
QE, main strategies of parallelization and levels of parallelisms

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SCAI - Cineca

Quantum ESPRESSO: introduction

Quantum ESPRESSO is an integrated software suite for atomistic simulations based on electronic structure, using density-functional theory(DFT), a plane waves (PW) basis set and pseudopotentials (PP)

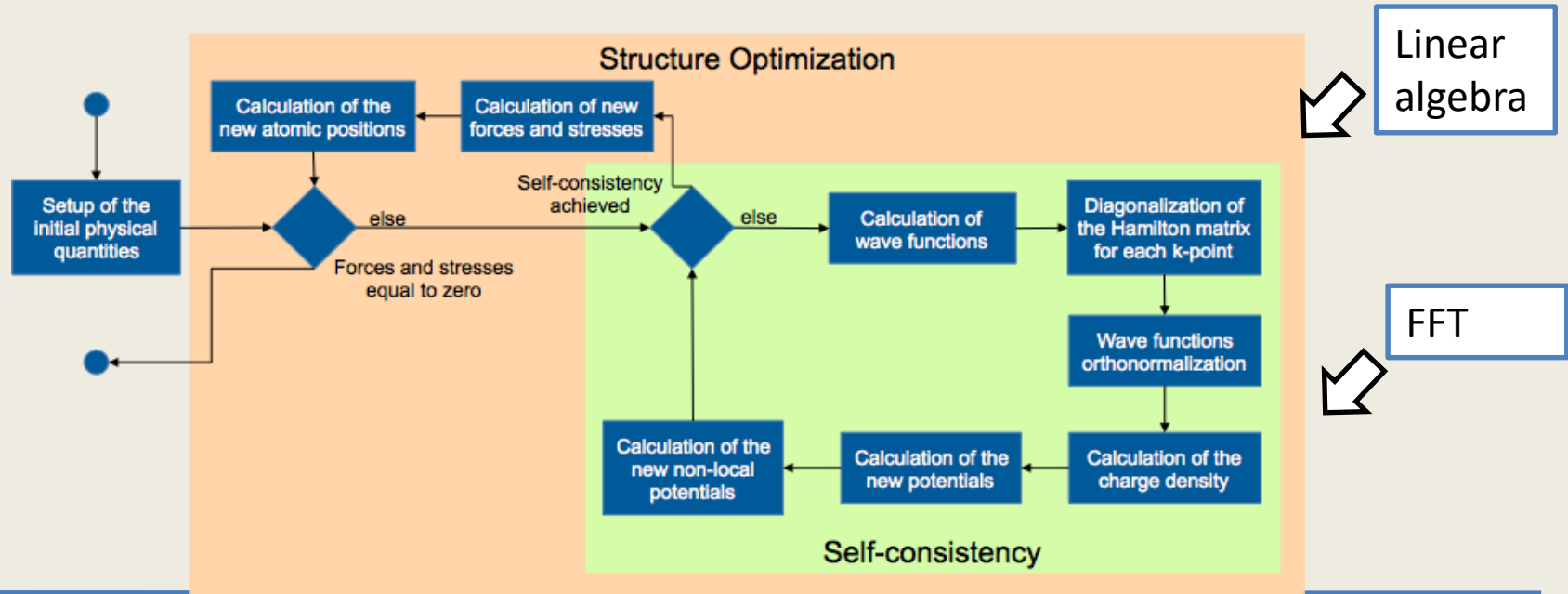
It is a collection of specific-purpose software, the largest being:

- PWSCF
- CP

plus many other applications able to post-process the wavefunctions generated by PWscf (for example PHonon, GW, TDDFPT, etc)

PWscf

As an example, let's watch at the structure of PWscf



Technical infos

Quantum ESPRESSO is released under a GNU-GPL license and it is downloadable from www.quantum-espresso.org

Mostly written in Fortran90

Ongoing effort to increase the modularization (MaX CoE funded)

