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Partition-of-unity finite element method for large, accurate electronic-structure calculations[1] JOHN PASK, Lawrence Livermore National Laboratory, NATARAJAN SUKUMAR, University of California, Davis — Over the past few decades, the planewave pseudopotential (PW) method has established itself as the method of choice for large, accurate, density-functional calculations in condensed matter. However, due to its global Fourier basis, the PW method suffers from substantial inefficiencies in parallel implementation and problems involving localized states. Modern real-space approaches, such as finite-difference (FD) and finite-element (FE) methods, resolve these problems but have until now required much larger bases to attain the required accuracy. Here, we present a new real-space FE based method which employs modern partition-of-unity FE techniques to substantially reduce the number of basis functions required. Initial results show order-of-magnitude improvements relative to current state-of-the-art PW and adaptive-mesh FE methods for systems involving localized states such as d- and f-electron metals.

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