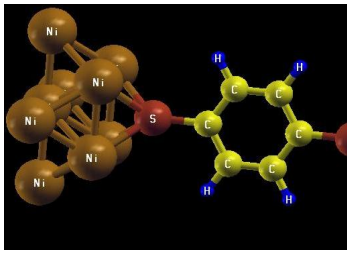
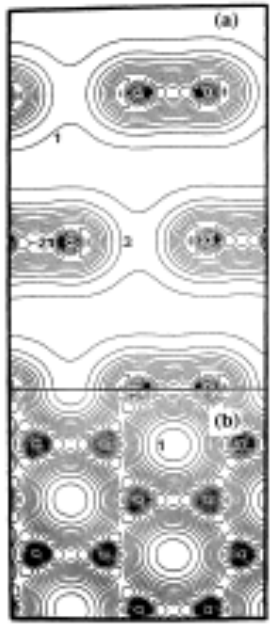
Guided tour of ABINIT : First-principles study of material properties

> 40 ABINIT contributors yearly …

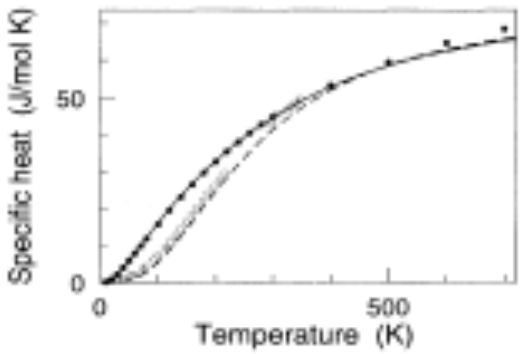
Properties from first principles

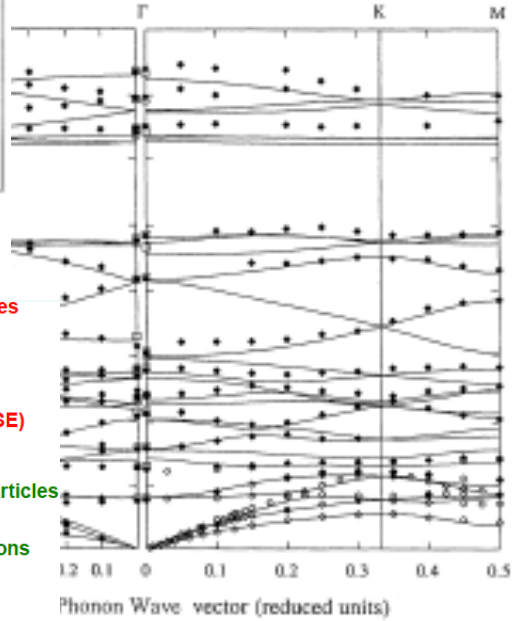
Computation of simple properties …
- interatomic distances, angles, total energies
- electronic charge densities, electronic energies

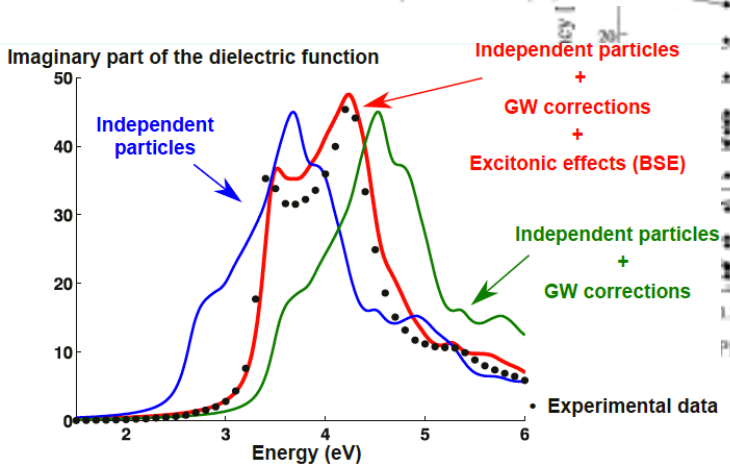




Followed by more complex ones ...
- vibrational properties
- thermal capacity
- dielectric behaviour
- optical response
- superconductivity
- surface properties
- spectroscopic responses
- piezoelectricity
- electronic transport
- ...







ABINIT software project

Ideas (1997) :

1) Software applications for first-principles simulations are more and more sophisticated :
   one needs a worldwide collaboration,
   of specialized, complementary, groups
2) Linux software development : ‘free software’ model

Now (2017) :

>1700 registered people on the forum
800 kLines of F90
about 60 contributors to ABINITv7

ABINIT milestones

- 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 – May 2017 : 8 international ABINIT developer workshops
  (between 35 and 60 participants each)
- Jan 2010 : launch of the Forum

Participants to the Frejus 2017 Int. ABINIT developer workshop

A few references

- Description of the ABINIT project and ABINIT capabilities

  X. Gonze et al, Comput. Mat. Science 25, 478 (2002)

  X. Gonze et al, Z. Kristallogr. 220, 558 (2005)

  X. Gonze et al, Comp. Phys. Comm. 180, 2582 (2009)

  X. Gonze et al, Comp. Phys. Comm. 205, 106 (2016)

- Software engineering and management techniques used in ABINIT

  Y. Pouillon et al, Computing in Science and Engineering 13, 62 (2011)

- File format description (ETSF-IO)

  X. Gonze et al, Comput. Mat. Science 43, 1056 (2008)

- Focused papers on specific implementations within ABINIT

  (e.g. PAW, parallelism)

  M. Torrent et al, Comput. Mat. Science 42, 337 (2008)

  F. Bottin et al, Comp. Mat. Science 42, 329 (2008)

Guided tour …

1. Capabilities
2. License
3. Reliability, portability
4. Documentation
5. Miscellaneous

Capabilities

ABINIT v8 capabilities (I)

Methodologies

Pseudopotentials/Plane Waves
+ Projector Augmented Waves (for selected capabilities)
    Many pseudopotential types, different PAW generators
        (ATOMPAW is shipped with ABINIT)

Density functionals : LDA, GGA (many : PBE and variations, HCTH, ...),
    LDA+U (or GGA+U)
    hybrid functionals + some advanced functionals (exact exchange + RPA or ...)
LR-TDDFT for finite systems excitation energies (Casida)
GW for accurate electronic eigenenergies
    (4 plasmon-pole models or contour integration ; non-self-consistent / partly self-consistent / quasiparticle self-consistent ; spin-polarized)
Bethe-Salpeter for accurate optical properties calculations
Dynamical mean field-theory for strongly-correlated materials

ABINIT v8 capabilities (II)

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

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

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

Path-Integral Molecular Dynamics, String / NEB method for saddle points

Susceptibility matrix by sum over states (Adler-Wiser)

