The ABINIT code

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Thanks to the > 50 ABINIT contributors, and especially to GM Rignanese for contributions to the slides

ABINIT software project

Ideas (1997) :

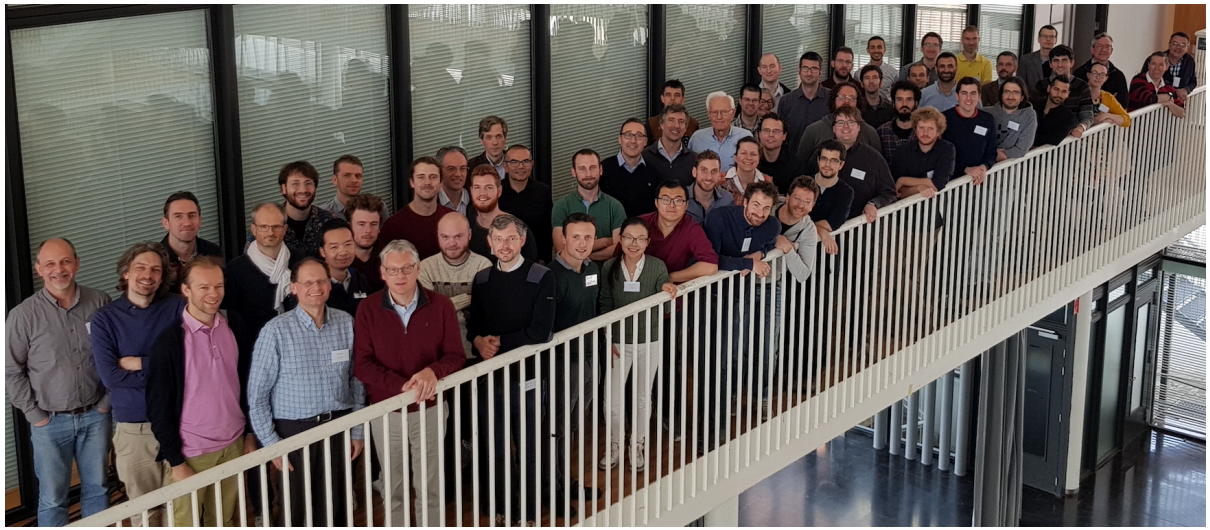
1) Software for first-principles simulations are more and more complex : needs a worldwide collaboration, of specialized, complementary, groups
2) Linux software development : 'free software' model

Now (2019) :

>2000 registered people on the forum
>800 kLines of F90 + many python scripts (abipy)
about 50 contributors to ABINITv8

Last release v8.10.3,
used in this school
http://www.abinit.org

Available freely
(GPL, like Linux).

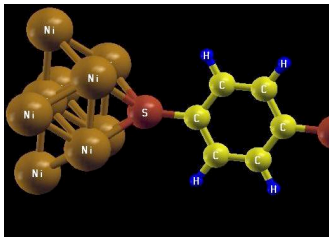


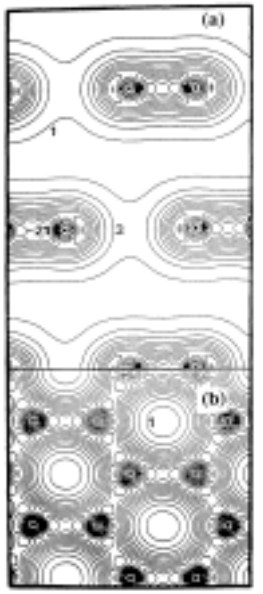
Properties from DFT+MBPT+ ...

