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Iterative solver for Density Functional Theory calculations on composite meshes by quadratic Finite Elements

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Density Functional Theory (DFT) is a simplified quantum model that has proved very successful in real applications. It introduces an independent particles description of the electronic structure of molecules or materials which is much simpler to treat that the original Schroedinger equations. Simulating realistic physical systems by DFT however is still computationally very demanding. More efficient numerical algorithms to reduce computer time and enable larger simulations are always in demand by chemists and physicists who are studying phenomenon at the molecular level.

The finite element (FE) method, a very popular approach to solve partial differential equations, has only recently started being used for solving the Kohn-Sham equations of Density Functional Theory for realistic 3D applications. Traditionally, the pseudo-spectral approach has been the most popular in the field under the denomination Plane Waves method. The regular usage of periodic boundary conditions with simple geometries explains this preference. However with the increase in computer power and the growing interest in studying larger and more diverse systems, more flexible real-space discretizations by finite difference or finite elements have recently attracted more interest.

In this work we focus on FE discretizations with local mesh refinement for the Kohn-Sham equations, and propose an efficient iterative solver and preconditioner for this problem. We present a hierarchical quadratic Finite Elements approach to discretize the equations on structured non-uniform meshes. A multigrid FAC preconditioner is proposed to iteratively minimize the energy functional associated to the Kohn-Sham equations. It is based on an accelerated steepest descent-based scheme. The method has been implemented using SAMRAI, a parallel software infrastructure for general AMR applications. Numerical results of electronic structure calculations on small atomic clusters show in particular a mesh-independent convergence rate for the iterative solver.