# FOMMS 2009

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One of the major accomplishments of the MMTF has been the establishment of a triennial series of international conferences, Foundations of Molecular Modeling and Simulation (FOMMS). The scope of the conference series is theory and applications of computational quantum chemistry and molecular simulation, and the forum is unique in its aim to bring together industrial and academic researchers from the quantum to the process scale. The inaugural meeting was organized by Peter Cummings and Phil Westmoreland at Keystone Resort in July 2000, and meetings were subsequently held in 2003 (again at Keystone) and 2006, the latter held at the beautiful and relaxing Semiahmoo Resort in Blaine, WA. The FOMMS 2009 Conference will be held July 12-16, again at Semiahmoo. In addition to outstanding lectures and discussion on a range of topics in molecular modeling and simulation, the conference will include a mini-workshop on open-source code development for molecular simulation, tutorial sessions on massively multicore chip architectures and GPUs for scientific simulation, and a special, inaugural FOMMS Award banquet.

FOMMS 2009 boasts a very impressive international list of invited speakers:

New perspectives in molecular simulation:
Daan Frenkel (Cambridge)
Berend Smit (UC Berkeley)

- Proteins and biological systems:
- David Baker (U. Washington)
- Charlie Brooks (U. Michigan)
- Linking process scale simulation and molecular modeling:
- Linda Broadbelt (Northestern U.)
- Dion Vlachos (U. Delaware)
- Rare events: acceleration algorithms and transition path sampling:
- Baron Peters (UCSB)
- Giovanni Ciccotti (La Sapienza, Rome)
- Phil Geissler (UC Berkeley)
- Soft materials and complex fluids:
- Ilja Siepmann (U. Minn)
- Clare McCabe (Vanderbilt)
- Lev Gelb (Wash U.)
- Simulation-based engineering & science - Novel materials and industrial applications:
- Caroline Mellot (UCL, UK)
- Shinichiro Nakamura (Mitsubishi, Japan)
- Herve' Toulhoat (IFP, France) and roundtable

- Petascale computing and emerging architectures for modeling and simulation:
- David Shaw (D.E. Shaw Research & Columbia)
- Klaus Schulten (UIUC)
- George Karniadakis (Brown U.)

Additional information about the conference can be found at www.fomms.org.

# Molecular Simulation Modules

A major activity of the CACHE Molecular Modeling Task Force is the development of molecular simulation modules for undergraduate and graduate instruction. Each module consists of an interactive molecular simulation and written supporting material related to it. The molecular simulation is written in the Java programming language, and it can be run as an applet in a browser, or as a standalone application. The supporting material provides an introduction to the concepts demonstrated by the applet, with some detailed background about what is being modeled. There are also examples describing the use of the simulation, and exercises suitable to use as homework assignments. The supporting material is set up on a wiki, which permits users of the modules to develop and improve the documentation.

Modules are developed with support from a CCLI grant from NSF. We think that the best source of ideas for such modules would come from the community of engineers and scientists who are engaged in research and education. In consultation with parties we do the development needed to design, produce, and assess the module in the classroom, while the module consultant provides the idea and background information that guides the students in the use of the modules. Thus we request proposals for ideas and assistance in developing new molecular simulation modules. Our NSF CCLI grant is structured to permit us to award up to $5000 for the support of the efforts of such “module consultants” whose proposals are selected for development.

So far we have completed five modules, with one more nearly finished:

- Virial-VLE: Molecular parameters are fit to experimental equation-of-state data and vapor-liquid coexistence behavior of the model defined by these parameters is studied by molecular simulation. These VLE data can be compared to experimental VLE data for the system used to fit the model.
- Molecular dynamics: Provides an introduction to the basic modeling and simualtion ideas that are used in many of the other simulations. It is useful as a background to understand how the other modules operate
- Osmosis: Demonstrates molecular phenomena underlying osmosis and reverse osmosis. Water or simpler solvents are simulated in the presence of membranes permeable to it but not to solutes that are also present in the system.
- Basic polymerization reactions: This simulation models two fundamental polymerization reaction types—stepwise growth and chain addition. Both of these sub-modules help students visualize how the different polymerization reactions function and how they result in significantly different polymers. This module

helps the student develop an understanding of molecular weight distributions and polymer structures.

- Vapor-liquid interface: This is intended to model the thermodynamic properties of an explicit vapor-liquid interface, with and without the presence of surfactant molecules. the module introduces the concept of interfacial modifications (via surfactants) and thermal effects on interfacial properties. In this way, there is a direct connection established between the specific intermolecular interactions in the system and the emergent thermodynamic properties of a vapor-liquid interface.
- Monolayer: Simulates the behavior of a tethered layer of alkane-like chain molecules as they are put under mechanical stress.

Development of two more is now beginning. We further anticipate selecting four more to develop before the term of our grant is expired. The deadline for the final module proposal solicitation is June 15, 2009. Details may be found here: http://www.etomica.org/app/modules/solicitation.html.

Completed modules may be found at http://rheneas.eng.buffalo.edu/wiki/Modules