

QUANTUM ESPRESSO: first-principles simulations at the nanoscale (and towards the exascale)

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First HPC workshop, Master in High Performance Computing
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What is QUANTUM ESPRESSO?

QUANTUM ESPRESSO stands for *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization*

QUANTUM ESPRESSO is a *distribution* (an integrated suite) of software for atomistic calculations based on electronic structure, using density-functional theory, a plane-wave basis set, pseudopotentials.

It is freely available under the terms of the GNU General Public License

Main goals of QUANTUM ESPRESSO are

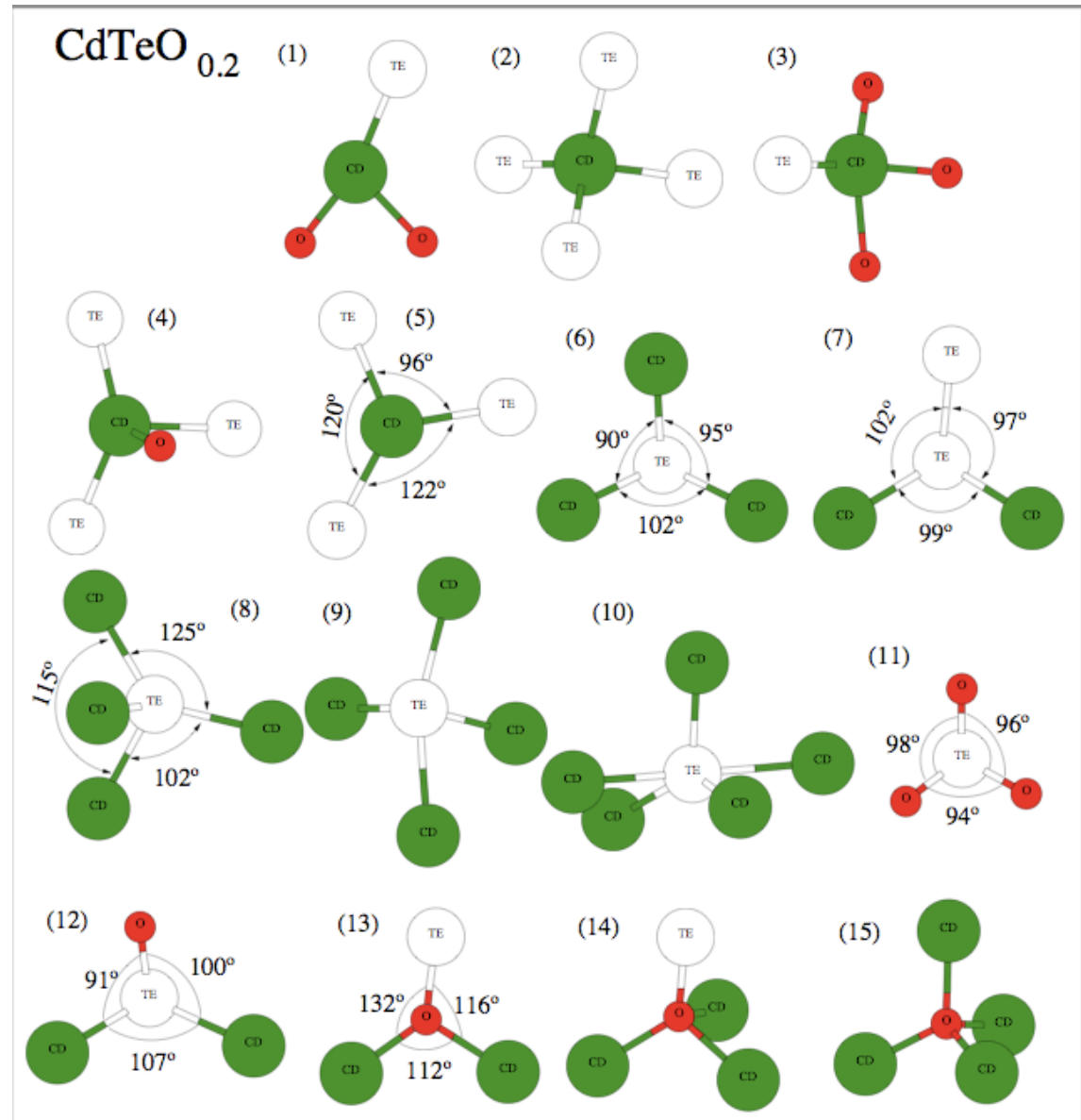
- *innovation* in theoretical methods and numerical algorithms
- *efficiency* on modern computer architectures

A great effort is also devoted to *user friendliness* and to the formation of a *users' and developers' community*

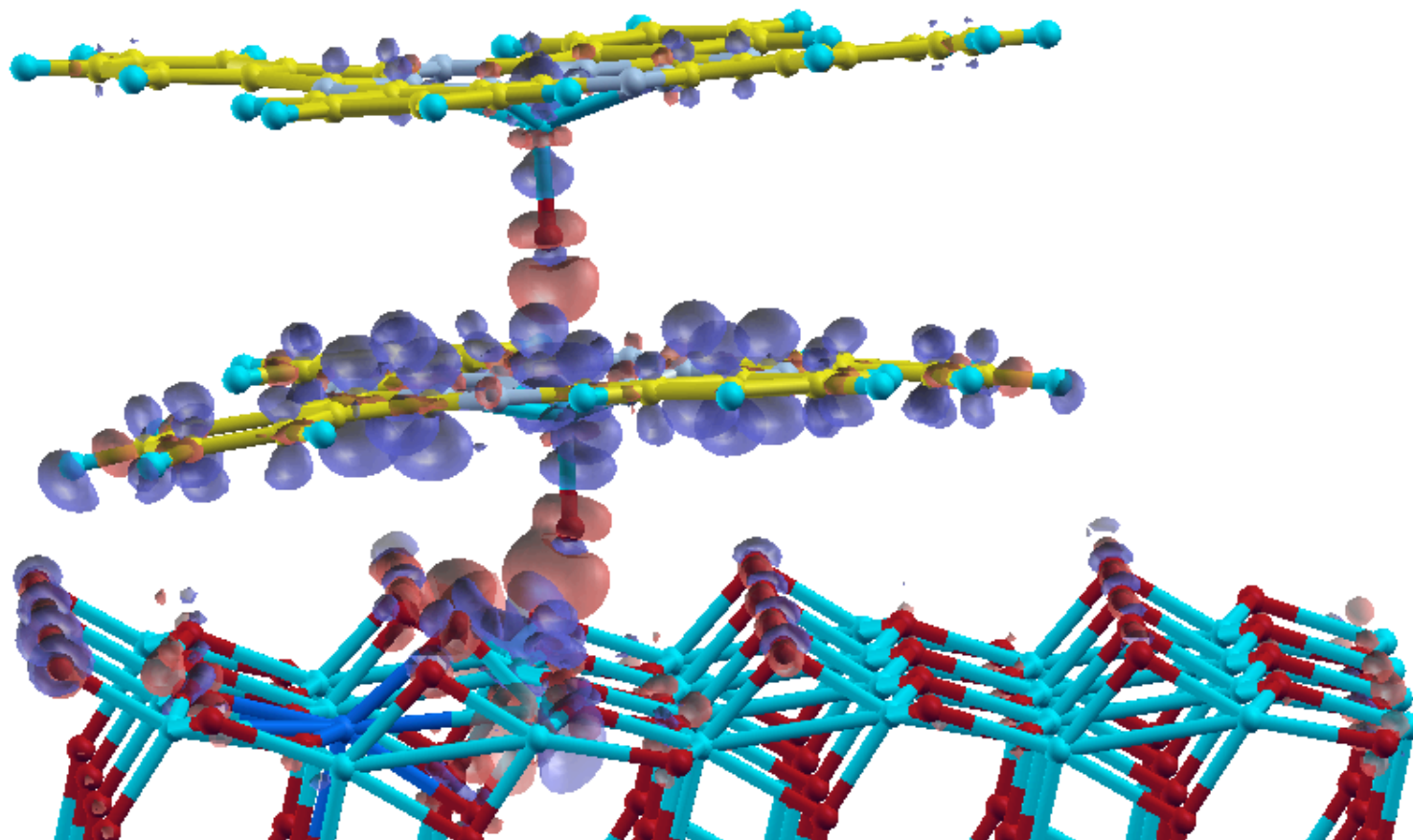
QUANTUM ESPRESSO exists since 2002, resulting from the merge of pre-existing packages; some core components have been under development for ~ 30 years

