Input and Output description

Where can I find useful information about Quantum-ESPRESSO ?

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```
prompt > ls  $espresso_dir/Doc/*.html

INPUT_BANDS.html   INPUT_DOS.html     INPUT_PH.html         INPUT_PWCOND.ht
INPUT_CPPP.html    INPUT_GIPAW.html   INPUT_PP.html         INPUT_pw_export
INPUT_D3.html      INPUT_LD1.html     INPUT_PROJWFC.html    INPUT_PW.html
```

We will examine to some extent the input of PWscf

The input file for PWscf is structured in a number of NAMELISTS and INPUT_CARDS.

```
&NAMELIST1 ... /

 &NAMELIST2 ... /

 &NAMELIST3 ... /

 INPUT_CARD1
   ....
   ....
 INPUT_CARD2
   ....
   ....
```

NAMELISTS are a standard input construct in fortran90.

The use of NAMELISTS allows to specify the value of an input variable only when it is needed and to define default values for most variables that then need not be specified. Variable can be inserted in any order.

```
&NAMELIST
   needed_variable2=XX, needed_variable1=X,
 /
```

NAMELISTS are read in a specific order

NAMELISTS that are not required are ignored

INPUT_CARDS are specific of ESPRESSO codes and are used to provide input data that are always needed and would be boring to specify with the `variable_name=variable_value` syntax used by NAMELIST.

INPUT_CARDS require data in specific order (which may depend on the situation and on the value of a card_format_specifier)

For instance:

```
INPUT_CARD   card_format_specifier
 data(1,1) data(1,2) data(1,3) ...
 data(2,1) data(2,2) data(2,3) ...
 data(3,1) data(3,2) data(3,3) ...
 ... ... ...
```

Logically independent INPUT_CARDS can be given in any order

There are three mandatory NAMELISTS in PWscf:

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```
&CONTROL    input variables that control the flux of the
            calculation and the amount of I/O on disk and
            on the screen.
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`&CONTROL`	`input variables that control the flux of the calculation and the amount of I/O on disk and on the screen.`
`&SYSTEM`	`input variables that specify the system under study.`

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`&CONTROL`	input variables that control the flux of the calculation and the amount of I/O on disk and on the screen.
`&SYSTEM`	input variables that specify the system under study.
`&ELECTRONS`	input variables that control the algorithms used to reach the self-consistent solution of KS equations for the electrons.

There are three additional NAMELISTS in PWscf that must be specified under certain circumstances:

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&IONS      needed when ATOMS MOVE! IGNORED otherwise !
           input variables that control ionic motion in
           molecular dynamics run or structural relaxation
```

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```
&IONS      needed when ATOMS MOVE! IGNORED otherwise !
           input variables that control ionic motion in
           molecular dynamics run or structural relaxation

&CELL      needed when CELL MOVES! IGNORED otherwise !
           input variables that control the cell-shape
           evolution in a variable-cell-shape MD or
           structural relaxation
```

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```
&IONS      needed when ATOMS MOVE! IGNORED otherwise !
           input variables that control ionic motion in
           molecular dynamics run or structural relaxation

&CELL      needed when CELL MOVES! IGNORED otherwise !
           input variables that control the cell-shape
           evolution in a variable-cell-shape MD or
           structural relaxation

&PHONON    needed when preparing input for PHONON !
           IGNORED otherwise!
           will be described with the PHONON code.
```

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```
ATOMIC_SPECIES    name, mass and pseudopotential used for
                  each atomic species present in the system
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ATOMIC_POSITIONS  type and coordinates of each atom in the
                  unit cell
```

There are three mandatory INPUT_CARDS in PWscf

`ATOMIC_SPECIES`	`name, mass and pseudopotential used for each atomic species present in the system`
`ATOMIC_POSITIONS`	`type and coordinates of each atom in the unit cell`
`K_POINTS`	`coordinates and weights of the k-points used for BZ integration`

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They are

```
CELL_PARAMETERS

OCCUPATIONS

CLIMBING_IMAGES   will be described with NEB
```

The &CONTROL namelist

```
&CONTROL    input variables that control the flux of the
            calculation and the amount of I/O on disk and
            on the screen.
```

```
FLUX       : calculation
I/O        : title, verbosity, iprint, outdir, prefix,
             pseudo_dir, tprnfor, tstress, disk_io
RECOVER    : restart_mode, max_seconds
MISC       : dt, nstep, etot_conv_thr, forc_conv_thr, tefiel
```

The &CONTROL namelist (FLUX)

