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A Discontinuous Galerkin Framework for Electronic Structure Calculations ANDREW BACZEWSKI, BALASUBRAMANIAM SHANKER, SUBHENDRA MAHANTI, BENJAMIN LEVINE, Michigan State University — It is generally accepted that a good basis set for any calculation should possess a number of salient features, including systematic improvability, adaptive resolution of multiscale features, and fidelity in capturing the pertinent physics. Considering the progenitors of most modern electronic structure basis sets to be Gaussian-type orbitals or planewaves, descendants of these methods have inherited features that address either systematic improvability (planewaves) or adaptive resolution (Gaussians) separately, and use a variety of tricks to differentiate the core and valence physics. Discontinuous Galerkin methods provide a framework for defining adaptive local basis sets, that may be based on these canonical basis sets, that can be mixed and matched to simultaneously achieve all of these goals. Our group is presently developing a new electronic structure code to enable Density Functional and Hartree-Fock calculations within this framework, particularly in the context of all-electron formulations wherein the accurate resolution of both core and valence states is necessary. Numerous implementation details will be addressed, including the incorporation of hardware- and software-based acceleration, such as GPU-based parallelism, and fast electrostatics solvers.

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