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

Polarization, finite electric field calculations

Electric field gradients

Positron lifetime

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

ABINIT v8 capabilities (III)

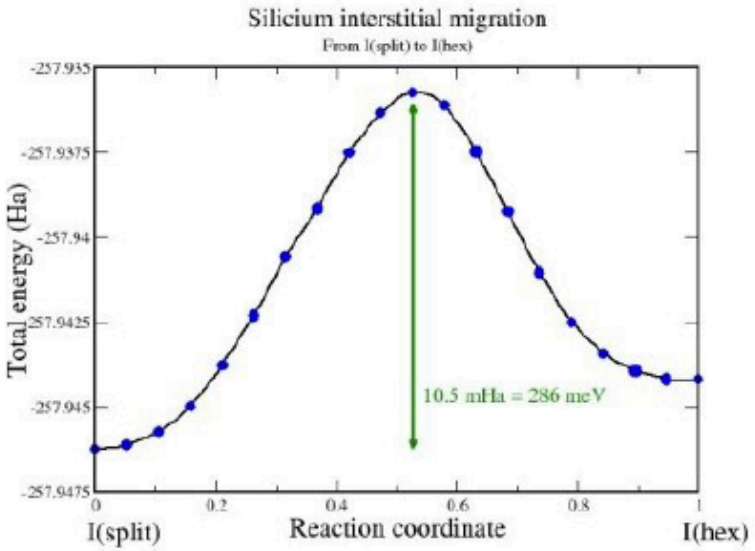
Density-Functional Perturbation Theory :

- Responses to atomic displacements, to static homogeneous electric field, to strain perturbations

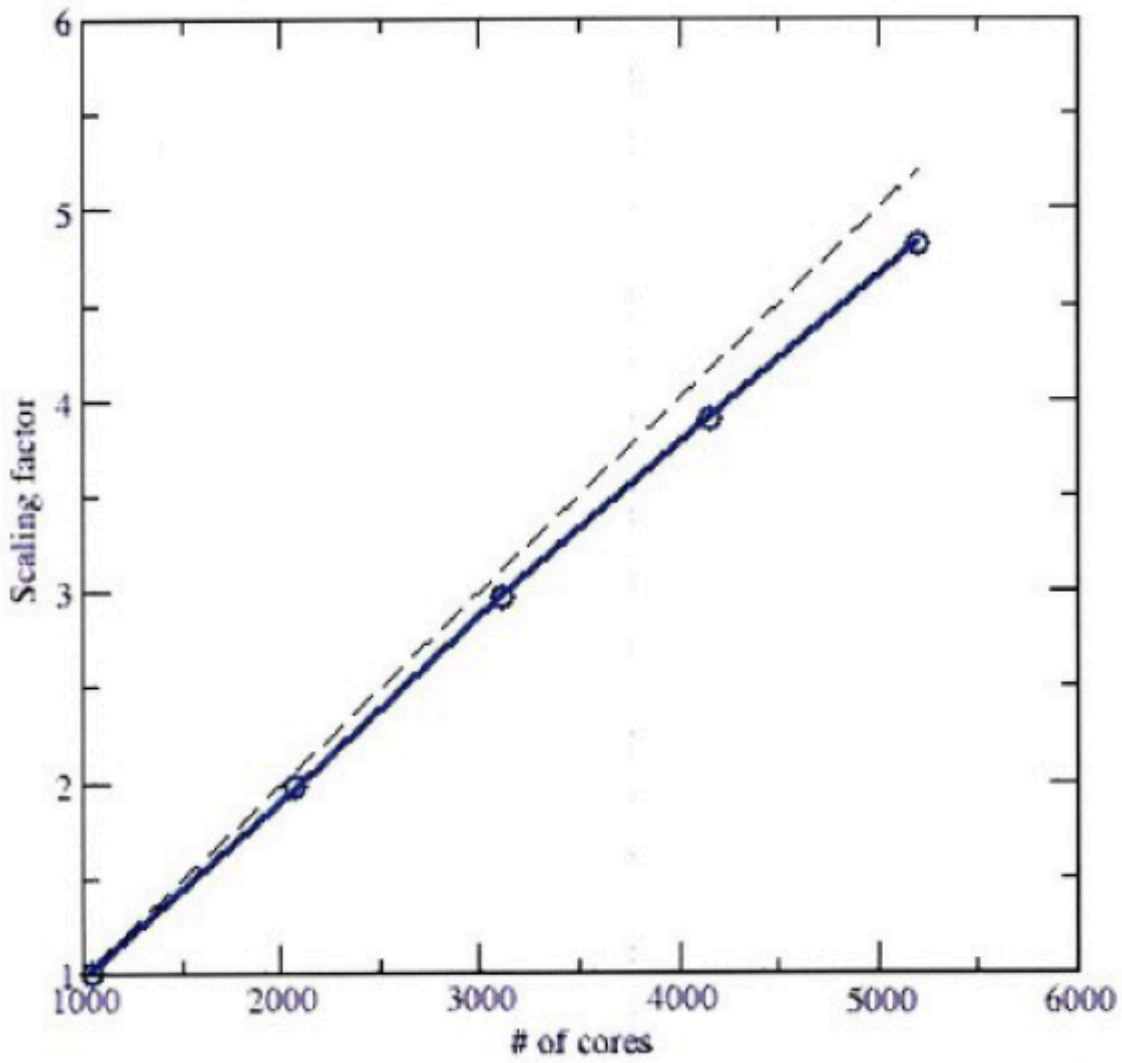
- Second-order derivatives of the energy, giving direct access to :
  dynamical matrices at any q, phonon frequencies, force constants ;
  phonon DOS, thermodynamic properties (quasi-harmonic approximation) ;
  dielectric tensor, Born effective charges ;
  elastic constants, internal strain ;
  piezoelectric tensor ...
- Matrix elements, giving direct access to :
  electron-phonon coupling, deformation potentials, superconductivity,
  temperature-depedence of the electronic structure
- Non-linear responses thanks to the 2n+1 theorem - at present :
  non-linear dielectric susceptibility; Raman cross-section ;
  electro-optic tensor

Parallelisation : four levels

Parallelisation over space, bands, wavevectors, images can be used simultaneously



Test case: calculation of the energy barrier between two positions of a silicon interstitial atom
65 silicon atoms ; 20 images of the cell
4 *k-points*; 130 bands; PAW method



ABINIT goes high-throughput : Abipy

Abipy is a library for launching ABINIT jobs,
and analysing/plotting the results
http://pythonhosted.org/abipy

=> connecting ABINIT with tools for high-throughput calculations developed in the Materials Project context (e.g. Pymatgen, Fireworks).

