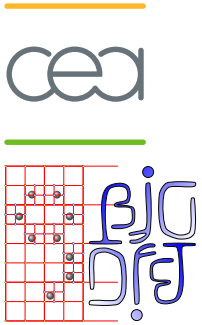


BigDFT hands-on 2012

Oak Ridge, Tennessee, USA

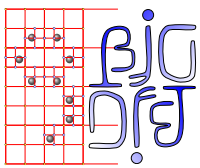
All you need to know about BigDFT

Damien Caliste, Luigi Genovese & Thierry Deutsch

L_Sim - CEA Grenoble

8 February 2012

Outline



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   - Definition of the basis-set
   - Structure of the calculation
     - The electronic minimisation loop
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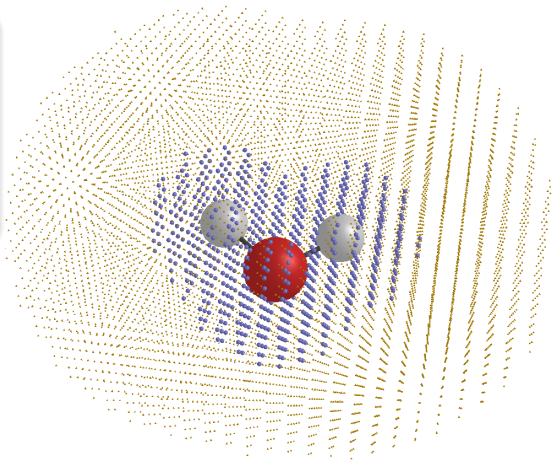
     - Possible add-on calculations after fix point is reached
2. A quick look from the user point of view
   - The input parameters and atomic data
   - How to compile BigDFT
   - How to run BigDFT

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

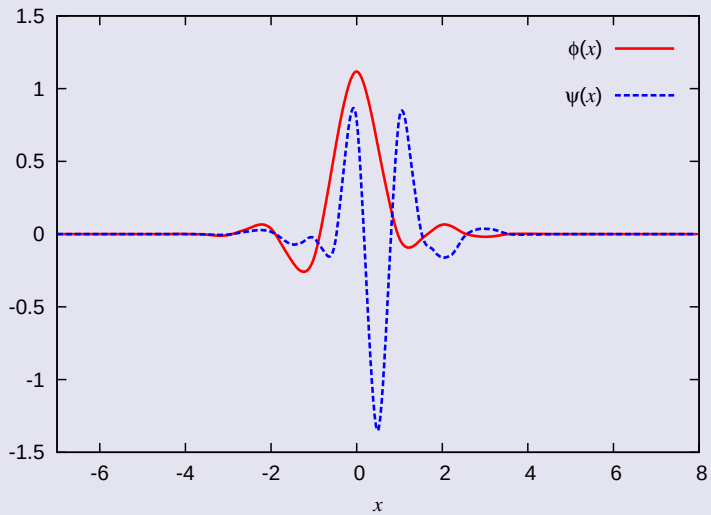
$$\tilde{c}_\ell = \sum_j a_j \, c_{\ell-j}$$

- Peculiar numerical properties

Real space based, highly flexible

Big & inhomogeneous systems

Daubechies Wavelets

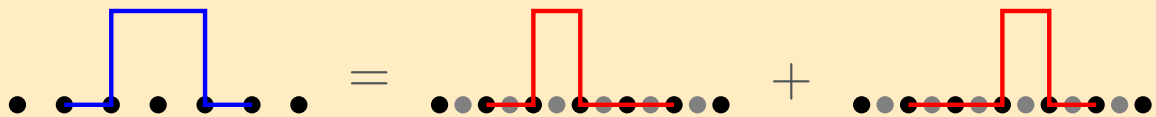


Wavelet properties: multi-resolution

Example of two resolution levels: step function (Haar Wavelet)

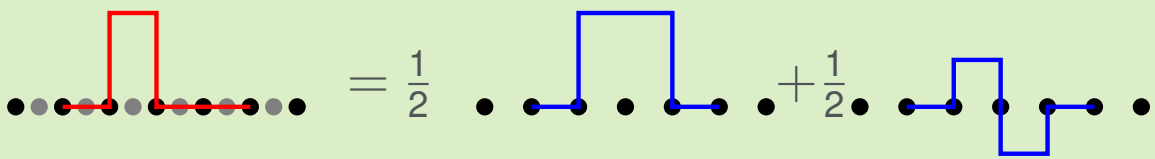
Scaling Functions: Multi-Resolution basis

