

The ABINIT web site and package :
How to explore the «Jungle» for very beginners

Masayoshi Mikami

Mitsubishi Chemical Group
Sci. & Tech. Research Center, Inc.

Contents

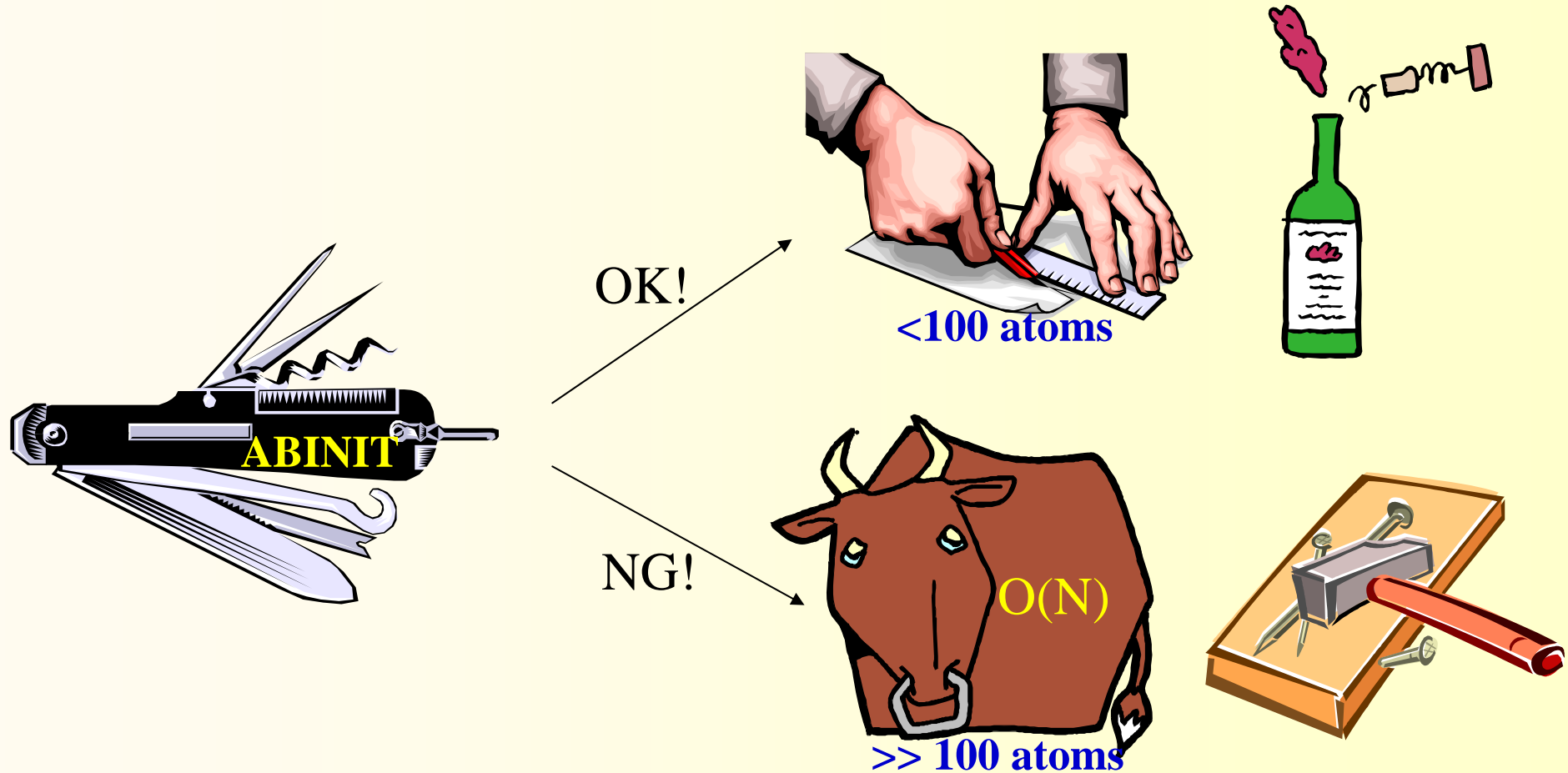
- 1. As an ABINITioner ...***
- 2. How to browse the WEB site ? – Quick tour***
- 3. How to explore the tar.gz ? – Demonstration***
- 4. Wrap-up***



***Acknowledgments: Yann Pouillon, Jean-Michel Beuken (WEB!)
and ABINITioners who posted e-mails on the MLs !***

*“Oh! ABINIT seems versatile !”
Thus, here is a typical FAQ:*

“Can we do ... with ABINIT ?”



Let us learn “What is ABINIT?”, “How to use ABINIT”
by reading documents inside ABINIT WEB page/package !



