A Posteriori Analysis for Nonlinear Eigenvalue Problems, Application to Electronic Structure Calculations

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ABSTRACT

Many mathematical models aiming at the determination of electronic structures give rise to nonlinear eigenvalue problems whose resolutions require very large computational resources [1]. The complexity of these computations reflects, among others, the chosen discretization and the chosen (possibly iterative) algorithm. The *a posteriori* analysis of such problems enables to reduce the computations involved to solve the problem by first giving a guaranteed upper bound on the total error and second by separating the error components stemming from the different sources and controlling each of them. This makes possible to iteratively fit these discretization parameters leading to small error at low computational cost [3].

We shall first present a full *a posteriori* analysis for a simple but representative one-dimensional Gross-Pitaevskii type equation, in a periodic setting with planewave (Fourier) approximation. The nonlinear discretized problem is solved with a Self-Consistent Field (SCF) algorithm, which consists in solving a linear eigenvalue problem at each step. To start with, we provide a computable upper bound of the energy error. We then separate this bound into two components, one of them depending mainly on the dimension of the discretized space, the other one on the number of iterations done in the SCF algorithm. This enables to adaptively choose between refining the discretization and performing SCF iterations, as we try to balance the error components. We also illustrate numerically the coherent performances of this *a posteriori* analysis. We then postprocess the approximate solution (eigenvalue and eigenfunction) using a linear perturbation theory based on residual computation [2]. This theoretically and numerically reduces the error significantly both for the eigenvalue and the eigenfunction.

This work is a first step towards an *a posteriori* analysis and postprocess of more complex electronic structure models like Hartree-Fock or Kohn-Sham models. We shall present the first results for the extension of our results in this framework.

REFERENCES

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