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     Program PWSCF v.6.3 starts on 16Apr2019 at 16:20:10

     This program is part of the open-source Quantum ESPRESSO suite
     for quantum simulation of materials; please cite
         "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
         "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
          URL http://www.quantum-espresso.org",
     in publications or presentations arising from this work. More details at
     http://www.quantum-espresso.org/quote

     Parallel version (MPI), running on     2 processors

     MPI processes distributed on     1 nodes
     R & G space division:  proc/nbgrp/npool/nimage =       2
     Waiting for input...
     Reading input from standard input
Warning: card  &IONS ignored
Warning: card  / ignored
     Message from routine read_cards :
     DEPRECATED: no units specified in ATOMIC_POSITIONS card
     Message from routine read_cards :
     ATOMIC_POSITIONS: units set to alat

     Current dimensions of program PWSCF are:
     Max number of different atomic species (ntypx) = 10
     Max number of k-points (npk) =  40000
     Max angular momentum in pseudopotentials (lmaxx) =  3
               file H.pz-kjpaw_psl.1.0.0.UPF: wavefunction(s)  1S renormalized

     Subspace diagonalization in iterative solution of the eigenvalue problem:
     a serial algorithm will be used


     Parallelization info
     --------------------
     sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
     Min         558     442    110                14128    10002    1258
     Max         559     443    111                14129    10003    1259
     Sum        1117     885    221                28257    20005    2517



     bravais-lattice index     =            1
     lattice parameter (alat)  =       7.5000  a.u.
     unit-cell volume          =     421.8750 (a.u.)^3
     number of atoms/cell      =            1
     number of atomic types    =            1
     number of electrons       =         1.00
     number of Kohn-Sham states=            5
     kinetic-energy cutoff     =      50.0000  Ry
     charge density cutoff     =     250.0000  Ry
     convergence threshold     =      1.0E-06
     mixing beta               =       0.2000
     number of iterations used =            8  plain     mixing
     Exchange-correlation      = SLA PZ NOGX NOGC ( 1  1  0  0 0 0)

     celldm(1)=   7.500000  celldm(2)=   0.000000  celldm(3)=   0.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000
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  crystal axes: (cart. coord. in units of alat)
            a(1) = (   1.000000   0.000000   0.000000 )
            a(2) = (   0.000000   1.000000   0.000000 )
            a(3) = (   0.000000   0.000000   1.000000 )

  reciprocal axes: (cart. coord. in units 2 pi/alat)
            b(1) = (  1.000000  0.000000  0.000000 )
            b(2) = (  0.000000  1.000000  0.000000 )
            b(3) = (  0.000000  0.000000  1.000000 )


  PseudoPot. # 1 for H  read from file:
  /qe-6.3/pseudo/H.pz-kjpaw_psl.1.0.0.UPF
  MD5 check sum: e55d7dbf3dbca295ac73bb1eaf3feab1
  Pseudo is Projector augmented-wave, Zval =  1.0
  Generated using "atomic" code by A. Dal Corso v.6.3MaX
  Shape of augmentation charge: PSQ
  Using radial grid of  929 points,  2 beta functions with:
             l(1) =   0
             l(2) =   0
  Q(r) pseudized with 0 coefficients


  atomic species   valence    mass     pseudopotential
     H              1.00     1.00000     H ( 1.00)

  48 Sym. Ops., with inversion, found



Cartesian axes

  site n.     atom                  positions (alat units)
      1           H   tau(   1) = (   0.5000000   0.5000000   0.5000000  )

  number of k points=     1  Marzari-Vanderbilt smearing, width (Ry)=  0.0500
                   cart. coord. in units 2pi/alat
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   2.0000000

  Dense  grid:    28257 G-vectors     FFT dimensions: (  40,  40,  40)

  Smooth grid:    20005 G-vectors     FFT dimensions: (  36,  36,  36)

  Estimated max dynamical RAM per process >       9.73 MB

  Estimated total dynamical RAM >      19.46 MB

  Initial potential from superposition of free atoms

  starting charge    0.99999, renormalised to    1.00000
  Starting wfcs are    1 atomic +    4 random wfcs
  Checking if some PAW data can be deallocated...

  total cpu time spent up to now is        1.5 secs

  Self-consistent Calculation

  iteration #  1     ecut=    50.00 Ry     beta= 0.20
  Davidson diagonalization with overlap
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     ethr =  1.00E-02,  avg # of iterations =  7.0

     Threshold (ethr) on eigenvalues was too large:
     Diagonalizing with lowered threshold

