



Welcome!

# Daubechies Wavelets in Electronic Structure Calculation: BigDFT Code Tutorial

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

*Welcome to BigDFT code tutorial*

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L\_Sim – CEA Grenoble

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# The (enlarged) BigDFT group



Welcome!

## CEA Grenoble – Group of **Thierry Deutsch**

LG, D. Caliste, B. Videau, I. Duchemin, P. Boulanger,  
E. Machado-Charry, F. Cinquini, B. Natarajan

## Basel University – Group of **Stefan Goedecker**

S. A. Ghazemi, A. Willand, M. Amsler, S. Mohr, A. Sadeghi,  
N. Dugan, H. Tran, S. De, D. Nafday

## And also

- Laboratoire d'Informatique de Grenoble:  
J-F. Méhaut, M. Ospici
- European Synchrotron Radiation Facility:  
Y. Kvashnin, A. Mirone, A. Cerioni
- CEA-DAM, Bruyères-le-Châtel:  
T. Rangel, M. Torrent

# A basis for nanosciences: the BigDFT project



Welcome!

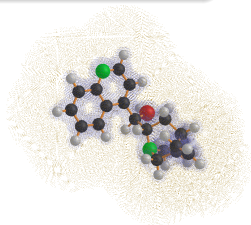
## STREP European project: BigDFT(2005-2008)

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 → January 2008



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

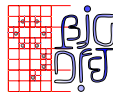
- Test the potential advantages of a new formalism
- A lot of outcomes and interesting results
- A lot can be done starting from present know-how



Welcome!

## Aim of the project

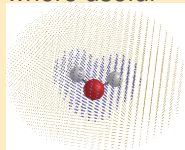
To develop a DFT code based on **wavelets** to treat large systems such as found in nanoscience or biology



FORTRAN 90 + C + OpenCL + CUDA Code:

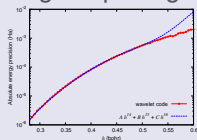
### Adaptive

Resolution can be **refined** only where useful



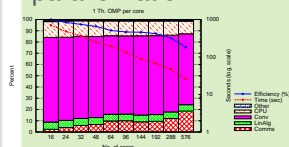
### Systematic

**Precision** can be arbitrarily reduced wrt grid spacing



### Fast

Intensively **optimized**, multi-level (MPI+OMP+GPU) parallelization



Moreover, such a real-space based approach allows for:

- ✓ Different choices of boundary conditions, flexibility
- ✓ Assess the pertinence of Quantum Chemistry Models

# How this tutorial is organized



Welcome!

## First day: The basis concepts

- From DFT to BigDFT ideas
- From massively parallel architectures to BigDFT code

## Second day: The present of the code

- High Performance Computing panorama
- Methods for exploration of Potential Energy Surfaces

## Third day: (Some of) the Future of the code

- Present techniques and Advanced applications
- BigDFT suitability for  $O(N)$  approaches

Hands On throughout the whole afternoons

# Who this tutorial is addressed for?



Welcome!

## Code Users

- The code is not a gaussian code (different approach)
- The code is not a plane waves code (different behaviour)

## Code Developers

- A formalism with new potentialities
- A code “modularly” conceived for integrating building-blocks

## A multi-audience orientation

Both the viewpoints will be presented during the tutorial  
It would be **normal** not feeling comfortable everywhere



Welcome!

WiFi only available via edu-roam portal

## The USB key (*very important*)

- ✓ **Needed** for executing the Hands On
- ✓ Contains a live UBUNTU 11.04 which **needs a login and a password** (check behind your badge)
- ✓ Contains BigDFT, V\_Sim and all programs needed for the (basic) Hands On

## Social dinner

Thursday, "Restaurant la Bastille" (Téléphérique de Grenoble at 19:30)

... via Ferrata also available...

