Adaptively restrained simulations in LAMMPS

The computational cost of particle simulations can be significantly reduced with the help of the Adaptively Restrained Molecular Dynamics (ARMD).
This approach modifies the Hamiltonian dynamics governing the motion of particles by switching positional degrees of freedom on and off during simulations.
ARMD allows to speed up calculations by either decreasing precision or focusing on select subsystems. Precisely, a part of the system of interest may remain frozen awhile throughout ARMD simulations. Therefore, incremental algorithms may enable an efficient calculation of interaction forces that govern the evolution of the system.

In order to combine ARMD with a large panoply of interaction potentials, we implemented ARMD in LAMMPS simulation package. We validated the method on several benchmarks and showed that the equilibrium statistics have been preserved.

Several incremental force update algorithms were developed to take advantage of adaptive restraints. We proposed and validated a general treatment of short-ranged interactions, which in turn reduces the computational cost of ARMD simulations. The method can be applied to any pairwise short-ranged interactions since it relies on a manipulation of neighbor lists. For completeness, we introduced several algorithms that accelerate the evaluation of pairwise long-range forces when some particles are restrained. Those algorithms allow us to benefit from ARMD on systems where electrostatics play an important role.