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 2017

In This Issue

Shell Winner of 2017 CoMSEF Impact Award

Professor M. Scott Shell from the Department of Chemical Engineering at the University of California, Santa Barbara is the winner of the 2017 CoMSEF Impact Award. He is cited, "***For the development of a powerful statistical mechanical theory of coarse-graining and associated multiscale algorithms to understand complex bio-molecular, liquid, and soft material systems***". Scott has been a member of the faculty at UC Santa Barbara since 2007. Prior to this appointment, he served as a postdoctoral scholar within the Department of Pharmaceutical Chemistry at UC San Francisco, completed a PhD at Princeton University, and earned a BS at Carnegie Mellon University. Scott will receive his award during the CoMSEF Plenary Session at the 2017 AIChE Annual Meeting, where he will also deliver a presentation 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.

Wilmer Winner of the 2017 CoMSEF Young Investigator Award

Professor Christopher E. Wilmer from the Department of Chemical and Petroleum Engineering at the University of Pittsburgh is the 2017 winner of the CoMSEF Young Investigator Award. He is cited, "***For his pioneering work on generating hypothetical metal-organic frameworks, and screening them on a large-scale for energy and environmental applications***". Chris has been a member of the faculty at the University of Pittsburgh since 2014. Prior to this appointment, he served as a postdoctoral fellow within the Department of Chemistry and Chemical Biology at Harvard University, completed a PhD at Northwestern University, and earned a BASc in Engineering Science at University of Toronto. Chris will receive his award during the CoMSEF Plenary Session at the 2017 AIChE Annual Meeting, where he will also deliver a presentation describing his research. The CoMSEF Young Investigator Award is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

2017 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded at the annual AIChE Meeting in Minneapolis. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees will be selected based on the nomination letters received from each student's advisor, their CV, and a poster presented at the CoMSEF poster session to be held Monday afternoon from 3:15 to 4:45 PM in Exhibit Hall B. The winners will be announced at the CoMSEF/Area 1a annual General Meeting (Wednesday, from 6:15-7:15 pm).

CoMSEF General Meeting in Minneapolis

CoMSEF will hold its annual General Meeting on Wednesday November 1 from 6:15-7:15 pm in room L100H of the Minneapolis Convention Center during the Fall 2017 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 and Liaison Directors elections 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 and select a logo for CoMSEF. Information about the candidates and the duties of the office can be found at http://comsef.org/elections-2017. 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 Monday October 30th.

Annual Meeting Sessions

CoMSEF has an exciting range of programming at the upcoming 2017 AIChE Annual Meeting in Minneapolis. Of special note are the "Hands On With Molecular Simulation" workshop on Sunday, the Plenary Session at 12:30 PM on Wednesday, and the CoMSEF Poster Session on Monday from 3:15-4:45 pm.

With regard to the workshop, CoMSEF members Eric Jankowski (Boise State) and Coray Colina (U of Florida) have organized an all day workshop on Sunday (link) entitled, "Workshop: Hands On With Molecular Simulation". The workshop is a ticketed event with a very reasonable cost for student attendees The workshop will feature seven different sessions with topics including basic computational skills, software usability, and reproducibility in computational science. Please contact Prof. Eric Jankowski ericjankowski@boisestate.edu with further questions.

All CoMSEF session are in the Convention Center.

