QE developers' meeting 2019 - summary

On Jan. 7th and 8th 2019 a meeting of developers of Quantum ESPRESSO was held at SISSA Trieste. Upon request received by some developers[1], and following what was done in previous editions, the meeting was made available online via "google meet" sessions to interested people.

The first session, on Jan.7th afternoon, was dedicated to the new "maintainable" GPU porting based on CUDA Fortran and aligned with the current development branch. The session was attended by 10 developers, either locally or remotely, including the CINECA team most directly involved in the new GPU porting.

The second session, on Jan.8th morning, was dedicated to the current status of the development and to problems to be solved in the near future. The final session, on Jan.8th afternoon, was dedicated to actual steps and actions to be taken to continue and extend the development of Quantum ESPRESSO, with particular emphasis on MaX activities, deliverables and deadlines. The last two sessions were attended by about **20?** developers, half of which coming from Trieste and surroundings, the other half from other Italian and EU institutions, with 5 more remotely connected via google meet.

Two preliminary documents were made available on the developers mailing list, containing an overview of problems and proposed solutions. These documents[2] are also based on a survey of problems and suggestions expressed by the community of users[3] and developers of (and around) Quantum ESPRESSO.

The agenda of the discussion can be found in **(link to be verified)**
http://www.quantum-espresso.org/news-events/news/qe-developers-meeting-2019
The outcomes of the discussion are summarized in the following document **(to be put somewhere on web)**.

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[1] https://lists.quantum-espresso.org/pipermail/developers/2019-January/002007.html, https://lists.quantum-espresso.org/pipermail/developers/2019-January/002008.html
[2] https://lists.quantum-espresso.org/pipermail/developers/2019-January/002003.html, https://lists.quantum-espresso.org/pipermail/developers/2019-January/002005.html
[3] See e.g. the following messages and related threads in the users mailing list: http://lists.quantum-espresso.org/pipermail/users/2018-December/041785.html, http://lists.quantum-espresso.org/pipermail/users/2018-December/041883.html,

QE developers' meeting 2019 - report

Day 1: discussion on the status and perspectives of the GPU porting, and actions to be taken also in view of MaX activities. (chair Pietro Bonfà)

Pietro Bonfà presents the status of the GPU version of Quantum Espresso **(link slides)**.
List of agreed upon actions from the meeting:

- Refactoring of some use associated variables to become *PROTECTED* thus promoting code modularization.
- Investigation of strategies to refactor exchange and correlation functionals.
- Enhancement of testing suite to increase code coverage, in particular with respect to the various modes of parallel execution.
- Cleanup of exact-exchange code, with removal of likely obsolete *_loc and *_exx copies of variables and FFT descriptors.
- Release of alpha (or maybe beta) version of QE-GPU together with next stable QE version.

Day 2 - Morning: Round table on plans for the future (Chair Paolo Giannozzi)

Most important actions to be taken for Quantum ESPRESSO are introduced by Paolo Giannozzi **(link slides, TODO list** https://lists.quantum-espresso.org/pipermail/developers/2019-January/002005.html) with some more (see https://lists.quantum-espresso.org/pipermail/developers/2019-January/002003.html) communicated by Nicola Marzari:

- **Reorganization of MD, structural optimization, NEB and the like**: better disentangle the various "ion-moving" steps implemented in PW from the electronic "quantum engine", unify where possible the algorithms available in PWscf with those used in CP. This will make implementation of other approaches easier, providing a clearer pathway for future developers.
- **Algorithms for self-consistency and diagonalization.** New algorithms for diagonalization like PPCG have been recently added to PWscf. These new techniques are very promising in terms of a more efficient usage of band parallelism. More work is going to be started to introduce new techniques based on conjugate gradients both for diagonalization and direct optimization of the charge density.

- More work is needed in the **Linear Response suite**, continuing the effort done on the wake of the LR developer's meeting of 2016, also with some attention to code performances. Within the work planned in the MaX project, developers in SISSA have started profiling the linear response codes and leveraging on this. During the discussion the importance of existing packages (in particular, SternheimerGW) that to some extent rely on Quantum Espresso libraries has also been stressed. A meeting aimed towards common work with Yambo is planned for the following week (Jan.14) .
- **ASCII and binary output data** will be, starting with the next release, available only in the new format. Compatibility issues are solved, except for three "corner cases" of little-used unmaintained utilities. Dropping the old format will allow to complete the replacement of IOTK by the FoX library. The usage of HDF5 for binary output data will remain, at least in the near future, optional in order to avoid a rigid dependence on hdf5 libraries. The availability of the HDF5 library in many HPC center as well as in many workstations will allow a broader adoption of this format, improving its verification and maintenance.
- The **postQE** suite must be finalized, methodologies for contribution documented and there should be more activity in advertising it for usage and contributions.
- Most **pseudopotentials** are now used in the UPF v.2.0.1 formats, which is XML-compliant, but cannot be described by a schema. A new schema-based format, which reproduces the contents and mostly the semantics of UPF v2.0.1 is available and usable since version 6.2.1. For the moment it does not seem advisable to distribute pseudopotentials in the new format because distributed files must be accessible also by previous versions.
- Various proposals for streamlining the **reading of pseudopotentials** have been discussed.
    - Reading could be done on the main node on start and then UPF data structures could be broadcast to all nodes.
    - Provide hard-coded pseudopotentials that can be used as default; or, provide a tool for building the hard-coded library that should the be linked by the code.

Day 2 - Afternoon: identification of actions to be taken, resources, duties to assign. (chair Paolo Giannozzi)

A few immediate actions and directions have been identified.

- Oscar Baseggio in SISSA will be the contact person for anybody willing to contribute to linear-response maintenance. He will also take care, in the framework of the MaX project, of profiling and benchmarking the DFPT part of the Quantum ESPRESSO suite.
- Pietro Delugas will follow the release of postQE.
- Pietro Bonfà will be the reference person for the QE-GPU porting and next release.
- Carlo Cavazzoni will follow the efforts in CINECA to unify the various band parallelization, replacing the current clumsy "task groups" with OpenMP tasks.

- Paolo Giannozzi will continue some work recently started on pseudopotential reading
- Stefano de Gironcoli will start working, in collaboration with applied mathematicians in China, on direct minimization of the energy functional as an alternative to the current self-consistency + diagonalization algorithm of PWscf.
- Paolo Giannozzi and Fabrizio Ferrari will work on functionals.
- Uwe Gerstmann will work, in collaboration with Davide Ceresoli, towards porting the simplified spin-orbit band structure calculation (already presented in a previous developer meeting) and the new zero-field splitting calculation.
- All: improve developer and user documentation.
- The date of the next stable release is set to **February 28**.