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Title: Spectral element formulation of density functional theory

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Although density functional theory is the de-facto standard for quantum materials simulations, current state-of-the-art, production software packages do not scale well on modern high-performance computing platforms --- often to only 10--100 processor cores for the leading planewave and molecular orbital based packages. This is a result of their underlying algorithms, which require global parallel communication, and improving the scaling of these methods is a challenging topic of current research. In contrast, so-called real-space methods, such as those using finite difference, finite element, or wavelet techniques, have demonstrated efficient parallel scaling to 10,000 processor cores. These techniques thus represent the likely evolution of density functional theory software in order to solve future grand challenge problems on exascale computing architectures. Unfortunately, one disadvantage of many real-space methods is the large number of degrees of freedom required to achieve chemical accuracy. The time to solution (CPU time) for these techniques is often slower on a practical number of processors even though the methods scale well. The advantage of planewaves in this respect is the spectral (or exponential) convergence of the error with respect to the number of basis functions. In this work, a real-space, spectral element formulation of density functional theory is presented. The spectral element method is an extension of the finite-element method to high-order polynomial basis sets. It retains the parallel efficiency of other real-space methods by requiring only local, nearest-neighbor communications, but unlike most other real-space methods, the error converges spectrally. This leads to a dramatic reduction in the number of basis functions needed to achieve chemical accuracy. In this talk both the reduction of degrees of freedom and parallel scaling will be presented, making direct comparisons to planewave, pseudopotential density functional theory approaches.