Adaptive parareal algorithms for molecular dynamics problems

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A central objective in molecular dynamics (MD) is the computation of ensemble averages and dynamical quantities, which both involve averages over very long trajectories of stochastic dynamics. Reducing the computational time of these large time-scales simulations is thus of great interest. One possible way to speed up such computations is to develop accelerated MD approaches based on the parallelization of problems in the temporal domain.
A popular parallel in time method for integrating ordinary differential equations is the parareal algorithm that has been first introduced in [3]. The algorithm aims to compute iteratively an approximation of the exact solution of the time-dependent problem. At each iteration, the parareal algorithm utilizes a coarse solver to quickly step through the time domain by computing relatively cheap approximate solutions for all time intervals of interest, and then simultaneously refines all of these approximate solutions using an accurate fine solver over small time subdomains. Since the fine propagator corrections (which are expensive to compute) are applied in parallel over each subinterval, the associated wall-clock time remains limited. In contrast, the coarse propagator is applied in a sequential manner but its cost is often negligible.
In the MD contex, it is convenient to consider parareal algorithms where the coarse and the fine propagators integrate dynamics based on different potential energies, using the same time-step (the difference in cost stemming from the different complexity for evaluating the potential). In this setting, an adaptive version of the parareal algorithm has recently been introduced [2], which leads to significant improved gains on some toy examples. Our aim here is to investigate the feasibility of this adaptive algorithm for realistic problems, in the high performance computing context. We shall present some preliminary numerical results [1] when applying this algorithm to the Langevin dynamics, using LAMMPS [1] - a popular molecular dynamics software with a focus on materials modeling. The simulations are performed with the machine-learning interatomic potentials SNAP (spectral neighbor analysis potentials) [4] for fine and coarse propagators.

[1] O. Gorynina, F. Legoll, T. Lelievre. in preparation.

[2] F. Legoll, T. Lelievre, U. Sharma. *An adaptive parareal algorithm : application to the simulation of molecular dynamics trajectories.* arXiv preprint.

[3] J.-L. Lions, Y. Maday, G. Turinici. *Résolution d'edp par un schéma en temps pararéel* . Comptes Rendus de l'Académie des Sciences-Series I-Mathematics, **332(7)**, 661–668, 2001.

[4] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, G. J. Tucker. *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials.* Journal of Computational Physics, **285**, 316–330, 2015.

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1. https ://lammps.sandia.gov/