It can use optimized libraries for LA and FFT (i.e. MKL, FFTW3, etc), but it can be also compiled without any external library

MPI based parallelization: multiple communicators, hierarchical strategy

OpenMP fine grained parallelization + usage of threaded libraries (OpenMP tasks will be soon implemented)

Relevant quantities

N_w : number of plane waves (used in wavefunction expansion)

N_g : number of G-vectors (used in charge density expansion)

N_1, N_2, N_3 : dimensions of the FFT grid for charge density (for Ultrasoft PPs there are two distinct grids)

N_a : number of atoms in the unit cell or supercell

N_e : number of electron (Kohn-Sham) states (bands)

N_p : number of projectors in nonlocal PPs (sum over cell)

N_k : number of k-points in the irreducible Brillouin Zone

Parallelization strategy

Goals:

- Load balancing
- Reduce communication
- Fit the architecture (intranode/internode)
- Exploit asynchronism and pipelining

SEARCH

[Forum](#)

NEWS

25.04.16

QUANTUM ESPRESSO V5.4.0

Version 5.4.0 of Quantum ESPRESSO is available for download. You can find all archives uploaded on QE-FORGE here.

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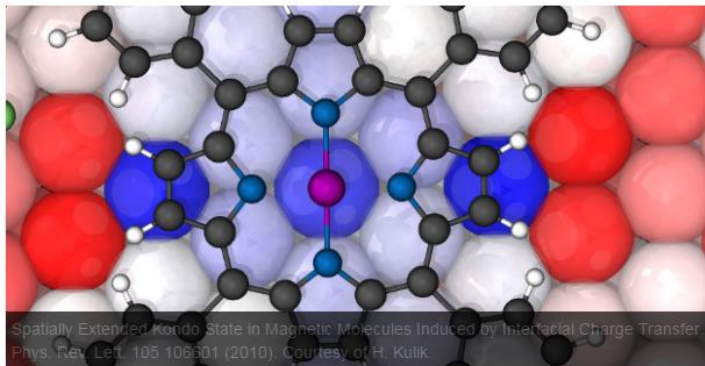
THE WALTER KOHN PRIZE

A prize for outstanding contributions in the field of quantum-mechanical materials and molecular modeling. More information here.

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QUANTUM ESPRESSO V5.3.0

Version 5.3.0 of Quantum ESPRESSO is available for download.



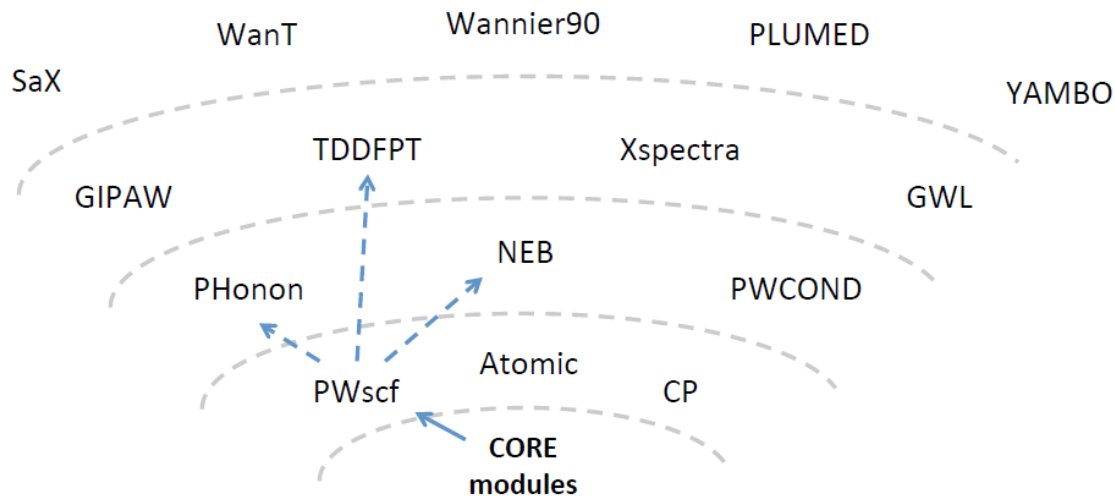
Spatially Extended Kondo State in Magnetic Molecules Induced by Inertial Charge Transfer. Phys. Rev. Lett. 105 106501 (2010). Courtesy of H. Kulk.

