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

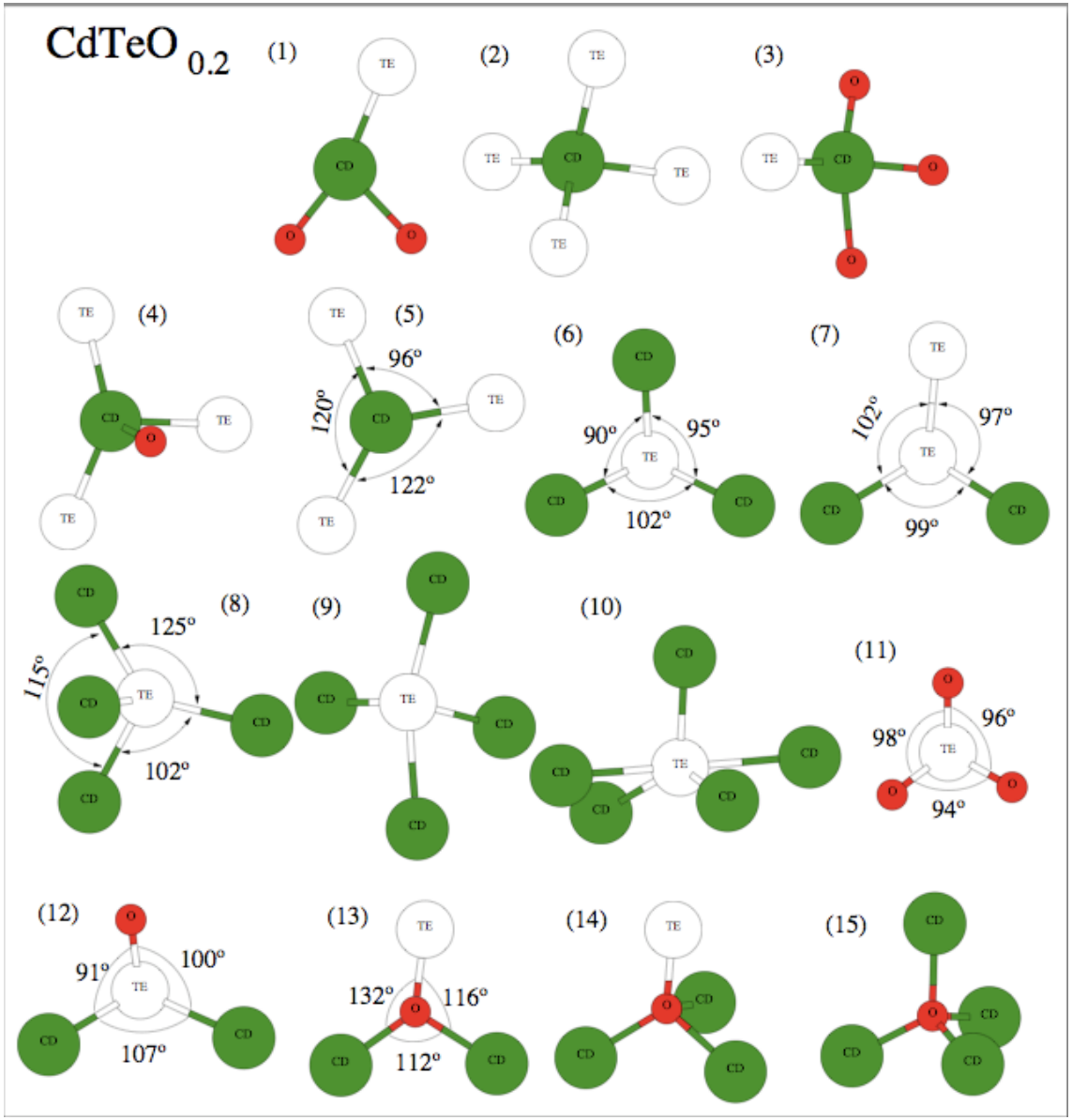
- *innovation* in theoretical methods and numerical algorithms
- *efficiency* on modern computer architectures

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

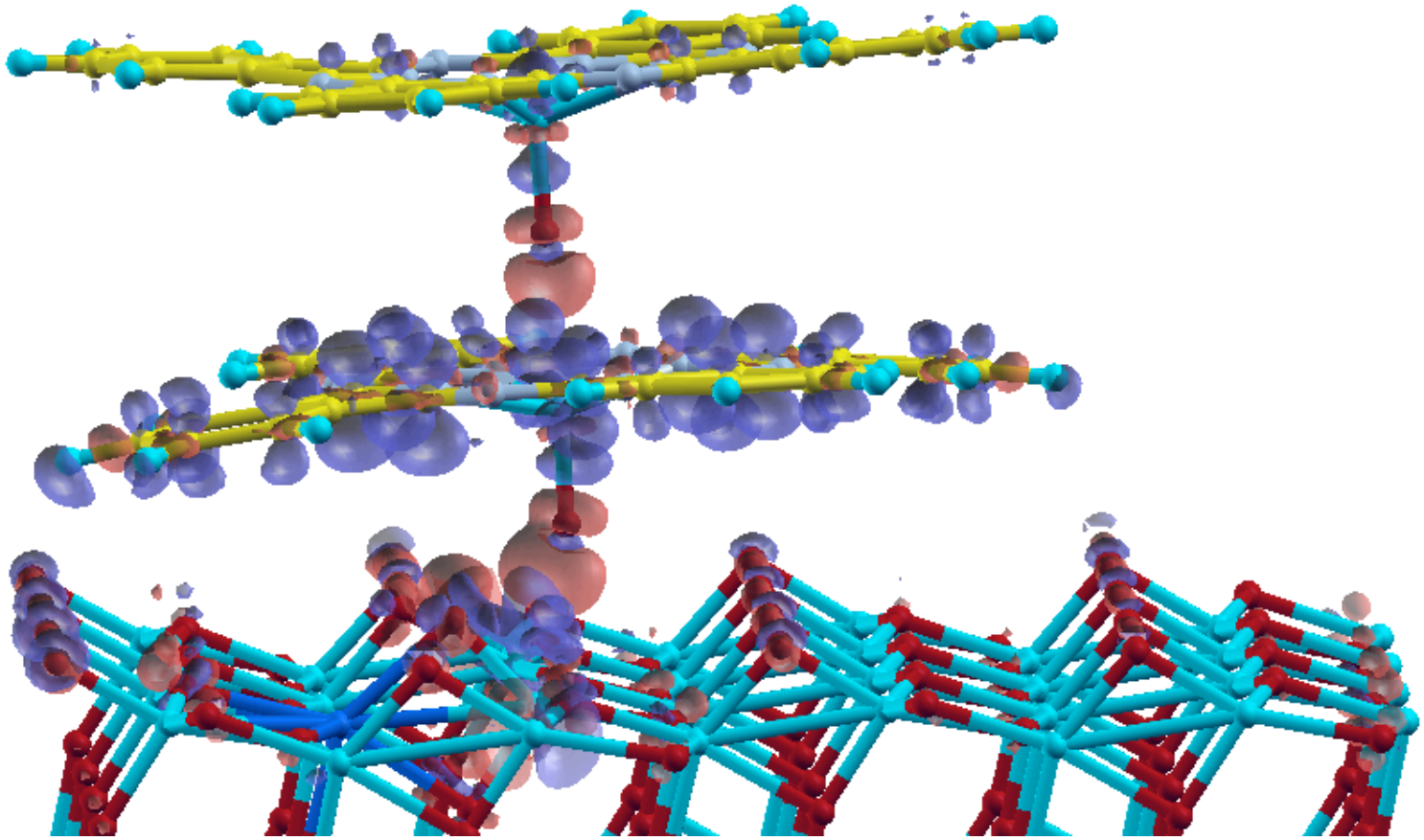
QUANTUM ESPRESSO exists since 2002, resulting from the merge of pre-existing packages; some core components have been under development for ~ 30 years

