QE, main strategies of parallelization and levels of parallelisms

Fabio AFFINITO

SCAI - Cineca

QUANTUM ESPRESSO FOUNDATION

«*What I cannot compute, I do not understand.*» (adapted from Richard P. Feynman)

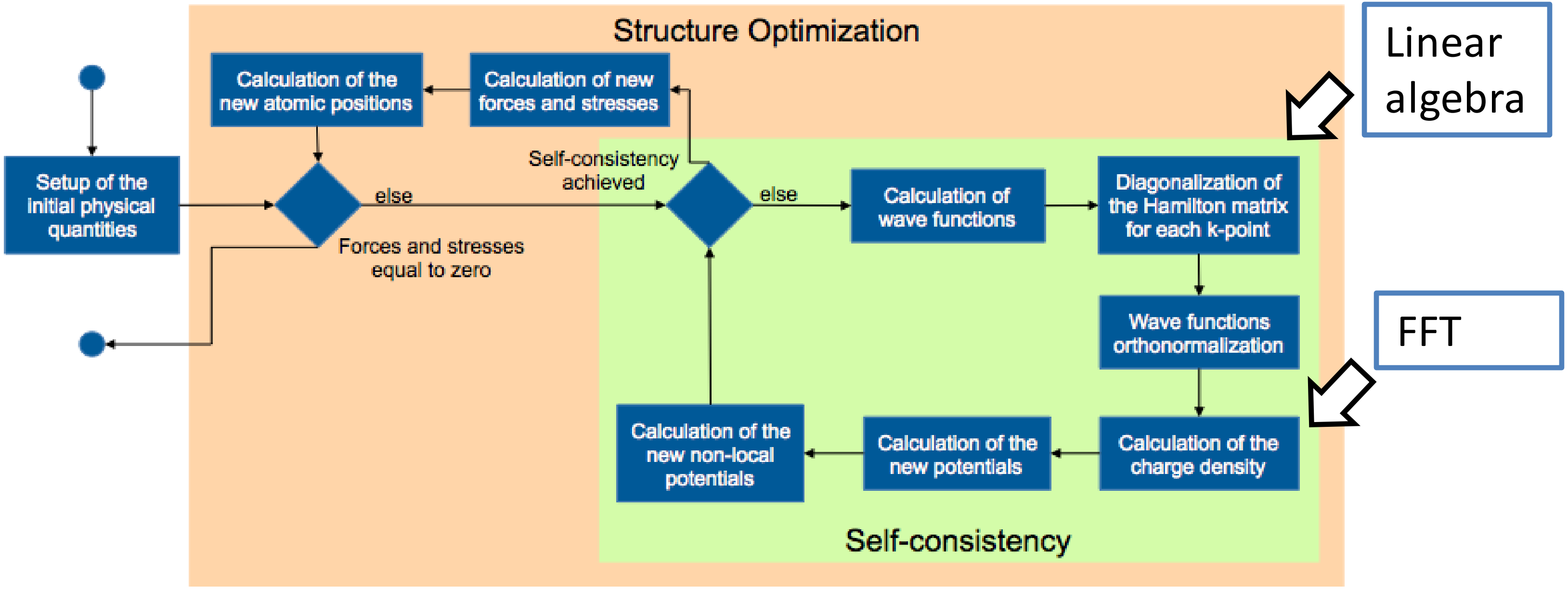
Quantum ESPRESSO: introduction

- 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

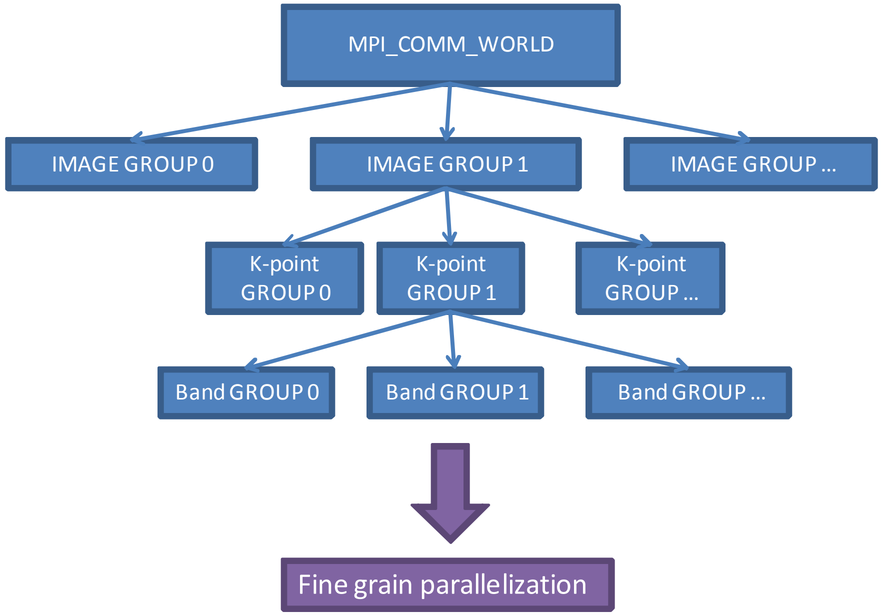
- Goals:
  - Load balancing
  - Reduce communication
  - Fit the architecture (intranode/internode)
  - Exploit asynchronism and pipelining