1. As an ABINITioner ...



- *Expect the ABINIT package moderately (not too extremely high/low)*
*Documentation has limitation: **NO PERFECT** for all kinds of users*
(ABINITioners are encouraged to read standard textbooks, reviews...)
- *Documentation has been piled up, and will be, in **self-assembly** way*
 - *Dilemma between completeness and simplicity (never 100% solved)*
 - *Difficulties to find relevant documents will remain for newcomers*
- *You may ask questions on the ML, but try to **save our "Humanwares"**:
i.e. try to find documents in the ABINIT source & WEB pages
before you ask your questions ... most of them may be found !*

*Learn ab initio methods & Improve your search skill, “**Googling**”,
to find documents to answer your questions by yourself (as possible)*

*Believe “**Those who help themselves will be helped**”*

2. How to browse the WEB site ?

- *Where to start ?*

The front page: [What is ABINIT ?](#) → [Short presentation](#),
→ [README](#) → Register [the ML](#) ([Netiquette](#), [FAQ](#))

- *Before running your jobs, why not try [this Suggestion](#) ?* (*New user guide, Tutorials, Help_files, running Test_*, ...*)

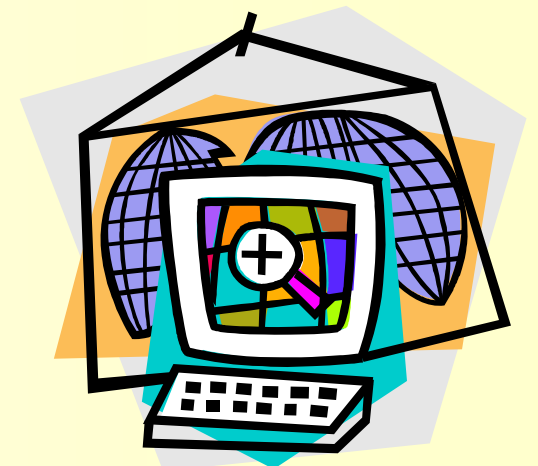
- *Consult with standard reviews and textbooks (c.f. [this FAQ](#))* *to know the concepts → good keywords for “Googling”*

- *How to search documents on the WEB ?*

www.abinit.org/about/?text=search

- *How to search relevant posts in MLs ?*

www.abinit.org/wws/



Let us have a quick tour !

About ABINIT

- What is ABINIT?
- Latest news
- Partners / Sponsors
- [Contact us](#)
- [Help ABINIT](#)

ABINIT Package

- [Sources, help files](#)
- Binaries (summary)
- Browse latest sources

Extra Packages

- Pseudopotentials
- PAW Atomic Data
- Atomic Densities
- Input Files

Documentation

- [Help files](#)
- [Input variables](#)
- [FAQ](#)
- Benchmarks
- Gallery

Community

- [Netiquette](#)
- [Mailing lists](#)
- Events
- [Bibliographical database](#)
- Job openings
- [Problem reports](#)
- Links
- Miscellaneous info

Other sections

- [Developer's corner](#)

What is ABINIT ?

ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulations using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (the GW approximation). In addition to the main ABINIT code, different utility programs are provided.

ABINIT is a project that favours development and collaboration ([short presentation of the ABINIT project - 10 pages in pdf](#)).

Getting started

- Welcome to new users ! Please read the [Readme](#) and subscribe to the [ABINIT users mailing list](#).
- Starting from version 3, ABINIT is distributed under the [GNU General Public Licence](#).
- If you plan to write a scientific article in which ABINIT was used, please read the [acknowledgments](#) suggestions. When your article is published, please [register](#) it in the ABINIT database.
- There are [many ways](#) to help the ABINIT project, including sponsoring.
- If you want to report a problem, please use [the problem report template](#).

About ABINIT

What is ABINIT?
Latest news
Partners / Sponsors
Contact us
Help ABINIT

ABINIT Package

[Sources, help files...](#)
Binaries (summary)
Browse latest sources

Extra Packages

Pseudopotentials
PAW Atomic Data
Atomic Densities
Input Files

Documentation

Help files
Input variables
FAQ
Benchmarks
Gallery

Community

Netiquette
Mailing lists
Events
Bibliographical database
Job openings
Problem reports
Links
Miscellaneous info

Other sections

[Developer's corner](#)

Available versions of the code (and associated help files) :

◆ **ABINIT v4.6**

- Help files : [installation notes](#), [release notes](#), [features](#), [new user guide](#), [abinis help](#), [input variables](#), [tutorial](#)
- Download :
 - [ABINIT v 4.6.2](#) (only for developers)
 - [ABINIT v 4.6.1](#) (only for reference)

◆ **ABINIT v4.5**

- Help files : [installation notes](#), [release notes](#), [features](#), [new user guide](#), [abinis help](#), [input variables](#), [tutorial](#)
- Download :
 - [ABINIT v 4.5.3](#) (production version)
 - [ABINIT v 4.5.2](#) (only for reference)
 - [ABINIT v 4.5.1](#) (only for reference)

◆ **ABINIT v4.4**

- Help files : [installation notes](#), [release notes](#), [features](#), [new user guide](#), [abinis help](#), [input variables](#), [tutorial](#)
- Download :
 - [ABINIT v 4.4.4](#) (preferred production version, robust)
 - [ABINIT v 4.4.3](#) (only for reference)
 - [ABINIT v 4.4.2](#) (only for reference)
 - [ABINIT v 4.4.1](#) (only for reference)

