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Advances in Real Space Methods to Solve the Kohn-Sham Equation[1] CHALRES LENA, JAMES R. CHELIKOWSKY, The University of Texas at Austin, ARIEL BILLER, LEEOR KRONIK, Weizmann Institute of Science — We will discuss advances in solving the Kohn-Sham equation using pseudopotentials implemented in real space. A solution is often limited by the high computational demand in solving an eigenvalue problem at each self-consistent-field. Our code replaces the explicit eigenvalue calculations by an approximation of the desired invariant subspace, refined with well-selected Chebyshev polynomial filters. The subspace iteration at each step is notably faster than solving a corresponding eigenproblem by the most efficient algorithms. Moreover, the subspace iteration reaches self-consistency within roughly the same number of steps as an eigensolver-based approach. We will discuss some advances in data partitioning. These advances include improvements to sparse matrix vector multiplication, which makes up the large computational component of the filtering process. We demonstrate an efficient scaling of the Laplacian component to more than 10^8 grid points and of the Rayleigh-Ritz component to 10^5 electronic states. As an application, we consider nanocrystals of silicon containing over 10,000 atoms.

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