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/

Newsletter

AIChE

June 2021

In This Issue

CoMSEF Executive Committee Elections

Congratulations to Jeetain Mittal (Vice Chair, Lehigh), Joe Golab (Secretary-Treasurer, Illinois Mathematics and Science Academy), Kayla Sprenger (Liaison Director, Colorado), and Poornima Padmanabhan (Liasison Director, RIT) who were elected to the CoMSEF Executive Committee in the fall of 2020! Thanks to Rebecca Lindsey (Liaison Director, LLNL), Neeraj Rai (Liaison Director, Mississippi St.), and Jeff Errington (Past Chair, Buffalo) who completed their terms on the executive committee.

Two Liaison Directors are elected each year and serve two-year terms. Their responsibilities include identifying opportunities for co-sponsorship and communicating and advocating CoMSEF activities with other organizations. Liaison Directors also aid the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter. The Vice Chair is elected every two years to formulate and implement long-term plans and strategic activities for the forum, implement projects in coordination with the Chair, serve as the forum's liaison to the Institute, and to be responsible for the programming activities of the Forum.

Call for Nominations

****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.

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.** The student should have already submitted an abstract to the CoMSEF poster session at the AIChE annual meeting.

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.

2020 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were awarded at the annual AIChE Meeting. 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:

- **Sarah Alamdari** (Washington, Advisor: Jim Pfaendtner)
- **Ryther Anderson** (Colorado School of Mines, Advisor: Diego Gomez-Gualdron).

This year the forum also named two Honorable Mentions:

- **Andrew S. Rosen** (Northwestern, Advisor: Randall Q. Snurr)
- **Karun Kumar Rao** (Houston, Advisor: Lars Grabow)

* Opinions presented in the newsletter are the authors' and do not necessarily represent the view of the CoMSEF organization.

Research Highlight: Pushing the Boundaries of MD Simulations with Deep Learning AI

Kayla Sprenger, Colorado

The ongoing global pandemic has highlighted the need for novel approaches to elucidate the complex molecular-scale mechanisms through which viruses interact with host cell proteins and gain entry into host cells to propagate infection. Such a deep mechanistic understanding is crucial to the design of effective vaccines and therapeutics, especially against viruses like SARS-CoV-2 that can rapidly evolve mutations that may otherwise affect vaccine efficacy. Experiments can provide only limited insight into the underlying molecular mechanisms of infection, due to the difficulty of resolving the structures of flexible loop regions on the viral proteins, as well as of the highly flexible glycans that coat their surfaces and that have been shown to play an important role in viral infection [1]. Additionally, experiments generally only provide static snapshots of viral components in action, leading to an incomplete understanding of virus entry pathways. Molecular dynamics (MD) simulations of fully-glycosylated viral surface proteins in their native membrane-bound environments offer a solution to overcome these structural limitations. Yet, the large system sizes inherent to performing such atomistic simulations renders them computationally prohibitive for broadly sampling the large-scale conformational transitions that many viruses undergo in order to bind to host cell receptors. In addition, the enormous amounts of data generated by these simulations circumvents the use of traditional analysis techniques to identify key conformational states along the transition pathway, and to detect undersampled regions of conformational phase space that may require more attention [1].

To address this problem, Casalino et al. recently applied artificial intelligence (AI)-based methods to drive conformational sampling of multiscale simulations of the SARS-CoV-2 spike protein, embedded in a lipid membrane and interacting with the human cellular receptor ACE2, also in its membrane-bound form [1]. Prior to performing these more complicated simulations, the authors perfomed an unbiased microseconds-long simulation of a truncated version of the spike protein and created an AI learning model trained on the trajectory data from this simulation. They then learned embeddings from this model that, when the model was instead employed to analyze trajectories from the more complicated spike-ACE2 membrane simulations, enabled them to efficiently cluster the conformations based on root mean squared deviation (RMSD). An outlier detection method was then used to identify regions of conformational phase space that had been undersampled, and new MD simulations were directly initiated from these regions, thereby greatly enhancing sampling. This adaptive sampling method, called DeepDriveMD, was previously developed by the authors [2] and here enabled them to 'drive' sampling in a large-scale simulation with many tens of millions of atoms, based on knowledge gained from a smaller-scale simulation. The authors were able to form novel hypotheses about the viral-cell membrane fusion process [3] and the active role of viral surface glycans in initiating/propagating infection [4]. Other recently developed adaptive sampling MD techniques utilize alternative AI-based methods, such as a method called AdaptiveBandit, which is based on reinforcement learning [5].

