MATLAB Tutorial on Chemical Kinetics Simulation

Introduction

There are four types of molecules in this simulation, namely A, B, C and D. Every time a pair of A and B molecules collide, they may react to form a pair of C and D molecules. A pair of C and D molecules may in turn decompose back into a pair of A and B molecules. The reaction system can be represented as follows:

$$A + B \underset{k_b}{\overset{k_f}{\rightleftarrows}} C + D$$

The double arrows indicate that both the forward and reverse reactions are possible. The probabilities of reaction per collision are called the **reaction rate constants**, which are abbreviated k_f and k_b for the forward and reverse reactions respectively.

Thus, the number of possible combinations by which the forward reaction can occur is given by

$$r_f = k_f x_A x_B$$

Similarly, for the backward reaction,

$$r_b = k_b x_C x_D$$

Here, x_A, x_B, x_C and x_D are the number of A, B, C and D molecules respectively. Note that this is similar to the expression for the rate expression in the deterministic model. The total number of combinations by which reactions can take place is given by

$$r_{total} = r_f + r_b$$

Now, we define $f = \frac{r_f}{r_{total}}$ and generate a random number p_1 from the interval (0,1).

If $0 < p_1 \leq f$, we choose the forward reaction to take place at that particular time step. Otherwise, we choose the reverse reaction to take place at that particular time step.

To update the time, we generate another random number p_2 from the interval (0,1), and define