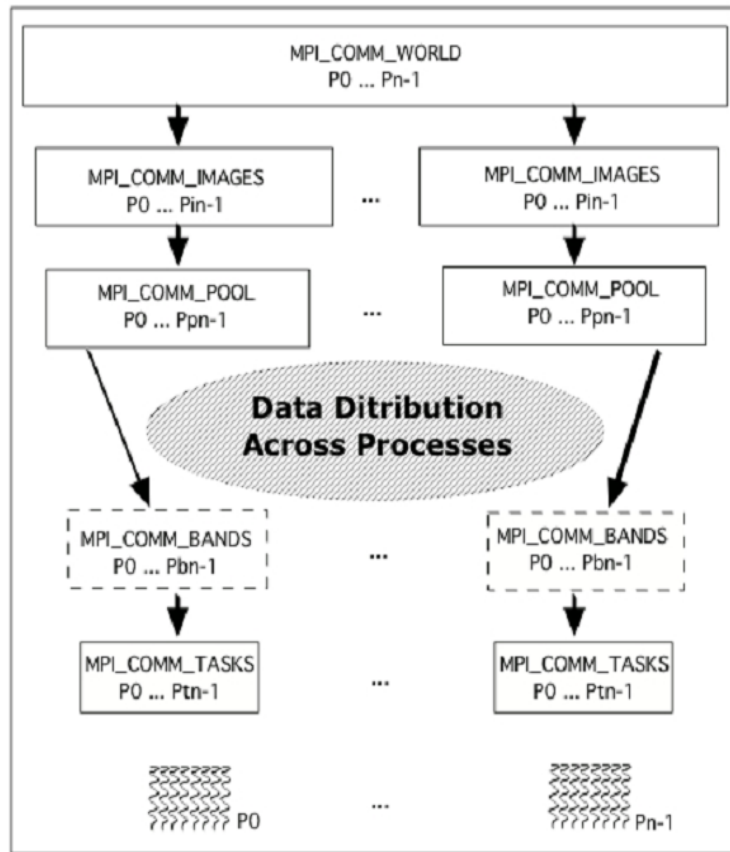
QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

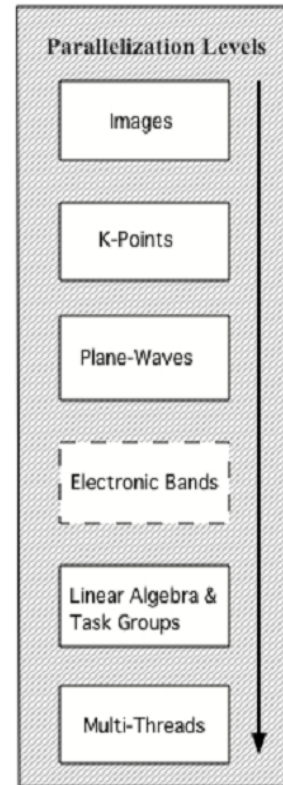
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Quantum ESPRESSO package portfolio





