

# QUANTUM ESPRESSO

## 2015 Developers' Meeting

Paolo Giannozzi

ICTP Trieste, 14 Jan. 2015

- *One year later:* status of planned activities, what has been done, what is going on, what hasn't been done, what should be done, ...

# 2014 news and achievements

- *New developments:*

- Hybrid functionals for CP have percolated to the stable release
- Wyckoff positions and space groups are recognized
- A few more functionals have been implemented
- First (very limited) interface with libxc is available
- GWW upgraded to GWL (with Lanczos chains)
- More and more pseudopotentials/PAWsets available

- *Funding:*

- (at least) two projects involving QE submitted (or about to be submitted): one FET-HPC and one Center of Excellence

## 2014 news and achievements (2)

- *The never-ending XML saga has taken a new turn:*
  - A company is willing to fund the definition and implementation of a XML file format, with schemas and whatnot, to be used together with their (proprietary) UI. Definition phase to be completed soon.
- *QE Tutorials and Schools:*
  - Usual, successful end-user schools and tutorials in 2014 (Penn State, Tokyo, others?), with at least two more planned or proposed or hoped for 2015 (ICHEC Ireland, Argentina)
  - A new edition of the developers schools is going to be held in ICTP in the next two weeks. Same format as last year's school.

# 2014 bad news and non-achievements

No significant progresses in

- Documentation (both user's and developer's)
- Porting of EPW and/or other electron-phonon stuff
- Actually *using* the new framework for QMMM and for binding to other codes
- Extending and making usable the ASE interface
- Hybrids with USPP/PAW still half-baked (PAW doesn't work)

# To be done in 2015

Major tasks:

- Finish definition and implementation of new xml file format
- Move to portable binary files, rethink the entire I/O machinery
- ... plus many other open issues listed in
  - the previous page
  - the [qe-forge.org](http://qe-forge.org) tracker page (“bugs” and “Feature Requests”)
  - the [quantum-espresso.org](http://quantum-espresso.org) “Roadmap” page

# Suite of the meeting

10:30-10:50 Iurii Timrov

Update on linear-response codes: TD-DFPT, EELS,

11:00-11:20 Paolo Umari

BSE without conduction states, hybrid functional

11:30-11:50 Fabio Affinito

Intel Parallel computing

12:00-12:30 Anton Kozhevnikov

Ongoing work at CSCS

Lunch break

14:00-14:20 Filippo Spiga  
QE-GPU + git/buildbot/test-suite

14:30-14:50 Andrea Cepellotti  
Latest on Aiida

15:00-15:20 Marco Govoni  
GW and hybrid functionals

15:30-15:50 Oliviero Andreussi  
Status of Environ

15:50-16:00 Tone Kokalj  
PWtk - a tcl scripting interface for QE