MOOSE GUI

How to use the Graphical User Interface for MOOSE
Version 1.3

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This manual is for MOOSE (version 1.3), The Multiscale Object-Oriented Simulation Environment.

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Executive Summary

It contains an overview of how to use the PyMOOSE/PyQT GUI for MOOSE.

1 Getting Started

The script to start the GUI for MOOSE is moosegui.py. Depending on where it is installed, you can enter the following in a command prompt:

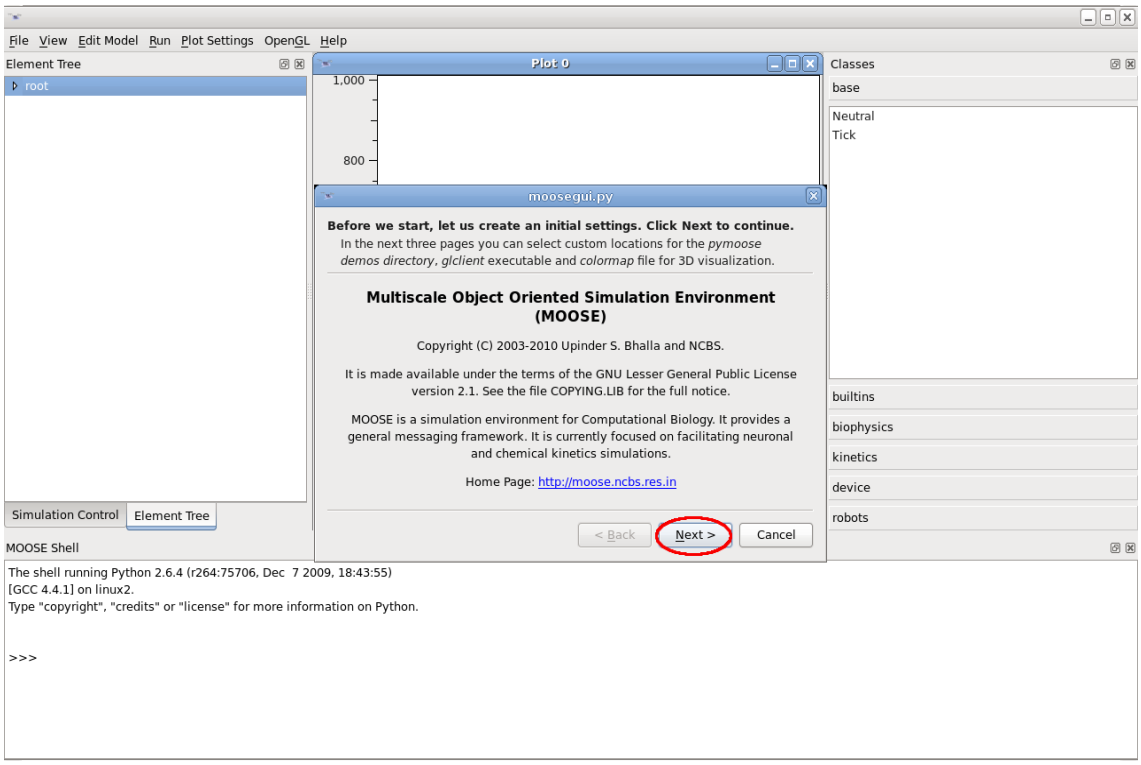
python {full path of moosegui.py}

If you install it from a binary package, it should already be in your path and have execute permission set. In that case just entering

moosegui.py

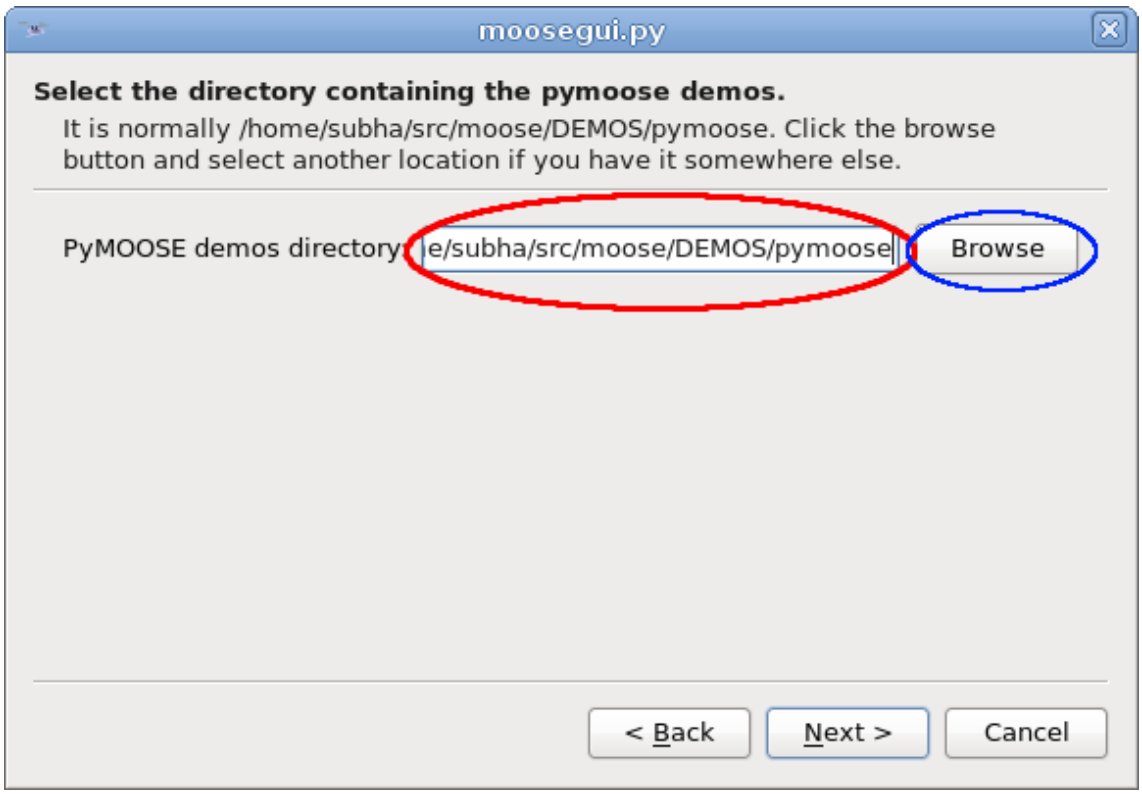
should fire up the GUI.

If you are running it for the first time, a graphical wizard will appear to confirm some details. It has three pages. Verify if the details in these pages are correct. Other wise select the appropriate values. The initial page contains general information about MOOSE and the wizard itself.



