Parallelization of DFT calculations within the real space grid approach

Maciej Marchwiany and Jacek A. Majewski

Faculty of Physics, University of Warsaw, ul. Hoża 69, 00-681 Warszawa, Poland

Modern computer architectures allow for realization of computational tasks in parallel and open new possibilities in computational materials science. However, the full facilitation of this technological advantage requires the special construction of the computer codes. It is well know that the parallelization process is very difficult in the case of quantum-mechanical approaches based either on the Hartree-Fock or Kohn-Sham realizations of the density functional theory (DFT) methods. The crucial role in the effectiveness of the parallelization plays the type of basis functions used for expansion of Kohn-Sham orbitals. It is commonly believed that direct solution of the Kohn-Sham equations on the numerical grid in real space is the most promising for highly effective parallelization of DFT based numerical packages.

In this communication, we share our experience concerning the effective use of multi-core computers for DFT type of calculations. Our studies of the parallelization algorithms are based on the newly developed method for the solution of the Kohn-Sham equations directly on a grid in the r-space. This method, in contrast to the majority of available commercial and under GNU license available computer codes, allows the employment of the periodic boundary conditions only along physically periodic directions, i.e., without the necessity of placing partly periodic systems into an artificial three-dimensional supercell. Our parallelization approach is based on MPI library (Message Passing Interface) and distributed memory model. It can be successfully use on each super computer and reaches also good performance on the biggest computer clusters. We show the basic idea of solver parallelization, memory and computing tasks distribution. Scalability of the whole application and the most time consuming functions will be also presented. We present results of numerous tests for real molecular and crystal systems.

As it turns out, the biggest advantage of the developed method is that it gives good scalability for thousands of computer nodes without lost of accuracy. Therefore, parallelization of the computer DFT codes can speedup computations many times and, what is equally important, can allow for studies of systems containing several thousand of atoms on the DFT level.