Overview of the ABINIT project

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Thanks to all of you !

ABINIT community : some dates

- Precursor : the Corning PW code (commercialized 92-95 by Biosym)
- 1997 : beginning of the ABINIT project
- Dec 2000 : release of ABINITv3 under the GNU General Public License
- Nov 2002 : 1st int. ABINIT dev. workshop (Louvain-la-neuve)
- May 2004 : 2nd int. ABINIT dev. workshop (Paris)
- Jan 2007 : 3rd int. ABINIT dev. workshop (Liège)
- Mar 2009 : 4rd int. ABINIT dev. workshop (Autrans)
- April 2011 : 5th int. ABINIT dev. workshop (Han-sur-Lesse)
- April 2013 : 6th int. ABINIT dev. workshop (Dinard)
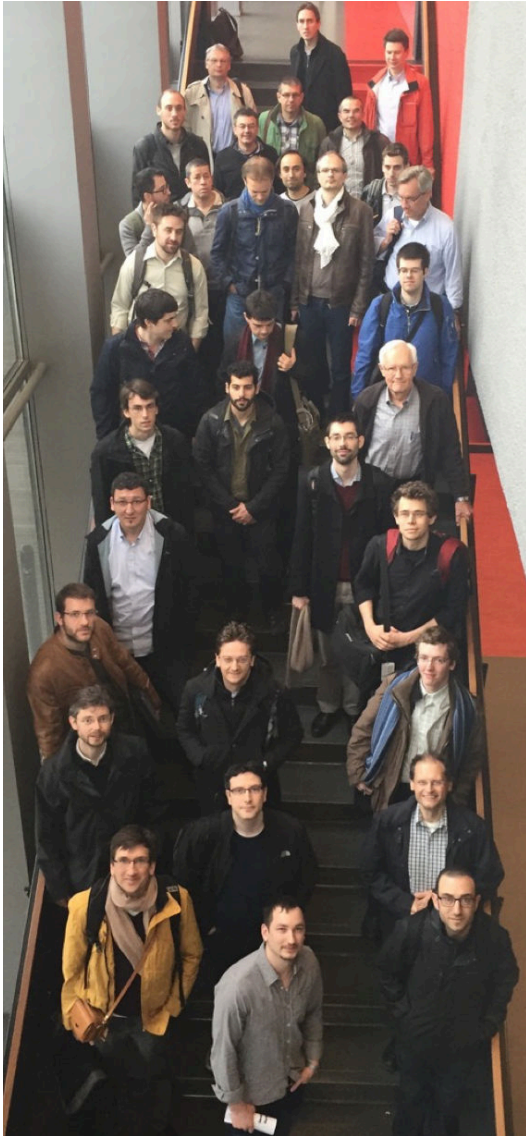- April 2015 : 7th int. ABINIT dev. workshop (Liège)

2007

2009

2011
(Han-sur-Lesse)

2013
(Dinard)

2015 (Liège)

Apr 2015 – now : main events for ABINIT

April 2015 : Developer workshop, Liège

May 2015 : CECAM School "Theoretical Spectroscopy", Lausanne

Nov 2015 : Launch of ABINITv8 (incl. database for the input variable documentation, cleaning of input files, of sources, switch testf-abiref)

March 2016 : Tutorial on "Many-body perturbation theory with ABINIT", APS March meeting, Baltimore

April 2016 : Publication of the ABINIT paper Comput. Phys. Comm.