At the nanoscale: new materials

Most common atomic configurations in amorphous CdTeO_x , $x = 0.2$; Phys. Rev. **B** 79, 014205 (2009).

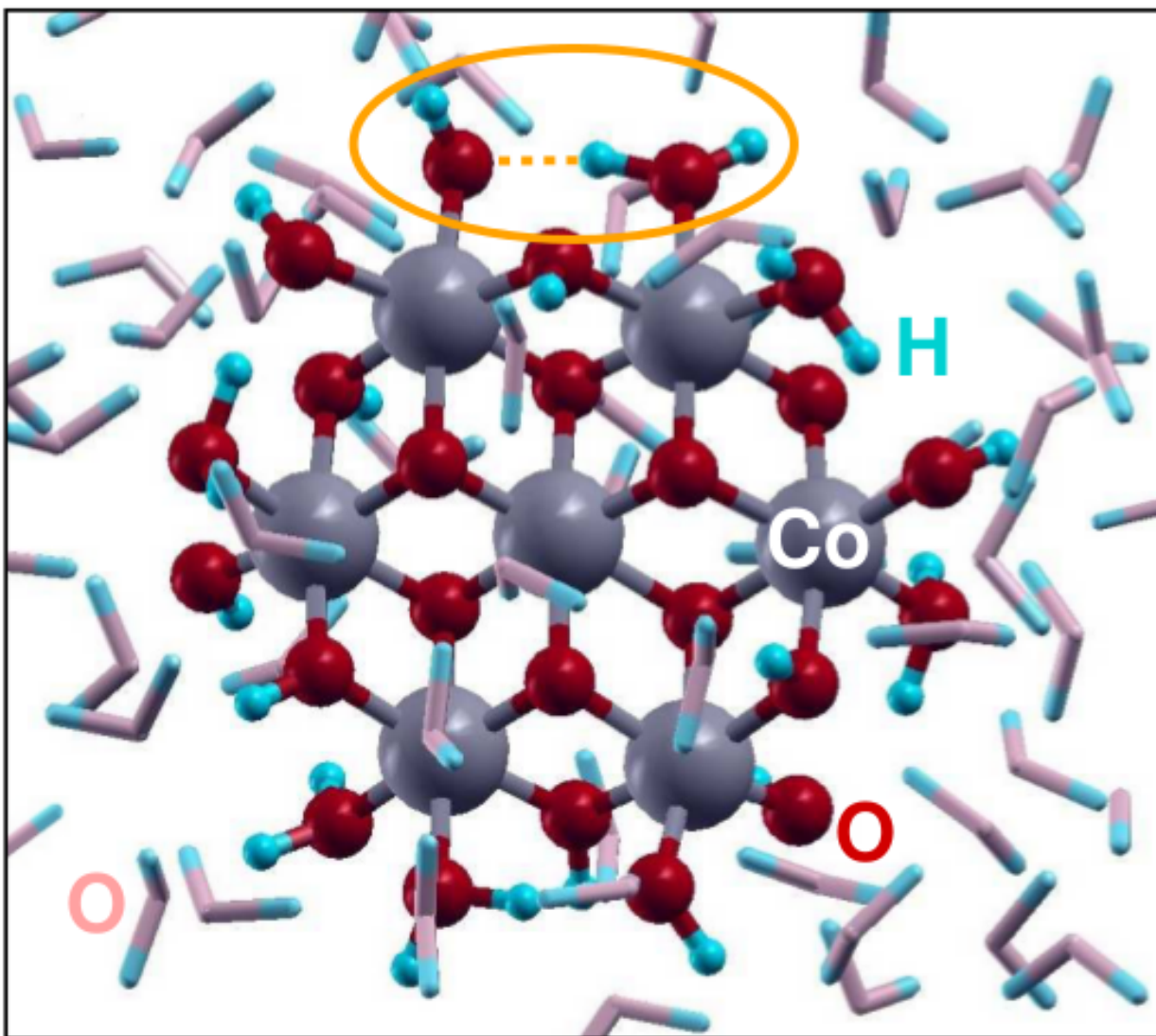


At the nanoscale: new devices



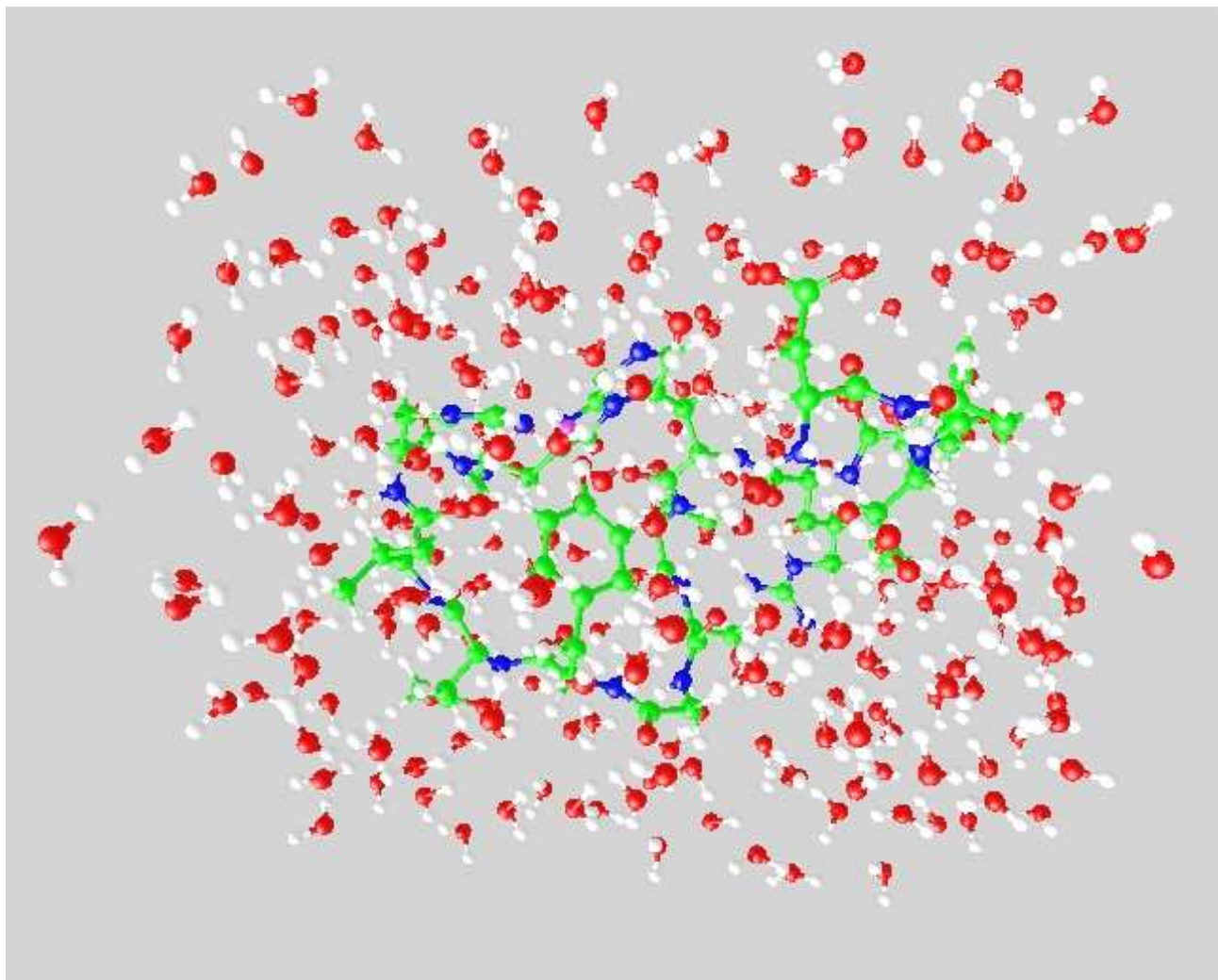
Organic-inorganic semiconductor heterojunction, phthalocyanine over TiO_2 anatase surface; Chem. Mater. **21**, 4555 (2009).

At the nanoscale: nanocatalysis



Cobalt-base catalyser for water splitting: J. Am. Chem. Soc. **135**, 15353 (2013)

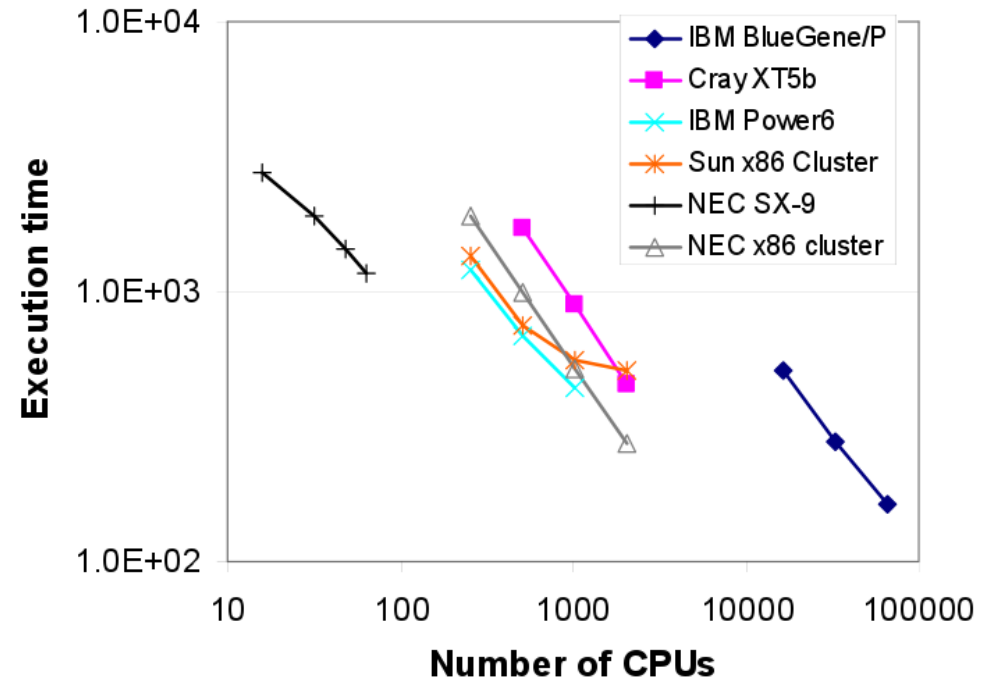