At the nanoscale: new materials

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

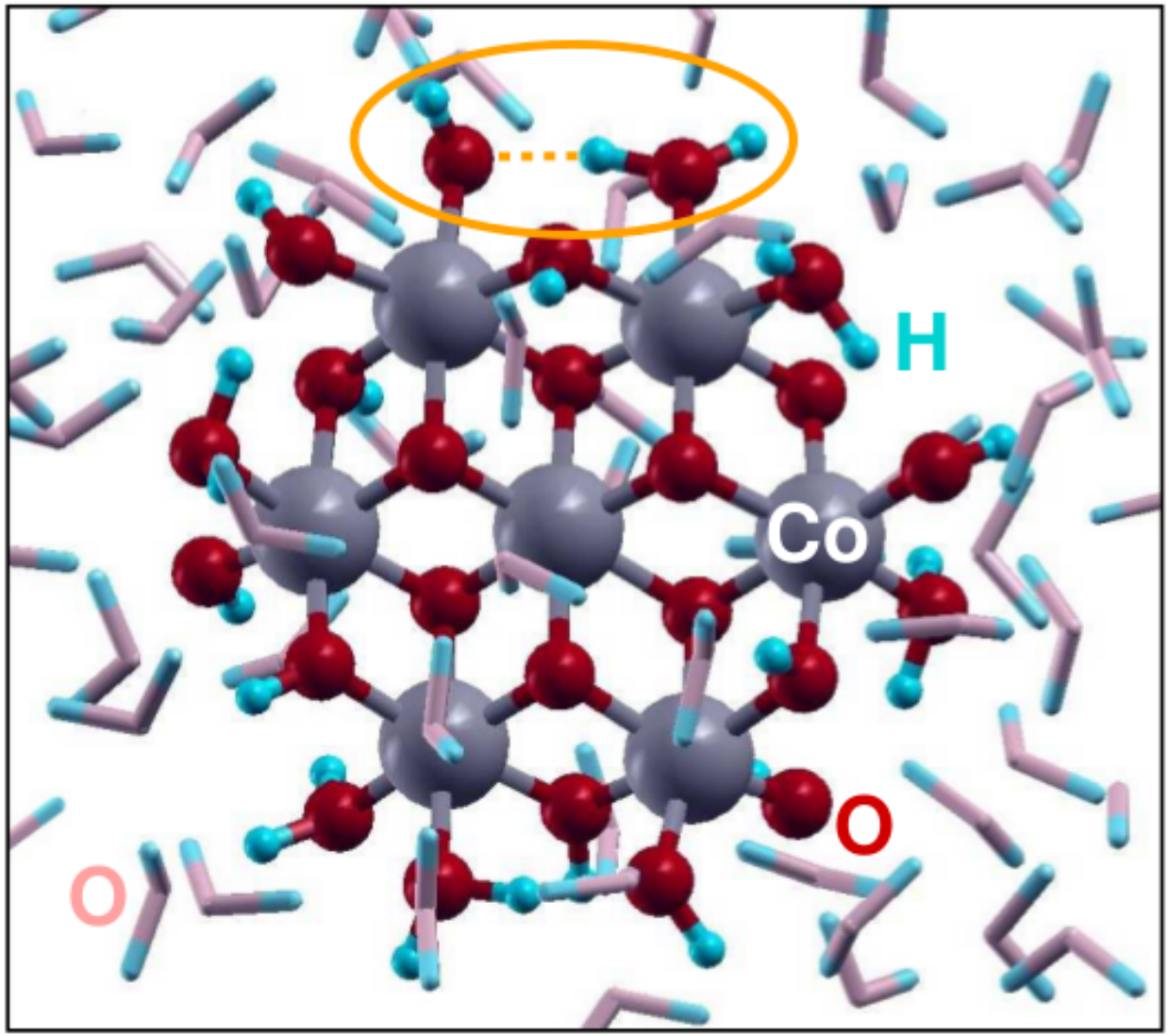


At the nanoscale: new devices



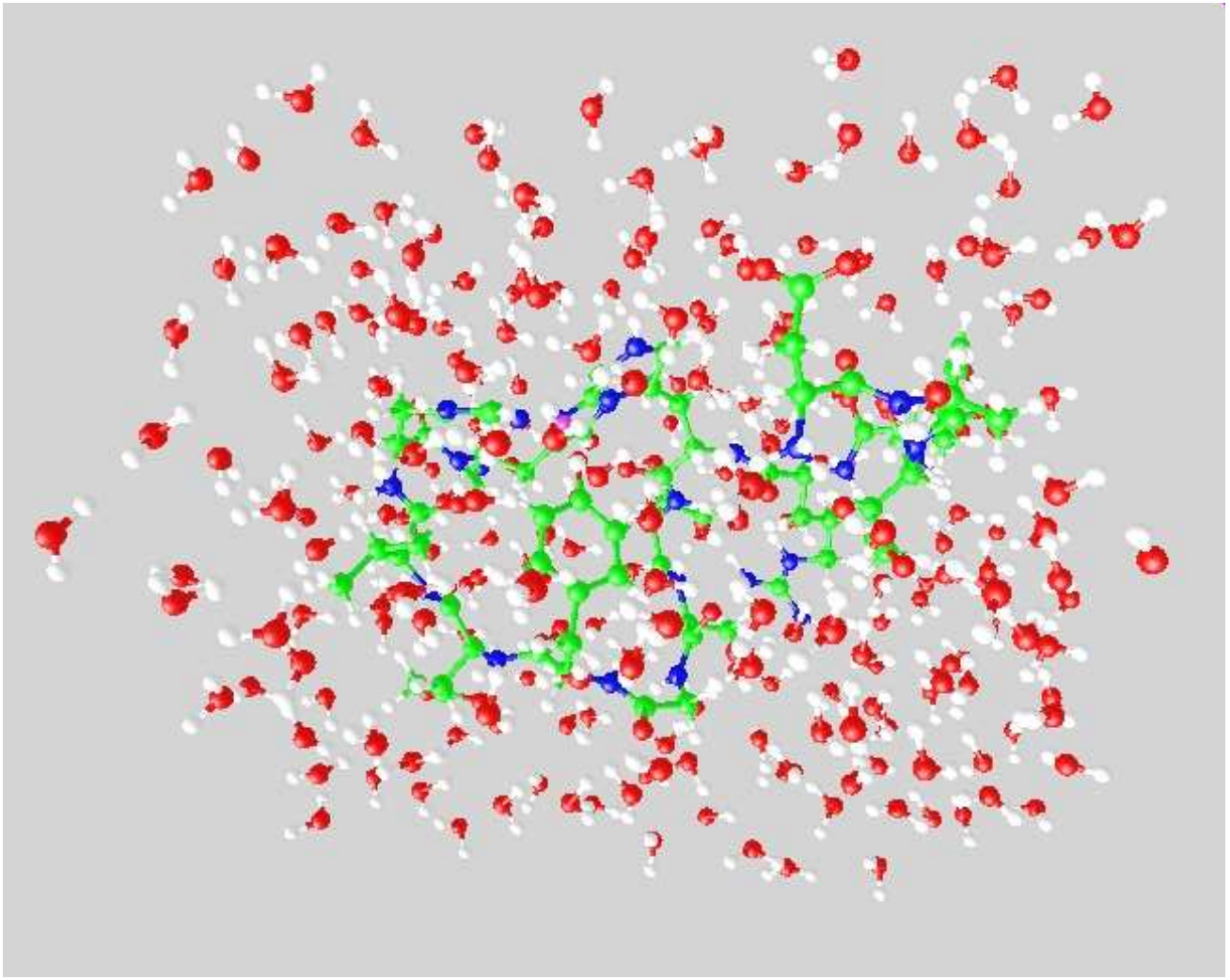
Organic-inorganic semiconductor heterojunction, phtalocyanine over TiO_2 anatase surface; Chem. Mater. **21**, 4555 (2009).

