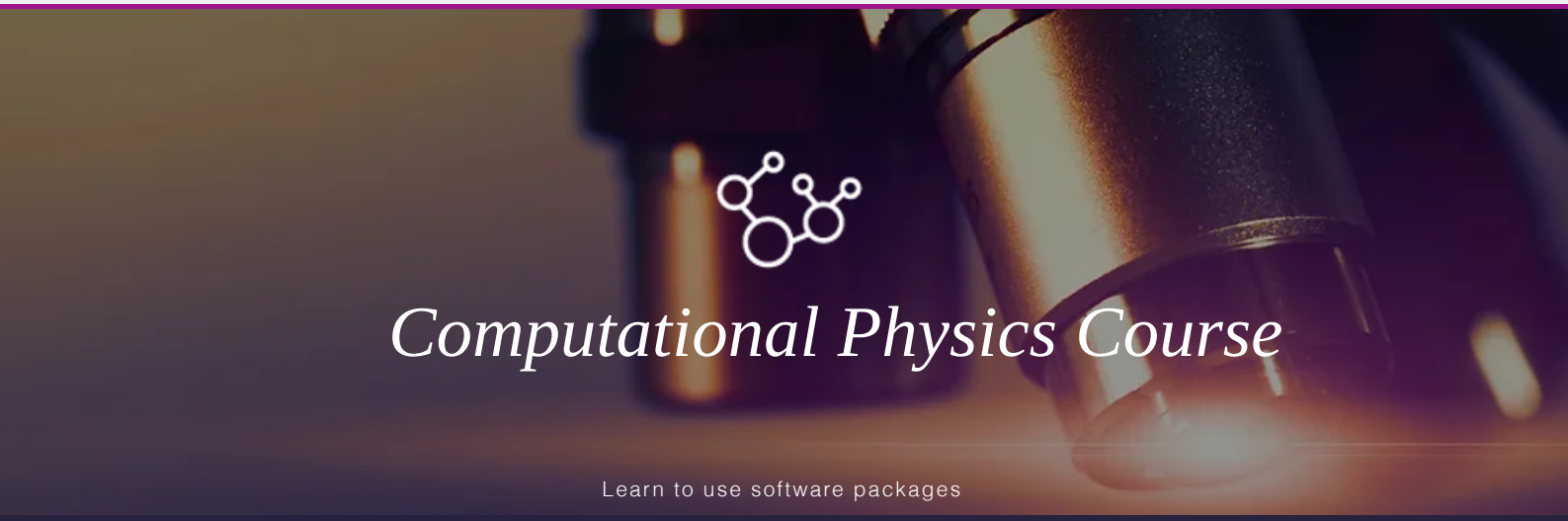

Computational Physics Course

Learn to use software packages

Electronic structure calculation

In the field of condensed matter physics, the software packages are most advanced for the electronic structure calculation. This is not only because the electronic structure is the most 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. Therefore, the electronic structure calculation is important for chemistry and material science as well.

There are several different ways to access to 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 with increasing speed of computers. Now, DFT has become the most popular approach, while others are mostly used for high-precision calculation.

In this course, we will learn DFT and the following packages.

DFT | Quantum Espressp | OpenMX | PIMD

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

The University of Tokyo