```
calculation CHARACTER  (default = 'scf')
            a string describing the task to be performed:
            'scf', 'nscf', 'phonon', 'relax', 'md',
            'vc-relax', 'vc-md', 'neb' (vc=variable-cell).
```

Input structure for a SCF run

```
&CONTROL ... /
&SYSTEM ... /
&ELECTRONS ... /
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
```

```
&CONTROL ... /
&SYSTEM ibrav=0 ... /
&ELECTRONS ... /
CELL_PARAMETERS
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
```

```
&CONTROL ... /
&SYSTEM ... /
&ELECTRONS occupations=fixed ... /
OCCUPATIONS
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
```

Input structure for a RELAX / MD run

```
&CONTROL calculation='relax' ... /
&SYSTEM ... /
&ELECTRONS ... /
&IONS ... /
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS

&CONTROL calculation='vc-relax' ... /
&SYSTEM ... /
&ELECTRONS ... /
&IONS ... /
&CELL ... /
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
```

An example

```
&control
    pseudo_dir = './',
    outdir='/scratch/stefano/Be0001/',
    prefix='be0001'
    tprnfor = .true.
 /
 &system
    ibrav=4, celldm(1)=4.247, celldm(3)=16.0, nat=12, ntyp=1, nbnd=20,
    occupations='smearing', smearing='methfessel-paxton', degauss=0.05
    ecutwfc=22.0, nr1=16, nr2=16,
 /
 &electrons
 /
ATOMIC_SPECIES
Be   1.0   Be.vbc2
ATOMIC_POSITIONS alat
Be   0.000000000  -0.288675135   4.359667099
Be   0.000000000   0.288675135   3.548485449
Be   0.000000000  -0.288675135   2.754655986
..   ...........   ...........   ...........
```

```
..    ............    ............    ............
Be    0.000000000     0.288675135    -2.754655986
Be    0.000000000    -0.288675135    -3.548485449
Be    0.000000000     0.288675135    -4.359667099
K_POINTS tpiba
  30
     0.000000000  0.000000000  0.000000000   1.00
     0.062500000  0.036084392  0.000000000   6.00
     0.125000000  0.072168784  0.000000000   6.00
     0.187500000  0.108253175  0.000000000   6.00
     ...........  ...........  ...........   ....
     ...........  ...........  ...........   ....
     0.250000000  0.433012702  0.000000000   6.00
     0.312500000  0.469097094  0.000000000  12.00
     0.375000000  0.505181486  0.000000000   6.00
     0.312500000  0.541265877  0.000000000   6.00
```

```
prompt> $espresso_dir/bin/pw.x < pw.in > pw.out
```

The output

```
Program PWSCF     v.2.0    starts ...
Today is 16Feb2004 at 16: 6:28

Ultrasoft (Vanderbilt) Pseudopotentials

Current dimensions of program pwscf are:
ntypx =10   npk =40000  lmax = 3
nchix = 6  ndim = 2000  nbrx = 8 nqfm = 8

bravais-lattice index     =            4
lattice parameter (a_0)   =       4.2470  a.u.
unit-cell volume          =    1061.4448 (a.u.)^3
number of atoms/cell      =           12
number of atomic types    =            1
kinetic-energy cutoff     =      22.0000  Ry
charge density cutoff     =      88.0000  Ry
convergence threshold     =      1.0E-06
beta                      =       0.7000
number of iterations used =            8  plain     mixing
Exchange-correlation      = PZ (1100)
iswitch =  0
```

```
celldm(1)=   4.247000  celldm(2)=   0.000000  celldm(3)=  16.00000
celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.00000

crystal axes: (cart. coord. in units of a_0)
          a(1) = (  1.000000  0.000000  0.000000 )
          a(2) = ( -0.500000  0.866025  0.000000 )
          a(3) = (  0.000000  0.000000 16.000000 )

reciprocal axes: (cart. coord. in units 2 pi/a_0)
          b(1) = (  1.000000  0.577350  0.000000 )
          b(2) = (  0.000000  1.154701  0.000000 )
          b(3) = (  0.000000  0.000000  0.062500 )
```

