Gollum2 Quick Start

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The aim of this document is to provide step by step help to run Gollum for a very simple example, one-dimensional chain shown in figure 1.

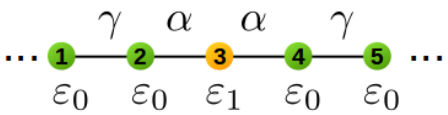

Figure 1. One-dimensional chain with two leads (1,2 and 4,5) and scattering region (3).

1- Download the relevant Matlab MCR as explained in the section 4 of Gollum manual and install it.

2- Create a test folder called “Test”.

3- Copy the “input” and “Extended_Molecule” files from the “Quick Start/input files” folder into the “Test” folder.

4- Copy the Gollum executable from the gollum.X folder (X = linux, windows or mac) into the “Test” folder:

- In Windows, copy “gollum.exe” from gollum.windows folder to the “Test” folder.
- In Linux, copy “run_gollum.sh” and “gollum” from gollum.linux folder to the “Test” folder.
- In Mac, copy “run_gollum.sh” and “Gollum.app” from gollum.mac folder to the “Test” folder.

Note that you may need to change the permission of the files to make them executable in Linux or Mac as follows:

Open a terminal, go to the “Test” directory and type “chmod 700 run_gollum.sh gollum”.

5- To run Gollum:
- In Windows, double click on the “gollum.exe” file.
- In Linux or Mac, Open a terminal, go to the “Test” directory and type “./run_gollum.sh path_to_mcr”

Instead of “path_to_mcr” type your MCR installation folder path e.g. /usr/local/MATLAB/R2017a/

6- Gollum should run and when it finishes the output will be written in the “Test” folder in a series of files with “.gdat” extensions such as:

- Open_channels_per_spin1.gdat
- Open_channels_per_spin2.gdat
- T_per_spin1.gdat
- T_per_spin2.gdat

Note that 1 and 2 in the end of the files refer to the lead number.
- The open channels are written for each lead X. The first column is the energy range and the second column is the number of the open channels in lead X.
- The transmission coefficient are also written for each lead X. The first column is the energy range. The second column is the transmission from lead X to the 1st lead ($T_{X,1}$). The third column is the transmission from lead X to the 2nd lead ($T_{X,2}$) and so on.

6- You need a plotting software to plot the outputs. Examples include gnuplot, gromacs, qtplot, xmgrace, Origin or Matlab.

7- Plot the number of open channels. They should look like as follows:

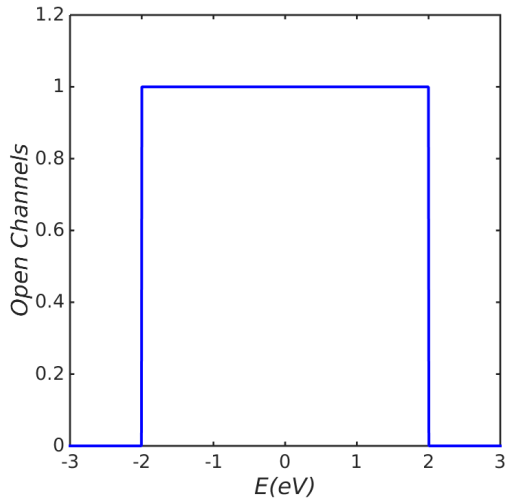

Figure 2. Number of open conduction channels for one-dimensional leads.

8- Plot the transmission coefficient. Here you have T_{11}, T_{12} from file "T_per_spin1.gdat" and T_{21}, T_{22} from file "T_per_spin1.gdat". Note that T_{11} (T_{22}) is in fact the reflection from lead 1 (2) to lead 1 (2). They should look like as follows:

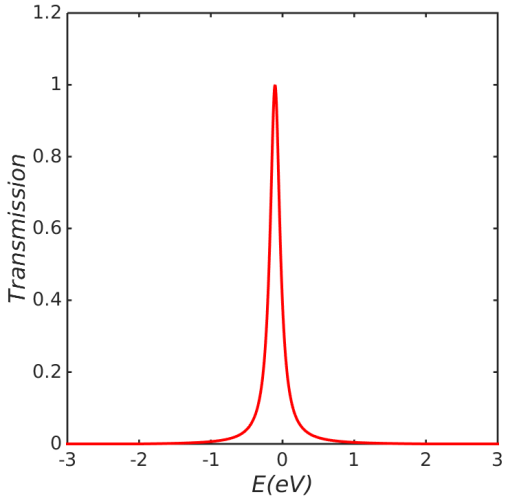

Figure 3. Transmission coefficient for electrons with energy E pathing from the first lead to the second through scattering region shown in figure 1.

9- This example is a chain of 5 atoms with an impurity in site 3 (see fig. 1). The on-site energies are $\varepsilon_0 = 0$, and the nearest neighbour coupling is $\gamma = -1$ in the leads. The on-site energy of the impurity is $\varepsilon_1 = -0.1$ and it couples to the left and the right leads with couplings $\alpha = -0.2$.

Now let's modify the Hamiltonian of the system by changing the impurity on-site energy to $\varepsilon_1 = -0.3$. To do this, open the "Extended_Molecule" file and change -0.1 in line 27 to the -0.3. Run Gollum for this new Hamiltonian and plot the transmission coefficient.

Note that a complete explanation of the format of the "Extended_Molecule" file can be found in section 9.2 of the manual.

Gollum needs an input file where the parameters, leads and scattering region atoms are defined. A complete explanation of the format of the "input" file can be found in section 5.1 and 8 of the manual.

This is a very simple tight-binding calculation. In Gollum you may use the leads Hamiltonian from the "Extended_Molecule" file or from a separate file called Lead_X, where X = 1,2,… is the lead number. A complete explanation of the format of the "Lead_X" file can be found in section 10 of the manual.

Gollum can compute transport properties of either user-defined systems described by a tight-binding Hamiltonian such as explained above, or more material-specific properties of systems composed of real atoms described by DFT Hamiltonians as explained in section 6 of the manual.