See ABINIT Github Web site
http://github.com/abinit

The broader picture ... couplings ...

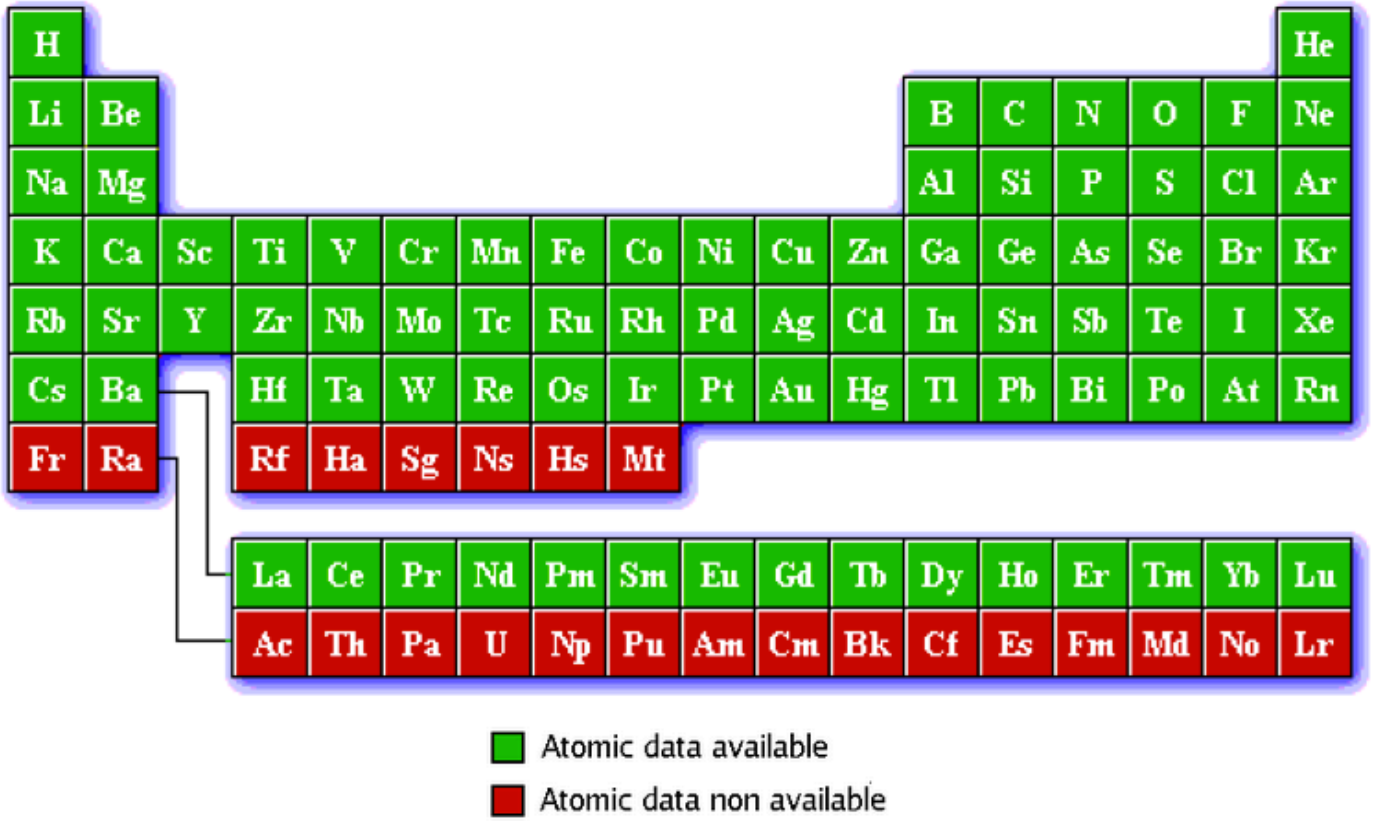
- Through files :
  - With pseudopotential generators
    (FHI98PP, OPIUM, APE, ATOMPAW, ONCVPSP, USPP, UPF ...)
  - With file “postprocessors”
    (EXC, DP, YAMBO, V_SIM, XCRYSDEN, Pymatgen)
- Through libraries :
  - LibXC (from OCTOPUS), WANNIER90
- Also with packagers :
  - Debian, Gentoo, Ubuntu

Pseudopotentials/PAW data in ABINIT

- Preferred PAW atomic dataset table : JTH v1.0

  http://www.abinit.org/download/atomic-data-files

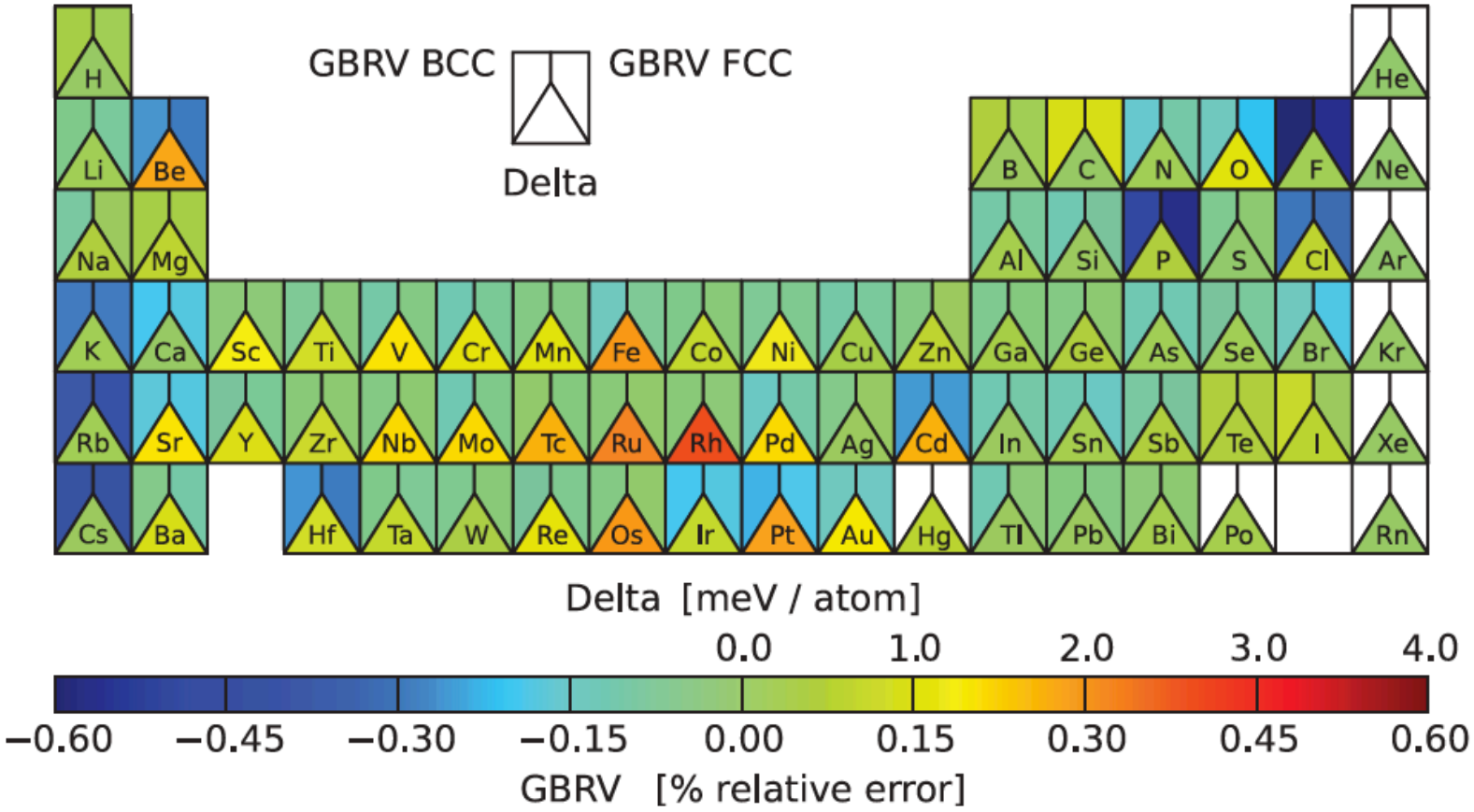
  See Jollet, Torrent, Holzwarth, Computer Physics Comm. 185, 1246 (2014)



