

Abstract Submitted
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Fast molecular dynamics simulations using high-order forces and nonlocal operators in real space¹ GRADY SCHOFIELD, N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We present a new modification to the finite-difference based real space pseudopotential density functional theory method as implemented in the code PARSEC. By using a high-order treatment of the nonlocal pseudopotential terms in the Hamiltonian, as well as integration performed during post-processing the wave functions, we improve the accuracy of total energy and interatomic forces. We perform molecular dynamics simulations for several systems, including organic molecules and small clusters. We demonstrate significant reduction in energy drift owing to the accuracy of our improved force calculations. Furthermore, the reduction in numerical noise as atoms move over the grid permits a larger grid spacing than would be possible with a conventional discretization.

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