

ABINIT Developer skype meeting 23 June 2020

Program

14:00 to 18:30

A. Global discussions (extracted from the proposal of topics below - estim. duration 1h45 to 2h50 ?)

- (1) ABINITv9 installation : status/difficulties/planned adaptation for ABINITv9.2; the ABINIT fallback project (tentatively 40-60 minutes)
- (2) Removing the files.file : status/planned adaptation/ possible beautification of selected tests (?tutorials) (tentative 20-30 minutes)
- (3) Beautification : tutorials, usage of XML for most test pseudopotentials, and/or other topics for beautification ? (tentatively 20-30 minutes)
- (4) Status of the test farm (info / questions / suggestions) (tentatively 15-25 minutes)
- (5) Next events (tentatively 15-25 minutes)

Break (15 minutes - coffee/tea/soft drink - well make your choice ... from your coffee machine or your fridge ...)

B. Specific personal projects (less than one hour ; see the list below, follow the alphabetic order, suggestion of one slide/three minutes per person willing to speak - well, more slides/time if you feel it is worth)

C. Other issues (if time left ...)

Contributions

Please, if you intend to participate to the event, indicate in the table below your name + possible topics or comments (e.g. suggestion of topics, or if restricted availability between 14:00-18:30 Europe or 8:00-12:30 East coast).

In case I do not have your SkypeID, I will contact you a few days before the meeting. Xavier.

Last name	SkypeID	Topics/Comments
Amadon	with MT	Update on cRPA and new projects. (I have to leave at 17h40)
Baguet	with MT	??
Beuken	OK	abinit-fallbacks project & test farm
Bieder	Testing	
Bousquet	Testing	Reshape of berryphase_new (+ applied E-, D-field) and higher parall level
Bruneval	OK	GW density matrix implementation
Côté	OK	To discuss: Can we remove the file.file file? Installation of ABINIT with Easybuild.

Last name	SkypeID	Topics/Comments
Gonze	OK	Build system of ABINIT : difficulty of installation (e.g. modifying ABINIT v9.0 for solving practical issues encountered on diverse machines) ; beautification end of August ?
Giantomassi	OK	Density/Potential in NetCDF by default (#90), refactoring of ddb_t to support dynamical quadrupoles #93, tutorials, runtests.py and \$ABI_PSPDIR #91, New syntax for sharing the documentation of vars common to different executables #74, Fix tests with FAILS_IFMPI tag #92, Using MPI_INPLACE version as default #89
Guster	OK	??
He	OK	brief update on development of TB2J and SCDM-k method for lattice and electron Wannier function.
Jollet	with MT	PAW tutorials update 5 '
Pouillon	OK	Build system
Rignanese	OK	??
Romero	OK	PyProcar status. Cleaning Berry phase modules (with E. Bousquet)
Torrent	OK	BS v9 experience on various architectures + Abinit dev workshop in May/June 2021
Van Bever	OK	??
Verstraete	OK	EPC update with Matteo, GPU enabling + followup on abstraction layer from CEA
Zwanziger	OK	Brief update on progress on orbital magnetization

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<https://wiki.abinit.org/> - **Tips for ABINIT users and developers**

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