

QUANTUM ESPRESSO

2017 Developers' Meeting

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ICTP Trieste, 9 Jan. 2017

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

2016 news and achievements (1)

- *New developments in v.5.4 and 6.0 of QE:*
 - Major speedup of hybrid functionals in PW using ACE
 - Hybrid functionals in PW with USPP and PAW now work (also with ACE)
 - Phonons with vdw-DF
 - Bethe-Salpeter equation added to GWL
 - Simplified and more modular FFT/grid management
 - I/O cleanup: new XML data file with schema, optional HDF or (simplified) binary files, simplified output directory, with less files and no subdirectories
 - No files written during PWscf runs, $k+G$ indices are stored in memory
 - Modularization of Linear-Response codes started
 - EPW completely integrated into QE
 - D3Q released as an add-on package
 - Improved real-space treatment of Q and beta functions with Fourier filtering
 - Socket interface with i-PI universal force engine (ipi-code.org)
 - Support for QM-MM using MPI
 - ... did I forget anything else?

2016 news and achievements (2)

- *Contributed developments to be (or not to be?) included:*
 - Improved tetrahedron method (Mitsuaki Kawamura) - DONE
 - Changes to postprocessing (Leopold Talirz) - DONE
 - DFT-D3 (Miha and Layla)
 - Improved band parallelization for hybrid XC (Taylor Barnes et al)
 - QM-MM (Damien Scherlis) (aligned 17 october 2017 to v.6.0)
 - 3D-RISM-SCF (Satomichi Nishihara) in branches/espresso-3drismscf/espresso
see also qe-forge.org/pipermail/q-e-developers/2015-May/000874.html
 - Constrained DFT(Matthew Goldey, U. Chicago)
qe-forge.org/pipermail/q-e-developers/2016-October/001461.html
 - Topological Numbers (Hyungjun Lee, EPFL)
qe-forge.org/pipermail/q-e-developers/2016-October/001462.html

The above list is far from being complete!

2016 news and achievements (3)

- *New QE paper is (slowly) converging*
- *MAX CoE in full activity, first “MaX” release of QE end of August 2016 (a pre-release of v.6.0 that was released end of September).*
- *Collaboration with Schrödinger: QE now works together with the Maestro interface.(note: we have received several other requests for collaboration on interfaces to QE, but no further activity has been started)*
- *QE Trademark registration completed*
- *QE Tutorials and Schools: Nothing during 2016, apart from Linear-Response Developers’ Meeting in Jan.2016. Advanced Workshop to be held in January 2017, likely another workshop in Penn State in 2017.*

2016 bad news and non-achievements

- *The QE IT Infrastructure is crumbling*

The QE infrastructure, currently hosted at Spin, consists of

- Domains quantum-espresso.org, qe-forge.org, pwscf.org
- www.quantum-espresso.org web site, currently running WordPress
- qe-forge.org, currently running the community edition of GForge

There are multiple problems with these services:

- Web site: the WordPress version is obsolete, the template is messy and buggy. No upgrade path without a disproportionate effort.
- qe-forge: as above. GForge is obsolete and not upgradable, the setup is messy and buggy, the entire machinery is slow.

Some hard decisions have to be taken, keeping in mind future maintainability, no later than yesterday.

- *Slow progress on:*
 - Optimization and parallelization. There have been some improvements but ACE for hybrid functionals seems to me the only significant one
 - Linear-Response codes. After an initial impulse, there hasn't been much activity, especially when compared with the amount of work to be done
 - Documentation. Apart from introduction of Ford into EPW, the state of both user and developer documentation is still, uhm, unsatisfactory?
 - Tools for Continuous Integration, apart from the test farm of EPW
 - Solving some problems that persist since years:
 - * "not enough space allocated for fft",
 - * "scf/phonon does not converge"
 - * "error in Cholesky: S matrix not positive definite"
 - * miscellaneous phonon problems, e.g.:
 - <http://qe-forge.org/pipermail/q-e-developers/2016-November/001496.html>
 - <http://qe-forge.org/pipermail/q-e-developers/2016-September/001361.html>
 - Solving recently reported problems, e.g.:
 - <http://qe-forge.org/pipermail/q-e-developers/2016-October/001471.html>

To be done in 2017 (IMHO)

- Input/Output:
 - Finalize the new xml- and hdf5-based file format, in particular reducing the number of binary files, improving their format
 - Extend new xml file to CP. This is a prerequisite for next item:
 - Make the new xml file the default, remove the old one soon
 - Design a schema-based pseudopotential file replacing UPF
 - Replace iotk with FoX
- Optimization and Performances:
 - Iterative diagonalization with reduced dense-matrix diagonalization
 - Exact exchange exploiting localization
 - Automatic estimate of optimal parallelization parameters
- Modularization and Documentation:
 - Standard header to all routines
 - Automatic documentation using FORD or whatever other solution

Suite of the meeting

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|---------------|---|
| 09:30 - 09:50 | New XML I/O in QE, Pietro Delugas (SISSA) |
| 09:50 - 10:10 | New FFT data distribution to improve scalability, Stefano de Gironcoli (SISSA) |
| 10:10 - 10:30 | How developing QE using GIT/GitHub will look like, Filippo Spiga (U.Cambridge) |
| 10:30 - 11:00 | Break |
| 11:00 - 11:20 | Status report on AiiDA, and the Materials Cloud portal for QE data, Nicola Marzari (EPFL) |
| 11:20 - 11:50 | Quantum Espresso enabling on Marconi, Fabio Affinito (CI) |
| 11:50 - 12:20 | Optimizing EXX calculations in QE for Intel Xeon Phi Thorsten Kurth/Taylor Barnes (NERSC) |
| 12:30 - 13:00 | Discussion |
| 13:00 - 14:00 | Lunch |
| 14:00 - 14:20 | Progress in EPW and discussion on test-farm & automatic documentation, Samuel Ponce (U.Oxford) |
| 14:20 - 14:40 | Using QE as a library: Lessons learned by developing the Sternheimer GW code, Martin Schlipf (U.Oxford) |
| 14:40 - 15:00 | thermo_pw: a Fortran driver for Quantum ESPRESSO routines |

Andrea Dal Corso (SISSA)

15:00 - 15:20 WEST: large-scale excited states calculations,
Marco Govoni (U.Chicago)

15:30 - 17:30 Discussion

Tuesday January 10th:

9:30 - 9:50 DFT and DFPT for two-dimensional systems: implementation
of 2D Coulomb cutoff in PW and PH, Thibault Sohier (EPFL)

9:50 - 10:10 Hubbard interactions from density functional perturbation
theory, Iurii Timrov (EPFL)

10:10 - 10:30 New development in exact exchange calculation,
Ivan Carnimeo (SISSA)

10:30 - 11:00 Break

11:00 - 11:20 XML data validation and Python tools for QE,
Davide Brunato (SISSA)

11:30 - 13:00 Discussion

14:00 - 18:00 QE Code Fest

Wednesday January 11th:

09:00 - 13:00 QE Code Fest

14:00 - 18:00 QE Code Fest (breaks anytime someone needs one)

Work Groups:

- A. Improving testing coverage and compilers support
- B. Working on improving and extending XML and HDF5 I/O support
- C. Enabling QE parallelism enhancements in FFT's and eigensolvers
- D. Using QE as a library