Low and High resolution functions related each other



Wavelets: complete the low resolution description

Defined on the same grid as the low resolution functions



Scaling Function + Wavelet = High resolution

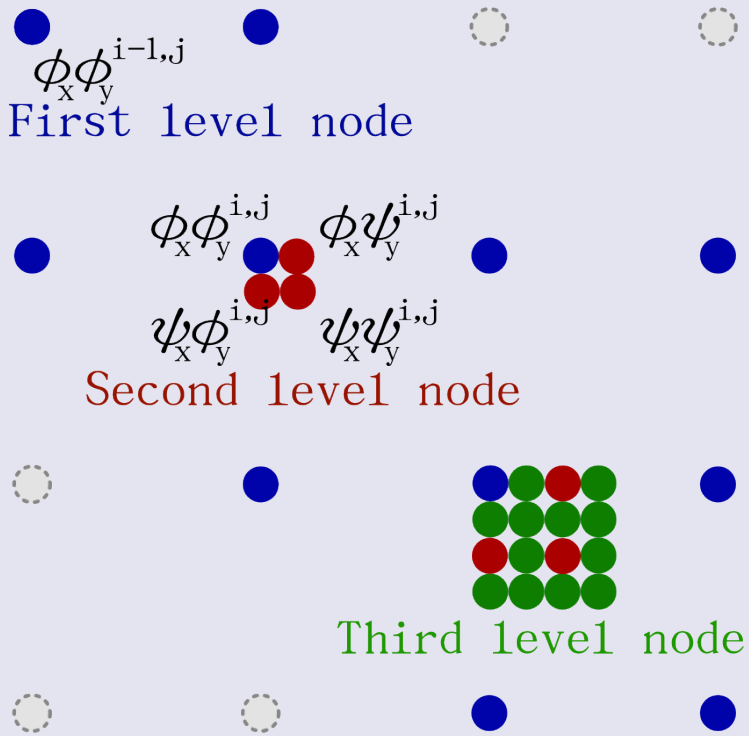
We increase the resolution without modifying the grid spacing

Going to a 3D basis-set

On a discretised mesh $[i,j,k]$ for one reslution:

$$f(i,j,k) = \sum_{l,m,n} c_{l,m,n} \Phi_l^{N_x}(i) \Phi_m^{N_y}(j) \Phi_n^{N_z}(k)$$

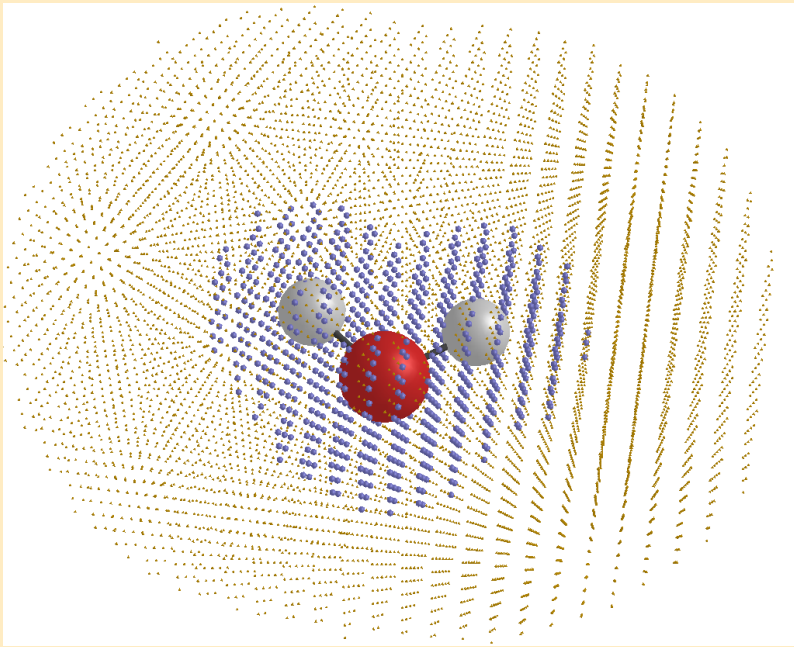
Schematic view for a multi-resolution grid in 2D