$$\delta t = \frac{\ln\left(\frac{1}{p_2}\right)}{r_{total}}$$

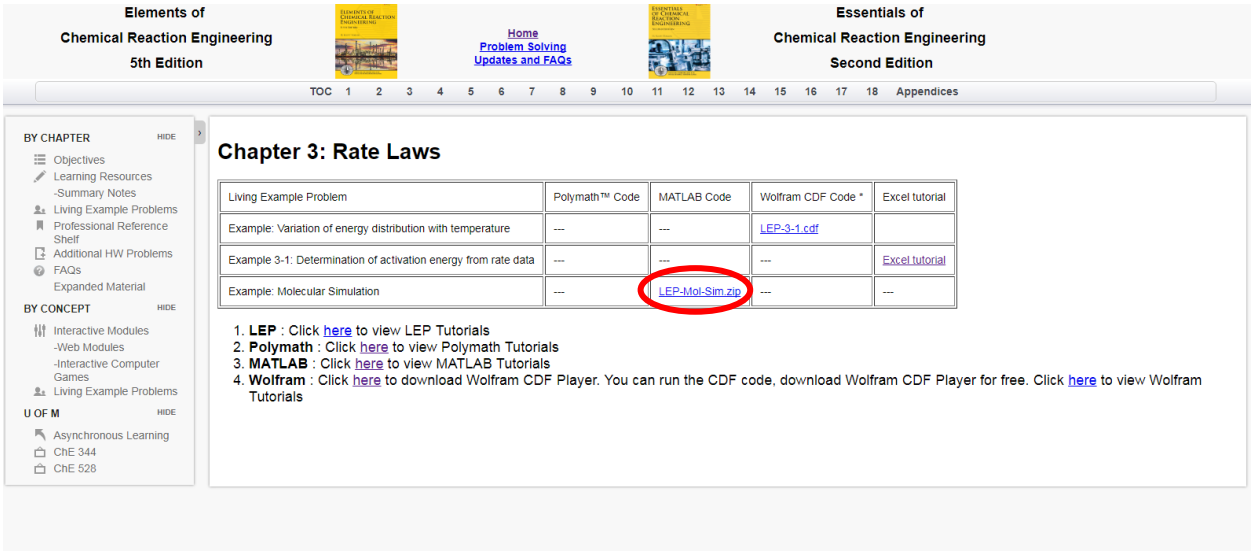
Now, we update the time step as

$$t_{j+1} = t_j + \delta t$$

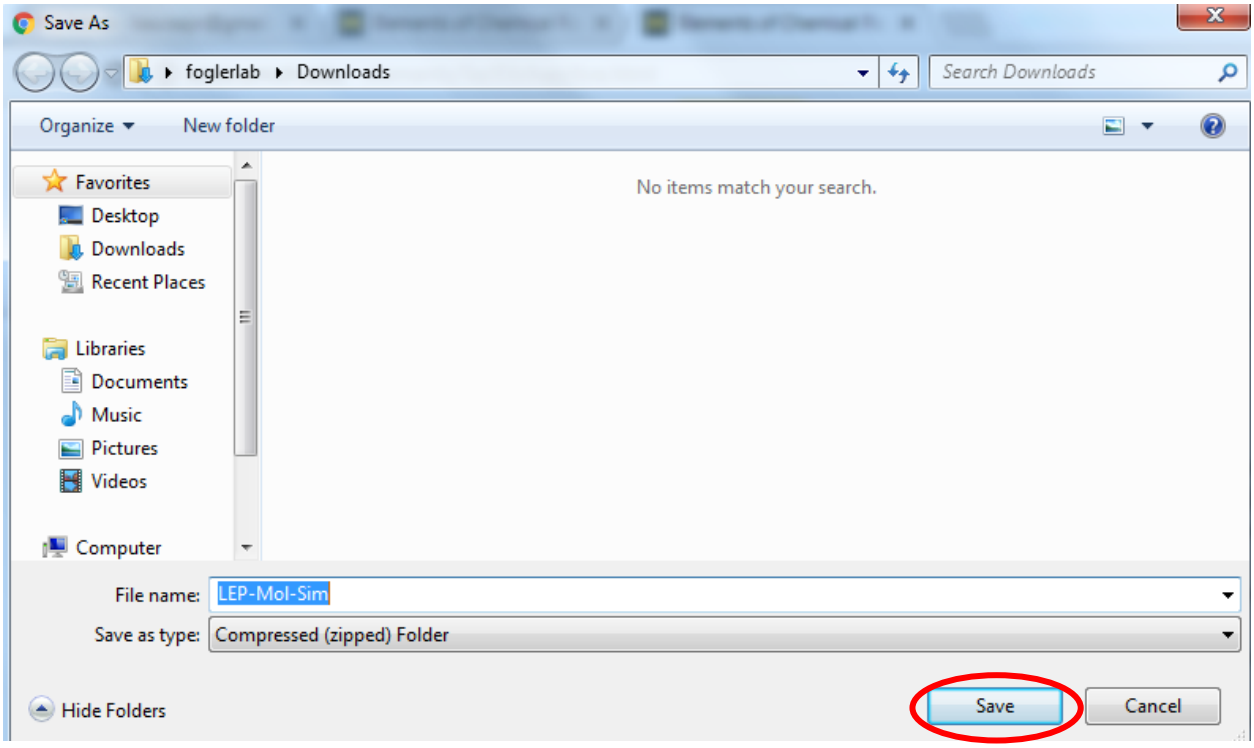
Tutorial

Step 1: Accessing and downloading the file

a) Open Chapter 3 on the CRE Web Site and go to "Living Example Problems"
b) Click on LEP-Mol-Sim.zip

