In this demonstration lecture of April 6, let me explain the Hartree-Fock theory and in addition installation of MateriApps to your PC.

MateriApps

Do you know MateriApps? To know that, please visit the site:

<https://ma.issp.u-tokyo.ac.jp/en/>

Here, many software packages for materials science are introduced. You may find those for condensed matter physics, those for molecular science and so on. By using them, you can rather easily go to the frontier of research. For simulation, it is important to learn with practice. For that purpose, let us make a computational environment.

On the page, you will find “new version MateriApps Live! 2.5”. This provides you with a linux environment where several important software packages are preinstalled. We have to learn linux because many of them are provided for linux.

If you go to

<https://ma.issp.u-tokyo.ac.jp/en/2414>

you will find updated software packages important for simulation and visualization of the simulation. If you further go to

<https://cmsi.github.io/MateriAppsLive/release.html>

you are at portal site of MateriApps Live!

Click “Setup” and see the installation slide. In the slide, USB memory is assumed to be provided but that is not necessary. Here we download from the site README, installer, and diskimage. You may take a while to finish downloading them because of the size of the files. In the meanwhile, please look at the page 7. You see that Quantum Expresso is preinstalled. If you have finished downloading, see the instruction to install the MateriApps Live!

If you have done, click the start menu to start System Tools / LXTerminal. If you type “pw.x” and send return key, you will find the program PWSCF to start. Then you have successfully installed MateriApps Live! Then send control-c to stop the program and end MateriApps! with start / logout / shutdown.