```
PSEUDO 1 is Be (vbc)   zval =  2.0   lmax= 1   lloc= 1
          i=       1              2          3
 core
 alpha =      0.99964        0.0000
 a(i)  =       1.0000        0.0000

 l =  0
 alpha =       1.7068        0.0000        0.0000
 a(i)  =       5.4710        0.0000        0.0000
 a(i+3)=      -1.6312        0.0000        0.0000

 l =  1
 alpha =      0.78031        0.0000        0.0000
 a(i)  =      -1.6972        0.0000        0.0000
 a(i+3)=      0.48457        0.0000        0.0000

 nonlinear core correction: rho(r) = ( a + b r^2) exp(-alpha r^2)
 a    =    0.95153E-01
 b    =    0.24127
 alpha=     2.7594
```

```
 atomic species   valence    mass     pseudopotential
    Be              2.00     1.00000     Be( 1.00)

  12 Sym.Ops. (with inversion)

Cartesian axes

  site n.     atom                  positions (a_0 units)
      1           Be  tau(  1) = (  0.0000000 -0.2886751  4.3596671  )
      2           Be  tau(  2) = (  0.0000000  0.2886751  3.5484854  )
      3           Be  tau(  3) = (  0.0000000 -0.2886751  2.7546560  )
      4           Be  tau(  4) = (  0.0000000  0.2886751  1.9655547  )
      5           Be  tau(  5) = (  0.0000000 -0.2886751  1.1789015  )
      6           Be  tau(  6) = (  0.0000000  0.2886751  0.3929197  )
      7           Be  tau(  7) = (  0.0000000 -0.2886751 -0.3929197  )
      8           Be  tau(  8) = (  0.0000000  0.2886751 -1.1789015  )
      9           Be  tau(  9) = (  0.0000000 -0.2886751 -1.9655547  )
     10           Be  tau( 10) = (  0.0000000  0.2886751 -2.7546560  )
     11           Be  tau( 11) = (  0.0000000 -0.2886751 -3.5484854  )
     12           Be  tau( 12) = (  0.0000000  0.2886751 -4.3596671  )
```

```
number of k points= 30  gaussian broad. (ryd)= 0.0500  ngauss = 1
                     cart. coord. in units 2pi/a_0
   k(  1) = (  0.0000000  0.0000000  0.0000000), wk =  0.0078125
   k(  2) = (  0.0625000  0.0360844  0.0000000), wk =  0.0468750
   k(  3) = (  0.1250000  0.0721688  0.0000000), wk =  0.0468750
   k(  4) = (  0.1875000  0.1082532  0.0000000), wk =  0.0468750
   ..  .. . .  .........  .........  ........... .. .  .........
   ..  .. . .  .........  .........  ........... .. .  .........
   k( 27) = (  0.2500000  0.4330127  0.0000000), wk =  0.0468750
   k( 28) = (  0.3125000  0.4690971  0.0000000), wk =  0.0937500
   k( 29) = (  0.3750000  0.5051815  0.0000000), wk =  0.0468750
   k( 30) = (  0.3125000  0.5412659  0.0000000), wk =  0.0468750

G cutoff =   40.2057  ( 14795 G-vectors)   FFT grid: ( 16, 16,216)

nbndx  =    80  nbnd   =   20  natomwfc =  12  npwx   =    1887
nelec  =   24.00 nkb   =   12  ngl    =   943
```

```
warning: negative or imaginary core charge    -0.000003    0.000000

   Initial potential from superposition of free atoms
   Starting wfc are atomic +   8 random wfc

   total cpu time spent up to now is     31.14 secs

   iteration #  1     ecut=    22.00 ryd     beta=0.70
   Davidson diagonalization (with overlap)
   ethr =  1.00E-02,  avg # of iterations =  8.0
   total energy              =   -29.14912003 ryd
   estimated scf accuracy    <     0.47112901 ryd

   total cpu time spent up to now is    220.47 secs

   iteration #  2     ecut=    22.00 ryd     beta=0.70
   Davidson diagonalization (with overlap)
   ethr =  1.96E-03,  avg # of iterations =  9.2
   total energy              =   935.30786090 ryd
   estimated scf accuracy    <   979.55647128 ryd
```

```
 .......

 total cpu time spent up to now is   1635.03 secs

 iteration # 15     ecut=    22.00 ryd     beta=0.70
 Davidson diagonalization (with overlap)
 ethr =  2.32E-08,  avg # of iterations =  3.6

      k = 0.0000 0.0000 0.0000 ( 1883 PWs)  bands (ev):
-8.6594 -8.3732 -8.0061 -7.5629 -7.0379 -6.4263 -5.7252 -4.9375
-4.0779 -3.1891 -2.3981 -0.2625 -0.2366  4.3785  5.4202  6.5117
 7.1274  7.7717  7.8515  9.1438

