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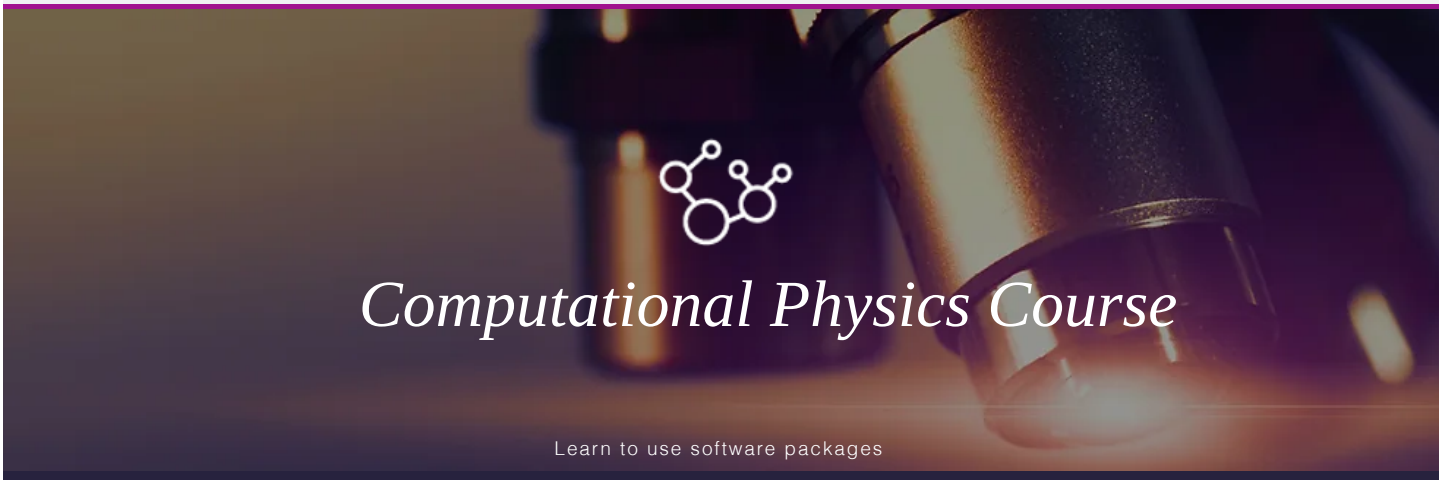
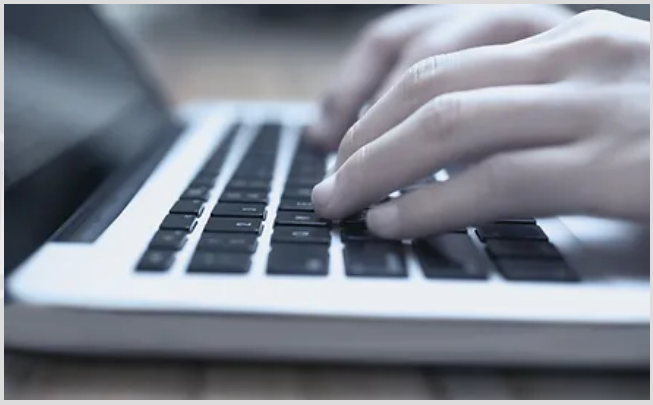


1. Day 1 (installation)

There are several ways to prepare your computational environment in your laptop PC.

1. Use Materiapps.
2. Use virtual machine (VMware or Virtual Box) and install LINUX (ubuntu), where packages are to be installed.
3. Use your own way.

In this course, I focus only on "ubuntu" installed on "VMware".



How to install VMware Workstat...

How to install Ubuntu 15 (using ...

Preparing ubuntu environment

1. Install VMware player (free) from http://www.vmware.com
2. Install ubuntu into VMware.
   - Download ubuntu from https://www.ubuntu.com/desktop
   - Use installer of VMware. Follow instruction appearing in a web site.

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Install Quantum Espresso

(a) First of all, install the following basic software by typing
$sudo apt-get install build-essential fftw3-dev gfortran

(b) Then, install software to be used for graphical analysis. Type the following command and follow the instruction thereby appearing.
$sudo apt-get install xcrysden
$sudo apt-get install gnuplot

(c) VMD is also a powerful graphical analysis tool. Download VMD from the site
http://www.ks.uiuc.edu/Research/vmd/
and follow the instruction for installation.

(d) OPENMPI: This software enables you to use all the CPU cores available in your PC. Download VMD from the site
https://www.open-mpi.org/
and download the most recent version.
Download openmpi
$ tar xvf openmpi-3.0.0.tar.gz
$ cd openmpi-3.0.0/
$ ./configure --prefix=/usr/local/openmpi-3.0.0
$ make install
Then openmpi is installed at the directory indicated by prefix. Next, add the following two lines to your ./bashrc file, which is located at your home directory.
PATH=$PATH:/usr/local/openmpi-3.0.0/bin
export PATH
When you open the terminal window next time, you can use openmpi. Make it sure by typing
$which mpirun

(e) LAPACK: Download package from
http://www.netlib.org/lapack/
Unpack the tgz file using the command
$tar -xzvf
Then you will see a newly constructed directory lapack-3.7.1
$cd lapack-3.7.1
$cp make.inc.example make.inc
$make blaslib
$make lapacklib
$make tmglib
$sudo cp librefblas.a /usr/local/lib/libblas.a
$sudo cp liblapack.a /usr/local/lib/liblapack.a
$sudo cp libtmglib.a /usr/local/lib/libtmg.a

(f) Quantum Espresso: Download from the site
http://www.quantum-espresso.org/
and then
$tar -xzvf qe-6.1.tar.gz
$cd qe-6.1
$./configure --enable-parallel=no --enable-openmp=yes
$make all
$cd ~
Next, add the line
export PATH=$PATH:/home/username/qe-6.1/bin/
at the end of .bashrc located at the home. You can use it next time when you open terminal window.

(g) Wannier90: Download wannier90 from the site
http://www.wannier.org/
$tar -xzvf wannier90-2.1.0.tar.gz
$cp ./config/make.inc.gfort ./make.inc
$make
add the line to your .bashrc
export PATH=$PATH:/home/username/qe-6.1/bin/

Now you have installed the minimal environment.

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

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