

CCPBioSim Training Week

BigDFT Session

Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations

Luigi Genovese

L_Sim - CEA Grenoble - France

September 23, 2022

Leeds (and remotely), England

Some ab initio Codes



Large-Scale DFT

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Plane Waves

- ABINIT — Louvain-la-Neuve — <http://www.abinit.org>
- CPMD — Zurich, Lugano — <http://www.cpmd.org>
- PWSCF → QE — Italy — <http://www.pwscf.org>
- VASP — Vienna — <http://cms.mpi.univie.ac.at/vasp>

Gaussians

- Gaussian — <http://www.gaussian.com>
- DeMon — <http://www.demon-software.com>
- CP2K — <http://cp2k.berlios.de>

Numerical-like basis sets

- Siesta — Madrid — <http://www.uam.es/siesta>
- Wien2K — Vienna — <http://www.wien2k.at>
(FPLAPW, all electrons)

Real space basis set

- ONETEP — <http://www.onetep.soton.ac.uk>
- **BigDFT** — www.bigdft.org

The BigDFT
project

Wavelets

PES exploration

$\mathcal{O}(N)$ BigDFT

BigDFT
compilation

BigDFT : increase
reach

Why a container

Perspectives

In Practice

Covid19 Outbreak

Opportunities

Basis sets for DFT calculations



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Plane Waves

ABINIT, CPMD, VASP, ...
Systematic convergence

- ✓ Accuracy increases with the number of basis elements
- ✓ Non-localised, optimal for periodic systems
- ✗ Non adaptive

Gaussians, Slater Orbitals

CP2K, Gaussian, AIMPRO, ...
Real space localized

- ✓ Small number of basis functions for moderate accuracy
- ✓ Well suited for molecules and other open structures
- ✗ Non systematic

FFT

Robust, easy to parallelise

Analytic functions

Kinetic and overlap matrices are calculated analytically

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Origin of the BigDFT project



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STREP European project: BigDFT(2005-2008)

In the beginning: Four partners, 15 people

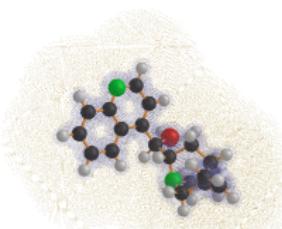
Now: around 10 active developers, Grenoble, Basel, Bristol, Catania, Trieste, Kobe

Used in production since twelve years.

Aim: To develop an ab-initio DFT code based on **Daubechies Wavelets**, to be integrated in ABINIT.

BigDFT 1.0 → January 2008

Why have we done this?



- Test the potential advantages of a new formalism
- A lot of outcomes and interesting results
- Future opportunities and ideas

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Daubechies wavelets



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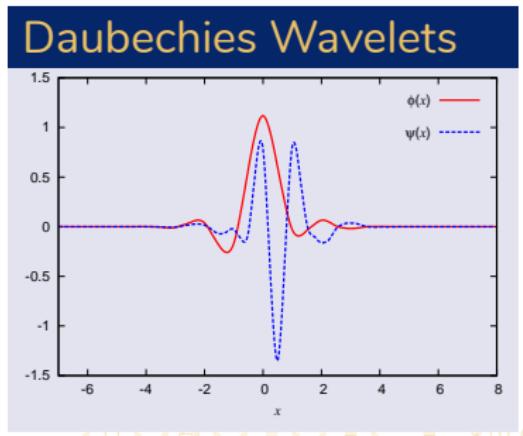
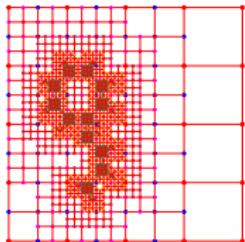
Wavelets

A basis with optimal properties for expanding localised information

- Localised in real space
- Smooth (localised in Fourier space)
- Orthogonal basis
- Multi-resolution basis
- Adaptive
- Systematic

From early 80's

Applied in several domains
Interesting for DFT



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A brief description of wavelet theory



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A Multi-Resolution real space basis

All functions w/ compact support, centered on grid points.
In the wavelet theory we have two kind of basis functions.

Scaling Functions (SF)

The functions of low resolution level are a linear combination of **high-resolution functions**.

$$\dots \square \square \dots = \dots \square \dots + \dots \square \dots$$

Wavelets (W)

Contain the DoF needed to complete the information lacking due to the coarseness of the resolution.

$$\dots \square \dots = \frac{1}{2} \dots \square \square \dots + \frac{1}{2} \dots \square \square \dots$$

Increase the resolution without modifying grid space

SF + W = Degrees of Freedom of SF of higher resolution

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Wavelet properties: adaptivity

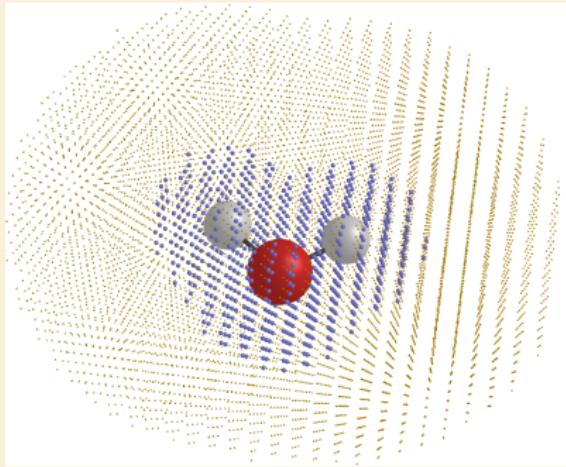


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Adaptivity

Resolution can be refined following the grid point.