[1] L. Casalino *et al.*, "AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics," *Int. J. High Perform. Comput. Appl.*, p. 109434202110064, Apr. 2021, doi: 10.1177/10943420211006452.
[2] H. Lee, M. Turilli, S. Jha, D. Bhowmik, H. Ma, and A. Ramanathan, "DeepDriveMD: Deep-learning driven adaptive molecular simulations for protein folding," 2019, doi: 10.1109/DLS49591.2019.00007.
[3] E. P. Barros *et al.*, "The flexibility of ACE2 in the context of SARS-CoV-2 infection," *Biophys. J.*, 2021, doi: 10.1016/j.bpj.2020.10.036.
[4] L. Casalino *et al.*, "Beyond shielding: The roles of glycans in the SARS-CoV-2 spike protein," *ACS Cent. Sci.*, 2020, doi: 10.1021/acscentsci.0c01056.
[5] A. Pérez, P. Herrera-Nieto, S. Doerr, and G. De Fabritiis, "AdaptiveBandit: A Multi-armed Bandit Framework for Adaptive Sampling in Molecular Simulations," *J. Chem. Theory Comput.*, 2020, doi: 10.1021/acs.jctc.0c00205.

A broader view: Diversity, Inclusion and Equity - Words and Actions

Natasha N. Croom, PhD
Associate Professor of Higher Education
College of Education

Note from Chair: In the conversations about diversity, equity and inclusion (DEI), it is often easy to get lost in the terminology. This can become often become overwhelming. However, incorrect usage of terminology can lead to unfortunate discussions. Thus, I invited an expert in this area to provide some clarity on the key terminology related to DEI. Dr. Natasha N. Croom is an Associate Professor of Higher Education and Student Affairs and the Special Advisor to the Dean for Diversity and Inclusive Excellence in the College of Education at Clemson University. Her scholarship focuses on disrupting intersecting systems of oppression (i.e., racism, sexism, classism, etc.) at the individual, group, institutional, systemic, and ideological levels of higher education. She is particularly interested in (a) issues of access, equity, and success for womyn of colour faculty and students, (b) dismantling interlocking systems of oppression in higher education institutional policy and practice, and (c) expanding the use of critical race feminist and intersectionality theory in higher education research and practice. As a critical race feminist qualitative scholar-practitioner, her goal is to identify and disrupt systems of oppression that operate throughout higher education organizations in the U.S. in an effort to construct equitable spaces, opportunities, policies, and practices that extend beyond post-secondary education.

Article:

College and university campuses have been a consistent site of advocacy, activism, and protest. The persistent physical and psychological violence enacted against Black, Latinx/Hispanic, Indigenous, Asian, and transgender communities in the U.S. (see for example, George Floyd, Breonna Taylor, Pedro Villanueva, Delaina Ashley Yaun, Nina Pop) has awoken many members of our campus communities to the myriad realities of minoritized communities. Faculty and students are paying

closer attention to state and federal legislation that has maintained and/or created inequity for queer, trans, and racially and ethnically minoritized communities (see for example, anti-trans bills in TN; Trump administration international student COVID policy; voting rights bills in GA; partisanship curriculum legislation in SC). Campus academic administrators are also now more aware of previous, and on-going, federal and state agency policy and legislation condemning particular explorations and teachings of diversity, inclusion, and equity as "divisive" and "anti-American" (see Trump administration memo M-20-34 memo). Moreover, we cannot forget about the global health pandemic that is disproportionately impacting racially and economically minoritized communities (Harper, 2020). While one could assume that these issues are beyond the scope of the university, I would offer that the privilege and subordination manifested beyond campus borders are present within them as well – as institutions of higher education are a microcosm of our greater society. As such, now is the time for more educators, students, staff, and administrators to engage with ideas, theories, and practices that can be used to disrupt inequality and inequity. As a scholar-practitioner who often engages in equity-minded work, I often come across well-intentioned people and groups who conflate really important ideas – ideas that have the ability to guide our actions. The purpose of this Broader View is to explore the differences between commonly conflated ideas and surface some ways in which the ideas can limit and/or expand our opportunities for social change. Continued and stalwart commitment to educating ourselves, as well as our colleagues, students, families, and community members we learn, work, and live alongside is one step towards ensuring that everyone in society has what they need to participate in this world.

Diversity, Inclusion, Equity – Oh My!

