

ABINIT : 3.5 Years of GNU GPL

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Collaborators : all of you !

Outline

Purpose :

Facts/statistics about the ABINIT project, starting from the release under GNU General Public License

- Chronology
- Bibliometry
- The user/developer community

Also, comments about on-going projects not presented at this workshop

The GNU GPL (just in case ...)

“The licences for most softwares are designed to take away your freedom to share and change it. By contrast, the GNU GPL is intended to guarantee your freedom to share and change free software - to make sure the software is free for all its users”
(www.gnu.org/copyleft/gpl.html)

- 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 freedom
- «accination»

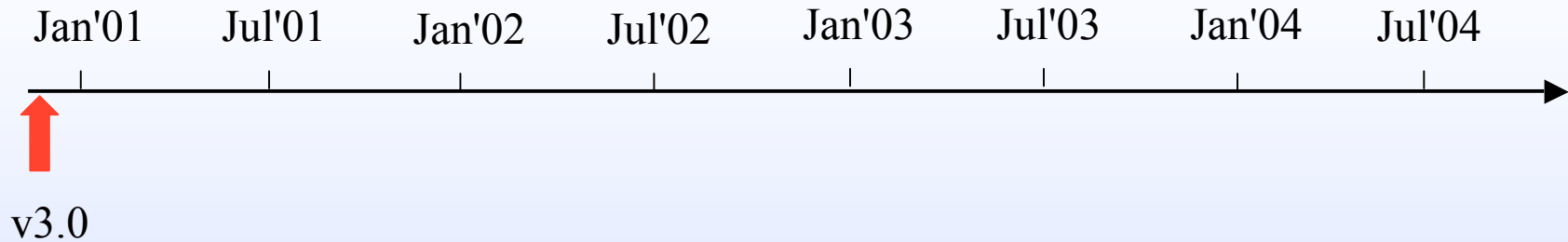
Chronology

- Precursor : the Corning PW code (commercialized 1992-1995 by Biosym)
- 1997 : beginning of the ABINIT project
- Dec 2000 : release of ABINITv3.0 under the GNU GPL
- Nov 2002 : 1st int. ABINIT developer workshop, Louvain-la-neuve
- May 2004 : 2nd int. ABINIT developer workshop, Paris

Dec 2000-May 2004

- New versions (v3.0 to v4.3)
- Computational Materials Science paper (submitted Feb. 2002, published Dec. 2002)
- Fast growing user community