Computation of ...

interatomic distances, angles, total energies

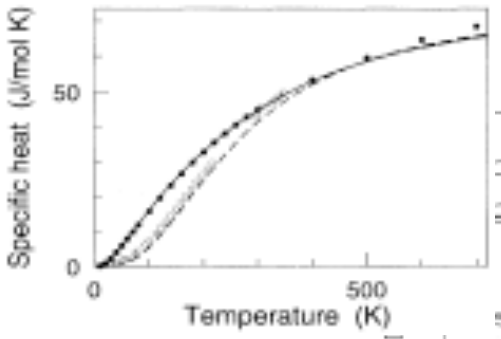
electronic charge densities, electronic energies

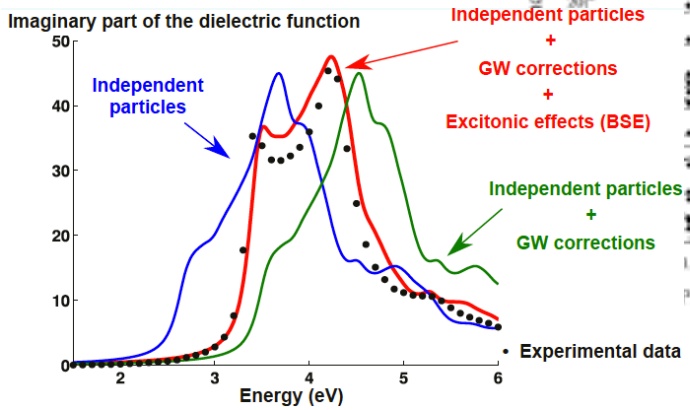


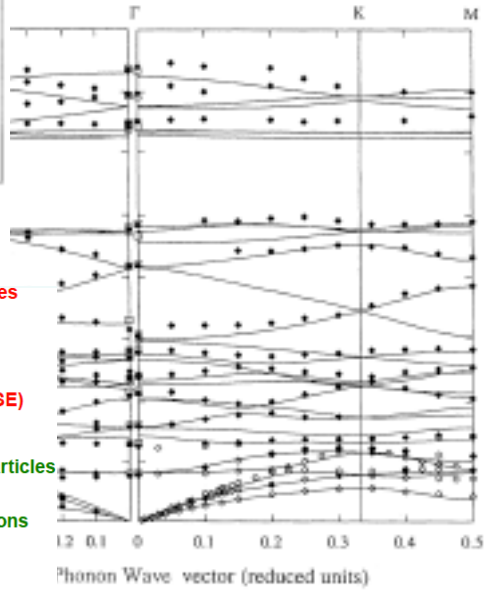


A basis for the computation of ...

- chemical reactions
- electronic transport
- vibrational properties
- thermal capacity
- dielectric behaviour
- optical response
- superconductivity
- surface properties
- spectroscopic responses
- ...







