

# How to install/compile

Quantum Espresso Tutorial 2019

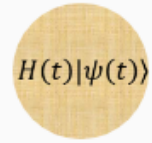
Quick start guide



QUANTUM ESPRESSO

# Be prepared...

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- Compilation/installation is perhaps the most painful/annoying part of using Quantum Espresso in Linux
  - Be patient
    - Consult official documentation, search on google, or just try around
    - Start clean
- Why so difficult?
  - Requires different compiler
  - Parallel computing library
  - Depend on the specific case of each machine
- However, the compilation highly influences the speed of the code!

# Necessary besides the code

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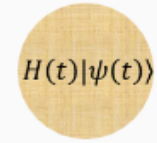
- Two possibilities: serial (easy to compile) or parallel version (efficient)
- Three things needed for the installation:
  - Compiler: GNU or Intel compiler
    - C compiler: gcc or icc
    - Fortran compiler: gfortran or ifort
  - Math library: internal or Intel MKL (for Intel CPUs. For AMD CPUs it is ACML)
    - BLAS and LAPACK
    - FFTW
  - Parallel computing library (not needed if compiling a serial version)
    - openmp or MPI
    - In case of MPI: MPICH or Intel MPI



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# General guideline

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- Serial compilation: easiest to compile but inefficient when running. Only use as test/nothing else works.
- Parallel compilation better, but potential conflicts with other libraries
- Vendor specific libraries much more efficient at run-time than GNU ones, but generally more problematic during compilation
  - Intel compilers better than GNU compilers
  - Intel MKL better than internal math libraries
  - Intel MPI around the same as MPICH, but openmpi is worse and also difficult to handle



QUANTUM ESPRESSO

# General steps

- Compilation

- Download q-e-qe-6.4.1.tar.gz from official website
- tar -zxvf q-e-qe-6.4.1.tar.gz
  - A directory of "q-e-qe-6.4.1/" will be created
- cd q-e-qe-6.4.1/
- ./configure
- (Tune the parameters of compilation by either passing arguments during ./configure or modifying the file make.inc directly)
- make pw (or make all)

- Test and benchmark

- cd test-suite/ (under q-e-qe-6.4.1/ folder)
- make run-tests-pw-serial (or make run-tests-serial)
- make run-tests-pw-parallel (or make run-tests-parallel)
  - How much time needed to run a certain test



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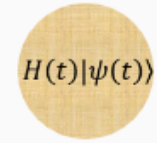
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## Next

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- Hands-on: install/compile quantum espresso on Linux
  - Default/Serial with GNU
  - Parallel with GNU
  - With Intel
  - ...
- Basic examples

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