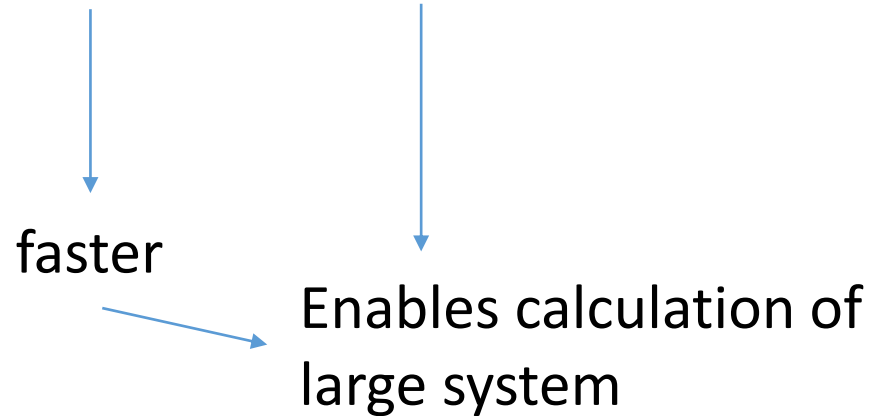


System requirements

Quantum Espresso Tutorial 2019

Quick start guide

- Any laptop/desktop will work
 - Both Intel and AMD
- Server/Cluster/supercomputer
 - Much more CPU cores and RAM



Operating system

- Can run on: Linux, Mac-OS X, Windows
- Linux (e.g. Ubuntu)
 - Designed to be used and mostly used in
 - *This tutorial is based on QE in Linux*
 - Pros: full control and features, parallel computation well supported
 - Cons: need to get used to Linux
- Windows
 - CMD
 - Virtual machine (e.g. Quantum Mobile virtual machine)
 - GUI: Burai (free), Amsterdam Modeling Suite (commercial)

Windows or Linux?

- If just curious/very small calculation
 - Windows, GUI (Burai, free)
- If your target system is larger/want to get the best out of your computer
 - Linux
- If very serious calculation/large system
 - Server/cluster -> Linux

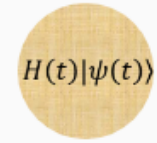


Important for performance

- the compilation highly influences the speed of the code!
- Compiler
- Math library
- Parallel computing library



Next



QuantumNerd



- Installation and compilation of QE
- Hands-on:
 - How to install Ubuntu
 - Basic commands in Linux

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