Dec. 2000 : Version 3.0

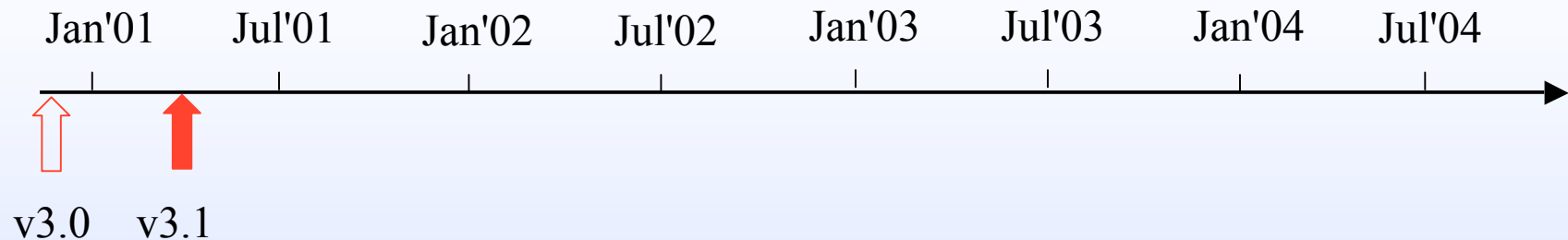


Opening of the Web site
GNU GPL
Robodoc formatting

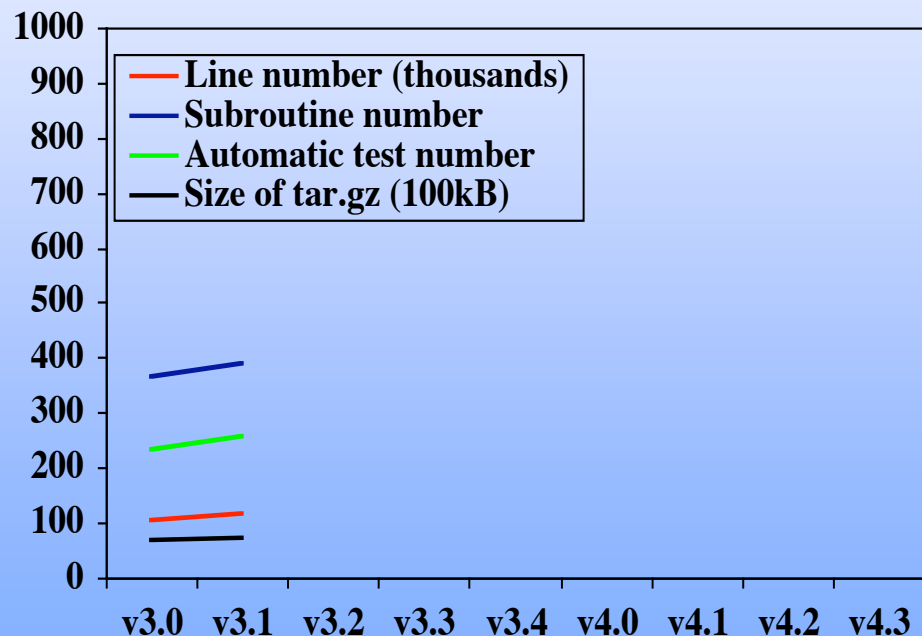
Included already many GS
features + RF features

105 kLines
364 subroutines
234 automatic tests
6.7 MBytes tar.gz package

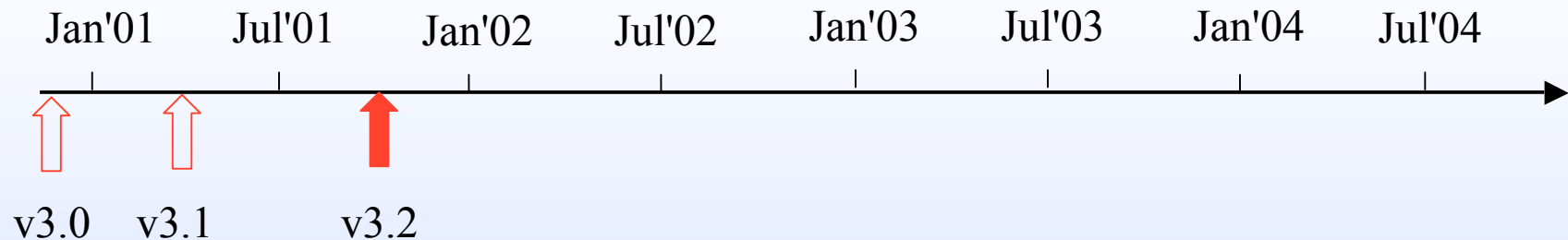
Apr. 2001 : Version 3.1



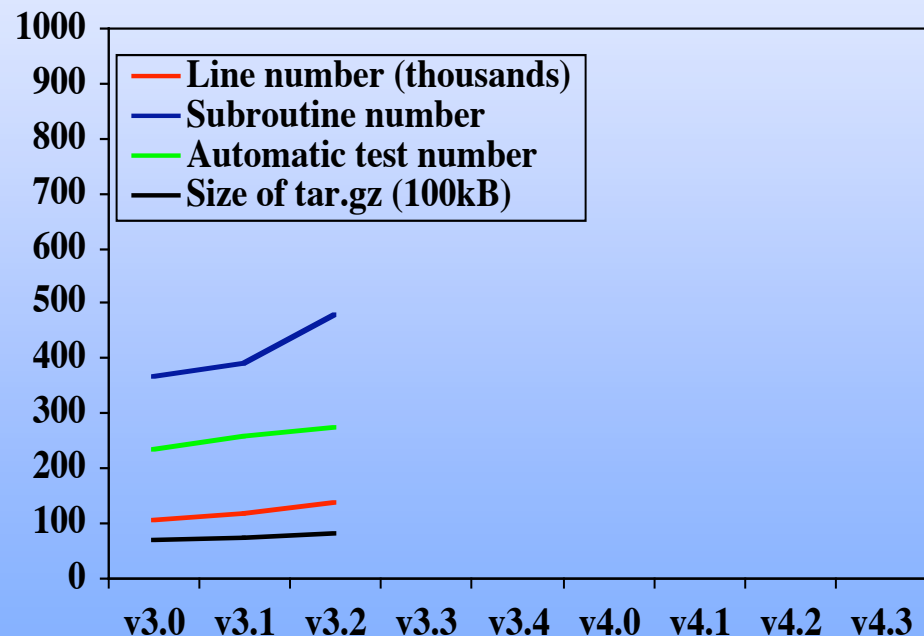
Spin-orbit coupling :
stresses and phonons
Scripts : parents & abirules
Spin MPI parallelism



