Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 342 (2018) 224–239
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Orbital-enriched flat-top partition of unity method for the Schrödinger eigenproblem

Clelia Albrecht[a,*], Constanze Klaar[a], John Ernest Pask[b], Marc Alexander Schweitzer[a,c], N. Sukumar[d,*], Albert Ziegenhagel[a]

[a] *Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Schloss Birlinghoven, 53757 Sankt Augustin, Germany*
[b] *Physics Division, Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, CA 94550, USA*
[c] *Institute for Numerical Simulation, Rheinische Friedrich-Wilhelms-Universität, Wegelerstr. 6, 53115, Bonn, Germany*
[d] *Department of Civil and Environmental Engineering, University of California, Davis, CA 95616, USA*

Received 15 February 2018; received in revised form 29 May 2018; accepted 31 July 2018
Available online 6 August 2018

Highlights

- New application of orbital-enriched flat-top partition of unity method: Schrödinger equation.
- Local orthogonalization on each patch is performed to construct a stable basis.
- Variational lumping scheme is used to deliver a standard eigenproblem.
- Established the accuracy, efficiency and stability of the method on benchmark Schrödinger eigenproblems.

Abstract

Quantum mechanical calculations require the repeated solution of a Schrödinger equation for the wavefunctions of the system, from which materials properties follow. Recent work has shown the effectiveness of enriched finite element type Galerkin methods at significantly reducing the degrees of freedom required to obtain accurate solutions. However, time to solution has been adversely affected by the need to solve a generalized rather than standard eigenvalue problem and the ill-conditioning of associated system matrices. In this work, we address both issues by proposing a stable and efficient orbital-enriched partition of unity method to solve the Schrödinger boundary-value problem in a parallelepiped unit cell subject to Bloch-periodic boundary conditions. In the proposed partition of unity method, the three-dimensional domain is covered by overlapping patches, with a compactly-supported weight function associated with each patch. A key ingredient in our approach is the use of non-negative weight functions that possess the *flat-top* property, i.e., each weight function is identically equal to unity over some finite subset of its support. This flat-top property provides a pathway to devise a stable approximation over the whole domain. On each patch, we use pth degree orthogonal (Legendre) polynomials that ensure pth order completeness, and in addition include eigenfunctions of the radial Schrödinger equation. Furthermore, we adopt a variational lumping approach to construct a (block-)diagonal overlap matrix that yields a standard eigenvalue problem for which there exist efficient eigensolvers. The accuracy, stability, and efficiency of the proposed method is demonstrated for the Schrödinger equation with a harmonic potential as well as a localized Gaussian potential. We show that the proposed approach delivers optimal rates of convergence in the energy, and the use of orbital enrichment

* Corresponding authors.
E-mail addresses: clelia.albrecht@scai.fraunhofer.de (C. Albrecht), nsukumar@ucdavis.edu (N. Sukumar).

https://doi.org/10.1016/j.cma.2018.07.042

significantly reduces the number of degrees of freedom for a given desired accuracy in the energy eigenvalues while the stability of the enriched approach is fully maintained.

Keywords: Quantum mechanics; Partition of unity method; Bloch boundary conditions; Variational mass lumping; Enrichment functions; Stability

1. Introduction

The Kohn–Sham (KS) equations of density functional theory (DFT) are the dominant theoretical formulation in quantum mechanical simulations of condensed matter (solids and liquids). The KS equations require the repeated solution of the steady-state Schrödinger and Poisson equations on a parallelepiped unit cell with Bloch-periodic boundary conditions [1]. The solution of the Schrödinger equation is the most time-consuming part in KS-DFT calculations. The current state-of-the-art approach to solve the equations of KS-DFT is the planewave (PW) pseudopotential method that uses a Fourier basis set, and requires the solution of a discrete standard eigenproblem. It has been appreciated in recent years that enriched Galerkin methods [2–13] can be very competitive with PW methods in attaining the desired accuracy with comparable or far fewer degrees of freedom (basis functions). While early formulations [2,6,7,10] employed direct enrichment, more recent approaches have employed discontinuous Galerkin [3,4,11] or partition of unity finite element [2,5,9,13] formulations in order to strictly localize orbital enrichments, thus facilitating flexible approximation and efficient parallel implementation. In [5] it was shown that an enriched partition of unity finite element method (PUFEM) [14,15] requires an order of magnitude fewer basis functions than current state-of-the-art PW based methods to attain the desired 1 mHa/atom accuracy in total energy calculations. However, the ill-conditioning of the resulting system matrices and the need to solve a generalized rather than standard eigenvalue problem were key issues identified as adversely affecting time to solution in practice. In this work, we use a *flat-top* partition of unity method (PUM) [16–18] to address these issues in the approximation of the Schrödinger equation. Our flat-top PUM produces well-conditioned system (Hamiltonian and overlap) matrices and yields a standard eigenvalue problem via variational lumping. The approximation quality of our flat-top PUM is comparable to that reported in [2], but it overcomes the two main shortcomings of the PUFEM that arise in the solution of the Schrödinger eigenproblem. In addition to the electronic Schrödinger equation, the flat-top PUM with Bloch boundary conditions also holds promise in areas such as acoustic scattering [19], elastodynamics [20] and electromagnetics [21], where large-scale eigenproblems are solved and useful *a priori* information is available.

In condensed matter calculations, the Schrödinger equation is solved in a unit cell (parallelepiped domain Ω) subject to Bloch-periodic boundary conditions (see Fig. 1). In the flat-top partition of unity method, the domain Ω is covered by overlapping patches (see Fig. 2) and each patch i is associated with a weight function $\varphi_i(\boldsymbol{x})$ with support ω_i such that $\sum_i \varphi_i(\boldsymbol{x}) = 1$ and $\varphi_i(\boldsymbol{x}) \equiv 1$ on $\omega_i^{\mathrm{FT}} \subset \omega_i$ (see Fig. 3). The local basis set V_i on each patch consists of polynomials and/or non-polynomial (orbital enrichment) functions, and the global approximation is formed by linear combinations of the products of $\varphi_i(\boldsymbol{x})$ and functions from V_i. We perform local orthogonalization to ensure that all functions on a patch are linearly independent and thereby obtain global stability [17], and adopt the variational lumping scheme [18] to realize a standard eigenproblem.

The remainder of the paper is organized as follows. In the next section, we state the strong and weak forms of the Schrödinger eigenproblem. In Section 3, we introduce the partition of unity method, where we present the proposed flat-top PUM in Section 3.1. The key steps in the local orthogonalization procedure to construct a stable global approximation are discussed in Section 3.2, and we describe the variational lumping scheme in Section 3.3. Numerical examples for the Schrödinger equation are presented in Section 4, where we show that the system matrices are well-conditioned and that the use of orbital-enrichment provides a very efficient solution vis-à-vis solely using polynomials over each patch. In addition, we also provide comparisons in the eigenspectrum when using the consistent overlap matrix versus the lumped overlap matrix, and the results reveal that the variational lumping scheme does not adversely affect the accuracy of the energy eigenvalues. We close with a few concluding remarks in Section 5.