Day	Title	Time	Location
Sunday	Workshop: Hands On With Molecular Simulation (Ticketed Event)	8 - 6	101I
Sunday	Recent Advances in Molecular Simulation Methods I	3:30 - 6	200A
Monday	Faculty Candidates in CoMSEF I: Biomolecules, Soft Materials, and Algorithms	8 - 10:30	L100H
	Molecular Simulation of Surface, Interface and Confinement Effects - In Honor of Keith Gubbins' 80th Birthday I (Invited Talks)	8 - 10:30	L100I
	Fundamental, Theory, and Model Development - In Honor of Keith Gubbins' 80th Birthday II (Invited Talks)	12:30 - 3	L100H
	In Honor of Stuart W. Churchill I (Invited Talks)	12:30 - 3	101E
	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)	12:30 - 3	101I
	Faculty Candidates in CoMSEF II: Energy, Catalysis, and Interfaces	3:15 - 4:45	L100H
	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	3:15 - 4:45	Exhibit Hall B
Tuesday	Applications of Molecular Modeling to Study Interfacial Phenomena	8 - 10:30	L100H
	New Developments in Computational Catalysis I	8 - 10:30	L100E
	New Developments in Computational Catalysis II	12:30 - 3	L100E
	The Industrial Fluid Properties Simulation Challenge	12:30 - 3	L100H
	Computational Catalysis I: Fundamentals	3:15 - 4:45	L100E
	Industrial Applications of Computational Chemistry and Molecular Simulation	3:15 - 4:45	L100H
Wednesday	Computational Catalysis II: Metal and Alloy Catalysis	8 - 10:30	L100E
	Recent Advances in Molecular Simulation Methods II	8 - 10:30	L100H
	Computational Catalysis III: Electrocatalysis	12:30 - 3	L100E
	Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)	12:30 - 3	L100H
	Data Mining and Machine Learning in Molecular Sciences I	3:15 - 4:45	L100H
	Molecular Simulation of Adsorption I - In Honor of Keith Gubbins' 80th Birthday III (Invited Talks)	3:15 - 4:45	M100E
Thursday	Computational Catalysis IV: Biomass Chemistry and Chemicals Production	8 - 10:30	L100E
	Molecular Modeling of Industrially Relevant Interfacial Phenomena	8 - 10:30	L100H
	Recent Advances in Molecular Simulation III: Free Energy and Phase Equilibrium	8 - 10:30	L100J
	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, Etc.	12:30 - 3	L100E
	Software Engineering in and for the Molecular Sciences	12:30 - 3	L100H
	Data Mining and Machine Learning in Molecular Sciences II	3:15 - 4:45	103A
Friday	Molecular Simulation of Protein Adsorption and Molecular Recognition Processes	8 - 10:30	103A

Upcoming Conferences of Interest to CoMSEF Members

AIChE Annual Meeting
Minneapolis, MN
October 29 - November 3, 2017
https://www.aiche.org/conferences/aiche-annual-meeting/2017

Quantum-chemistry methods for materials science
CECAM-HQ-EPFL, Lausanne, Switzerland
November 8-10, 2017
https://www.cecam.org/workshop-1387.html

Supercomputing 2017
Denver, CO
November 12-17, 2017
http://sc17.supercomputing.org/

MRS Fall Meeting
November 26-December 1, 2017
Boston, Massachusetts
http://www.mrs.org/fall-2017-exhibit

Physics and Chemistry at Fluid/Fluid Interfaces
CECAM-AT
December 11-13, 2017
https://www.cecam.org/workshop-1459.html

Data-driven Discovery and Design in Soft and Biological Materials
January 7-13,2018
Aspen, CO
http://ferguson.matse.illinois.edu/page/index.html

MolSim-2018
CECAM-NL
January 8-19, 2018
https://www.cecam.org/workshop-1494.html

Anharmonicity and thermal properties of solids
CECAM-FR-MOSER
January 10-12, 2018
https://www.cecam.org/workshop-1397.html

ICCMSE 2018: 14th International Conference of Computational Methods in Sciences and Engineering
Thessaloniki, Greece
March 14-18, 2018
http://www.iccmse.org/

Structure-Activity Relationships
Cardiff, Wales
April 11-12, 2018
http://ukqsar.org/index.php/2017/06/20/structure-activity-relationships-11-12-april-2018-university-of-cardiff/

2018 AIChE Spring Meeting
Orlando, FL
April 22-26, 2018
https://www.aiche.org/conferences/aiche-spring-meeting-and-global-congress-on-process-safety/2018

Nanotech 2018
Anaheim, CA
May 13-16, 2018
http://www.techconnectworld.com/Nanotech2018/

3rd Conference on Multiscale Modelling of Condensed Phase and Biological Systems - CCPBioSim & CCP5
Manchester, UK
May 21-23, 2018
http://www.ccpbiosim.ac.uk/events/upcoming/eventdetail/106/-/3rd-conference-on-multiscale-modelling-of-condensed-phase-and-biological-systems-ccpbiosim-ccp5

Tenth Liblice Conference on the Statistical Mechanics of Liquids
Cesky Krumlov, Czech Republic
June 17-22, 2018
http://liblice.icpf.cas.cz/2018/2018.php

16th International Congress of Quantum Chemistry
Menton, France
June 18-23, 2018
https://icqc16.sciencesconf.org/

Symposium of Thermophysical Properties
Boulder, CO
June 24-29, 2018
http://thermosymposium.nist.gov/

FOMMS 2018
Delavan, WI (Lake Lawn Resort)
July 15-20, 2018
http://fomms.org

Hermes Summer School in Materials Modelling and Science Communication
Windsor, UK
July 19-23, 2018
http://hermessummerschool.org/

