Molecular Simulation Module Development Project Update

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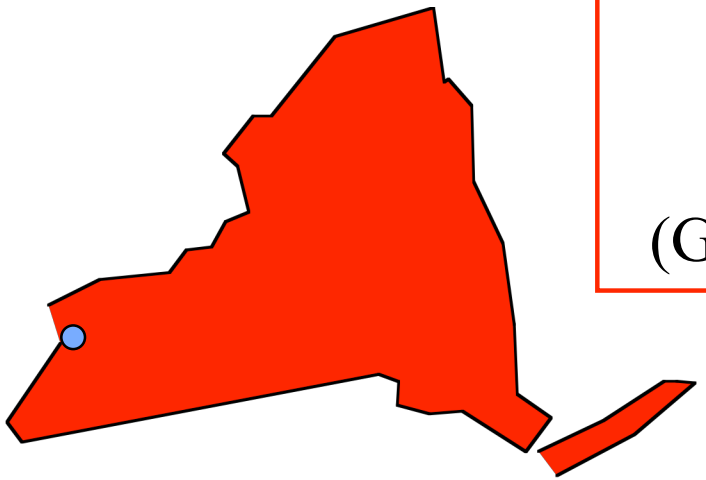

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Molecular Simulation as a Teaching Tool

- Molecular simulation provides a virtual laboratory for molecular mechanics
  - Physically accurate (for the choice of molecular model)
- Many interesting, nontrivial behaviors can be demonstrated
  - Open ended
  - No simple underlying model that directly programs behavior
- The molecular picture is completely accessible
  - Possible to observe how a macroscopic outcome results from collective molecular actions
- Quantitative measurements can be taken
  - Molecular behaviors analyzed with tools of thermodynamics and continuum mechanics

Obstacles 1.

- Educational activities must focus on the *use* of simulation, not its development
  - Don't bog students down in complex coding tasks
- Simulations should be interactive and graphically-oriented
  - Manipulate in real time, like an experiment
- Results should be readily accessible and amenable to post-simulation analysis
  - Like an experiment
- Simulations need to be presented as a complete, fully-functional integrated package

Obstacles 2.

- Broad range of application areas
  - Chemical thermodynamics
    - Boiling, freezing, miscibility, self-assembly, osmosis, etc.
  - Transport phenomena
    - Heat transfer, diffusion, sound, viscosity,…
  - Kinetics
    - Chemical reactions, polymerization, nucleation,…
  - Materials science
    - Elasticity, strength, electronics, photonics,…
  - Biology
    - Protein folding, ion channels,…
- No single person can develop simulations to encompass all the potentially relevant phenomena

Obstacles 3.

- Graphical programming is a tedious skill that few researchers otherwise need
  - Most content experts cannot develop graphical tools
- Educationally effective graphically-oriented simulations are difficult to develop
  - Pedagogical skill varies among practitioners
  - Interest and/or skill to do assessment is not widespread
- In summary
  - A broad range of people are needed to cover the breadth of application
  - The skills needed to develop effective modules are not found among this same group
- Also are obstacles that confront research applications
  - Accessible length and time scales
  - Long CPU time needed to gather some types of results
  - Accuracy of molecular model

Module Development Project

- A community effort to develop molecular simulation teaching modules
- Solicit short proposals for module designs from the science/engineering community at large
- Select several from this pool
- Develop modules
  - We produce graphical-oriented molecular simulation
  - Module consultant produces background documentation
- Assess effectiveness of the modules
  - Involve multiple groups
- Supported by NSF CCLI grant

Definition of "Module"

- Interactive, graphically oriented molecular simulation
- Supporting material to help instructor and student to use module
  - *Introduction*, describing physical ideas
  - *Background*, containing technical information
  - *Examples*, with step-by-step instructions on use of simulation
  - *Problems*, relevant to module for assignment by instructor
  - *Instructor Material*, describing particular points or caveats
  - *Assessment Material*, to be completed by student and/or instructor for use in formative and summative evaluations
  - *Simulation Instructions*, giving details on how to set up and run simulation in various ways, with source code to permit modification

