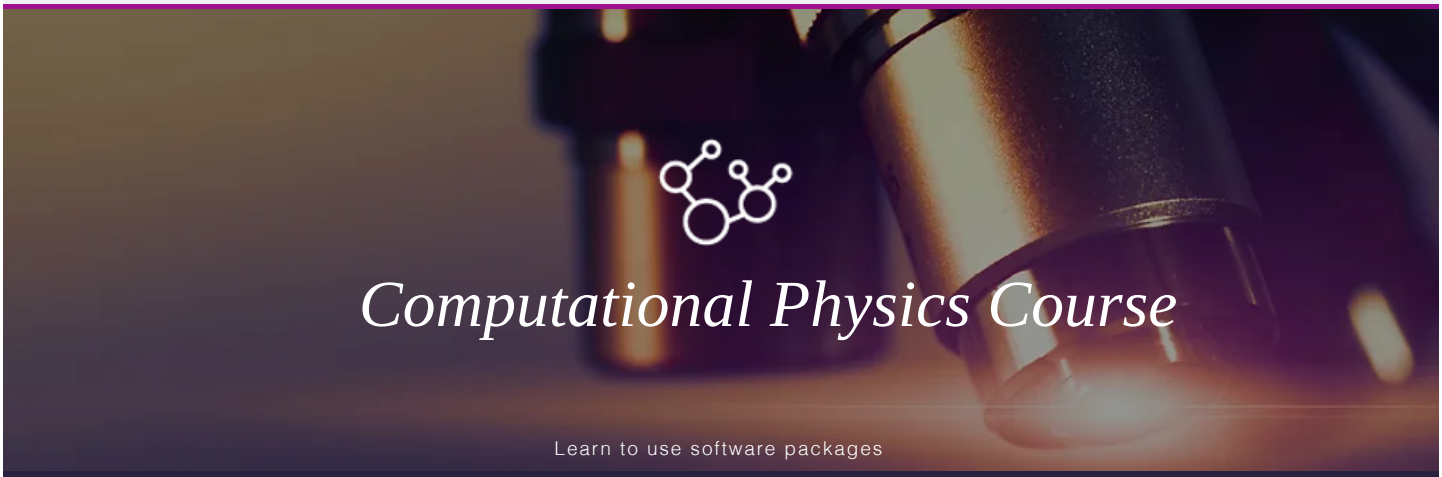

This is a copy of a QE homepage. You will find that you can do various calculations with QE.

The full Quantum ESPRESSO distribution contains the following core packages for the calculation of electronic-structure properties within Density-Functional Theory (DFT), using a Plane-Wave basis set and pseudopotentials:

- PWscf (PW) : Plane-Wave Self-Consistent Field,
- CP (CPV): Car-Parrinello Molecular Dynamics.

It also includes the following more specialized packages:

- PWneb (NEB) : energy barriers and reaction pathways through the Nudged Elastic Band method,
- PHonon : phonons with Density-Functional Perturbation Theory,
- PostProc (PP) : various utilities for data postprocessing,
- PWcond : ballistic conductance,
- GWL: GW calculations and solution of the Bethe-Salpeter Equation,
- XSPECTRA : K-edge X-ray adsorption spectra,
- TDDFPT : calculations of spectra using Time-Dependent Density-Functional Perturbation Theory,
- EPW : electron-phonon calculations using Wannier functions.

The following auxiliary codes are included as well:

- PWgui : a Graphical User Interface, producing input data files for PWscf,
- atomic : a program for atomic calculations and generation of pseudopotentials.

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

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