May-June 2016 : ABINIT user survey

June 2016 : Int. Summer school on "Comput. methods for quantum materials" , Sherbrooke, Québec, Canada

July 2016 : Switch from bzr to git(lab)

January 2017 : "ABINIT hands-on 2017", Bruyères-le-châtel, France

History : some quantitative indicators

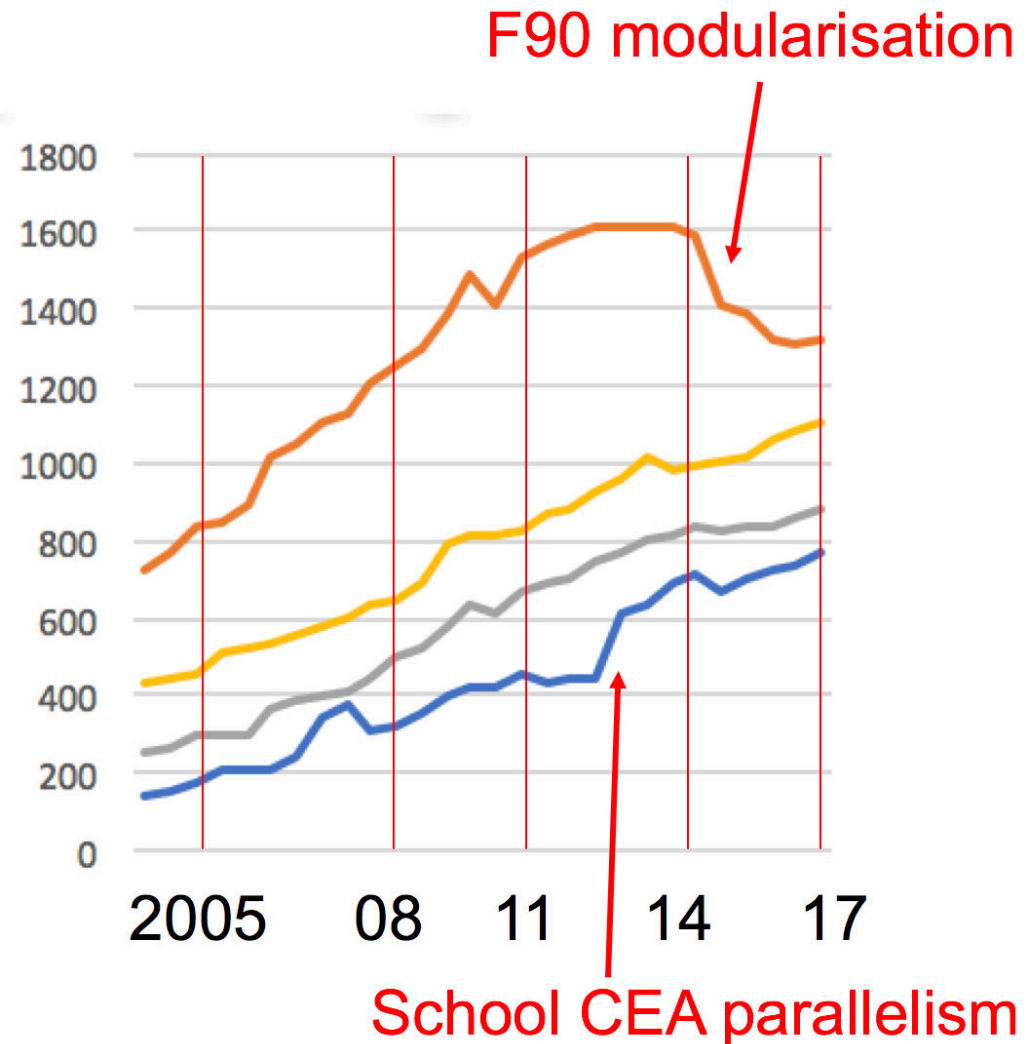As of May 2017 :
1321   F90 files
1102   autom. tests
878   kLines of F90
76.4   MBytes tar.gz
            package

F90 modularisation

School CEA parallelism

Highlights from 2015-2017

v8.0 (May 2016) :

-Van der Waals D3 functionals, including DFPT for D2 and D3.
-NC pseudopotential tables (PAW previously)
-DMFT framework with cRPA, CTHYB solver
-Bethe-Salpeter : Haydock recursion, Rohlfing-Louie interp.
-Fold2Bloch (unfolding of electronic structure from supercells)
-Direct computation of effective mass tensors from DFPT
-GW Lanczos-Sternheimer
-Strain perturbation in PAW+DFPT
-Electron-positron Doppler broadening
-Linear electro-optic coefficients (in the IPA)
-Electronic Stopping power
-qpSCGW with bootstrap kernel
-Progresses : Fock, hybrids, ZPR and T-dep of the electronic structure