Wavelet properties: adaptivity

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

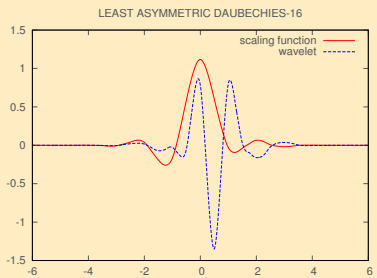
Optimal for big & inhomogeneous systems, highly flexible

Overview of wavelet families used in BigDFT code

Daubechies $f(x) = \sum_\ell c_\ell \phi_\ell(x)$

Orthogonal set

$$c_\ell = \int dx\, \phi_\ell(x) f(x)$$



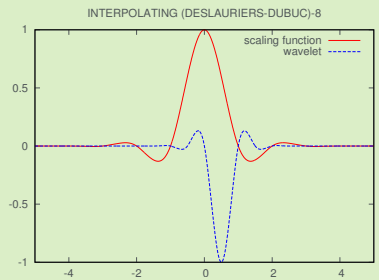
No need to calculate overlap matrix of basis functions

Used for wavefunctions, scalar products

Interpolating $f(x) = \sum_j f_j \varphi_j(x)$

Dual to dirac deltas

$$f_j = f(j)$$



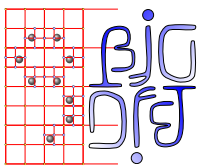
The expansion coefficients are the point values on a grid

Used for charge density, function products

Magic Filter method (A.Neelov, S. Goedecker)

The passage between the two basis sets can be performed without losing accuracy

Basis set features



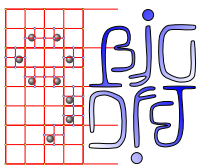
BigDFT features in a nutshell

- ✔ Arbitrary absolute precision can be achieved
  Good convergence ratio for real-space approach ($O(h^{14})$)
- ✔ 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

The DFT framework



The ground state is obtained by solving:

Schrödinger equation

$$H\Psi = E\Psi$$

- Expressed only for the electrons, using the Born-Oppenheimer approximation ;
- Solved in the framework of Kohn-Sham, using one particule wavefunctions ;
- Use of a self-consistency loop since the Hamiltonian H depends on Ψ.

What about wavelets?

Wavelets are the basis set for the representation of the wavefunctions. Thus things like XC approximation or Hellmann-Feynman theorem are still usable.

Elements of the Hamiltonian H

All classical parts present in plane-waves, can also be treated with wavelets.

The kinetic operator $\nabla^2\Psi$

Computed from the wavefunctions Ψ, applying a local filter.
Length for Daubechies is 28, see `isf_to_daub_kinetic()`.

Finite differences in 1D:
$\Delta f(x_n) = \frac{f(x_{n-1})-2f(x)+f(x_{n+1})}{h^2}$
is a filter of $(1,-2,1)$.

Precision is $O(h^{14})$ for arbitrary function. Even exact for linear combination of Daubechies functions:

$$f(x) = \sum_\ell c_\ell \phi_\ell(x), \qquad \nabla^2 f(x) = \sum_\ell \tilde{c}_\ell \phi_\ell(x),$$

$$\tilde{c}_\ell = \sum_j c_j a_{\ell-j}, \qquad a_\ell \equiv \int \phi_0(x)\partial_x^2\phi_\ell(x),$$

Elements of the Hamiltonian H

The non-local part of pseudo-potentials

Computed from the scalar product of wavefunctions Ψ and the projectors, in routine `applyprojectorsonthefly()`.

$$V_{\text{nonloc}} = \sum_{\ell} \sum_{ij} \sum_{m=-\ell}^{\ell} h_{ij}^{(\ell)} |p_i^{\ell,m}\rangle \langle p_j^{\ell,m}|$$

$$\langle \mathbf{r}|p_i^{\ell,m}\rangle = Y_{\ell,m}(\theta,\varphi) f_i^{(\ell)}(r_\ell) e^{-\frac{1}{2}\left(\frac{r}{r_\ell}\right)}$$

This is possible for GTH and HGH pseudo-potentials because of the spatial separability in their analytic expression.