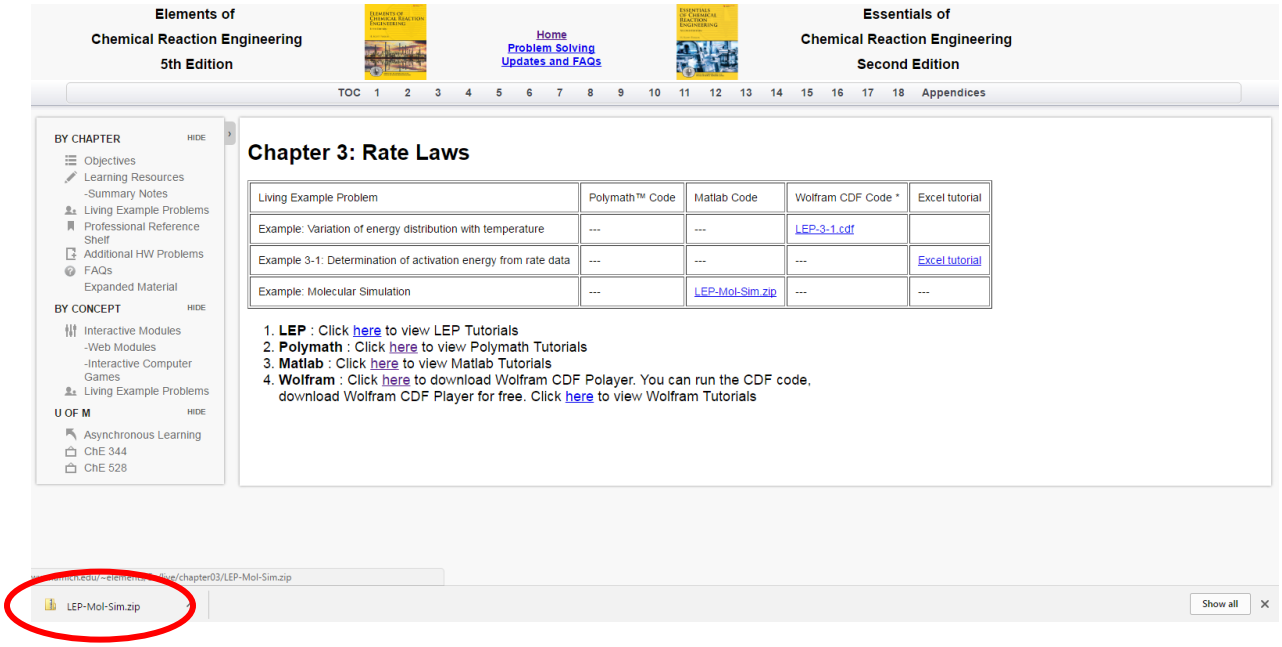


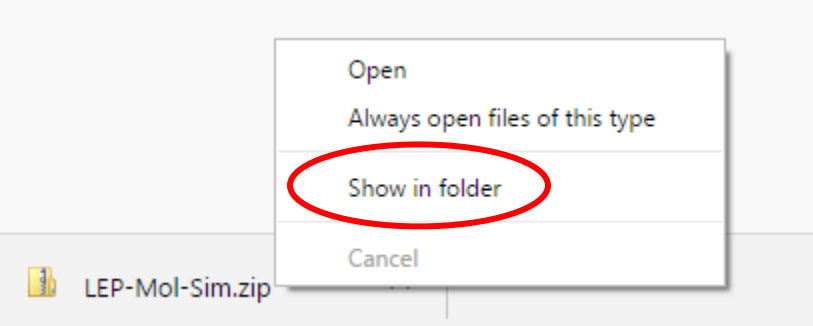
Troubleshooting: On clicking the file, if the following window pops up, click on "Save"



c) You should have the file downloaded at the bottom of your browser window.

