Tutorial to use Quantum Espresso

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- ## Installation:

First download the Quantum Espresso from the website *www.**quantum-espresso**.org* from the download section.
Like: espresso-5.2.1.tar.gz
Then extract the file in the folder where you want to install it.
Go to terminal: **Ctrl+ Alt+ T** or using .
Like we have extract it in **src** folder then
cd src/ espresso-5.2.1
then
ls *//it will give all the list of files and folders under it.*

Install gfortran in the system to compile the setup file.

To install the Quantum ESPRESSO source package, run the configure script.

./configure --enable-openmp
make all

This will install Quantum Espresso in the system.

- ## Introduction to Pwscf

PWscf (Plane-Wave Self-Consistent Field) package, a core component of the Quantum ESPRESSO distribution.

What can PWscf do:

PWscf performs many different kinds of self-consistent calculations of electronic-structure prop- erties within Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials (PP). In particular:
• ground-state energy, atomic forces, stresses;
• structural optimization;
• molecular dynamics on the Born-Oppenheimer surface;

• macroscopic polarization and finite electric fields via the modern theory of polarization
• modern theory of orbital magnetization;
• free-energy surface calculation at fixed cell through meta-dynamics, if patched with PLUMED.

- **How to run calculations using Pwscf:**

Input data:
Input data is organized as several namelists, followed by other fields (“cards”) introduced by keywords. The namelists are

&CONTROL: general variables controlling the run
&SYSTEM: structural information on the system under investigation
&ELECTRONS: electronic variables: self-consistency, smearing
&IONS (optional): ionic variables: relaxation, dynamics
&CELL (optional): variable-cell optimization or dynamic

&CONTROL:
This block contains:

calculation= '.....' //calculation to perform
restart_mode='from_scratch',
pseudo_dir = '.....', //path of pseudo file
outdir='./tmp/', //path of output directory
prefix='xx' //prefix

Some of the important blocks under &CONTROL *:*

calculation
Default: CHARACTER

a string describing the task to be performed:
'scf',
'nscf',
'bands',
'relax',
'md',
'vc-relax',
'vc-md'
(vc = variable-cell).

restart_mode
Default: 'from_scratch'

CHARACTER
'
: from scratch. This is the normal way to perform a PWscf calculation

'restart' : from previous interrupted run. Use this switch only if you want to continue an interrupted calculation, not to start a new one, or to perform non-scf calculations. Works only if the calculation was cleanly stopped using variable "max_seconds",

nstep *INTEGER*
Default: 1 if calculation = 'scf', 'nscf', 'bands';
50 for the other cases

“number of ionic + electronic steps”

tstress *LOGICAL*
Default: .false.

calculate stress. It is set to .TRUE. automatically if calculation='vc-md' or 'vc-relax'

tprnfor *LOGICAL*
calculate forces. It is set to .TRUE. automatically if calculation='relax','md','vc-md'

outdir *CHARACTER*
Default: current directory ('./')

input, temporary, output files are found in this directory,

prefix *CHARACTER*
Default: 'pwscf'

prepended to input/output filenames

max_seconds *REAL*
Default: 1.D+7, or 150 days, i.e. no time limit

jobs stops after "max_seconds" CPU time. Use this option in conjunction with option "restart_mode" if you need to split a job too long to complete into shorter jobs

pseudo_dir *CHARACTER*
directory containing pseudopotential files

&SYSTEM

&system
ibrav= ...., //Bravais lattice index
celldm(1) =....., //Lattice parameter
nat=..... , //Number of atoms
ntyp=....., //Types of atoms in unit cell
ecutwfc =....., //Kinetic energy cutoff for wavefunctions
occupations='.....' //Depends on the type of calculations

ibrav INTEGER

Bravais-lattice index

ibrav strucuture

0 Free
1 SC
2 FCC
3 BCC
4 Hexagonal and trigonal P.

celldm(i), i=1,6 REAL
Crystallographic constants

nat INTEGER
number of atoms in the unit cell

ntyp INTEGER
number of types of atoms in the unit cell

nbnd INTEGER
number of electronic states (bands) to be calculated.

tot_charge REAL
Default: 0.0
total charge of the system. Useful for simulations with charged cells.
By default the unit cell is assumed to be neutral (tot_charge=0).
tot_charge=+1 means one electron missing from the system,
tot_charge=-1 means one additional electron, and so on.

ecutwfc REAL
kinetic energy cutoff (Ry) for wavefunctions

occupations CHARACTER
'smearing': gaussian smearing for metals see variables 'smearing' and 'degauss'
'tetrahedra' : especially suited for calculation of DOS
'fixed' : for insulators with a gap

These blocks(**degauss and smearing**)will are used when we use
occupation= smearing.