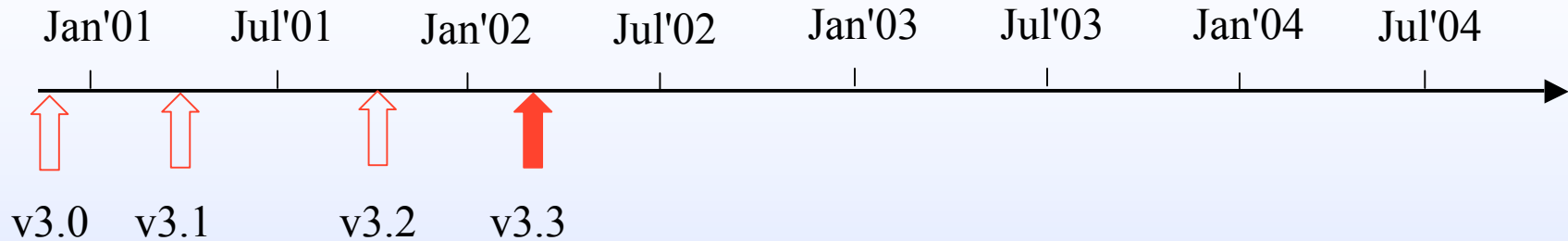
Oct. 2001 : Version 3.2



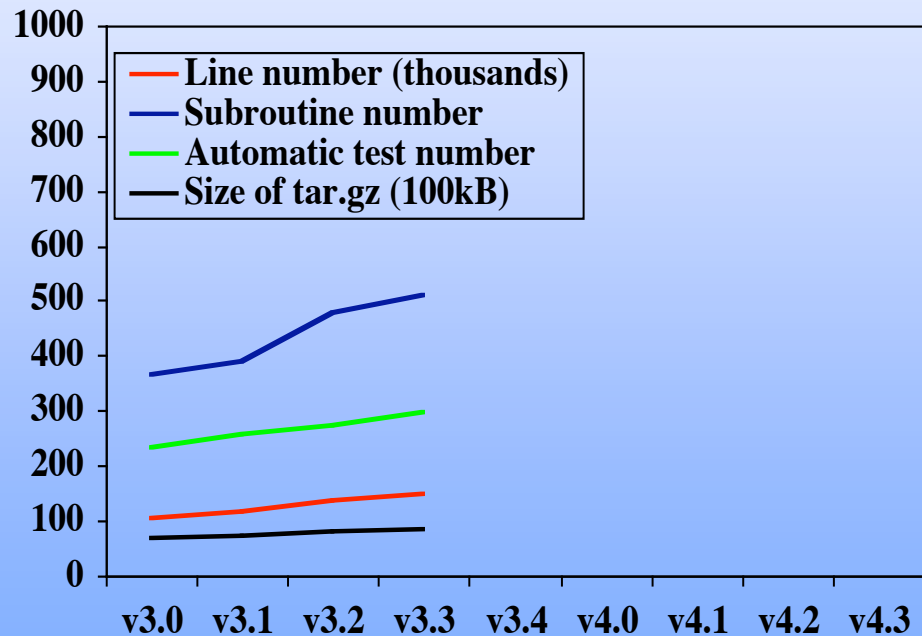
GW as 2 separate mains
(60 routines)
Recognition of space groups
Spin-polarized responses
Shubnikov symmetries
Non-collinear spin
magnetization