The grid is divided in **Low** (1 DoF) and **High** (8 DoF) resolution points.

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

Empty regions must not be “filled” with basis functions.

Localization property, real space description

Optimal for **big & inhomogeneous** systems, **highly flexible**

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Systematic basis set



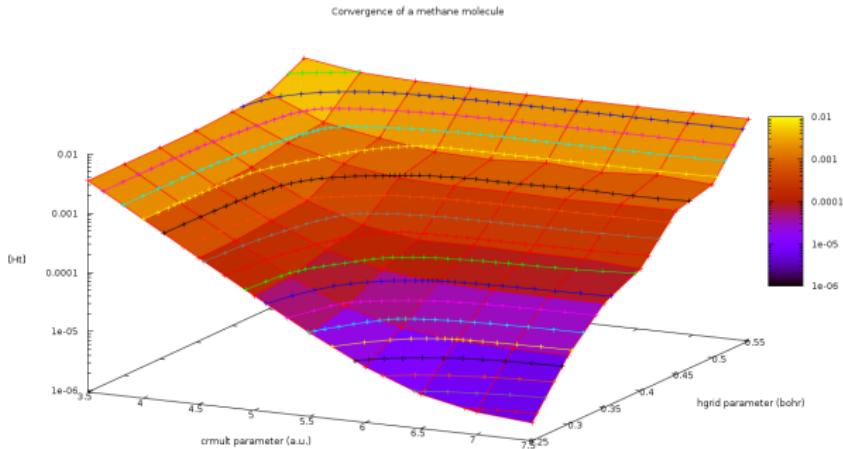
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The absolute accuracy of the calculation is directly proportional to the number of the basis functions

Two parameters for tuning the basis

- The grid spacing `hgrid`
- The extension of the Low resolution points `crmult`



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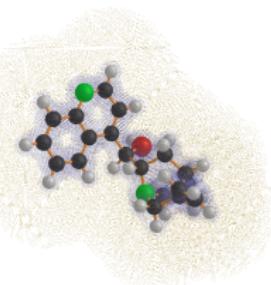
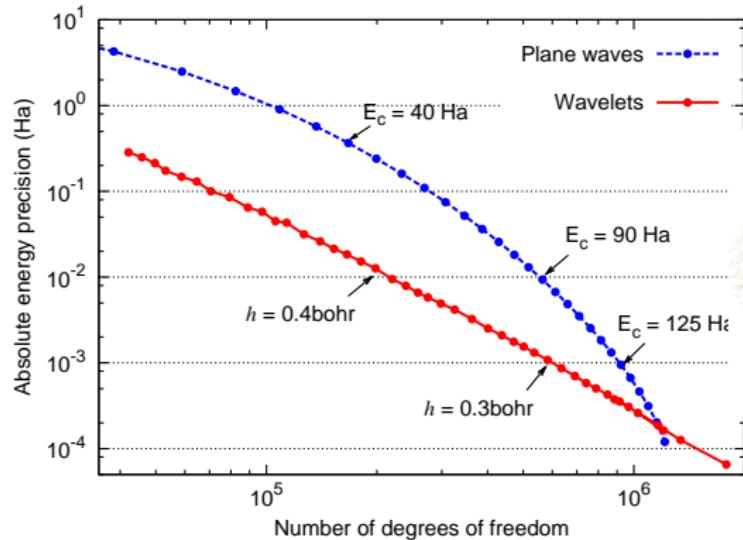
Optimal for inhomogeneous systems



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Test case: cinchonidine molecule (44 atoms)



Enables a systematic approach for molecules

Considerably faster than Plane Waves codes.
the above run :10 (5) times faster than ABINIT (CPMD)
Charged systems can be treated explicitly with the same time

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Non-linear core correction

J. Chem. Phys. **138**, 104109 (2013)

- Simple analytic form (a single gaussian as ρ_c)
- Same hardness as HGH
 - a systematic localized basis is **fundamental**

Precision considerably improved

(Atomization energies)

G2-1 test set (Atomization

kcal/mol	MAD	RMSD	MSD	maxAD	minAD
Old HGH	6.85	9.13	-6.76	23.94	0.10
NLCC-HGH	0.51	0.63	0.16	1.50	0.03
PAW Paier	0.46	0.56	-0.43	1.13	0.01
Δ AE (geopt)	0.29	0.70	-0.29	4.21	0.00

AE precision for quantities in different environments

Bond lengths, Pressure (Bulk systems),

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Opportunities

A DFT code conceived for HPC (www.bigdft.org)

- DFT calculations up to many thousands atoms
- 👉 An award-winning HPC code
- BigDFT has been conceived for massively parallel heterogeneous architectures since more than 10 years (MPI + OpenMP + GPU)



Code able to run routinely on different architectures

- GPU accelerators since the advent of double-precision GPGPU (2009)
- Various large calculation projects since 10 years
- ✓ A code conceived for supercomputers