At the nanoscale: nanocatalysis



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

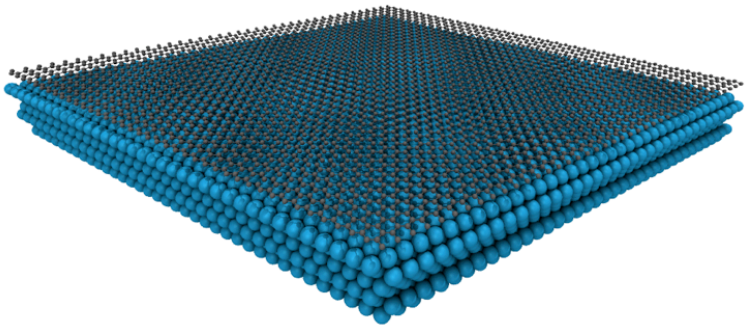
At the nanoscale: biological systems

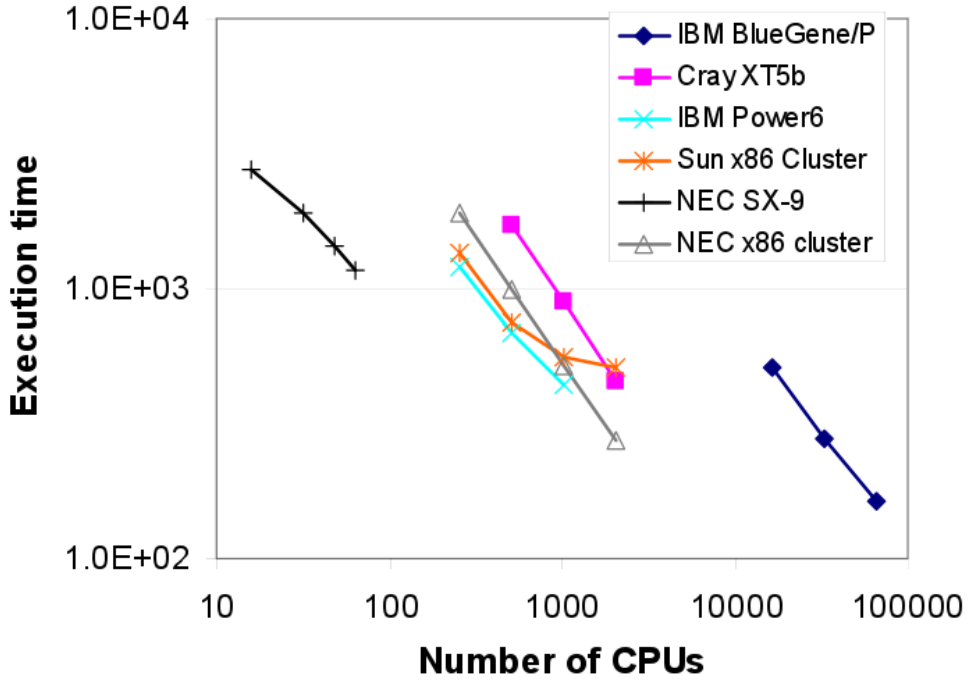


Metal-β-amyloid interactions; Metallomics **4**, 156 (2012).

