New implementations of the orbital minimization method in the SIESTA code

Fabiano Corsetti[a], Emilio Artacho[a,b]

[a] CIC nanoGUNE Consolider, E-20018 Donostia-San Sebastián, Spain
[b] Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, United Kingdom
f.corsetti@nanogune.eu

Abstract

The orbital minimization method (OMM) is the general name given to a class of iterative minimization algorithms devised for solving the generalized eigenvalue problem in the context of linear-scaling DFT [1]. The central idea of the method is to find the Wannier functions of the electronic system that describe the occupied subspace by direct unconstrained minimization of an appropriately constructed functional [2,3]. The method is made to scale linearly with system size by imposing a localization radius on the Wannier functions, which in turn determines the truncation range of the density matrix.

Unfortunately, the OMM suffers from a serious problem of multiple local minima, requiring in practice that the initial guess reflect the correct bonding properties of the system. Alternatively, Kim *et al.* [4] have proposed to work with more orbitals than those needed to span the occupied subspace, leading to a linearly dependent basis. This eliminates the local minima problem, but introduces the electronic chemical potential as an unknown parameter.

We report on several new implementations of the OMM in the SIESTA [5] DFT code, that aim to exploit the efficiency and stability of the method while circumventing the limitations described above.

Firstly, we show the potential of the original OMM method as a conventional DFT solver (without the linear-scaling approximation), as the local minima are no longer present when the Wannier functions are allowed to extend over the whole system. The algorithm is therefore both accurate and efficient, due to the fact that no explicit orthogonalization operation is required between orbitals, and that the solution from each minimization can be reused iteratively for multiple self-consistent field steps and *ab initio* MD steps. We also show that the sparsity pattern of the Hamiltonian matrix in SIESTA can be used in this context to significantly reduce the computational cost; in conclusion, the method has proven to be competitive with explicit diagonalization even in small systems despite the large ratio of occupied states to total basis size that is used in SIESTA and other atomic orbital codes.

Secondly, we discuss a number of approaches for imposing the correct electron number in the augmented OMM of Kim *et al.* that can be used with Wannier localization for linear-scaling DFT calculations; we report on an automated adjustment of the chemical potential to preserve electron number, a projected gradient method and a normalization transformation of the Wannier function coefficients. We discuss the connection between our approaches and those used in density matrix methods; in particular, the OMM presents further challenges in this respect due to the fact that we do not have direct access to the density matrix in the Wannier basis. Finally, we present initial results for a modified OMM functional that allows for smeared Fermi level calculations (pseudo finite temperature), opening up the possibility of performing linear-scaling DFT for metallic systems in SIESTA.

References

[1] D. R. Bowler and T. Miyazaki, Rep. Prog. Phys., **75** (2012) 036503.
[2] P. Ordejón, D. A. Drabold, R. M. Martin, and M. P. Grumbach, Phys. Rev. B, **51** (1995) 1456.
[3] F. Mauri, G. Galli, and R. Car, Phys. Rev. B, **47** (1993) 9973.
[4] J. Kim, F. Mauri, and G. Galli, Phys. Rev. B, **52** (1995) 1640.
[5] J. M. Soler *et al.*, J. Phys.: Condens. Matter, **14** (2002) 2745.