QUANTUM ESPRESSO: porting to GPGPUs and towards exascale HPC

Webinar: Fabio Affinito
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Welcome: MAX codes Webinar Series

How to use Quantum ESPRESSO on new GPU based HPC systems

Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive.
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
• 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

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 …
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 mailing list archives:
  https://www.mail-archive.com/users@lists.quantum-espresso.org/
Developers

• Main repository on GitLab [https://gitlab.com/QEF/q-e](https://gitlab.com/QEF/q-e)
  • Merge requests
  • Issues
• CUDA-GPU version on [https://gitlab.com/QEF/q-e-gpu](https://gitlab.com/QEF/q-e-gpu)
• Mirror on GitHub: [https://github.com/QEF/q-e](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
• www.quantum-espresso.org

• http://www.max-centre.eu/codes-max/quantum-espresso

• Papers:

• MAX libraries:
  http://www.max-centre.eu/product/libraries
THANKS

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