/

VIIth Brazilian Meeting on Simulational Physics
August 5-10, 2013
João Pessoa - Brazil
http://www.fisica.ufpb.br/bmsp/

International Materials Research Congress 2013
August 11-15, 2013
Cancun, Mexico
http://www.mrs.org/imrc2013/

Gordon Conference: Nanoporous Materials & Their Applications
August 11-16, 2013
Holderness, NH
http://www.grc.org/programs.aspx?year=2013&program=nanopor

Sixth Annual NIST Workshop on Atomistic Simulations for Industrial Needs
August 13-14, 2013
National Institute of Standards and Technology, Gaithersburg, MD
http://www.ctcms.nist.gov/potentials/

Gordon Conference: Soft Condensed Matter Physics
August 18-23, 2013
New London, NH
http://www.grc.org/programs.aspx?year=2013&program=softcond

EUPOC 2013: Polymers and Ionic Liquids
Sept 1-5, 2013
Gargnano, Italy
http://www.dcci.unipi.it/eupoc2013/scope.html

CPMD-Meeting 2013: Matter, life, light from ab initio molecular dynamics simulations
September 2-6, 2013
Leipzig, GER
http://www.uni-leipzig.de/~cpmd2013/

Thermodynamics 2013
The University of Manchester, Manchester, UK
September 3-6, 2013
https://www.meeting.co.uk/confercare/thermodynamics2013/

2013 GROMACS USA conference
University of Virginia, Charlottesville, VA
Sep 13-15, 2013
http://faculty.virginia.edu/gromacsworkshop/

23rd International Workshop on Computational Mechanics of Materials
October 2-5, 2013
Singapore
http://www.iwcmm23.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/