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Finite elements for accurate, large-scale quantum mechanical materials calculations: from classical to enriched to discontinuous

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ABSTRACT

We discuss recent developments in finite-element (FE) based methods for the solution of the Kohn-Sham equations that have made possible smaller basis sets and larger calculations than possible by current state-of-the-art planewave based methods, in some cases by an order of magnitude or more. We begin with classical FE based approaches, demonstrating optimal convergence rates and micro-Hartree agreement with established PW based methods. We then discuss recent enriched partition-of-unity FE methods, which build known atomic physics into the basis while retaining strict locality and systematic improvability. By incorporating known physics, these bases can achieve the required accuracies with an order of magnitude fewer degrees of freedom (DOF) than required by traditional PW based methods, for “hard atom” calculations in particular. However, with such enrichment comes more expensive quadrature and some degree of ill-conditioning, which must be addressed. By incorporating not only local-atomic but also environmental physics into the basis, recent Discontinuous Galerkin (DG) based approaches can achieve larger reductions in DOFs still, while retaining both strict locality and systematic improvability. Crucially, however, the DG formulation allows for orthonormality as well, alleviating conditioning issues and allowing for the solution of standard rather than generalized discrete eigenproblems in the critical N_3 scaling step of the Kohn-Sham solution. Accurate quantum mechanical forces have also been demonstrated. We conclude with an outlook and particular applications interests going forward.