Using a Hybrid Mixing in Fixed-Point Self-Consistent Iterations to Accelerate Electronic Structure Calculations

Matyáš Novák
Department of Mechanics, Faculty of Applied Sciences, University of West Bohemia &
Institute of Physics, The Czech Academy of Sciences
novakmat@fzu.cz

Robert Cimrman
New Technologies - Research Centre, University of West Bohemia
cimrman3@ntc.zcu.cz

Radek Kolman, Jiří Plešek
Institute of Thermomechanics, The Czech Academy of Sciences
kolman@it.cas.cz, plesek@it.cas.cz

Jiří Vackář
Institute of Physics, The Czech Academy of Sciences
vackar@fzu.cz

Abstract

In ab-initio calculations of electronic states within the density-functional theory (DFT) framework, a self-consistent state is sought by a fixed-point iteration, the so called DFT loop. One of the key components needed for fast convergence is to apply a suitable mixing of new and previous states in the DFT loop. In this contribution we discuss the standard Broyden [1] and Pulay [2] mixing algorithms as well as a newly proposed adaptable hybrid scheme that combines those two approaches in a way that accelerates the convergence. The scheme is used within our computer implementation of a new robust ab-initio real-space code based on (i) density functional theory [3], (ii) finite element method and (iii) environment-reflecting pseudopotentials [4] — this approach to solving Kohn-Sham equations and calculating electronic states, total energy, Hellmann-Feynman forces and material properties brings a new quality particularly for non-crystalline, non-periodic structures [5].

References

1. C. G. Broyden. A class of methods for solving nonlinear simultaneous equations. Math. Comp. 19 (1965), 577-593 .
2. P. Pulay. Improved SCF convergence acceleration. J. Comput. Chem., 3: 556–560 (1982). doi:10.1002/jcc.540030413.
3. R. M. Dreizler and E. K. U. Gross. Density Functional Theory. Springer-Verlag, 1990.
4. J. Vackář and A. Šimůnek. Adaptability and accuracy of all-electron pseudopotentials. Phys. Rev. B 67 (2003) 125113.
5. J. Vackář and O. Čertík and R. Cimrman and M. Novák and O. Šipr and J. Plešek. Finite Element Method in Density Functional Theory Electronic Structure Calculations. In "Advances in the Theory of Quantum Systems in Chemistry and Physics", Prog. Theoretical Chem. and Phys. (22), Springer, 2011.