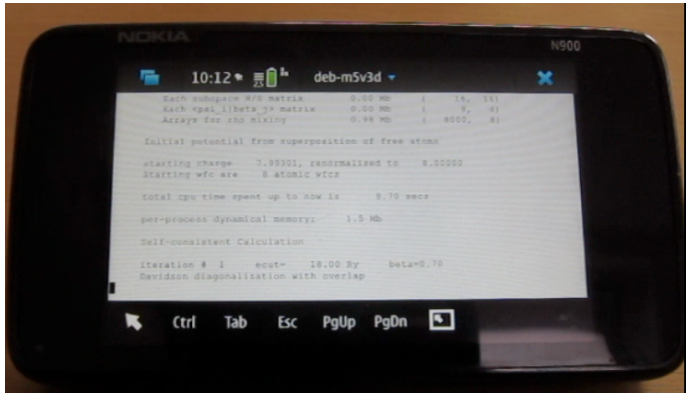
Towards the exascale: massive parallelization

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`

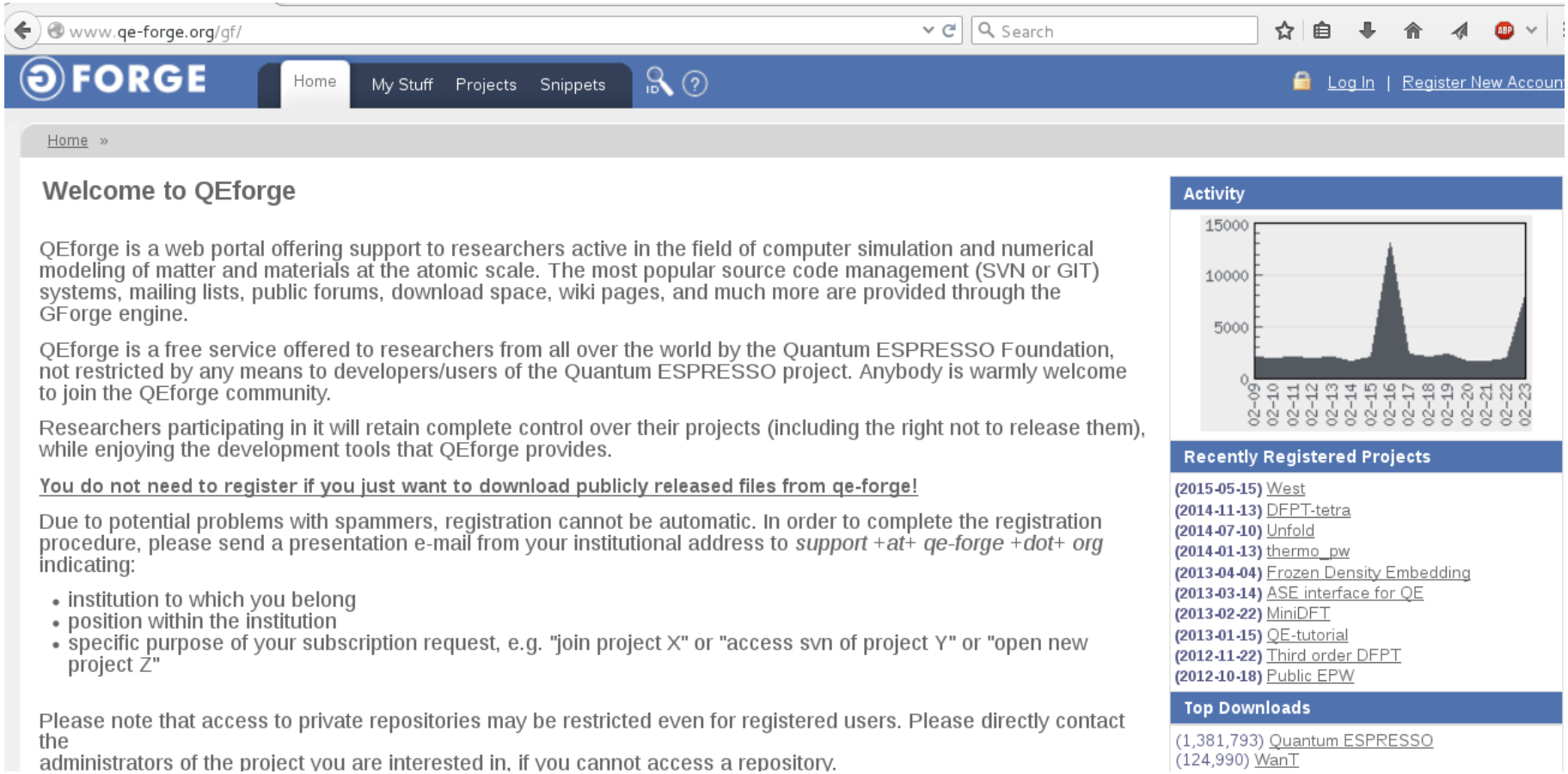
Mailing list (public):

