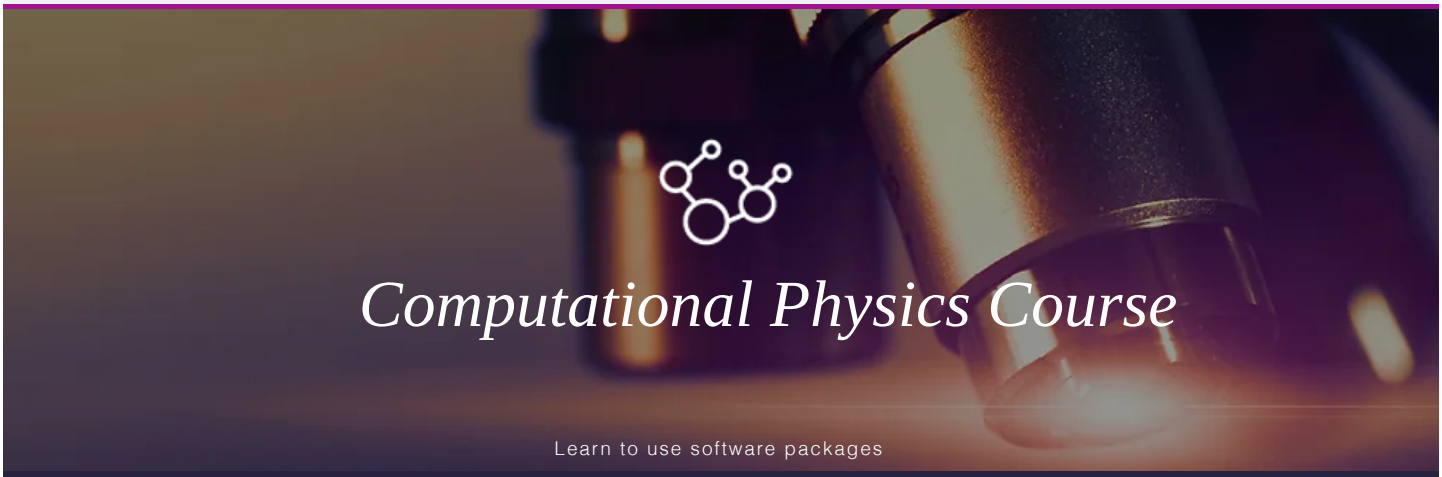

2. Day 1-3 (Electronic structure theory)

Electronic structure calculation

There are several different ways to access the electronic structures

1. Compute the wave function as a superposition of basis functions
2. Compute the wave function stochastically
3. Compute the Green's function
4. Compute the electron density and apply density functional theory

Historically, 1 is the oldest; it started in 1920s as Hartree-Fock theory. In 1960s, density functional theory (DFT) and the many-body Green's function theory started. The quantum Monte Carlo method has attracted attention as speed of computers increases. Now, DFT has become the most popular approach, while others are mostly used for high-precision calculation.

In the field of condensed matter physics, the software packages for the electronic structure calculation are most advanced . This is not only because the electronic structure is very important target itself but also because the inter-atomic interactions (or the atomic forces), essential for dynamics of atoms, can be derived from the electronic structure. Because of this, the electronic structure calculation is important for chemistry and materia science as well.

In this course, we will learn DFT using the package "Quantum Espresso".

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

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