BigDFT adventure

5th International ABINIT Developer Workshop

DOMAINE DES MASURES – HAN-SUR-LESSE, BELGIUM

The BigDFT project: Results, Advancements and Potentialities

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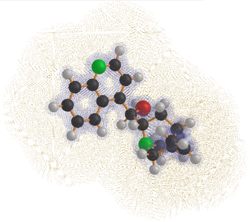
A basis for nanosciences: the BigDFT project

STREP European project: BigDFT(2005-2008)

Four partners, 15 contributors:
CEA-INAC Grenoble (T.Deutsch), U. Basel (S.Goedecker), U. Louvain-la-Neuve (X.Gonze), U. Kiel (R.Schneider)

Aim: To develop an ab-initio DFT code based on Daubechies Wavelets, to be *integrated in ABINIT*.
BigDFT 1.0 $\longrightarrow$ January 2008



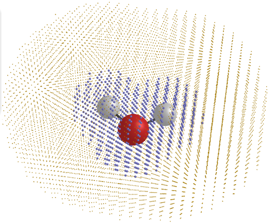
. . . why have we done this? Was it worth it?

- Test the potential advantages of a new formalism
- A lot of outcomes and interesting results
- What can (will) we do starting from present know-how

A DFT code based on Daubechies wavelets

BigDFT: a PSP Kohn-Sham code

A Daubechies wavelets basis has unique properties for DFT usage



- Systematic, Orthogonal
- Localised, Adaptive
- Kohn-Sham operators are analytic

Short, Separable convolutions

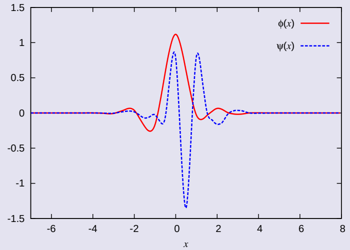
$$\tilde{c}_\ell = \sum_j a_j \, c_{\ell - j}$$

- Peculiar numerical properties

Real space based, highly flexible

Big & inhomogeneous systems

Daubechies Wavelets



A new phase for the BigDFT code

Half of 2009: End of first development phase

Since then ($\sim$ 18 months):

- 8(+4) papers in different fields
  (Phys. Rev. B, J. Chem. Phys., PCCP)
- 1 Patent, 3 Book chapters, Grand Prix Bull-Fourier 2009

BigDFT has become not only a DFT adventure

The code is an ideal case study for a number scientific and computational questions. Two categories:

- Validation of present-day theoretical approaches in complex situations
- Study of optimisation strategies of High Performance Computing in modern machines

Basis set features

BigDFT features in a nutshell

- ✔ Arbitrary absolute precision can be achieved
  Good convergence ratio for real-space approach ($\mathcal{O}(h^{14})$)
- ✔ Optimal usage of the degrees of freedom (adaptivity)
  Optimal speed for a systematic approach (less memory)
- ✔ Hartree potential accurate for various boundary conditions
  Free and Surfaces BC Poisson Solver
  (present also in CP2K, ABINIT, OCTOPUS)
- ☛ Data repartition is suitable for optimal scalability
  Simple communications paradigm, multi-level parallelisation possible (and implemented)

Improve and develop know-how

Optimal for *advanced* DFT functionalities in HPC framework

Exploration of configuration space

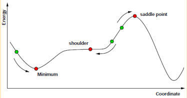
Benefit from high precision

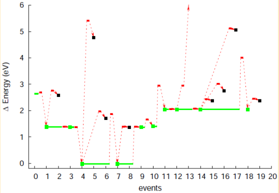
Different methods linked with BigDFT:

- Minima Hopping (S. Goedecker)
- Activation-Relaxation Technique (N. Mousseau)