- `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

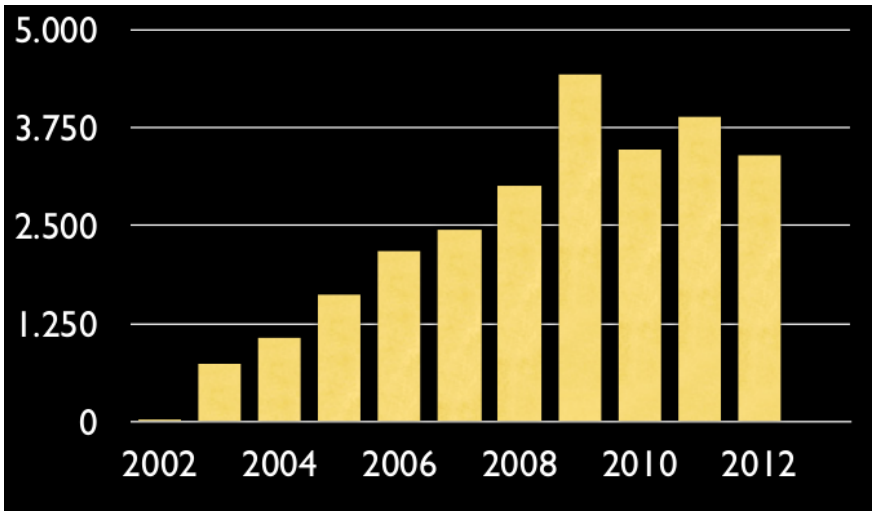
Developers' portal: qe-forge



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

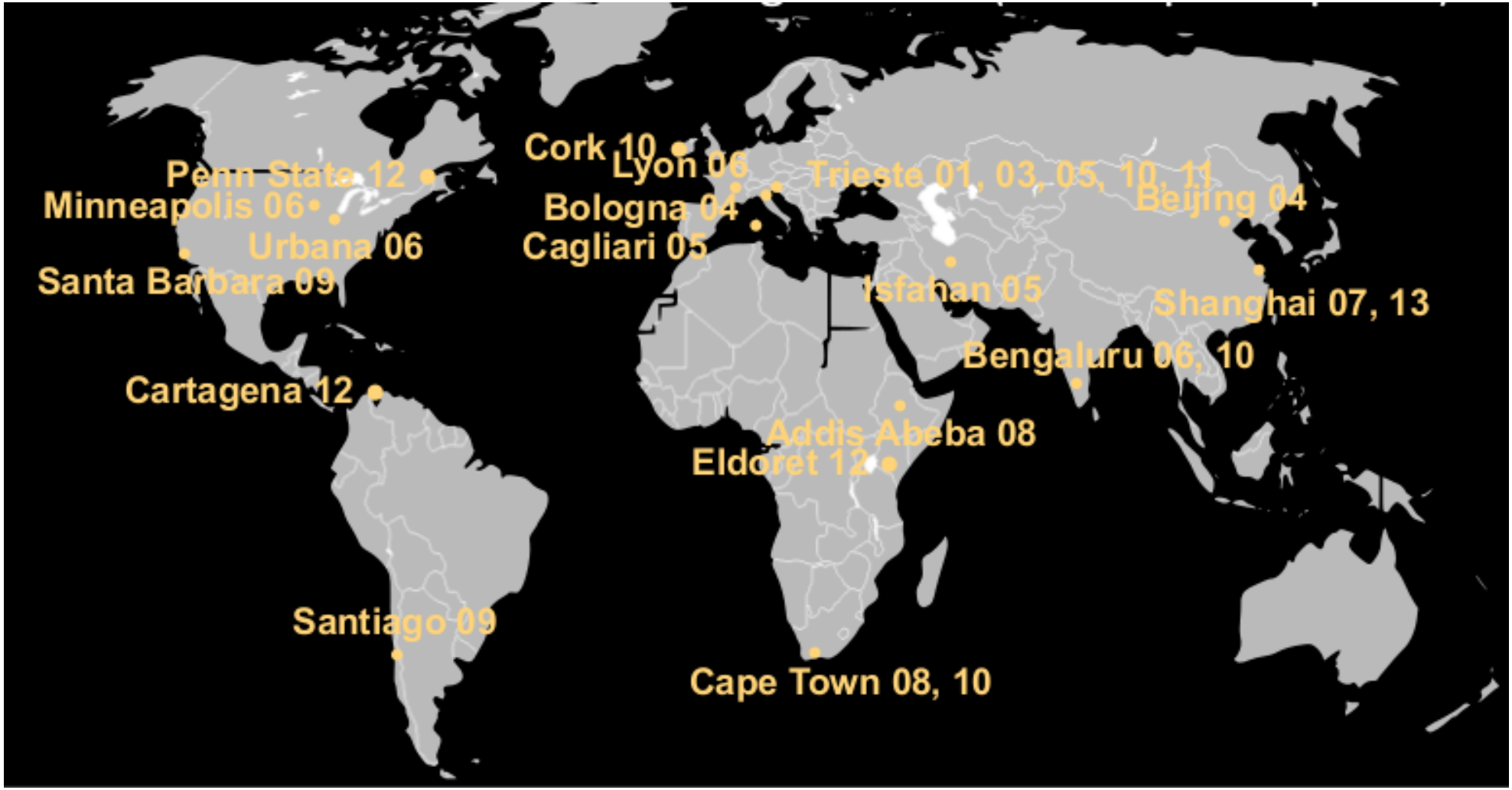
- About 1800 registered users for the pw_forum mailing list
- An average of $\sim$ 10 messages a days on pw_forum
- latest version (5.3.0) downloaded 6700 times [*] since release date (Jan.9)



- 30 Schools or tutorials since 2002, attended by $\sim$ 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

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **21** (2009) 395502 (19pp) doi:10.1088/0953-8984/21/39/395502

