

New implementation of Chebishev filtering inside ABINIT

B.Sataric¹, Bieder², M. Torrent³ and W.Jalby¹

¹ University of Versailles UVSQ, France

² University of Liege, Belgium

³ CEA, DAM, DIF, Arpajon, France

We consider the problem of improving the parallelization of electronic structure computations in plane-wave Density Functional Theory. In such computations, parallelism has to be found at two levels: the iterative eigensolver and the application of the Hamiltonian operator.

We show how the algorithm based on Chebyshev polynomials, implemented in ABINIT in 2015 [1], can be improved according to recent improvements made inside the LOPBCG solver [2].

Improvements include rewriting existing Chebishev filtering module using newly formed ABINIT abstract layer (Xg datatypes and functions). Xg module hides and improves OpenMP and MPI parallelization within linear and matrix algebra as well as memory management of wave functions arrays.

References

[1] A. Levitt, M. Torrent, *Comp. Phys. Communications* **187**, 98-105 (2014).

[2] F. Bottin, S. Leroux, A. Knyazev, G Zérah, *Comp. Mat. Sc.* **42**, 329-336 (2008).