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



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Fine grain parallelization levels

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

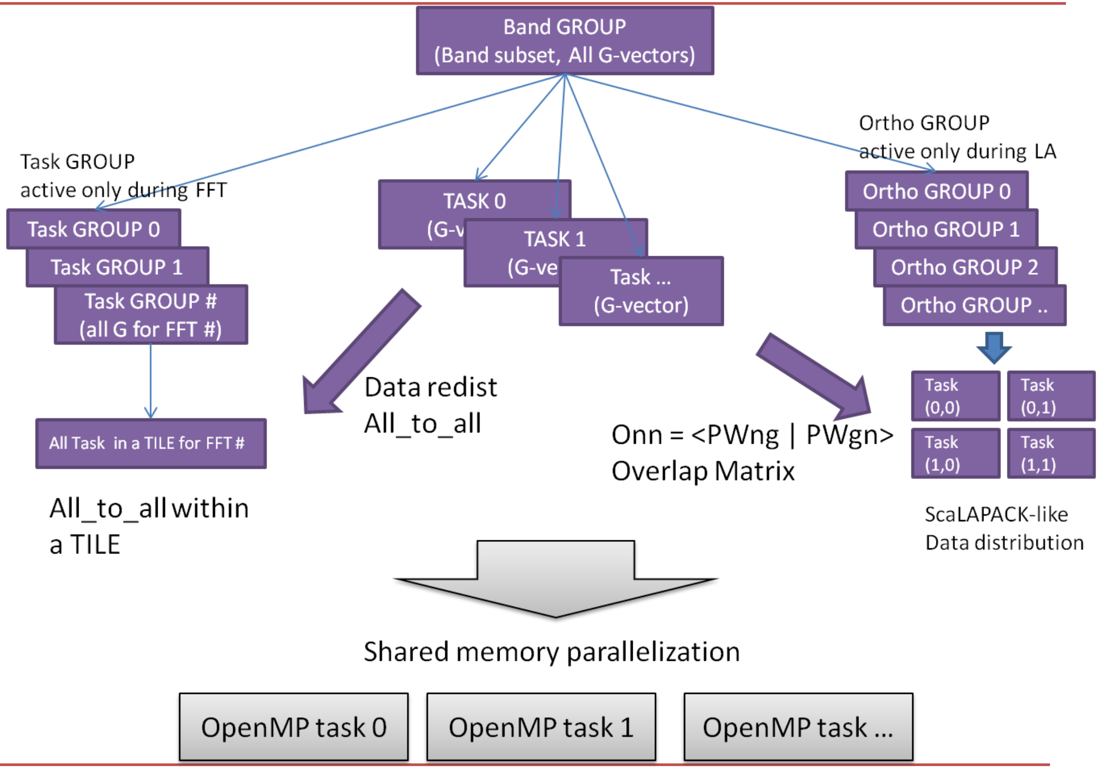


Image parallelization

- 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 tipically 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. $n_{diag} = m^2$, where m is an integer such that $m^2 \leq n_{PW}$.
- 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 $n_{task} \times n_{FFT} = n_{PW}$;
- 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 $n_{pool} = 4$ pools of $n_{PW} = 256$ processors,
  - divided into $n_{task} = 8$ tasks of $n_{FFT} = 32$ processors each;
  - Subspace diagonalization performed on a subgroup of $n_{diag} = 144$ processors :

