

Instructions on insilicoSim 1.4.2

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Abstract

This document describes how to use insilicoSim 1.4.2. You can also find some OS-specific notes and trouble-shooting techniques which you would like to know when using insilicoSim 1.4.2.

1 Running insilicoSim

On Windows, double-clicking “insilicoSim.exe” in the start menu starts the insilicoSim program. On Mac OS X, double-clicking “insilicoSim.app” in the “insilicoPlatform” directory works similarly. Shortcut `Ctrl+Q` in order to quit insilicoSim.

2 Executing a simulation

2.1 Markup languages representing models

Currently the following three languages are available to represent models:

- insilicoML(ISML)
- CellML
- SBML

2.2 Calculation methods for ordinary differential equations(ODE)

Currently the following two algorithms are available to solve ODEs numerically:

- Euler method
- Runge-Kutta 4th order method

2.3 Procedure

How to simulate a model is that:

1. Open an existing xml file representing a model to be simulated (Shortcut **Ctrl+O**). Then you have a subwindow to arrange options of the simulation process.
2. Select the calculation method of ODE in the “Numerical Integration Method” option.
3. Specify the total length of simulation in the “Simulation Length” option.
4. Specify the step length of simulation in the “Simulation Time Step” option.
5. Push button “Run” or **Alt+R**.

2.4 Messages

Some messages about the simulation process will appear on the text area in each subwindow. They consists of elapsed time in second for each kind of processing, e.g.,

- Total time
- Init and Cleanup: time for initialization and cleanup
- Euler calc: time to solve ODE by Euler method
- Runge-Kutta calc: time to solve ODE by Runge-Kutta 4th order method
- Output: time to write data to the **.dat** file (see below)
- Multivariate: time to write data to the **.csv** file (see below)

2.5 Output

A successful simulation generates files as its result. Let us say that **/path/of/x** is the path of file of the model to be simulated. The following three files will be created during simulation:

- **/path/of/x.csv**: one line per step

- `/path/of/x.dat`: one line per step and physical quantity (optional)
- `/path/of/x.map`: describing the mapping of variables/indices in `x.csv`
- `/path/of/x.plt`: gnuplot script for visualization (see below)

Note that all of them are just of plain texts.

3 Visualizing a result

3.1 Preference

With simulating a model you can visualize its result as a line graph. Current `insilicoSim` uses `gnuplot` for this purpose. It means that you have to install `gnuplot` at first. And also you need to specify the location of the `gnuplot` executable on your system; edit the preference in the top menu of `insilicoSim`, and select the path of `gnuplot` (or `pgnuplot.exe` on Windows), e.g., `"/usr/bin/gnuplot"`. On Mac OS X, if you have, say, `/Applications/gnuplot.app` as an application bundle of `gnuplot`, its value should be

`/Applications/gnuplot.app/bin/gnuplot.`

3.2 Procedure

After simulating all you need to plot the result is as follows:

1. select Tab "Plotting".
2. choose the abscissa and ordinates from the left side frame by dragging and dropping variables corresponding to physical quantities.
3. if there are so many variables that some of them scroll out on a frame, a scroll bar appears on the left edge of the frame. Besides scrolling them by wheeling with mouse, especially on the left side frame, you can jump to a variable by typing an alphabet key (i.e., [A-z]) which specifies the first character of the variable's name.
4. push button "Plot" or `Alt+P`.

Now you have a line graph in another window.

3.3 Writing to a file

It is also possible to write the line graph to some file, as follows:

- choose Tab “Target”.
- check the “file” button.
- select a file format and path to be written.
- push button “Plot”.

Then a dialog will inform you of the resulting status.

3.4 Options for gnuplot

You can control the following options for gnuplot in Tab “Range” or “Legend”:

- Minimum and/or maximum value(s) for the abscissa (X) and/or ordinates ($Y1/Y2$)
- Labels for the abscissa (X) and/or ordinates ($Y1/Y2$)
- With or without the title

These will be enabled on next time plotting.

3.5 Trouble shooting

- Pushing button “Plot” with no response, you may want to check the gnuplot initialization file to load. It is called `.gnuplot` on Unix and Mac OS X, and `GNUPLOT.INI` on other systems.