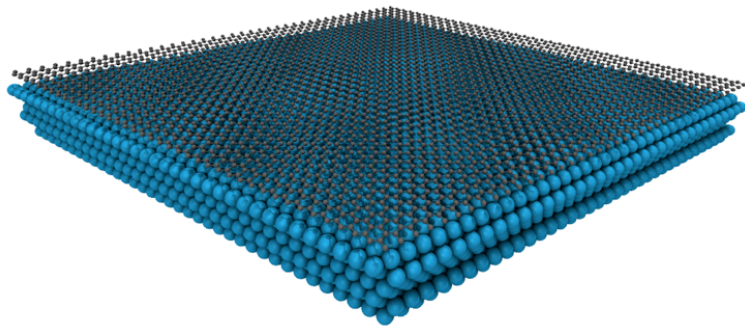
At the nanoscale: biological systems



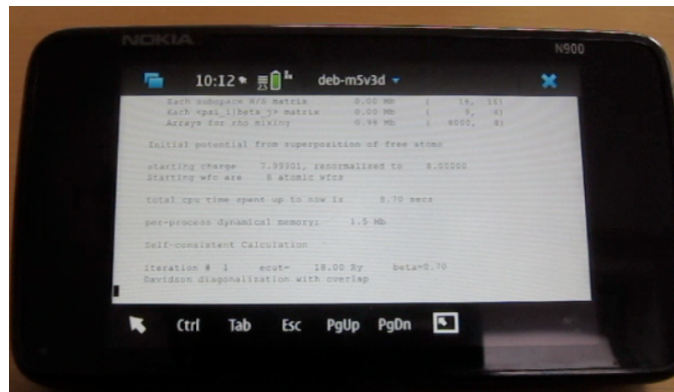
Metal- β -amyloid interactions; Metallomics **4**, 156 (2012).

Towards the exascale: massive parallelization

C@Ir(001)
443 atoms
2987 electrons



... still not forgetting smaller machines! In the figure, Nicola Marzari's smartphone running QUANTUM ESPRESSO



QUANTUM ESPRESSO contributors



QUANTUM ESPRESSO receives contributions from many individuals and partner institutions in Europe and worldwide. Who “owns” QUANTUM ESPRESSO?