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A flexible formalism

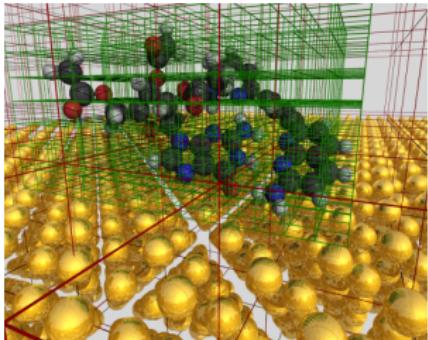


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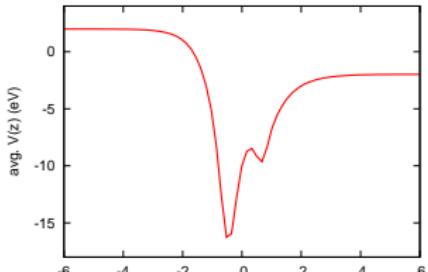
Flexible Boundary Conditions

- Isolated (free) BC
- Wires BC
- Surfaces BC
- Periodic (3D) BC



Systematic approach

Only relevant degrees of freedom are taken into account
Boundary conditions can be implemented explicitly



E.g.: Surfaces BC

2D Periodic + 1D isolated
Optimal to treat dipolar
systems **without** corrections



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A code **both** for Solid-State and Quantum Chemistry

- 3D periodic, Surfaces and Free BC (\leftarrow Poisson Solver)
- Very high precision (analytic KS operators)
- Usage of analytic HGH pseudopotentials
- AE accuracy, benchmarked in G2-1, S22, DeltaTest

Present functionalities

Traditional functionalities for GS Kohn-Sham DFT (including metals, Hybrid Functionals), LR-TDDFT, empirical VdW

Exhaustive library of Structural Prediction, $O(N)$ calculations

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Exploration of configuration space



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Benefit from high precision

Different methods linked with BigDFT:

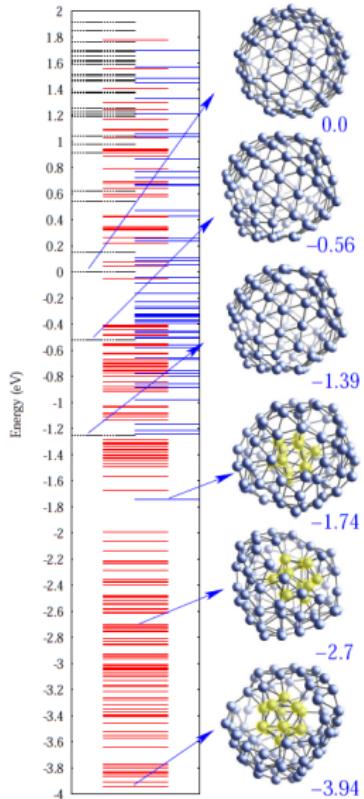
- Minima Hopping (S. Goedecker)
- Activation-Relaxation Technique (N. Mousseau)

Applied on different systems

Benefit from high flexibility and performances



Interesting for potential synthesis pathways



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Use locality of the basis set

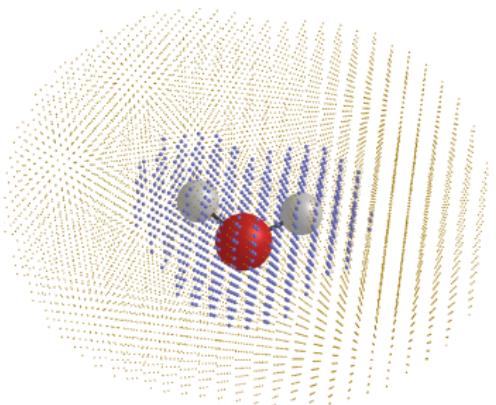


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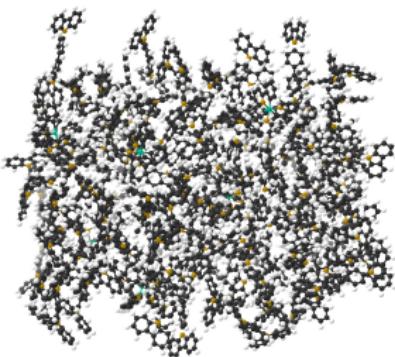
Wavelets

an ideal basis for electronic structure calculations – flexible, systematic **and** localized



Linear-scaling DFT

allows us to access very large system sizes via the use of a localized minimal basis set



Combining the two is now possible!

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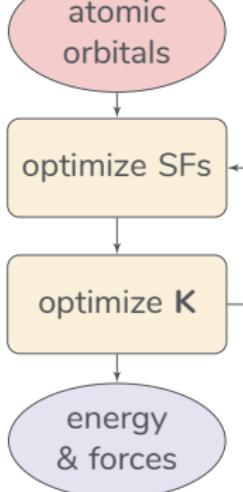
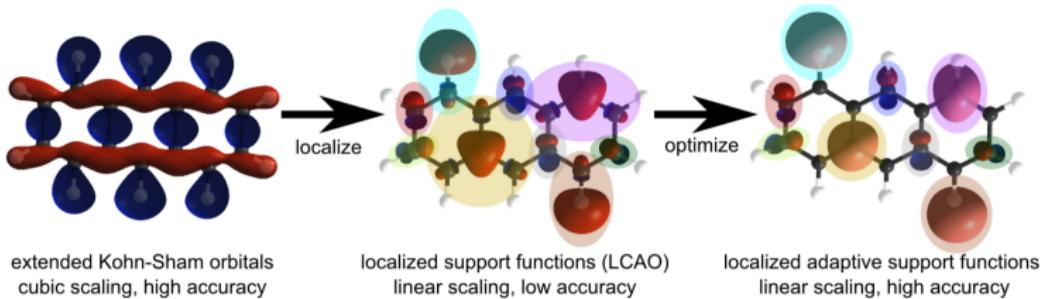
Opportunities

A Linear Scaling Algorithm



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Accurate Minimal Basis

- Employs optimized DoF to express accurately and efficiently the DFT solution
- Able to treat systems up to tens of thousand atoms
- Ideal framework to reduce the complexity of the description

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O(N) Codes In Practice

- O(N) codes have been able to compute large systems for many years now.
- And yet, how often do you encounter research being done with DFT involving systems of many tens of thousands of atoms?

