MAX DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO: porting to GPGPUs and towards exascale HPC

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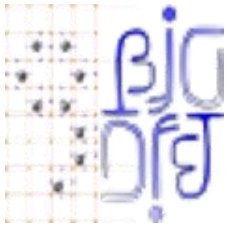
Welcome: MAX codes Webinar Series



Outline:

The webinar will present the version of Q.E. for CUDA-GPU systems

Pietro Delugas (SISSA, Trieste): Introduction and general information about QUANTUM ESPRESSO

Fabio Affinito (CINECA, Bologna): Introduction to Marconi100

Pietro Bonfà (University of Parma): How to compile and run Quantum Espresso on CUDA-GPU systems

What is QUANTUM ESPRESSO

- Main goals of QUANTUM ESPRESSO are:
  - **innovation** in theoretical methods and numerical algorithms
  - **efficiency** on modern computer architectures
- Started in 2002 from the merge of pre-existing packages; some core components have been under development for about 30 years
  - **PWscf** and **PHonon** (Baroni, De Gironcoli, Dal Corso, Giannozzi and others …)
  - **CP/FPMD** (Pasquarello, Laasonen, Trave, Car, Marzari, Cavazzoni, Scandolo and others …)

The Quantum ESPRESSO foundation

The Quantum ESPRESSO Foundation

foundation.quantum-espresso.org

- is a non profit organization.
- coordinates and supports research, education, and outreach within the QE community
- owns the trademarks and protects the open-source character of QE
- raises funds to foster the QE project and its development
- Current member of the Foundation are:

  SISSA, EPFL, ICTP, IOM-CNR, CINECA

What is inside QUANTUM ESPRESSO

Libraries:

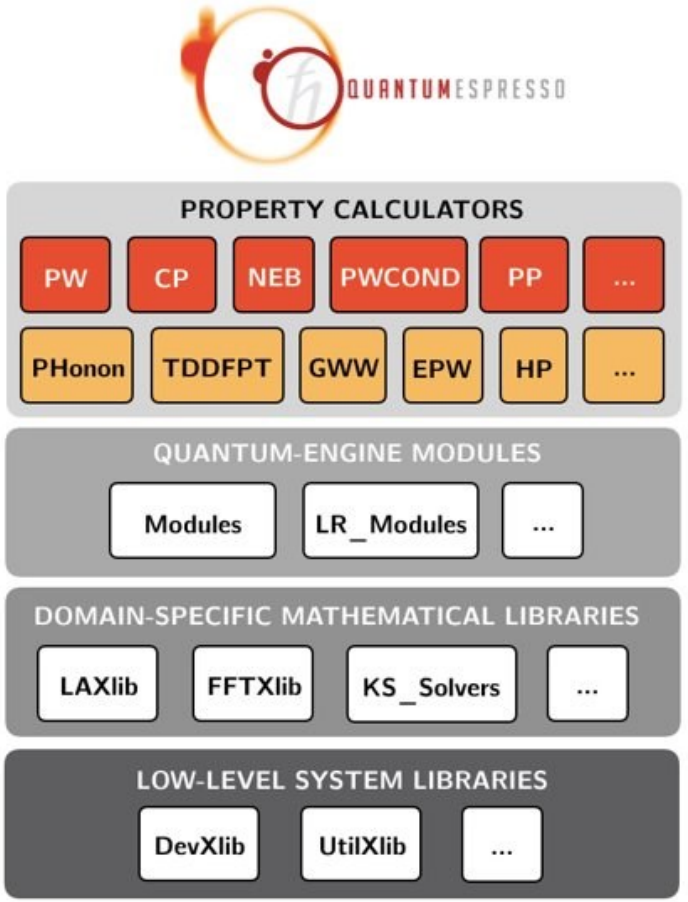
- Completely encapsulated can be easily reused in other codes.
- Are distributed by the MAX centre.

Modules:

- Encapsulated and self contained but still dependent on Q.E. datastructure
- Mostly fitted to be used for internal development in Q.E. of packages with similar data structure

Applications:

- Quantum engines
- Property calculators



Applications:

- **PWscf**:
  - Total energies, forces stresses using plane waves + pseudopotentials or PAW
  - L(S)DA , GGA , metaGGA and many other advanced functionals
  - collinear and noncollinear spin density
  - much more …
- **CP -** Car-Parrinello molecular dynamics
- **PHonon**: vibrational frequencies, dielectric response, anharmonic terms and many more with linear response
- **TDDFPT**: Optical spectra and collective excitations.
- **EPW**: electron phonon with Wannier Function
- Interoperability with many other external packages …

Users

Mostly researchers and students in academia, but also industry.