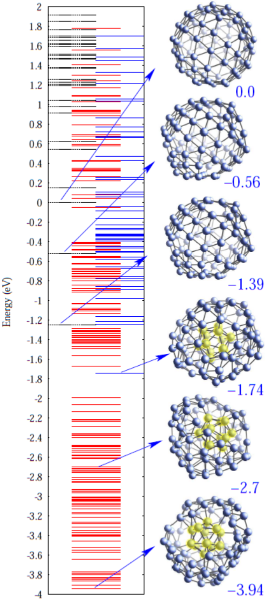
Applied on different systems

Benefit from high flexibility and performances





Interesting for potential synthesis pathways



BigDFT version 1.5.2: (ABINIT-related) capabilities

http://inac.cea.fr/L_Sim/BigDFT

- Isolated, surfaces and 3D-periodic boundary conditions (k-points, symmetries)
- All XC functionals of the ABINIT package (libXC library)
- Hybrid functionals, Fock exchange operator
- Direct Minimisation and Mixing routines (metals)
- Local geometry optimizations (with constraints)
- External electric fields (surfaces BC)
- Born-Oppenheimer MD, ESTF-IO
- Vibrations
- Unoccupied states
- Empirical van der Waals interactions
- Saddle point searches (NEB, Granot & Bear)
- All these functionalities are GPU-compatible

Operations performed

The SCF cycle

Orbital scheme:

- Hamiltonian
- Preconditioner

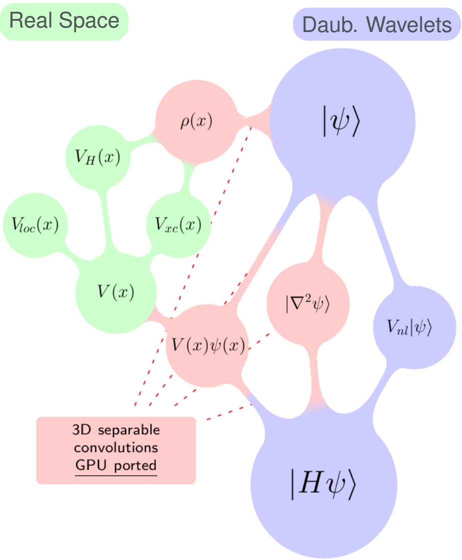
Coefficient Scheme:

- Overlap matrices
- Orthogonalisation

Comput. operations

- Convolutions
- BLAS routines
- FFT (Poisson Solver)

Why not GPUs?



Hybrid Supercomputing nowadays

GPGPU on Supercomputers

- Traditional architectures are somehow saturating
  More cores/node, memories (slightly) larger but not faster
- Architectures of Supercomputers are becoming hybrid
  3 out to 4 Top Supercomputers are hybrid machines
- Extrapolation: In 2015, No. 500 will become petafloppic
  Most likely it will be a hybrid machine

Codes should be conceived differently

- # MPI processes is limited for a fixed problem size
- Performances increase only by enhancing parallelism
- Further parallelisation levels should be added (OpenMP, GPU)

Does electronic structure calculations codes are suitable?

Using GPUs in a Big systematic DFT code

Nature of the operations

- Operators approach via convolutions
- Linear Algebra due to orthogonality of the basis
- Communications and calculations do not interfere
- ☛ A number of operations which can be accelerated

Evaluating GPU convenience

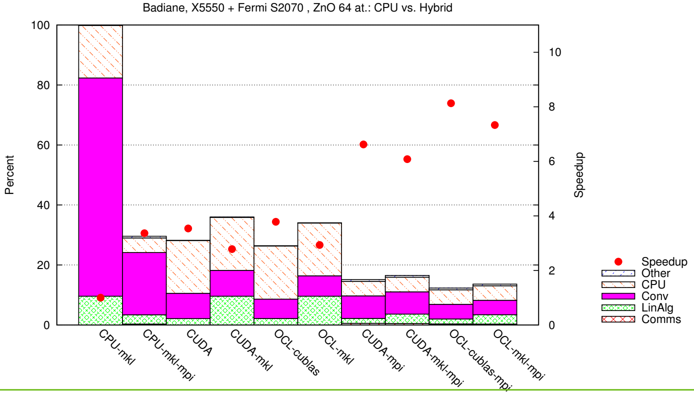
Three levels of evaluation

1. Bare speedups: GPU kernels *vs.* CPU routines
   Does the operations are suitable for GPU?
2. Full code speedup on one process
   Amdahl's law: are there hot-spot operations?
3. Speedup in a (massively?) parallel environment
   The MPI layer adds an extra level of complexity

BigDFT in hybrid codes

Acceleration of the full BigDFT code

- Considerable gain may be achieved for suitable systems
  Amdahl's law should always be considered
- Resources can be used concurrently (OpenCL queues)
  More MPI processes may share the same card!