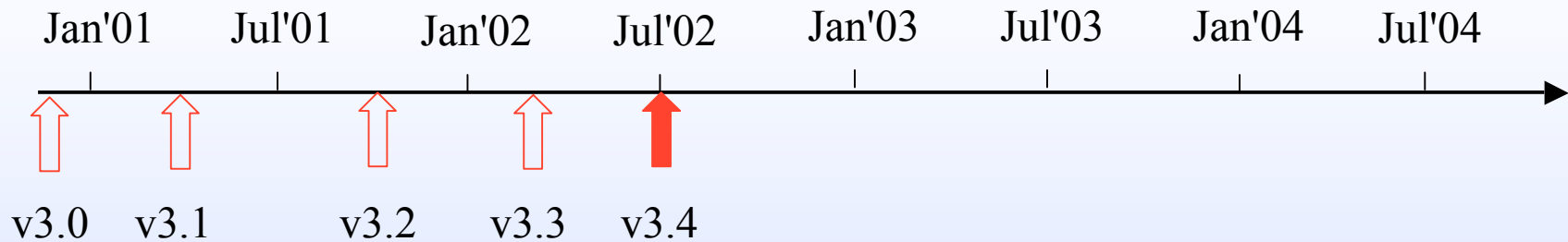
Mar. 2002 : Version 3.3



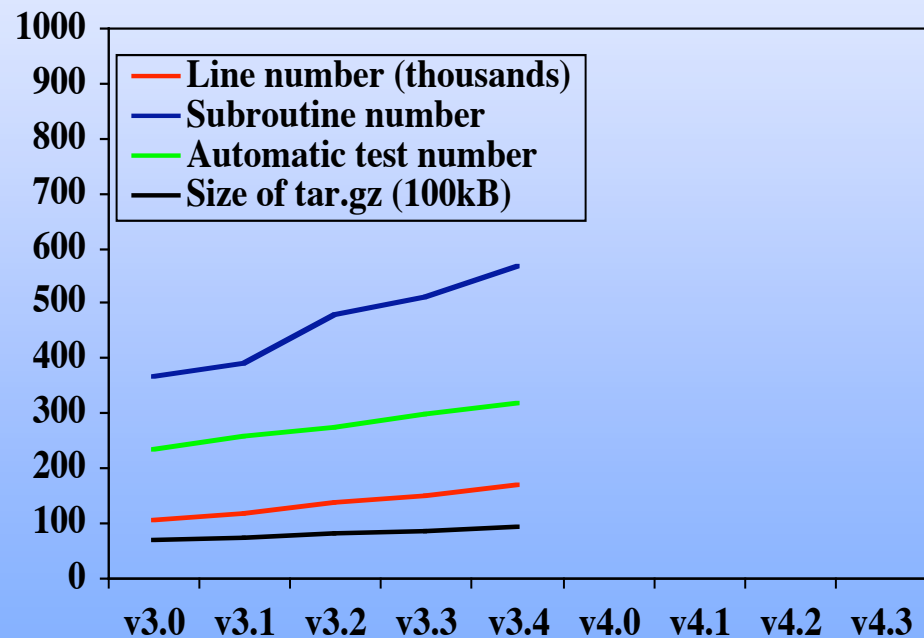
GGAs for responses
MPI band-by-band
parallelism for ground state
Localization tensor
Optical conductivity tensor



