Multilevel domain decomposition for electronic structure calculations

M. Barrault[1], G. Bencteux[1], E. Cancès[2], W. W. Hager [3] and C. Le Bris[2]

[1] EDF R&D, 1 avenue du Général de Gaulle, 92141 Clamart Cedex, France

{maxime.barrault,guy.bencteux}@edf.fr

[2] CERMICS, École Nationale des Ponts et Chaussées,

6 & 8, avenue Blaise Pascal, Cité Descartes,

77455 Marne-La-Vallée Cedex 2, France {cances,lebris}@cermics.enpc.fr

[3] Department of Mathematics, University of Florida,

Gainesville FL 32611-8105, USA, hager@math.ufl.edu

June 12, 2006

We introduce a new multilevel domain decomposition method (MDD) for electronic structure calculations within semi-empirical and Density Functional Theory (DFT) frameworks. This method iterates between local fine solvers and global coarse solvers, in the spirit of domain decomposition methods. Using this approach, calculations have been successfully performed on several linear polymer chains containing up to 40,000 atoms and 200,000 atomic orbitals. Both the computational cost and the memory requirement scale linearly with the number of atoms. Additional speed-up can easily be obtained by parallelization. We show that this domain decomposition method outperforms the Density Matrix Minimization (DMM) method for poor initial guesses. Our method provides an efficient preconditioner for DMM and other linear scaling methods, variational in nature, such as the Orbital Minimization (OM) procedure. In order to deal with more realistic systems such as thin films or bulk crystals (two or three-dimensional), the extension of the method and its effective parallelization are subject to ongoing works.

References

[1] M. Barrault, E. Cancès, W. W. Hager and C. Le Bris (2005), *Multilevel domain decomposition for electronic structure calculations*, Journal of Computational Physics, accepted in Journal of Computational Physics.

[2] E. Cancès, M. Defranceschi, W. Kutzelnigg, C. Le Bris, and Y. Maday, *Computational Quantum Chemistry: a Primer*, in: Handbook of Numerical Analysis, Special volume, Computational Chemistry, volume X, North-Holland 2003.

[3] S. Goedecker, *Linear scaling electronic structure methods*, Rev. Mod. Phys. 71 (1999) 1085-1123.

[4] C. Le Bris, Computational chemistry from the perspective of numerical analysis, Acta Numerica,volume 14, 2005, pp 363-444.

[5] Y. Saad, *Numerical methods for large eigenvalue problem : theory and algorithms*, Manchester University Press 1992.