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

OpenMP parallelization

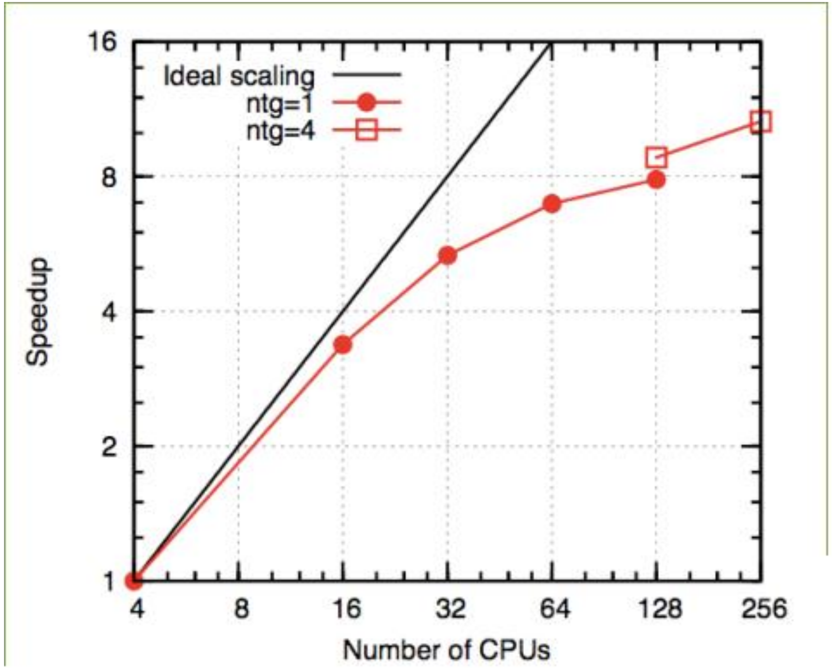
- Explicit with workshare directives on computationally intensive for-loops
- Implicit, when using external thread-safe libraries, e.g.
  - MKL for linear algebra and fft (DFTI interface)
  - FFTW/FFTW3

- 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

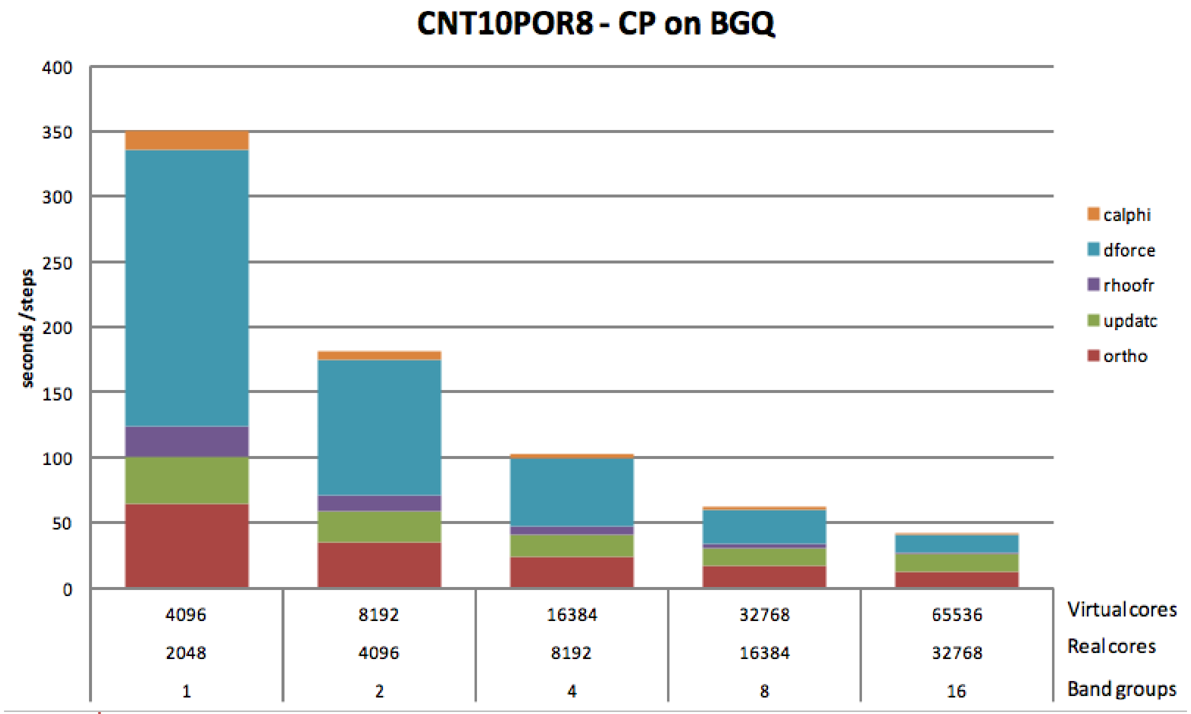
Some examples

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

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



Some examples



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