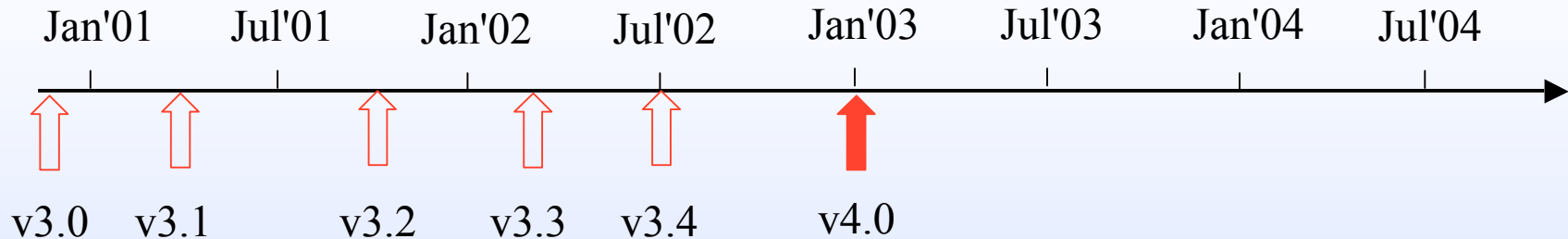
Jul. 2002 : Version 3.4



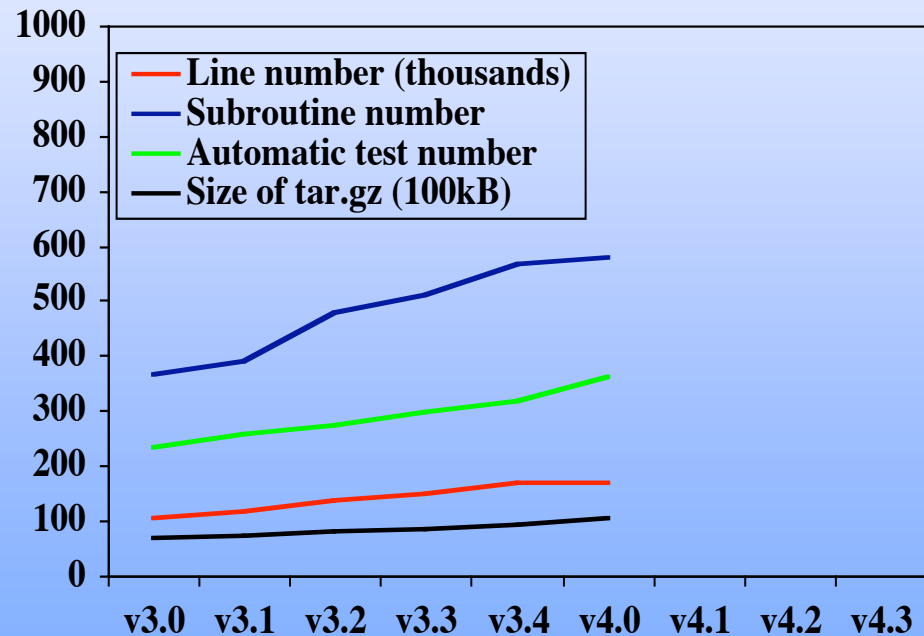
Bader analysis
(atom-in-molecule)
GW merged in main driver
Alchemical mixing of psp



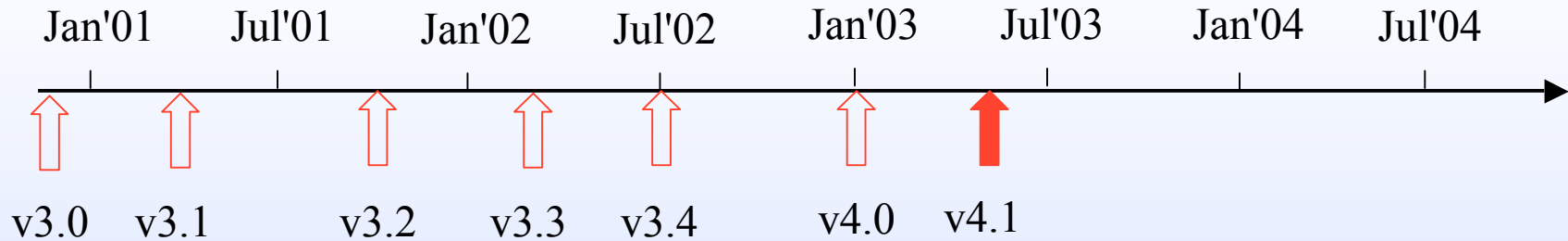
Jan. 2003 : Version 4.0



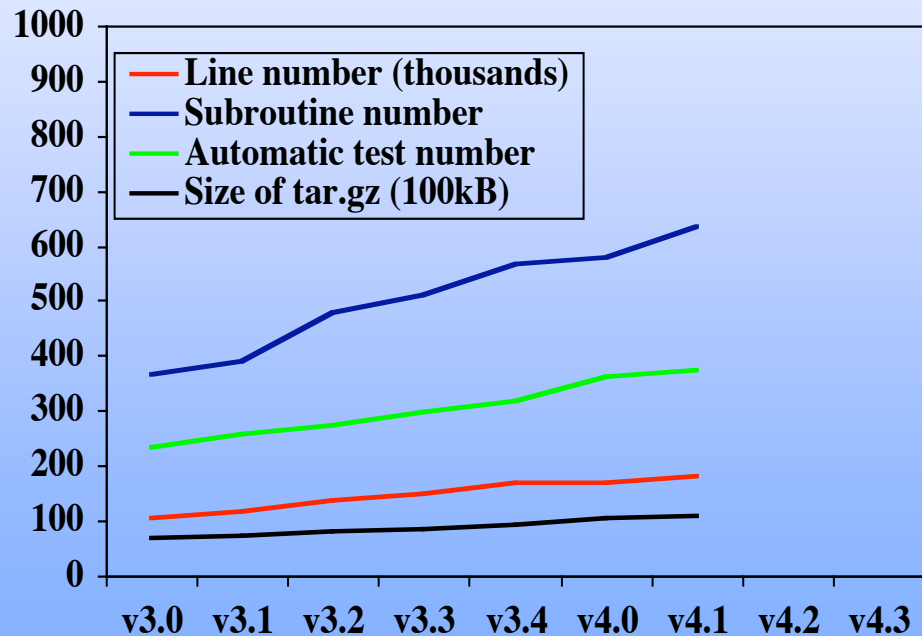
First self-consistent PAW
Electronic DOS
 $2n+1$ theorem : Raman and
non-linear susceptibility
Shubnikov group recognition
Parallel TDDFT
CML I/O