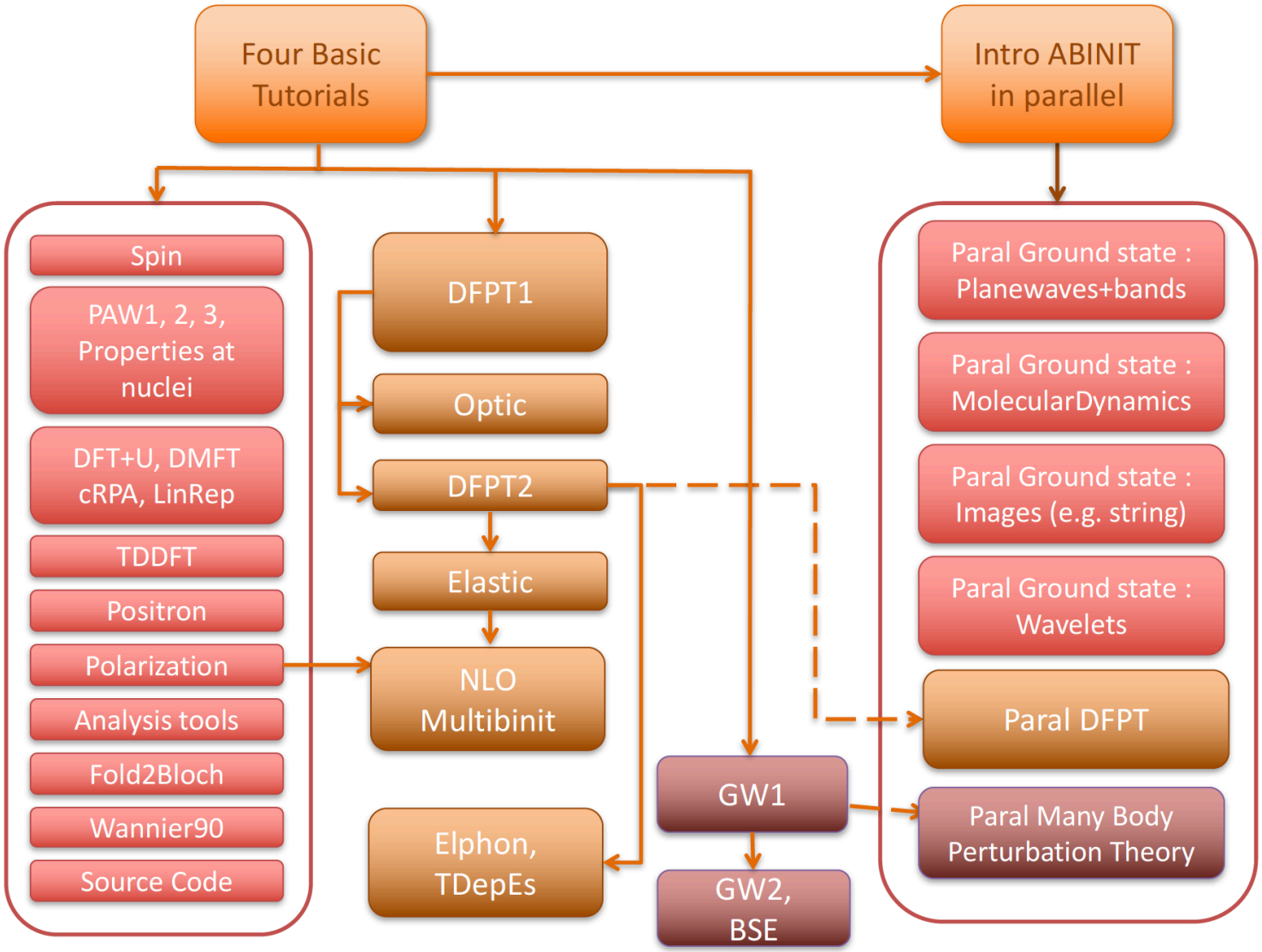
Basic Documentation

Web site http://www.abinit.org ; http://docs.abinit.org

- User's guides
- Installations notes
- List of input variables + description
- List of topics = a hub to input variables, files, tutorial, bibrefs
- over 800 example input files
- >30 tutorial lessons (each 1-2 hours)
  https://docs.abinit.org/tutorial