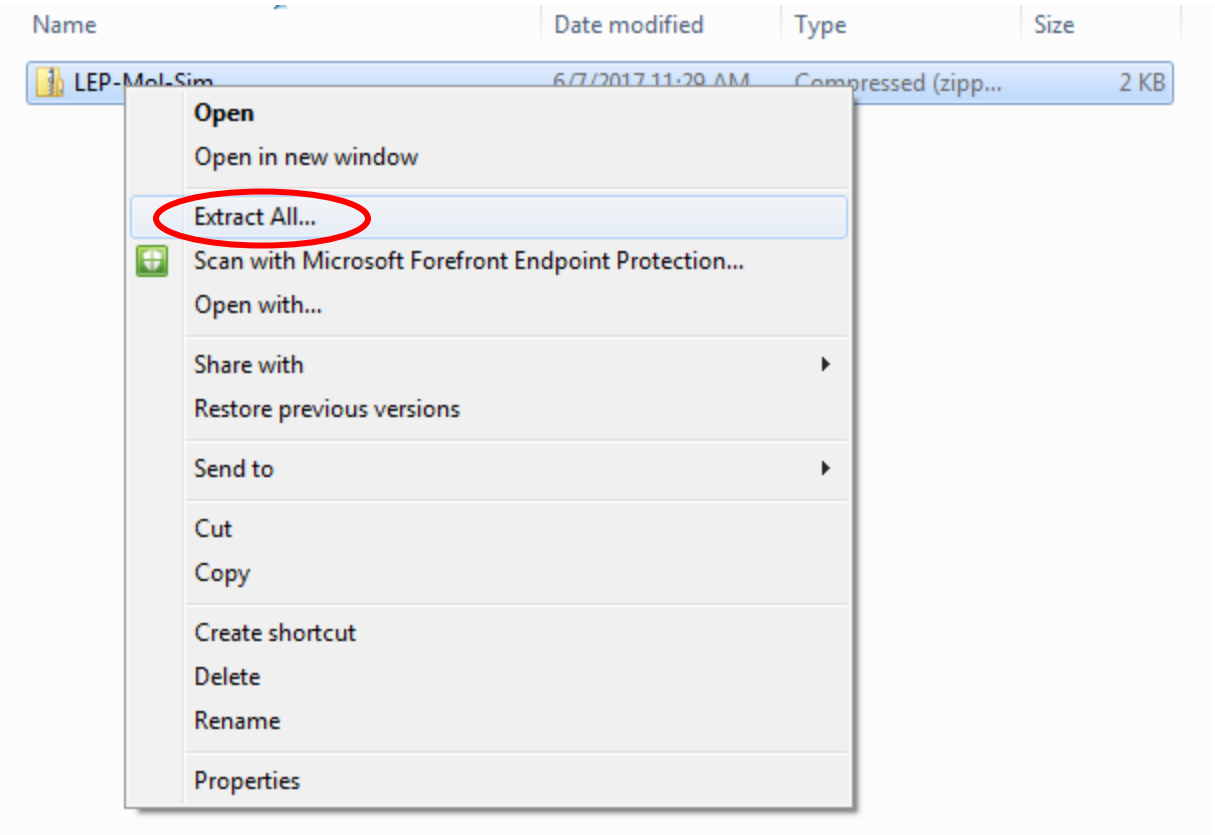
d) Right click on the downloaded file and click “Show in Folder“. This will show the folder location where your zip file is downloaded