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

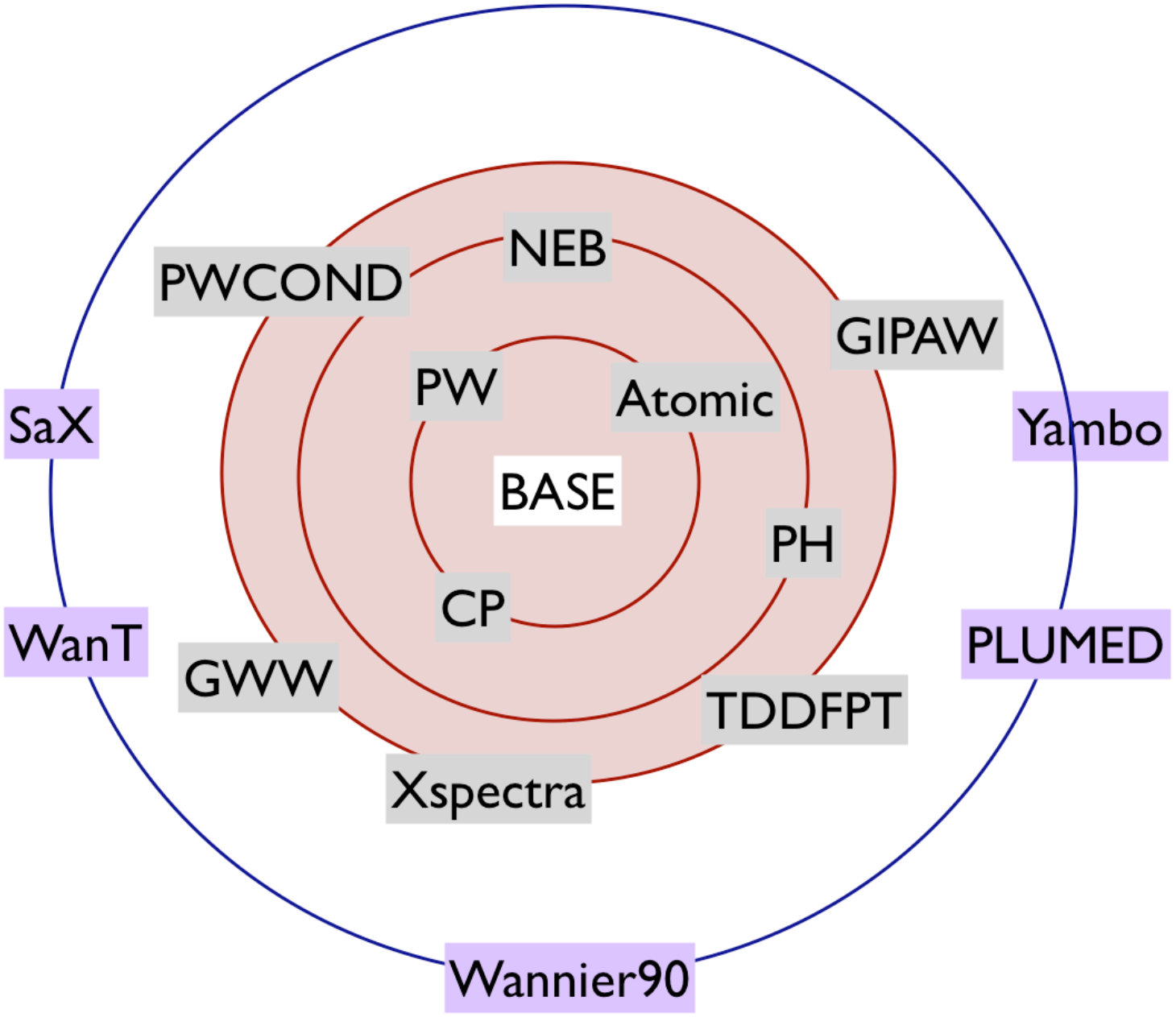
Paolo Giannozzi[1,2], Stefano Baroni[1,3], Nicola Bonini[4], Matteo Calandra[5], Roberto Car[6], Carlo Cavazzoni[7,8], Davide Ceresoli[4], Guido L Chiarotti[9], Matteo Cococcioni[10], Ismaila Dabo[11], Andrea Dal Corso[1,3], Stefano de Gironcoli[1,3], Stefano Fabris[1,3], Guido Fratesi[12], Ralph Gebauer[1,13], Uwe Gerstmann[14], Christos Gougoussis[5], Anton Kokalj[1,15], Michele Lazzeri[5], Layla Martin-Samos[1], Nicola Marzari[4], Francesco Mauri[5], Riccardo Mazzarello[16], 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 Seitsonen[5], Alexander Smogunov[13], Paolo Umari[1] 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**
- Finaly, scientific ethics requires that **results should be reproducible** and **algorithms susceptible of validation**

Structure of the distribution



Technical characteristics (coding)

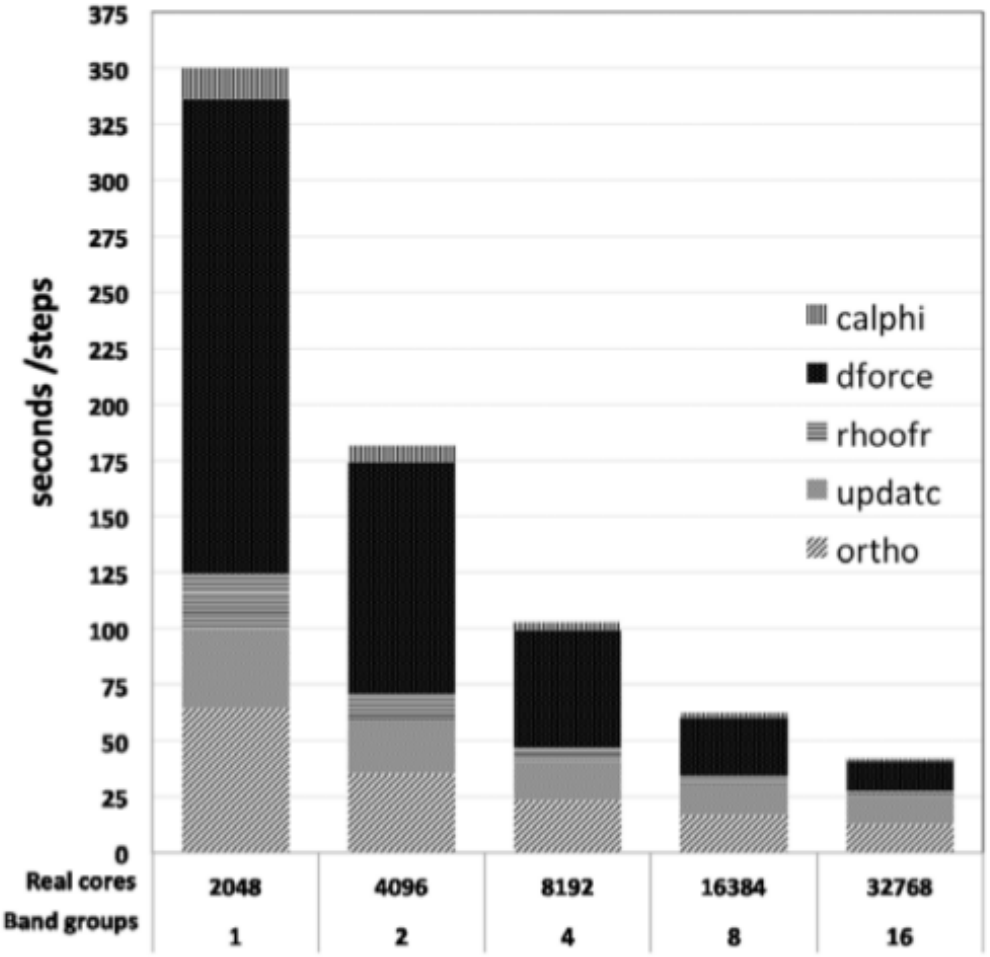
- 380000+ Fortran-95 lines, with various degrees of sophistication (i.e. use of advanced f95 features) – no "dusty decks" any longer
- use of standard library routines (lapack, blas, fftw) to achieve portability – Machine-optimized libraries can (should) (*must!*) be used if available
- C-style preprocessing 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.

