MAX DRIVING THE EXASCALE TRANSITION

BigDFT

Description

Starting in 2005, the BigDFT EU project aimed to test the advantages of Daubechies wavelets as a basis set for DFT using pseudopotentials. This led to the creation of the BigDFT code, which has optimal features of flexibility, performance and precision. In addition to the traditional cubic-scaling DFT approach, the wavelet-based approach has enabled the implementation of an algorithm for DFT calculations of large systems containing many thousands of atoms, with a computational effort which scales linearly with the number of atoms. This feature enables electronic structure calculations of systems which were impractical to simulate even very recently.

Level of theory

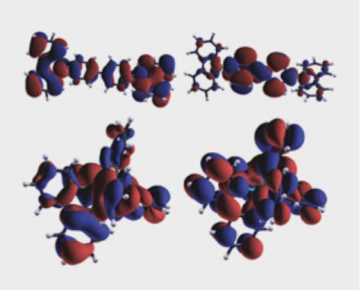
BigDFT has rapidly become a mature and reliable package suite with a wide variety of features, ranging from ground-state quantities up to potential energy surface exploration techniques. BigDFT uses dual space Gaussian type norm-conserving pseudpotentials including those with non-linear core corrections, which have proven to deliver all-electron precision on various ground state quantities. Its flexible poisson solver can handle a number of different boundary conditions including free, wire, surface, and periodic. It is also possible to simulate implicit solvents as well as external electric fields. Such technology is employed for the computations of hybrid functionals and time-dependent (TD) DFT.

Features

The unique features of BigDFT are well-suited for chemical applications such as

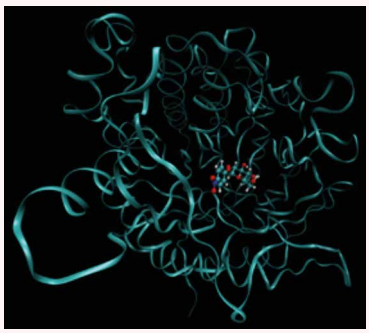
- Adsorption on surfaces and adhesion: corrosion inhibition, surface impregnation of dyes, wettability, rubber adhesion, adsorption of catalyzers.
- Heterogeneous catalysis: catalytic reaction, conformation of van-der-Waals complexes.
- Nanoclusters, oligomers, organic crystals, hypothetical MOFs, zeolite cages.
- OLEDs: electronic properties.
- Defects/Dopants in semiconductors, inorganic crystals or metals.

Case studies



Enzymes

Enzymes are proteins that promote chemical reactions, i.e., they act as biological catalysts and act upon substrates, which are the molecules that undergo the desired chemical reaction in the presence of the enzyme. An important property is the selectivity, i.e., the ability to act only on a specific substrate. BigDFT has been used to perform a full Quantum Mechanical calculation of a complex enzyme-substrate system and to identify those fragments of the enzyme that most interact with the substrate.
[Dawson et al., J. Chem. Theory Comput (2020)]



OLEDs

BigDFT has been used to study a supramolecular structure that can be employed as organic light-emitting diode (OLED). The material was composed of a host transport matrix doped with optically active centres (guests), and the charge transport parameters were calculated on the basis of a CDFT method implemented in the linear-scaling approach of BigDFT.
[Ratcliff et al., J. Chem. Theory Comput. (2015)]

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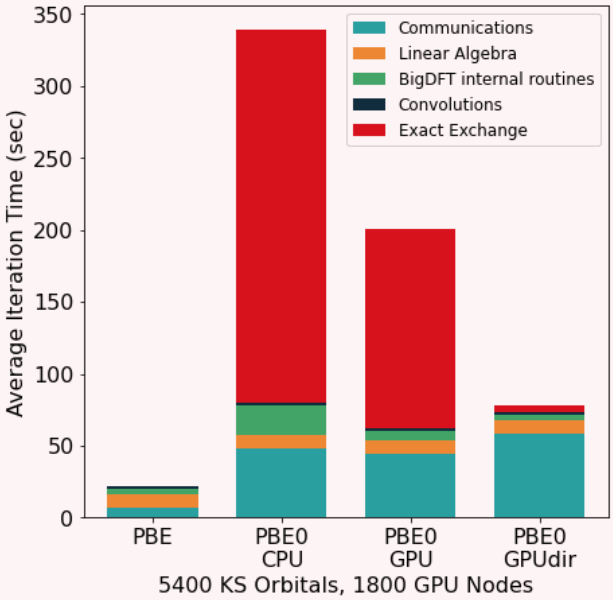
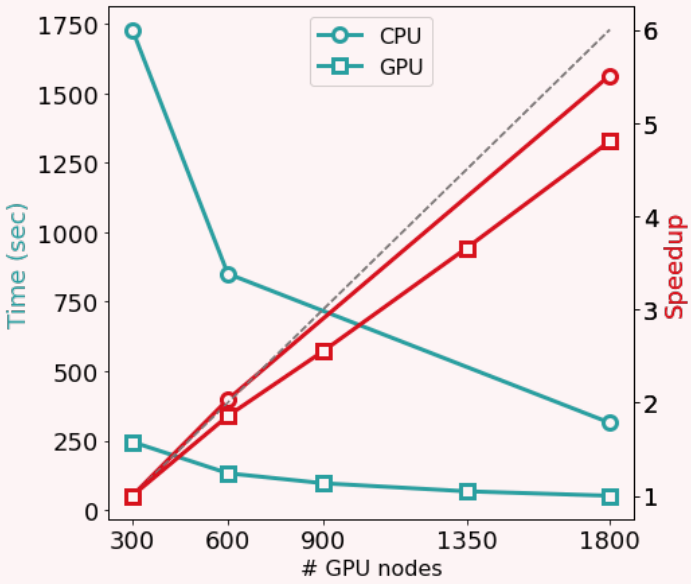
Parallelization and HPC performance

BigDFT is a award-winner DFT code, recipient of the first edition (2009) of the Bull-Fourier prize for its "ground-breaking usage of wavelets and the adaptation to hybrid architectures, combining traditional processors and graphic accelerators, leading the path for new major advancements in the domain of new materials and molecules". It is parallelized using a combination of MPI and OpenMP and has supported GPU acceleration since the early days of GPGPU computing. Such supports involve both CUDA and OpenCL computing kernels, and can be routinely applied to large systems. For example, the calculation of a 12,000 atom protein system requires about 1.2 hours of wall-time on 16 nodes of the Irene-ROME supercomputer. This calculation can be further accelerated for systems composed of repeated sub-units using a fragment approach for molecules, or in the case of extended systems, a pseudo-fragment approach.





Support

Website

References

- *S. Mohr, et al., Accurate and efficient linear scaling DFT calculations with universal applicability, Phys. Chem. Chem. Phys.* ***17****, 31360-31370 (2015).*
- *L. E. Ratcliff et al., Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations, J. Chem. Phys.* ***152****, 194110 (2020).*