Hoobas: A highly object-oriented builder for molecular dynamics

Computational Materials Science 167, 25-33 (2019)

Polydispersity and random sequences are ubiquitous features of polymers, and molecular dynamics simulations can help elucidate the impact of disorder in polymer systems. However, currently available packages for building polymer topologies do not enable the user to include randomness in a straightforward fashion. Here, we introduce Hoobas, a molecular builder package that easily handles polydispersity using a prototype-builder design pattern. This enables fast and easy building of systems comprised of thousands of distinct objects. It is written in the Python programming language, which ensures compatibility with a wide range of molecular dynamics packages and tools, as well as easy integration into most workflows.

Significance and Impact

In this paper, we presented Hoobas, a topology builder for molecular dynamics based on a prototype-builder design pattern. This strategy allows for simple syntax for topology generation, including easy incorporation of polydispersity in systems of arbitrary size. The use of Python as a programming language also allows Hoobas to integrate with different molecular dynamics packages in a straightforward manner. For instance, Hoobas can be combined with backmapping to run coarse-grained simulations in one package, such as HOOMD-blue, and atomistic simulations in another, such as openMM, to take advantage of optimizations inherent to different packages.

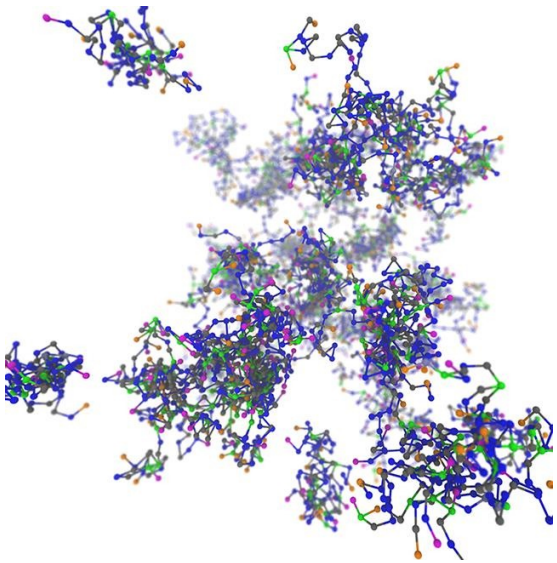

Figure: A cubic simulation box with 12.5 nm sides, filled with 50 polyethylenimine molecules generated procedurally. The random orientation of attachment sites used results in a random walk that includes overlaps between particles, and will require an energy minimization procedure. Particles are colored by bond number and charge.

Northwestern

Funding: Sherman Fairman Foundation (to M.O.d.I.C.), Natural Science and Engineering Research Council of Canada (NSERC, PGS-D #6799-459278-2014), Center for Computation and Theory of Soft Materials (DOE), grant number DE-FG02-08ER46539.