

Parallel research of numerous eigenvalues in ABINIT

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In ABINIT, the research of N orthonormal wave functions for the Kohn-Sham model is associated with an algorithm which owes a $O(N^3)$ complexity. We propose a new parallel algorithm, based on a spectral partitionning of an energy band which is to be determined. We calculate independently clusters of eigenvalues with local orthogonalizations. We give a partitionning criterium of the energy band adapted to the kind of eigenvalue algorithm used. In collaboration with the CEA, this method should lead to an algorithm of complexity $O(N^2)$ in the ABINIT project.