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Highlights from 2015-2017

v8.2 (released February 2017) :

-Limited memory BFGS optimization algo (ionmov=22).
-Tutorial computation of effective U and J using cRPA for DFT+DMFT
-Temperature-dependent spectral functions (due to el-ph coupling)
-qpSCGW with bootstrap kernel
-Progresses : creation of the main executable « multibinit », new « driver » (optdriver=7) for el-ph calculations, Raman intensities for PAW, non-collinear DFPT …

v8.4 … soon to be released

To be presented
or announced here !

The user/developer community

As of May 2017 :

1829 registered addresses at forum.abinit.org (started 2009)

1050 registered addresses in the "announce" mailing list

45 names in "contributors" file ABINIT v8 (Sep 14-Jan17)

50 ABINIT Gitlab users (Merge requests from 20 users)

Forum :

started in 2009

587 in April 2011

1011 in Jan 2013

1433 in Jan 2015

1829 in May 2017

ABINIT Discussion Forums
The meeting place for ABINIT users and developers

Main site | Download | Documentation | Tutorials

⌂ Board index

👤 User Control Panel • View your posts

WHO IS ONLINE

In total there are **17** users online :: 3 registered, 0 hidden and
Most users ever online was **187** on Mon Aug 01, 2016 11:58 pm

Registered users: cennanaradipa, gonze, Google [Bot]
Legend: Administrators, Global moderators

STATISTICS

Total posts **10049** • Total topics **3166** • Total members **1829** •

Bibliometry

Some measure of usefulness of ABINIT : citations of the four papers co-authored by all active developers in the period

Comput. Mat. Science 25, 478 (2002) - 16 authors
As of May 2017 : 2092 citations (124 in 2016)

Z. für Kristallogr. 220, 558 (2005) - 20 authors
As of May 2017 : 807 citations (70 in 2016)

Comp. Phys. Comm. 180, 2582 (2009) - 33 authors
As of May 2017 : 1181 citations (225 in 2016)

Comp. Phys. Comm. 205, 106 (2016) - 55 authors
As of May 2017 : 12 citations (5 in 2016)

Bibliometry : where is ABINIT cited ?

Analysis of papers #1-100 in 2016 citing the 2009 ABINIT paper, from Scopus.

Phys. Rev. B   17 cit. (22.6% in 2013 census)
Phys. Rev. Lett   7 cit. (4.4% in 2013)
J. Chem. Phys.   5 cit. (2.2% in 2013)
Sci. Reports   5 cit.
Phys. Rev. E   4 cit.
J. Phys. Chem. C   4 cit. (1.6% in 2013)
(others are at 3 cit. or below, and account for 68% citations)

High impact (IF>7)   12 citations (7.5% in 2013)

With respect to major material codes ...

Citation analysis from NOMAD, period 2011-2015
https://nomad-coe.eu/index.php?page=codes

VASP	16500
CASTEP	5970
WIEN2K	4880
Quantum Espresso	4810
Siesta	4040
Crystal	2225
ABINIT	1870
CP2K	1190
CPMD	938
TB-LMTO-ASA	840
GPAW	624
FPLO	459
FHI-Aims	407
Elk	225
FLEUR	212

2017 ABINIT Workshop

The most important : interactions between the developers !!

Discussion sessions + social activity

Tuesday : ABINIT survey discussion
Wednesday : ABINIT ecosystem (perhaps already Monday)
Wednesday : Underwater vision (in Agay) + dinner in Frejus
Thursday : Gitlab / github / test farm
              ABINIT build system

Friday : Preparing the future. Discussion groups.
(topics ? documentation, wiki, Web site, Gitlab …
   ? adjust ABINIT to standard usage –defaults,test cases ...)