     Davidson diagonalization with overlap
     ethr =  6.20E-04,  avg # of iterations =  1.0

     total cpu time spent up to now is        1.7 secs

     total energy              =      -0.95451949 Ry
     Harris-Foulkes estimate   =      -0.95502351 Ry
     estimated scf accuracy    <       0.00619770 Ry

     iteration #  2     ecut=    50.00 Ry     beta= 0.20
     Davidson diagonalization with overlap
     ethr =  6.20E-04,  avg # of iterations =  1.0

     total cpu time spent up to now is        1.8 secs

     total energy              =      -0.95350766 Ry
     Harris-Foulkes estimate   =      -0.95453792 Ry
     estimated scf accuracy    <       0.00359518 Ry

     iteration #  3     ecut=    50.00 Ry     beta= 0.20
     Davidson diagonalization with overlap
     ethr =  3.60E-04,  avg # of iterations =  4.0

     total cpu time spent up to now is        1.8 secs

     total energy              =      -0.95374670 Ry
     Harris-Foulkes estimate   =      -0.95374109 Ry
     estimated scf accuracy    <       0.00001131 Ry

     iteration #  4     ecut=    50.00 Ry     beta= 0.20
     Davidson diagonalization with overlap
     ethr =  1.13E-06,  avg # of iterations =  2.0

     total cpu time spent up to now is        1.9 secs

     total energy              =      -0.95374254 Ry
     Harris-Foulkes estimate   =      -0.95375220 Ry
     estimated scf accuracy    <       0.00003781 Ry

     iteration #  5     ecut=    50.00 Ry     beta= 0.20
     Davidson diagonalization with overlap
     ethr =  1.13E-06,  avg # of iterations =  1.0

     total cpu time spent up to now is        1.9 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (  2517 PWs)   bands (ev):

    -7.0443   0.6863   5.7449   5.7449   5.7450

     the Fermi energy is    -6.9495 ev

!    total energy              =      -0.95374481 Ry
     Harris-Foulkes estimate   =      -0.95374481 Ry
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estimated scf accuracy    <       0.00000003 Ry

total all-electron energy =        -0.953742 Ry

The total energy is the sum of the following terms:

one-electron contribution =      -0.30707669 Ry
hartree contribution      =       0.16830084 Ry
xc contribution           =      -0.42020949 Ry
ewald contribution        =      -0.37830633 Ry
one-center paw contrib.   =      -0.00004399 Ry
smearing contrib. (-TS)   =      -0.01640914 Ry

convergence has been achieved in   5 iterations

Writing output data file H.save/

init_run     :      0.44s CPU      0.47s WALL (       1 calls)
electrons    :      0.41s CPU      0.46s WALL (       1 calls)

Called by init_run:
wfcinit      :      0.01s CPU      0.01s WALL (       1 calls)
potinit      :      0.06s CPU      0.08s WALL (       1 calls)
hinit0       :      0.13s CPU      0.14s WALL (       1 calls)

Called by electrons:
c_bands      :      0.18s CPU      0.20s WALL (       6 calls)
sum_band     :      0.09s CPU      0.09s WALL (       6 calls)
v_of_rho     :      0.08s CPU      0.09s WALL (       6 calls)
newd         :      0.01s CPU      0.02s WALL (       6 calls)
PAW_pot      :      0.00s CPU      0.00s WALL (       6 calls)
mix_rho      :      0.02s CPU      0.04s WALL (       6 calls)

Called by c_bands:
init_us_2    :      0.00s CPU      0.00s WALL (      13 calls)
cegterg      :      0.18s CPU      0.19s WALL (       6 calls)

Called by sum_band:
sum_band:bec :      0.00s CPU      0.00s WALL (       6 calls)
addusdens    :      0.01s CPU      0.01s WALL (       6 calls)

Called by *egterg:
h_psi        :      0.16s CPU      0.18s WALL (      23 calls)
s_psi        :      0.00s CPU      0.00s WALL (      23 calls)
g_psi        :      0.00s CPU      0.00s WALL (      16 calls)
cdiaghg      :      0.00s CPU      0.00s WALL (      21 calls)

Called by h_psi:
h_psi:pot    :      0.16s CPU      0.18s WALL (      23 calls)
h_psi:calbec :      0.00s CPU      0.00s WALL (      23 calls)
vloc_psi     :      0.16s CPU      0.18s WALL (      23 calls)
add_vuspsi   :      0.00s CPU      0.00s WALL (      23 calls)

General routines
calbec       :      0.00s CPU      0.00s WALL (      29 calls)
fft          :      0.07s CPU      0.06s WALL (      35 calls)
ffts         :      0.01s CPU      0.01s WALL (      12 calls)
fftw         :      0.17s CPU      0.19s WALL (     204 calls)
interpolate  :      0.02s CPU      0.02s WALL (       6 calls)
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     Parallel routines
     fft_scatt_xy :      0.01s CPU      0.02s WALL (     251 calls)
     fft_scatt_yz :      0.06s CPU      0.07s WALL (     251 calls)

     PWSCF        :     1.72s CPU         2.02s WALL


   This run was terminated on:  16:20:12  16Apr2019

=------------------------------------------------------------------------------=
   JOB DONE.
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