The Issues

- Enthalpy challenge: are DFT functionals really more accurate than a well tuned forcefield?
- Entropy challenge: can DFT capture the full set of conformations of a large system?
- The key value added of DFT is not accuracy, but insight.

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Advanced Review

Challenges in large scale quantum mechanical calculations

Laura E. Ratcliff,¹ Stephan Mohr,² Georg Huhs,² Thierry Deutsch,^{3,4} Michel Masella⁵ and Luigi Genovese^{3,4*}



During the past decades, quantum mechanical methods have undergone an amazing transition from pioneering investigations of experts into a wide range of practical applications, made by a vast community of researchers. First principles calculations of systems containing up to a few hundred atoms have become a standard in many branches of science. The sizes of the systems which can be simulated have increased even further during recent years, and quantum-mechanical calculations of systems up to many thousands of atoms are nowadays possible. This opens up new appealing possibilities, in particular for interdisciplinary work, bridging together communities of different needs and sensibilities. In this review we will present the current status of this topic, and will also give an outlook on the vast multitude of applications, challenges, and opportunities stimulated by electronic structure calculations, making this field an important working tool and bringing together researchers of many different domains. © 2016 John Wiley & Sons, Ltd

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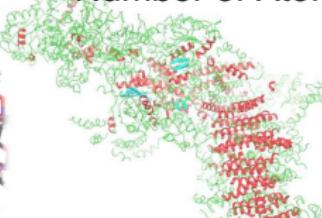
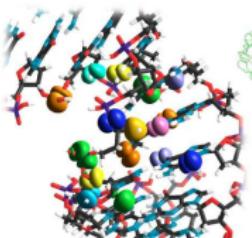
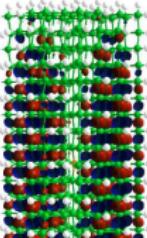
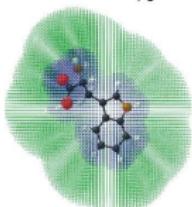
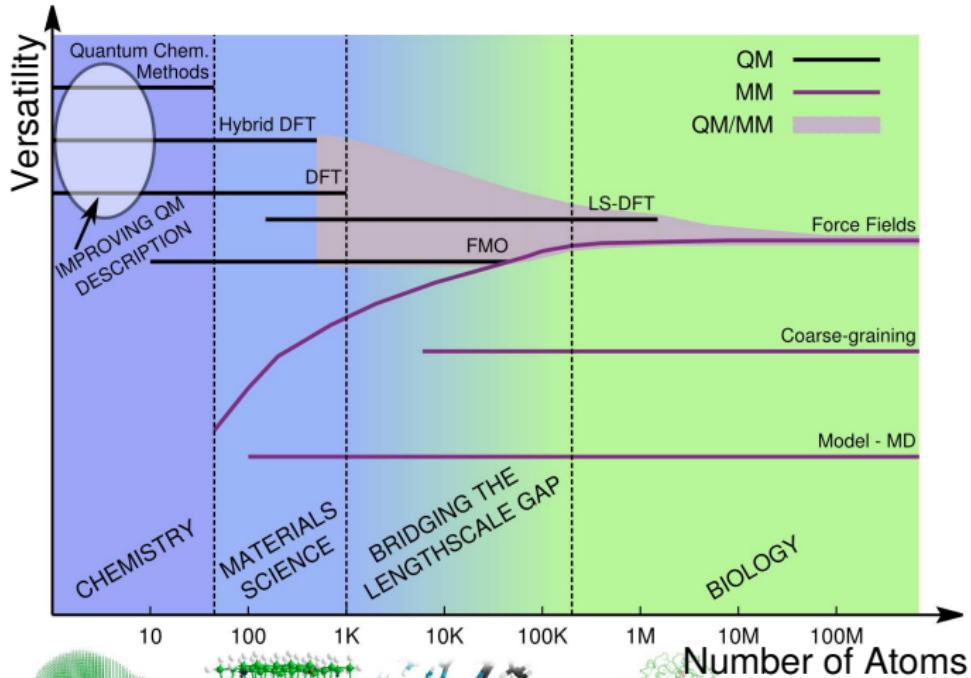
New calculation paradigms are emerging

Why Large Scale DFT? Present-day situation



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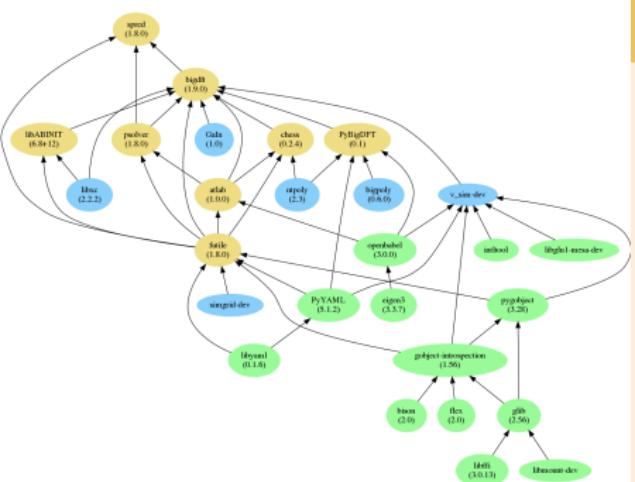
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Opportunities



Modularity first

BigDFT-suite : collection of different independent libraries with own build system.