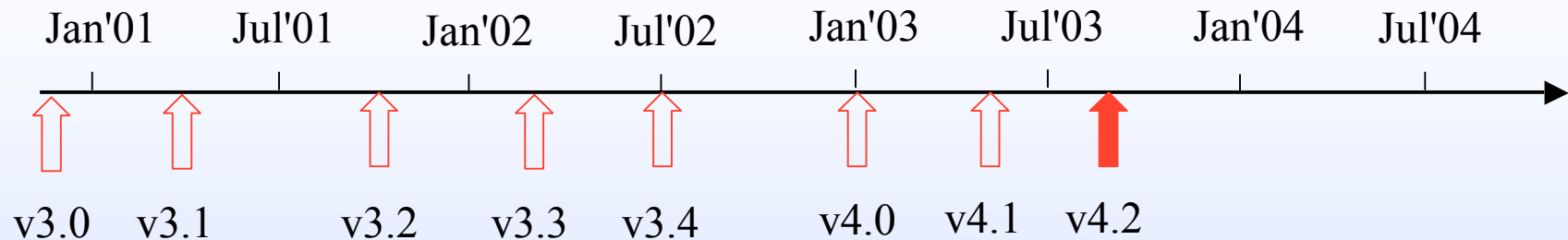
May 2003 : Version 4.1



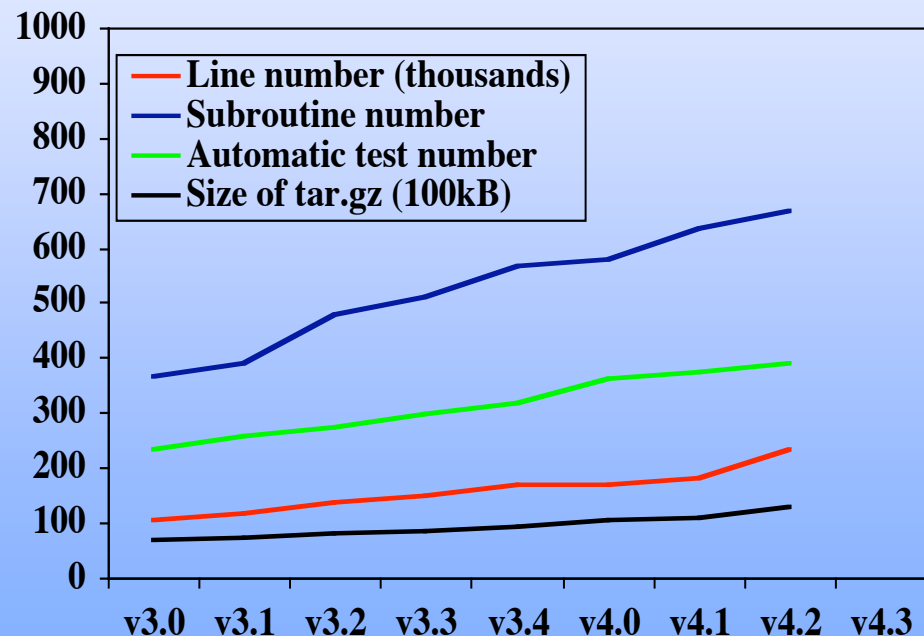
PAW beta testing
New FAQ
ANADDB/MRGDDB
treat 3rd order derivative