Ongoing developments are done to include PAW pseudo-potentials.

Elements of the Hamiltonian H

The local potentials, V_H V_{xc} V_{psploc} & V_{ionic}

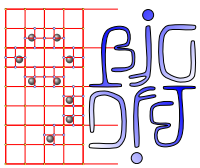
Hartree and ionic potentials are computed with a Poisson solver from the density $\rho(\vec{j})$.

$$V_H(\vec{j}) = \int d\vec{x}\, \frac{\rho(\vec{x})}{|\vec{x}-\vec{j}|}, \quad V_{xc}(\vec{j}) \text{ with LibXC routines and}$$
$$V_{\text{ionic}}(\vec{j}) = \sum_\kappa \int d\vec{x}\, \frac{Z_\kappa}{|\vec{x}-\vec{j}|}$$

This Poisson solver is:

- ✔ very fast and accurate, with optimal parallelisation ;
- ✔ can be used independently from the DFT code ;
- ✔ integrated quantities (energies) are easy to extract ;
- ✔ correct treatment of isolated boundary conditions and of charge offset ;
- ✘ non-adaptive, needs data uncompression.

Finding the fix point in Schrödinger equation



Two possible methods: the diagonalisation and the direct minimisation. The latter is fast and simple but restricted to systems with a non-zero HOMO-LUMO gap.

Direct minisation (systems with gap)

Classical gradient algorithms are applied for electronic minimisation: steepest descent or DIIS.

Diagonalisation (metallic systems)

Done within two loops, the inner one, non self consistent to find wavefunctions of a given hamiltonian, the outer one mixing either potential or density.

To improve convergency, preconditioning is done on the gradients $H\Psi$ using the routine `preconditionall()`. $(\frac{1}{2}\nabla^2 + C)\vec{p} = \vec{g}$ $\vec{p}$ is computed in an iterative way (CG).

The input guess, take a good start!

On the contrary to plane waves, wavelet representation requires a good input start for the minimisation loop.

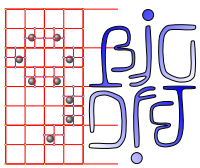
Using atomic orbitals

The input guess is based on atomic orbitals, using the following scheme:

- project gaussian atomic orbitals in a Daubechies wavelet basis set (see the `inputguess_gaussian_orbitals()` routine) ;
- compute the associated hamiltonian ;
- diagonalise it in this basis set ;
- use the lowest states as input for the calculation.

This is done in `input_wf_diag()` routine.

Additional computation after minimisation



Getting the Kohn-Sham wavefunctions

A diagonalisation is done on output of the minimisation loop by the `last_orthon()` routine.

