The ABINIT software project : a very brief description

ABINIT in brief

Chronology :

- Precursor : the Corning PW code (commercialized 1992-1995 by Biosym)
- 1997 : beginning of the ABINIT project
- Dec 2000 : release of ABINITv3 under the GNU General Public License (GPL)
- Nov 2002 : 1st int. ABINIT developer workshop (Louvain-la-Neuve, Belgium)
- May 2004 : 2nd int. ABINIT developer workshop (Paris)
- As of Sept 2004 : 600 addresses in the main mailing list, 150 addresses in the developers mailing list

A "free" software : comes under the GNU General Public Licence (GPL)

- freedom 1 : unlimited use for any purpose
- freedom 2 : study and modify for your needs (need source access !)
- freedom 3 : copy
- freedom 4 : distribute modifications

+ protection of these freedoms (http://www.gnu.org/copyleft/gpl.html)

ABINIT v4.4 capabilities (I)

Pseudopotentials/Plane Waves

(soon, Projector Augmented Waves in production)

Many pseudopotential types, but no ultra-soft psps

Density functional : LDA, GGA (PBE and variations, HCTH)

+ some advanced functionals (exact exchange + RPA or ...)

TDDFT (following Cassida) / GW for excitation energies

Periodic systems / finite systems in the supercell geometry

Insulators/metals - smearings : Fermi, Gaussian, Gauss-Hermite ...

Automatic k-point sampler

Symmetry analyser (database of the 230 spatial groups, and the 1191 Shubnikov magnetic groups)

Collinear spin / non-collinear spin / spin-orbit coupling

ABINIT v4.4 capabilities (II)

Forces, stresses, automatic optimisation of atomic positions and unit cell parameters (Broyden and Molecular dynamics with damping)

Molecular dynamics (Verlet or Numerov), Nosé thermostat, Langevin dynamics

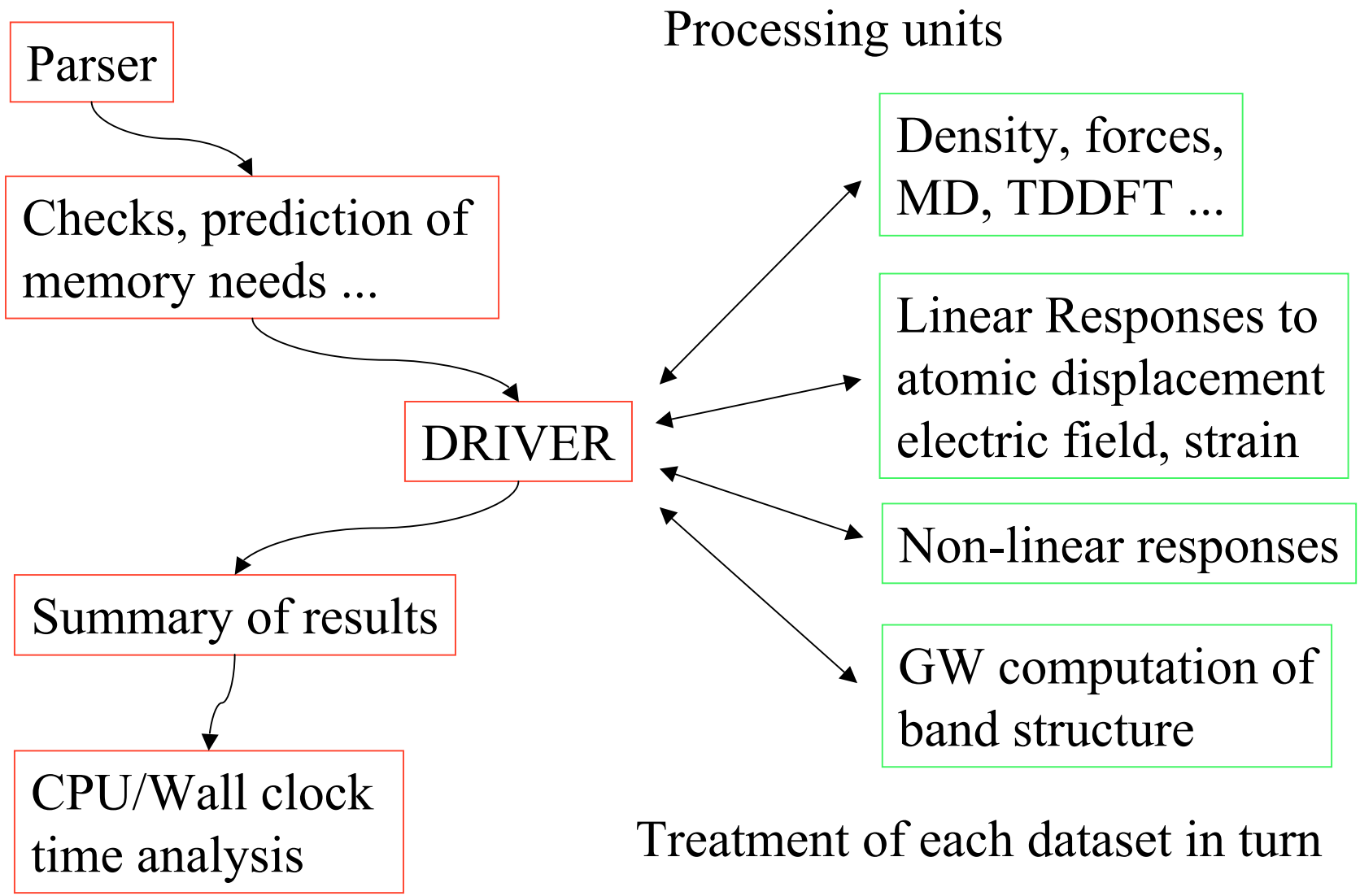
Density-Functional Perturbation Theory :

