
The Comsuite VM and the Hands-on Sessions

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1. Purpose of this School

The Purpose of this School is to teach you how to use Comsuite to calculate strongly correlated systems. Also you will need to learn how to install Comsuite. The best way for you to learn how to do this is by experience; by really doing it.

- We supply the Comsuite Virtual Machine to provide a soft start. It allows you to:
 - Run Comsuite even when you have not yet learned to install it.
 - Experiment with materials that are interesting to you.
 - Compile Comsuite for a first time in an environment (the VM) where everything about compilation is already understood and no troubleshooting is required.
- The Hands-On Sessions are designed to give you a dedicated time and space with:
 - A VM easing your learning process.
 - Tutorials guiding you through many calculations using Comsuite.
 - The Comsuite team will be present, ready for discussion and troubleshooting.
 - We will also encourage and support you as you install on other computers besides the VM.

2. What is a Virtual Machine?

A Virtual Machine is a second computer which runs on your host computer (your PC or laptop).

- The VM and Comsuite do not know they are being hosted; they don't know anything about the host.
- The VM and Comsuite do not have interaction with the host; there is a wall keeping the two apart. (There is a way of sharing a directory with the host, but this is turned off at the start.)
- The VM and Comsuite do consume resources: memory, CPU, disk space, Internet.
- A Virtual Machine is:
 - Memory, CPU, disk space, Internet.
 - The operating system, which we have installed for you. [Ubuntu 18.04.5 LTS]
 - All of the configuration which we have done on the Virtual Machine, including installing compilers and libraries.
 - The Comsuite software.
 - Many other ab initio software packages, because the Comsuite VM is based on the Quantum Mobile VM.

3. How to Set Up the Virtual Machine

- Make sure there is 30+ Gigabytes of free disk space on your computer.
 - Know how much RAM and how many CPUs your computer has. Of that, how much do you want to allow the VM to use? Some should be left over for the host.
 - Download and Install and Start VirtualBox from <https://www.virtualbox.org/wiki/Downloads>
 - Download the Comsuite Virtual Machine from dropbox or google drive:
 - <https://www.dropbox.com/s/417n7uv6xx88o1q/Comsuite.Virtual.Machine.2021.ova?dl=0>
 - <https://drive.google.com/file/d/19JazSHiiL3gEcsBZWfrOHw3DKgOzpSqY/view?usp=sharing>
 - In VirtualMachine, use “Import Appliance” to install the Virtual Machine on your computer.
 - Configure CPU and memory usage options.
 - Start the Virtual Machine! Comsuite is in the codes directory. (Compiled and Uncompiled versions.)
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- More details are in the “Getting.Started.With.Comsuite.Virtual.Machine” document.
 - We will help with any problems via the Slack channel.
 - More troubleshooting docs at <https://quantum-mobile.readthedocs.io/en/latest/users/faq.html> and <https://quantum-mobile.readthedocs.io/en/latest/users/troubleshoot.html> .
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4. What is in Comsuite?

- **flapmbpt** - extended systems (crystals), using techniques suitable for systems without strong correlations: dft, hartree-fock, hybrids, self-consistent GW, qsGW, and vertex corrections.
- **ctqmc** - dmft solver for the single-site impurity problem.
- **cygutz** - uses the gutzwiller approximation to solve the single-site impurity problem
- **comsuite** - python code tying together rspflapw and ctqmc . Also includes utilities for choosing wannier functions, for calculating the hubbard interaction U from first principles using cRPA, and for calculating the double-counting correction from first principles.
- **comrisb** - python code tying together rspflapw and cygutz

5. Our support for your use of comsuite

6. Why Use Comsuite?