Also, possibility to use : GPAW table, GBRV v1.0 table, or norm-conserving pseudopotentials (e.g. ONVC pseudo generator), or many other pseudos …

Assessment of precision : NC, PAW

ONCVPSP PBE table



License

The “Free” software concept

Free for freedom (also price ...)

- 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

From copyright to freedom (“copyleft”)

- copyright allows licensing
- licenses grants freedom

Terminology : Free software=Open source=Libre software

ABINIT pioneered the use of the GPL « Free software license » in the computational condensed matter community (2000)

http://www.abinit.org : download, documentation ...

Reliability / portability

Quality control : test suite + test farm

How to secure existing capabilitites despite the development efforts (by diverse groups) and associated bug generation ?

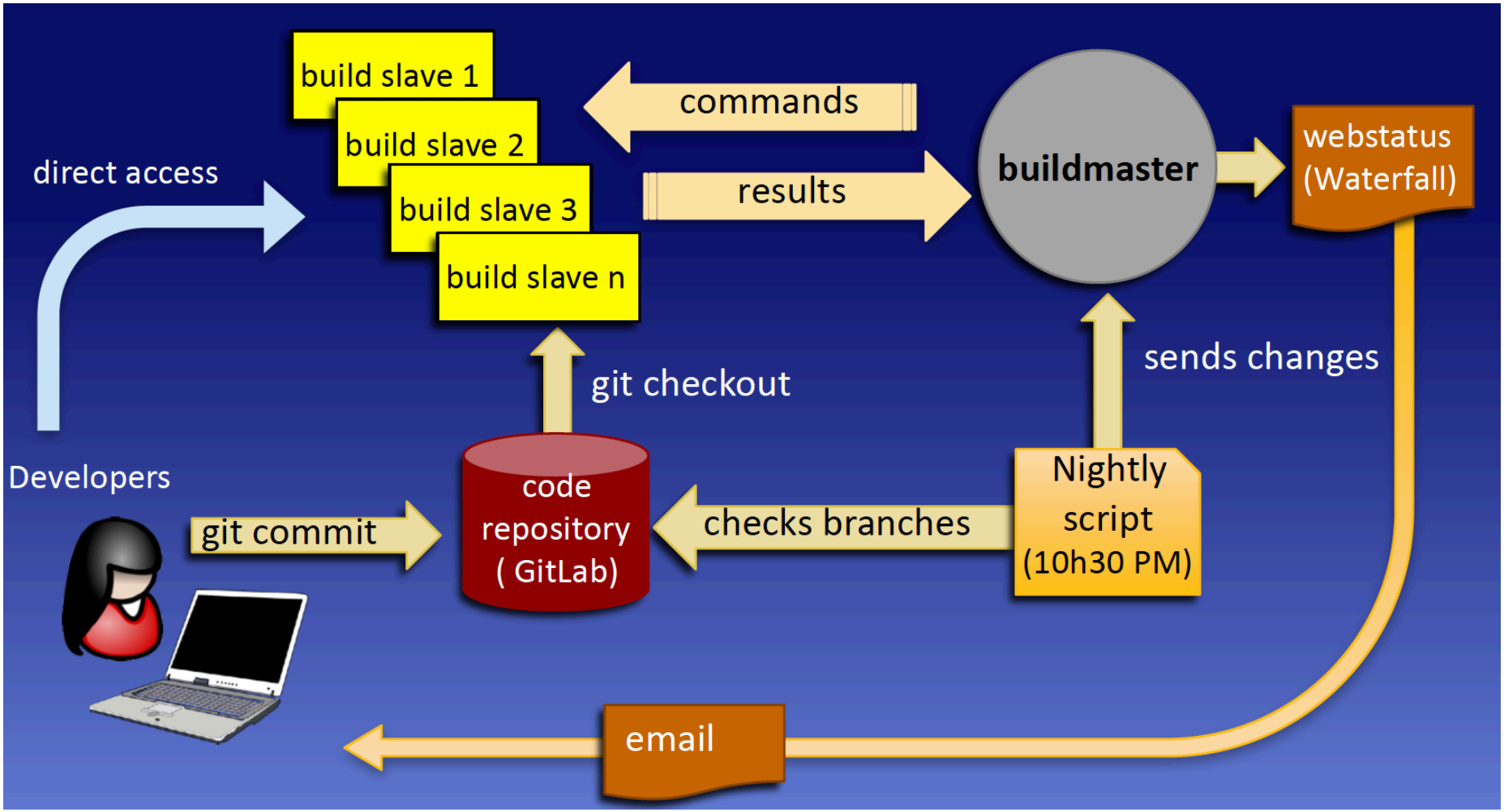
Test suite : >1000 automatic tests (+ new added for each capability)

Test farm : >12 computers (4 to 48 cores)

with 4 compilers (gfort, Intel, NAG, XLF) => over 20 'builders'