 ......  ......  ......  ......  ......  ......  ......  ......

      k = 0.3125 0.5413 0.0000 ( 1887 PWs)  bands (ev):
-0.4220 -0.1336  0.2091  0.5662  0.9013  1.1965  1.4595  1.6954
 1.7326  1.8983  1.9058  1.9856  2.1627  2.4288  2.6712  2.9470
 3.2659  3.6570  4.2349  5.0255
```

```
     the Fermi energy is     2.3995 ev

!    total energy              =   -29.53349448 ryd
     estimated scf accuracy    <     0.00000041 ryd

     band energy sum           =    -3.75904228 ryd
     one-electron contribution =  -847.59119742 ryd
     hartree contribution      =   431.32053221 ryd
     xc contribution           =   -16.79591716 ryd
     ewald contribution        =   403.53337095 ryd
     correction for metals     =    -0.00028305 ryd

     convergence has been achieved
```

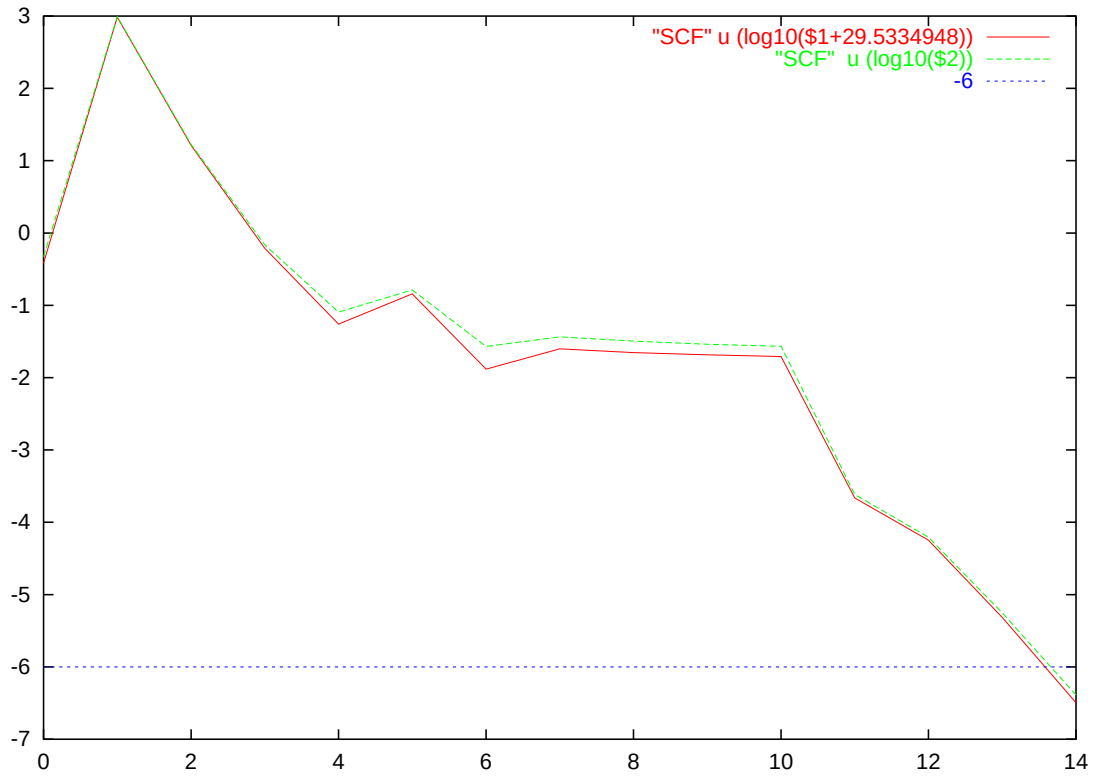
```
Forces acting on atoms (Ry/au):

 atom    1 type  1   force =   0.00000000  0.00000000 -0.00004555
 atom    2 type  1   force =   0.00000000  0.00000000  0.00003219
 atom    3 type  1   force =   0.00000000  0.00000000 -0.00011340
 atom    4 type  1   force =   0.00000000  0.00000000  0.00007865
 atom    5 type  1   force =   0.00000000  0.00000000  0.00005442
 atom    6 type  1   force =   0.00000000  0.00000000 -0.00001113
 atom    7 type  1   force =   0.00000000  0.00000000  0.00001113
 atom    8 type  1   force =   0.00000000  0.00000000 -0.00005442
 atom    9 type  1   force =   0.00000000  0.00000000 -0.00007865
 atom   10 type  1   force =   0.00000000  0.00000000  0.00011340
 atom   11 type  1   force =   0.00000000  0.00000000 -0.00003219
 atom   12 type  1   force =   0.00000000  0.00000000  0.00004555