Compute the forces

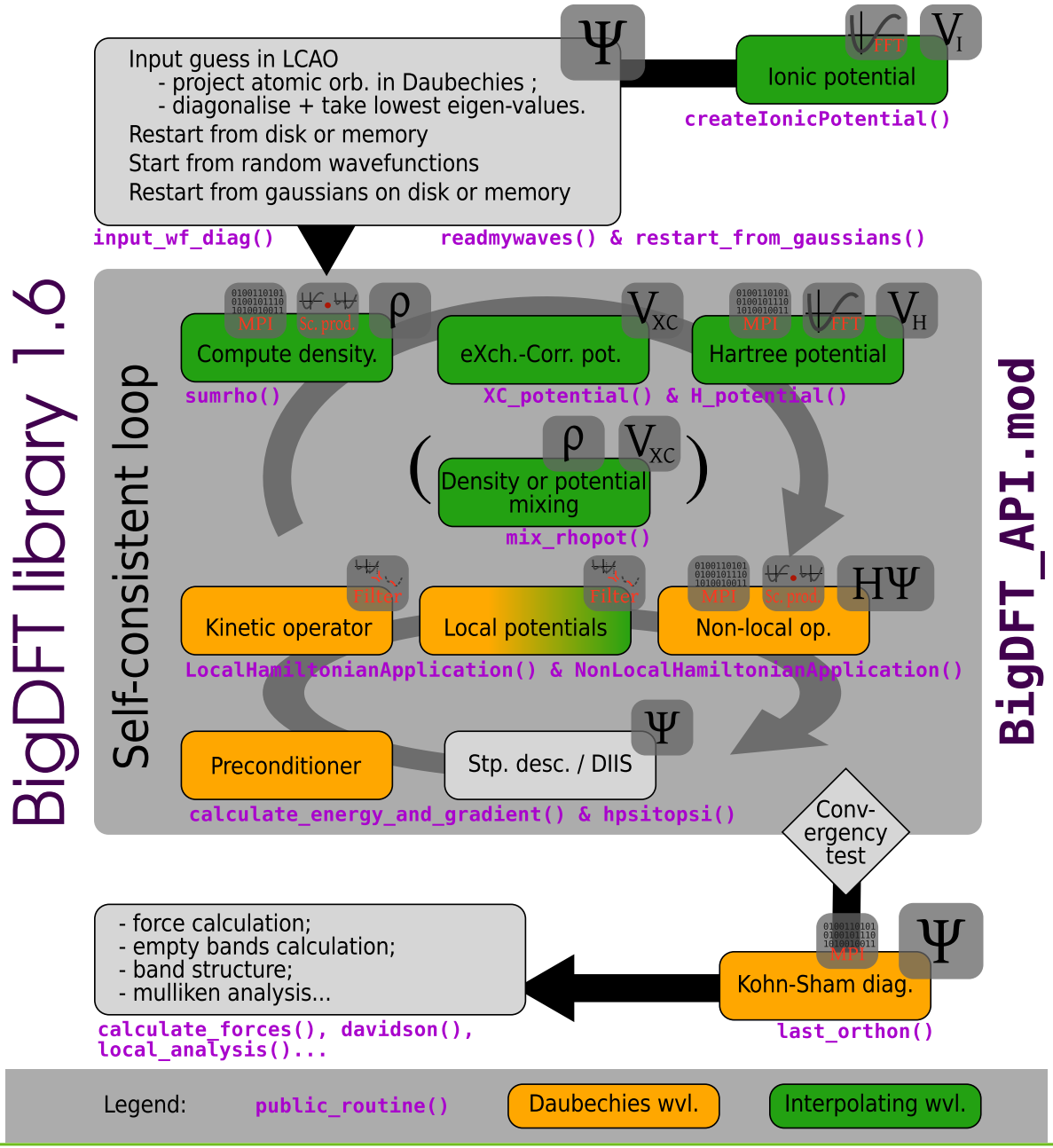
The forces are sum of three parts:

- the local contribution, computed with the Poisson solver, see `local_forces()` routine ;
- the non-local part, coming from the first derivatives of projectors, see `nonlocal_forces()` routine ;
- an optional contribution to to the non-linear core correction, see `rhocore_forces()` routine.

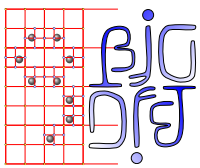
Finite-size effects - an error estimation

After convergency, the basis set can easily be expanded to estimate these effects.

Overview (code)



Outline



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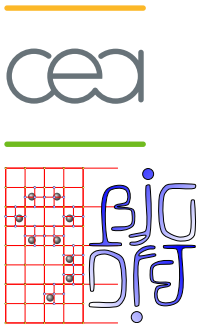
The BigDFT input files (or not)



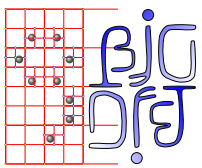
- `input.dft`: DFT related parameters;
- `input.geopt`: geometrie relaxations and MD;
- `input.kpt`: the *k*-point mesh and band structure path;
- `input.mix`: diagonalisation mechanism;
- `input.sic, tddft, occ, perf`: other parameters;
- `psppar.Element`: pseudo-potentials for each element;
- `posinp.xyz`: the atomic coordinates and box definition.

Only the coordinates are mandatory.
All lines of different input files are mandatory and output on BigDFT log. When BigDFT is run, all default values are output in files called `default.xxx`.

Naming scheme

All input files may be renamed by providing a `name` argument to the command line.

