Quantum Espresso

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Installation

- Requirements: Unix-like environment (here we assume Ubuntu is installed) / fortran compiler (gfortran) / Openmpi for parallel computing (if you need)
- First, in terminal, type “sudo apt-get update” and “sudo apt-get install build-essential”
- gfortran: build-essential will install gcc, so you may already have gfortran compiler. Check its version: “gfortran --version”. If not, type “sudo apt-get install gfortran”

Installation

- Download Quantum-Espresso (QE) file (tar file; here we use 6.0 version)
- Untar the source file: “tar –xzvf qe-6.0.0.tar.gz”
- Go to the extracted folder: “cd qe-6.0.0”
- Now we will install QE. In this example, we just install a serial version.
- Configure: “./configure”
- Make: “make all”
- Now wait installation process.

Running an Example QE Simulation

- Executable files are located in “bin” folder
- We will use **PWscf (PW) package**: self-consistent calculation using Plane-Wave (PW) basis set and pseudopotentials (PP). In particular:
  1. ground-state energy and one-electron (Kohn-Sham) orbitals, atomic forces, stresses;
  2. structural optimization, also with variable cell;
  3. molecular dynamics on the Born-Oppenheimer surface, also with variable cell;
  4. macroscopic polarization (and orbital magnetization) via Berry Phases;
  5. various forms of finite electric fields, with a sawtooth potential or with the modern theory of polarization;
  6. Effective Screening Medium (ESM) method;
  7. self-consistent continuum solvation (SCCS) model, if patched with ENVIRON (http://www.quantum-environment.org/).
- PWscf works for both insulators and metals, in any crystal structure, for many exchange-correlation (XC) functionals (including spin polarization, DFT+U, meta-GGA, nonlocal and hybrid functionals), for norm-conserving (Hamann-Schluter-Chiang) PPs (NCPPs) in separable form or Ultrasoft (Vanderbilt) PPs (USPPs) or Projector Augmented Waves (PAW) method. Noncollinear magnetism and spin-orbit interactions are also implemented.

Running an Example QE Simulation

- Set the path for the executable file, pw.x, in your environmental file: “cd ~”, “gedit .bashrc”, and add a line (“export PATH=“/to/your/QE_bin folder/: $PATH”)
- In terminal, type: “source .bashrc”
- Make a folder for a case simulation in out of qe-6.0.0 folder: “cd ..” and “mkdir qe_trial”
- Move to that folder: “cd qe_trial”
- Locate an input file (in this class, we use “Cu.in”) to that folder
- Locate a pseudopotential file (we use “Cu.UPF”) to that folder
- Type command to run PW executable (“pw.x”) with these inputs: “pw.x –in Cu.in > Cu.out”
- Simulation results are contained in Cu.out file

Energy Vs. Lattice Parameter Curve

- Make a folder for a simulation and move to that folder: “mkdir qe_trial2” and “cd qe_trial2”
- Locate the input file (“Cu.in”) and a pseudopotential file (“Cu.UPF”) to that folder
- Locate a fortran file (“evfit.f”) and a shell file (“ev_curve”) to that folder
- Make “ev_curve” file to executable: “chmod +x ev_curve”
- Compile “evfit.f” file using gfortran: “gfortran –O2 evfit.f –o evfit”
- Change the name of input file (“Cu.in”) to “fcc.ev.in” which “evfit” can read
- Run “ev_curve” shell in this format (./ev_curve (structure) (lattice paramter)): “./ev_curve fcc 3.6”

Input of Quantum Espresso

- Full input guide can be found from the following: https://www.quantum-espresso.org/Doc/INPUT_CP.html