+ Forum Web site http://forum.abinit.org

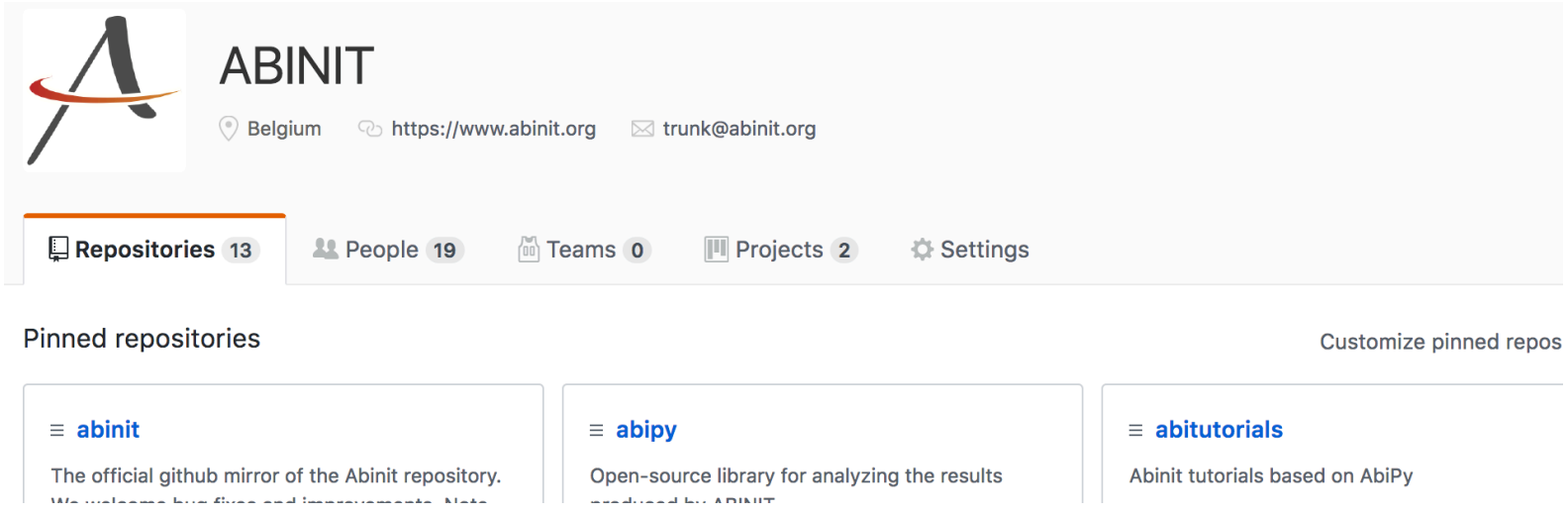
ABINIT tutorial : layout + dependencies



ABINIT + python : Abipy, Abitutorials …

ABINIT organization on GitHUB https://github.com/abinit

Abipy : python library for launching ABINIT jobs,
and analysing/plotting the results http://pythonhosted.org/abipy
=> e.g. connecting ABINIT with tools for high-throughput calculations developed in the Materials Project context (like Pymatgen, Fireworks).
Abitutorials : tutorial based on Jupyter notebooks ABINIT+python



Running ABINIT : basics

Density Functional Theory calculations

In ABINIT …

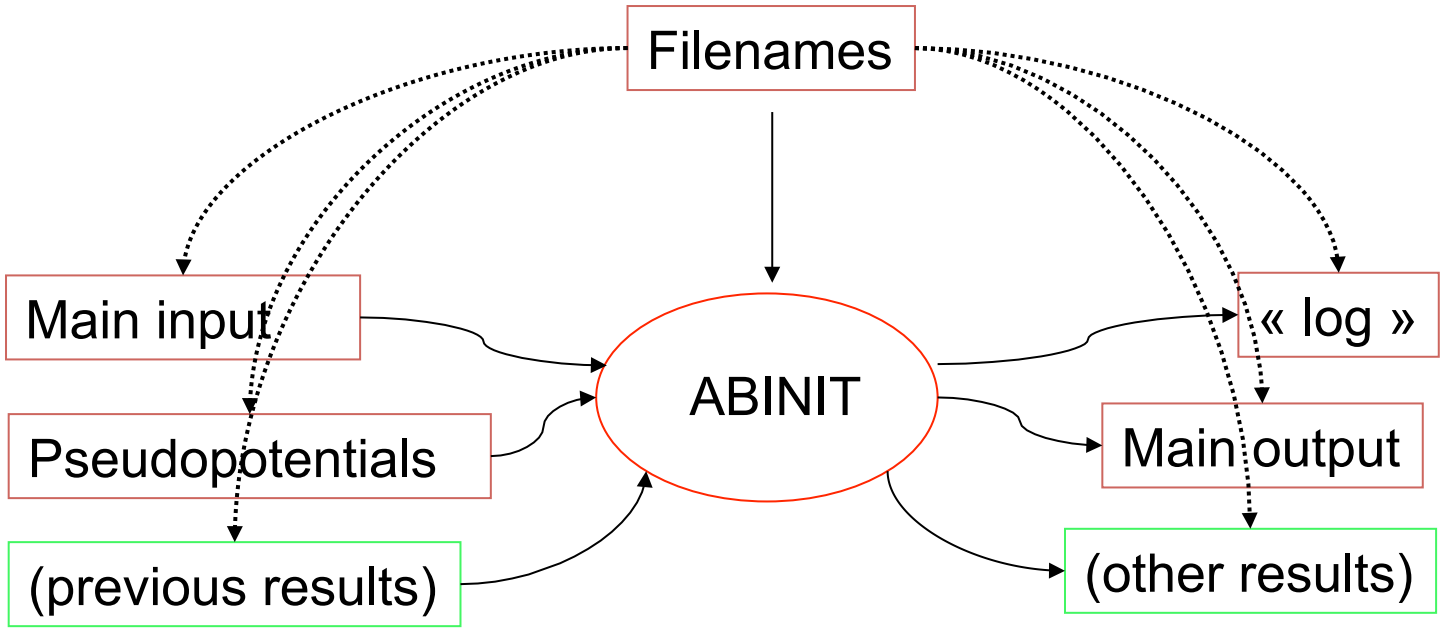
Representation of mathematical formalism
with a Plane Wave basis set :
- wavefunctions
- density, potential