About ABINIT

- What is ABINIT?
- Latest news
- Partners / Sponsors
- [Contact us](#)
- Help ABINIT

ABINIT Package

- Sources,help files...
- Binaries (summary)
- Browse latest sources

Extra Packages

- Pseudopotentials
- PAW Atomic Data
- Atomic Densities
- Input Files

Documentation

- Help files
- Input variables
- FAQ
- Benchmarks
- Gallery

Community

- Netiquette
- Mailing lists
- Events
- Bibliographical database
- Job openings
- Problem reports
- Links
- Miscellaneous info

Other sections

- Developer's corner

Contact information

- ◆ **For new users**
 - ◇ [Read Me First](#)
 - ◇ Consult [FAQ](#)
- ◆ **For users with problems**
 - ◇ First, read the [Netiquette](#)
 - ◇ Consult [FAQ](#)
 - ◇ Search in the [forum archive](#)
- ◆ **For developers**
 - ◇ [How to contribute](#)

Please notice & read this !

- ◆ **Projet leader**

Prof. Xavier Gonze
Catholic University of Louvain-la-Neuve
Lab PCPM (Physico-Chemistry and Physics of Materials)
1, Place Croix du Sud
Louvain-la-Neuve, BELGIUM
Tel : +3210472076 Fax : +3210473452

- ◆ **Webmaster** : [Jean-Michel Beuken](#)
- ◆ **GNU Arch manager** : [Yann Pouillon](#)

About ABINIT

What is ABINIT?
Latest news
Partners / Sponsors
Contact us
Help ABINIT

ABINIT Package

Sources,help files...
Binaries (summary)
Browse latest sources

Extra Packages

Pseudopotentials
PAW Atomic Data
Atomic Densities
Input Files

Documentation

Help files
Input variables
FAQ
Benchmarks
Gallery

Community

Netiquette
Mailing lists
Events
Bibliographical database
Job openings
Problem reports
Links
Miscellaneous info

Other sections

Developer's corner

Netiquette for ABINIT forum/developer MLs

Copyright (C) 2003-2004 ABINIT group (MMikami, JMBeuken, XGonze)
This file is distributed under the terms of the GNU General Public License,
see ~ABINIT/Infos/copyright or <http://www.gnu.org/copyleft/gpl.txt>.
For the initials of contributors, see ~ABINIT/Infos/contributors .

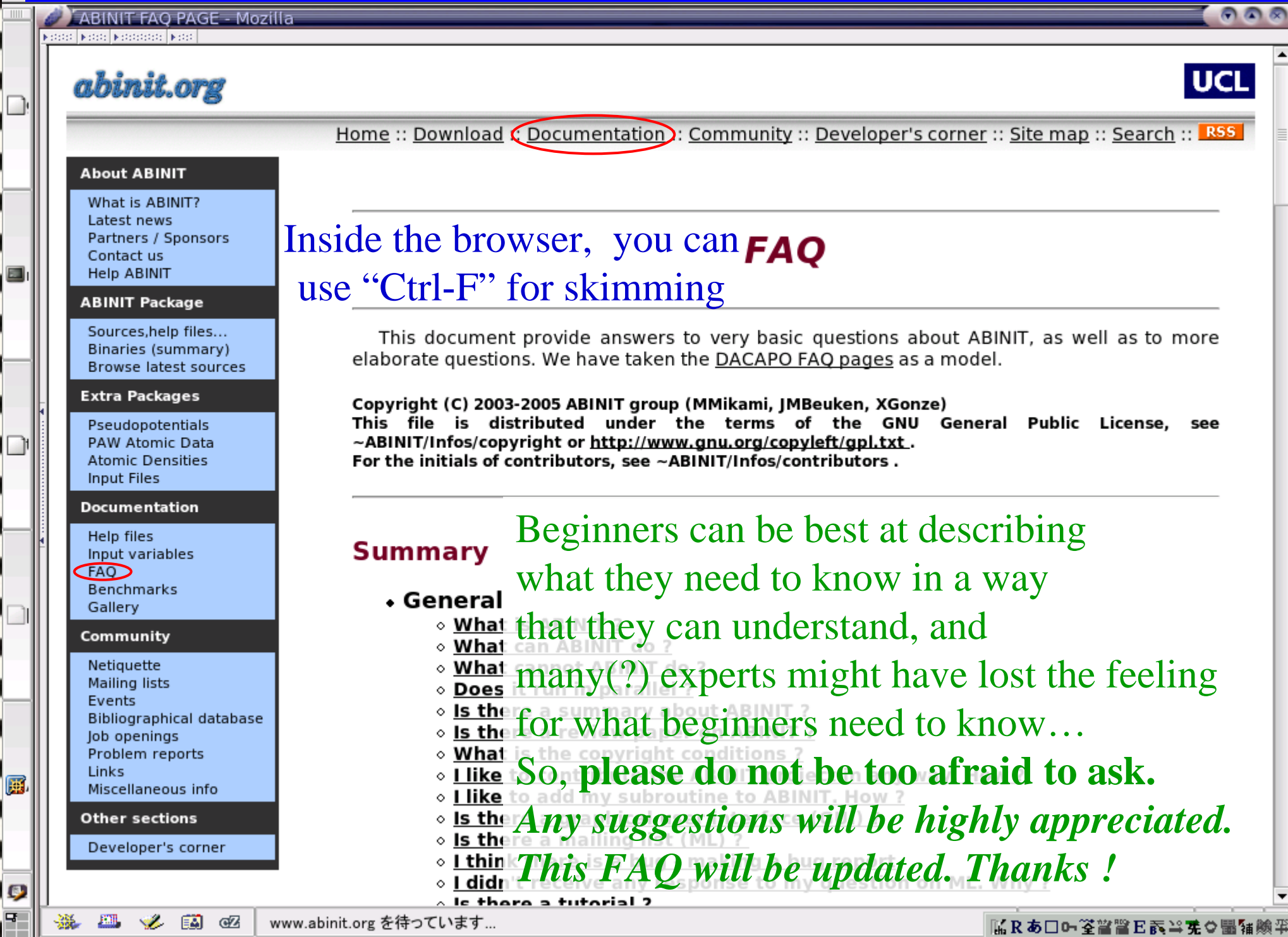
The ABINIT MLs are available for fruitful information exchange among ABINITioners, thanks to the UCL system and the administrators' hard work.