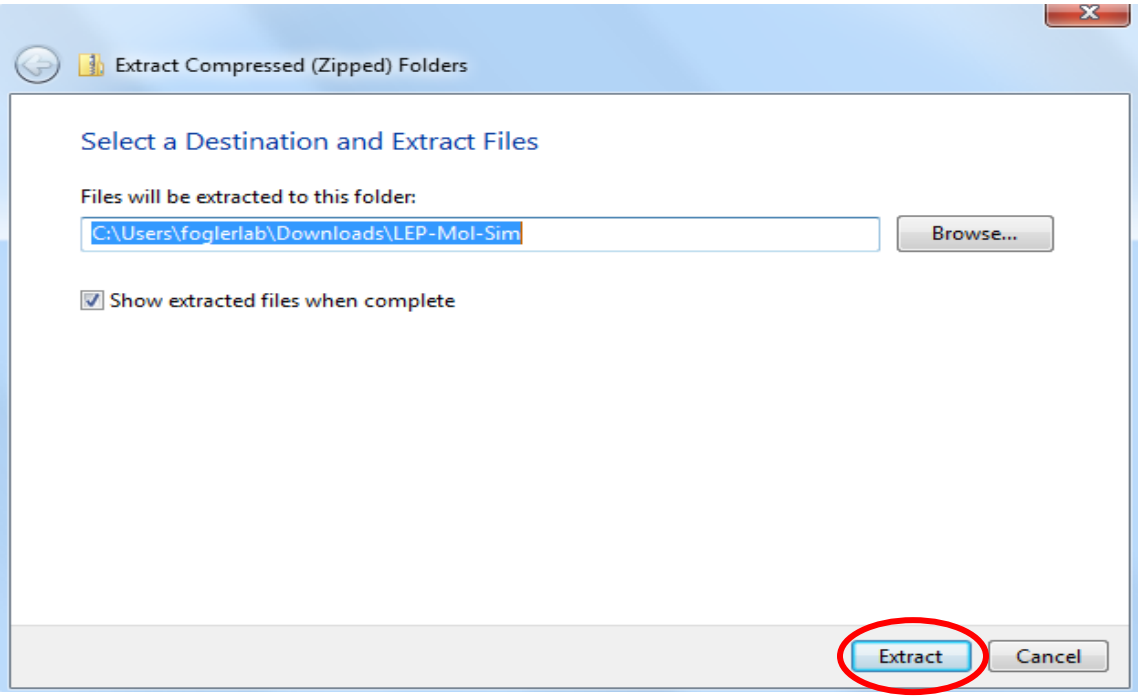


Step 2: Extracting the contents of the file

The following folder will appear. Right click on the zip folder “LEP-Mol-Sim” and select “Extract All…”. This will extract the files from zip folder.

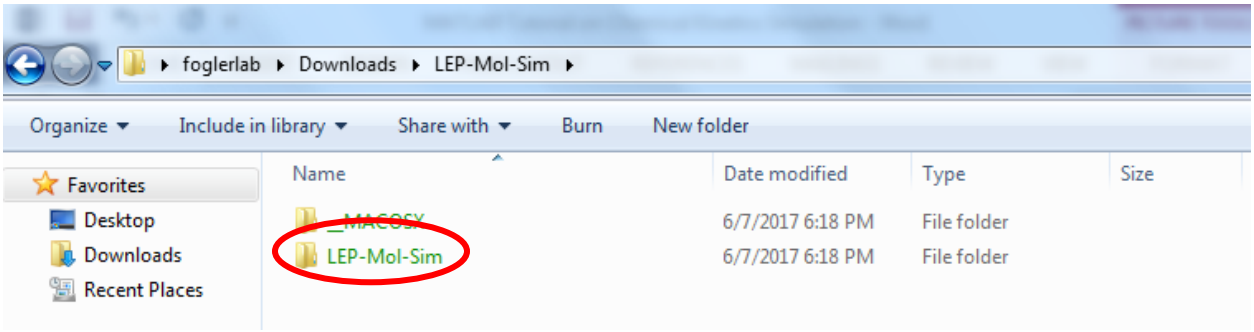


A new window will open up where you can select the location you want the files to be extracted. By default, it will extract the contents to the same directory in which your zip file resides. Just click **Extract**

