Convergence study of isogeometric analysis in electronic structure calculations

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

[a] New Technologies Research Centre, University of West Bohemia,
Univerzitní 8, Pilsen 306 14, Czech Republic
e-mail: {cimrman; logic}@ntc.zcu.cz

[b] Institute of Physics, The Czech Academy of Sciences,
Na Slovance 1999/2, Prague, Czech Republic
Email: {novakmat;vackar}@fzu.cz

[c] Institute of Thermomechanics, The Czech Academy of Sciences,
Dolejškova 5, Prague 182 00, Czech Republic
Email: {kolman;plesek}@it.cas.cz

[d] Institute of Computer Science, The Czech Academy of Sciences,
Pod Vodárenskou věží 2, 182 07 Prague, Czech Republic
Email: tuma@cs.cas.cz

ABSTRACT

We present a study of convergence and accuracy properties of isogeometric analysis applied for electronic structure calculations [1]. A new method [2] for non-periodic electronic structures based on the density functional theory, environment-reflecting pseudopotentials and the isogeometric analysis with Bézier extraction has been developed and tested. The approach is especially suitable for calculating the total energy and its second derivatives and mainly for evaluation of atomic forces based on the Hellmann-Feynman theorem.

Within the contribution, convergence study for isogeometric analysis vs. standard finite-element approach is carried out and illustrated on sub-problems that appear in our electronic structure calculations method: the Poisson problem, the generalized eigenvalue problem and the Kohn –Sham self-consistent solution problem within density functional theory. The effect of order and continuity of spline shape function is analyzed [3]. It seems that the isogeometric analysis is an excellent tool for accurate calculations of electronic structure behavior.

ACKNOWLEDGMENTS

The work was supported by the Czech Science Foundation, grant projects GA17-12925S. The second author acknowledges the support by CEDAMNF project, reg. no. CZ.02.1.01/0.0/0.0/15_0 03/0000358, co-funded by the ERDF as part of the Ministry of Education, Youth and Sports OP RDE programme. The work of R. Kolman and J. Plešek was supported by the European Regional Development Fund under Grant No. CZ.02.1.01/0.0/0.0/15_003/0000493 (Centre of Excellence for Nonlinear Dynamic Behaviour of Advanced Materials in Engineering), within institutional support RVO: 61388998.

REFERENCES

[1] R.M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, (2005).

[2] R. Cimrman, M. Novák, R. Kolman, M. Tůma and J. Vackář, Isogeometric analysis in electronic structure calculations, *Math. Comput. Simul*., in press, doi: 10. 340 1016/j.matcom.2016.05.011 (2017).

[3] R. Cimrman, M. Novák, R. Kolman, M. Tůma, J. Plešek and J. Vackář, Convergence study of isogeometric analysis based on Bézier extraction in electronic structure calculations, *Applied Mathematics and Computation*, in press, http://dx.doi.org/10.1016/j.amc.2017.02.023, (2017).