Now the number of the accounts in the forum ML gets over 500 from many countries, i.e. **GLOBAL**. Since our "common sense" may differ from country to country, we strongly feel that we need set up our etiquette to keep the MLs effective. Thus those who want to post e-mails (esp. questions) to the MLs should follow a sort of etiquette ("netiquette") to make the MLs most effective, and the burden of our limited resource ("humanware" as well as hardware) little as possible.

*beautiful & small post
positive feedback !*

Our netiquette will be :

1. Before posting, **please check relevant documents** (the [FAQ](#) etc.) in ABINIT source archives (src_tests_*.tar.gz) as well as [the ML archives](#).
 - Q: How to find relevant documents for my questions ?"
 - A: Follow [this FAQ](#) !
2. **Try to make your post "beautiful" as possible**. Specifically speaking,
 1. Give a meaningful Subject to your e-mail that may help us to find/remember your post easily. We should avoid "HELP","PLEASE","Question", (BLANK), ...
 2. Do not cite e-mails that are not relevant to your post. When you want to start a new thread, please do not post by follow-up (reply). This is important, for Mailers/ML web pages make the most use of "thread" idea.
 3. Please avoid two-byte characters in your e-mails. (Especially for Asian subscribers, e.g. Chinese characters for "month", "date", "year" etc.).
 4. Please stick to PLAIN TEXT format for posting. About "HOW TO SEND YOUR E-MAIL in PLAIN TEXT ?". you can consult with the online help of your Mailer. The following



Inside the browser, you can **FAQ** use “Ctrl-F” for skimming

This document provide answers to very basic questions about ABINIT, as well as to more elaborate questions. We have taken the [DACAPO FAQ pages](#) as a model.

Copyright (C) 2003-2005 ABINIT group (MMikami, JMBeuken, XGonze)
This file is distributed under the terms of the GNU General Public License, see [~ABINIT/Infos/copyright](#) or <http://www.gnu.org/copyleft/gpl.txt>.
For the initials of contributors, see [~ABINIT/Infos/contributors](#).

Summary

• General

- ◊ **What** can ABINIT do ?
- ◊ **What** does it run in parallel ?
- ◊ **Does** it run in parallel ?
- ◊ **Is there** a summary about ABINIT ?
- ◊ **Is there** a tutorial ?
- ◊ **What** is the copyright conditions ?
- ◊ **I like** to add my subroutine to ABINIT. How ?
- ◊ **I like** to add my subroutine to ABINIT. How ?
- ◊ **Is there** a mailing list (ML) ?
- ◊ **Is there** a mailing list (ML) ?
- ◊ **I think** I have a bug report
- ◊ **I didn't** receive any response to my question on ML. Why ?
- ◊ **Is there** a tutorial ?

Beginners can be best at describing what they need to know in a way that they can understand, and many(?) experts might have lost the feeling for what beginners need to know... So, please do not be too afraid to ask. Any suggestions will be highly appreciated. This FAQ will be updated. Thanks !

About ABINIT

- What is ABINIT?
- Latest news
- Partners / Sponsors
- Contact us
- Help ABINIT

ABINIT Package

- Sources,help files...
- Binaries (summary)
- Browse latest sources

Extra Packages

- Pseudopotentials
- PAW Atomic Data
- Atomic Densities
- Input Files

Documentation

- Help files
- Input variables
- FAQ
- Benchmarks
- Gallery

Community

- Netiquette
- Mailing lists
- Events
- Bibliographical database
- Job openings
- Problem reports
- Links
- Miscellaneous info