 Total force =     0.000225   Total SCF correction =  0.001059

 Writing file be0001.pun    for program phonon
```

```
PWSCF        : 28m48.18s CPU time

 init_run     :    31.12s CPU
 electrons    :  1696.01s CPU
 forces       :     0.95s CPU

 electrons    :  1696.01s CPU
 c_bands      :  1496.42s CPU (      15 calls,  99.761 s avg)
 sum_band     :   195.59s CPU (      15 calls,  13.039 s avg)
 v_of_rho     :     2.04s CPU (      31 calls,   0.066 s avg)
 mix_rho      :     1.91s CPU (      15 calls,   0.127 s avg)

 c_bands      :  1496.42s CPU (      15 calls,  99.761 s avg)
 init_us_2    :     1.40s CPU (     960 calls,   0.001 s avg)
 cegterg      :  1493.49s CPU (     450 calls,   3.319 s avg)

 sum_band     :   195.59s CPU (      15 calls,  13.039 s avg)
```

```
wfcrot        :    30.20s CPU (      30 calls,   1.007 s avg)
cegterg       :  1493.49s CPU (     450 calls,   3.319 s avg)
h_psi         :  1398.80s CPU (    2473 calls,   0.566 s avg)
g_psi         :     3.22s CPU (    1993 calls,   0.002 s avg)
overlap       :    46.05s CPU (    1993 calls,   0.023 s avg)
cdiaghg       :    14.71s CPU (    2023 calls,   0.007 s avg)
update        :    26.08s CPU (    1993 calls,   0.013 s avg)
last          :    18.87s CPU (     586 calls,   0.032 s avg)

h_psi         :  1398.80s CPU (    2473 calls,   0.566 s avg)
init          :     2.32s CPU (    2473 calls,   0.001 s avg)
firstfft      :   669.67s CPU (   32391 calls,   0.021 s avg)
secondfft     :   653.82s CPU (   32391 calls,   0.020 s avg)
add_vuspsi    :     6.94s CPU (    2473 calls,   0.003 s avg)

 General routines
ccalbec       :     8.00s CPU (    2503 calls,   0.003 s avg)
cft3          :     2.74s CPU (     126 calls,   0.022 s avg)
cft3s         :  1432.65s CPU (   73782 calls,   0.019 s avg)
davcio        :     2.67s CPU (    1410 calls,   0.002 s avg)
```

```
 prompt>  grep -e 'total energy' -e ' scf ' pw.out | \
          awk '/l e/{e=$(NF-1)}/ scf /{print e, $(NF-1)}'

-29.14912003 0.47112901
935.30786090 979.55647128
-13.21357118 16.83007169
-28.92055625 0.68658733
-29.47844813 0.08060113
-29.38920267 0.16317196
-29.52040351 0.02695532
-29.50844717 0.03671080
-29.51131284 0.03206405
-29.51277583 0.02891886
-29.51395038 0.02707970
-29.53327797 0.00024233
-29.53343821 0.00006216
-29.53348998 0.00000557
-29.53349448 0.00000041
```

```
prompt>  grep -e 'total energy' -e ' scf ' pw.out | \
         awk '/l e/{e=$(NF-1)}/ scf /{print e, $(NF-1)}' > SCF
```



Where can I find some useful information about PWscf ?

```
prompt > ls  $espresso_dir/Doc/
```

In particular INPUT_PW.html contains a rather complete description of the input of PWscf.

Similarly INPUT_PP.html, INPUT_PH.html,... contain descriptions of post processing, phonon...

```
prompt > ls  $espresso_dir/examples/
```

This directory contains a number of example scripts that illustrate (some) of the features implemented in PWscf and related codes.

There is a GUI for PWscf and the other codes in the package.
It can be used in order to have on-line help and to prepare well-formed input files.

When everything else fail read the manual at `http:\\www.quantum-espresso.org/wiki`

THE END