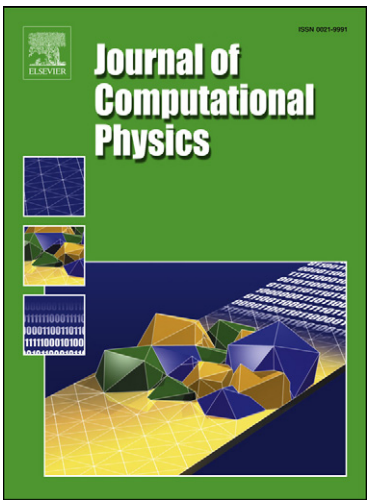

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P. Motamarri, M.R. Nowak, K. Leiter, J. Knap, V. Gavini

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Higher-order adaptive finite-element methods for Kohn-Sham density functional theory

P. Motamarri [a], *M. R. Nowak* [b], *K. Leiter* [c], *J. Knap* [c], *V. Gavini* [a*]

[a] Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA

[b] Department of Electrical Engineering, University of Michigan, Ann Arbor, MI 48109, USA

[c] U.S. Army Research Labs, Aberdeen Proving Ground, Aberdeen, MD 21001, USA

Abstract

We present an efficient computational approach to perform real-space electronic structure calculations using an adaptive higher-order finite-element discretization of Kohn-Sham density-functional theory (DFT). To this end, we develop an *a priori* mesh adaption technique to construct a close to optimal finite-element discretization of the problem. We further propose an efficient solution strategy for solving the discrete eigenvalue problem by using spectral finite-elements in conjunction with Gauss-Lobatto quadrature, and a Chebyshev acceleration technique for computing the occupied eigenspace. The proposed approach has been observed to provide a staggering $100 - 200$ fold computational advantage over the solution of a generalized eigenvalue problem. Using the proposed solution procedure, we investigate the computational efficiency afforded by higher-order finite-element discretizations of the Kohn-Sham DFT problem. Our studies suggest that staggering computational savings—of the order of $1000-$fold—relative to linear finite-elements can be realized, for both all-electron and local pseudopotential calculations, by using higher-order finite-element discretizations. On all the benchmark systems studied, we observe diminishing returns in computational savings beyond the sixth-order for accuracies commensurate with chemical accuracy, suggesting that the hexic spectral-element may be an optimal choice for the finite-element discretization of the Kohn-Sham DFT problem. A comparative study of the computational efficiency of the proposed higher-order finite-element discretizations suggests that the performance of finite-element basis is competing with the plane-wave discretization for non-periodic local pseudopotential calculations, and compares to the Gaussian basis for all-electron calculations to within an order of magnitude. Further, we demonstrate the capability of the proposed approach to compute the electronic structure of a metallic system containing 1688 atoms using modest computational resources, and good scalability of the present implementation up to 192 processors.

*Corresponding author