ABINIT Developer Workshop

LIÈGE

Abilint and some adverts

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L_Sim

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First goal of abilint

Build automatically interfaces:
Compiler can check all arguments (help for the robustness of ABINIT)

- Detect call and functions:
  `48 directories, 1114 files, 23 modules, 1292 routines (from which 60 functions)`
- Create interfaces (src/defs/interfaces_03paw.F90)

```
interface
      function clp(x)
            use defs_basis
            real(dp) ::  clp
            real(dp),intent(in) ::  x
      end function clp
end interface
```

- Add `use interfaces_03paw` for each routines using the function `clp`

Features (Help of abilint)


```
abilint [options] <source> <dest>
-beautify beautify the code (experimental)
-graph=<routine1,routine2,...> or -graph=all
     build the graph of calls of the <routine>
in the file routine.ps
-graph=directories
     build the graph of interdependences
between directories
-help display this message
-libraries build the files lib/xxx/_xxx_
-lint complete analysis (experimental)
-nofatal no fatal message:  always generate
interfaces
-only=src/<dir> or -only=lib/<dir>
     build src/defs/interfaces_<dir>.F90
     only for the directory <dir>
-verbose display more information
```

Dependencies of directories


```
abilint.py -graph=directories .  .
dot -Tps -o directories.ps directories.dot
```

Need graphviz package

Perpectives

- Improve documentation
- Any suggestions are welcome

BigDFT: European project

Daubechies wavelets for electronic structure calculations

- T. D., A. Bergman, L. Genovese (CEA Grenoble)
- S. Goedecker, A. Ghazemi, A. Neelov, M. Rayson (Uni Basel)
- X. Gonze, P.M. Anglade, D. Caliste (Uni Louvain La Neuve)
- R. Schneider, F. Krüger, J. Piwonski (Uni Kiel)

http://www-drfmc.cea.fr/sp2m/L_Sim/BigDFT

Aim

To develop a linear scaling electronic structure code based on wavelets that can do density functional calculations for large systems such as found in nanosciences or biology

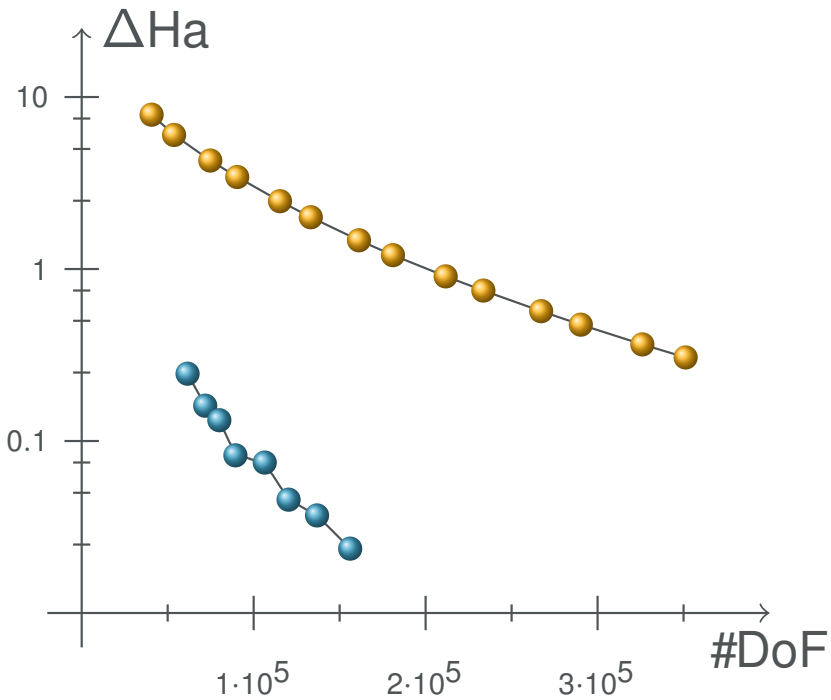
ABINIT 5.3

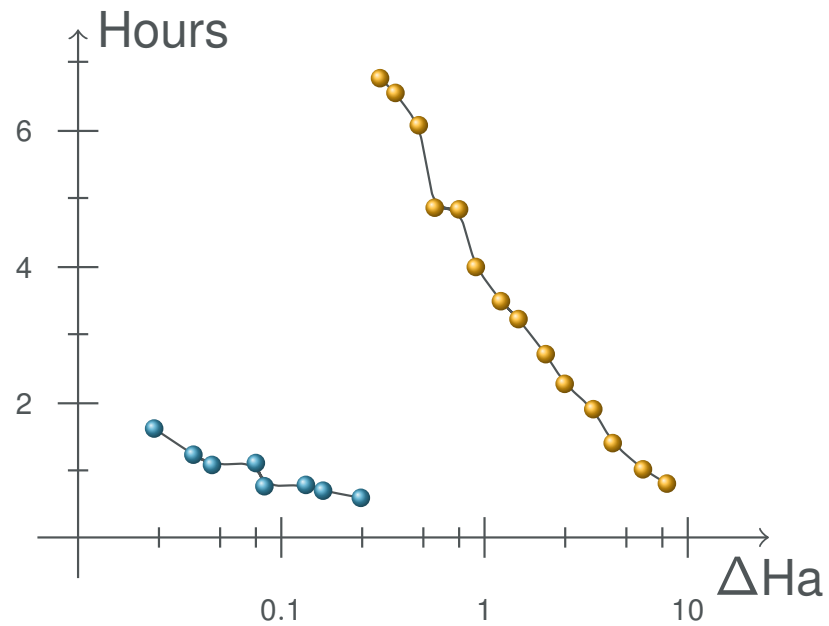
BigDFT INSIDE

- a talk from Damien Caliste and Luigi Genovese
- a poster about the BigDFT project
- a poster about adaptive Poisson solver

$C_{19}H_{22}N_2O$ (44 atoms, ∼30 Bohr)

Absolute precision tests: ABINIT BigDFT





Wiki

- Easy to install (apache, PHP, MySQL)
- Easy to use
- Easy to modify (authentification can be required)
  It is a kind of parallelisation

- Aim:
  - Complement of the forum
  - Complement of the documentation (code, tutorials)
  - About test or special cases