QUANTUM ESPRESSO
2018 Developers' Meeting, Sissa, 1 Feb. 2018

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February 1, 2018

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

2017 news and achievements (1)

- *New developments in v.6.1/6.2/6.2.1 of QE:*

    - Hybrid functionals with localization
    - Pair-of-bands parallelization for hybrid XC (incompatible with localization)
    - SCAN and meta-GGA functionals working (sort of)
    - DFT+D3
    - Two-dimensional phonons
    - New QE-GPU using CUDA Fortran
    - I/O cleanup almost finished
    - More "librarization" of QE: Kohn-Sham solvers ...
    - .. and more FFT revolutions !

2017 news and achievements (2)

Contributed developments to be (or not to be?) included:

- QM-MM in CP (Damien Scherlis) (aligned end 2017 to v.6.2)

- Various DFT+U stuff: DFT+U+V, phonons with DFT+U

- The new QE-GPU

- Magnons with TD-DFPT?

- Some mentioned last year, whose state is unclear:
  - 3D-RISM-SCF (Satomichi Nishihara)
  - Constrained DFT(Matthew Goldey, U. Chicago
  - Topological Numbers (Hyungjun Lee, EPFL)
  - OEP

- ...

2017 news and achievements (2)

- *New QE paper published*

- *Move to new IT infrastructure started* (limited to the repository, though)

- *Development moved to gitlab*, continuous integration tools more or less set up

- *MAX CoE in full activity*, closing in 2018, application to new CoE is brewing

- *Collaboration with Schrödinger is ongoing*

- *QE Tutorials and Schools*:
  Advanced Workshop, January 2017. Next:
  School on electron-phonon interactions, March 2018 Workshop at Penn State,
  June?

2017 bad news and non-achievements

- *Slow progress on:*

  - Optimization and parallelization. The many changes to FFT's and the many pieces of codes transformed into libraries haven't (yet) translated into significant speed and parallelization improvements
  - Modularization of linear-response codes. There have been some significant developments in LR codes, but modularization hasn't progressed in 2017
  - Documentation. The state of user documentation is as bad as it used to be, while developer's documentation is even worse because badly obsolete
  - Solving some problems that persist since years (see last year's list!)

To be done in 2018 (IMHO)

- Organization:

  – Define procedures for the proper usage of git
  – Update developer documentation

- Input/Output:

  – Finalize the new xml- and hdf5-based file format, removing all remaining bugs
  – Remove old xml files and `iotk`, leaving only the new format and `FoX`

- Optimization and Performances:

  – Iterative diagonalization with reduced dense-matrix diagonalization
  – Automatic estimate of optimal parallelization parameters
  – OpenMP parallelization must be redone from scratch
  – Include QE for GPU into main distribution

- Modularization and Documentation:

  – Standard header to all routines
  – Automatic documentation using FORD or whatever other solution

Suite of the meeting

10:00-10:25 Andrea Dal Corso: Thermo_pw, a fortran driver for
            Quantum ESPRESSO routines - progress report.
10:30-10:55 Samuel Ponce': Updates on EPW and the test-farm/test-suite
11:00-11:25 Martin Schlipf: Progress in the Sternheimer GW code

14:30-14:45 Ivan Carnimeo: updates and perspectives on hybrid functional
14:50-15:05 Pietro Delugas: updates on I/O and on git
15:10-15:25 Pietro Bonfa': state of QE-GPU
15:30, or when he arrives: Paolo Umari
After: General discussion