O.7 Abinit performances for systems with many atoms : some analyses and perspectives

Lucas Baguet[1] and Marc Torrent[1]

[1] *CEA, DAM, DIF, F-91297 Arpajon, France, and Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France.*

In the context of a DFT plane-wave basis code, to efficiently compute the ground-state properties of systems with dozens or even hundreds of atoms is a challenging task. Because of the complexity of the underlying mathematical problem, there are many ways to minimise the total energy. Furthermore, parallelisation schemes are not trivial as a lot of data has to be frequently communicated between processes. Even details about the implementation can have an huge impact on the performances, without changing any digit of the final result. At last, compilation options should also be considered carefully.

In a first part we will present the performances obtained in various conditions. In particular we will show that, with a fixed number of cores, transferring MPI processes to openMP threads significantly improves the performances.

At last we will propose an alternative implementation of the conjugate-gradient algorithm which use less non-local operations. As non-local operations are the most expensive terms to compute in big systems, it is a serious option to consider for improving the efficiency of other algorithms implemented in Abinit.