Since 2002 more than 30 training events all around the world (schools, tutorials, developers' schools)

Last stable version: quantum-espresso.org/downloads

More than 9000 **downloads from for the last version (6.5)**

Resources for users.

- You can find the documentation at :

  http://www.quantum-espresso.org/resources/users-manual

- Subscribe to the user forum

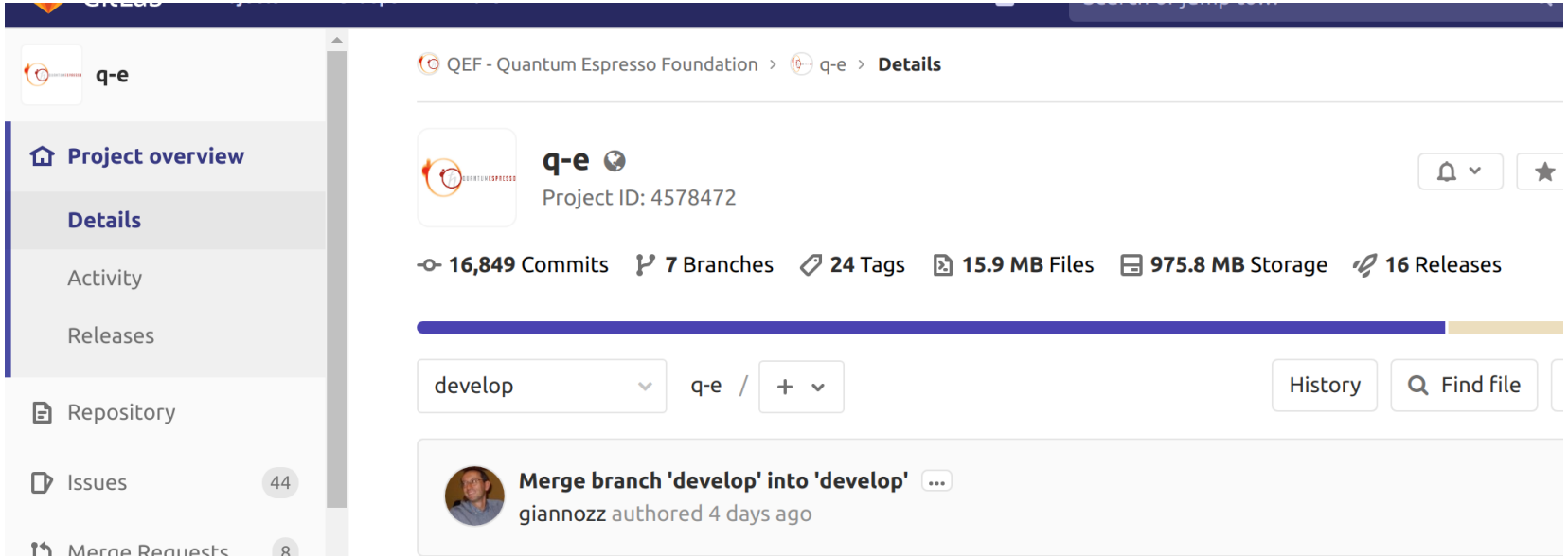
  https://lists.quantum-espresso.org/mailman/listinfo/users

- Browse mailining list archives:

  https://www.mail-archive.com/users@lists.quantum-espresso.org/

Developers

- Main repository on GitLab https://gitlab.com/QEF/q-e
  - Merge requests
  - Issues
- CUDA-GPU version on https://gitlab.com/QEF/q-e-gpu
- Mirror on GitHub: https://github.com/QEF/q-e



Interoperable data formats for I/O

- Standard hierarchical data formats:
  - XML small data collected in one data file described by a XSD schema
  - HDF5 files for charge density and wavefunctions

- Python packages for reading and converting data files
  - qeschema: available on pip and on GitHub: https://github.com/QEF/qeschema
  - postqe: https://github.com/QEF/postqe

More info

- www.quantum-espresso.org
- http://www.max-centre.eu/codes-max/quantum-espresso
- Papers:
  - J. Chem. Phys. **ESS2020**, 154105 (2020); https://doi.org/10.1063/5.0005082@jcp.2020.ESS2020.issue-1
  - J.Phys.:Condens.Matter **21**, 395502 (2009) http://dx.doi.org/10.1088/0953-8984/21/39/395502
- MAX libraries:

  http://www.max-centre.eu/product/libraries

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THANKS

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