- Responses to atomic displacements
- Responses to static homogeneous electric field
- Responses to strain perturbations
- Altogether, giving access to : dielectric tensor, Born effective charges, dynamical matrices at any wavevector, phonon frequencies, force constants, phonon DOS, thermodynamic properties in the quasi-harmonic approximation, elastic constants, internal strain, electron-phonon coupling ...
- Non-linear responses thanks to the 2n+1 theorem - at present : non-linear dielectric susceptibility; Raman cross-section ; electro-optic tensor

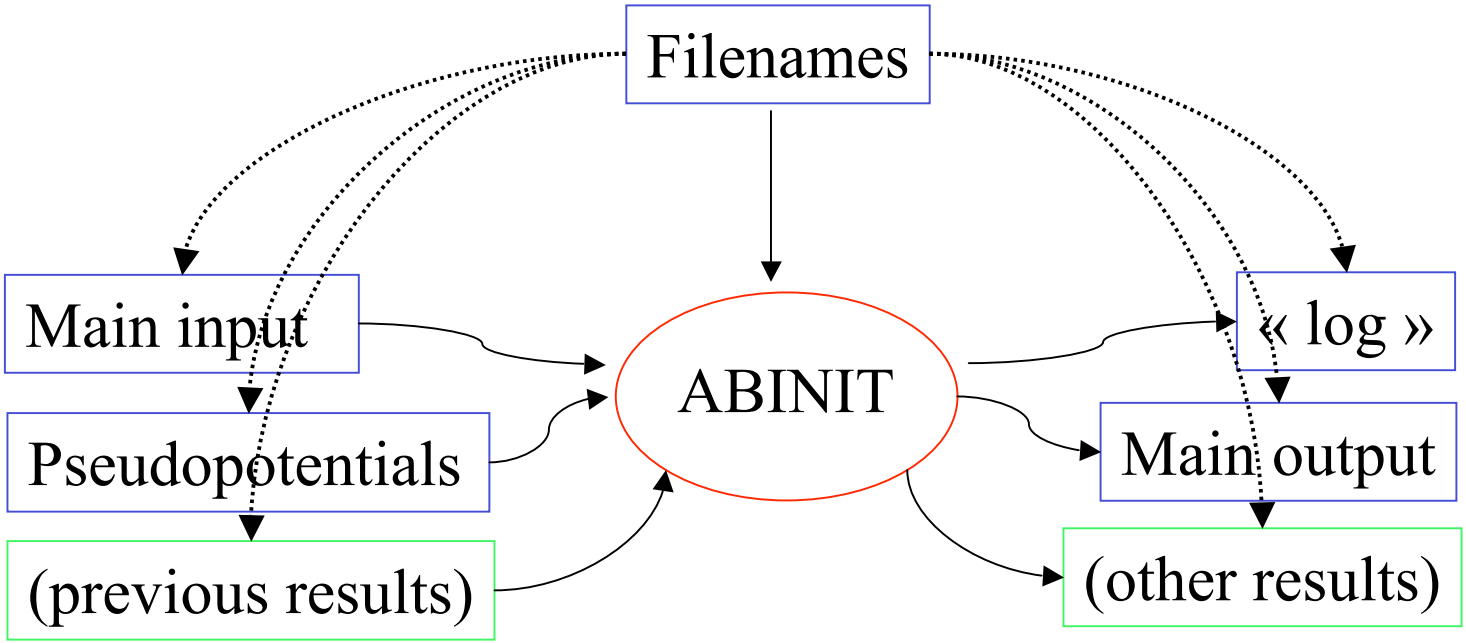
Susceptibility matrix by sum over states (Adler-Wiser)

Optical (linear + non-linear) spectra by sum over states

ABINIT : the pipeline and the driver



External files in a ABINIT run



Results : density (_DEN), potential (_POT),
wavefunctions (_WFK ; _KSS), ...

Then : post-processing (density analysis, wavefunction analysis,
dynamical matrix analysis, electron-phonon coupling,
optical spectra ...)

Distributed development : the groups

Major active contributors :

- Louvain-la-neuve, Belgium (JM Beuken, J Bouchet, F Detraux, X Gonze, Y Pouillon, GM Rignanese, L Sindic, M Verstraete ...)
- CEA Bruyères Paris, France (M Boulet, G Jomard, F Jollet, V Recoules, A Roy, M Torrent, G Zérah ...)
- Liège, Belgium (Ph Ghosez, JY Raty, M Veithen)
- Mitsubishi Chem. Corp., Japan (Mikami-san)
- Palaiseau Paris, France (V. Olevano, F. Bruneval ...)
- Rutgers, USA (D. Hamann, D. Vanderbilt)

also :

- Corning Inc. USA (DC. Allan)

+ Many other contributors

http://www.abinit.org