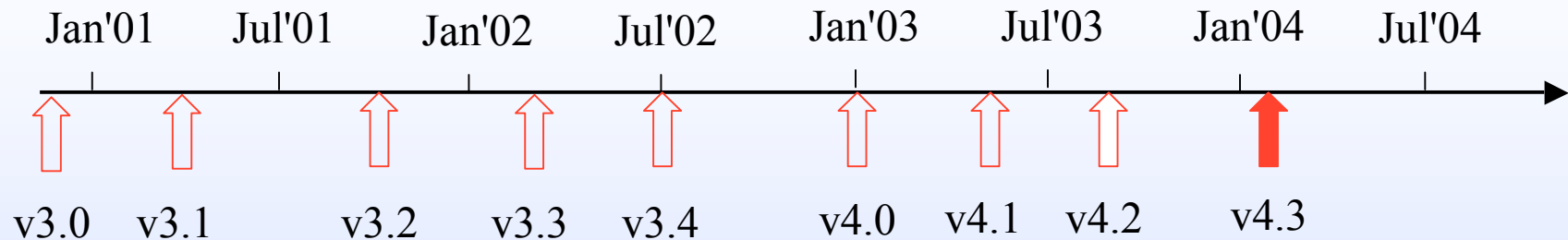
Sep. 2003 : Version 4.2



Strain perturbation (47kLines)
Macroave utility
PAW-potential generator



Feb. 2004 : Version 4.3



Piezoelectricity

ANADDB analysis of strain

Finite electric field

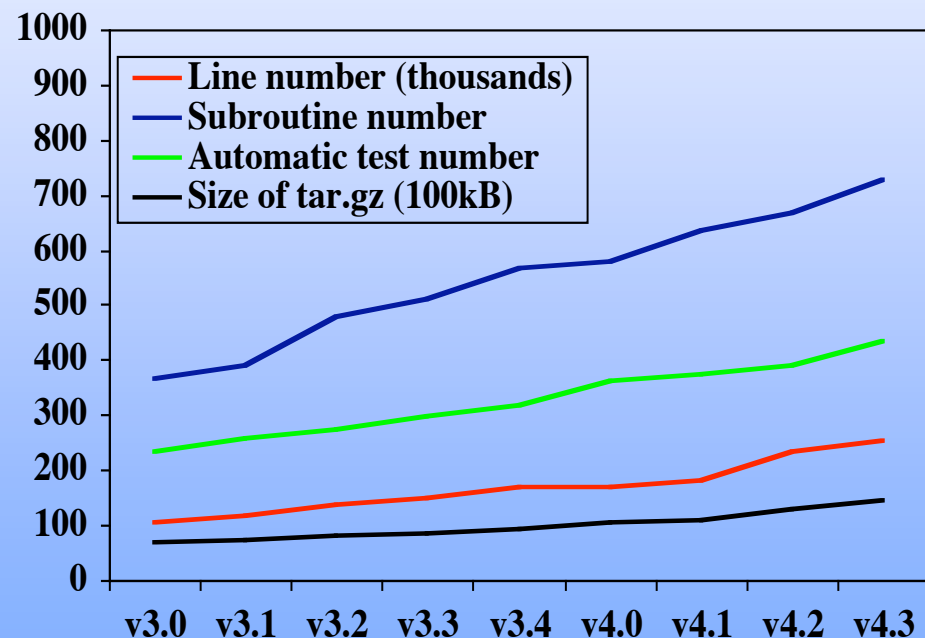
GW tutorial

252 (105) kLines

726 (364) routines

432 (234) automatic tests

14.5 (6.7) MBytes tar.gz package



Bibliometry (I)

Some measure of usefulness of ABINIT ...

Comput. Mat. Science 25, 478 (2002)

submitted Feb. 2002, published Dec. 2002

40 citations in 1.5 years, among which

1 Science

6 Phys. Rev. Lett.

16 Phys. Rev. B

then, Chem. Phys. Lett, J. Phys Cond. Mat., Comp. Mat. Sc., Comp. Phys. Comm.,
J. Chem. Phys., Surf. Sc., Acta Crystall., Phys. Stat. Solid., J. Lumin., Microelec., ..

Ground-state only : 20 citations

Response-function : 16 citations

Method papers : 2 citations

Reference to the project, without use : 2 citations

Bibliometry (II)

Before Dec. 2002 : the bibliographical database
(actually, the existence of this database has not been mentioned
to the users in 2003 and 2004 => rather incomplete by now)

38 publications mentioned in 2001 and 2002

2 Science

3 Phys. Rev. Lett.

12 Phys. Rev. B

then, J. Phys Cond. Mat., Comp. Mat. Sc., Phys. Rev. E, Jap. J. Appl. Phys.,
Appl. Surf. Sc., Phys. Stat. Solid., J. Non-cryst. Solids, Int. Mass Spectr., ...