degauss REAL
Default: 0.D0 Ry
value of the gaussian spreading (Ry) for brillouin-zone integration in metals.

smearing CHARACTER
Default: 'gaussian'
'gaussian', 'gauss': ordinary Gaussian spreading (Default)
'methfessel-paxton', 'm-p', 'mp': Methfessel-Paxton first-order spreading
(see PRB 40, 3616 (1989)).
'marzari-vanderbilt', '*cold'*, *'m-v'*, *'mv*' : Marzari-Vanderbilt cold smearing
(see PRL 82, 3296 (1999))
'fermi-dirac', *'f-d'*, *'fd'*: smearing with Fermi-Dirac function

nspin Integer
Default: 1
nspin = 1 : non-polarized calculation (default)
nspin = 2 : spin-polarized calculation, LSDA
(magnetization along z axis)

Namelist: ELECTRONS

```
&electrons
  diagonalization='cg'
  mixing_beta = 0.7
```

electron_maxstep INTEGER
Default: 100
maximum number of iterations in a scf step

mixing_beta REAL
Default: 0.7D0
mixing factor for self-consistency

diagonalization CHARACTER
Default: 'david'
'david': Davidson iterative diagonalization with overlap matrix (default). Fast, may in

some rare cases fail.
'cg' : conjugate-gradient-like band-by-band diagonalization . Typically slower than 'david' but it uses less memory and is more robust (it seldom fails) .

For more Namelist and blocks refer to Quantum espresso User Guide.

Card: ATOMIC_SPECIES
Syntax:
ATOMIC_SPECIES
X(1) Mass_X(1) PseudoPot_X(1)
X(2) Mass_X(2) PseudoPot_X(2)
. . .
X(n) Mass_X(n) PseudoPot_X(n)

X CHARACTER
label of the atom.

Mass_X REAL
Mass of atomic species.

PseudoPot_X CHARACTER
File containing PP for this species.

CARD:ATOMIC_POSITIONS

Syntax:
ATOMIC_POSITIONS { alat | bohr | angstrom | crystal | crystal_sg }
X(n) x(1) y(1) z(1)
X(n) x(1) y(1) z(1)
.....
X(n) x(n) y(n) z(n)

Description of items:
alat : atomic positions are in cartesian coordinates, in units of the lattice parameter.
bohr : atomic positions are in cartesian coordinate, in atomic units (i.e. Bohr radii)
angstrom: atomic positions are in cartesian coordinates, in Angstrom
crystal : atomic positions are in crystal coordinates,
crystal_sg : atomic positions are in crystal coordinates, i.e.
in relative coordinates of the primitive lattice.

X CHARACTER
label of the atom as specified in ATOMIC_SPECIES
x, y, z REAL
atomic positions

Card: K_POINTS { tpiba | automatic | crystal | gamma | tpiba_b | crystal_b | tpiba_c | crystal_c }

Syntax
K_POINTS tpiba | crystal | tpiba_b | crystal_b | tpiba_c | crystal_c
nks
xk_x(1) xk_y(1) xk_z(1) wk(1)
xk_x(2) xk_y(2) xk_z(2) wk(2)
.....
xk_x(nks) xk_y(nks) xk_z(nks) wk(nks)

Syntax:
K_POINTS automatic
nk1 nk2 nk3 sk1 sk2 sk3

Syntax:
K_POINTS gamma

Description of items:

tpiba : read k-points in cartesian coordinates, in units of 2 pi/a (default)
automatic: automatically generated uniform grid of k-points,
crystal : read k-points in crystal coordinates, i.e. in relative coordinates of the reciprocal lattice vectors .
gamma : use k = 0 (no need to list k-point specifications after card) . In this case wavefunctions can be chosen as real, and specialized subroutines optimized for calculations at the gamma point are used (memory and cpu requirements are reduced by approximately one half).
tpiba_b : Used for band-structure plots. k-points are in units of 2 pi/a.

nks*: Number of supplied special k-points.*

So after all this input file look like the following.
Here Iam taking input file for 'Al'

```
&control
   calculation='scf'
   restart_mode='from_scratch',
   pseudo_dir = '/home/abhi/src/espresso-5.2.1/pseudo/',
   outdir='./tmp/',
   prefix='al'

 /
 &system
   ibrav=  2, celldm(1) =7.50, nat=  1, ntyp= 1, ecutwfc =15.0,
   occupations='smearing', smearing='marzari-vanderbilt', degauss=0.05
 /
 &electrons
   diagonalization='cg'
   mixing_beta = 0.7
 /
ATOMIC_SPECIES
 Al  26.98 Al.pbe-n-van.UPF
ATOMIC_POSITIONS
 Al 0.00 0.00 0.00

K_POINTS (AUTOMATIC)
 15 15 15 0 0 0
```