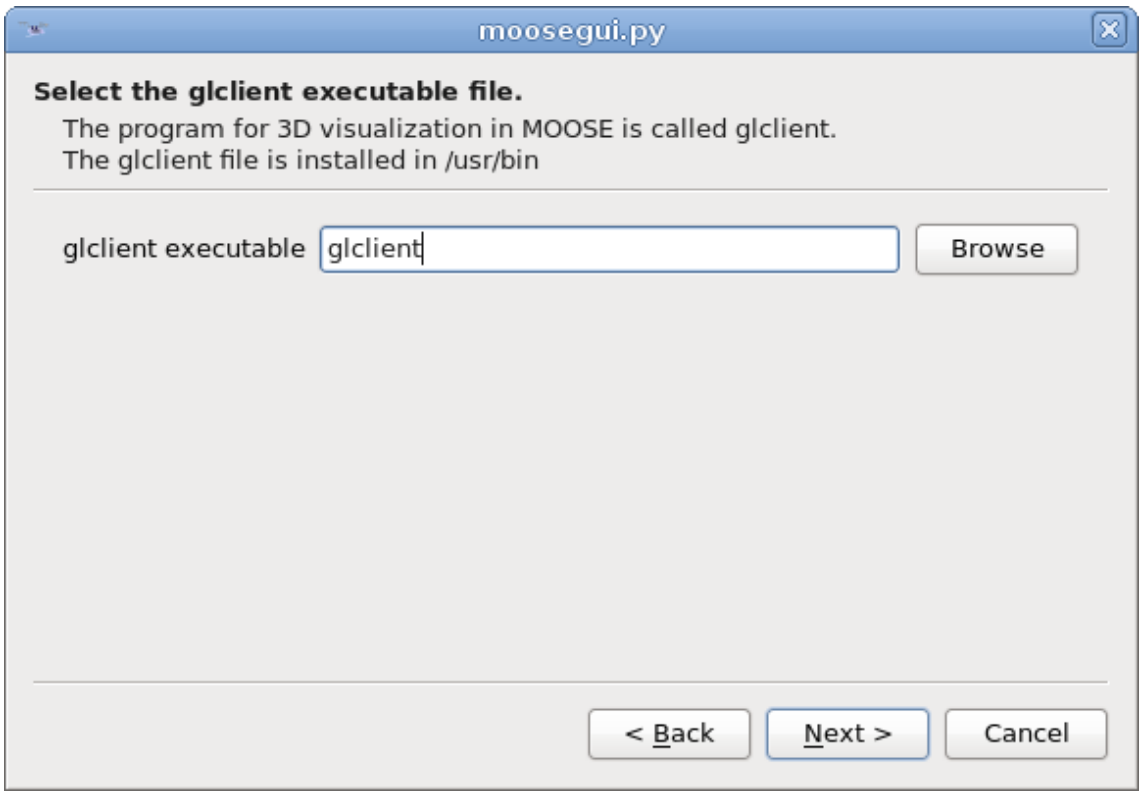
Click *next* and you will be prompted to select the directory containing the PyMOOSE demos. On Linux systems, these are installed in `usr/share/doc/moose1.3/DEMOS/pymoose`. Verify that the contents of the text box labeled ``PyMOOSE demos directory''(encircled in red) has the correct location of the PyMOOSE demos. Otherwise, click the `Browse` button

(encircled in blue) next to it and browse to the appropriate directory and click `Open` button on the pop-up dialog.



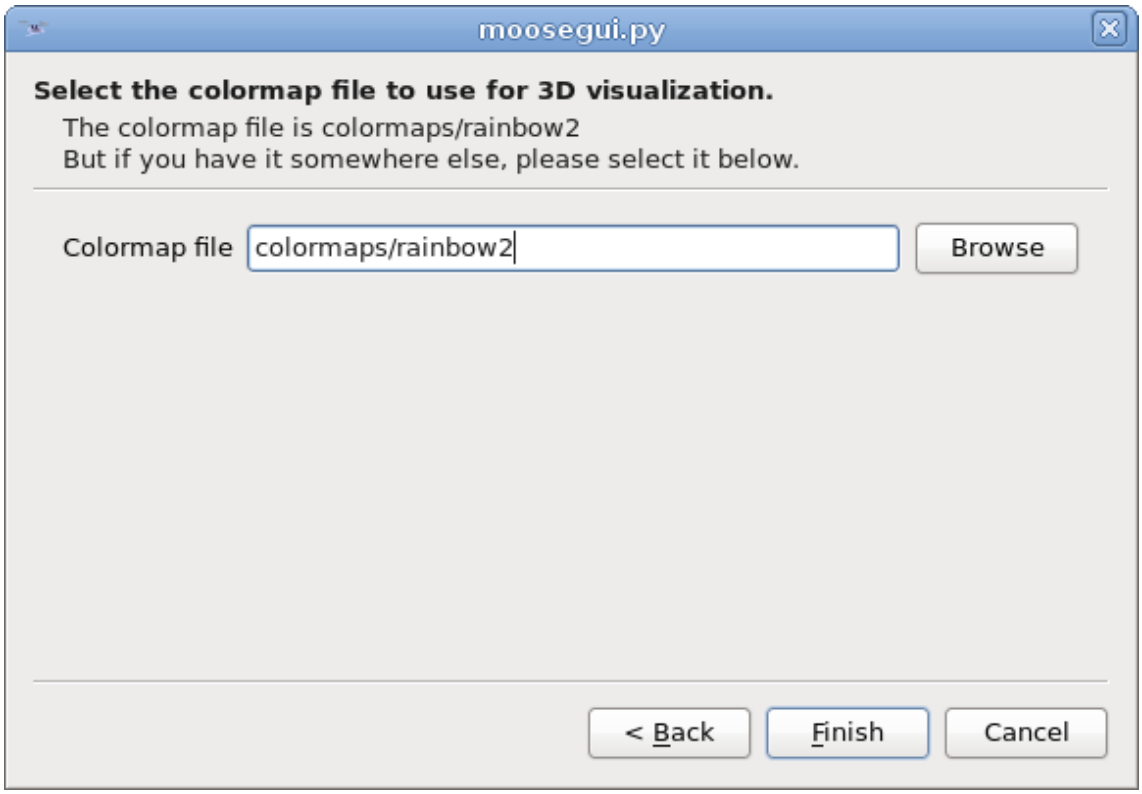
Clicking *next* will take you to the next page to select the `glclient` executable. If this is installed in some location in your `${PATH}` (which is the case for installation from binary packages), then just glclient in the textbox will do. Otherwise, you will have to browse and

select the executable file. If you compiled MOOSE from source with the `USE_GL=1` option to `make`, it will be located in `{moose-source}/gl/src/glclient`.



