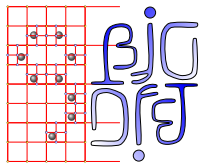

BigDFT
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Daubechies Wavelets in Electronic Structure Calculation: BigDFT Code Tutorial

CECAM RHÔNE ALPES - ST. MARTIN D'HÈRES, FRANCE

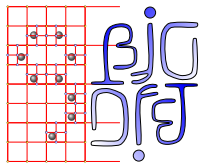
BigDFT Code Overview, Future Perspectives

Luigi Genovese

L_Sim – CEA Grenoble

October 20, 2011

A basis for nanosciences: the BigDFT project



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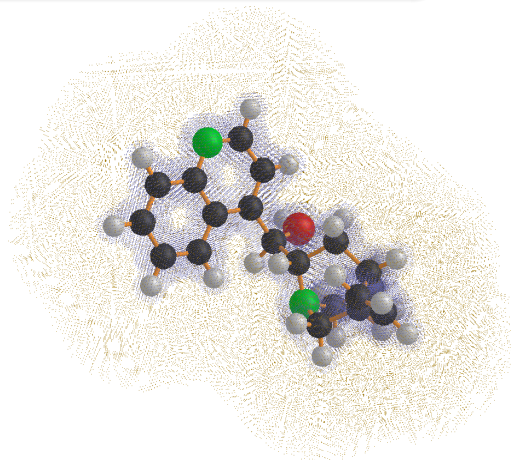
STREP European project: BigDFT(2005-2008)

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

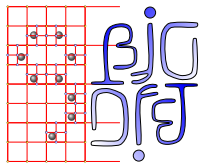
Aim: To develop an ab-initio DFT code based on Daubechies Wavelets, to be *integrated in ABINIT*.
BigDFT 1.0 $\longrightarrow$ January 2008



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

- Test the potential advantages of a new formalism
- ☛ A lot of outcomes and interesting results
- A lot can be done starting from present know-how

A new formalism for DFT: which advantages?



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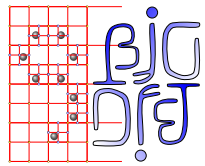
Interesting features

- Systematic treatment
  The basis does not depend of the particular system
- Real-space, localised basis
  Allows optimal flexibility for complex environments and BC
- Compact operator expressions
  Operators expressed analytically (3D convolutions)

Implementation Questions (end of 2005)

- What are the actual convergence properties?
  Number of degrees of freedom wrt other systematic basis
- Is the formalism easy to handle?
  Treat similarly “Simple” and “Complex” environments
- Does the computing behaviour is good?
  Parallel and massively parallel environments

Adaptivity on the grid mesh



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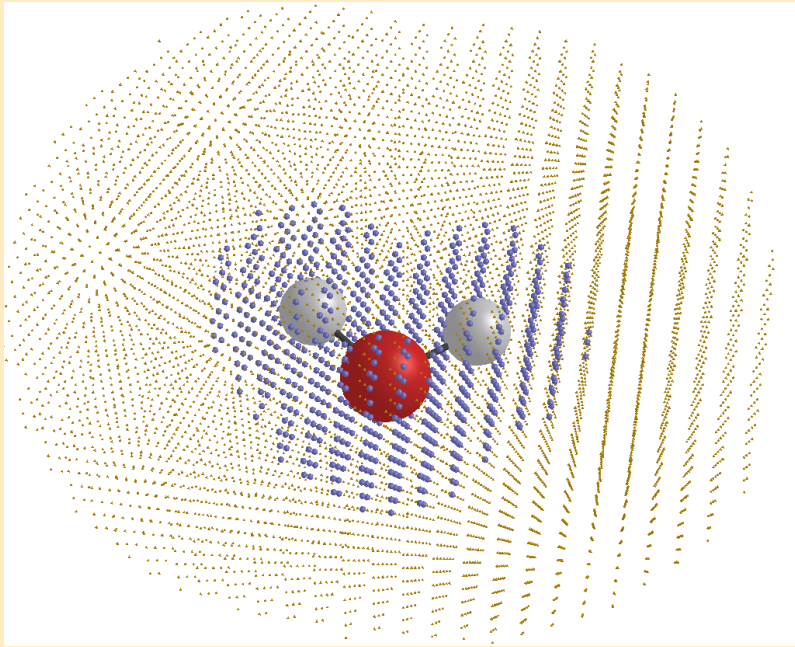
Main Feature: Adaptivity

Resolution can be refined following the grid point.