The user's community : analysis of mailing lists

As of May 5, 2004 :

585 registered addresses in "announce" mailing list

517 registered addresses in "forum" mailing list

170 registered addresses in "developper" mailing list

(from "contributors" file : 95 adresses)

Growth of the main list:

about 100 in Dec. 2000

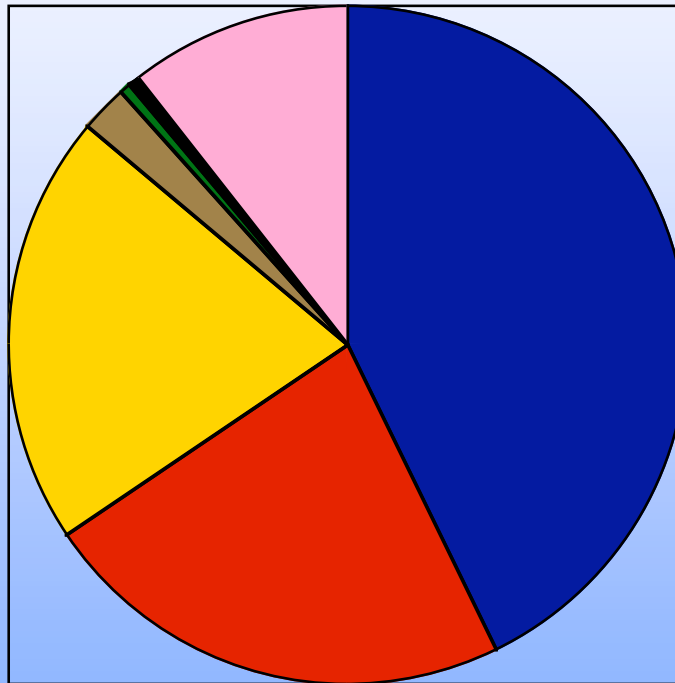
about 300 in Feb. 2002

Compare : GAMESS, GAUSSIAN > 10k

WIEN : 400 + 400 (users with fee)

Vasp : 1000 ??

Announce mailing list : geographical repartition



251	■ Europe
133	■ N. America
120	■ Asia+FSU
12	■ S. America
4	■ Africa
3	■ Oceania
62	■ Other

Announce mailing list : geographical repartition (II)

Total : 585 mailing addresses

251 Europe	: 82 .fr ; 37 .de ; 31 .be ; 24 .it ; 20 .uk ; 11 .es ; 10 .ch ; 5 .pl ; 5 .se ; 5 .pt ; 3 .fi ; 3 .yu ; 3 .cz ; 2 .no ; 2 .dk ; 2 .gr ; .at ; .hu ; .ee ; .si ; .ie ; .ro
133 N. America	: 95 .edu ; 18 .gov ; 11 .ca ; 5 .mil ; 4 .mx
120 Asia+FSU	: 42 .jp ; 27 .cn ; 12 .ru ; 9 .tr ; 9 .in ; 8 .tw ; 5 .kr ; 3 .ua ; 2 .hk ; .sg ; .ir ; .su
12 S. America	: 9 .br ; 3 .ar
4 Africa	: 2 .cm ; .za ; .tn
3 Oceania	: 3 .au
62 Other	: 53 .com ; 6 .net ; 3 .org

Actual contributors : geographical repartition

(From the Infos/contributors file)

96 contributors

61 Europe	: 24 .fr ; 17 .be ; 6 .it ; 4 .es ; 3 .nl ; 3 .uk ; 2 .at ; 1 .ch ; 1 .de
26 N. America	: 12 .edu ; 5 .ca ; 4 .gov ; 3 .com (US) ; 2 .mil
9 Asia	: 6 .jp ; 2 .com (China) ; 1 .tw

ABINIT capabilities, or ABINIT on-going projects, not presented here

Actually, several of these topics were presented in previous workshop, with description of planned steps ... now done ... or still going on !

- TDDFT (now, parallel)
- Shubnikov group recognition
- parallel FFT

There are also some rather specialised improvements like advanced functionals (RPA, HCTH), and a whole set of small achievements (e.g. charge density of state near Fermi level, for STM)

Still, many other features / improvements are needed !
... For next workshop ...