MPI Communicators Hierarchy

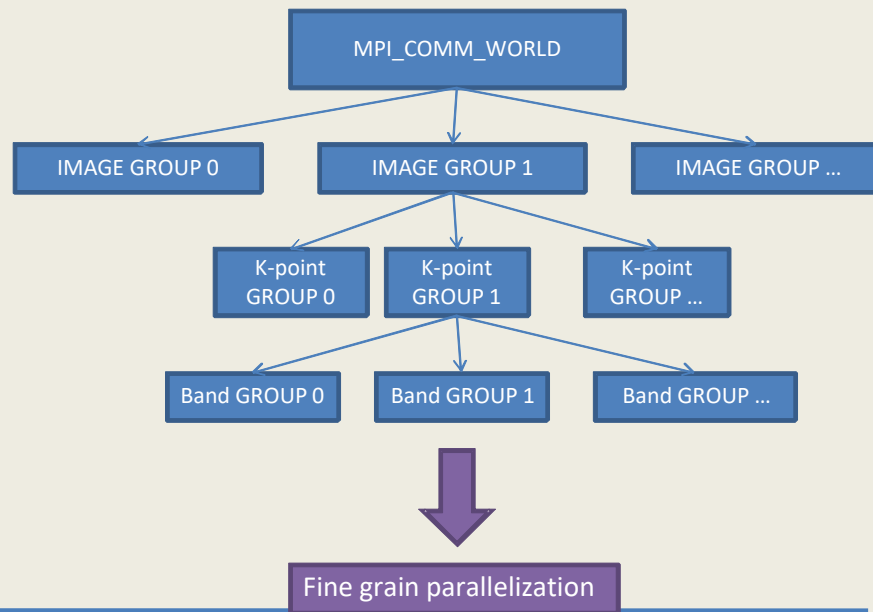


Coarse grain parallelization levels

1. Plane-waves (MPI_Comm_World)
2. Images
3. K-points
4. Bands

+ a finer grain data distribution

Coarse grain, high level QE data distribution



Fine grain parallelization levels

Data can be furtherly redistributed in order to accomplish specific tasks, such as FFT or linear algebra (LA) routines

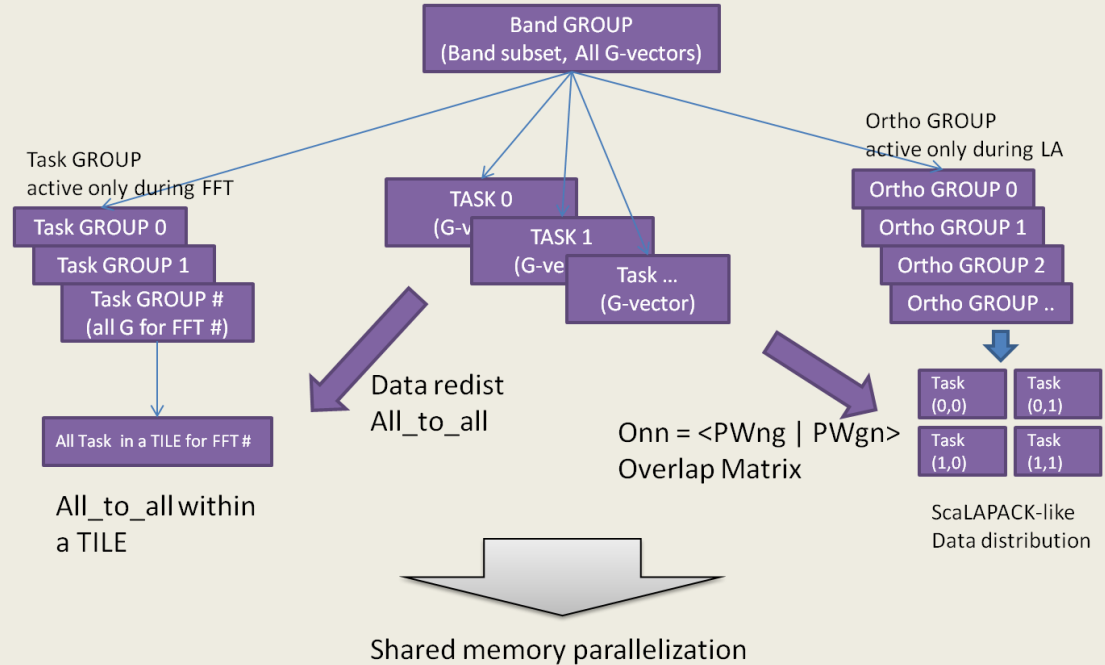


Image parallelization

A trivial parallelization can be made on images. Images are loosely coupled replica of the system and they are useful for

