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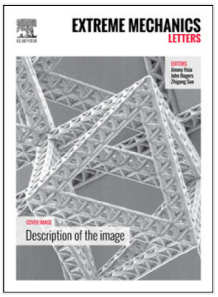

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J.E. Pask, N. Sukumar

PII: S2352-4316(16)30204-8
DOI: http://dx.doi.org/10.1016/j.eml.2016.11.003
Reference: EML 235

To appear in: *Extreme Mechanics Letters*

Received date: 26 September 2016
Revised date: 28 October 2016
Accepted date: 2 November 2016

Please cite this article as: J.E. Pask, N. Sukumar, Partition of unity finite element method for quantum mechanical materials calculations, *Extreme Mechanics Letters* (2016), http://dx.doi.org/10.1016/j.eml.2016.11.003

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Partition of unity finite element method for quantum mechanical materials calculations

J. E. Pask[a,*], N. Sukumar[b,*]

[a]*Lawrence Livermore National Laboratory, Livermore, CA 94550, USA.*
[b]*Department of Civil and Environmental Engineering, University of California, Davis, CA 95616, USA.*

Abstract

The current state of the art for large-scale quantum-mechanical simulations is the planewave (PW) pseudopotential method, as implemented in codes such as VASP, ABINIT, and many others. However, since the PW method uses a global Fourier basis, with strictly uniform resolution at all points in space, it suffers from substantial inefficiencies in calculations involving atoms with localized states, such as first-row and transition-metal atoms, and requires significant nonlocal communications, which limit parallel efficiency. Real-space methods such as finite-differences (FD) and finite-elements (FE) have partially addressed both resolution and parallel-communications issues but have been plagued by one key disadvantage relative to PW: excessive number of degrees of freedom (basis functions) needed to achieve the required accuracies. In this paper, we present a real-space partition of unity finite element (PUFE) method to solve the Kohn-Sham equations of density functional theory. In the PUFE method, we build the known atomic physics into the solution process using partition-of-unity enrichment techniques in finite element analysis. The method developed herein is completely general, applicable to metals and insulators alike, and particularly efficient for deep, localized potentials, as occur in calculations at extreme conditions of pressure and temperature. Full self-consistent Kohn-Sham calculations are presented for LiH, involving light atoms, and CeAl, involving heavy atoms with large numbers of atomic-orbital enrichments. We find that the new PUFE approach attains the required accuracies with substantially fewer degrees of freedom, typically by an order of magnitude or more, than the PW method. We compute the equation of state of LiH and show that the computed lattice constant and bulk modulus are in excellent agreement with reference PW results, while requiring an order of magnitude fewer degrees of freedom to obtain.

Keywords: electronic structure calculations, density functional theory, Kohn-Sham equations, finite elements, partition of unity enrichment, adaptive quadrature

*Corresponding authors
Email addresses: pask1@llnl.gov (J. E. Pask), nsukumar@ucdavis.edu (N. Sukumar)

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