After clicking next you will reach the final page in the wizard. Here you specify a colormap file for OpenGL-based 3D visualization. Select any of the files in the `colormaps`

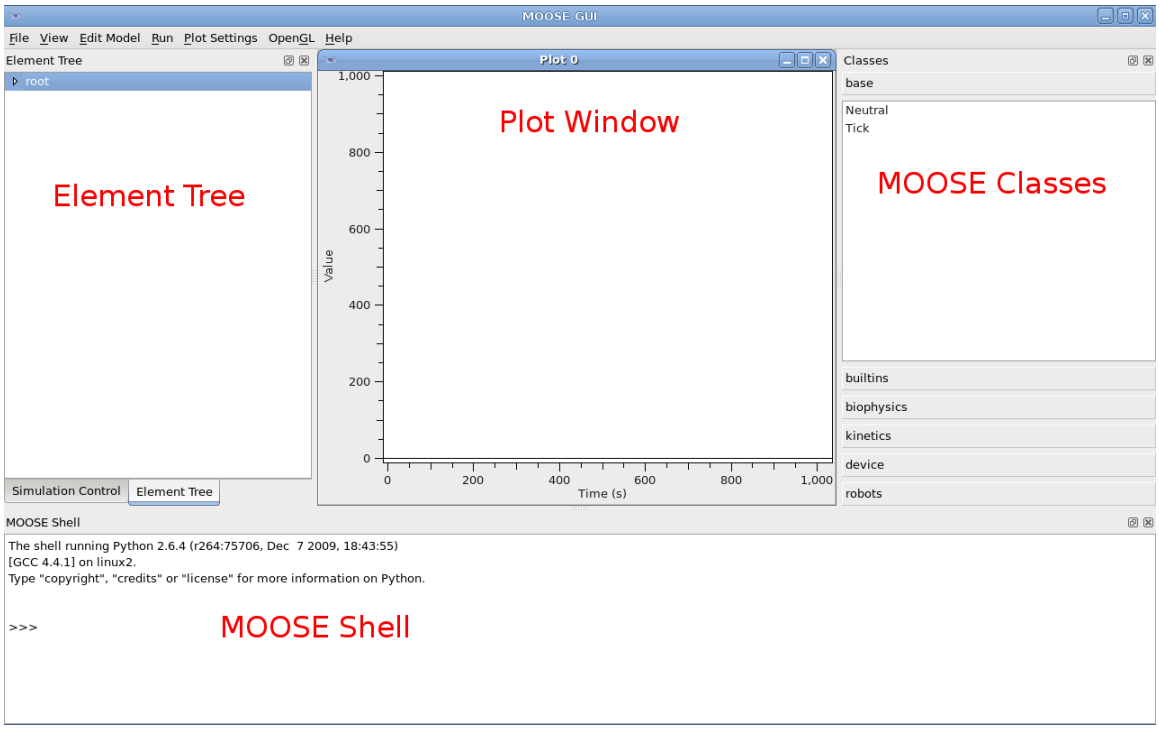
directory (which is `/usr/share/moose1.3/colormaps/` for binary packages and `{moose-source}/gl/colormaps` when compiled from source) and click `Finish`.



2 Overview of the GUI window

Once you are finished with the `First-time Wizard`, you will be working with the *moosegui*. Even if you cancel the wizard the first time, you can go back to it and change the settings. It can be accessed from the `File->First time wizard` menu.

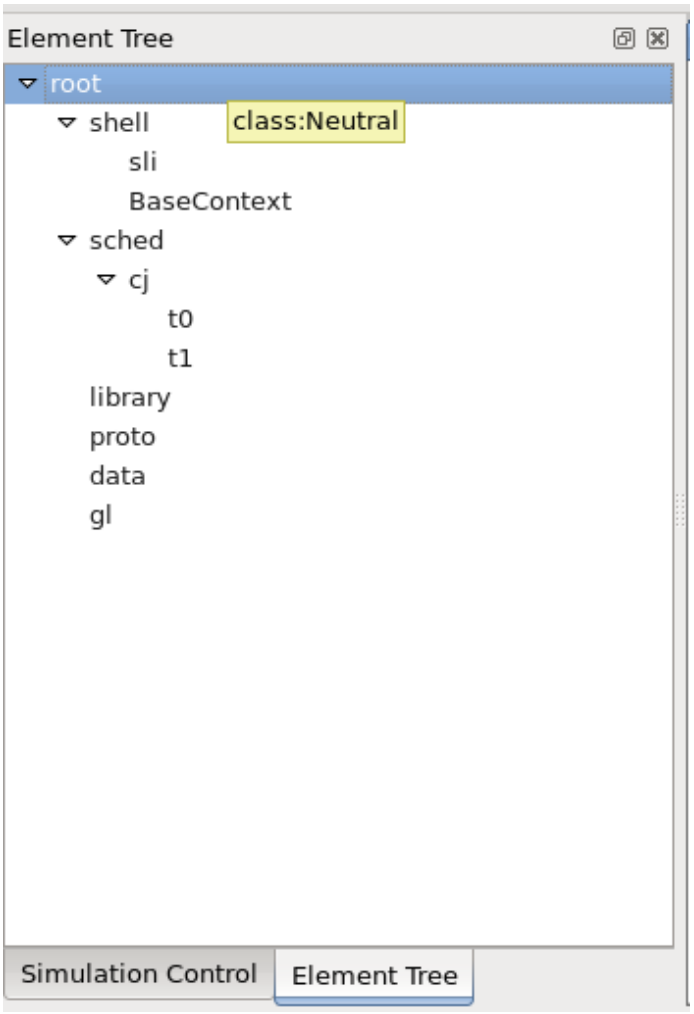
We discuss the different parts of this window below.



Element Tree

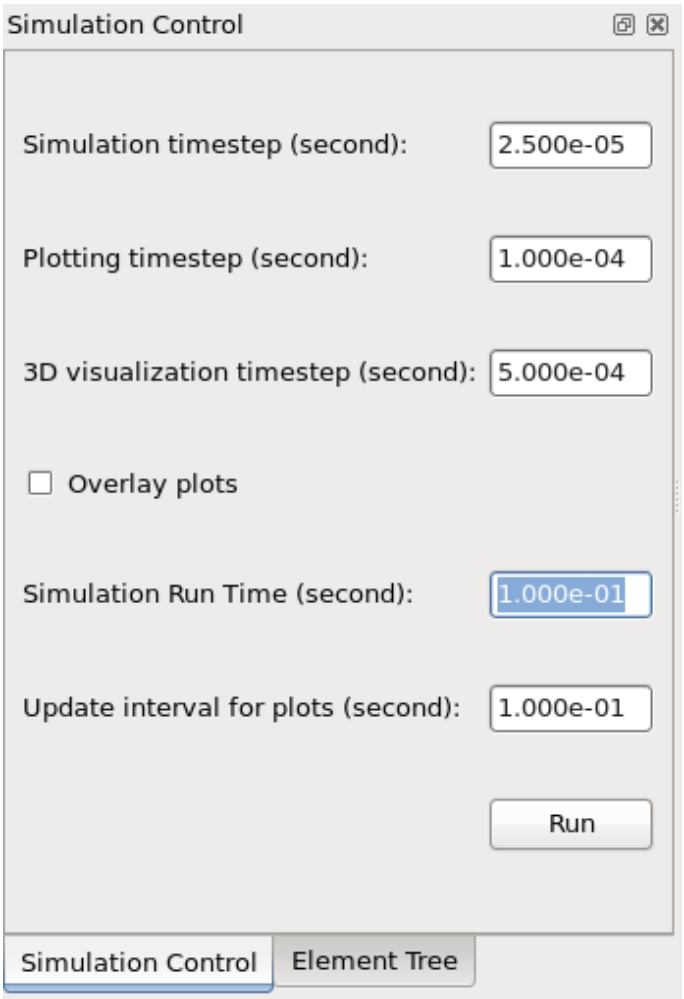
The left-most dock area of the moosegui contains two tabs. The one titled `Element Tree` contains the complete tree structure of the MOOSE elements. The elements(objects) in MOOSE models are part of a tree structure similar to the folder structure in your PC.