QUANTUM ESPRESSO Foundation

The QUANTUM ESPRESSO Foundation: a non-profit (“limited by guarantee”) company, based in London, that

- coordinates and supports research, education, and outreach within the QUANTUM ESPRESSO community
- owns the trademarks and protects the open-source character of QUANTUM ESPRESSO
- raises funds to foster the QUANTUM ESPRESSO project and its development



QUANTUM ESPRESSO Foundation Members

Current QEF members:

- Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste
- Ecole Polytechnique Fédérale de Lausanne (EPFL)
- International Centre for Theoretical Physics (ICTP), Trieste
- Consiglio Nazionale delle Ricerche (IOM-CNR), Italy
- CINECA supercomputing center, Bologna
- University of North Texas
- Duke University

Development

The distribution is maintained as a single SVN (Subversion) tree. Slowly moving towards a less centralized development model based on git.

- Web site: <http://www.quantum-espresso.org>
- Developers' portal: <http://www.qe-forge.org>

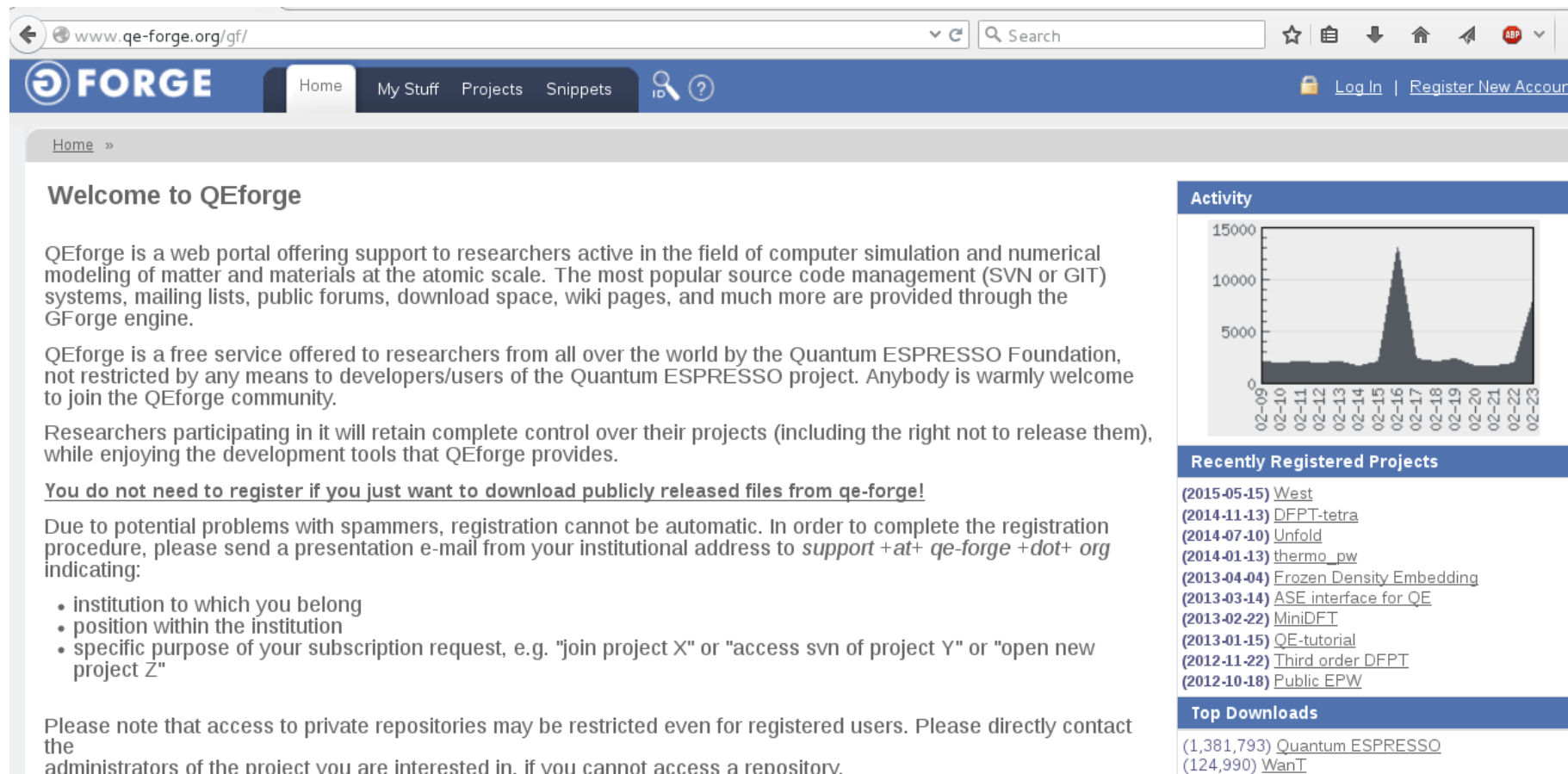
Mailing list (public):

- pw_forum@pwscf.org: for general discussions

More mailing lists (for developers only):

- qe_developers@qe-forge.org: for technical discussions
- qe_commits@qe-forge.org: receives commit messages

Developers' portal: qe-forge



The screenshot shows the homepage of the Qe-forge website. The browser address bar displays 'www.qe-forge.org/gf/'. The website has a blue header with the 'Q FORGE' logo and navigation links: 'Home', 'My Stuff', 'Projects', and 'Snippets'. A search bar is located in the top right. Below the header, the main content area is titled 'Welcome to QEforge'. It contains a paragraph about the portal's purpose, a paragraph about its free service nature, and a paragraph about user control. A bolded instruction states: 'You do not need to register if you just want to download publicly released files from qe-forge!'. Below this, it explains the registration process and lists required information: institution, position, and specific purpose. A 'Top Downloads' section lists 'Quantum ESPRESSO' and 'WanT'. An 'Activity' graph shows a peak in activity around 2016. A 'Recently Registered Projects' list includes 'West', 'DFPT-tetra', 'Unfold', 'thermo_pw', 'Frozen Density Embedding', 'ASE interface for QE', 'MiniDFT', 'QE-tutorial', 'Third order DFPT', and 'Public EPW'.

www.qe-forge.org/gf/

Q FORGE Home My Stuff Projects Snippets

Home »

Welcome to QEforge

QEforge is a web portal offering support to researchers active in the field of computer simulation and numerical modeling of matter and materials at the atomic scale. The most popular source code management (SVN or GIT) systems, mailing lists, public forums, download space, wiki pages, and much more are provided through the GForge engine.

QEforge is a free service offered to researchers from all over the world by the Quantum ESPRESSO Foundation, not restricted by any means to developers/users of the Quantum ESPRESSO project. Anybody is warmly welcome to join the QEforge community.

Researchers participating in it will retain complete control over their projects (including the right not to release them), while enjoying the development tools that QEforge provides.