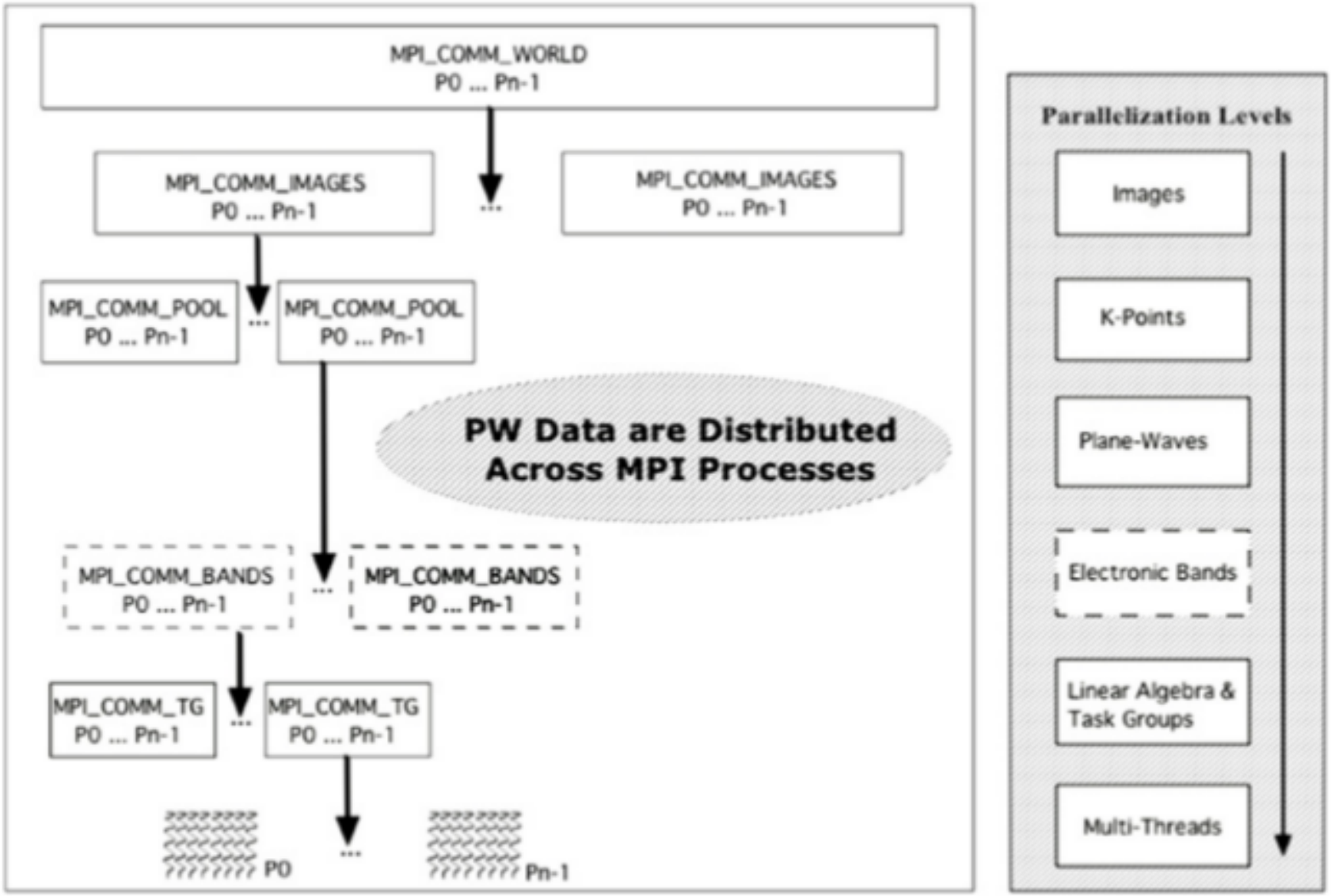
Careful optimization of nonscalable RAM and computations required! Scalability *strongly depends upon the kind and size of system*!



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



MPI Communicators Hierarchy

Summary of parallelization levels (2)

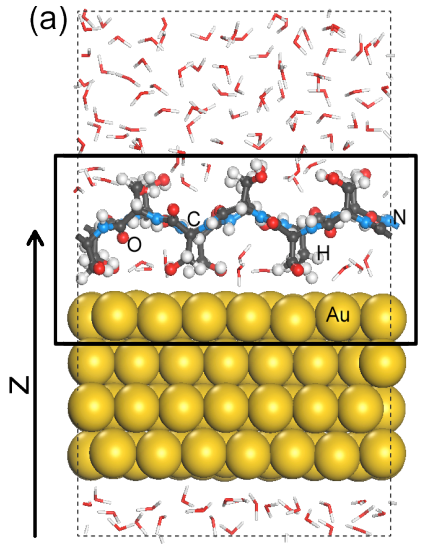
group	distributed quantities	communications	performances
image	NEB images, phonon modes	very low	linear CPU scaling, fair to good load balancing; does not distribute RAM
pool	$\mathbf{k}$-points	low	almost linear CPU scaling, fair to good load balancing; may distribute some RAM
bands	Kohn-Sham orbitals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

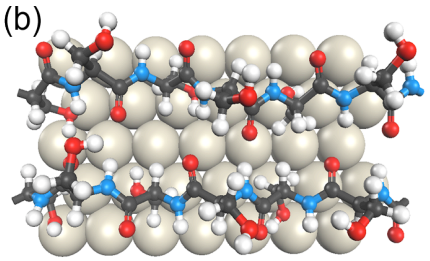
Importance of collaboration with computing centers

