

Abstract Submitted
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Partition-of-unity finite elements for electronic structure: have planewaves finally met their match?¹ JOHN PASK, LLNL — Over the past few decades, the planewave (PW) pseudopotential method has established itself as the dominant method for large, accurate, density-functional calculations in condensed matter. However, due to the underlying Fourier representation of the required quantum mechanical wavefunctions, the PW method suffers from substantial inefficiencies in parallelization and applications involving highly localized states, such as those with 1st-row, transition-metal, or other atoms at extreme conditions. Modern real-space approaches, such as finite-difference (FD), finite-element (FE), and wavelet based methods, can address these deficiencies but have until now required much larger bases to attain the required accuracy. In this talk, we discuss our recent work on a new real-space FE based method which employs modern partition-of-unity FE techniques to substantially reduce the number of basis functions required by building known atomic physics into the basis, while retaining both locality and systematic improvability. 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 and/or other atoms at extreme conditions.

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