MAX DRIVING THE EXASCALE TRANSITION

QUANTUMESPRESSO

The QE suite

QUANTUM ESPRESSO™ (QE) is a suite of applications for ab-initio electronic structure calculations using plane waves and pseudopotentials. With a constantly increasing number of citations of the main relevant articles (Fig1a), and a share of 32% of total PRACE allocations in the "Chemical Sciences and Materials" domain, among all the electronic structure codes (Fig1b), the QE suite is by far one of the most popular solutions currently available for simulations in chemistry and material science. The estimated user community includes nearly 45000 researchers, distributed in more than 110 countries, who have tsuccessfully used QE to achieve their scientific results and publish around 18000 articles on international peer-reviewed journals indexed by ISI Web of Science database.
When downloading the code, many users declare to work in some of the currently most strategic scientific and technological fields, such as green technologies (e.g. organic electronics, energy storage and conversion, heterogeneous catalysis), device engineering (e.g. quantum transport, semiconductors), spectroscopy and electrochemistry (Fig1c).

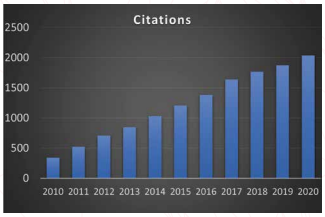

Fig1a

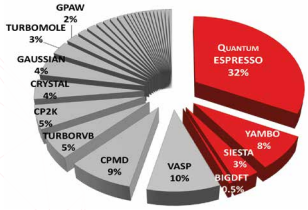

Fig1b

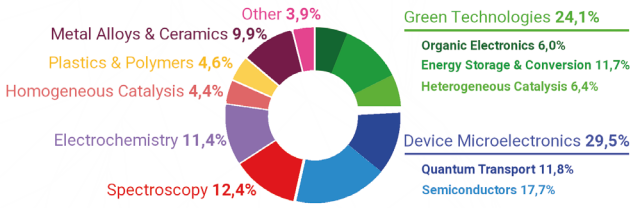

Fig1c

Some selected features of the QE suite

PWSCF:

- Solution of Kohn-Sham equations with different methods
- Energies, forces, stress of molecules and materials
- Born-Oppenheimer molecular dynamics
- Band structures (e.g. Fig2a) and DOS
- Magnetic properties

CP:

- Car-Parrinello molecular dynamics

Phonon:

- Phonon frequencies
- IR and Raman spectra (e.g. Fig2b, Fig2c)
- Dielectric properties

TDDFPT:

- UV-Vis absorption
- Electron energy loss spectroscopy
- Spin wave spectroscopy

NEB:

- Reaction paths

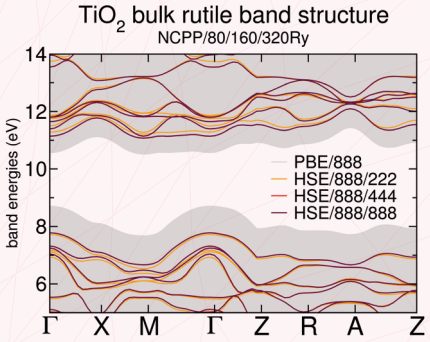

Fig2a

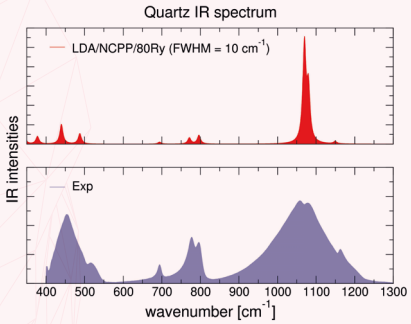

Fig2b

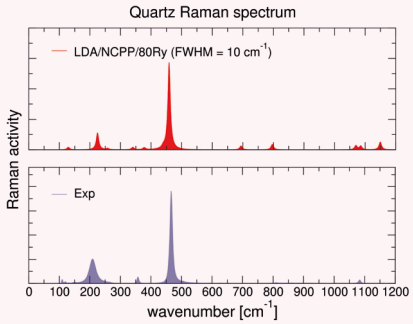

Fig2c

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QUANTUMESPRESSO

High Performance Computing with QE

Most of the applications of the QE suite are designed for the efficient usage of the state-of-the-art HPC machines using multiple parallelization levels.

The basal workload distribution can be done using MPI + OpenMP multithreading, possibly combined with GPU offloading, depending on the nodes' architecture, allowing computational treatment of systems with up to several thousands atoms. In Fig3a performance of PWSCF for a simulation of a mid-size system (a Carbon nanotube functionalized with two porphyrine molecules, about 1500 atoms, 8000 bands, 1 k-point) is shown on an HPC homogeneous nodes' cluster.

Additionally, auxiliary MPI parallelization levels allow to obtain further scaling. The band parallelization level distributes the operations on wave functions of different basal groups.

The two upper parallelization levels -- pools and images -- are very efficient because they distribute the computations in concurrent quasi-independent blocks; as shown in Fig3b for a Ph onon calculation on 72 atoms quartz, executed on an heterogeneous nodes' HPC cluster equipped with Ampere GPGPUs.

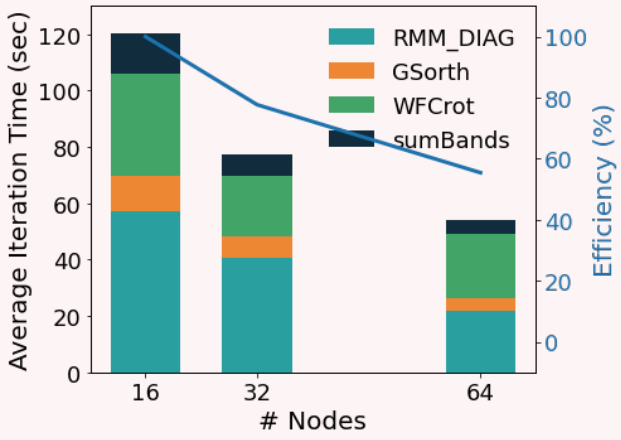

Fig3a

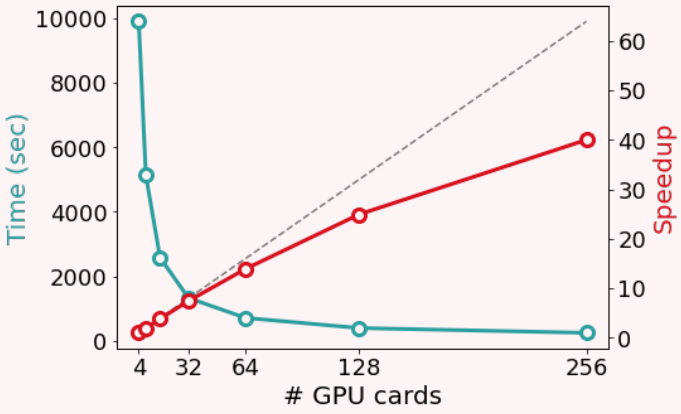

Fig3b

Support

Website | Latest release | Forum | Source code | Tutorials

References

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- *P. Giannozzi et al., Advanced capabilities for materials modelling with Quantum ESPRESSO, J. Phys.: Condens. Matter* ***29****, 465901 (2017).*
- *P. Giannozzi et al., QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter* ***21****, 395502 (2009).*
- *S. Scandolo et al., First-principles codes for computational crystallography in the Quantum-ESPRESSO package, Zeitschrift fur Kristallographie* **220**, *574-579 (2005).*