The grid is divided in:

- Low resolution pts (SF, 1 DoF)
- High resolution pts (SF + W, 8 DoF)

Points of different resolution belong to *the same* grid.

We can expand the information only where needed

Localization property

Empty regions must not be “filled” with basis functions.
Optimal for big inhomogeneous systems, $O(N)$ approach.

BigDFT performances

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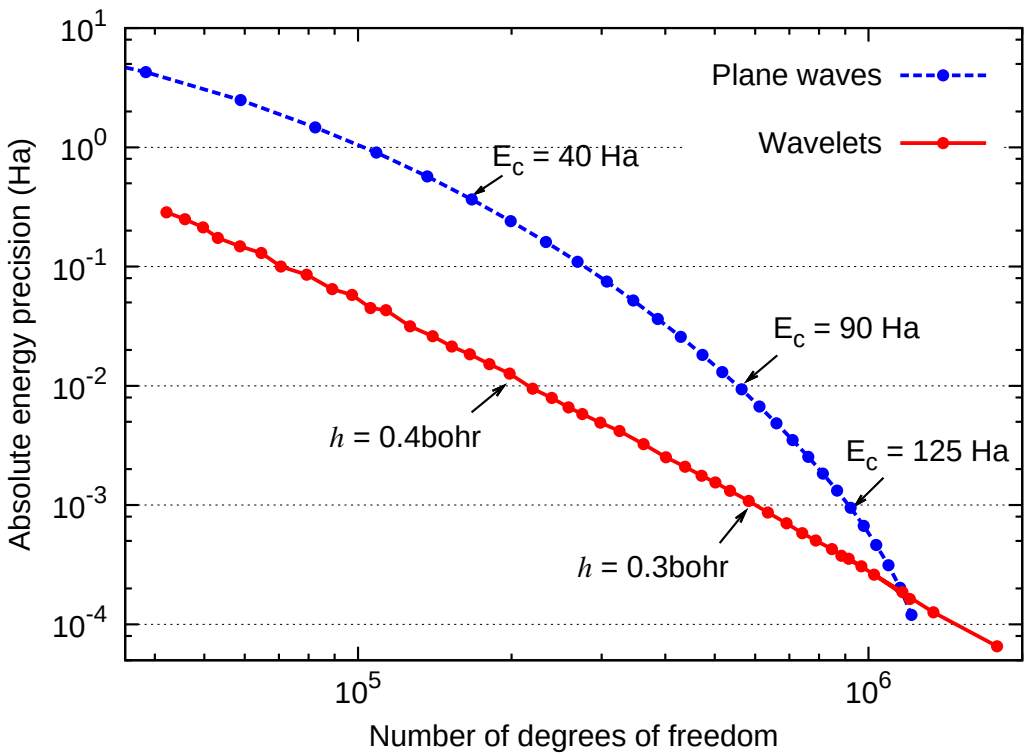
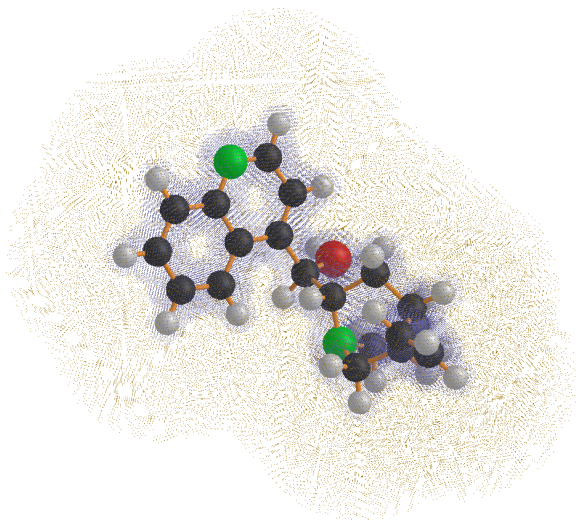
Optimal convergence, charged and polarised systems

