

# QUANTUM ESPRESSO

## 2018 Developers' Meeting, Sissa, 1 Feb. 2018

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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, 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, 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

## 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