Other sections

- Developer's corner

Search



Google Search

Search WWW Search www.abinit.org

About ABINIT

What is ABINIT?
Latest news
Partners / Sponsors
Contact us
Help ABINIT

ABINIT Package

Sources,help files...
Binaries (summary)
Browse latest sources

Extra Packages

Pseudopotentials
PAW Atomic Data
Atomic Densities
Input Files

Documentation

Help files
Input variables
FAQ
Benchmarks
Gallery

Community

Netiquette
Mailing lists
Events
Bibliographical database
Job openings
[Problem reports](#)
Links
Miscellaneous info

Other sections

[Developer's corner](#)

Problem Report

This is the description of the ABINIT problem report format. Please refer to the ABINIT [Netiquette](#) list as well, before sending your report via e-mail. Copyright (C) 2000-2004 ABINIT group (MM,XG)

This file is distributed under the terms of the GNU General Public License, see [-ABINIT/Infos/copyright](#) or <http://www.gnu.org/copyleft/gpl.txt>

For the initials of contributors, see [-ABINIT/Infos/contributors](#) .

In case of a problem with ABINIT, what can you do ?

First, please refer to [-ABINIT/Infos/known_problems.*](#) to see if your problem is reported or not. If you think that you have found a bug, you should report it. The best is of course when you have a bug fix. However usually, you will ask for help to the ABINIT group.

Note that on the side of the developpers, there is no obligation to look at your problem, it is a pure courtesy ... (You know, ABINIT is free ...)

In the case where you have a bug fix, please send by mail (to [Xavier Gonze](#)) :

1. A short description of the problem (do not forget the description of the platform, if it is platform-dependent, as well as the version of code in which this problem appeared)
2. The modified routine(s), in the form of a tar.gz file, if there is more than one routine.

If you have a problem without bug fix and ask us to solve it, we would like you to make a first effort :

- ◆ First, examine the log file, to see whether there might be a WARNING or COMMENT message suggesting that you have made a mistake in your input file.
- ◆ Second, try to reduce the run so as to make the problem appear within two minutes on your machine. Basically, you should reduce ecut, and reduce the k point sampling. You might as well try with a smaller cell, if the problem allows it. If the problem disappear when trying to reduce these, or if the run becomes meaningless, you should signal it to us. Note that some bugs seen in production runs at 20

About ABINIT

What is ABINIT?
Latest news
Partners / Sponsors
Contact us
Help ABINIT

ABINIT Package

Sources,help files...
Binaries (summary)
Browse latest sources

Extra Packages

Pseudopotentials
PAW Atomic Data
Atomic Densities
Input Files

Documentation

Help files
Input variables
FAQ
Benchmarks
Gallery

Community

Netiquette
Mailing lists
Events
Bibliographical database
Job openings
Problem reports
Links
Miscellaneous info

Other sections

Developer's corner

Input Variables

- ◆ For the latest developer's version :
[list of automatic tests](#) that use each input variable (script written by T. Deutsch).
- ◆ [For ABINIT v4.5](#) → next page
- ◆ [For ABINIT v4.4](#)
- ◆ [For ABINIT v4.3](#)
- ◆ [For ABINIT v4.2](#)

Useful to find template files
for your own jobs

Main ABINIT code, input variables:

Complete list.

This document lists the names (keywords) of all input variables to be used in the main input file of the abinis code.

The new user is advised to read first the [new user's guide](#), before reading the present file. It will be easier to discover the present file with the help of the [tutorial](#).

When the user is sufficiently familiarized with ABINIT, the reading of the `~ABINIT/Infos/tuning` file might be useful. For response-function calculations using abinis, the complementary file `~ABINIT/Infos/respfn_help` is needed.

Copyright (C) 1998-2005 ABINIT group (DCA,XG,RC)

This file is distributed under the terms of the GNU General Public License, see `~ABINIT/Infos/copyright` or <http://www.gnu.org/copyleft/gpl.txt>.

For the initials of contributors, see `~ABINIT/Infos/contributors`.

Goto : [ABINIT home Page](#) | [Welcome](#) | [Suggested acknowledgments](#) | [List of input variables](#) | [Tutorial home page](#) | [Bibliography](#)

Help files : [New user's guide](#) | [Abinis \(main\)](#) | [Abinis \(respfn\)](#) | [Mrgddb](#) | [Anaddb](#) | [AIM \(Bader\)](#)

Files which describe the input variables:

- Basic variables, [VARBAS](#)
- Developpement variables, [VARDEV](#)
- Files handling variables, [VARFIL](#)
- Geometry builder + symmetry related variables, [VARGEO](#)
- Ground-state calculation variables, [VARGS](#)
- GW variables, [VARGW](#)
- Internal variables, [VARINT](#)
- Parallelisation variables, [VARPAR](#)

About ABINIT

[What is ABINIT?](#)
[Latest news](#)
[Partners / Sponsors](#)
[Contact us](#)
[Help ABINIT](#)

ABINIT Package

[Sources,help files...](#)
[Binaries \(summary\)](#)
[Browse latest sources](#)

Extra Packages

[Pseudopotentials](#)
[PAW Atomic Data](#)
[Atomic Densities](#)
[Input Files](#)

Documentation

[Help files](#)
[Input variables](#)
[FAQ](#)
[Benchmarks](#)
[Gallery](#)

Community

[Netiquette](#)
[Mailing lists](#)
[Events](#)
[Bibliographical database](#)
[Job openings](#)
[Problem reports](#)
[Links](#)
[Miscellaneous info](#)

Other sections

[Developer's corner](#)

What is ABINIT ?

ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulations using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (the GW approximation). In addition to the main ABINIT code, different utility programs are provided.

ABINIT is a project that favours development and collaboration ([short presentation of the ABINIT project - 10 pages in pdf](#)).

Getting started

- ◆ Welcome to new users ! Please read the [Readme](#) and subscribe to the [ABINIT users mailing list](#).
- ◆ Starting from version 3, ABINIT is distributed under the [GNU General Public Licence](#).
- ◆ If you plan to write a scientific article in which ABINIT was used, please read the [acknowledgments](#) suggestions. When your article is published, please [register](#) it in the ABINIT database.
- ◆ There are [many ways](#) to help the ABINIT project, including sponsoring.
- ◆ If you want to report a problem, please use [the problem report template](#).

[Login](#)

[Pref](#) [Your subscriptions](#) [Home](#) [Help](#)

ABINIT PROJECT Mailing Lists Service

This server provides you access to your environment on mailing list server **sympa@abinit.org**. Starting from this URL, you can perform subscription options, unsubscription, archives, list management and so on.

To subscribe, click on one of the mailing lists below.

Mailing lists

Announce List (announce@abinit.org - *Announce of new ABINIT release*)

Forum List (forum@abinit.org - *The ABINIT Users Mailing List*)

Advisory Committee List (advisory@abinit.org - *The ABINIT Advisory Committee Mailing List*)

Developer List (developer@abinit.org - *The ABINIT Developer Mailing List*)

GNU Arch List (gnuarch@abinit.org - *The Mailing List for Developer using GNU Arch*)

In order to benefit from the full services provided by this server, you probably need to identify yourself first : enter below your email address and password.

email

password :

Login


email is your subscriber email address and **password** is your password.

If you never had a password from that server or if you don't remember it :

[Send me a password](#)

Listmaster : [Jean-Michel Beuken](#)

[ABINIT home page](#)

Powered by 

Logout

ABINIT Project

Create list Preferences Your subscriptions Home Help

mmikami@rc.m-kagaku.co.jp
Subscriber

forum@abinit.org
The ABINIT Users Mailing List

List info

Subscribers: 651

Owners
Jean-Michel
Beuken
Moderators

Subscriber Options

Unsubscribe

Archive

Post

Shared web

Search

Advanced search

→ next page

2002	01	02	03	04	05	06	07	08	09	10	11	12
2003	01	02	03	04	05	06	07	08	09	10	11	12
2004	01	02	03	04	05	06	07	08	09	10	11	12
2005	01	02	03	04	05	06	07	08	09	10	11	12

08 2005

page n° 1 / 1

Chronological Thread

- **Re: Re: [abinit-forum] Dynamical Matrix (for Copper and other metals) for Runtime problem on Opteron Cluster with Pathscale/mvapich.** fer
 - **Re: [abinit-forum] Runtime problem on Opteron Cluster with Pathscale/mvapich.** Steven Homolya
- **Re: [abinit-forum] Runtime problem on Opteron Cluster with Pathscale/mvapich.** Xin, Liu
- **Installation of 4.5.3 on 64-bit Opteron running PGI 6.0 mlusk version 4.5.3** Nuno A. G. Bandeira
 - **RE: [abinit-forum] version 4.5.3** Mark T. Lusk
 - **Re: [abinit-forum] version 4.5.3** Nuno A. G. Bandeira
 - **GPL Re: [abinit-forum] version 4.5.3** Scott P. Beckman
 - **Re: GPL Re: [abinit-forum] version 4.5.3** Nuno A. G. Bandeira
- **total energy calculation** occupierliu
 - **Re: [abinit-forum] total energy calculation** Rajdeep Saha
 - **Re: [abinit-forum] total energy calculation** Masayoshi Mikami
 - **Re: [abinit-forum] total energy calculation** Fernando D. Vila
- **PAW potential for Hf** Kyeongjae Cho
- **GW calculations** fabrizio cleri
- **how to compile abinit parallelly with HP-MPI + Intel Fortran 8.0** Hai-Ping Lan
- **Re: Re: [abinit-forum] total energy calculation** occupierliu
- **Compilation/Declaration error in rherformi 590** Paul Fene

[Logout](#)

ABINIT Project

[Create list](#)

[Preferences](#)

[Your subscriptions](#)

[Home](#)

[Help](#)

mmikami@rc.m-kagaku.co.jp
Subscriber

forum@abinit.org
The ABINIT Users Mailing List

[List info](#)

Search field : **2005-08**

Subscribers: **651**

Owners
[Jean-Michel Beuken](#)
Moderators

Search
Prefer
Case
Check
Layout
Search area

- this **sentence**
- newest** messages
- insensitive**
- part** of word
- 10** results by page
- Sender**
- Date**
- all of** this words
- oldest** messages
- sensitive**
- entire** word
- 25** results by page
- Subject**
- one of** this words
- 50** results by page
- Body**