Allows a systematic approach for molecules

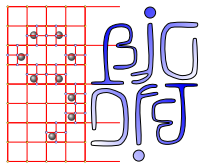
Charged systems, electric fields, can be treated *explicitly*

Test case: cinchonidine molecule (44 atoms)





High Performance Computing



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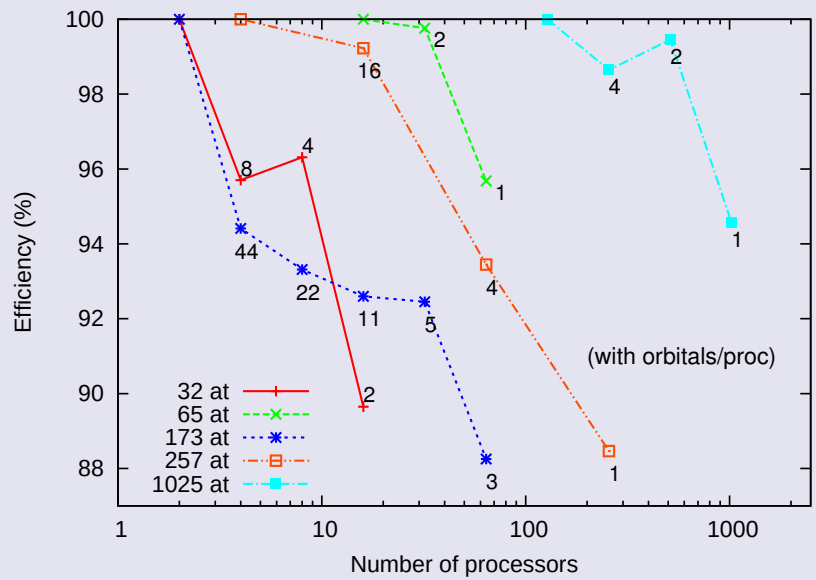
Localisation & Orthogonality → Data locality

- ✔ Principal code operations can be intensively optimised
- ✔ Parallelisation scheme conceived for supercomputers
- ☛ A HPC oriented code

Calculation on massively parallel architectures

Optimal efficiency in parallel calculations

- ✔ Time-to-solution enormously reduced
- ✔ Large systems become accessible in short time
- ☛ A different approach to calculations



