QUANTUMESPRESSO

How to run

Quantum Espresso Tutorial 2019

Quick start guide

Different subprograms

- Quantum Espresso consists of multiple subprograms including:
  - PW: Plane-wave self-consistent calculation. “pw.x”
  - CP: Molecular dynamics
  - NEB: Energy barrier and reaction pathway calculations
  - PP: Data postprocessing
  - …
- See official website for the detailed format of the input files for different subprograms
  - PW: https://www.quantum-espresso.org/Doc/INPUT_PW.html
- For now, just PW for example (pw.x)

Basic command

Serial computation

- pw.x < si.in > si.out

executable program (need full path)

input file

output file

Parallel computation

- mpirun –np 4 pw.x < si.in > si.out

Parallel computing command

number of CPU cores used

input file

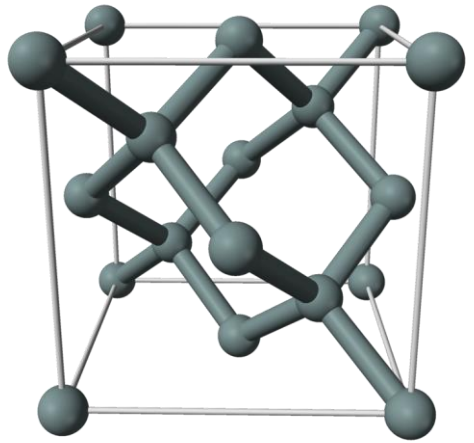
output file

Better way (e.g. Intel compiled version):

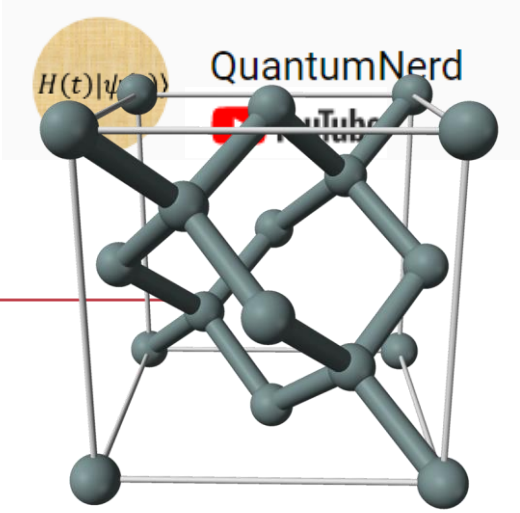
- pw.x -input si.in > si.out
- pw.x -inp si.in > si.out

Input file for pw.x

```
&control
    calculation = 'scf'
    prefix = 'si'
    pseudo_dir = '/home/anonymous/quantumEspresso_2019/q-e-qe-6.4.1_2_MPICH/pseudo'
/
&system
    ibrav=2, celldm(1) =10.20,
    nat=2, ntyp=1,
    ecutwfc=20.0
/
&electrons
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS (alat)
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 0 0 0
```



Input file for pw.x




```
&control
    calculation = 'scf'
    prefix = 'si'
    pseudo_dir = '/home/anonymous/quantumEspresso_2019/q-e-qe-6.4.1_2_MPICH/pseudo'
/
&system
    ibrav=2, celldm(1) =10.20,
    nat=2, ntyp=1,
    ecutwfc=20.0
/
&electrons
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS (alat)
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 0 0 0
```

Calculation type: ‘scf’, ‘nscf’, ‘bands’, ‘relax’, ‘vc-relax’, ‘md’, ‘vc-md’

how to name the temporary file

directory containing the pseudopotential file

- ibrav: Bravis-lattice index. 2 is fcc.
- celldm: lattic constants in Bohr (~0.5Å).
- nat: number of atoms in one unit cell. Must equal the number of atoms specified in the ATOMIC_POSITIONS card
- ntyp: number of types of atoms in one unit cell
- ecutwfc: kinetic energy cutoff (Ry). The larger, the more expensive, but more precise

Si	28.086	Si.pz-vbc.UPF
element	atomic mass	pseudopotential file

atomic positions. “alat” means relative to celldm

k points in reciprocal space. 6*6*6=216 points without offset

QUANTUMESPRESSO

Next

- Hands-on: run the example calculation in the last slide
- Next: project oriented tutorial on different systems
  - Molecules: structures, energy
  - Solids: band structure, density of state, structure
  - …

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