Combining cheap and expensive forces in ab initio molecular dynamics

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We present an efficient method to mix well converged ab initio forces with simpler and faster ones in molecular dynamics [1]. The integration method is similar to that used previously to split classical force fields into slow and fast components [2]. Like in the 'learn on the fly' scheme [3], ab initio forces are computed only rarely, but our method does not involve any learning process. While the cheap forces are evaluated every time step, the converged ones correct the trajectory only every n time steps. For convenience, both types of forces are calculated with the SIESTA method, using density functional theory, norm conserving pseudopotentials, and a basis set of numerical atomic orbitals [4]. The cheap forces are evaluated with a short-range minimal basis set and the non-selfconsistent Harris functional. Since these evaluations are hundreds of times faster than those of the converged forces, they add a neglegible cost, and the boost in computational efficiency is approximately a factor n. Using 'quick and dirty' ab initio forces for the cheap forces avoids having to parametrize a classical potential for every new system to be simulated. Our results indicate that the method is very robust with respect to inaccuracies of the cheap forces, and that one can use values of n of up to 10, without affecting significantly the calculated structural and dynamical magnitudes.

PACS numbers:

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