The words "diversity," "inclusion," and "equity" are literally everywhere nowadays. And while these terms have become more common place in our lexicon, much of the time they are used interchangeably or used as coded language (for example, people use the words "diversity/diverse" to mean race (and really just Black people in some places)). It is important that we know the difference between these basics as they have the ability to communicate more clearly (a) what is meant and (b) particular practices we can employ to enhance each. Let's parse out these words.

Diversity simply means that difference is present. For example, if everyone on a research team held the same racial identity, there would still be diversity – difference in socioeconomic backgrounds, religious/spiritual affiliations, age, gender, etc.

Inclusion means that there is purposeful and thoughtful inclusion of particular groups/people. For example, one might notice that their lab has no women and might seek to add women to the lab.

Equality means that everyone has access to the same thing. Let's say the department offers a virtual professional development seminar in the summer and everyone is invited and has access to the link – we could say there is equal opportunity to participate in the seminar.

Equity refers to everyone having access to what they need to meet their goals. Taking the example above of the seminar -- perhaps students have returned to their home communities for the summer where there is unreliable wifi. Working with CCIT to ensure that those folks have hotspots and other hardware and service to connect would be an equitable practice.

Social justice requires diversity, inclusion, equality, ***and*** equity as it refers to the process of "full and equal participation of all groups in a society that is mutually shaped to meet their needs…[where] all members are physically and psychologically safe and secure" (Adams, Bell, & Griffin, 2007). The important thing to note here is that "justice", in any form, is a process and NOT a destination.

Ensuring that we know the differences between these words, may ensure that when we act, we are actually addressing the concerns at hand. Looking at equality and equity and the example of the virtual seminar. While ensuring that everyone is invited and has the connection information could be an example of equality – equality has its limitations. Namely, equality efforts tend to come from an assumption that everyone is starting from the same set of circumstances – which is often not the case in educational settings (and really any social setting because of diversity – there's always likely some difference). Thus, we must also consider equity to account for the myriad sets of circumstances at play (i.e., underresourced communities likely have more connectivity issues than more fully resourced communities).

Privilege and Oppression

Another set of terms that we hear often, but get very little formal understanding around, are privilege and oppression. Usually accompanied by the prefix systemic – systemic means that the "thing" is pervasive or ingrained within the entire structure. Sometimes people conflate systemic with systematic in conversations of oppression and privilege. Systematic refers to the specificities of how the "thing" gets ingrained; it's referring to a methodical process. For example, to say systemic racism is to suggest that racism is throughout a structure, but it does not communicate how it became so. Moreover, in thinking about how our social world functions we must consider how resources, experiences, and outcomes of targeted groups are controlled by the actions of dominant groups. Further, we must understand that everyone belongs to social groups (i.e., we all have a race, gender, class, ability status, etc.) – it is how our social world is organized. Thus, when referring to privilege and oppression, the conversation should not only be situated in an individual's experiences, but must also be considered in a larger social perspective that recognizes a social system at play. Here are some ways to consider oppression and privilege.

Oppression has historically been defined solely based on the exercise of tyranny, or an absolute abuse of power (e.g., Holocaust, South African Apartheid); however, oppression is also "the disadvantage and injustice some people suffer not because a tyrannical power coerces them, but because of the everyday practices of a well-intentioned society" (Young, 2000, p. 5). Iris Young (2000) categorized five types of oppression. First, ***exploitation*** is the transfer of the benefits of labor from one social group to another group. In higher education, think about the ways faculty might more greatly benefit from the work of graduate students or how adjunct/contingent faculty are often undercompensated but provide a larger percentage of the teaching role in a large university. Second, ***marginalization*** happens when groups are excluded from useful participation in social life and deprived of material goods or removed all together. In education, for example, federal and state laws excluding enslaved people's from a formal education (i.e., it was literally illegal to teach an enslaved person

to read or write and there were consequences for enslaved peoples caught reading and writing for more than two centuries) and formal tracking programs (i.e., segregated schools for racially minoritized communities often had limited curricula across P-16 contexts) created generational educational marginalization – leading to much of the current exclusion of U.S.-born Black and Latinx communities in certain fields now. The third form of oppression is <u>*powerlessness*</u>, which points to groups inability to control and make decisions about their own living and working conditions. In the book, *The Lives of Campus Custodians: Insights into Corporatization and Civic Disengagement in the Academy* (2016), Peter Magolda surfaced the ways in which job security, benefits, and autonomy have taken a downward turn for this campus population – a group which tends to come from working class backgrounds – leaving them feeling a sense of inability to control their professional destinies. Fourthly, <u>*cultural imperialism*</u> refers to the ways privileged social group ways of knowing and doing get valued and enforced over others. In discussing the experiences of first-generation poor and working-class student experiences, Oldfield (2007) illuminated the ways in which these student populations ways of knowing were often critiqued based on a standardization of middle class and more affluent ways of knowing the world in college. Lastly, <u>*violence*</u> captures the threat of or actual manifestations of physical, sexual, emotional assaults enacted upon bodies and/or through policies, practices, and structures. Consider the ways in which groups (i.e., faculty, staff, students) on campus communicate that racially minoritized students/faculty or queer students/faculty are not welcomed (see: Clemson University Sikes Sit-In).

