A Molecular Simulation Module Development Community

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David Kofke at the University at Buffalo is leading a project to develop molecular simulation modules with support from a CCLI grant to CAChE from the National Science Foundation.

The aim of a molecular-simulation module is to provide a microscopic perspective on macroscopic phenomena with the purpose of improving the instruction of topics often encountered in engineering and science curricula. With simulation the students may interact with and observe molecular phenomena and conduct “measurements” that can then be interpreted with the macroscopic tools taught in their classes.

Prof. Kofke is soliciting ideas for modules from the community of engineers and scientists who are engaged in research and education. This community has a good understanding of the molecular origins of macroscopic phenomena, but often lacks the skills or interest needed to develop a robust, user-friendly, and pedagogically sound molecular simulation module that can help to convey this understanding. Kofke aims to team with these parties to design, produce, and assess in the classroom molecular simulation modules conceived from members of this community.

The project is structured such that persons with ideas for modules can submit a proposal for its development to the group led by Kofke. The NSF CCLI grant provides funds to award up to $5000 for the support of the efforts of each such “module consultant” whose proposals are selected for development. So far, six modules are being developed through this process, summarized here:

* Virial-VLE (with Jochen Autschbach of the University at Buffalo Department of Chemistry). Demonstrates the connection between different thermodynamic behaviors (viz, gas-phase equation of state, and vapor-liquid equilibria) exhibited by a common molecular model.

* Square-Well Molecular Dynamics (with J. Richard Elliott of the University of Akron). Provides a laboratory for studying thermodynamic behaviors directly from a molecular model.

* Osmosis (with Sohail Murad of the University of Illinois - Chicago). Demonstrates the phenomenon of osmosis and reverse osmosis via a semipermeable membrane.

* Mechanical Properties at Golden Interfaces (with Redhouane Henda of Laurentian University). Shows some of the phases, stress-strain relations, and other behaviors exhibited by chain molecules tethered to a surface.

* Vapor-Liquid Interface (with C. Heath Turner of the University of Alabama). Provides a window on the nature of the interface between gas and liquid phases.

* Basic Polymerization Reactions (with William Chirdon of the University of Louisiana at Lafayette). Models free-radical chain polymerization and stepwise-growth polymerization.

Documentation for the modules is being developed on a wiki, and in this manner the community at large can not only help to develop ideas for modules, but they can also contribute to their documentation. The web site hosting the modules and their documentation is located here: www.etomica.org/wiki/Modules.

Prof. George Bodner, of the Department of Chemistry at Purdue University, is a co-PI on the CCLI grant, with responsibilities for overseeing the assessment of the modules in the classroom.

Plans include the development of six more modules before this phase of the project is co mplete. Anyone with ideas for a module is encouraged to submit a proposal for develop ment. Details may be found at www.etomica.org.