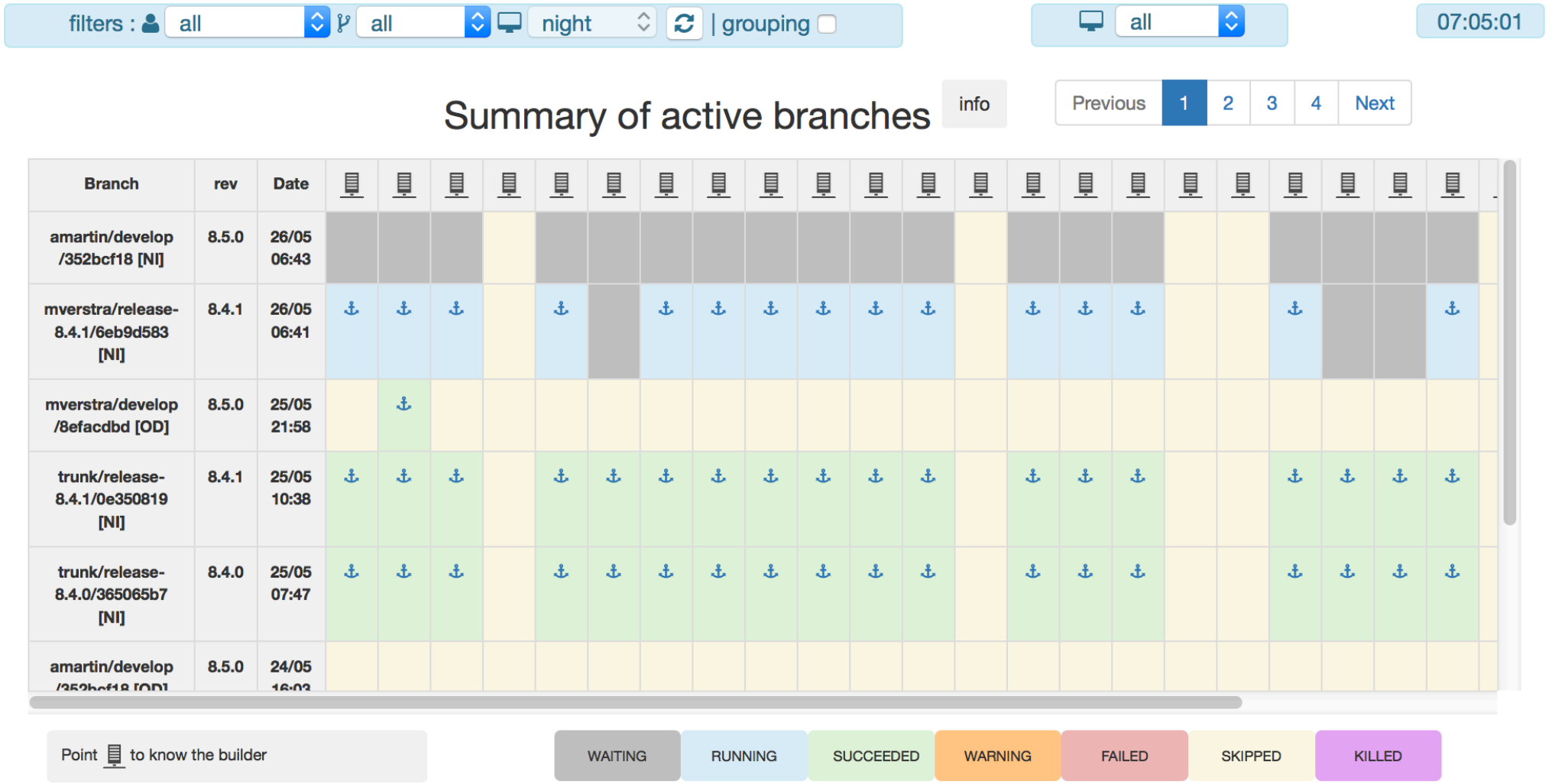
Name	Brand	CPU / Freq	# cores	RAM	OS	misc
abiref	HP DL360 gen9	Xeon E5-2670v3/ 2.30	2 x 24	32GB	CentOS 7.2	Ref
bob	Dell R430	Xeon E5-2603v3/ 1.60	2 x 6	8GB	Fedora 23	
buda	SuperMicro	Xeon X5570/ 2.7	2 x 4	12GB	CentOS 6.8	2xGPU K40 2xGPU C1060
coba2	HP Z400	Xeon W3520/ 2.7	4	12GB	CentOS 6.5	
cronos	HP DL185 G7	AMD Opteron 6276/ 2.3	2 x 16	16GB	Debian 5.0	
graphene	Apple MacPro	Xeon E5-2697/ 2.7	1 x 12	64GB	MacOS X 10.12	
ibm8	IBM Power S824	Power8/ 3.0	4	8GB	AIX 7.2	
inca	virtual machine	Opteron 6276/ 2.3	12	30GB	CentOS 6.9	
max2	HP DL185	Opteron 6140/ 2.6	2 x 8	12GB	Slinux 6.1	
petrus	Intel	Core i7 3930/ 3.2	6	16GB	openSUSE 12.1	
testf	Bull Novascale	Xeon X5570/ 2.9	2 x 4	12GB	CentOS 5.11	
tikal	Dell T5500	Xeon X5647/ 3.0	8	8GB	Slinux 6.9	
ubu	HP DL360 gen9	Xeon E5-2670v3/ 2.30	2 x 24	32GB	Ubuntu 16.04	