Third-party libraries (green) and upstream modules (blue)

☞ Dependencies expressed easily in the jhbuild-based bundler.

- Lots of possible options
- Very versatile
- Python configuration files can be shared, many provided
- Good or Expert knowledge often required

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Opportunities

Provide new alternatives to users

- Packaged versions
- Virtual machines
- Containers

Which users ? which usages ?

- Development
- HPC
- Analysis

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Opportunities

We need

- System packages (`bison`, `flex`, `cmake`,...)
- Linear algebra packages (`blas`, `lapack`, `MKL?`,...)
- Upstream packages (`libyaml`, `glib`, `libffi`,...)
- Community packages (`simgrid`, `ntpoly`, `libxc`,...)
- BigDFT packages

Moreover

- CUDA has to be installed
- The MPI layer should be CUDA-aware (GPUdirect)
- On workstation and frontends we use jupyter notebooks
- The compilation instructions are cumbersome. Difficult to control all these things for non-expert developers.

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Containers as a possible solution



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Our container history

- Development of GPU acceleration for exact exchange with GPUdirect
- Development of PyBigDFT API
- CI

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Opportunities

Flavours

- SDK: large, with everything to build, no BigDFT
- runtime: stripped, with bigdft/MPI built from SDK
- Also available on Nvidia NGC repository

▶ SDK

▶ runtime

▶ NGC

Features

- Built using Nvidia HPC container maker toolkit :
- Comes with CUDA/OpenCL, MKL, either MVAPICH2 or OpenMPI, Jupyter server
- Works on non-GPU systems, ARM/x86 platforms, Windows (using WSL2).
- BigDFT libraries with/without vectorized instructions, dynamically selected
- Tested with GPUDirect on singularity and shifter

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Virtual Machine

- BigDFT is part of MaX flagship codes, is available on the Quantum Mobile virtual machine.
- Great for training/schools

► QM

Package

- Debian package in the making: Easy to install, less optimized.
- Python package for BigDFT run analysis
BigDFT client (futile and PyBigDFT)
- Conda package recipe (release candidate)

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Opportunities

In this training you will...

- Get acquainted with BigDFT code API
- Have an overview of how to employ some of the functionalities of this code
- Work to some pre/post processing of the code data/results

In this training you will **not**...

- Run BigDFT in a production environment (supercomputer)
- Have a realistic idea of the performance of the code
- Have too much time to play with the code runs

👉 bring BigDFT back home!

Available Functionalities



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Non-Exhaustive List of Functionalities

	$O(\mathcal{N}^3)$	$O(\mathcal{N})$	fragment
MPI and OpenMP	✓	✓	✓
GPUs	✓	✗	✗
free/wire/surface boundary conditions	✓	✓	✓
periodic orthorhombic cells	✓	✓	✓
periodic non-orthorhombic cells		in progress	
k -points	✓	✗	✗
forces (geometry optimizations, MD)	✓	✓	✗
metals	✓	✓	✓
hybrid functionals (no k -points)	✓	✗	✗
spin polarization	✓	✓	in progress
explicit charges (free BC only)	✓	✓	✓
external electric field (free/surface BC only)	✓	✓	✓
electrostatic embedding	✓	✓	✓
structure searching	✓	✓	✓
empirical Van der Waals (free BC only)	✓	✓	✓
Raman spectra		in progress	
time-dependent DFT	✓	✗	✗
constrained DFT (no spin or forces)	✗	in progress	✓

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From Cubic Scaling to Multiscale

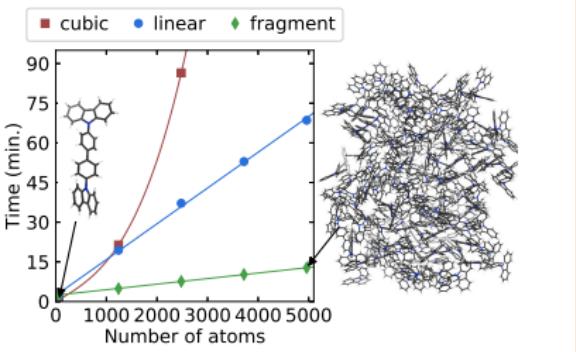
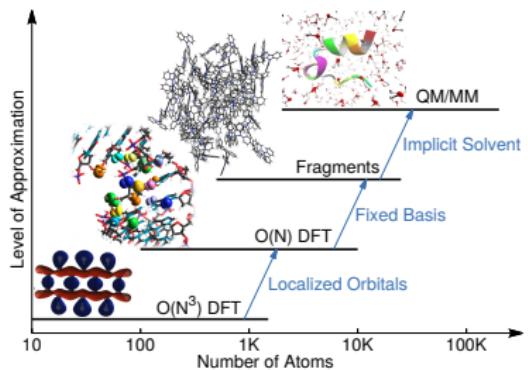


