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A Fourier Multi-level Hybrid OpenMP/MPI Approach for Eigenvalue Problems in First-principles Materials Science Calculations

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We present a multi-level approach in Fourier space to solve the Kohn-Sham equations from Density Functional Theory (DFT) using a plane wave (Fourier) basis and replacing the ionic cores by pseudopotentials. By increasing the cutoff energy and associated other parameters in subsequent levels, we demonstrate that this approach efficiently speeds up solving the Kohn-Sham equations. The method was implemented in the PARATEC first principles plane wave code. Examples of multi-level calculations for bulk silicon, quantum dots and an aluminum surface are presented. In some case using the multilevel approach the total computation time is reduced by half compared to the original single level approach. We will also discuss the advantages of our hybrid OpenMP/MPI implementation over a pure MPI version for running on multi-core architectures.