

SED-ED editor tutorial

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SED-ED tutorial

Welcome to this tutorial, which will explore the features of the SED-ED viewer and editor for SED-ML level 1 version 1.

SED-ED is available as a standalone application, a plugin for Eclipse, or as a plugin for SBSI.

This tutorial will cover:

- Installation and getting started.
- Creating new SED-ML documents *de novo*.
- Working with existing SED-ML files
- Editing SED-ML (creating and viewing changes).

The features listed above exist in all versions of SED-ED. If you run SED-ED as an SBSI plugin, then you will also be able to execute SED-ML files and run simulations as well. We'll cover this at the end of the tutorial.

Installation and getting started.

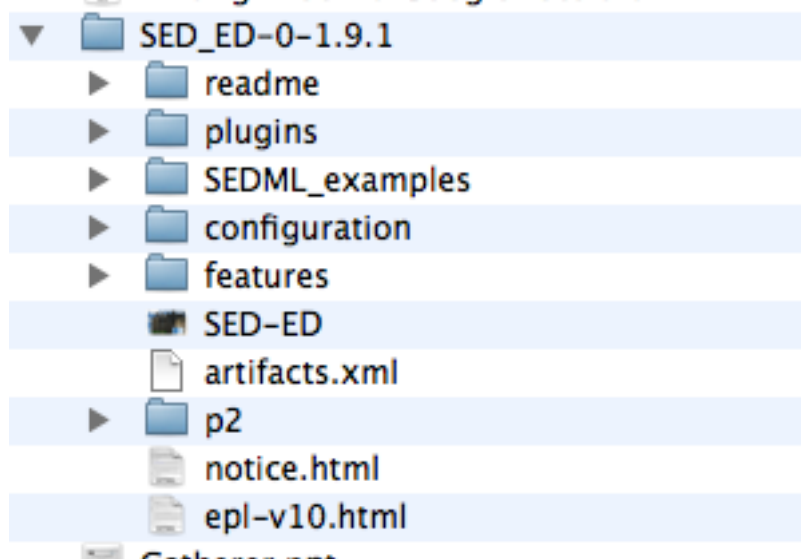
In this section, we'll describe how to get SED-ED up and running on your machine. You only need to use one of these installation mechanisms.

Installing the standalone application

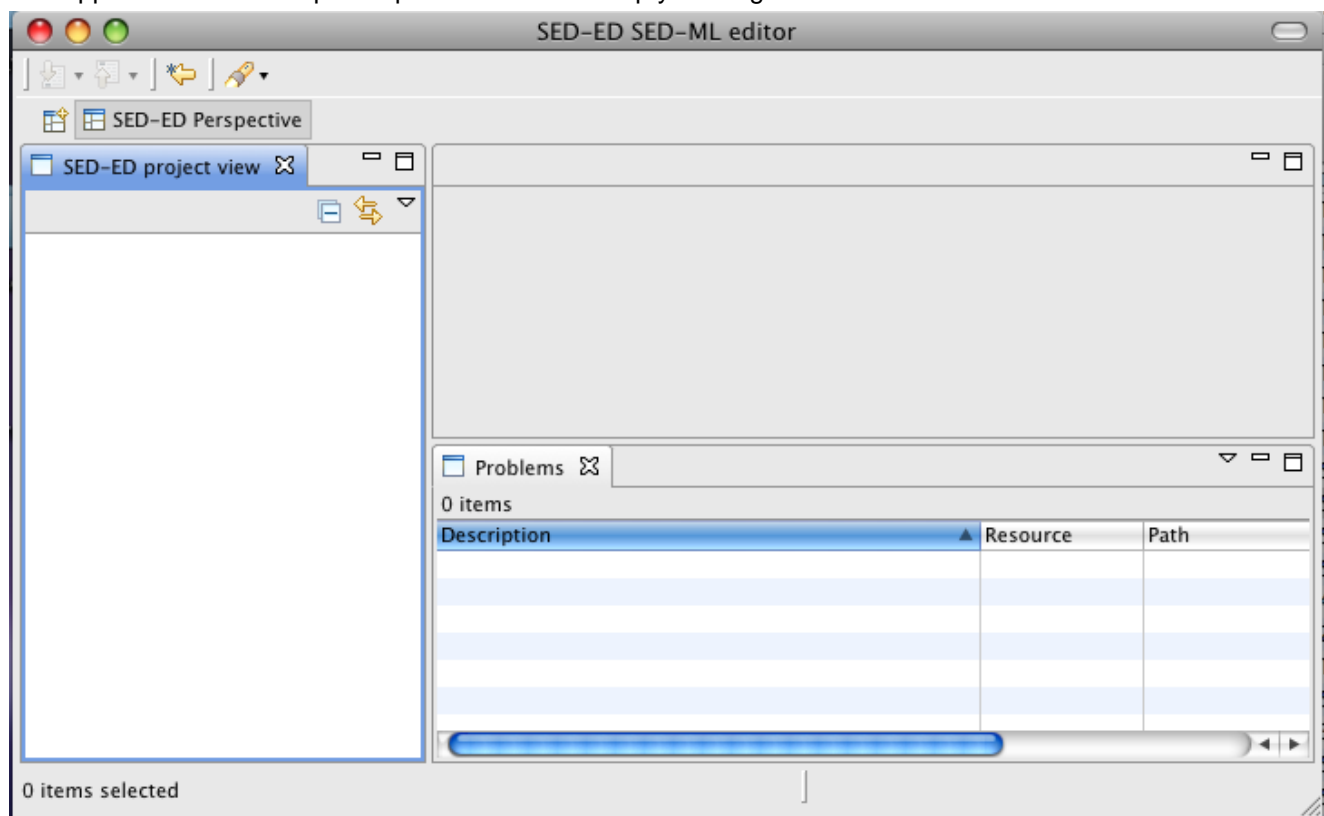
This is the most straightforward installation:

1. Go to the SED-ED download site at <http://sourceforge.net/projects/jlibsedml/files/SED-ED/> and download the version for your platform.