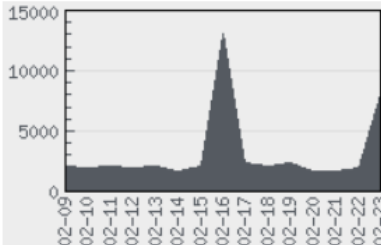
You do not need to register if you just want to download publicly released files from qe-forge!

Due to potential problems with spammers, registration cannot be automatic. In order to complete the registration procedure, please send a presentation e-mail from your institutional address to support+at+qe-forge+dot+org indicating:

- institution to which you belong
- position within the institution
- specific purpose of your subscription request, e.g. "join project X" or "access svn of project Y" or "open new project Z"

Please note that access to private repositories may be restricted even for registered users. Please directly contact the administrators of the project you are interested in, if you cannot access a repository.

Activity



Recently Registered Projects

- (2015-05-15) [West](#)
- (2014-11-13) [DFPT-tetra](#)
- (2014-07-10) [Unfold](#)
- (2014-01-13) [thermo_pw](#)
- (2013-04-04) [Frozen Density Embedding](#)
- (2013-03-14) [ASE interface for QE](#)
- (2013-02-22) [MiniDFT](#)
- (2013-01-15) [QE-tutorial](#)
- (2012-11-22) [Third order DFPT](#)
- (2012-10-18) [Public EPW](#)

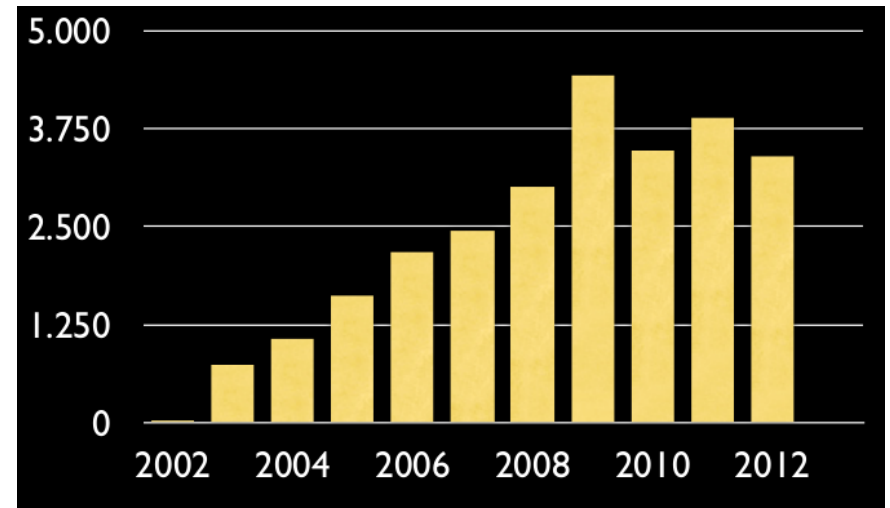
Top Downloads

- (1,381,793) [Quantum ESPRESSO](#)
- (124,990) [WanT](#)

Currently 45 public projects, 570 registered users, 66 QE developers registered
QE-forge will undergo a significant overhaul in the near future

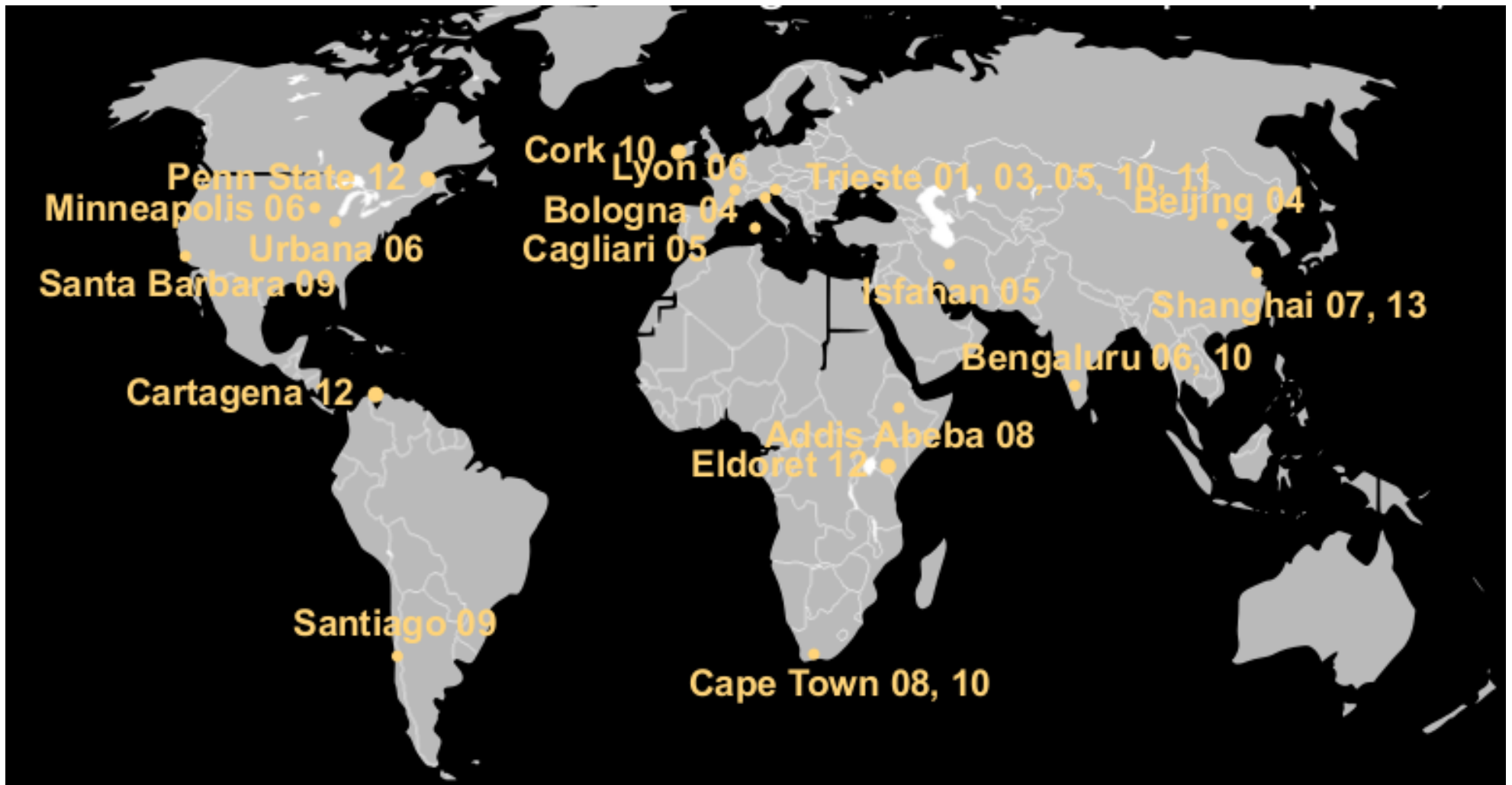
Users' community: factoids

- About 1800 registered users for the pw_forum mailing list
- An average of ~ 10 messages a days on pw_forum
- latest version (5.3.0) downloaded 6700 times [*] since release date (Jan.9)
- 30 Schools or tutorials since 2002, attended by ~ 1200 users
- 3 developers' schools since 2013, latest in January 2015
- annual developers' meeting since 2010, latest in January 2016