Periodic boundary conditions
=> wavefunctions characterized by a wavevector (k-vector)

PseudoPotentials (or Projector Augmented Waves – PAW)

Iterative techniques to solve the equations
(Schrödinger equation ; DFT Self-consistency ; optimisation of atomic positions)

External files in a ABINIT run



Results :

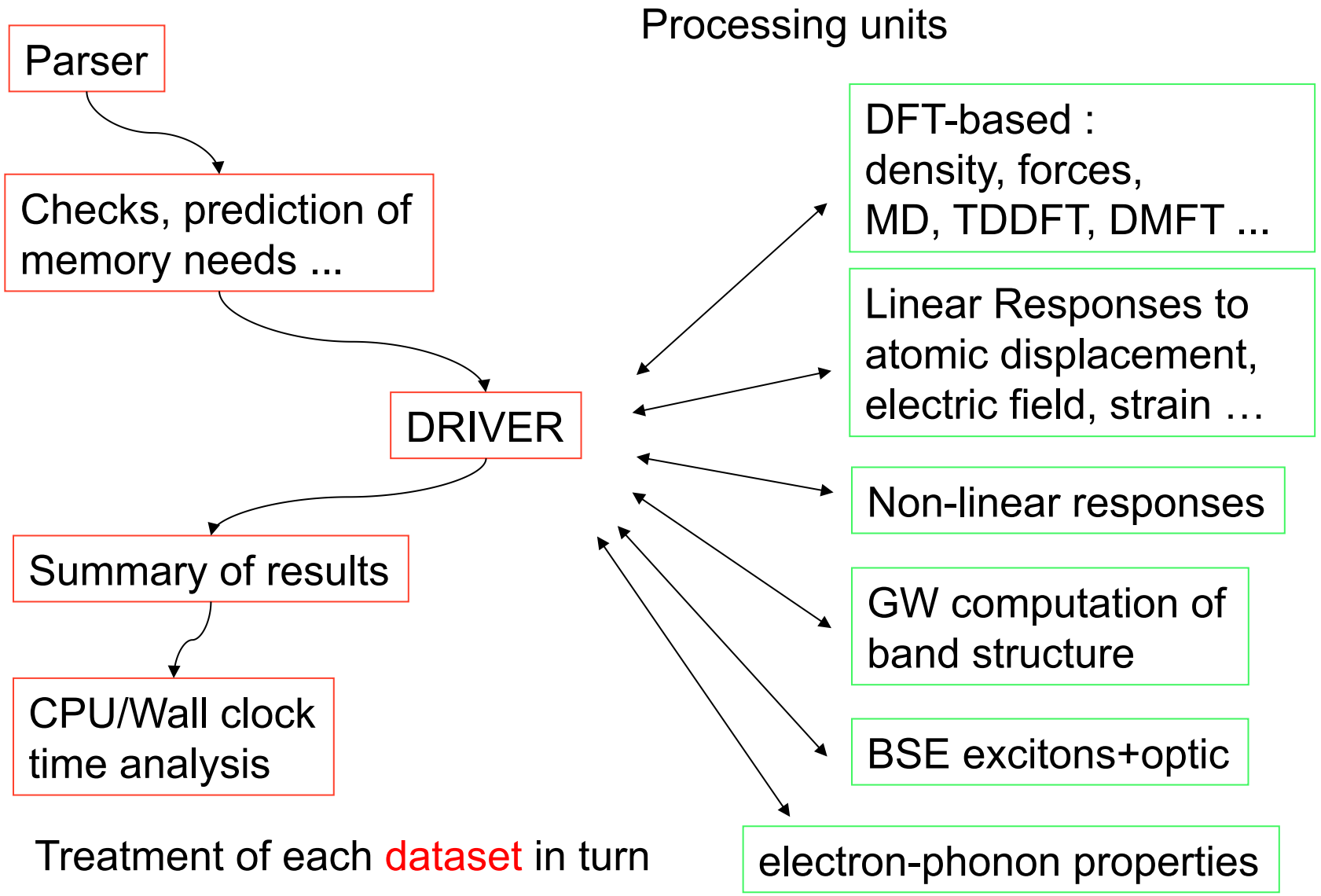
log, main output, energy derivatives (_DDB), ... – text files