You can click the little arrows to the left of the tree items to expand the tree. When fully expanded, the element tree looks like this:



Simulation Control

This is the other tab in the left-most dock window.



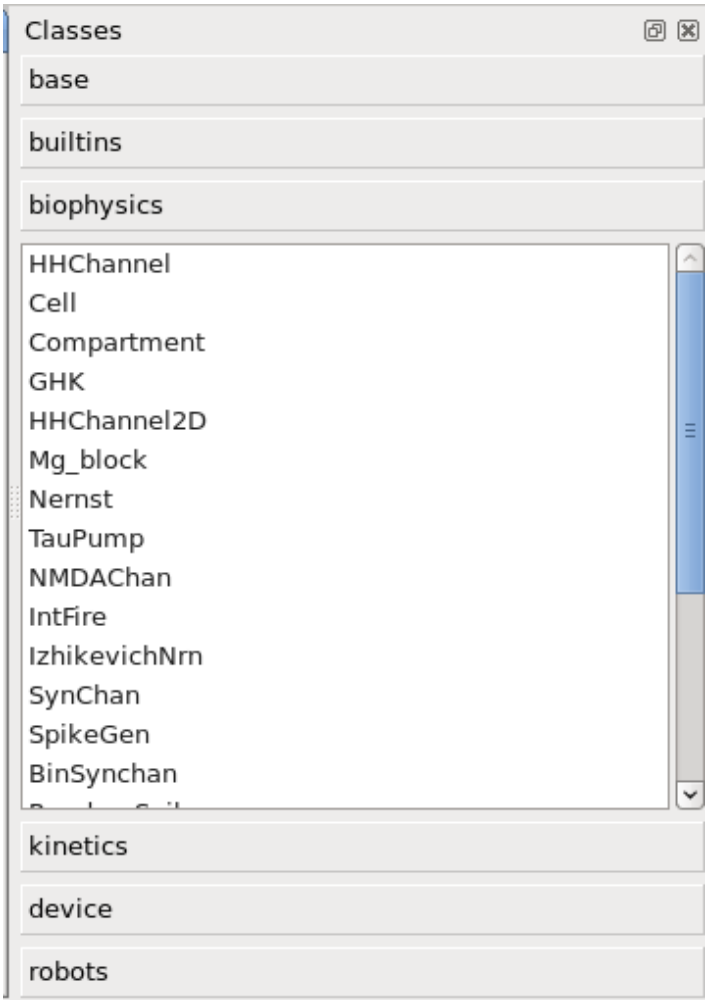
Here you can specify the simulation time step, the time step used for plotting and the timestep when using the 3D visualization. The total run time of the simulation and the update interval for plots is also specified here. When you are ready to run a model, you can click the `Run` button here to carry out the simulation for the specified time.

Plot Window

In the centre of the main moosegui window is the plot window. When you run a simulation, you can plot the variables of interest in this area. This will be discussed in connection with the `Object Editor` later.

MOOSE Classes

The right dock area contains a list of classes available in MOOSE. They are categorized under different headings.



Clicking a heading will expand that category. Below is a short description of the categories:

base	Basic classes.
builtins	Classes for some builtin utility functions.
biophysics	Classes used in simulation of biophysical entities. It includes compartments for cable models of neurons, ion channels, synaptic channels, etc.
kinetics	Classes for simulating biochemical entities. Includes molecule pool, reaction, enzyme, etc.
device	Classes for simulating instrumentation. It includes rc-circuit, pulse-egenrator, differential amplifier, PID controller.

robots These are special purpose classes used in multiscale models.

If you hover the cursor over any class name in the list, a tool-tip text with a brief documentation of the class will show up.

