BigDFT: Large-Scale ab initio methods based on wavelets

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Daubechies wavelets are a powerful systematic basis set for electronic structure calculations because they are orthogonal and localized both in real and Fourier space. We describe in detail how this basis set can be used to obtain a highly efficient and accurate method for density functional electronic structure calculations. This code, BigDFT, shows high systematic convergence properties, very good performances, and an excellent efficiency for parallel calculations alos in hybrid architectures based on CPU and graphical processing units.

References

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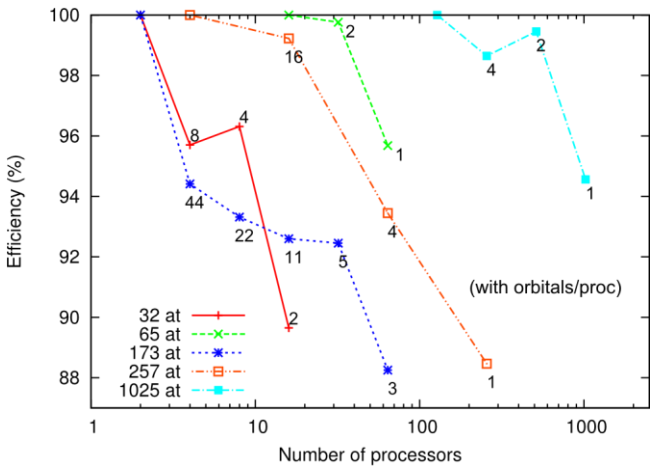

Efficiency of BigDFT versus the number of cores. The number near the points are the distribution of orbitals per core.