- Nudged Elastic Band calculations
- Atomic Displacement patterns for linear response calculation

and in general for all the cases in which you want to replicate N times your system and perform identical simulations (ensemble techniques).

```
mpirun -np 64 neb.x -nimage 4 -input inputfile.inp
```

k-point parallelization

If the simulation consists in different k-points, those can be distributed among n_{pools} pools of CPUs

K-points are typically independents: the amount of communications is small

When there is a large number of k-points this layer can strongly enhance the scalability

By definition, n_{pools} must be a divisor of the total number of k-points

```
mpirun -np 64 pw.x -npool 4 -input inputfile.inp
```

Band parallelization

Kohn-Sham states are split across the processors of the band group. Some calculations can be independently performed for different band indexes.

In combination with other levels of parallelism can improve performances and scalability

For example, in combination with k-points parallelization:

```
mpirun -np 64 pw.x -npool 4 -bgrp 4 -input inputfile.inp
```

Linear algebra parallelization

Distribute and parallelize matrix diagonalization and matrix-matrix multiplications needed in iterative diagonalization (SCF) or orthonormalization (CP). Introduces a linear-algebra group of n_{diag} processors as a subset of the plane-wave group. $n_{\text{diag}} = m^2$, where m is an integer such that $m^2 \leq n_{\text{PW}}$.

Should be set using the `-ndiag` or `-n_ortho` command line option, e.g.:

```
mpirun -np 64 pw.x -ndiag 25 -input inputfile.inp
```

Task-group parallelization

Each plane-wave group of processors is split into n_{task} task groups of n_{FFT} processors, with $n_{\text{task}} \times n_{\text{FFT}} = n_{\text{PW}}$;

each task group takes care of the FFT over N_e/n_t states.

Used to extend scalability of FFT parallelization.

Example for 1024 processors

- divided into $n_{\text{pool}} = 4$ pools of $n_{\text{PW}} = 256$ processors,
- divided into $n_{\text{task}} = 8$ tasks of $n_{\text{FFT}} = 32$ processors each;
- Subspace diagonalization performed on a subgroup of $n_{\text{diag}} = 144$ processors :

```
mpirun -np 1024 pw.x -npool 4 -ntg 8 -ndiag 144  
-input inputfile.inp
```


OpenMP parallelization

Explicit with workshare directives on computationally intensive for-loops

Implicit, when using external thread-safe libraries, e.g.

- MKL for linear algebra and fft (DFTI interface)
- FFTW/FFTW3

Usually scalability on threads is quite poor (no more than 8 threads).

