

QUANTUMESPRESSO

Quantum ESPRESSO is an **open-source** suite of computer codes that implements state-of-the-art electronic-structure methods for **materials modelling** at the atomic/nano-scale.

QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials Author(s): Giannozzi, P; Baroni, S; Bonini, N, et al.

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www.quantum-espresso.org







Ecole Polytechnique Fédérale

de Lausanne

DEMOCRITOS

DEmocritos MOdeling Center for Research In aTOmistic Simulation

Massachusetts Institute of Technology Princeton University DEMOCRITOS National Simulation Center of Trieste

CINECA National Supercomputing Center of Bologna



Material modelling

Questions that one would like to answer ...

- Why some material has a particular behavior?
- Would some material exhibit some particular property?
- Would this material work if submitted to ... ?
- Which material/materials do I have in my sample?

without the need of making experiments or going beyond the experimental sensitivity

Steps

- Finding of the equilibrium structure (ions and electrons)
- "Post-processing":
 - STM images
 - Density of States
 - plot of the electronic density and/or states
 - Absorption spectra
 - etc

FEATURES

espresso-4.1

- Structure optimisation
- Phonons
- Elastic constants
- Quantum transport
- Ab-initio molecular dynamics
- Dielectric and Raman tensors
- Infrared spectra
- NMR spectra

access to development version is open

- Electronic excitations: absorption spectra, ionisation potentials, electron affinities
- Distributed together:
 - Quantum transport WanT

www.want-code.org

Electronic excitations YAMBO

www.yambo-code.org

 coming soon Free energy reaction paths PLUMED http://merlino.mi.infn.it/~plumed/PLUMED/home.html

PERFORMANCES

ionic and electronic degree of freedom \rightarrow big objects \rightarrow relatively big communication between process

 Parallel computers : homogeneous architecture, fast communication between process → versatile

- Different parallelization levels
- Hybrid MPI-OPENMP

BENCHMARK CODE FOR:





http://www.prace-project.eu/

scalable on thousand of procs



Speed-up 3.5 3,25 2,75 2,5 2,25 -STD 3 -SCALAPACK 1,75 1,5 1,25 1 512 1024 2048 4096

HECToR - CNT10POR8 (CINECA benchmark)

BCX - W256 (CINECA benchmark)



http://www.deisa.eu/science/benchmarking/results

Courtesy of C. Cavazzoni, CINECA



DEISA EXTREME COMPUTING INITIATIVE



Ab-initio simulations of Protein-Surface Interactions mediated by WATer



S. Corni, A. Calzolari, G. Cicero, C. Cavazzoni, A. Catellani and R. Di Felice

DEISA EXTREME COMPUTING INITIATIVE

Distributed European Infrastructure for Supercomputing Applications

ElectroLuminescent Efficiency in polymers based Light Emitting Diodes



Identification of surface equilibrium structures

Model

Experiment



phthalocyanine + Zn or phthalocyanine+Fe16Zn on Ag substrate

pw.x + **pp.x**

A. Calzolari, W. Jin, J. E. Reutt-Robey and M. Buongiorno Nardelli





F. Fabris et al

Solvated hybrid surfaces : equilibrium structure



- Dye sensitized solar cell
- Squarainel + TiO2 + water
- Equilibration : 20ps Car-Parrinello molecular dynamics

cp.x

Equilibrium structure and charge distribution



 Nano-structuration of substrate induced by absorption of organic molecules

C60 + Au surface

pw.x + **pp.x**

more applications at : www.quantum-espresso.org/samples.html or at www.quantum-espresso.org/wiki/index.php/Bibliography

EDUCATION

- Quantum ESPRESSO with DEMOCRITOS, SISSA and ICTP are strongly involved in educational and dissemination activities related to material modelling from first principles.
- past schools and tutorials:

http://www.quantum-espresso.org/wiki/index.php/Tutorials_and_Examples

- -June 2010 workshop in Ireland
- -July 2010 school at SISSA
- -July 2010 CECAM tutorial at SISSA
- -2011 School in Brazil

