Sakurai-Sugiura algorithm based eigenvalue solver for Siesta

Georg Huhs

Barcelona Supercomputing Center, c/ Gran Capita 2-4, 08034 Barcelona, Spain.
georg.huhs@bsc.es

In ab initio calculations based on density functional theory very often the most time consuming step is the solution of the generalized eigenvalue problem appearing in the self consistent loop. This applies also for Siesta, a DFT code currently using ScaLAPACK for this purpose.

This standard-package has two disadvantages. First, due to the atomic orbital basis set of Siesta, the matrices to deal with are sparse, whereas ScaLAPACK is meant for dense systems. Second, Siesta is meant for using thousands of processors for thousands of atoms, thus an even better scaling method is needed.

The Sakurai-Sugiura algorithm has the capability of solving this issue. This talk shows how:

- this method shifts the problem to solving linear systems, which is much easier to deal with

- it offers three levels of parallelization, giving the possibility of using many processing units efficiently

- also the fact of being applied inside of an iterative loop can be used to accelerate the computation

The Barcelona Supercomputing Center is currently working on implementations for both, CPU and GPU systems, so the most recent performance results for several configurations can be shown.

References

[1] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón and D. Sánchez-Portal, J. Phys.: Condens. Matter 14, **The Siesta method for ab initio order-N materials simulation** (2002) 2745-2779.

[2] E. Artacho, E. Anglada, O. Dieguez, J. D. Gale, A. García, J. Junquera, R. M. Martin, P. Ordejón, J. M. Pruneda, D. Sánchez-Portal and J. M. Soler, J. Phys.: Condens. Matter 20, **The Siesta method; developments and applicability** (2008)

[3] T. Sakurai, H. Sugiura, Technical Report ISE-TR-02-189 University of Tsukuba, **A projection method for generalized eigenvalue problems** (2002)

[4] I. Ikegami, T. Sakurai, U. Nagashima, Technical Report S-TR-08-13 University of Tsukuba, **A filter diagonalization for generalized eigenvalue problems based on the Sakurai-Sugiura projection method** (2008)