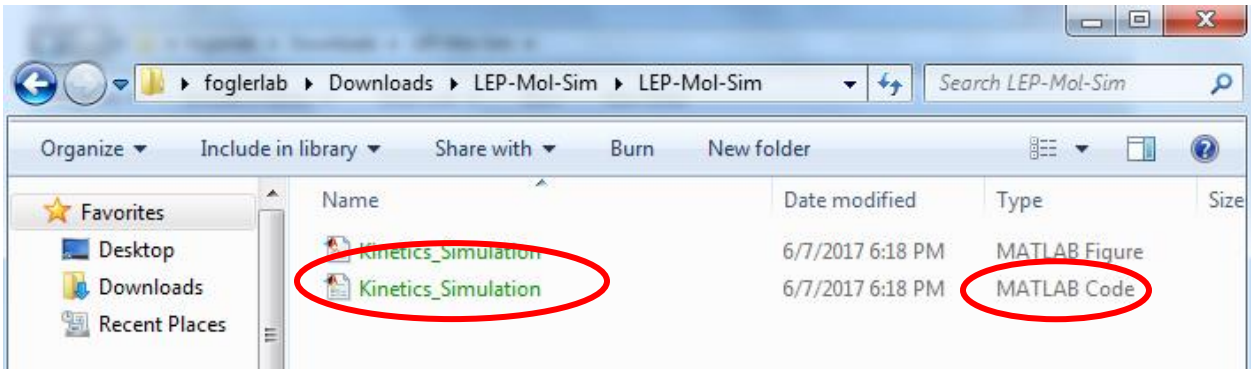


Step 3: Opening the MATLAB file

The following window opens. You will find that it contains two folders. Open the folder “LEP-Mol-Sim”.

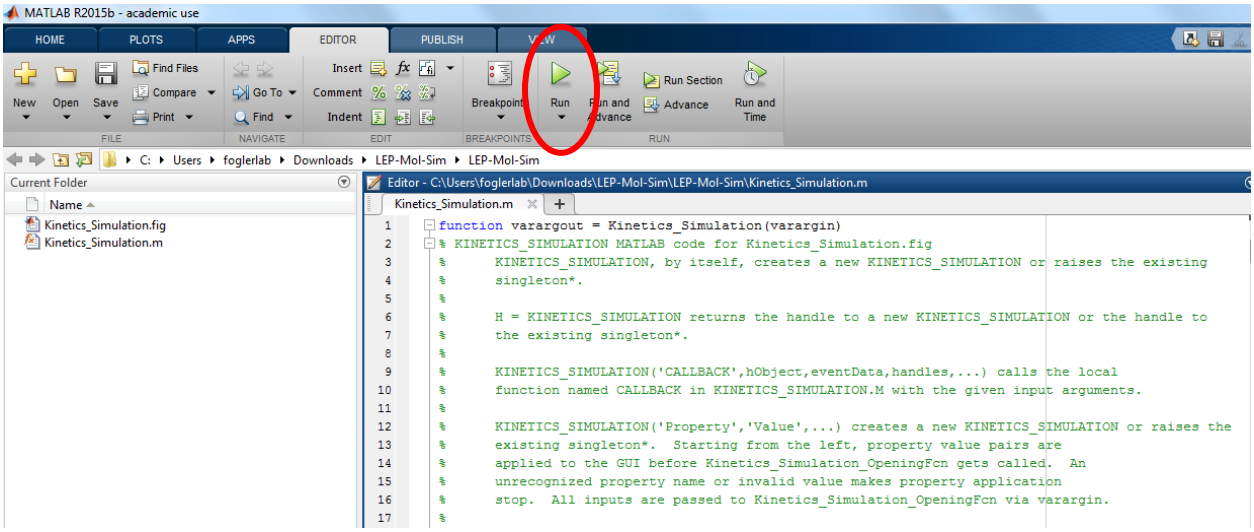


You will find that it contains two files with the same name (“Kinetics_Simulation”). Open the file which is of type “MATLAB Code”.