[Subscriber Options](#)

[Unsubscribe](#)

[Archive](#)


[Post](#)

[Shared web](#)

2005-08 ▲
2005-07
2005-06
2005-05 ▼

Extend search field

Listmaster : Jean-Michel Beuken

Powered by 

About ABINIT

- What is ABINIT?
- Latest news
- Partners / Sponsors
- Contact us
- Help ABINIT

ABINIT Package

- Sources,help files...
- Binaries (summary)
- Browse latest sources

Extra Packages

- Pseudopotentials
- PAW Atomic Data
- Atomic Densities
- Input Files

Documentation

- Help files
- Input variables
- FAQ
- Benchmarks
- Gallery

Community

- Netiquette
- Mailing lists
- Events
- Bibliographical database
- Job openings
- Problem reports
- Links
- Miscellaneous info

Other sections

- Developer's corner

ABINIT bibliographical database

This database contains information about papers in which scientific results have been produced thanks to ABINIT (for years 2000 and after) or its predecessors (for years 1999 or before : Corning, Plane_Wave, RESPFN, the MGDDDB8 and PPDDDB9 utilities). It might rather complete for ABINIT, RESPFN and the utilities, but is likely incomplete for Corning and Plane_Wave.

The authors of a paper based on ABINIT should register it, when it is published (no preprint, please !). The database can be searched : the whole listing can be printed, or the search can be done by years or by authors.

When you have clicked a button below, submit your action ...

- Search in the data base
- Add an article in a journal
- Add an article in conference proceedings
- Add a contribution to a book
- Add an abstract of conference

→ for search of papers

→ for registration

Submit

About ABINIT

- What is ABINIT?
- Latest news
- Partners / Sponsors
- Contact us
- Help ABINIT

ABINIT Package

- Sources,help files...
- Binaries (summary)
- Browse latest sources

Extra Packages

- Pseudopotentials
- PAW Atomic Data
- Atomic Densities
- Input Files

Documentation

- Help files
- Input variables
- FAQ
- Benchmarks
- Gallery

Community

- Netiquette
- Mailing lists
- Events
- Bibliographical database
- Job openings
- Problem reports
- Links
- Miscellaneous info

Other sections

- Developer's corner

Searching the ABINIT database.

To obtain the list of all papers in the database, submit the search as it is. For a restricted search, you can mention an author's name, or part of its name, or a year, or de-select some of the buttons.

Remember : papers in 1999 or before relates to Corning, Plane_wave or RESPFN, while in 2000 or after, ABINIT was used.

Author:

Title :

- Type: articles in journals
 articles in conference proceedings
 contributions to book
 abstracts of conferences

Year:

→ next page

About ABINIT

What is ABINIT?
 Latest news
 Partners / Sponsors
 Contact us
 Help ABINIT

ABINIT Package

Sources,help files...
 Binaries (summary)
 Browse latest sources

Extra Packages

Pseudopotentials
 PAW Atomic Data
 Atomic Densities
 Input Files

Documentation

Help files
 Input variables
 FAQ
 Benchmarks
 Gallery

Community

Netiquette
 Mailing lists
 Events
 Bibliographical database
 Job openings
 Problem reports
 Links
 Miscellaneous info

Other sections

Developer's corner

Search results ...

Note that they are ordered by reverse chronological order.

Back to the [ABINIT bibliographical database page](#).

Books

1. Oganov A.R.
"Theory of Minerals at High and Ultrahigh Pressures: Structure, Properties, Dynamics, and Phase Transitions."
 in **High-Pressure Crystallography, NATO Science Series II: Mathematics**
 edited by A.Katrusiak, P.F.McMillan,pp 199-215 (Kluwer Academic Publishers, Dordrecht., 2004)
 Contact : a.oganov@mat.ethz.ch
2. G.-M. Rignanese, X. Gonze, A. Pasquarello
"Ab-initio calculations of the structural, electronic and dynamical properties of high-k dielectrics"
 in **High-k gate dielectrics**
 edited by M. Houssa,pp 431-466 (Institute of Physics Publishing, 2004)
 Contact : gonze@pcpm.ucl.ac.be
3. P.C.H. Mitchell, S.F. Parker, A.J. Ramirez-Cuesta and J. Tomkinson
"Interpretation and Analysis of Spectra using Molecular Modelling"
 in **Vibrational Spectroscopy with Neutrons With Applications in Chem**
 edited by ,pp 137-182 (World Scientific, Series on Neutron Techniques and Applications, 2004)
 Contact : a.j.ramirez-cuesta@rl.ac.uk
4. L. Wirtz, M. Dallos, H. Lischka, and J. Burgdörfer
"Ab-initio Calculations of Charge Exchange in Ion-surface Collisions: An

About ABINIT

What is ABINIT?
Latest news
Partners / Sponsors
Contact us
Help ABINIT

ABINIT Package

Sources,help files...
Binaries (summary)
Browse latest sources

Extra Packages

Pseudopotentials
PAW Atomic Data
Atomic Densities
Input Files

Documentation

Help files
Input variables
FAQ
Benchmarks
Gallery

Community

Netiquette
Mailing lists
Events
Bibliographical database
Job openings
Problem reports
Links
Miscellaneous info

Other sections

[Developer's corner](#)

What is ABINIT ?

ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulations using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (the GW approximation). In addition to the main ABINIT code, different utility programs are provided.

ABINIT is a project that favours development and collaboration ([short presentation of the ABINIT project - 10 pages in pdf](#)).

Getting started

- ◆ Welcome to new users ! Please read the [Readme](#) and subscribe to the [ABINIT users mailing list](#).
- ◆ Starting from version 3, ABINIT is distributed under the [GNU General Public Licence](#).
- ◆ If you plan to write a scientific article in which ABINIT was used, please read the [acknowledgments](#) suggestions. When your article is published, please [register](#) it in the ABINIT database.
- ◆ There are [many ways](#) to help the ABINIT project, including sponsoring.
- ◆ If you want to report a problem, please use [the problem report template](#).



“Source tree” for the source archive → next page

Home :: [Download](#) :: [Documentation](#) :: [Community](#) :: [Developer's corner](#) :: [Site map](#) :: [Search](#) :: [RSS](#)

Developer's docs

[Source tree](#)

[Ongoing efforts](#)

[How to contribute](#)

[Miscellaneous](#)

GNU Arch pages

[TLA Tutorial for ABINIT](#)

[Getting started with TLA](#)

[Writing change logs](#)

[Advanced use of TLA](#)

[Switching to Bazaar](#)

Other sections

[Home](#)

Miscellaneous

- ◆ In September-October 2000, the ABINIT international collaboration was taking advantage of facilities provided by [SourceForge](#). However, the access was too slow, and only an old version of ABINIT is available there.
- ◆ [Self-documentation of source.](#)
- ◆ [MatLab environment to extract data from ABINIT output files.](#)

Copyright © 2004-2005 The ABINIT Group

This file is distributed under the terms of the GNU General Public License, see `~ABINIT/COPYING` or <http://www.gnu.org/copyleft/gpl.txt> for details.
For the initials of contributors, see `~ABINIT/Infos/contributors`.

This page is maintained by [Yann Pouillon](#) and [Jean-Michel Beuken](#).

Developer's docs

[Source tree](#)

[Ongoing efforts](#)

[How to contribute](#)

[Miscellaneous](#)

GNU Arch pages

[TLA Tutorial for ABINIT](#)

[Getting started with TLA](#)

[Writing change logs](#)

[Advanced use of TLA](#)

[Switching to Bazaar](#)

Other sections

[Home](#)

Directories and files

Introduction

This file provides a description of the organisation of the abinit package, in terms of subdirectories and their content.

See the files *welcome.html* and *new_user_guide* for an introduction to the abinit package. Instructions to install the code, make the executable and run some tests can be found in the *Installation_notes* directory.

The main directory of the abinit package is referred to as *~ABINIT* hereafter, independently of its absolute location. As an example, in Louvain-la-Neuve, there is one in */home2/pcpm/gonze/ABINIT/ABINITv4.4.3* on the machine Decci. From the Web site, a file *src_tests.4.4.3.tar.gz* can be dumped and, following the installation notes, a *~ABINIT* directory will be created for this version.

In the present 4.4 version of the ABINIT package, there are more than thirty subdirectories in *~ABINIT*:

- ◆ A. *Infos*: contains different information files.
- ◆ B. *Src **: they contain the source of ABINIT.
- ◆ C. *Lib **: they contain the source of different libraries.
- ◆ D. *Test **, *Tutorial*, *Pspis_for_tests*: they contain tests cases, the tutorial and the needed pseudopotentials.
- ◆ E. *Machine_dept_files*: contains machine dependent files, i.e. *makefile_macros* and *mpif.h*.
- ◆ F. *Utilities*.

~ABINIT also contains:

- ◆ a *README* file;



3. How to explore the tar.gz ?

- *First, try this Suggestion: (README, Tutorials, Test_*, ...)*
- *Refer to the Site Map for the archive :*
www.abinit.org/developers/?text=dirs_and_files

How to find relevant documents/input examples etc?

- **grep -ir (key word)** on most unix system
(or, find . -name ¥* -print | xargs grep (keyword))
- acrobat reader for PDF files

NB: The following may also help to find documents:

“Google desktop” on Windows*

Default function in the next Windows (“Vista”)

“Spotlight” on Tiger (MacOSX 10.4.x)

Let us demonstrate !

4. Wrap-up

**ABINITIONers, note Everything is developing,
so, let us learn everyday
and remember this prayer everyday...**

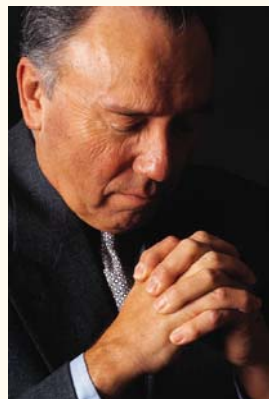


*Grant me the serenity
to accept the things I cannot change,*

Courage to change the things I can,

And the wisdom to know the difference ...

about ABINIT as well !



Thank you for your attention !