ETSF Test farm, under buildbot



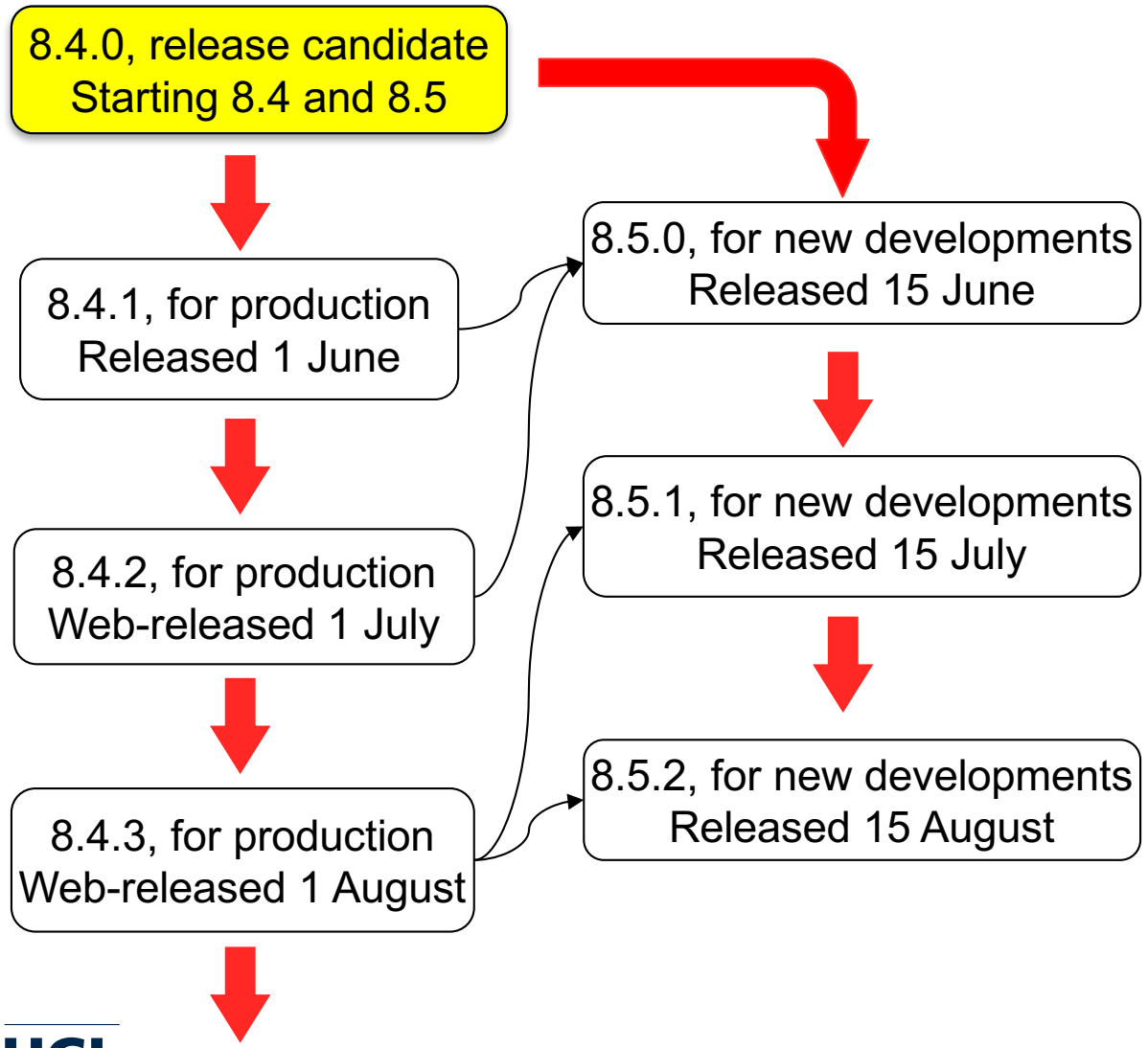
Web-delivered analysis of tests

Cross branch / builder success table



Distributed development: versioning scheme

Iterative procedure :



Version management :