GRC: Towards Next-Generation Challenges in Computational Chemistry: From Quantum Chemistry and Molecular Simulation to Data Discovery and Quantum Computing
West Dover, VT
July 22-27, 2018
https://www.grc.org/computational-chemistry-conference/2018/

GRC: Polymer Physics
South Hadley, MA
July 22-27, 2018
https://www.grc.org/polymer-physics-conference/2018/

XXVII International Materials Research Congress
Cancun, Mexico
August 19-24, 2018
https://www.mrs.org/imrc-2018

AIChE Annual Meeting
Pittsburgh, PA
October 28 - November 2, 2018
https://www.aiche.org/conferences/aiche-annual-meeting/2018

PPEPPD 2019
The 15th International Conference on Properties & Phase Equilibria for Product and Process Design
Vancouver, Canada
May 12-16, 2019

European Conference on Thermophysical Properties
Venice, IT
September 14-17, 2020

Research Highlight: Polymorphism at 129 dictates metastable conformations of the human prion protein N-terminal β-sheet

S. Alexis Paz, Eric Vanden-Eijnden, and Cameron F. Abrams
Chemical Science, Vol. 8, pp 1225-1232, 2017 | DOI: 10.1039/c6sc03275c

Comprehensive sampling of molecular simulation conformational space is a long-standing technological challenge and is one that is particularly important for calculating accurate and precise thermodynamic quantities such as free energy landscapes. In determining free energy landscapes of biomolecular processes using collective variable biasing methods, hidden variables (variables that are not explicitly biased and, thus, not ergodically sampled) pose one of the more significant sampling challenges. A multitude of methodological developments have sought to overcome the hidden variable sampling problem, typically in the form of either an orthogonal-space sampling method or a non-collective variable-based enhanced sampling (i.e., replica exchange) method coupled with an adaptive collective variable-based method. The former address only the hidden variables that are strongly coupled with the collective variables. The latter, adaptive collective variable methods, suffer from history-dependence as a result of the adaptivity. Thus, while all such methods achieve a level of enhanced hidden variable sampling, an efficient and history-independent enhanced hidden variable sampling method remained unavailable.

Co-authors Paz, Vanden-Eijnden, and Abrams tackled this methodological challenge in their recent *Chem. Sci.* article in which they describe the development, validation, and application of a new free energy calculation method, replica-exchange on-the-fly parameterization (RE-OTFP). The methodological development, itself, represents a significant advance in free energy landscape calculation, but the implementation of RE-OTFP toward understanding the thermodynamic stability of human prion proteins revealed interesting new hypotheses relevant to the origins of prion diseases. The described RE-OTFP method, a combination of replica-exchange molecular dynamics, temperature-accelerated molecular dynamics, and on-the-fly parameterization, is accompanied by detailed heuristics for identifying appropriate numbers of replicas, acceptance ratios, and auxiliary temperatures for each replica. Additionally, a standard protocol for RE-OTFP simulations is outlined, comprising stages of initialization, equilibration, reset, and production simulations. The level of detail Paz, et al. provide enables adoptees of RE-OTFP to easily implement this approach in their own research. Validation of RE-OTFP against prior alanine dipeptide and mouse prion protein free energy landscape determinations revealed extreme precision (<<1 kcal/mol) and remarkable computational efficiency on a per-unit-error basis. As proof-of-concept, the authors implemented RE-OTFP to examine the free energy landscapes of four different human prion protein genotypes arising from the M129V/D178N polymorph. The profiles, having the same ground state structure, exhibited unique variations in the form of metastable states. This finding led the authors to develop a new hypothesis regarding the possible relationship between transmissible spongiform encephalopathy strains and energetic accessibility of the metastable states. The precision of RE-OTFP in free energy landscape determination will likely prove useful in many other protein folding and aggregation-type studies, but perhaps more importantly, the ability to identify the existence of metastable protein states provides insight into folding and aggregation processes beyond the current capabilities of experimental techniques.

Research Highlight authored by Christina M. Payne, Chemical and Materials Engineering, University of Kentucky

Where are They Now?

Now that CoMSEF has been giving the graduate student awards for more than 10 years, we've started including a "where are they now?" section in the newsletter, catching up with the winners from ~ 10 years ago.