[*] *this number may be inflated by bots, failed downloads, etc.*

Schools and tutorial using QUANTUM ESPRESSO



More: Penn State, June 2014; University of Tokyo, April 2014; Pune, July 2014; Cordoba (Argentina), September 2015

QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials

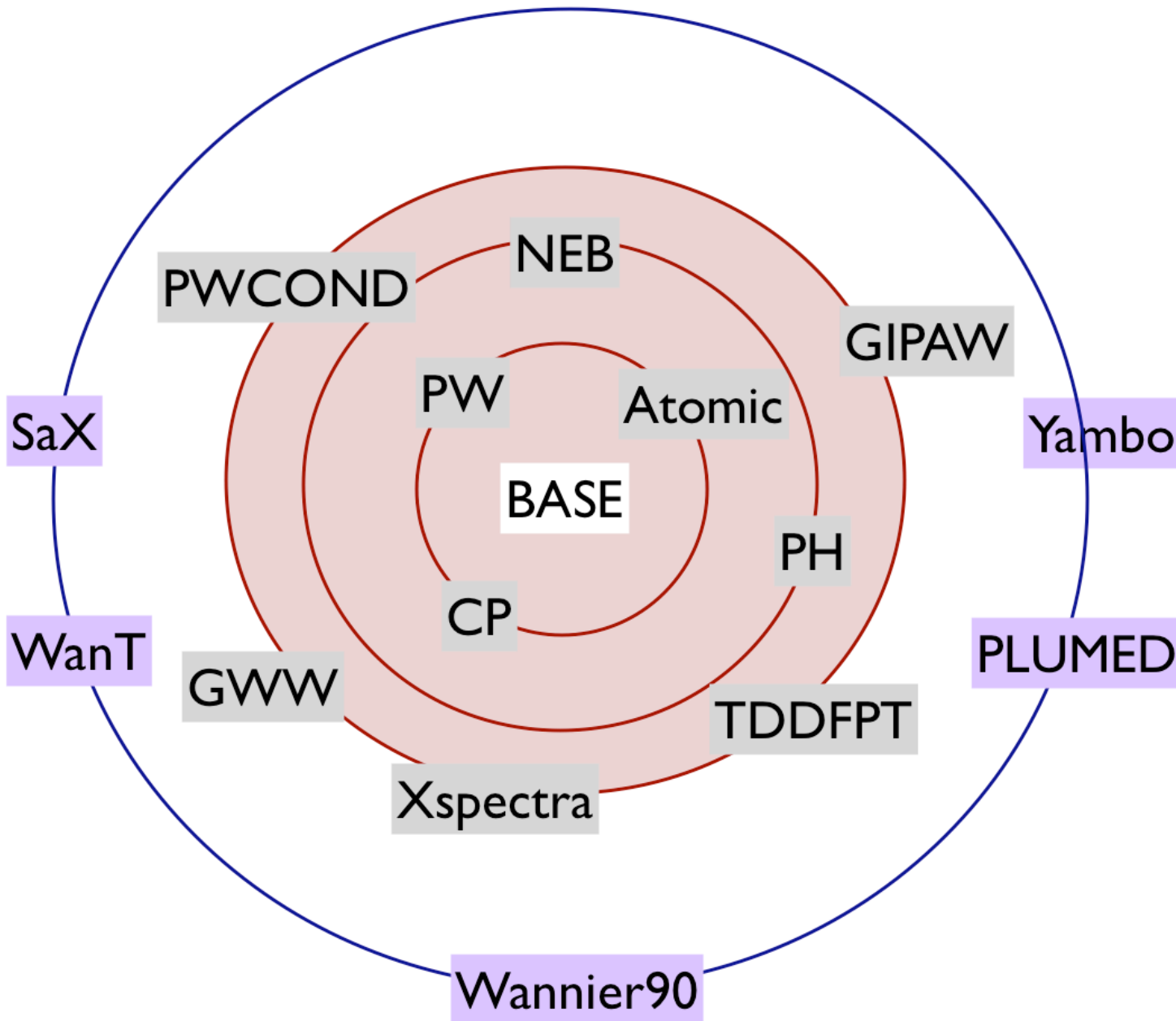
**Paolo Giannozzi^{1,2}, Stefano Baroni^{1,3}, Nicola Bonini⁴,
Matteo Calandra⁵, Roberto Car⁶, Carlo Cavazzoni^{7,8},
Davide Ceresoli⁴, Guido L Chiarotti⁹, Matteo Cococcioni¹⁰,
Ismaila Dabo¹¹, Andrea Dal Corso^{1,3}, Stefano de Gironcoli^{1,3},
Stefano Fabris^{1,3}, Guido Fratesi¹², Ralph Gebauer^{1,13},
Uwe Gerstmann¹⁴, Christos Gougoussis⁵, Anton Kokalj^{1,15},
Michele Lazzeri⁵, Layla Martin-Samos¹, Nicola Marzari⁴,
Francesco Mauri⁵, Riccardo Mazzarello¹⁶, Stefano Paolini^{3,9},
Alfredo Pasquarello^{17,18}, Lorenzo Paulatto^{1,3}, Carlo Sbraccia^{1,†},
Sandro Scandolo^{1,13}, Gabriele Sclauzero^{1,3}, Ari P Seitsonen⁵,
Alexander Smogunov¹³, Paolo Umari¹ and
Renata M Wentzcovitch^{10,19}**

4400 citations as of today

Requirements on effective software for quantum simulations at the nanoscale

- Challenging calculations stress the limits of available computer power: software should be **fast and efficient**
- Diffusion of first-principle techniques among non-specialists requires software that is **easy to use and** (reasonably) **error-proof**
- Introducing innovation requires new ideas to materialize into new algorithms through codes: software should be **easy to extend and to improve**
- Complex problems require a mix of solutions coming from different approaches and methods: software should be **interoperable with other software**
- Finally, scientific ethics requires that **results should be reproducible** and **algorithms susceptible of validation**

Structure of the distribution



Technical characteristics (coding)

