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-forg software:**
  The QE Foundation pays SPIN, a service provider based in Trieste, to host and manage QE web sites and QE-forg 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 Trieste

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 calculations

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