PARAREAL ALGORITHMS FOR MOLECULAR DYNAMICS SIMULATIONS

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Abstract. In this talk, we introduce parareal algorithms in the context of molecular dynamics, where we couple a fine propagator based on the reference potential energy landscape with a coarse propagator based on a surrogate potential. These algorithms allow parallel-in-time computations of the trajectory and often offer computational gains compared to a standard sequential integration. Although the parareal algorithm, in its original formulation, always converges, it suffers from various limitations in the context of molecular dynamics. In particular, it is observed that the algorithm does not provide any computational gain in the limit of increasingly long time-horizons. This numerical observation is backed up with theoretical discussions. We then introduce a modified version of the parareal algorithm wherein the algorithm adaptively divides the entire time-horizon into smaller time slabs. We numerically show that the adaptive algorithm overcomes the various limitations of the standard parareal algorithm, thereby allowing for significantly improved gains. We also discuss the implementation of the algorithm in LAMMPS, and the various adaptations we have to make in order to use LAMMPS in a non-intrusive manner. Numerical simulations of self-interstitial atoms diffusing in a tungsten lattice will be discussed.

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