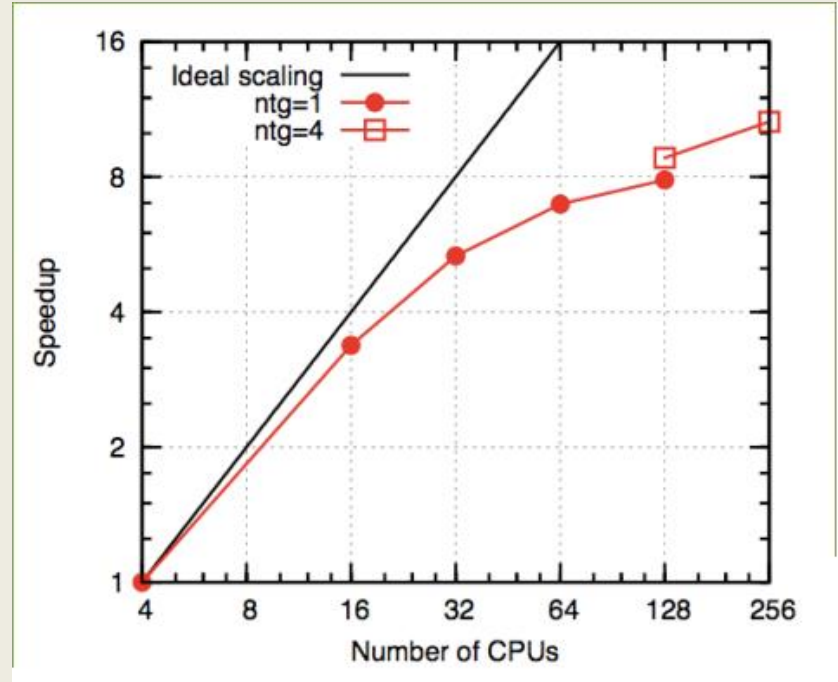
Ongoing effort to enhance OpenMP scalability using tasking techniques