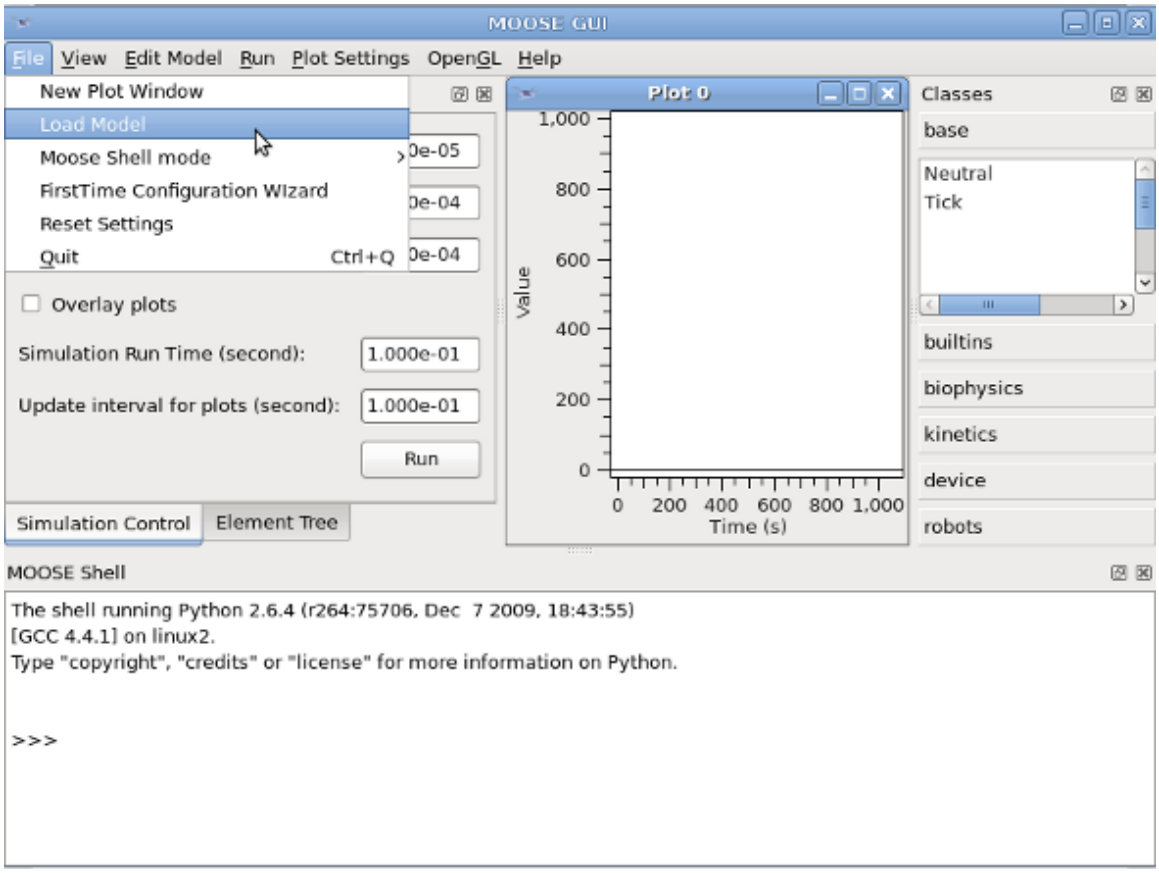
MOOSE Shell

The MOOSE Shell at the bottom dock area provides an interpreter where you can enter Python or GENESIS commands.

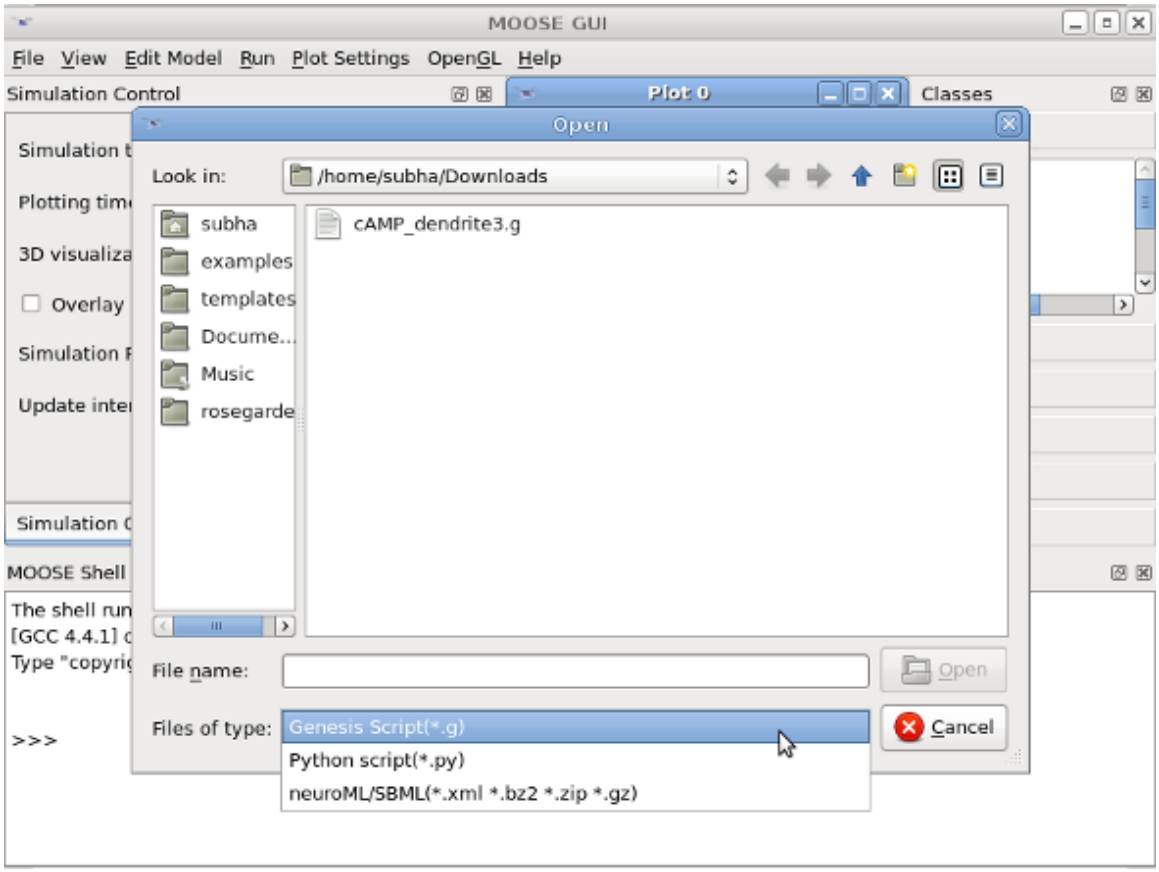
The default interpreter is the Python interpreter. You can switch to the GENESIS shell by selecting GENESIS from `File->MOOSE Shell Mode` from the menu.

3 Loading a file in the GUI

You can load an existing model into the GUI from the menu: File->Load Model.



This will pop-up a file browser in which you can select the file you want to load. At the bottom of the file-browser you can select what type of model file you want to load.



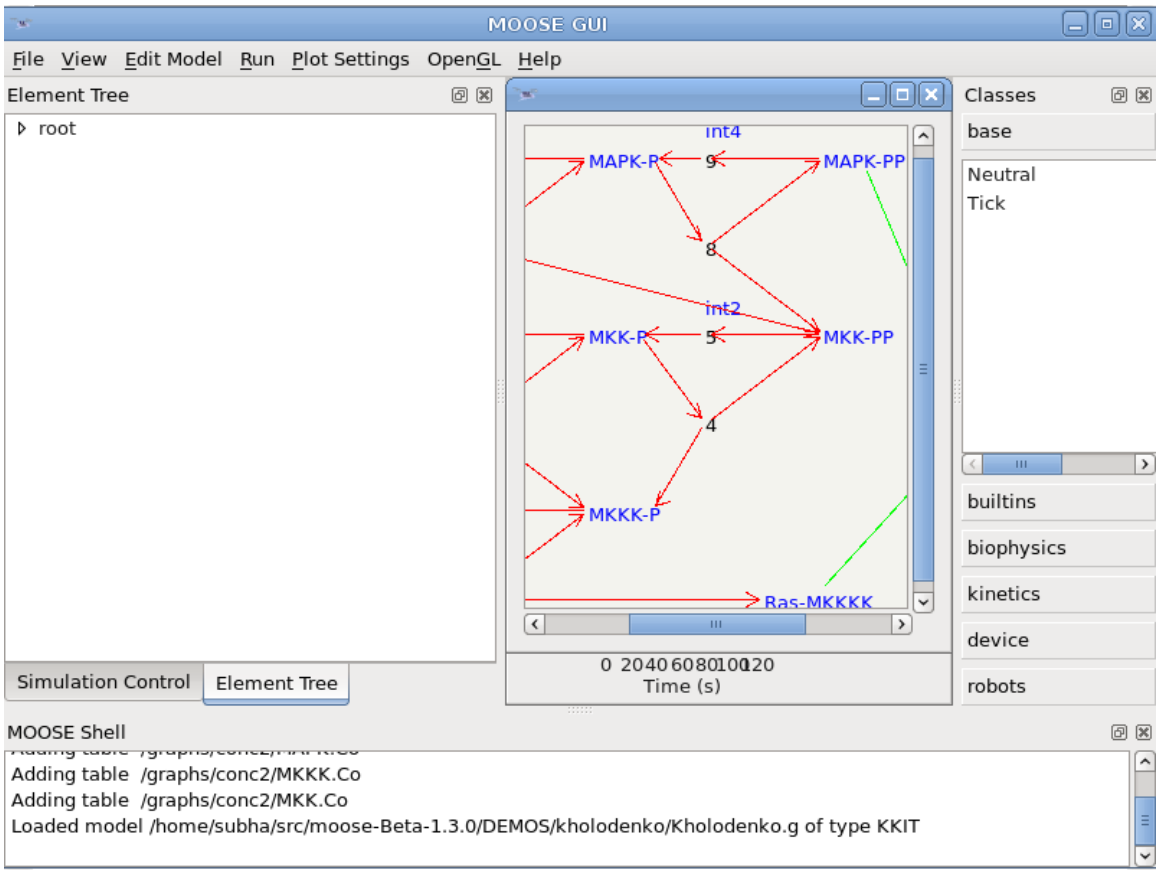
The default is GENESIS script (.g), you can also choose NeuroML or SBML files (extension .xml).