density (_DEN), potential (_POT), wavefunctions (_WFK), ... – binary F90 files

or similar files in netCDF (_DEN.nc, _POT.nc, _WFK.nc)

Advantage of netCDF : portable, addressed by content, extensible, Python-friendly

ABINIT : the pipeline and the driver



Basic ‘files’ file : delivers filenames

h2.in	Name of input file
h2.out	Name of main output file
h2i	‘Root’ name for possibly other input files
h2o	‘Root’ name for possibly other output files
h2	‘Root’ name for temporary files
hydrogen.hgh	Name for the pseudopotential file for atoms of type 1
[oxygen.pspnc	Name for the pseudopotential file for atoms of type 2]
[92u.psp	Name for the pseudopotential file for atoms of type 3]

Made of at least 6 lines (more if > 1 type of atoms) with one name/address specified on each of these lines.

A basic ‘input’ file : dihydrogen (I)

```
# H2 molecule in big cubic box
# Characters after  ’#’ or after ‘!’ are comments, will be ignored.
# Keywords followed by values. Order of keywords in file is not important.

# Definition of the unit cell
acell 10 10 10          # Keyword "acell" refers to
                        #  lengths of primitive vectors (default in Bohr)
# Definition of the atom types
ntypat 1                # Only one type of atom
znucl 1                 # Keyword "znucl" refers to atomic number of
                        # possible type(s) of atom. Pseudopotential(s)
                        # mentioned in "filenames" file must correspond
                        # to type(s) of atom. Here, the only type is Hydrogen.
# Definition of the atoms
natom 2                 # Two atoms
typat 1 1               # Both are of type 1, that is, Hydrogen
xcart                   # This keyword indicate that location of the atoms
                        # will follow, one triplet of number for each atom
  -0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 1, in Bohr
   0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 2, in Bohr
```

A basic input file : dihydrogen (II)

```
# Definition of planewave basis set
ecut 10.0          # Maximal plane-wave kinetic energy cut-off, in Hartree

# Definition of k-point grid
kptopt 0           # Enter k points manually
nkpt 1             # Only one k point is needed for isolated system,
                   # taken by default to be 0.0 0.0 0.0

#Definition of SCF (self-consistent field) procedure
nstep 10           # Maximal number of SCF cycles
toldfe 1.0d-6      # Will stop when, twice in a row, the difference
                   # between two consecutive evaluations of total energy
                   # differs by less than toldfe (default in Hartree)
diemac 2.0         # Although this is not mandatory, it is worth to precondition the
                   # SCF cycle. A model dielectric function, used as standard
                   # preconditioner, is described in "dielng" input variable section.
                   # Here, we follow prescriptions for molecules in a big box
## After modifying the following section, one might need to …
#%%<BEGIN TEST_INFO>          Metadata … to be ignored in the tutorial !
```