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Large-scale All-electron Density Functional Theory Calculations using Enriched Finite Element Method[1] BIKASH KANUNGO, VIKRAM GAVINI, Univ of Michigan - Ann Arbor — We present a computationally efficient method to perform large-scale all-electron density functional theory calculations by enriching the Lagrange polynomial basis in classical finite element (FE) discretization with atom-centered numerical basis functions, which are obtained from the solutions of the Kohn-Sham (KS) problem for single atoms. We term these atom-centered numerical basis functions as enrichment functions. The integrals involved in the construction of the discrete KS Hamiltonian and overlap matrix are computed using an adaptive quadrature grid based on gradients in the enrichment functions. Further, we propose an efficient scheme to invert the overlap matrix by exploiting its LDL factorization and employing spectral finite elements along with Gauss-Lobatto quadrature rules. Finally, we use a Chebyshev polynomial based acceleration technique to compute the occupied eigenspace in each self-consistent iteration. We demonstrate the accuracy, efficiency and scalability of the proposed method on various metallic and insulating benchmark systems, with systems ranging in the order of 10,000 electrons. We observe a 50-100 fold reduction in the overall computational time when compared to classical FE calculations while being commensurate with the desired chemical accuracy.

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