Adaptive two-stage integrators for sampling algorithms based on Hamiltonian dynamics

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We present an alternative to the standard velocity Verlet integrator, known to be the state-of-the-art method for numerical integration of the Hamiltonian equations in molecular dynamics (MD) and hybrid / Hamiltonian Monte Carlo (HMC) simulations.

The novel methodology, which we call the Adaptive Integration Approach, or AIA, offers, for any chosen simulation problem and step size, a system-specific two-stage splitting integrator, which provides the best conservation of energy for harmonic forces. The proposed new family of numerical integrators can be viewed as a one-parameter two-stage splitting integrators family, with the parameter being a function of the simulation step size and the highest angular frequency present in the simulated system. In contrast, all numerical integrators for Hamiltonian dynamics used to date belong to the fixed parameters families.

The AIA has been formulated for a range of algorithms, which simulate either constrained or unconstrained dynamics, and sample with Hamiltonians or modified Hamiltonians. It can be implemented in a MD / HMC software code, without introducing computational overheads in the simulations.

Numerical tests show that the method successfully realises the fail-safe strategy.
In all experiments, and for each of the criteria employed, the AIA is at least as good as, and often significantly outperforms the standard Verlet scheme, as well as fixed parameter, optimized two-stage integrators.

The ideas underlying the AIA can be also used for a rational choice of simulation parameters.