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Quantum dynamics integrators in a plane-wave implementation of time-dependent density functional theory ANDRÉ SCHLEIFE, ALFREDO CORREA, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina at Chapel Hill — In order to develop our understanding of various dynamical phenomena in materials at the electronic-structure level, computational methods based on first-principles theory are indispensable. Such approaches can make significant contributions to improving materials for a wide range of applications reaching from photovoltaic cells to nuclear reactors. Time-dependent density functional theory is an efficient approach for describing the real-time quantum dynamics of electronic systems. However, the numerical integration of the time-dependent Kohn-Sham equations, i.e., including a density-dependent effective Hamiltonian, is highly non-trivial. We studied various integrators for propagating the single-particle wave functions explicitly in time, in order to achieve a highly-scalable implementation based on plane-waves and pseudo-potentials. We show that the fourth-order Runge-Kutta scheme is conditionally stable and accurate within this framework. Moreover, the application of our scheme to a system consisting of several hundreds of electrons unveils its excellent scalability and, hence, its applicability for large-scale simulations.

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