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Across Lengthscales

- extended orbitals $\rightarrow O(N^3)$
- exploit locality $\rightarrow O(N)$
- exploit repetition $\rightarrow \downarrow \text{cost } O(N)$
- larger systems \rightarrow increasing complexity
- \rightarrow how to treat **complex systems?**



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Features of the approach

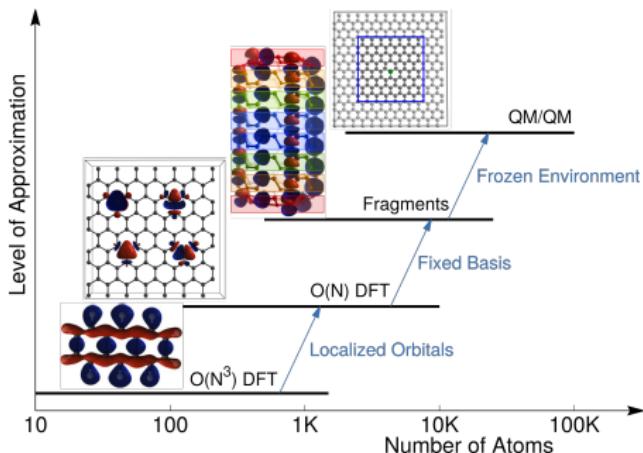


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Across Lengthscales with Wavelets

- three methods in BigDFT with differing levels of approximation fragment → linear → cubic
- approximations are controllable – can estimate or measure errors



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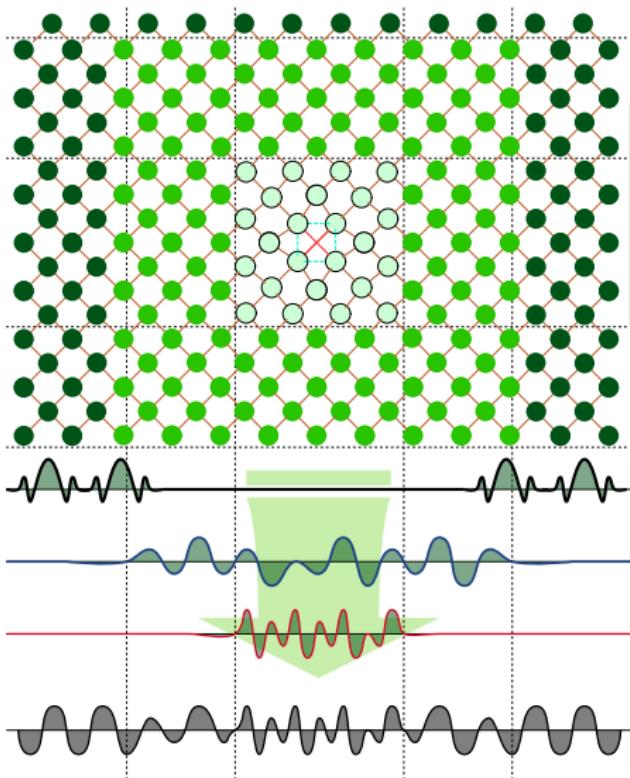
Opportunities

Perspectives (QM/QM)



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Region descr.

- active site
- full ab initio
- constrained-DFT approach
- tight-binding like environment

Wavefunc. descr.

- bulk-like frozen wavefunctions
- optimized wavefunc. on a frozen basis set
- optimized wavefunc. and basis set
- complete representation of the active site in bulk environment

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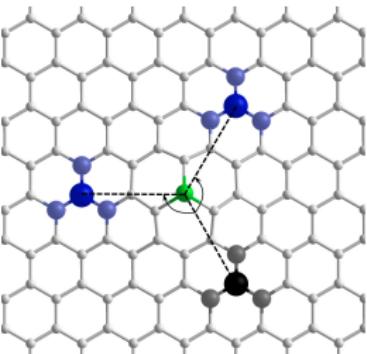
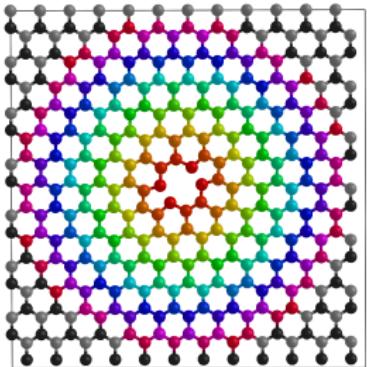
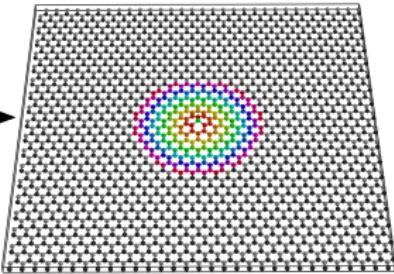
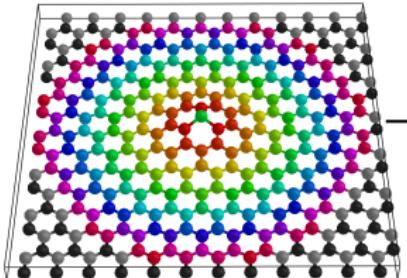
Opportunities