Systems of oppression are the structures in which the types of oppression above get operationalized based on the identity group. Moreover, each system is typically used to control resources, experiences, and outcomes for the targeted social group. While a full briefing of all systems of oppression are beyond the scope of this article, here are a few examples. Racism is a system of oppression connected to the social identity of race. Specifically, racially minoritized communities (i.e., Asian, Black, Hispanic/Latinx, and Indigenous peoples) *may* experience racism. Sexism and Genderism are systems of oppression connected to sex (biological) and gender (cultural). Ableism is a system of oppression connected to (dis)ability. Other examples of systems of oppression include nativism and xenophobia (nationality), ethnocentrism (ethnic culture), classism (socioeconomic status and class), heterosexism (sexuality), and ageism/adultism (age).

Privilege simply refers to the advantages available to some groups based on their social group membership and status of said group. Peggy McIntosh (1989) brought the term white privilege, for example, more firmly into our view with her work *White Privilege: Unpacking the Invisible Knapsack* – where she explained the often taken for granted norms, ideas, and practices of white racial communities as they navigate the world (i.e., flesh tone band-aids and nylons, buying cards with white people on them at any store, feeling safe in a traffic stop, etc.). Racial privilege, however, is just one form. There is also religious privilege, gender privilege, class privilege, and so on.

Systems of privilege are the structures, and the prevailing ideologies, that maintain privilege of hierarchically dominant social groups. Again, while a full briefing of all systems of privilege are beyond the scope of this article, here are a few examples. White supremacy (ideology) and whiteness (structure) are the systems of privilege connected to the social identity of race. Specifically, white racial communities *may* experience white privilege because the ideology of white supremacy suggests that white people are more deserving of the resources (i.e., entitlement reinforced by many of the forms of oppression shared above over time) and whiteness as a structuring function has created specific opportunity for privilege to manifest (i.e., federal and state law restricting access to education, jobs, participation in governance, and so forth). Another example is patriarchy – a system of privilege connected to the social identity of gender (and sometimes sex) that *may* benefit men communities. Patriarchy ideologically suggests that men have an innate right to assume power and authority (see Great Man leadership theory for example (an original leadership theory based in masculine traits)) and structurally has informed the ways in which they can operate in society (i.e., voting (see women's suffrage movements), schooling (see Title IX), working (see Yellen, 2020), etc.). Other examples of systemic privilege include Christian hegemony/privilege (religion/spirituality) and heteronormativity (sexuality).

Having a more sophisticated understanding of privilege and oppression is important, particularly if we are interested in using our voices and influence (whether that be in our personal or professional lives) to disrupt inequity. For example, in a U.S. context many people erroneously assume that Asian communities do not experience racism. Anti-Asian racism is not, however, new (see Japanese internment on U.S. soil). The COVID-19 pandemic has simply spurred a renewed sense of anti-Asian sentiments and violence in this country. Racisms manifest both similarly and differently for racially minoritized communities. That is to say, that Black women and Indian women may both experience racism, but they may experience them differently. Moreover, a more sophisticated understanding of privilege would help us understand how and why those groups experience racism differently!

While there is much more to be said and more ways to complicate the above, starting with some clear definitions is helpful. As we know, words mean things and the ideas connected to such words have a direct impact on our practices and behaviors. As I previously mentioned, now is the time to engage with ideas, theories, and practices that can be used to disrupt inequality and inequity in our classrooms and beyond. As educators, researchers, scholars, and practitioners, it is our responsibility to understand more deeply how the social world works and to situate ourselves within it so we can disrupt inequity.

