# Compiling

In its current state, the project is uncompiled. .cpp files prefixed with an underscore indicate that they are to be compiled into executables.

There are four main executable files, one for each section of the report:

* \_QB1.cpp Calculates results for a hydrogen-like lithium atom
* \_QB2.cpp Models an atom with greens function electron screening
* \_QB3.cpp Uses the Hartree iterative method
* \_QB4.cpp Uses the Hartree-Fock iterative method

As well as three additional files for testing other features:

* \_SingleHydrogen.cpp  
  A test file for solving the bare nucleus orbitals for any Z and l. Useful for validating results against hydrogen by using and
* \_QB3-fast.cpp   
  An alternative to \_QB3.cpp that uses an alternate implementation of the Hartree method that scales better with
* \_QB4-fast.cpp   
  An alternative to \_QB3.cpp that uses an alternate implementation of the Hartree-Fock method that scales better with

These files must be compiled alongside their dependencies:

* matrix.cpp A matrix class used in linear algebra systems
* LP\_solvers.cpp Functions for using LAPACK
* vector\_utils.cpp Utility functions and overloads for vectors
* spline\_eval.cpp Wrapper functions for bsplines.hpp
* potentials\_and\_solvers.cpp Atomic potentials & solvers (e.g. Hartree)

And must be compiled with the flags -llapack -lblas to allow the use of the Fortran LAPACK libraries in LP\_solvers.cpp, and the -O3 flag.

e.g., to compile \_QB1.cpp:

g++ \_QB1 \_QB1.cpp matrix.cpp LP\_solvers.cpp vector\_utils.cpp spline\_eval.cpp Potentials\_and\_Solvers.cpp -llapack -lblas -O3

All of these files can be compiled automatically by using the shell script “\_compile.sh”, and will compile to executables of the same name (including the underscore prefix).

# Running / Inputs

All compiled executables are set to take arguments from command line. Arguments must be given in order, and will defer to default values if not provided. E.g.

\_QB1 120 20001

Will run \_QB1 with and , and will use default values for and the output mode / folder. The “\_run.sh” shell script will run the main files (\_QB[1-4]) with the parameters used to generate the values in the report. Outputs will only save if the specified directory exists.

**\_QB1 and \_QB2**

|  |  |  |  |
| --- | --- | --- | --- |
| **Input** | **Type** | **Default** | **Desc** |
|  | Int | 60 | Number of modes to solve / splines to model with |
|  | Int | 5001 | Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration |
|  | Double | 0.001 | Minimum modelling radius |
|  | Double | 100 | Maximum modelling radius |
| Output | Bool | False | Whether or not to save results that are too big to save to the screen |
| Output Folder | String | ./outputs/B[i]/ | Folder to output results to if output=true |

**\_QB3, \_QB4 and Alternatives**

|  |  |  |  |
| --- | --- | --- | --- |
| **Input** | **Type** | **Default** | **Desc** |
|  | Int | 60 | Number of modes to solve / splines to model with |
|  | Int | 5001 | Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration |
|  | Double | 0.001 | Minimum modelling radius |
|  | Double | 100 | Maximum modelling radius |
| maxits | Int | 40 | Maximum number of iterations in Hartree and Hartree-Fock |
| Tol | double | 1E-6 | Energy change tolerance for |
| Ens\_to\_check | Int | 5 | Number of energy levels to check for convergence in iterative procedures |
| Output | Bool | False | Whether or not to save results that are too big to save to the screen |
| Output Folder | String | ./outputs/B[i]/ | Folder to output results to if output=true |

**\_SingleHydrogen**

|  |  |  |  |
| --- | --- | --- | --- |
| **Input** | **Type** | **Default** | **Desc** |
| Z | Int | 1 | Atomic number of hydrogen-like atom |
| L | int | 0 | ‘l’ number of orbital to model |
|  | Int | 60 | Number of modes to solve / splines to model with |
|  | Int | 1001 | Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration |
|  | Double | 0.001 | Minimum modelling radius |
|  | Double | 200 | Maximum modelling radius |
| Output | Bool | False | Whether or not to save results that are too big to save to the screen |
| Output Folder | String | ./outputs/single/ | Folder to output results to if output=true |

# Plotting

To generate the plots in the report, pythons scripts have been added to the pre-made output folders. Activating these should save the relevant plots to the folder.