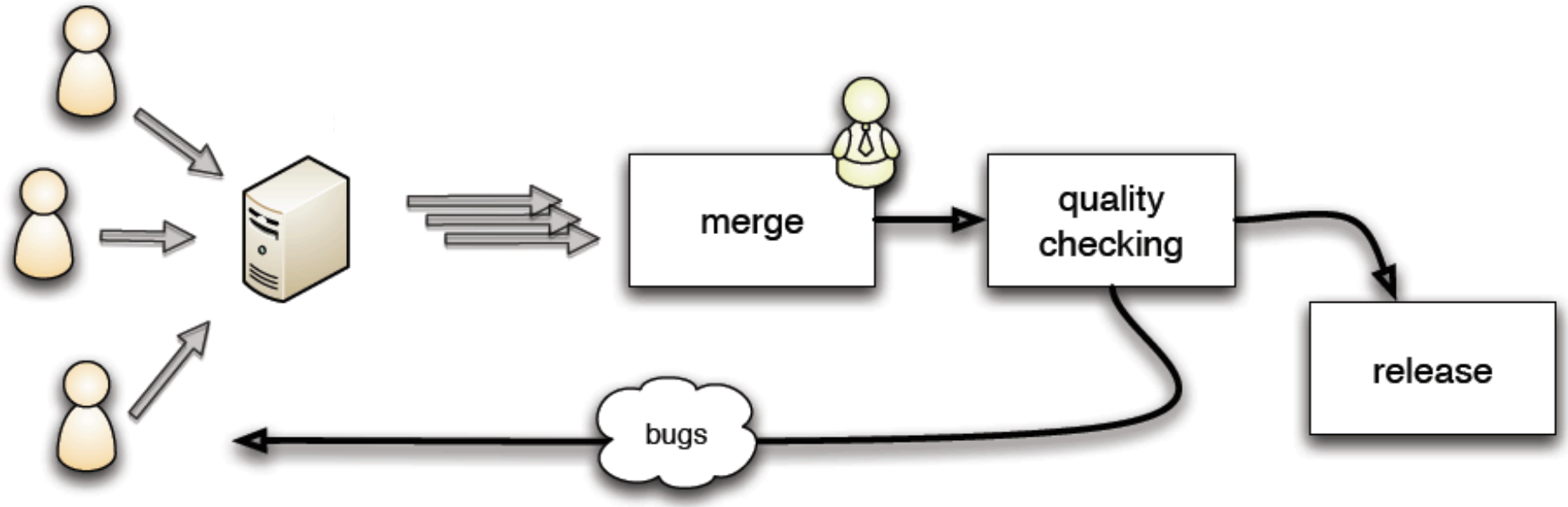
"git" software

Several git branches
for each developer,
for each ABINIT version

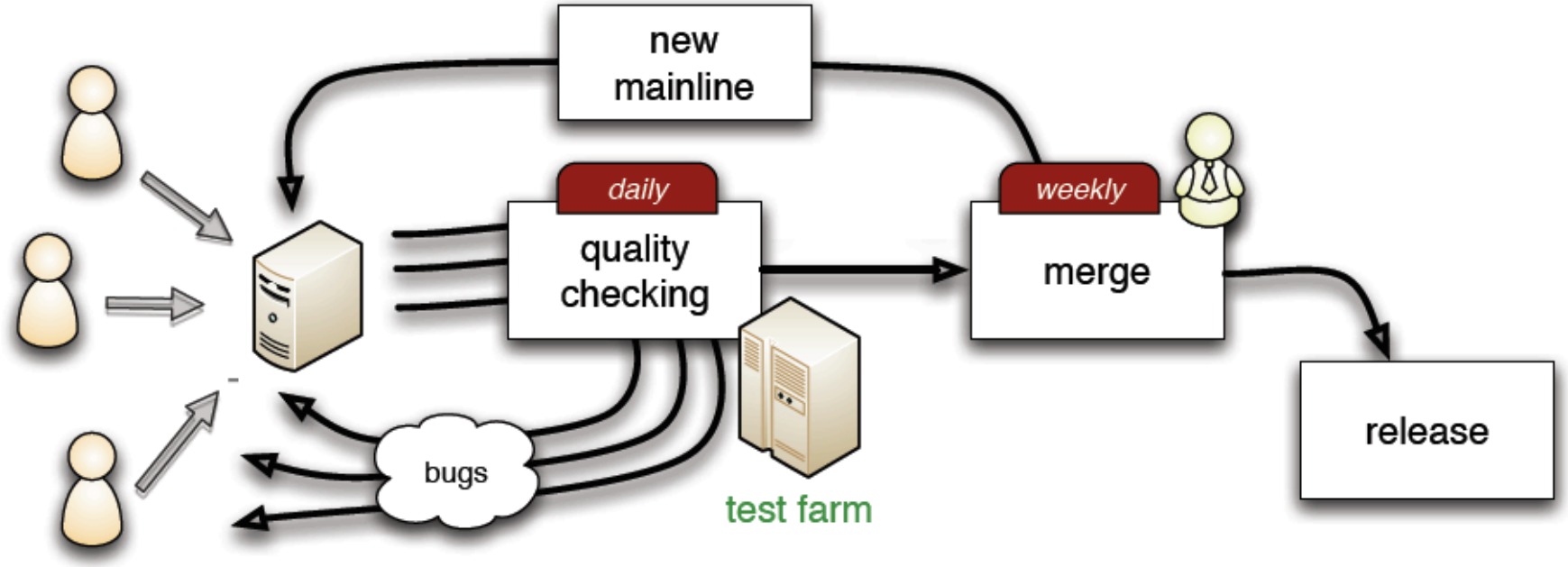
Worldwide access
of the repository

http://github.com/abinit

Testing : traditional workflow



Testing : continuous integration



Documentation

Documentation

Web site http://www.abinit.org

- User's guide
- Installations notes
- List of input variables
- >30 tutorials (each 1-2 hours)
  http://www.abinit.org/tutorials

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

Videos

How to install on Linux ?

http://www.youtube.com/watch?v=DppLQ-KQA68

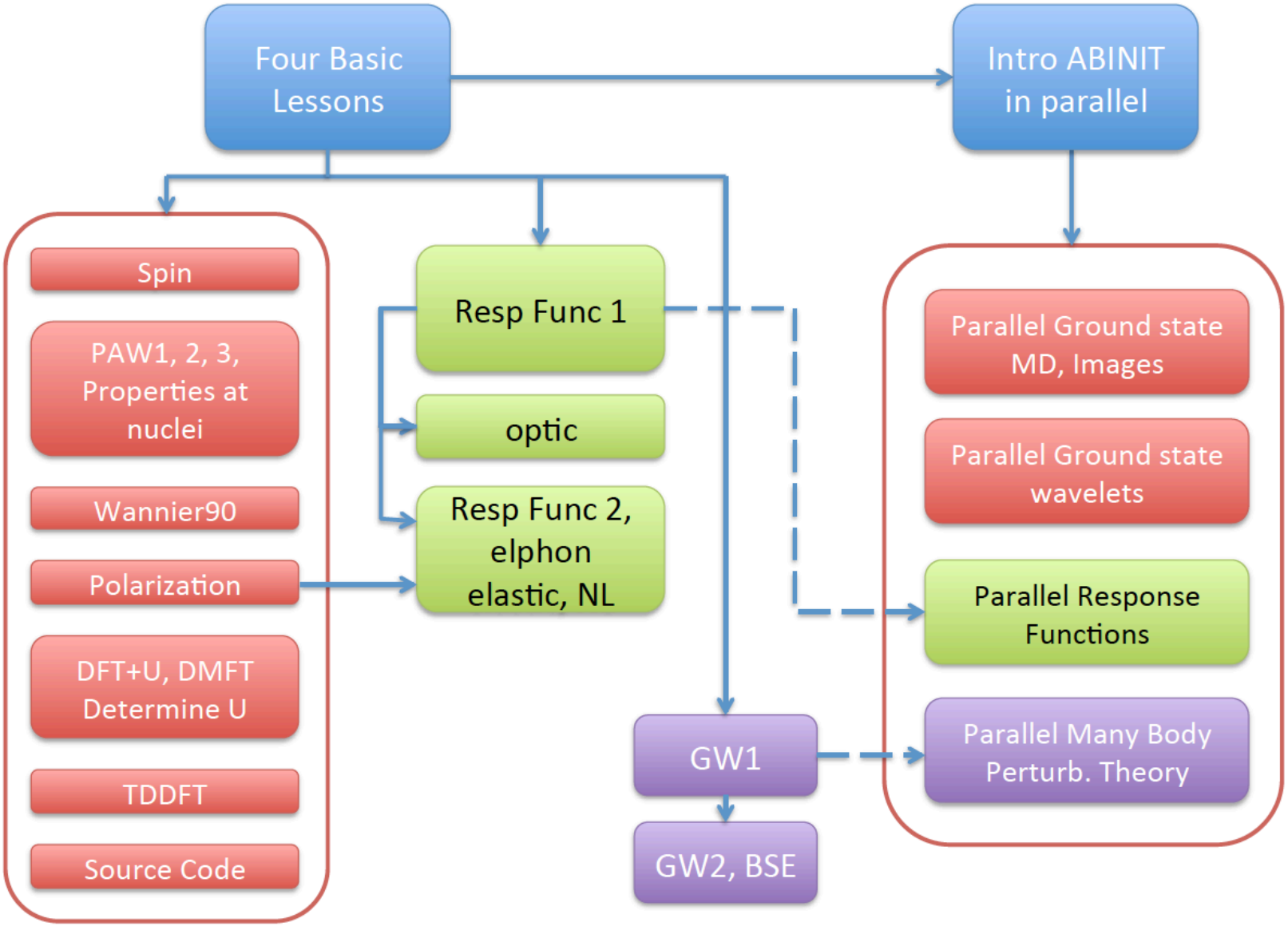
How to install on Windows 64bits ?

http://www.youtube.com/watch?v=EfJcYi1MNBg

First ABINIT tutorial (H2 molecule)