Chethan Acharya
University of Alabama, Advisor: C. Heath Turner
2007 Poster Title: Dft Investigation On The Stability Of Pt Clusters On Carbon Supports

Chethan Acharya joined Southern Company Services in 2011 as a Research Engineer. Since joining the group, he has worked on CO2 capture technologies, Mercury and Air Toxics Standards (MATS) and Effluent Limitations Guidelines (ELG). Chethan has worked on developing strategies and performed technology evaluations to provide solutions for different environmental regulations facing the coal industry. In addition to providing environmental solutions for Southern Company, his role is also to direct and influence the work performed by external organizations such as Electric Power Research Institute (EPRI) to provide industry wide environmental solutions.

Chethan received his B.S. in Chemical Engineering from Madras University in India and Ph.D. in Chemical Engineering from the University of Alabama. After graduation, Chethan joined University of California at San Diego as a Postdoctoral Scholar. He was there for three years working on biomass gasification before joining Southern Company Services.

YouTube: The Hydrogen Alternative
LinkedIn: Chethan Acharya

The Tenth Industrial Fluid Properties Simulation Challenge

The Industrial Fluid Properties Simulation Challenge is an open competition organized by employees of the Army Research Lab, the National Institute of Standards and Technology (NIST), The Dow Chemical Company, 3M, and United Technologies Research Center with support from CoMSEF and the ACS. The goals of the competition are to drive improvements in the practice of molecular modeling, formalize methods for the evaluation and validation of simulation results with experimental data, and ensure relevance of simulation activities to industrial requirements. The Simulation Challenge was initiated by the workshop on "Predicting the Thermophysical Properties of Fluids by Molecular Simulation" held at NIST in 2001.

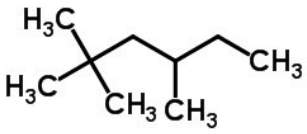
The 10th Industrial Fluid Properties Simulation Challenge will test the capability of molecular dynamics simulation to provide the property of liquids most important to elastohydrodynamic lubrication (EHL), the pressure-viscosity relation. The temperature dependence at elevated pressure could be the subject of a future challenge.

A fundamental requirement of elastohydrodynamic lubrication (EHL) is a description of the viscosity of the liquid as a function of pressure [1]. The classical film thickness formulas all require a value for a property known as a pressure-viscosity coefficient; although the definition of this property is not always clear [2]. The shape of a traction (friction) curve has been the subject of much speculation for at least forty years [3]. The shape of a traction curve when plotted as friction coefficient or average shear stress versus the logarithm of sliding speed or slide-to-roll ratio depends strongly on the pressure dependence of viscosity at the Hertz pressure [4], more fragile liquids having a less steep logarithmic portion. Although the pressure dependence of viscosity is clearly essential to the field, until about ten years ago, experimentally measured values of this property were not a typical part of EHL analysis. The reasons for the previous neglect may be debated, but the demand for this information is now growing.

Molecular dynamics simulations have the promise of generating pressure-viscosity data for liquids which have not yet been synthesized but only if the accuracy of the method can be validated. There has been a claim of success in predicting the pressure dependence of viscosity for squalane [5], although the temperature dependence is not accurately recovered in this example [6]. There has been extensive experimental work on squalane viscosity at elevated pressure [7,8] so that simulations have a known “target” value of viscosity. As of this time, there has been no success in recovering the super-Arrhenius pressure dependence that is important to friction [9].

A Lubricant Viscosity Simulation Challenge is now proposed to assess the possibility of employing molecular dynamics simulations to predict the pressure dependence of viscosity in a simple hydrocarbon molecule. This should be a material for which there is no presently published viscosity data, with the exception perhaps of viscosity at ambient pressure. It should, for simulation convenience, be composed of a minimum number of carbons. Linear alkanes are excluded because they are not glass-formers and would be crystallized at EHL pressures. The material should possess all of the pressure-viscosity trends of lubricating oil. A candidate fulfilling these requirements is 2,2,4 Trimethylhexane.

Prof. Scott Bair (Georgia Tech) has characterized the viscosity of 2,2,4 Trimethylhexane (>98%), Aldrich product number 92470, lot BCBR3588V. Pressures of 0.1, 25, 50, 100, 150, 250, 350, 400, 500, 600, 700, 800, 900, and 1000 MPa were investigated, all at temperature of 20°C (293K). It has not yet been decided exactly which pressures will be included in the challenge. The viscometers were calibrated with di (2ethylhexyl) sebacate based on the correlation of Paredes et al. [10]. Estimated uncertainties are 3% for viscosity, 0.3°C for temperature and the greater of 1MPa and 0.4% for pressure.



More information about previous challenges can be found at http://fluidproperties.org/simulation-challenge

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Why CoMSEF?

CoMSEF has over 230 dues-paying 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!