37g Molecular Simulation Using a Graphical User Interface

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One of the difficulties in teaching molecular simulation is the investment of time required for students to develop fully-functional codes from scratch. As a remedy, we have developed Etomica, a Java-based object-oriented library of components including graphical devices and displays. Students can assemble these components into a fully-functional simulation. The students can also include extra components to extend the simulation to accomplish a variety of complex tasks. Although the library often lacks some element needed for a particular simulation, the library can be extended to handle such additional functionality. We have used this package in the past to teach students from the high-school to the graduate level. In this presentation we demonstrate previously constructed simulations and how to assemble new simulations from scratch.