Software for the HKUST IAS Asian Winter School in Quantum Chemistry (7-11 Dec 2015)

Students are advised to have the software installed and ready for use **before the practice sessions**.

Please note: usage of the programs requires basic knowledge of Linux. Additional prerequisites are indicated in the respective sections.

1. Quantum chemistry (Chan)

Prerequisite: basic familiarity with Python.

We will use PySCF, a free software package available from:
http://chemists.princeton.edu/chan/software/pyscf/

Alternatively, you can pull directly from the git repository at:
https://github.com/sunqm/pyscf

Documentation can be found at:
http://sunqm.github.io/pyscf/

Some examples of inputs that we will run through can be found at:
https://github.com/sunqm/pyscf/tree/1.0/examples

Optional DMRG calculations will be performed using the BLOCK package. This is available through:
http://chemists.princeton.edu/chan/software/block-code-for-dmrg/

or optionally, can be pulled directly from the git repository at:
https://github.com/gkc1000/block

2. Green function calculations (Jiang)

We will use Abinit, available from:
http://www.abinit.org/

Some examples of inputs that we will use can be found at:
http://www.abinit.org/doc/helpfiles/for-v7.10/tutorial/lesson_gw1.html

3. Quantum Monte Carlo calculations (Wagner)

We will use Qwalk, available from:
http://qwalk.github.io/mainline/

Inputs will be provided so that users will not have to run their own quantum chemistry calculations for the QMC wavefunction input. However, if you would like to generate your own inputs, you may wish to install a compatible quantum chemistry software package (e.g. GAMESS)

4. Matrix Product State tutorial (Nakatani)

Prerequisite: familiarity with C++ programming.

This tutorial will focus on the basic implementation of matrix product state algorithms in C++, with a view to users developing their own ability to implement DMRG like algorithms.