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Beyond Verlet: Unlocking a 2x Speedup in Molecular Dynamics with Novel Time Integrators

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Molecular dynamics (MD) simulations constitute a central pillar of computational chemistry. While the methods for force computation have advanced significantly in recent decades, the underlying time integration algorithm is still mostly the same – namely, the Verlet integrator in its various (equivalent) formulations. Previous attempts to improve integration, such as those by Yoshida or Suzuki, have not translated into better efficiency for practical MD simulations. Here, we present a family of novel integration algorithms which we have optimized to substantially enhance the performance of MD simulations. Our algorithms are explicit 8-stage Runge–Kutta–Nyström methods that are both symmetric (i.e. time-reversible) and symplectic, ensuring excellent long-term stability and energy conservation. The performance gains are significant: Compared to a MD simulation with a Verlet time step of dt=0.5 fs, our methods deliver either a 2.5-fold increase in computational speed at the same accuracy, or a 150-fold increase in accuracy (measured in terms of energy conservation) at the same computational cost. Even compared to a Verlet time step of dt=1.0 fs, our approach still achieves a two-fold speedup at the same accuracy, or a six-fold increase in accuracy using the same resources. As a time integration algorithm, our approach is independent of the underlying computational model, and thus compatible with all flavors of MD, including ab initio MD (AIMD), force field MD, and machine learned interatomic potentials (MLIPs). Geometric constraints and modern thermostats (such as NHC) can easily be supported, albeit not yet implemented. The speedup directly translates to savings in computational time and energy consumption, making a significant contribution to a more environmentally friendly computational chemistry. Given that MD simulations are estimated to consume around 2 terawatt-hours per year, our methods could potentially save half of this energy. An initial implementation will soon be publicly available in the open-source simulation package LAMMPS.