Towards nanoscale DFT calculations with SIESTA and PEXSI

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Abstract
In computational nanoscience the desire to treat large structures as accurately as possible conflicts with the huge computational effort first principles electronic structure computations demand. This effort grows with the system size N like $O(N^3)$.
The availability of more and more powerful supercomputers allows in principle studies of systems with hundreds or thousands of atoms, but the developments in high performance computing can not overcome the $O(N^3)$ scaling. Moreover, the parallel algorithms currently applied can use only a number of processors far below the capabilities top supercomputers provide.

Thus it is clear that new algorithms are needed. One representative of a new class of algorithms is PEXSI, which stands for “Pole EXpansion and Selected Inversion”. Its main advantages are the ability to use thousands of cores efficiently and, notably, the reduction of the computational cost for calculating the density matrix to

- $O(N^2)$ for 3D systems
- $O(N^{3/2})$ for (quasi-) 2D systems
- $O(N)$ for (quasi-) 1D systems

The method does not imply any additional simplifications or assumptions, thus it is general and exact. The reduction of order is based on having a sparse density matrix, so only a suitable DFT implementation can take advantage of this feature.
SIESTA is a DFT code using strictly localized basis sets, implying that it works with sparse matrices. This is particularly efficient for systems with a lot of vacuum, like nanotubes and two-dimensional problems.

In this talk we show how using PEXSI in SIESTA enhances the performance for large systems and even allows dealing with 2D systems, like stacked layers of graphene and BN, in the 10nm scale. We also demonstrate that PEXSI can use a much larger number of processors than Scalapack efficiently. As a result this method pushes the size of the systems that can be solved in reasonable time to the range of tens of thousands of atoms.

References
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[2] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matter, 14 (2002), 2745–2779

Figures

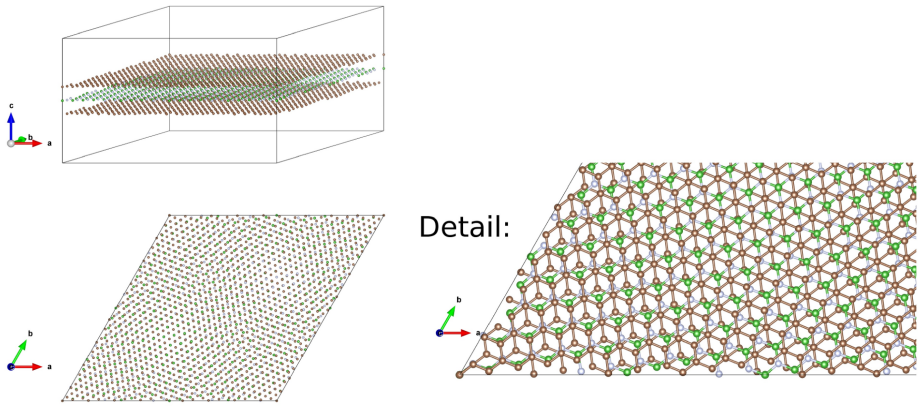

Figure 1: An example for quasi 2D systems under consideration: a layer of BN sandwiched between two graphene sheets. The Moire patterns emerging from the differing atomic distances need large unit cells. This example, consisting of about 2500 atoms, is still rather small compared to those SIESTA + PEXSI can deal with.