Activities of the Molecular Modeling Task Force

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The Molecular Modeling Task Force (MMTF) was formed by CACHE in 1996 and charged with the task of developing resources and activities that assist the introduction of molecular modeling methods into the chemical engineering curriculum and ultimately into chemical engineering practice. The task force is headed by Peter Cummings, and its membership includes CACHE trustees Warren Seider, David Kofke and Phil Westmoreland along with 16 other representatives from the molecular modeling research community. A full list is available at the MMTF web site, http://zeolites.cqe.nwu.edu/Cache/

Meetings of the MMTF have been facilitated by the generous support of the Department of Chemical Engineering at the Colorado School of Mines. The group last met there nearly two years ago, in March 2001, but many of the original activities of the Task Force are continuing or are reaching fruition. In this article we describe the latest news.

FOMMS 2003

One of the major activities of the MMTF has been the establishment of a new 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 (CO) in July 2000, and is widely viewed as a great success. Now the next one in the series is nearly upon us. It is being organized by Jim Ely and will take place July 6-11, 2003 again at Keystone. The web site for the meeting is http://www.mines.edu/academic/chemeng/fomms/

The content of the meeting is balanced between molecular simulation and computational chemistry. All talks are invited, and two poster sessions will provide opportunities for attendees to present their work. One afternoon will be devoted to a software/hardware demonstration session for providers to showcase their products and services. There will be large blocks of time available for informal discussions, and receptions will be held to facilitate interaction between conference participants. Each invited talk will represent a state-of-the-art review and will be rigorously reviewed and edited. All papers (both posters and invited) will be published in a combination of the journals *Molecular Physics* and *Molecular Simulation*.

The schedule of sessions and speakers is listed here:

Sunday, July 6
Keynote Address: Dominic Tildesley, Unilever

Monday, July 7
Industrial Applications (morning session)
Joseph Golab, BP
Cristina Thomas, 3M
Sami Karaborni, Merck

Biological Applications (evening session)
Sangtae Kim, Eli Lilly
Ken Dill, UCSF

Tuesday, July 8
Polymeric Materials (morning session)
Ron Larson, UMich
Masao Doi, Nagoya
Doros Theodorou, Patras

Nanoscience and Nanotechnology (evening session)
Alain Fuchs, UParis-LCP
Anabella Selloni, Princeton

Wednesday, July 9
Electronic Materials (morning session)
Krishnan Ragharvachari, IU
Dimitrios Maroudas, UMass
Roberto Car, Princeton

Advances in Molecular Simulation Techniques (evening session)
Dave Kofke, UB/SUNY
Patrick Warren, Unilever

Thursday, July 10
Reaction Engineering (morning session)
Thanh Truong, Utah
Matt Neurock, UVA
Tony Rappé, CSU
Bill Green, MIT

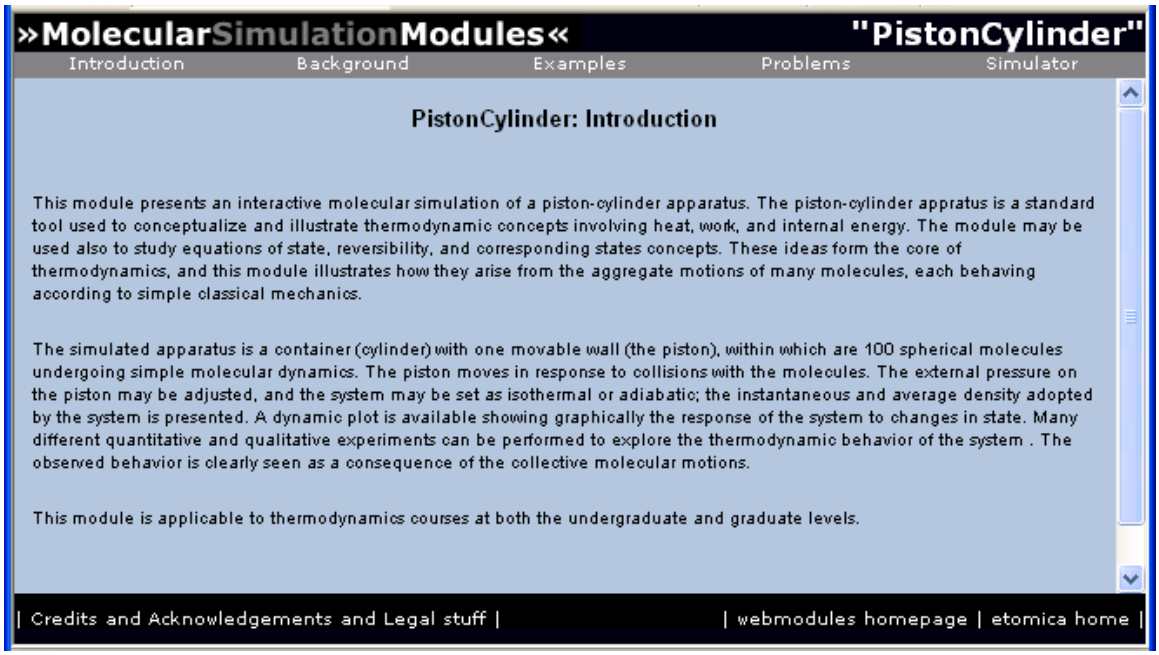
Friday, July 11
Future Vision (morning session)
Alex Bell, UCB
Costas Pantelides, Imperial College
Ellen Stechel, Ford

Molecular Simulation Modules

Another major activity of the MMTF 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 in most cases it can be run as an applet in a web browser. In all cases the simulation can instead be downloaded and run as an application on the user's machine. 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.