When you load a GENESIS script, it executes whatever is in the script using the built-in GENESIS-parser. Such a script can do much more than just loading the model. In particular, if the script contains `reset` and `step` commands, then the simulation will be executed and you will have to wait until the simulatioin is over to get control of the moosegui back. You may want to comment out the lines containing these commands from the `.g` file before loading in order to use the `Simulation Control` to run the simulation with custom time.

3.1 Kinetikit models

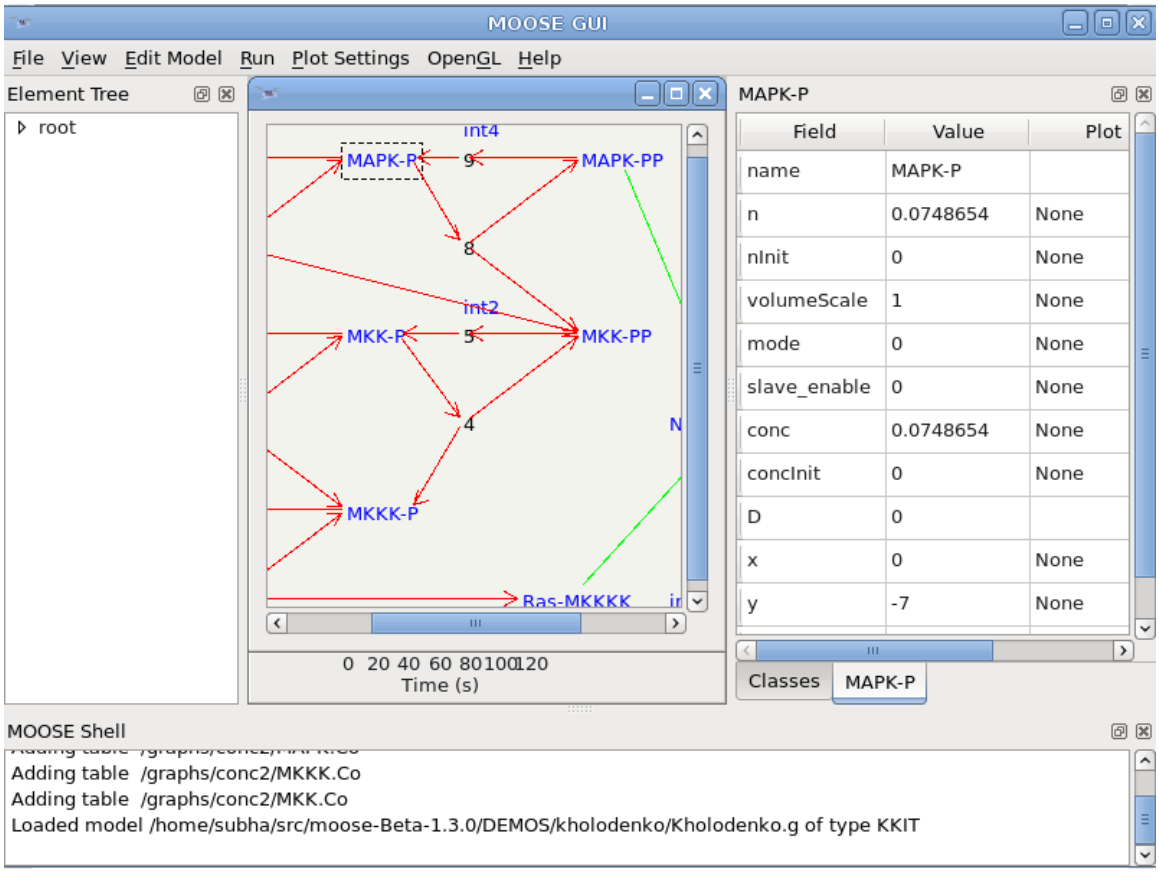
In addition to regular GENESIS scripts, the GUI recognizes `.g` files that contain kinetikit models. Kinetikit models have the commands to plot variables of interest. When you load the model, all these plots are added to the available plot window. Moreover, you get a graphical representation of the reaction network in the layout window and the plots in the

Plot window. For example, after I load `Kholodenko.g` from `DEMOS/kholodenko` directory I get the following:



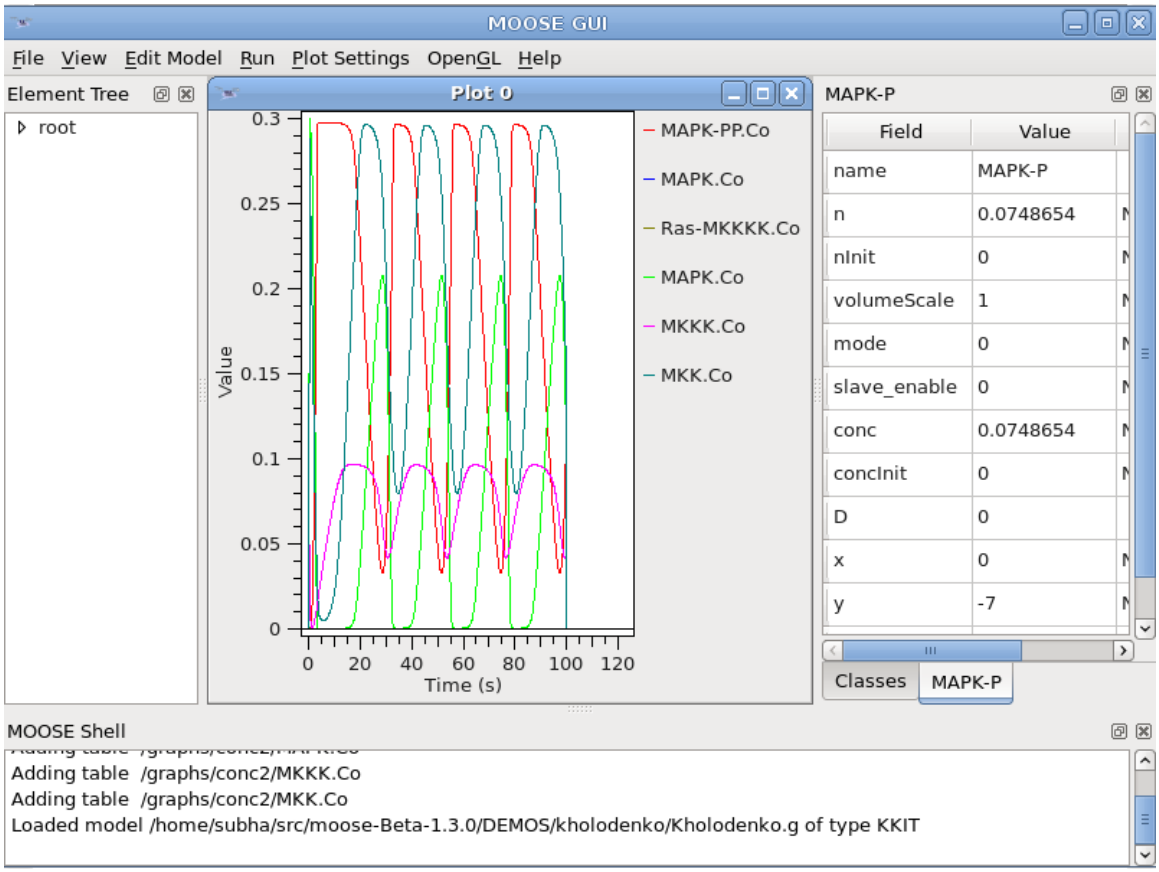
You can double click any item in the layout window and that will open an editor(`Object Editor`) for the underlying MOOSE object on the right hand dock (on top of the `Class`

`List`) will come up. The more general way of bringing up the `Object Editor` is to double click an item in the `Model Tree`.



You can modify the properties of the objects (for example the initial concentration of a substrate) in the object editor.

Normally the plot window is under the layout window. You can minimize the windows on top to view the ones below.



3.2 SBML models

Just like GENESIS models, you can select SBML model in the drop down and load an SBML file. The main difference is that here you don't get the reaction network layout. Also, GENESIS kinetikit files come with predefined plots. But SBML does not handle plotting and visualization.

3.3 NeuroML models

Currently MOOSE has partial support for NeuroML models. You can load a model from the "Load File" dialog and selecting NeuroML format from the file type drop down. The elements in the model are generated as children of the currently selected element in the `Model Tree`. So, you can create the model under a new element by

1. creating a new `Neutral` element
2. then selecting the newly created element.
3. then loading a model using the file menu

4 Recording and plotting field values over simulation time

Elements of the `Table` class are used in MOOSE are used for recording data. `Table` is a versatile class: it can serves as (1) an interpolation table, (2) a function generator (3) a recording table, depending on what stepmode you set. But in the **moosegui** you do not need to create the `Table` explicitly to record data. You can simply drag and drop fields in MOOSE elements to a plot window in order to plot it. The steps are:

1. You have to double click the object whose field you want to plot in the `Model Tree`. This will open the object editor with list of available fields.
2. Now you can plot a field by either left-clicking on the field and dragging it to the plot widget and releasing the mouse button,
3. or by clicking in the the `Plot` column twice and then selecting 'Plot 0' from the drop down. When you have multiple plot widgets, you can select where it should be plotted from this drop-down.

5 Adding elements in a model

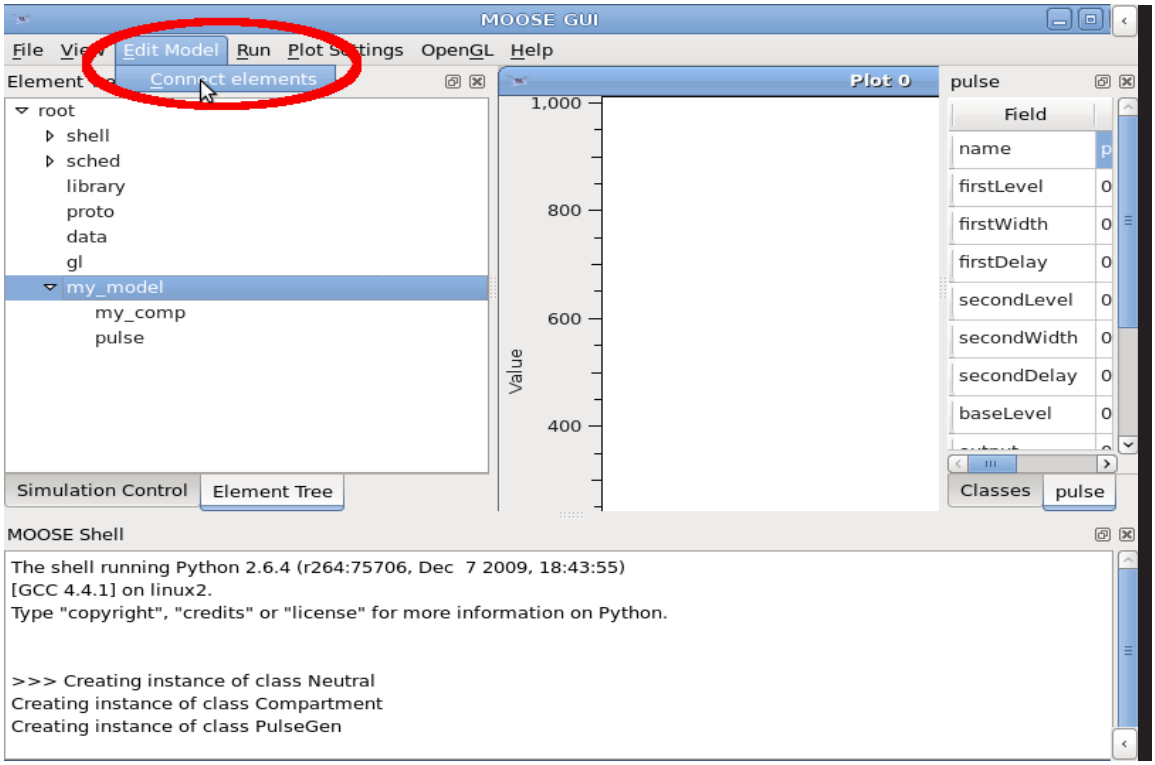
5.1 Adding a new element in the `Model Tree`

You can add a new element in a model by using the class list on the right hand side pane in moosegui see [Moose Classes], page 10. Double clicking the class name will create a new element in the `Model Tree` under the currently selected element and also open the `Object Editor` widget for the new element. The element will have the same name as the class name. It is up to you to rename it to something more appropriate. To do so edit the `name` field in the `Object Editor`.