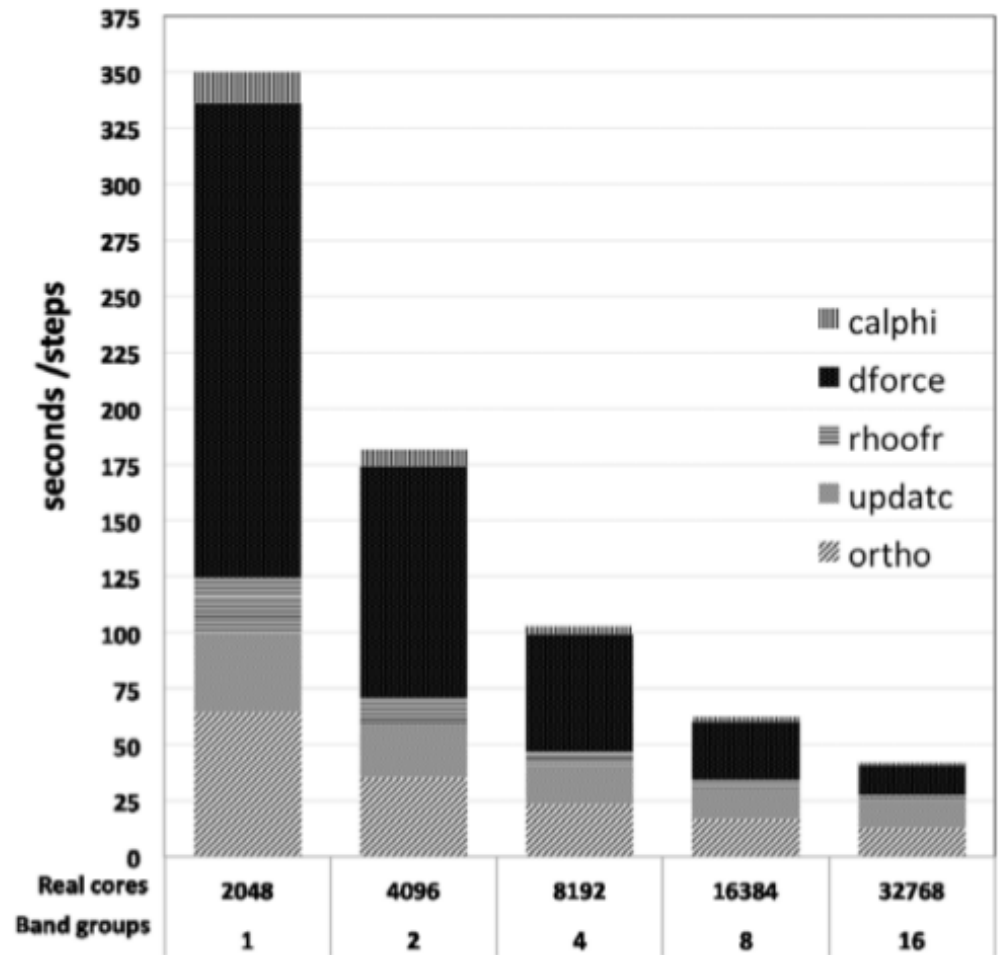
- 380000+ Fortran-95 lines, with various degrees of sophistication (i.e. use of advanced f95 features) – no “dusty decks” any longer
- use of standard library routines (lapack, blas, fftw) to achieve portability – Machine-optimized libraries can (should) (*must!*) be used if available
- C-style preprocessing options allow to keep a single source tree for (almost) architectures, from PC's to BG's (BlueGene)
- various parallelization levels via MPI calls or OpenMP directives, hidden into calls to a few routines – almost unified serial and parallel versions; parallel code can (usually) be written without knowing the details of how parallelism works.
- I/O based on an XML file plus binary files for large records (e.g. wavefunctions, charge density) – soon moving to schema-based, standard-compliant XML and portable (HDF5) binary files

Parallelization of QUANTUM ESPRESSO

Several *parallelization levels* are implemented; most of them require *fast* interprocess communications.

Scalability of realistic calculations on up to tens of thousands cores, using mixed MPI-OpenMP parallelization, has been demonstrated.

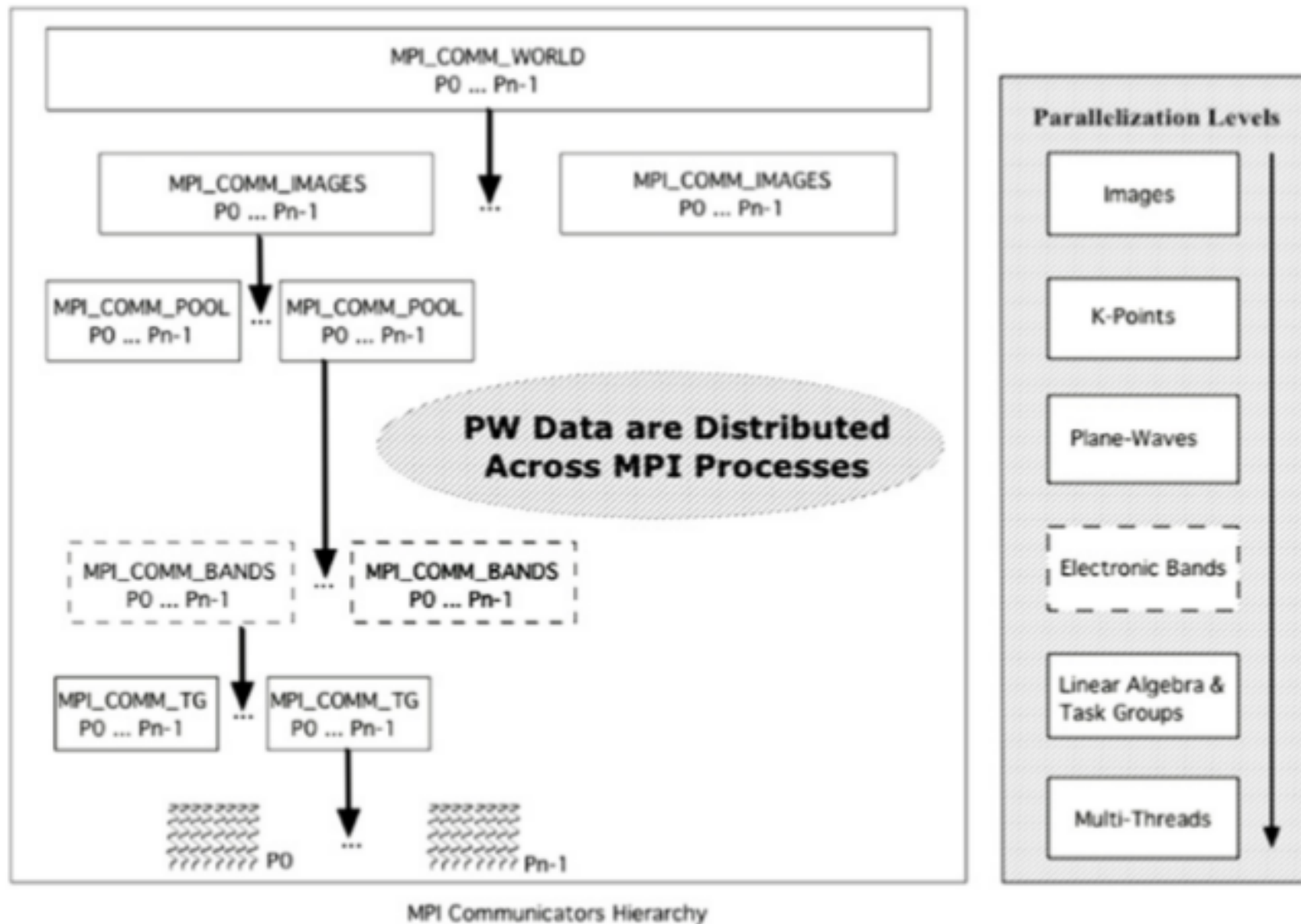
Careful optimization of nonscalable RAM and computations required!
Scalability *strongly depends upon the kind and size of system!*