A new approach for dimensioning the calculations

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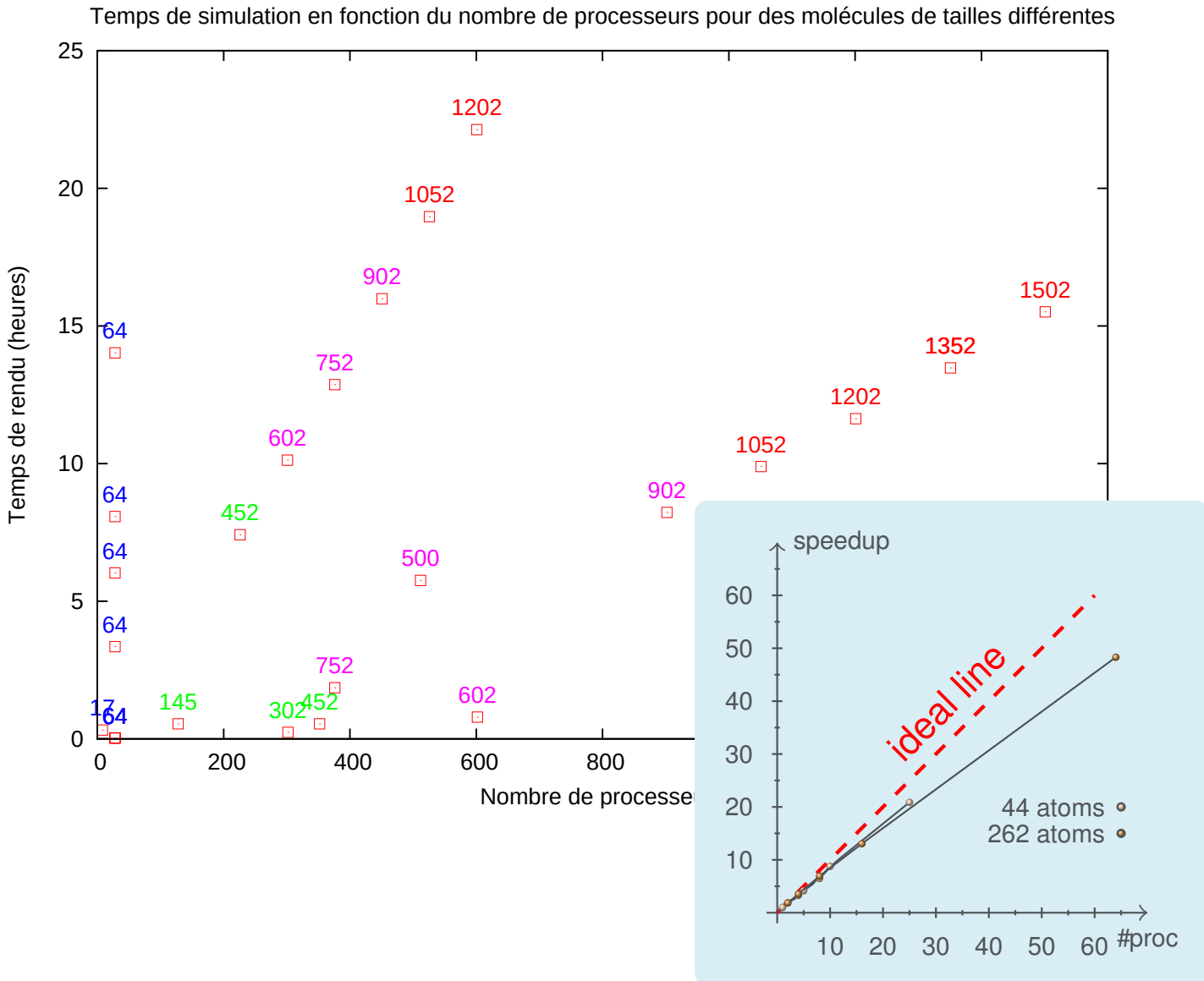
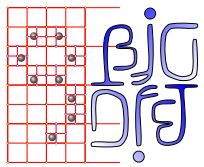
One day for a numerical experiment:



BigDFT version 1.6-tuto: (ABINIT-related) capabilities



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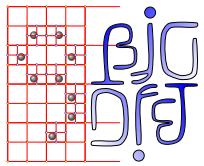
http://inac.cea.fr/L_Sim/BigDFT

- 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, Vibrations
- Unoccupied states, Wannier functions, Atomic charge analysis. . .
- Empirical van der Waals interactions
- Saddle point searches, ART, Minima Hopping
- All these functionalities are GPU-compatible

The second phase of the BigDFT project



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Half of 2009: End of first development phase

Since then ($\sim$ 18 months):

- Several 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

Exploration of configuration space

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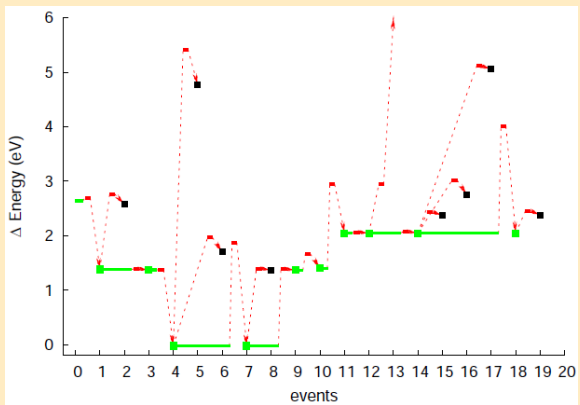
Benefit from high precision

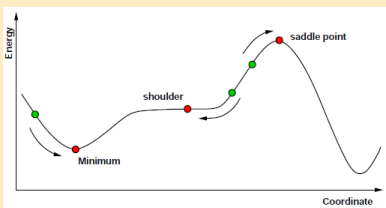
Different methods linked with BigDFT:

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

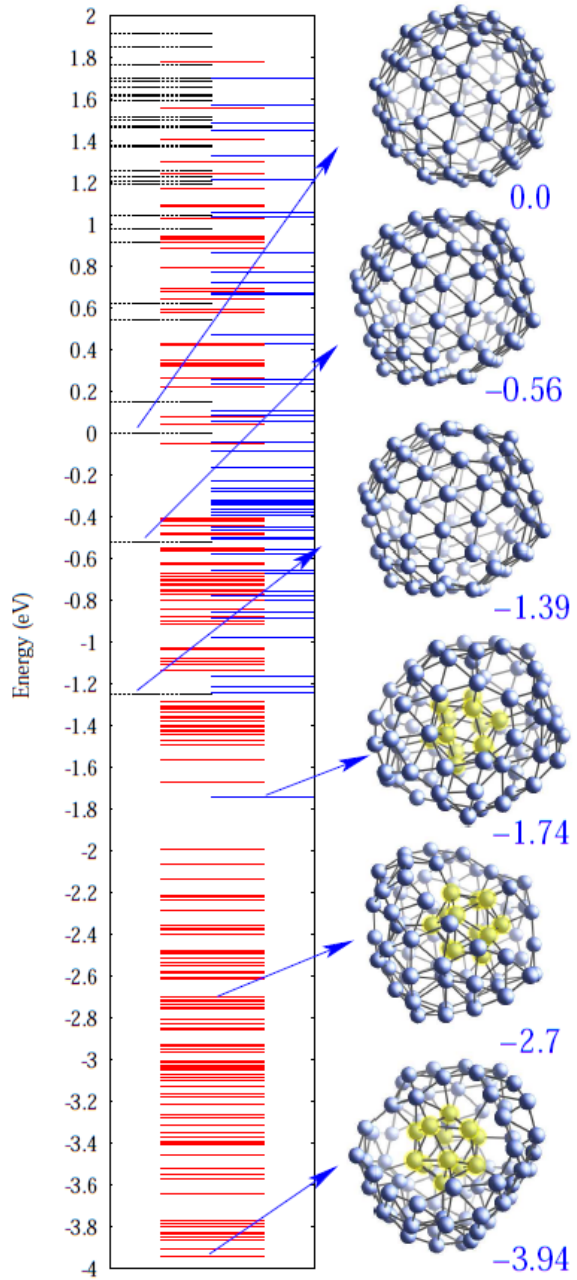
Applied on different systems

Benefit from high flexibility and performances

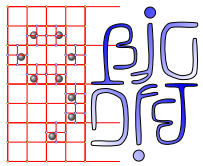




Interesting for potential synthesis pathways



A formalism continuously improved



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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)

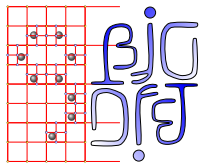
AE (G_{03})	PAW (VASP)	HGH-K	HGH	HGH+ NLCC
144.0*	143.3*	130.39	130.4	145.4

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

☛ A delicate quantity (e.g. PAW (ABINIT) $\rightarrow$ 137.5 kcal/mol)

Develop new solutions for large scale DFT calculations

A formalism continuously improved



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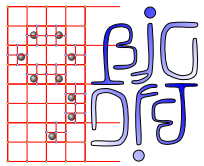
Introducing PAW formalism in BigDFT

Work has just started (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

Gaussian augmented Daubechies basis



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Basis set

with F. Longo (PhD thesis), Turin

$B = \{\phi_k\} \cup \{g_\mu\}_{\mu=1}^{N_g}$, with

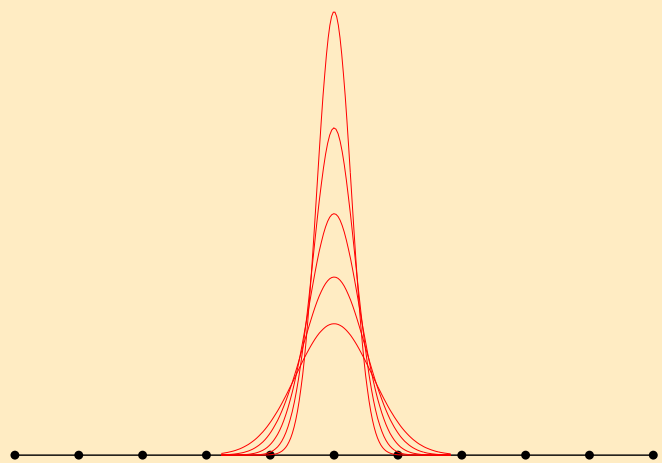
1. ϕ_k Daubechies SF/W on a grid with spacing h
2. $g_\mu = K_\mu e^{-\alpha_\mu r^2} r^\ell Y_\ell^m(\theta,\phi)$ centered on each atom

