# 11th International ABINIT developer workshop

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# ABINIT software project

Ideas (1997) – pioneer :

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 (2024) :
> 1 200 000 lines of F90
> 50 python scripts
about 60 contributors to ABINITv8/v9/v10

# 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)

○ 2010 : launch of the old Forum (up to 2500 registered people) / 2021 : launch of the discourse Forum

○ Nov 2002 – July 2024 : 11 international ABINIT developer workshops
    (between 35 and 80 participants each). Split 2021-2022 => COVID/hackathon



Now in Canada !

# Impactful capabilities of ABINIT

'ABINIT : Overview, and focus on selected capabilities'
J. Chem. Phys. 152, 124102 (2020)
A.    Romero et al – 43 authors
**To be updated !**

Non-exhaustive list :
Dynamical Mean-Field Theory
GW + PAW, **recently low-scaling GW**
Advanced capabilities in DFPT (strain perturbation, spin-magnetic field
      perturbation, flexoelectricity, dynamical quadrupoles, non-linear electric
      susceptibility, Raman intensity, natural optical activity ...)
Positron lifetime
aTDEP
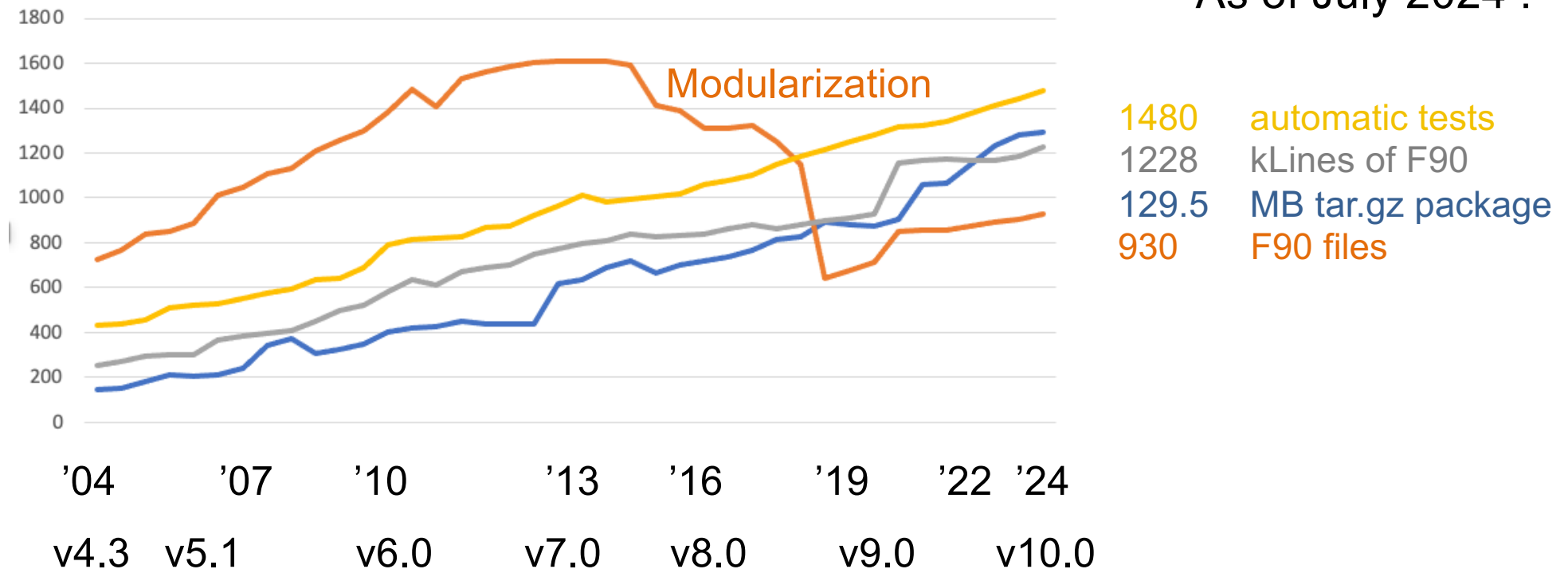Electron-phonon : zero-point renormalization, mobility calculations
Also :    Quality of documentation, especially tutorial
          Abipy script gallery
          Norm-conserving pseudos (pseudo-dojo) + JTH PAW atomic data

# Time evolution : indicators



As of July 2024 :

| | |
|---|---|
| 1480 | automatic tests |
| 1228 | kLines of F90 |
| 129.5 | MB tar.gz package |
| 930 | F90 files |