QE COMMUNITY

There is a vast open community behind us

- Users 1034 subscribers to the *forum*
- Developers 23, researchers with write access to the source code. Two ways for contributing:
 - Sending routines/changes to coordinators
 - Asking for write access on the cvs

THE FORUM

pw_users@pwscf.org

E-mails from the beginning of the forum



E-mails during 2009



E-mails during 2009



E-mails during 2009



THE QE-forge





Welcome to QEforge

QEforge is a web portal, using Gforge as engine, offering an integrated software development environment: CVS or SVN repository, mailing lists, public forums, download space, wiki pages and much more. QEforge is hosted and maintained by the Democritos National Research Center, in collaboration with SISSA eLab and is open to researchers worldwide active in the field of computer simulation of matter at the atomic scale. Researchers participating in the QEforge initiative will retain complete control over their project (including the right not to release it), while enjoing the advanced development tools that QEforge provides. Our goal is to make QEforge a prime source of scientific software for scientists all over the world

For more information on QEforge, please contact the management

Latest News

New files for download

Paolo Giannozzi - 2010-03-10 11:33 - Quantum ESPRESSO The following new or updated files are available for download: Almost final set of patches for v.4.1.3, to be applied to v.4.1.2 - Benchmarks (input modified to work with next version of QE) (0 Comment) [Read More/Comment]

PWTK submitted to ge-forge

Anton Kokalj - 2009-07-23 07:56 - PWTK The development of PWTK -- PWscf ToolKit -- has been migrated to ge-forge

(0 Comment) [Read More/Comment]

SaX tutorial pdf slides availables

Lavla Martin-Samos - 2009-04-28 16:01 - Self-energies And eXcitations The pdf slides of SaX tutorial at Sao Paolo University (july 2008) are availables at section Docs (0 Comment) [Read More/Comment]

SaX presentation article at http://tinyurl.com/ao9ghw Layla Martin-Samos - 2009-02-20 10:38 - Self-energies And eXcitations http://tinyurl.com/ao9ghw

(0 Comment) [Read More/Comment]

ISO image

Lorenzo Paulatto - 2009-02-11 16:12 - QE live distribution Please note that for technical reasons it is not possible to upload the pre-generated iso image of the distribution. Checkout the CVS instead and generate the image yourself, it is not difficult!

geForge Statistics

Hosted Projects: 21 Registered Users: 121

Top Project Downloads

(381)Quantum ESPRESSO (214)GW+Wannier (206)DMFT (195)Quasiharmonic Approximation (179)Self-energies And eXcitations (123)GRID lattice dynamics (79)PWTK More

Most Active This Week

(100.0%) Quantum ESPRESSO (90.0%) Yambo (80.0%) Multi Scale Modeling Simulation (70.0%) Quantum Monte Carlo (60.0%) GW+Wannier (50.0%) Self-energies And eXcitations (40.0%) PWTK (30.0%) Quasiharmonic Approximation (20.0%) DMFT (10.0%) GRID lattice dynamics [More] **Recently Registered Projects** (02/18) VIBrational TOOLS

(02/01) CHAMP (11/17) vdW-DF Exchange-Correlation Functional (11/12) Solvent Models and Electrochemistry (10/28) QE-GIPAW (10/19) Multi Scale Modeling Simulation (09/15) PSlibrary (09/10) Yambo (09/04) Wyckoff Positions Parser (08/24) Sergey Gusarov

> Fusion Forge

QE-forge

- Mailing lists
- Forums
- Wiki
- Version management (cvs svn)
- Web pages
- Doc
- etc

What we expect to do

- Enhance the linux-like distribution character of QE, inviting more people to contribute.
- Explore the porting on of some parts on GPU (ICHEC, NVIDIA), GRID (e-lab).
- Improve QE-forge
- Improve exchanges with R&D.

THANK YOU