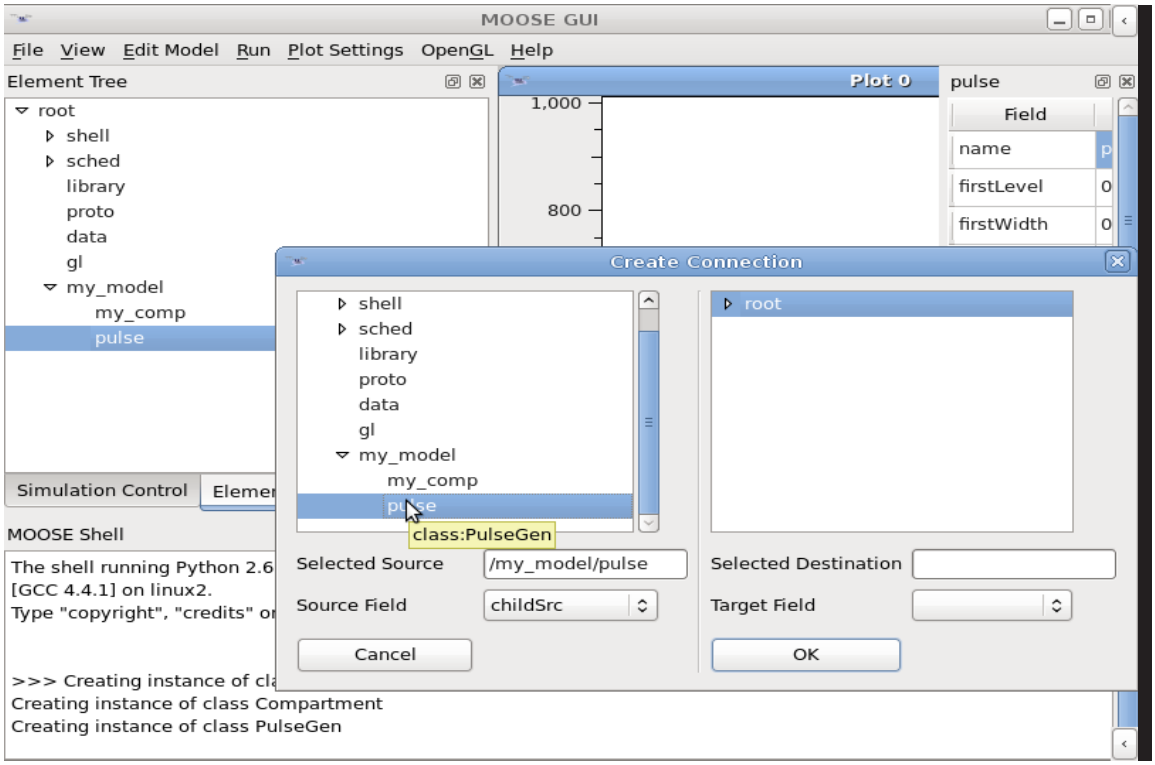
5.2 Connecting elements via messages

Just creating an element may not be sufficient for any complex model. You need to enable this model to talk to other elements during a simulation. This is done via messages. To do this,

1. Click `Edit Model` in the menu bar and select `Connect Elements`.

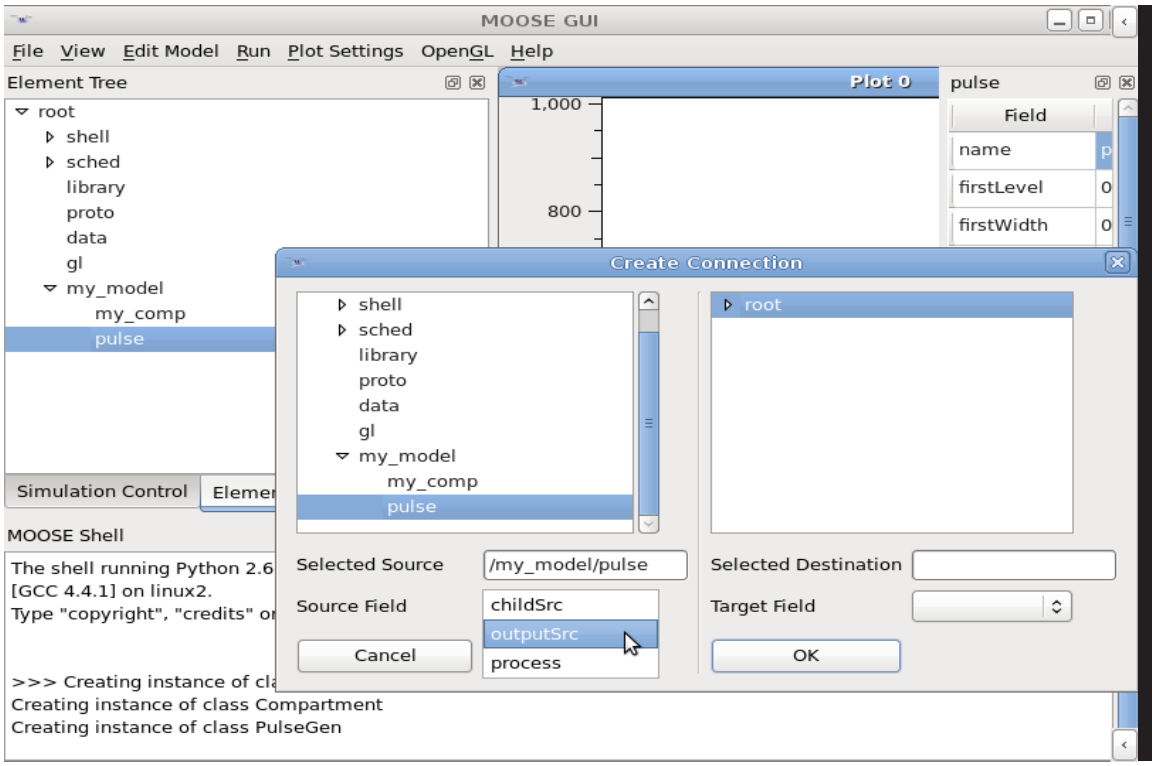


This will pop up a window with two panes. The left pane is for selecting the source of the message, the right for the destination of the message. Both has a model tree and drop-down menu for the message field.



2. Select source In the left pane, expand the `Model Tree` and select the element which will be the source of the message. Once you select the element, the drop-down menu

labeled `Source Field` will be populated. You have to select the appropriate source field here.



3. Select Destination Similar to selecting source, you have to select the destination element and the target field in the right pane.
4. Click OK to actually make the connection.