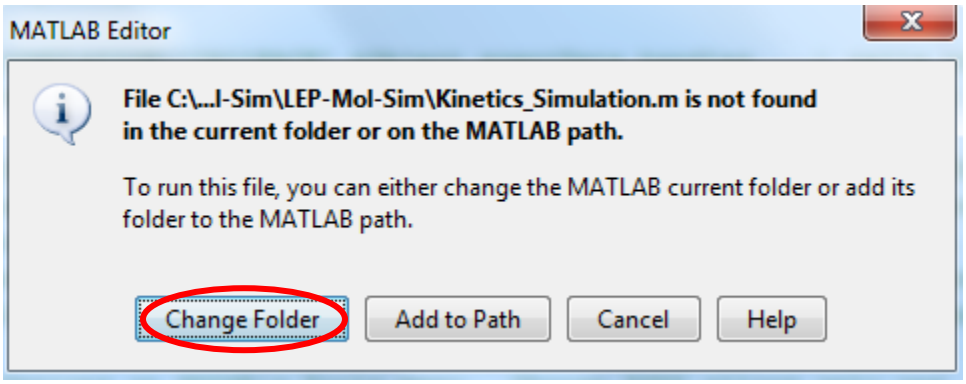


Step 4: Running the MATLAB file

You should see that the following window appears. To run the file, click on the Run button present on the menu bar

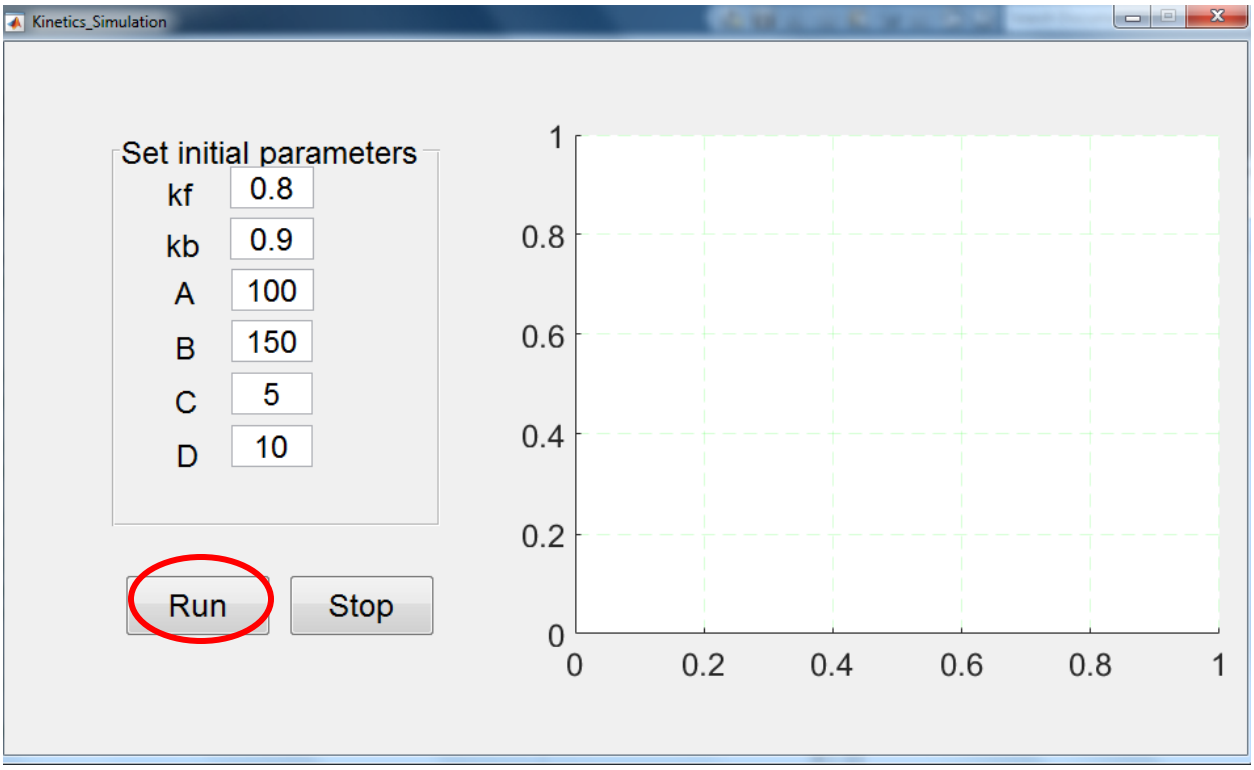


Troubleshooting: While running the script, if the following pop-up is generated, then select "Change Folder".



