

QUANTUM ESPRESSO

2014 Developers' Meeting

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

2013 news and achievements

- *New management of web sites and of QE-forge software:*
The QE Foundation pays SPIN, a service provider based in Trieste, to host and manage QE web sites and QE-forge software.
- *Trademark:*
The QUANTUM ESPRESSO trademark and logos have been registered by the QE Foundation.
- *QE Tutorials and Schools:*
 - Usual, successful end-user schools and tutorials, with more already planned for 2014 (Tokyo, Penn State, India, ...)
 - New: two developers schools have been held in March and in December 2013, both in Trieste. They have followed two rather different approaches: an experience to be carefully studied.

2013 news and achievements (2)

- *New developments:*

- New packages: GW-Lanczos (Umari), Frozen-phonon (Nardelli)
- COUPLE interface (Axel), together with new MPI initialization, makes calling QE from external packages *much* easier
- New GGA and vdW functionals (various authors), Tkatchenko-Scheffler (DiStasio), XDM (Otero de la Roza), GAU-PBE (Song)
- Improved (in my opinion) restart mechanism (PG)
- Improved mechanism for I/O to RAM (PG+Paulatto)
- Many other small or not-so-small improvements and extensions; cleanup of loops for hybrid functionals (PG)
- TD-DFPT with hybrid functionals (Ge?)
- Calculation of EELS (Timrov?)

2013 partial achievements

- Hybrid functionals with USPP/PAW (Paulatto + PG): partially working, must be finished
- Interface for ASE (Tornatore), the Atomistic Structure Environment developed at CAMP: released, but nobody is taking care of it
- XML data file format: work restarted, stalled, recently restarted again by Ziraldo
- Windows builds made available (Axel)

2013 bad news and non-achievements

No significant progresses in

- Finding some money (EU or national projects)
- Documentation (both user's and developer's)
- Testing
- Pseudopotential/PAW formats, setup of database of all-electron results
- Porting of EPW and/or other electron-phonon stuff
- Several other long-promised new developments

To be done in 2014

See preceding page! Also:

- Finish hybrids with USPP/PAW
- Finish new xml file format, move towards portable binaries
- ...

Suite of the meeting

- 9:30-10:00 Layla Martin-Samos
Integration of new modules and plugins into QE
Projects: Horizon 2020
- 10:00-10:30 Emine Kukucbenli
Report on the QE developer school just held in T
- 10:30-11:00 Break
- 11:00-11:30 Filippo Spiga
Update on QE on GPU
- 11:30-12:00 Fabio Affinito
Porting QE on Xeon Phi
- 12:00-12:30 Discussion: Horizon 2020 and psi-k projects
- 12:30-14:00 Lunch Break

- 14:00-14:30 Pizzi/Cepellotti
AiiDA: management of high-throughput calculation
- 14:30-15:00 Ferretti
New developments in CP: self-interaction/Koopman
functionals, complex wfcs
- 15:00-15:30 Uwe Gerstmann
New development in spin-orbit calculations with
- 15:30-16:30 General discussion