- Necessary when working on many-cores architectures

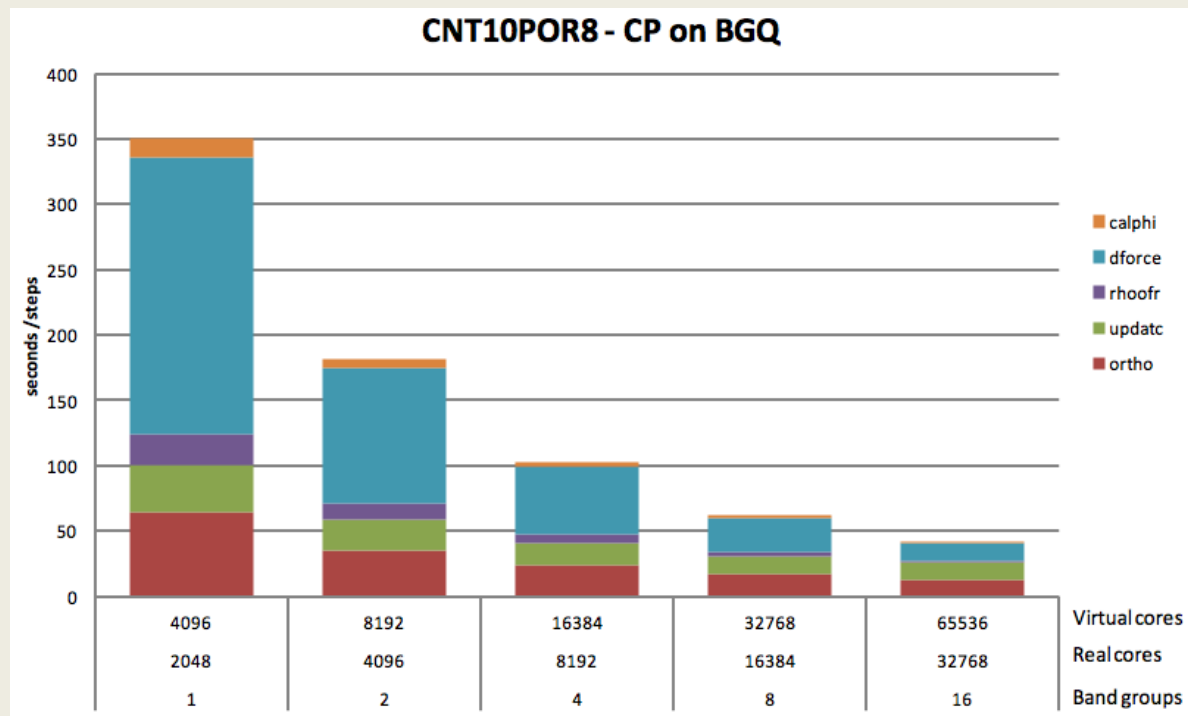
Some examples

128 water molecules, PW
calculation (IBM Power6),
MPI-only

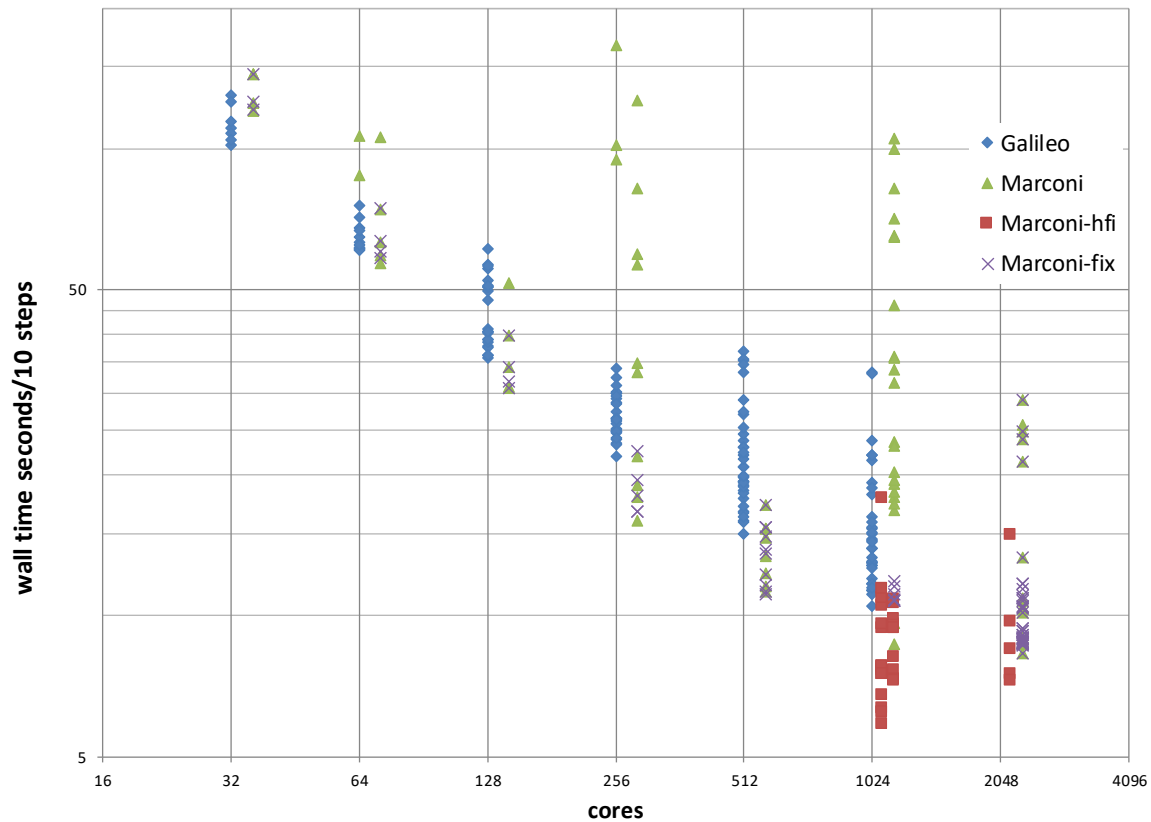
When scalability saturates,
using task-groups
permitted to push further..



