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DFT_3: An Efficient DFT Solver for Nanoscale Simulations and Beyond. XUECHENG SHAO, WENHUI MI, MICHELE PAVANELLO, Rutgers University, Newark — To date, there are two kinds of DFT algorithms: Kohn-Sham DFT (KS-DFT) and orbital-free DFT (OF-DFT). KS-DFT is most common, uses a prescription whereby the lowest N eigenvalues (where N is the number of electrons) of a one-particle Hamiltonian need to be computed. OF-DFT prescribes to compute just one state recovering the effect of the other states with pure density functionals. In this work, we propose a new DFT solver (DFT_3). From KS-DFT we borrow the self-consistent field iteration, so that computationally expensive density functionals are evaluated seldom. From OF-DFT we borrow the reliance on kinetic energy functionals, thus removing the need to diagonalize bringing strong computational savings. DFT_3 leverages recent advances in OF-DFT development to output a computationally cheap and accurate ab initio electronic structure method. The key aspect of DFT_3 is its still make use of an eigenvalue-like problem targeting just one solution while retaining the ability to sample ensemble N-representable electron densities. We implemented this method in DFTpy software. In comparison to OF-DFT and KS-DFT, DFT_3 cuts the timing down by orders of magnitude and maintains linear scalability with system size.

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