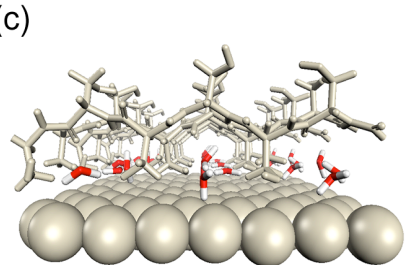
DEISA EXTREME COMPUTING INITIATIVE

Distributed European Infrastructure for Supercomputing Applications

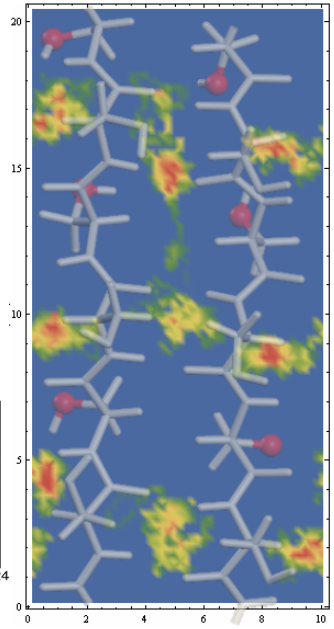
Ab-initio simulations of Protein-Surface Interactions mediated by WATer



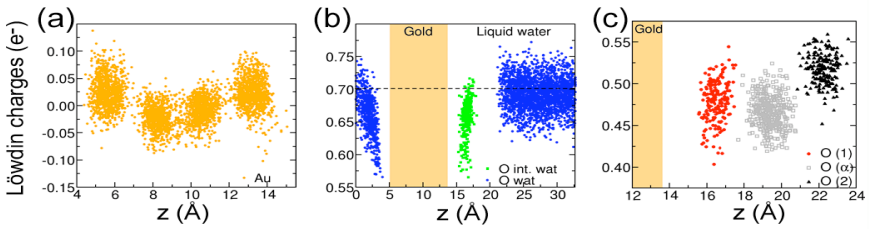




Density map of Oxygen in the hydration layers

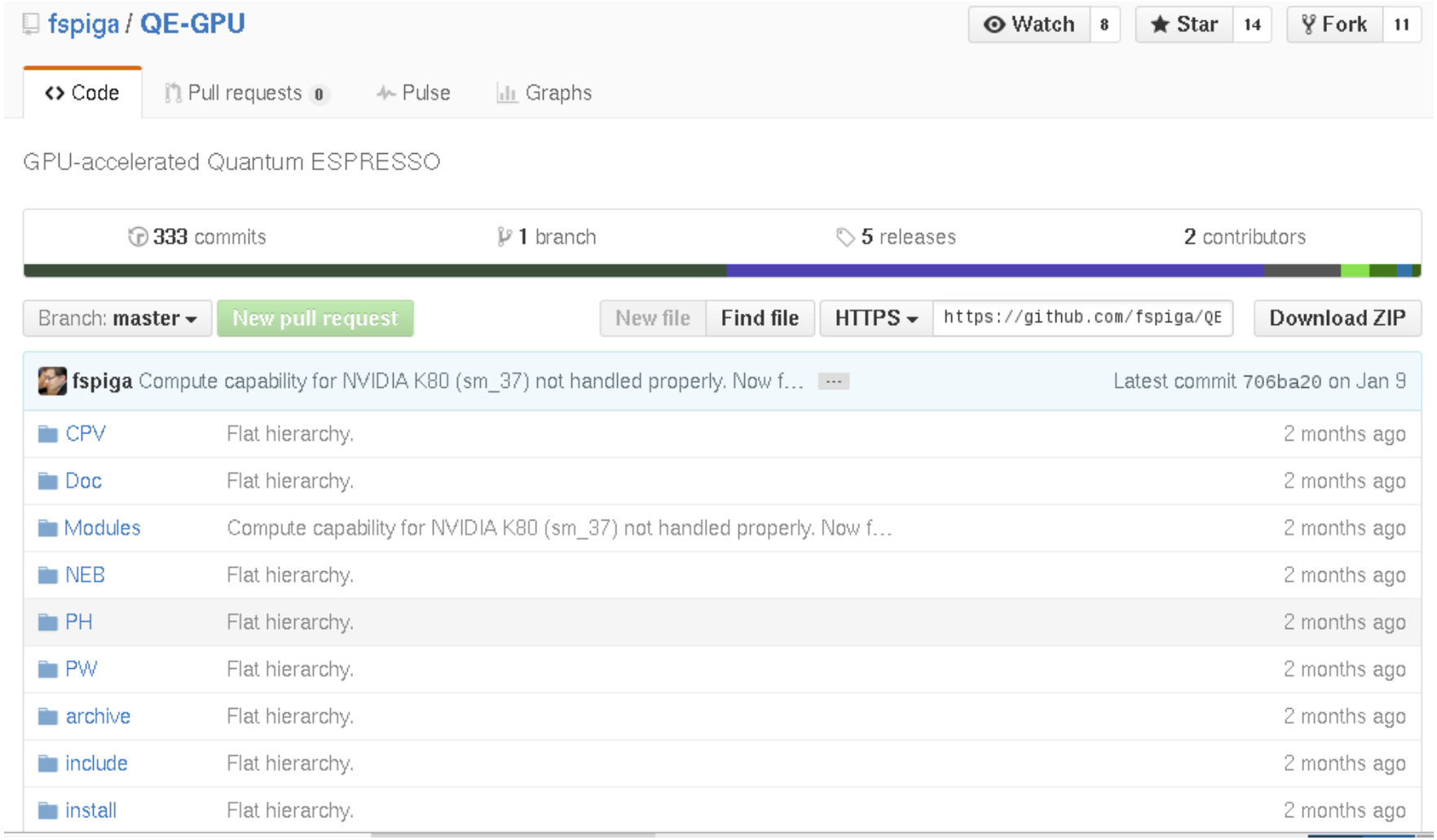


(a-c) Löwdin charges (dq) for selected atoms as a function of the positions, calculated with respect to the corresponding formal atomic values



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