Atomic coordinate format



BigDFT uses `XYZ` format plus additional modifications:

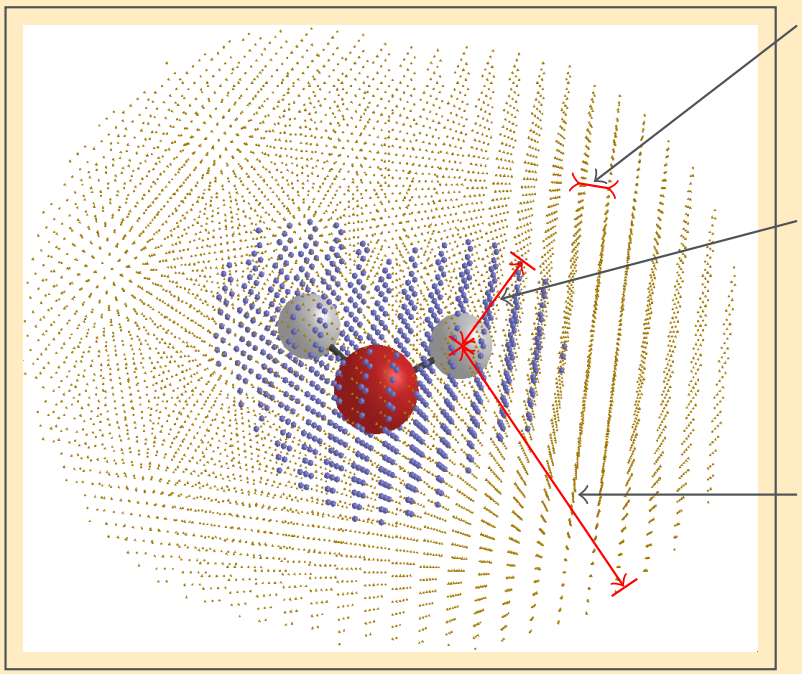
- physical unit, after the number of atoms on the first line put either `bohr` or `angstroem`.
- boundary conditions, on second line, start with one of `freeBC`, `surface` X_{lat} `0` Z_{lat} or `periodic` X_{lat} Y_{lat} Z_{lat}.
- frozen positions, add a `f`, `fy` or `fxz` at the end of an atom line.
- input polarisation, add values at the end of an atom line.

On output, forces are added for each element at the end of the XYZ file:

```
 2 angstroem
freeBC
Na -1 0 0
Cl +1 0 0
forces
Na 2.654367E-2 0 0
Cl -2.654367E-2 0 0
```

Defining the basis set in `input.dft`

Main specific variables to control the basis set



`hgrid` the grid size

`frmult` the expansion around atoms for fine grid

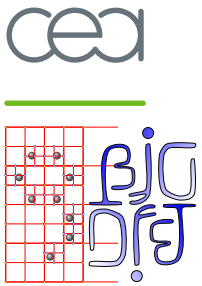
`crmult` the expansion around atoms for coarse grid

Convergence properties

- Decreasing `hgrid` $\rightarrow$ more degrees of freedom.
- Increasing `crmult` $\rightarrow$ less box constraint.

It is important to improve both parameters together to avoid error on one hiding improvement made on the other one.

How to compile BigDFT



Build system of BigDFT is based on *Autotools*.
BigDFT provides uncommon libraries (LibXC, LibABINIT) in its tar file and relies on *installed Lapack implementations*.

Compiling with Intel MKL

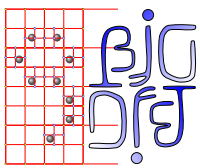
```
../configure -with-ext-linalg="-lmkl_intel_lp64
-lmkl_intel_thread -lmkl_core"
-with-ext-linalg-path="-L$MKLPATH" FC=mpif90
```

Comiling with OpenCL (or CUDA) support

```
../configure -enable-opencl
-with-ocl-path="/opt/cuda/4.1" FC=mpif90
```

CUDA is activated with equivalent options. Both can be activated at the same time.

How to run BigDFT



Some pre-processing

`bigdft-tool -n nprocs [name]`

Help to find the optimal number of processors for the run that fit into the computer memory. Also useful to check that all input files are without errors.

The main run

```
mpirun -np 6 bigdft [name] | tee [name].log
...
Number of MPI processes 5
MPI process does not use OpenMP

No material acceleration (iproc=0)
```

The outputs

- log is output on `stdout`, so redirect it.
- generated data are stored in a subdirectory called `data[-name]`.