Computational Tools for Monte Carlo Simulation: Applications to Aqueous Systems

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Using Java, Perl, and other cross-platform languages, several end-user tools are being developed to aid the presentation and propagation of computational chemistry research methods in educational and research environments. With a Monte Carlo FORTRAN program[1] as a basis, we are designing a graphical front-end and a real-time results interface aimed at the classroom and beginning research environments. Our goals for this project include: overcoming the generally steep learning curve involved in computational chemistry research and demonstrating that computational chemistry can be integrated into the classroom as easily as wet labs are currently. In addition to research applications, we plan to develop several experiments that could be used on a high school and early college level for teaching and introduction to research.

These tools have been applied to reproducing valid vapor-liquid coexistence curves and critical properties for a variety of water models. Gibbs-ensemble Monte Carlo simulations are performed for SPC/E, TIP4P, SPC-FQ, and TIP4P-FQ water models at several sub-critical temperatures. Despite the increased complexity of the fluctuating charge models with response to electronic degrees of freedom, the fixed-charge models are able to better reproduce the vapor-liquid coexistence curves. The critical temperature for the best model, SPC/E, was found to be 659 K, with a critical density of 0.31 g/mL. All models are in good agreement with literature values.[2]

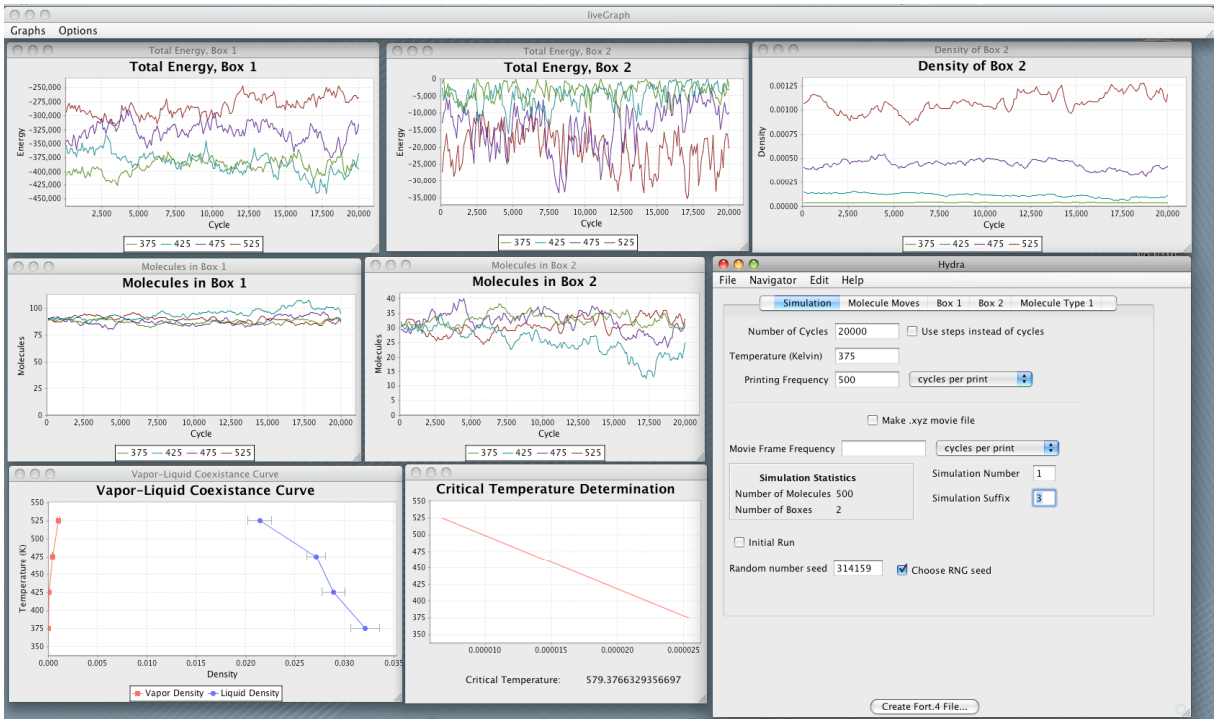

Figure 1: The graphical front-end, for use in educational and research environments.

[1] Monte Carlo for Complex Chemical Systems from the Siepmann Group at the University of Minnesota, http://www.chem.umn.edu/groups/siepmann/software.html

[2] B. Chen, J.J. Potoff, and J.I. Siepmann, *J. Phys. Chem. B* **104**, 2378-2390 (2000).