QE, main strategies of parallelization and levels of parallelisms

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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).
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](http://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

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-FORCE here.

31.01.18
THE WALTER KOHN PRIZE
A prize for outstanding contributions in the field of quantum-mechanical materials and molecular modeling. More information here.

11.01.18
QUANTUM ESPRESSO V5.3.0
Version 5.3.0 of Quantum ESPRESSO is available for download.

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.

READ MORE ➔
Quantum ESPRESSO package portfolio

courtesy of Stefano Baroni and Filippo Spiga
Coarse grain parallelization levels

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

+ a finer grain data distribution
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 \( n_{\text{pools}} \) 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, \( n_{\text{pools}} \) 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 $n_{\text{diag}}$ 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.:

```bash
mpirun -np 64 pw.x -ndiag 25 -input inputfile.inp
```
Task-group parallelization

Each plane-wave group of processors is split into $n_{\text{task}}$ task groups of $n_{\text{FFT}}$ 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)


Molecular Dynamics of Functionalized Carbon nanotube
1532 atoms
~7nm

~ 2PFlops!