The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

KOHN-SHAM DENSITY FUNCTIONAL THEORY CALCULATIONS WITH ISOGEOMETRIC ANALYSIS

Kaan Karaca*, **İlker Temizer**

Department of Mechanical Engineering, Bilkent University, 06800 Ankara, Turkey
{temizer,kaan.karaca}@bilkent.edu.tr

Keywords: *nonlocal pseudopotentials, higher-order finite element methods, isogeometric analysis, generalized eigenvalue problems, Chebyshev-filtered subspace iteration*

Kohn-Sham density functional theory is an *ab initio* framework for electronic structure calculation that offers a basis for nonphenomenological multiscale approaches. In this presentation, higher-order finite element methods [1] are discussed in the non-periodic setting of this theory, with a particular focus on the use of nonlocal pseudopotentials. Specifically, an accurate class of pseudopotentials which are based on the generalized gradient approximation of the exchange-correlation functional with nonlinear core corrections are targeted. To this end, the suitable weak formulation of the underlying nonlinear eigenvalue problem is derived and additionally cast in a radial form. The weak forms are discretized through traditional Lagrange elements in addition to isogeometric analysis based on B-splines [2] in order to explore alternative means of achieving faster routes to the solution of the resulting generalized eigenvalue problems with $\mathcal{O}(10^6\text{-}10^7)$ degrees of freedom via the Chebyshev-filtered subspace iteration method. Numerical investigations in the radial case demonstrate all-electron and local pseudopotential capabilities on single atoms. In the three-dimensional case, all-electron and nonlocal pseudopotential computations on single atoms and small molecules are followed by local and nonlocal pseudopotential studies on larger systems. At all stages, special care is taken to demonstrate optimal convergence rates towards the ground state energy with chemical accuracy. Comparisons with classical Lagrange basis sets indicate that cubic NURBS discretizations can offer a faster route to a prescribed accuracy than even sixth-order Lagrange discretizations on comparable meshes. Finally, the framework is further extended towards geometry optimization and features associated with his extension such as the variational consistency as well as the translational invariance of the forces are discussed.

REFERENCES

[1] N. Rufus and B. Kanungo and V. Gavini, Fast and robust all-electron density functional theory calculations in solids using orthogonalized enriched finite elements. *Physical Review B*, Vol. **104**, 085112, 2021.

[2] İ. Temizer, Radial and three-dimensional nonlocal pseudopotential calculations in gradient-corrected KohnSham density functional theory based on higher-order finite element methods. *Comput. Methods Appl. Mech. Engrg.*, Vol. **386**, 114094, 2021.