Also : AbiPy 0.9.0 gallery with >50 plotting scripts (python)
        >40 tutorial

# Bibliometry

Citations (scopus) of the six articles co-authored by all active developers
Total as of July 1, 2024 : 7546 citations ; 536 citations in 2023

Comput. Mat. Science 25, 478 (2002) – 16 authors
2858 citations ; 64 citations in 2023

Z. Kristallogr. 220, 558 (2005) – 20 authors
1196 citations ; 28  citations in 2023

Comp. Phys. Comm. 180, 2582 (2009) – 33 authors
2283 citations ; 117  citations in 2023

Comp. Phys. Comm. 205, 106 (2016) – 55 authors
637 citations ; 140  citations in 2023

Comp. Phys. Comm. 248, 107042 (2020) – 53 authors
385  citations ; 123 citations in 2023

J. Chem. Phys. 152, 124102 (2020) – 43 authors
187 citations ; 64 citations in 2023

# Abilogix

A consortium to manage the development of ABINIT.
Consortium agreement : 1/10/2021 – 30/9/2031.
Institutional value !
Members : UCLouvain, ULiège, UNamur, CEA (1/10/23).
In practice : meetings for coordination of the actions of permanent members incl. JMB, MG, HeXu

Composition of the board :
- Representatives of the 4 institutions
   (XG, GMR, PhG, MV, LH, MT, BA)
- Elected representative of the ABINIT advisory board (JZ)
- Elected representative of the developers (to be elected HERE)
- Elected representative of the users (still to be organized)

# Advisory board

The role of the ABINIT International Advisory Committee (IAC) is to help make decisions concerning broad policies of ABINIT implementation, use, and licensing, and to help coordinate international activities of the ABINIT community.

Examples of IAC activities include maintenance of the GPL licensing model within ABINIT, forging links to related coding projects, and coordinating ABINIT-sponsored Workshops and Schools.

D.C. Allan, F. Bruneval, D. Caliste, M. Côté, Ph. Côté, X. Gonze, N. Holzwarth, F. Jollet, M. Mikami, J. Rehr, G.-M. Rignanese, A. Romero (Chair), N. Spaldin, M. Stengel, M. Torrent, M. Verstraete, J. Zwanziger

# Lots of things to do at ABIDEV24 !

Presentations by developers, "external" invitees, expert users
          Discussion sessions / Hackathon
  +  Advisory board meeting / ABILOGIX consortium meeting/ Group picture

|  | Monday, July 1st | Tuesday, July 2nd | Wednesday, July 3rd | Thursday, July 4th |
|---|---|---|---|---|
|  |  |  |  |  |
|  |  |  |  | ABILogix (7h30) |
|  |  |  |  | ABILogix (continued) |
| 8h30 | Welcome (+Discussion topics) | Xu (visio) | Emmanuel | Samuel |
| 8h50 | Xavier: ABINIT overview | Romuald | Natalie | Guillaume |
| 9h10 | Marc | Olivier | Matthieu | Maxime |
| 9h30 | Lucas | Philippe | James | Vasilii (visio) |
| 9h50 | Lygatsika | Aldo | Lorien | Samare (visio) |
| 10h10 | Break (50min) | Break (50min) | Break (50min)+advisory (at 10:30) | Break (50min) |
| 11h00 | Eric | Fabien | Advisory committee or free | Web site (Maryam visio) |
| 11h20 | Josef | Augustin | Advisory committee or free | (c'ed) |
| 11h40 | Asier | Matteo | Advisory committee or free or talk ? | Other discussions |
| 12h00 | Miquel | Matteo (other things) | Advisory committee or free or talk ? | (c'ed) |
|  |  |  |  |  |
| 12h30 | Lunch | Lunch | Lunch | Lunch |
|  |  |  |  |  |
| 14h | Organization of discussions (5min) | Hackathon | Hackathon |  |
| 14h10 | Discussions (small groups) |  |  |  |
| 15h | Discussions (global) |  |  |  |
| 15h30 | Planning of hackathon + return (30m) |  |  |  |
| 16h | Break (30 min) |  |  |  |
| 16h30 | Discussion: test farm | Hackathon | Hackathon |  |
| 17h00 | Discussions (small groups) |  |  |  |
| 18h00 | Discussions (global) |  |  |  |
| 18h30 | Break |  |  |  |
| 19h00 | Dinner |  |  |  |

Try :
abinit.github.io/abinit_web