Defective Graphene with Fragments



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close to the defect:
strong perturbation

far from the defect:
bulk-like behaviour

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ADVANCED REVIEW



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Density functional theory calculations of large systems: Interplay between fragments, observables, and computational complexity

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Abstract

In the past decade, developments of computational technology around density functional theory (DFT) calculations have considerably increased the system sizes which can be practically simulated. The advent of robust high performance computing algorithms which scale linearly with system size has

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Wavelets

PES exploration

$O(N)$ BigDFT

BigDFT compilation

BigDFT : increase reach

Why a container

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Example: fragment in peptides



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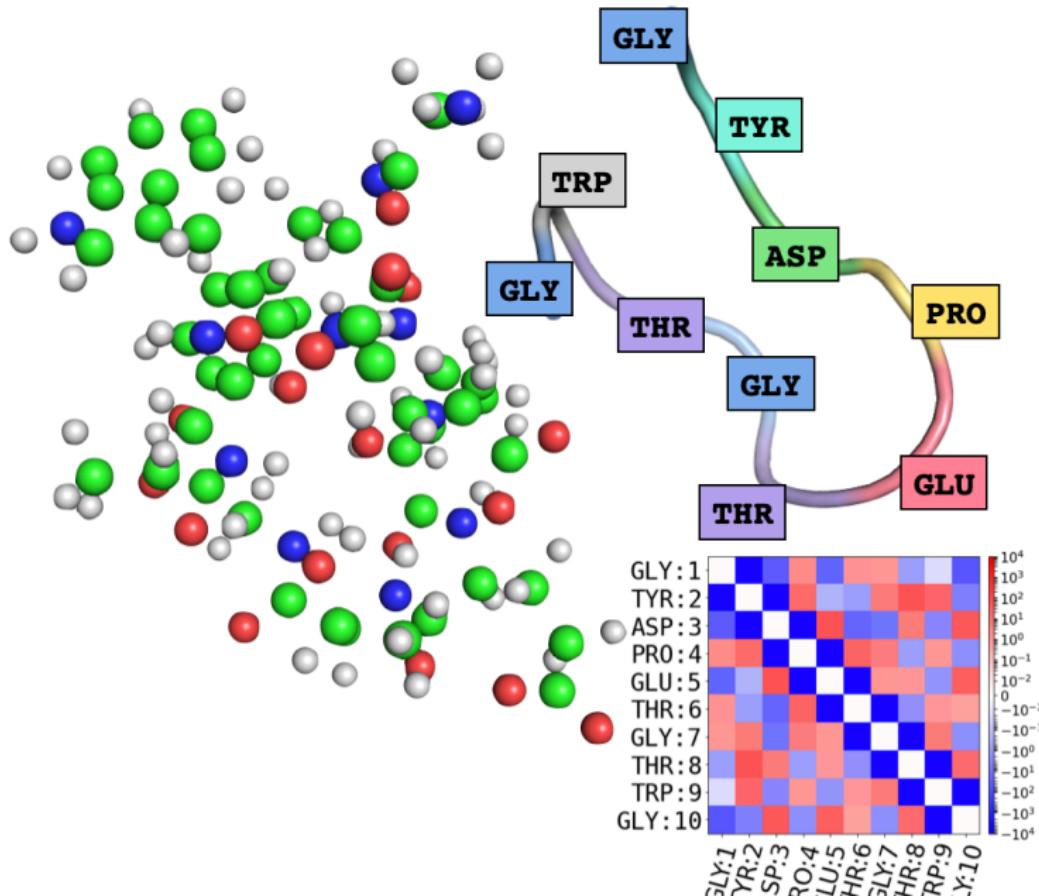
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Example 2: the same in protein



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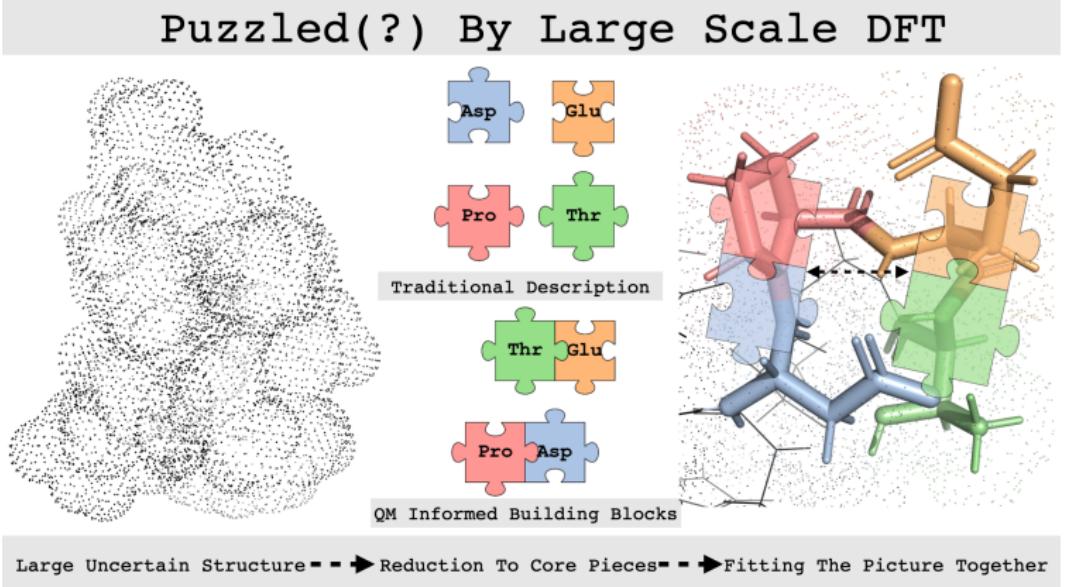
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Lots of Systems of interest in Biology