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CoMSEF Sponsored and Co-Sponsored Sessions at the 2021 Annual Meeting

Session CoMSEF	Chair(s) and co-chair(s)
Advanced batteries	John Ekerdt, Jane Chang, Charles Musgrave, & Griselda Bonilla
Applications of Molecular Modeling to Study Interfacial Phenomena	Cory Simon, Kaihang Shi, Yamil Colón, & Obioma Uche
Computational Studies of Early-Stage and Low-Dimensional Self-Assembly	Julia Dshemuchadse & Sumit Sharma
Data-Driven Design and Modeling	Stephanie Valleau, Yi He, & Qing Shao
Development of Intermolecular Potential Models	Neeraj Rai & Nav Nidhi Rajput
Faculty Candidates in COMSEF/Area 1a	Jeremy Palmer & Amir Haji-Akbari
Hybrid systems, halide perovskites, molecular modeling	Sapna Sarupria & Letian Dou
Molecular Simulations for Designing Adsorbents and Adsorption Processes	Alexander Neimark & Daniel Siderius
Nanoscale Behavior of Sustainable Processes	Jindal K. Shah & Joshua Howe
Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	Jeetain Mittal & Kayla Sprenger
Perovskites, spinels, energy conversion, modeling of these systems	Al Weimer & Gyeong S. Hwang
Plasma catalysis	Ryan Hartman & Maria Carreon
Plenary: CoMSEF	Sapna Sarupria & Jim Pfaendtner
Practical Application of Process Data Analytics and Machine Learning (Invited Talks)	Leo Chiang & Selen Cremaschi
Practical Applications of Computational Chemistry and Molecular Simulation	Martin Sanborn, Andrea Browning, Jonathan Moore, Phil Westmoreland, & Steven Arturo
Recent Advances in Molecular Simulation Methods	Harish Vashisth, Diego Gomez Gualdron, & Mona Minkara
Recent Advances in Multiscale Methodologies	Nathan Mahynski & Kayla Sprenger
Soft systems, molecular simulation, sustainability	Carissa Eisler & Janani Sampath
Software Engineering in and for the Molecular Sciences	Eric Jankowski & Utkarsh Kapoor
Special Session In Honor of Arup Chakraborty's 60th Birthday	Andrew Ferguson & Bernhardt Trout
Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)	M. Scott Shell & Arthi Jayaraman
Teaching Data Science to Students and Teachers	Martha Grover & Phil Westmoreland

Upcoming Conferences of Interest to CoMSEF Members

21st Symposium on Thermophysical Properties
Virtual
June 20-25, 2021
https://thermosymposium.org/

31st European Symposium on Applied Thermodynamics
Virtual
July 4-7, 2021
http://www.esat2020.com/

11th Liquid Matter Conference
Virtual
July 19-23, 2021
http://www.lmc2020.cz/

13th European Congress of Chemical Engineering and 6th European Congress of Applied Biotechnology
Virtual
Sep 19-23, 2021
http://ecce-ecab2021.eu/

PPEPPD
Tarragona, Spain
May 22-26, 2022
https://ppeppd.org/

Congress of the World Association of Theoretical and Computational Chemists
Vancouver, Canada
July 3-8, 2022
https://www.watoc.net/watoc.congress.html

FOMMS
Delavan, WI
July 2022
http://fomms.org

STATPHYS28
Tokyo, Japan
August 8-12, 2022
https://www.statphys28.org/

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.

Andrew Paluch
2011 Grad Student Award winner (University of Notre Dame, Advisor: Ed Maginn)
Poster Title: Predicting the Solubility of Pharmaceutical Solids by Molecular Simulation

I completed my PhD in Chemical Engineering from the University of Notre Dame under the supervision of Ed Maginn in April 2013. I then started my independent career as an Assistant Professor in the Department of Chemical, Paper, and Biomedical Engineering at Miami University in August 2013, and was promoted to Associate Professor in August 2019. (Miami University is the second oldest university in Ohio, founded in 1809 while Florida was a territory of Spain.) Since being at Miami, I have co-authored 26 peer reviewed journal articles and involved over 45 undergraduate students in my research program. A major goal of my current research efforts is to marry molecular simulation and electronic structure calculations with classical thermodynamic modeling for early stage process conceptualization and design applications. I am the recipient of the American Chemical Society Petroleum Research Fund (ACS PRF) Undergraduate New Investigator Award (2016), the inaugural Miami University Associated Student Government Affordable Education Leader Award (2018), was named an Emerging Investigator by the Journal of Chemical & Engineering Data (2018), and I am the recipient of the Miami University Junior Faculty Scholar Award (2020). I would additionally like to acknowledge Jeff Errington at SUNY University at Buffalo, from whom I caught the thermodynamic bug and who introduced me to molecular simulation. It was the passion that began there that has carried me to where I am today.

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. Our 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!