

# Comparison of Lagrangian and B-Spline Finite Element Basis in Electronic Structure Calculations

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## Abstract

Isogeometric analysis (IGA) is a spline modification of finite element method (FEM). The spline basis of IGA (B-splines, NURBS, etc.) allows to describe accurately the shape of a computational domain, and provides high degree of global continuity on domains consisting of a single NURBS patch. We compare convergence of IGA and FEM in the context of ab-initio electronic structure calculations. The technique of Bézier extraction was used to add the IGA capabilities to our FEM based real space code for calculations of electronic states of non-periodic systems within the density-functional framework, built upon the open source finite element package SfePy. The computations of the resulting highly non-linear generalized eigenvalue problem involve fixed point solver iterations with generalized eigenvalue problems solved each iteration. Numerical results for several quantum mechanical systems will be presented.

## References

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