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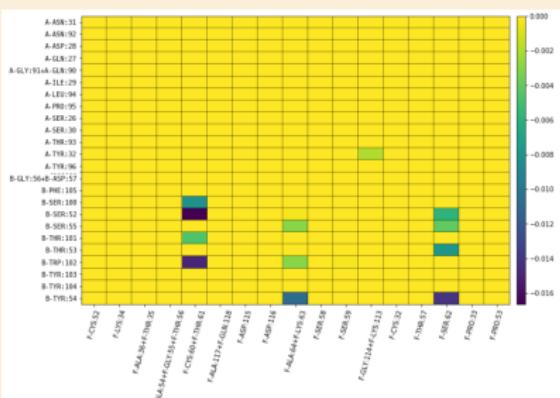
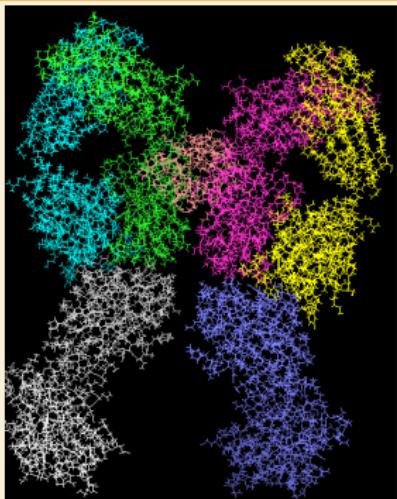
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Large systems are routinely accessible

Linear Scaling code → CPU time per atom

Example: 1400 Residues (One Monoclonal Antibody); 22 thousand atoms; 1.2h of walltime on 32 nodes of IRENE-Rome Machine

Reduce (identify) the interactors in a biological system



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Given this situation



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Pandemic Emergency

- A unprecedented emergency → no one had solutions
- The scientific world was *listening*
- The technology was there to help

The fundamental point

The investigation paradigms and ideas which were (almost) ready found new actors in the pandemic emergency



New (updated) contacts and collaboration

UK: Oxford, Bristol, Diamond Synchrotron, US: Scripps (Florida), Boston College (Virology Dept.), EU: Institut Joliot (CEA), SANOFI

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Quantum Mechanics (DFT) may be needed

- Whenever DFT is necessary to study the electronic structure of the systems, it is important to provide the tools to interpret experimental data
- Need of new tools developed especially for the study of biological systems
- The BigDFT code provide a new paradigm of analysis

Main ingredients

- PDB files from neutron crystallography, Cryo-TEM, MD simulations, ...
- Remotely accessible (super) computing platform
- A post-processing infrastructure easy-to-use

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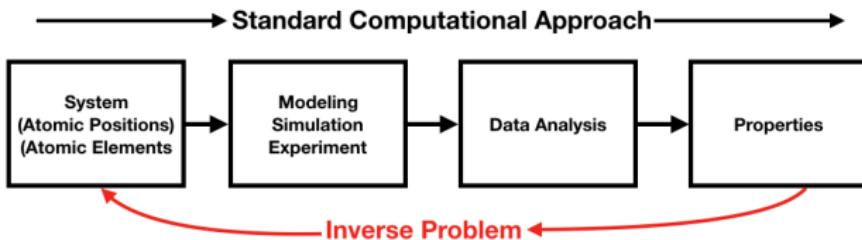
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The Inverse Problem of Computational Science

- Mechanistic models might be used to gain detailed insight into individual systems.
- However, the goal is not only understanding, but design (drugs, antibodies, enzymes).
- Inverse problem: given a set of desirable properties, how do we build a system that produces those properties?

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Quantum-as-a-Service approach



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A dedicated Users' platform ?

Collaboration L_Sim (CEA Grenoble) and CS Group (ILL)

PyBigDFT	HPC	Userclub	Database
Pre- and Post-processing of simulations are performed via a Python module	Calculations triggered remotely on a super-computer from a Jupyter notebook (AiiDA framework)	Simulation can be processed from a platform next to experimental data (ILL User Club access)	Large databases of biological systems can be created

New insights for (neutron) data analysis

- Dedicated routine for neutron crystallography data interpretation
- Possible improvement from other structural (e.g. SANS) data

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Summary

- DFT shouldn't be employed for large systems just on the hope of accuracy, but instead with the goal of insight.
- Complexity Reduction - We have developed a way to use information from DFT to generate coarse-grained views of a system by defining reliable fragments and measuring their interaction.

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From Material Science to other communities

- The complexity reduction framework presented here originate from our expertise on Physics and Material Science.
- Postprocessing can be performed even by non-specialists.
- This combination create interesting opportunities for interdisciplinair collaborations.

Interdisciplinary considerations



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Discussion with biologists

We are not referring to a set of established techniques:

- New objects, definitions, descriptors
- The Physico-Chemical outcome (and only this!) should be highlighted

Difference (I have found) in the approach: example

- For a Physicist the procedure is the ground basis for the result
- For Biologists the result is the ground basis for the procedure

Interdisciplinarity requires

Rigor, Trust, Vision, Commitment ➡ The right guys

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