CP Scalability on BG/Q, 1532-atom porphyrin-functionalized carbon nanotube
(data from paper appearing in next slide)

Summary of parallelization levels

N. Varini et al. / Computer Physics Communications 184 (2013) 1827–1833



Summary of parallelization levels (2)

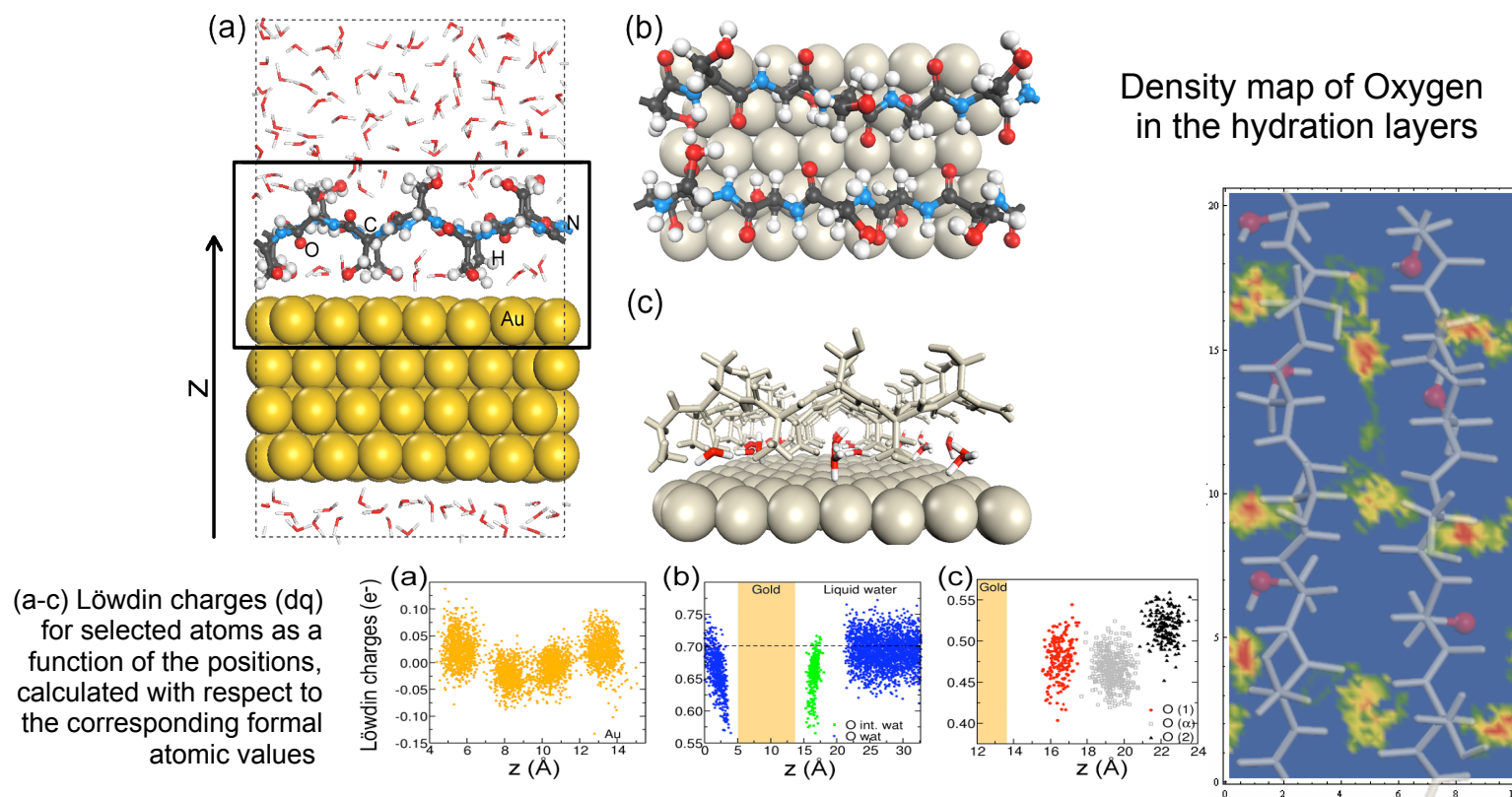
group	distributed quantities	communications	performances
<i>image</i>	NEB images, phonon modes	very low	linear CPU scaling, fair to good load balancing; does not distribute RAM
<i>pool</i>	k-points	low	almost linear CPU scaling, fair to good load balancing; may distribute some RAM
<i>bands</i>	Kohn-Sham orbitals	high	improves scaling
<i>plane-wave</i>	PW, G -vector coefficients, R -space FFT arrays	high	good CPU scaling, good load balancing, distributes most RAM
<i>task</i>	FFT on electron states	high	improves load balancing
<i>linear-algebra</i>	subspace hamiltonians and constraints matrices	very high	improves scaling, distributes more RAM
<i>OpenMP</i>	FFT, libraries	intra-node	extends scaling on multicore machines

Importance of collaboration with computing centers

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

QUANTUM ESPRESSO on GPU's

fspiga / QE-GPU

Watch

8

Star

14

Fork

11

<> Code

Pull requests

0

Pulse

Graphs

GPU-accelerated Quantum ESPRESSO

333 commits

1 branch

5 releases

2 contributors

Branch: master

New pull request


New file

Find file

HTTPS

https://github.com/fspiga/QE

Download ZIP

 fspiga

Compute capability for NVIDIA K80 (sm_37) not handled properly. Now f...

Latest commit 706ba20 on Jan 9

CPV	Flat hierarchy.	2 months ago
Doc	Flat hierarchy.	2 months ago
Modules	Compute capability for NVIDIA K80 (sm_37) not handled properly. Now f...	2 months ago
NEB	Flat hierarchy.	2 months ago
PH	Flat hierarchy.	2 months ago
PW	Flat hierarchy.	2 months ago
archive	Flat hierarchy.	2 months ago
include	Flat hierarchy.	2 months ago
install	Flat hierarchy.	2 months ago

Perspectives and Outlook

- More packages for advanced methodologies
- Better-structured distribution, with interfaces to external codes and to python scripting
- Porting to new hybrid and accelerated architectures
- More parallelization everywhere, communication-reducing and latency-hiding algorithms

QUANTUM ESPRESSO is one of the community codes involved into the recently funded MaX – Materials at the Exascale EU project (next talk)

Credits

- Thanks to all people whose slides and pictures I borrowed
- Thanks to all people who contributed to QUANTUM ESPRESSO
- ...and thanks to you all