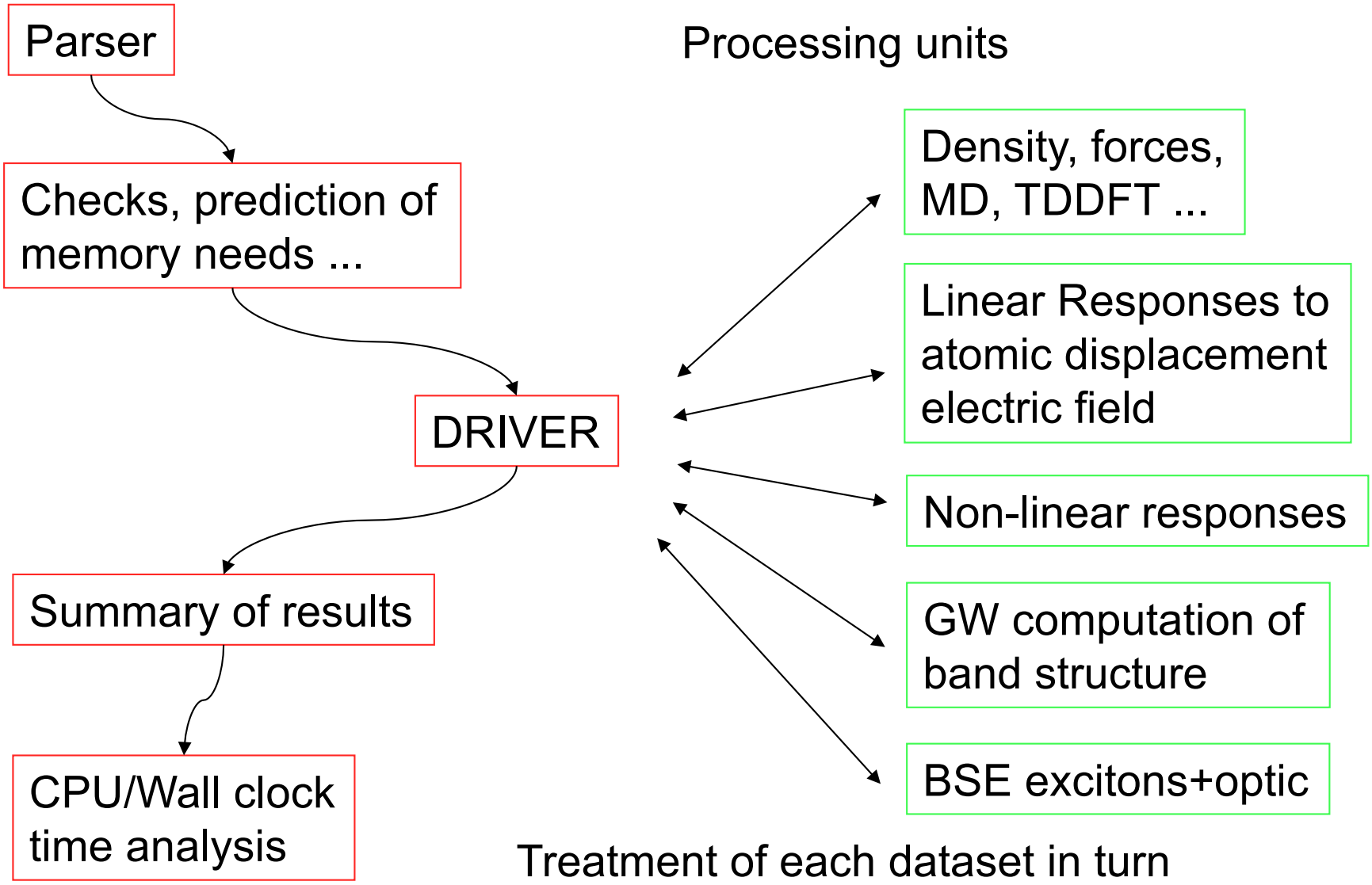
http://www.youtube.com/watch?v=gcbfb_Mteo4

ABINIT Tutorial :global view

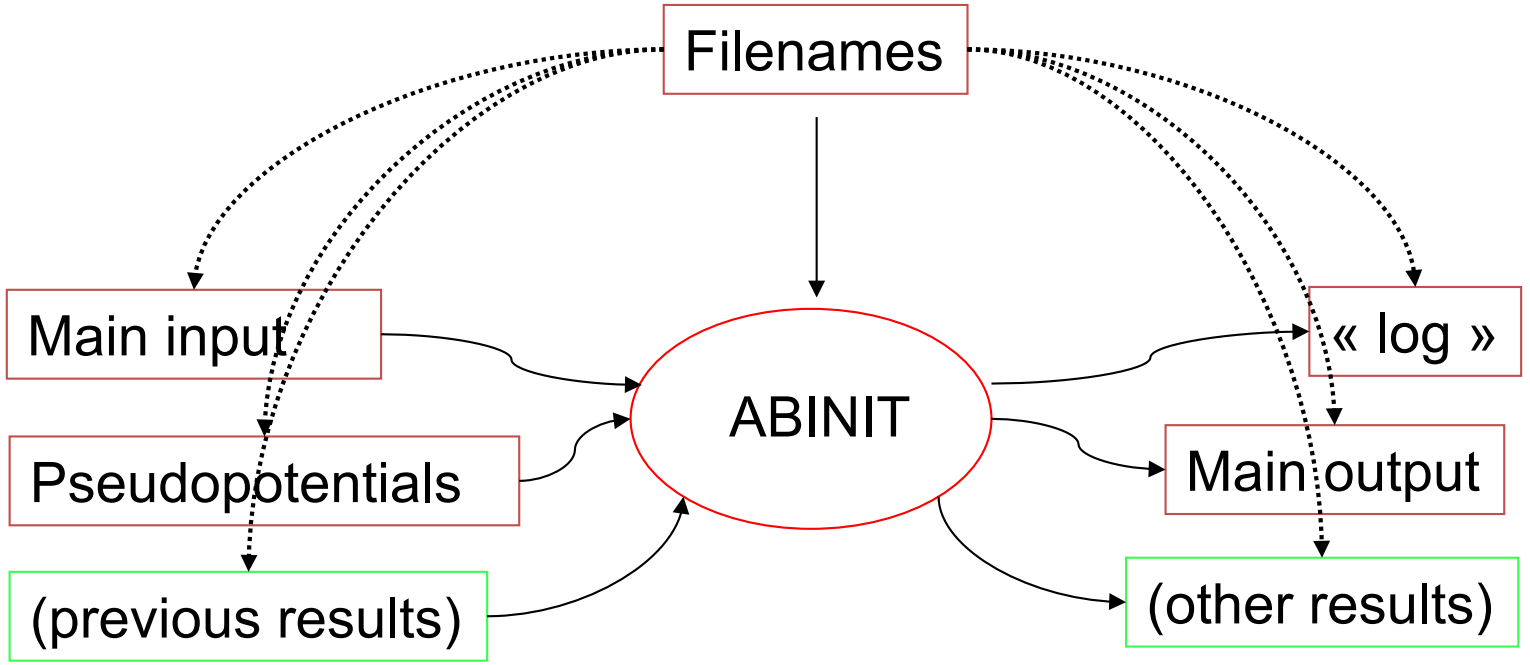


Miscellaneous

ABINIT : the pipeline and the driver



External files in a ABINIT run



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