Module Consultant Responsibilities

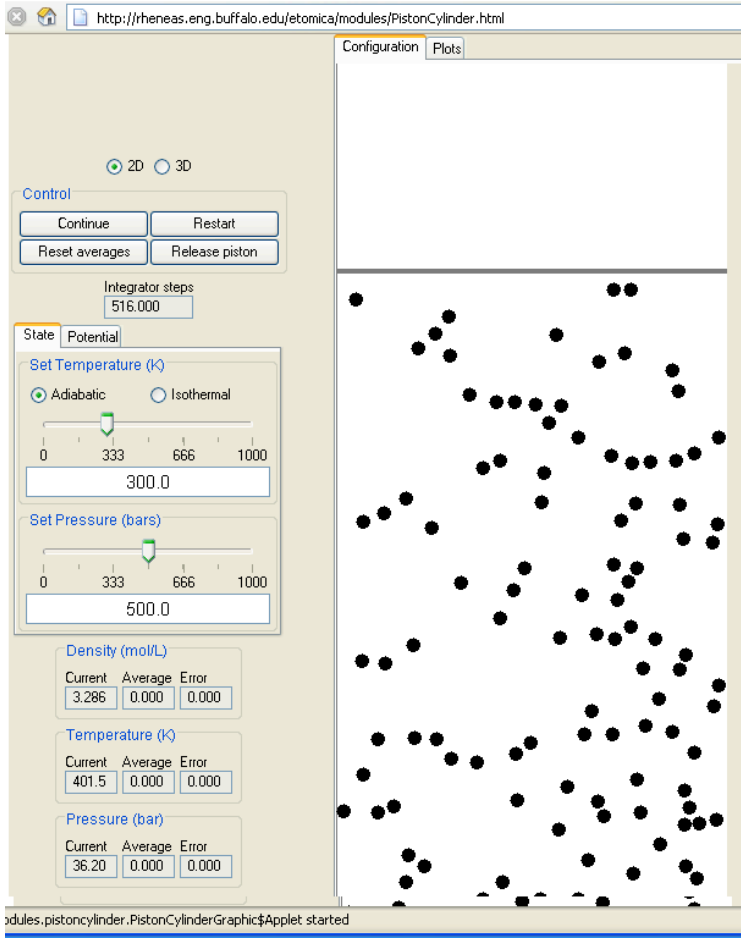
- Generate general idea for the module (via a proposal)
- Specify all aspects of the simulation (in consultation with simulation developers, as needed)
  - Choice of molecular models
  - Model parameters
  - Simulation algorithm
  - Accessible ranges of user-adjustable parameters
  - Values of other parameters
  - General layout of graphical interface
  - Identification of data to be recorded to file
- Preparation of all supporting materials (excluding general assessment material, and simulation instructions)
- Preparation of assessment material specific to the module (in consultations with pedagogy expert, if needed)
- Use and assess simulation module in a course setting, and report results
- Compensated up to $5000 for their efforts

Progress Report

- Modules used as focus in two workshops at ASEE Chemical Engineering Summer School
- One "initial module" under development
  - J. Autschbach, UB Dept of Chemistry
  - Expt measurement of virial coefficient of CO_2
  - VLE simulation of phase coexistence of model fit to data
- Two modules selected from first solicitation
  - Osmosis
  - Mechanical properties at a gold interface
- Pilot module used and assessed in classroom

Pilot Study

- Chemical engineering thermodynamics course
  - Spring 2005, 2006
  - Sophomore level, about 45 students
  - Prof. Mark Swihart, instructor
- Piston-cylinder simulation
  - Classical thermo from classical (statistical) mechanics
- Problem given in memo form
  - Assess suitability of molecular simulation for evaluating virial coefficients
  - Virial coefficients determined by regressing simulation PVT data
  - Results compared to data for real substances
  - Compared to ability to do same using off-the-shelf thermo correlations
- Results submitted in form of report



Likert-scale Responses

- students were strongly positive in responses to questions that dealt with the ease of operation of the simulation
- neutral in their responses to questions that probed whether the simulations enhanced their understanding of material
  - Qualitative interviews needed to clarify some inconsistencies
- strongly negative toward both the amount of time the simulation took
- strongly positive toward the general idea of simulations being a "good way to learn"
- strong agreement the simulation was well-designed and agreement that the simulation was a valuable experience

Open-ended Responses

- How many simulations would be appropriate for a course?
  - 1 (n=25) or 2 (n=9)
  - Complaint about time required for simulation
- What are the benefits of computer simulations?
  - Help to visualize molecules as well as perform experiments hard to duplicate in laboratory
  - It enables us students to focus on the concept behind the experiment
- What are the disadvantages of simulations?
  - Time required to complete simulation
  - Possible mistakes
  - Crashes
- Work by yourself, pairs, teams?
  - Group effort would make project more convenient to complete

Open-ended Responses

- Time spent on project and report?
  - Confused responses, but most (n=25) report more than five hours
- Did simulations provide insight into past learning?
  - Positive (n=12) fewer than negative (n=21)
- What should be changed?
  - Shorter simulations
  - More insight regarding expected values
- Other recommendations?
  - Faster simulation
  - Miscellaneous user interface suggestions

Summary

- Ideas for modules are being solicited from the community
- Modules comprise
  - Graphically-oriented molecular simulation developed by us
  - Supporting materials prepared by proposer of module
- Second solicitation underway
  - Current proposal period ends December 15
  - www.etomica.org

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- Etomica web site
  - www.etomica.org