Séminaire de Chimie Théorique

Salle conference 3eme Est, Bat. A12
Jeudi 02 Février 2012 à 16:00

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Linear scaling density functional theory for hundred thousands of atoms: An overview of CONQUEST and first steps towards exact exchange

Development of suite of programs (GPL or commercial) including computational material and molecular software demonstrate the increasing interest for advanced modelling solutions, such as research and development in pharma, biotech, chemicals or nanotechnologies. These emerging solutions are sustained by the development of high-performance computer market. The increasing availability of massively parallel processing systems combined to the hierarchy of computational methods enable researchers to perform routine simulations from the atomic to the mesoscale (~100 nanometers). Naturally, depending of the research interests and the size of the system, the level of theory is chosen accordingly. At present, the use of modeling for large size (~500,000 atoms) aperiodic systems, such as liquids, soft mater or glasses, encompasses molecular mechanics (MM) simulations based on force fields, as well as the use of quantum mechanical (QM) approaches typically embedded in QM/MM calculations, where the QM kernel is generally described on the basis of the density functional theory (DFT).
DFT has become the most widely used electronic structure theory, mainly because of the balance between computational cost and accuracy which can be achieved. The many-body Schrödinger equation is rewritten as a set of independent electron equations moving in an effective potential, which in principle includes all the many-body effects. The standard implementations of DFT, however, scale badly with the size of system being modelled: the computational effort increases with the cube of the number of atoms modelled, while the memory required increases with its square. This scaling effectively limits the size of systems which can be addressed to a few hundred atoms or, using high performance computing (HPC) resources, a thousand or so.

The cubic scaling seen for standard DFT codes is not required by the physics of the problem: indeed, chemistry suggests that electronic structure is localised within some region, which implies that it ought to be possible to solve the electronic structure problem in a way that scales linearly with system size, i.e. with the computer effort for each atom only depending on the number of atoms in its local neighbourhood. This is the idea which underlies linear scaling or O(N) DFT methods.[1] It has recently been shown that, given high performance computing (HPC) facilities and many thousands of computational cores, systems of over a million atoms can be modelled with DFT[2].
In talk we will give an overview of the linear scaling *machinery* as implemented in the HPC DFT code CONQUEST[3] along with some examples. Current developments dedicated to exact (Fock) exchange will be presented.[4]

[1] D. R. Bowler and T. Miyazaki, arXiv:1108.5976v5 [cond-mat.mtrl-sci]
[2] D. R. Bowler and T. Miyazaki, J. Phys.: Condens. Matter 22: 074207 (2010)
[3] http://www.order-n.org/ and D. R. Bowler, T. Miyazaki and M. J. Gillan, J. Phys.: Condens. Matter 14: 2781 (2004)
[4] D.R. Bowler and L. A. Truflandier, arXiv:1112.5989v1 [physics.chem-ph]

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