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Large scale parallel ab initio electronic structure calculations with the LOBPCG method.

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We present an implementation in the *ab initio* plane-wave code ABINIT, of a parallelization scheme based on the locally optimal block preconditioned conjugate gradient LOBPCG method, and using an optimized three-dimensional (3D) fast Fourier transform (FFT).

We will first compare, for various systems, the performance of the method with the more standard eigensolvers currently used in ABINIT.

Next, we present the parallelization scheme, which, in addition to the standard data partitioning over processors corresponding to different k-points, relies upon data partitioning with respect to blocks of bands and Fourier coefficients.

Finally we analyze the performances of the whole scheme on multiprocessor machines in terms of scalability and convergence speed.

Reference:

F. Bottin, S. Leroux, A. Knyazev, G. Zerah, Large scale ab initio calculations based on three levels of parallelization. (2007). Computational Material Science. http://dx.doi.org/10.1016/j.commatsci.2007.07.019