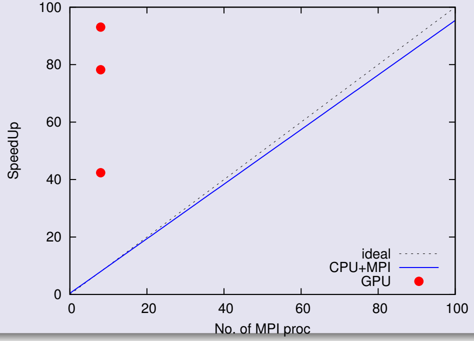
The time-to-solution problem

Good example: 4 C at, surface BC, 113 Kpts

Parallel efficiency of 98%, convolutions largely dominate.

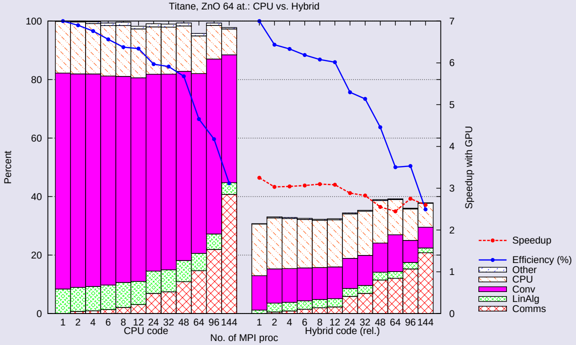
Node:
2× Fermi + 8 × Westmere
8 MPI processes

# GPU added	2	4	8
SpeedUp (SU)	5.3	9.8	11.6
# MPI equiv.	44	80	96
Acceler. Eff.	1	.94	.56



The time-to-solution problem

Not so good example: A too small system



- ✘ CPU efficiency is poor (calculation is too fast)
- ✘ Amdahl's law not favorable (5x SU at most)
- ✔ GPU SU is almost independent of the size
- ✔ The hybrid code *always* goes faster

Concrete examples with BigDFT code

MD simulation, 32 water molecules, 0.5 fs/step

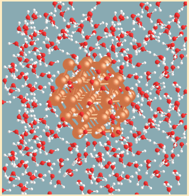
Mixed MPI/OpenMP BigDFT parallelisation *vs.* GPU case

MPI•OMP	32•1	128•1	32•6	128•6	128+128
s/SCF	7.2	2.0	1.5	0.44	0.3
MD ps/day	0.461	1.661	2.215	7.552	11.02

An example: challenging DFT for catalysis

Multi-scale study for OR mechanism on PEM fuel cells

- Explicit model of H_2O/Pt interface
- Absorbtion properties, reaction mechanisms



Outcomes from the understanding of catalytic mechanism at atomic scale:

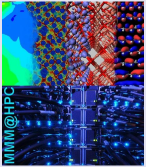
- Conception of new active and selective materials
- Fuels cell ageing, more efficient and durable devices

BigDFT in L_Sim projects

BigDFT-powered projects at L_Sim

Partner in several development and application projects

- SAMSON, ANR Cosinus
- ABSOR^2, MEDILEN (CEA)
- ELECMADE, BOLIDE, ANR Blanc
- NEWCASTLE (coord.), ANR Cosinus
- MMM @ HPC, European FP7 Project



2 PostDocs + 2 PhD to come

Explore new applications

These projects are based on the peculiarities of BigDFT code

- Heavier calculations and bigger systems
  (*at least* one order of magnitude)