Even-tempered exponents

$\alpha_\mu = \alpha\beta^{\mu-1}, \quad 1 \leq \mu \leq N_g,$
with optimal $\alpha(h)$
Combine the best of the formalisms

- Save Degrees of freedom
- To be tuned, needs practice

s-channel, $N_g = 5$



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Combine the best of the formalisms

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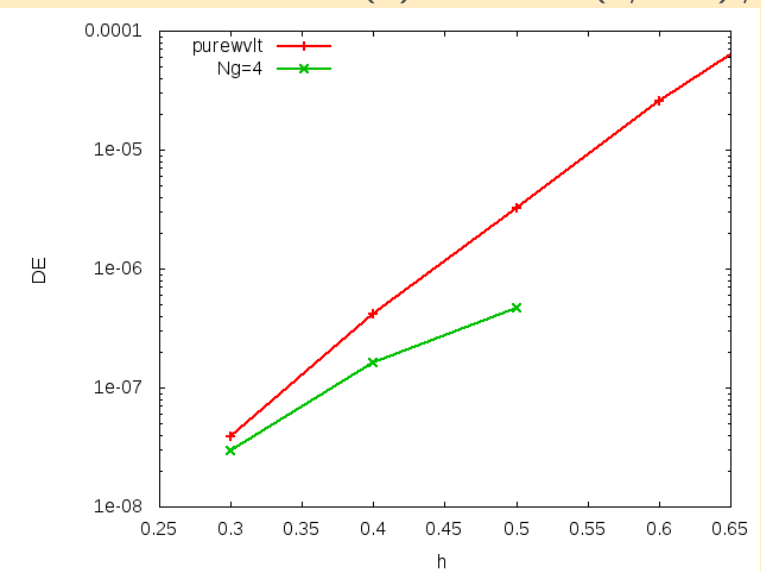
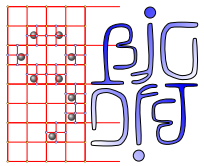
Test: $V(r) = \mathrm{erf}(r/0.3)/r$



The vessel: Ambitions from BigDFT experience



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Reliable formalism

- Systematic convergence properties
- Explicit environments, analytic operator expressions

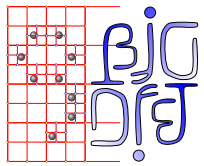
State-of-the-art computational technology

- Data locality optimal for operator applications
- Massive parallel environements
- Material accelerators (GPU)

New physics can be approached

- Enhanced functionalities can be applied relatively easily
- Limitation of DFT approximations can be evidenced
- A formalism of interest for Post-DFT treatments

A look in near future



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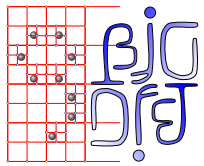
A concerted set of actions

- Improve BigDFT functionalities for present projects
- Test our know-how in other formalisms
- Insert BigDFT code in new workflows

Enhancing DFT functionalities

- PAW formalism
  Should further reduce computational overhead
- $\mathcal{O}(N)$ 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

A look in near future: science with HPC DFT codes



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A concerted set of actions

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- Insert BigDFT code in new workflows

The Mars "mission"

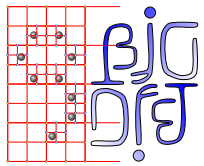
Is Petaflop performance possible?

- GPU acceleration $\rightarrow$ one order of magnitude
- Bigger systems, heavier methods $\rightarrow$ (more than) one order of magnitude bigger

BigDFT experience makes this feasible

An opportunity to achieve important outcomes and know-how

Conclusions



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BigDFT code: a modern approach for nanosciences

- ✔ 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 $\Leftarrow$ dimensioning of system wrt architecture

Still lots of things to be done