Some examples

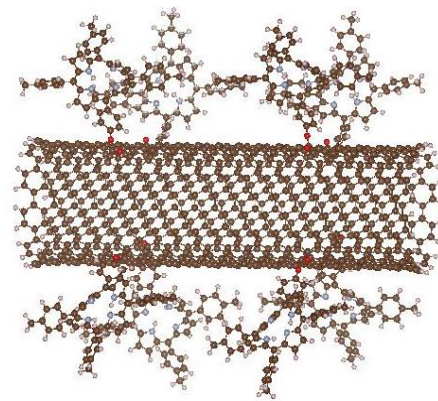
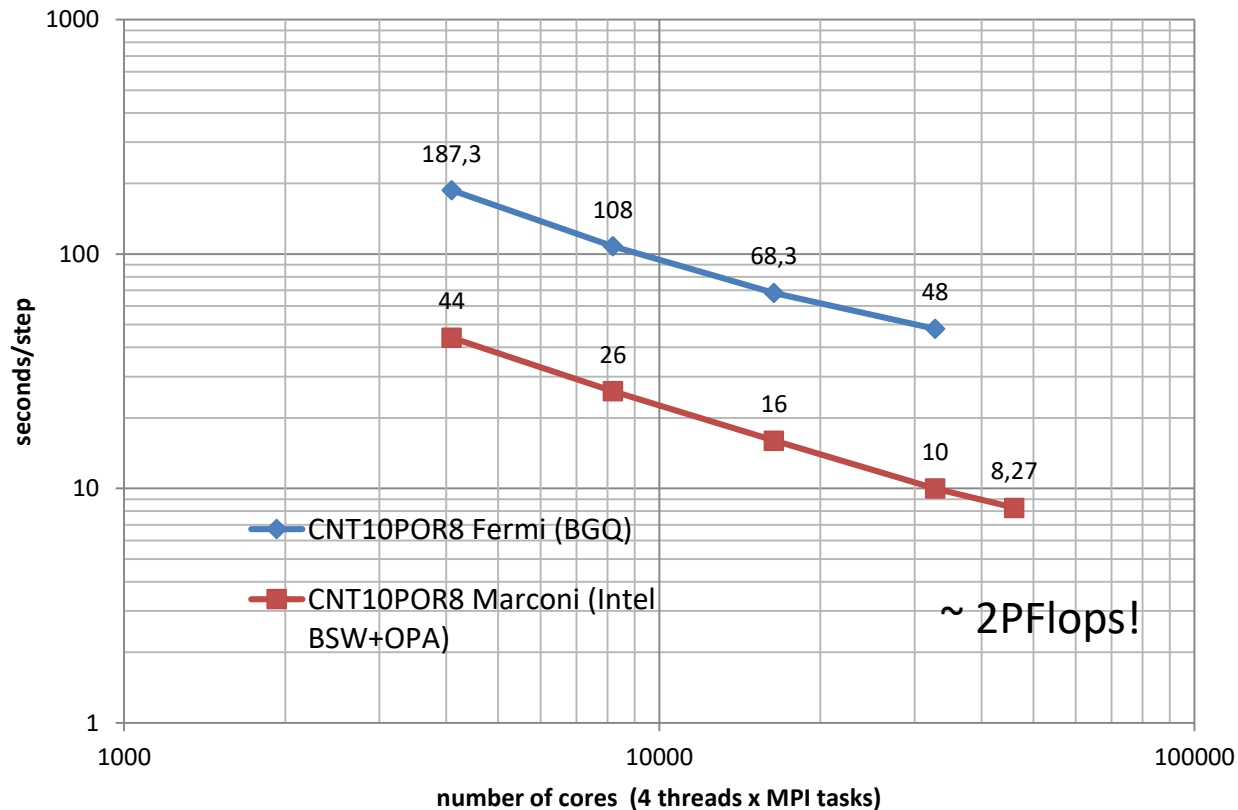


Dataset: PCBM_P3HT - Code: CP (QE 6) - Cluster: Marconi vs Galileo
(Dataset main sizes: 288 atoms, 794 electrons, 60Ryd)



QE scaling benchmark (cp.x)

Input dataset: <http://www.qe-forge.org/gf/download/frsrelease/49/63/CNT10POR8.tgz>



Molecular Dynamics of
Functionalized
Carbon nanotube
1532 atoms
~7nm