☛ The code must be more powerful

BigDFT beyond DFT

Casida TDDFT formalism

B. Natarajan, PhD thesis (M. Casida, T. Deutsch)

- Uses BigDFT Poisson Solver
  $\rightarrow$ Systematic, explicit treatment
- Comparison with Gaussian basis (DeMon2k)
- Easier formalism (e.g. no Pulay terms for gradients)

Real-Space approach for GW calculations

I. Duchemin, Post-Doc — Tests on small molecules

- Single-electron transition basis (analytic on ω)
- Number and kind of basis functions
  Reliability of the choice of the basis
- Influence of the virtual states
  ☛ Various cases under investigation

A formalism continuously improved

Pseudopotentials used

BigDFT uses HGH Norm-Conserving pseudopotentials:

- ✔ Transferable, reliable for a number of quantities
- ✔ Well known technique, almost all Periodic Table
- ✘ Hard pseudopotentials, require high precision
- ✘ Terms like Non-Linear core correction absent

☛ HGH PSP generator is under improvement (libXC, NLCC)

Example: Atomization energy of the O_2 molecule (kcal/mol)

AE (G_{03})	PAW (VASP)	HGH-K	HGH	HGH+ NLCC
144.0*	143.3*	130.39	130.4	145.4

* From Paier et al. J. Chem. Phys. 122, 234102 (2005)

☛ A delicate quantity (e.g. PAW (ABINIT) → 137.5 kcal/mol)

Develop new solutions for large scale DFT calculations

A formalism continuously improved

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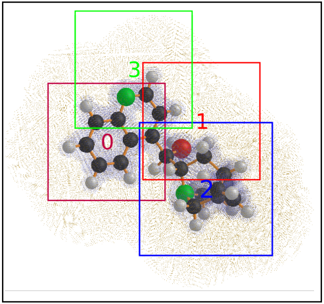
Introducing PAW formalism in BigDFT

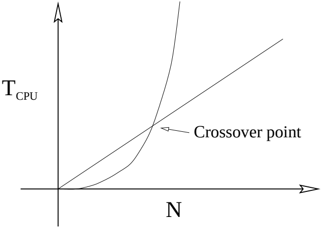
Work starting after summer (T. Rangel, M. Torrent)

- ✔ Modularize PAW ABINIT routines
  Identify basis-independent sections
- ✔ Define strategies to express PAW projectors
- ✔ Insert first wavelet PAW calculation within ABINIT

Develop new solutions for large scale DFT calculations

$O(N)$ approach (traditional $O(N^3)$)





P. Boulanger, S. Mohr

- Use locality of wavelets
- Localization regions
- Better flexibility
- Different schemes to localise wavefunctions

Where are we?

- A prototype version validated since 2007
- New localisation schemes already tested with cubic paradigm
- Underlying infrastructure under preparation

A look in near future

A concerted set of actions

- Improve BigDFT functionalities for present L_Sim projects (ABSOR^2, ELECMADE, NEWCASTLE)
- Provide BigDFT implementations of TDDFT and GW
- Insert BigDFT code in new workflows (MMM@HPC)

Enhancing DFT functionalities

- PAW formalism
  Should further reduce computational overhead
- $O(N)$ approach, production code
  Possible thanks to wavelets localisation and orthogonality
- New parallelisation scheme suitable for very large platforms
- Further refine formalims for Quantum Chemistry
  Systematic basis set extension for accurate treatment

Conclusions

BigDFT: solid state physics meets quantum chemistry

- ✔ Flexible, reliable formalism (wavelet properties)
- ✔ Easily fit with massively parallel architecture
- ✔ Open a path toward the diffusion of Hybrid architectures

Messages from GPU experience with BigDFT

- ✔ GPU allow a significant reduction of the time-to-solution
- ✔ Require a well-structured underlying code which makes multi-level parallelisation possible
- ✔ To be taken into account while evaluating performances
  Parallel efficiency $\Leftarrow$ system dimensioning wrt architecture

CECAM BigDFT tutorial next October

A tutorial on BigDFT code is scheduled!

Grenoble, 19-21 October 2011

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