Step 5: Entering the input parameters

Once you run the code, you will see that the following window appears. Enter the values of the rate constants, and the initial number of molecules of A, B, C and D in the space provided. Once you are done, click on "Run".



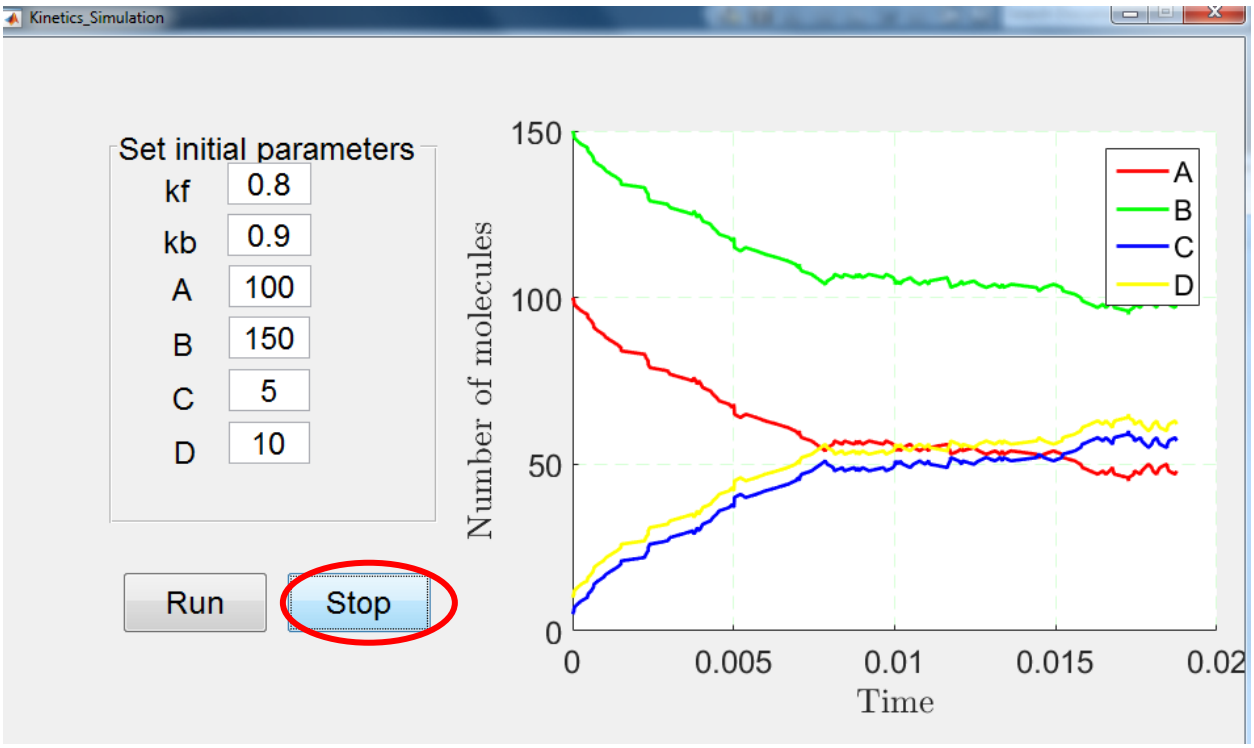
You will see that a graph is generated, similar to the one shown below. Please note that this is a dynamic graph and the simulation is being done in real time.

Step 6: Observing the trajectories

Observe the trajectories and wait for the system to attain equilibrium, i.e., when the concentrations of all the species are constant on average. There will however be momentary fluctuations in the concentrations.

Step 7: Stopping the simulation

Now, to stop the simulation, press the “Stop” button.



Step 8: Change the parameters

If you want to change any parameter values to analyze its effect on profile, all you need to do is to change the parameters in the spaces provided, and click on “Run”. Repeat Steps 5 to 7 to observe the change in trajectories for different values of the input parameters.