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Original articles

Isogeometric analysis in electronic structure calculations

Robert Cimrman[a,*], Matyáš Novák[b], Radek Kolman[c], Miroslav Tůma[d], Jiří Vackář[b]

[a] *New Technologies Research Centre, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic*
[b] *Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 1999/2, Prague, Czech Republic*
[c] *Institute of Thermomechanics, Academy of Sciences of the Czech Republic, Dolejškova 5, 182 00 Prague, Czech Republic*
[d] *Institute of Computer Science, Academy of Sciences of the Czech Republic, Pod Vodárenskou věží 2, 182 07 Prague, Czech Republic*

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Abstract

In electronic structure calculations, various material properties can be obtained by means of computing the total energy of a system as well as derivatives of the total energy w.r.t. atomic positions. The derivatives, also known as Hellman–Feynman forces, require, because of practical computational reasons, the discretized charge density and wave functions having continuous second derivatives in the whole solution domain. We describe an application of isogeometric analysis (IGA), a spline modification of finite element method (FEM), to achieve the required continuity. The novelty of our approach is in employing the technique of Bézier extraction to add the IGA capabilities to our FEM based code for ab initio calculations of electronic states of non-periodic systems within the density-functional framework, built upon the open source finite element package SfePy. We compare FEM and IGA in benchmark problems and several numerical results are presented.

Keywords: Electronic structure calculation; Density functional theory; Finite element method; Isogeometric analysis

1. Introduction

The electronic structure calculations allow to predict and understand material properties such as stable atomic arrangements by minimizing the total internal energy of a system of atoms, as well as to determine derived properties such as elasticity, hardness, electric and magnetic properties, etc.

We are developing a real space code [28] for electronic structure calculations based on

- the density functional theory (DFT), [10,22,18,23];
- the environment-reflecting pseudopotentials [29];
- a weak solution of the Kohn–Sham equations [15].

The code is based on the open source finite element package SfePy (Simple Finite Elements in Python, http://sfepy.org) [4], which is a general package for solving (systems of) partial differential equations (PDEs) by the finite element method (FEM), cf. [11,27].

* Corresponding author.
E-mail address: cimrman3@ntc.zcu.cz (R. Cimrman).

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The key required ability for practical computations is the calculation of the *Hellman–Feynman forces* (HFF), which correspond to the derivatives of the total energy w.r.t. atomic positions. The HFF can efficiently provide gradients in a gradient-based optimizer searching the total energy minimum. A major hurdle to overcome in computing the HFF is the requirement that the discretized charge density and wave functions should have continuous second derivatives in the whole solution domain—implementing a globally C^2 continuous basis in FEM is not easy. Therefore we decided to enhance the SfePy package with another PDE discretization scheme, the *Isogeometric analysis* (IGA), see [6,2].

IGA is a modification of FEM which employs shape functions of different spline types such as B-splines, NURBS (Non-uniform rational B-spline), T-splines [1], etc. It was successfully employed for numerical solutions of various physical and mathematical problems, such as fluid dynamics, diffusion and other problems of continuum mechanics [6].

IGA has been reported to have excellent convergence properties when solving eigenvalue problems connected to free vibrations in elasticity [17], where the errors in frequencies decrease in the whole frequency band with increasing the approximation order, so even for high frequencies the accuracy is very good. It should be noted that dispersion and frequency errors are reported to decrease with increasing spline order [13]. Moreover, IGA solution excellently approximates not only eigenvalues in the full frequency spectrum but also accurately approximates eigen-modes. There are no optical modes as in higher-order FEM, where the errors in higher frequencies grow rapidly with the approximation order and band gaps in the frequency band exist, see [7,16,12]. The Kohn–Sham equations are a highly non-linear eigenvalue problem so the above properties of IGA seem to further support our choice.

The drawbacks of using IGA, as reported also in [17], concern mainly the increased computational cost of the numerical integration and assembling. Also, because of the higher global continuity, the assembled matrices have more non-zero entries than the matrices corresponding to the C^0 FEM basis. A comparison study of IGA and FEM matrix structures, the cost of their evaluation, and mainly the cost of direct and iterative solvers in IGA have been presented by [5,25].

Recently, using FEM and its variants in electronic structure calculation context is pursued by a growing number of groups, cf. [8], where the hp-adaptivity is discussed, [20,21] where spectral finite elements as well as the hp-adaptivity are considered, or [19], where NURBS-based FEM is applied.

In the paper we first outline the physical problem of electronic states calculations in Section 2, then introduce the computational methods and their implementation in terms of both FEM and IGA in Section 3. Finally, we present a comparison of FEM and IGA using a benchmark problem and show some numerical results in Section 4.

2. Calculation of electronic states

The DFT allows decomposing the many-particle Schrödinger equation into the one-electron Kohn–Sham equations. Using atomic units they can be written in the common form

$$\left(-\frac{1}{2}\nabla^2 + V_{\mathrm{H}}(\boldsymbol{r}) + V_{\mathrm{xc}}(\boldsymbol{r}) + \hat{V}(\boldsymbol{r})\right)\psi_i = \varepsilon_i \psi_i, \tag{1}$$

which provide the orbitals ψ_i that reproduce, with the weights of occupations n_i, the charge density ρ of the original interacting system, as

$$\rho(\boldsymbol{r}) = \sum_i^N n_i |\psi_i(\boldsymbol{r})|^2. \tag{2}$$

$\hat{V}$ is a (generally) non-local Hermitian operator representing the effective ionic potential for electrons. In the present case, within pseudopotential approach, $\hat{V}$ represents core electrons, separated from valence electrons, together with the nuclear charge. V_{xc} is the exchange–correlation potential describing the non-coulomb electron–electron interactions. We use local-density approximation (LDA) of this potential [18]. V_{H} is the electrostatic potential obtained as a solution to the Poisson equation. The Poisson equation for V_{H} has the charge density ρ at its right-hand side and is as follows:

$$\Delta V_{\mathrm{H}} = 4\pi\rho. \tag{3}$$

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