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Partition of Unity Finite Element Method to Solve the Kohn-Sham Equations of Density Functional Theory

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ABSTRACT

Over the past few decades, the planewave pseudopotential (PW) method has established itself as the method of choice for large, accurate quantum-mechanical calculations in solids and liquids. However, due to its global Fourier basis, the PW method suffers from substantial inefficiencies in parallel implementation and in problems involving localized states. Modern real-space methods [1] such as finite-differences, finite elements (FE) [2], and wavelets, resolve these problems but have until now required a much larger number of basis functions to attain the required accuracy. For N degrees of freedom, the $\mathcal{O}(N^3)$ scaling of the eigensolution versus $\mathcal{O}(N)$ complexity of the Poisson solver renders the solution of the Schrödinger equations as the limiting step in *ab initio* calculations for large number of atoms.

In this work, we present a new real-space finite element method to solve the Kohn-Sham equations of density functional theory. The solution of the Kohn-Sham equations requires the solution of coupled Schrödinger and Poisson equations. We employ partition-of-unity (PU) enrichment techniques [3] to build the known atomic physics into the FE basis, thereby substantially reducing the degrees of freedom required. The unit cell is parallelepiped, and we consider Dirichlet boundary conditions for atoms and molecules, and Bloch boundary conditions for crystalline solids. A new approach to impose Bloch boundary conditions (arbitrary k-points) in FE and PUFE methods is also developed. Uniform meshes consisting of higher-order 'serendipity' finite elements (8-, 20-, and 32-node brick elements) are used to construct the FE basis, and trilinear finite elements are used to form the PU basis. The enrichment functions are pseudoatomic wavefunctions $\psi_{nlm}(\mathbf{x}) = R_{nl}(r)Y_{lm}(\theta,\phi)$, the product of radial solutions and spherical harmonics. A one-dimensional spectral finite element solver is used to compute $R_{nl}(r)$. Our initial results for the energy eigenvalues show order-of-magnitude improvements relative to current state-of-the-art PW and adaptive-mesh (AMR) FE methods for systems involving localized states such as first-row, d-, and f-electron systems. The finite element and PUFE potential solutions for localized charge densities via the Poisson equation will also be discussed.

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