We have designed a consistent web-based interface that organizes all of the material in each module. We have developed scripts using *perl* that ease the job of putting the written material into this common format. The developer of a module must construct simple text files, perhaps with HTML markup that permits inclusion of figures and tables. Then he or she runs the files through the *perl* script, which adds HTML formatting and links to put the set of files into the common configuration. We then upload the files to our module site for anyone to access. This site is perhaps best accessed through the *etomica* site. *Etomica* is a Java-based support environment we have developed for the modules project, and which has now been expanded for other applications: go to http://www.ccr.buffalo.edu/etomica and click on the "modules" link in the navigation bar on the left.

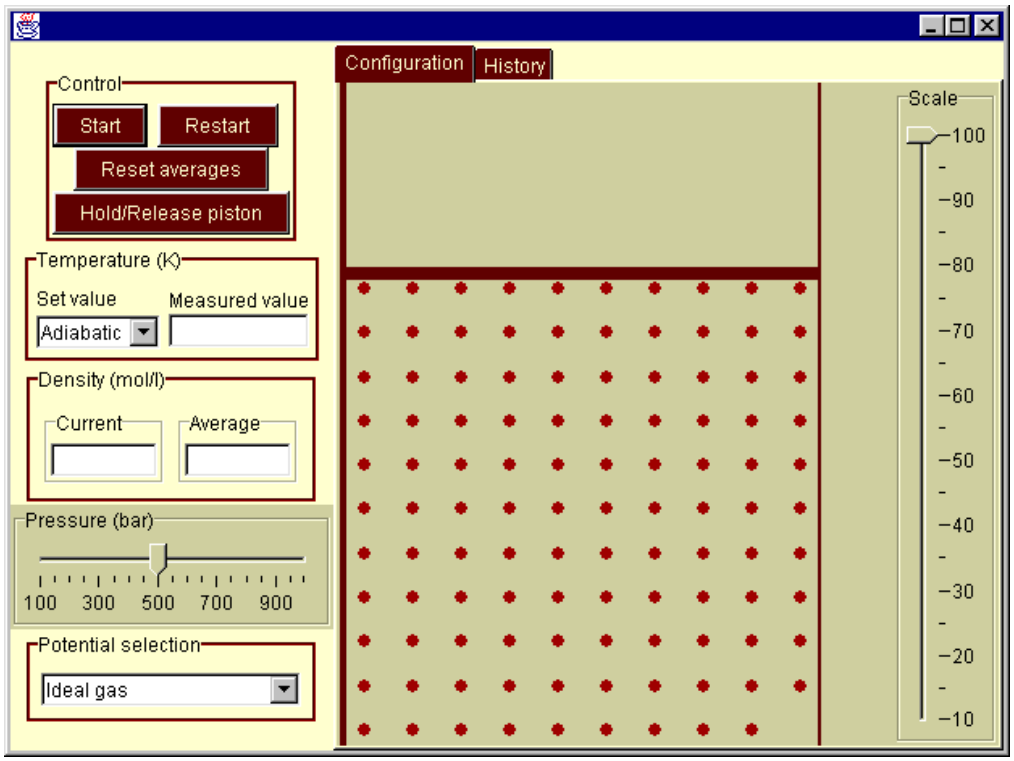
To exemplify the interface, we present the following screen shot from the introduction page for the piston-cylinder module:



This particular module presents an interactive molecular simulation of a piston-cylinder apparatus. The text on the introduction page describes its purpose, "The piston-cylinder

apparatus is a standard tool used to conceptualize and illustrate thermodynamic concepts involving heat, work, and internal energy. The module may be used also to study equations of state, reversibility, and corresponding states concepts. These ideas form the core of thermodynamics, and this module illustrates how they arise from the aggregate motions of many molecules, each behaving according to simple classical mechanics."

Here is a screen shot from the piston-cylinder simulation itself:



Again, as per the introduction, "The simulated apparatus is a container (cylinder) with one movable wall (the piston), within which are 100 spherical molecules undergoing simple molecular dynamics. The piston moves in response to collisions with the molecules. The external pressure on the piston may be adjusted, and the system may be set as isothermal or adiabatic; the instantaneous and average density adopted by the system is presented. A dynamic plot is available showing graphically the response of the system to changes in state. Many different quantitative and qualitative experiments can be performed to explore the thermodynamic behavior of the system. The observed behavior is clearly seen as a consequence of the collective molecular motions."

Following is a list of other phenomena and concepts for which modules are completed or planned for this year:

- Chemical reaction equilibrium
- Osmosis
- Diffusion
- Molecular dynamics
- Normal modes of a solid
- Chemical reaction kinetics

- Dissipative particle dynamics
- Surface tension
- Crystal viewer
- Joule-Thomson expansion
- Self assembly
- Chemical potential
- Multicomponent phase equilibrium
- Heat transfer
- Atomic billiards
- Viscosity

The success in using Java for development of these modules has led us to expand its capabilities further, and the Java-based codes are now the primary tool used for research applications in the author's group. Further development of the code for these purposes is being supported by a new 4-year grant from NSF, via the ITR program.