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Molecular dynamics simulation: A tool for exploration and discovery

DENNIS C. RAPAPORT, Physics Department, Bar-Ilan University

The exploratory and didactic aspects of science both benefit from the ever-growing role played by computer simulation. One particularly important simulational approach is the molecular dynamics method, used for studying the nature of matter from the molecular to much larger scales. The effectiveness of molecular dynamics can be enhanced considerably by employing visualization and interactivity during the course of the computation and afterwards, allowing the modeler not only to observe the detailed behavior of the systems simulated in different ways, but also to steer the computations in alternative directions by manipulating parameters that govern the actual behavior. This facilitates the creation of potentially rich simulational environments for examining a multitude of complex phenomena, as well as offering an opportunity for enriching the learning process. A series of relatively advanced examples involving molecular dynamics will be used to demonstrate the value of this approach, in particular, atomistic simulations of spontaneously emergent structured fluid flows (the classic Rayleigh–Bénard and Taylor–Couette problems), supramolecular self-assembly of highly symmetric shell structures (involved in the formation of viral capsids), and that most counterintuitive of phenomena, granular segregation (e.g., axial and radial separation in a rotating cylinder).