- Unzip and you should get a folder with the following contents:

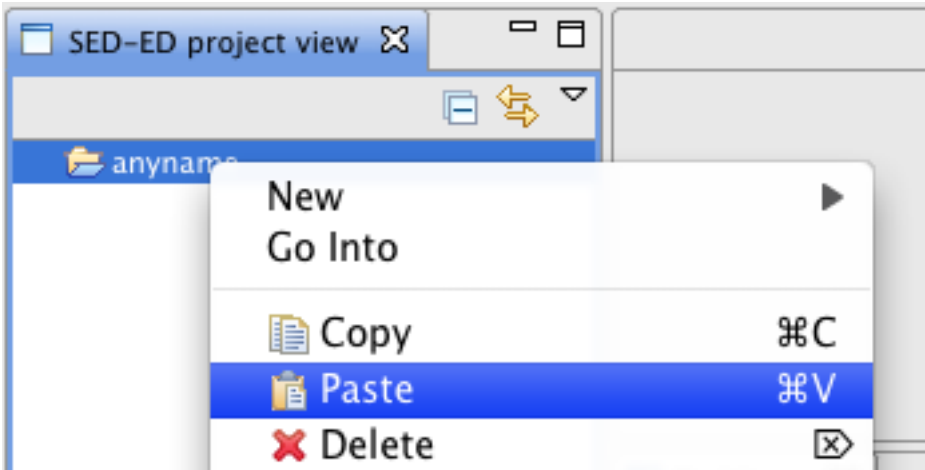


- To start the application, double-click the 'SED-ED' launch icon.
- The first time you run the application, you will be invited to choose a *workspace*. This should be a new folder on your filesystem that SED-ED will use to manage the files and resources you create.
- The application will now open to produce a rather empty-looking window



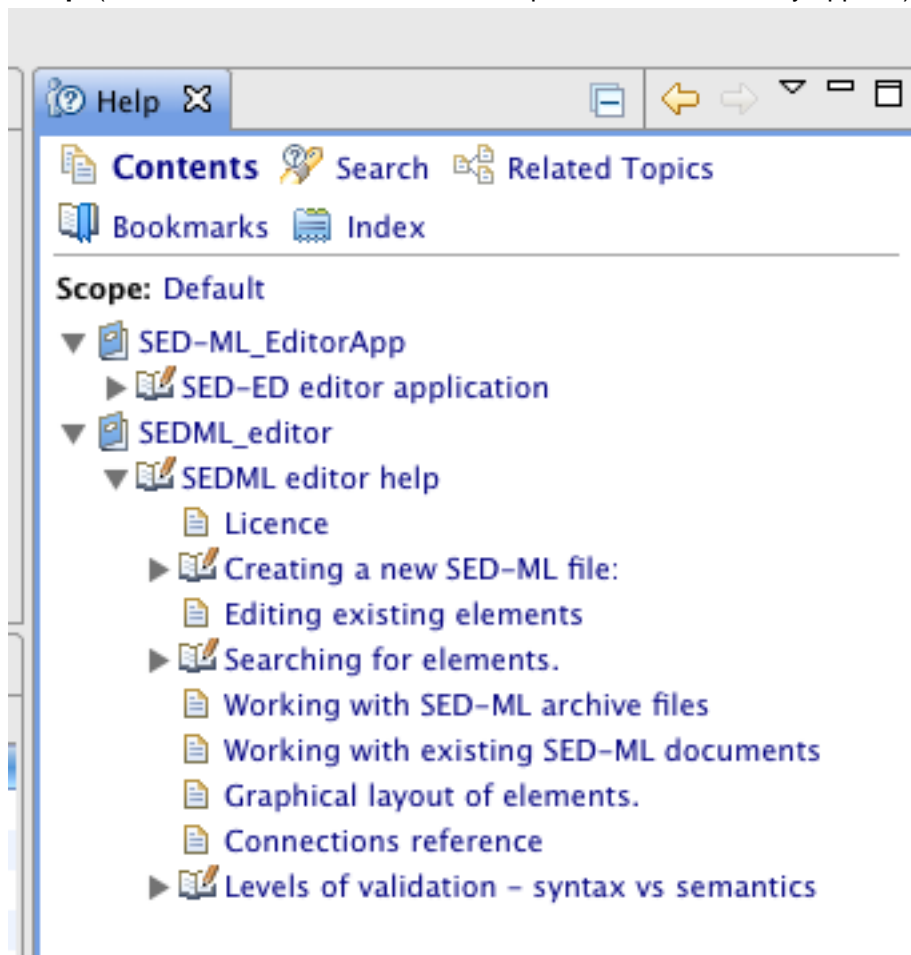
- Now, create a new project (**File->New->Other->General->Project**) and give it a name.

7. Copy the folder 'SEDML_examples' from your unzipped application folder from step 2, and paste it into the project. To perform the paste operation, select the project, right-click and then paste.



Alternatively, you can just drag-and-drop the folder into your new project.

You are now ready to start exploring the SED-ED editor. There are embedded Help files accessible via **Window->Help**. (Click on the 'Contents' link if the Help does not immediately appear). You should see Help pages appear :



Installing as an SBSIVisual plugin

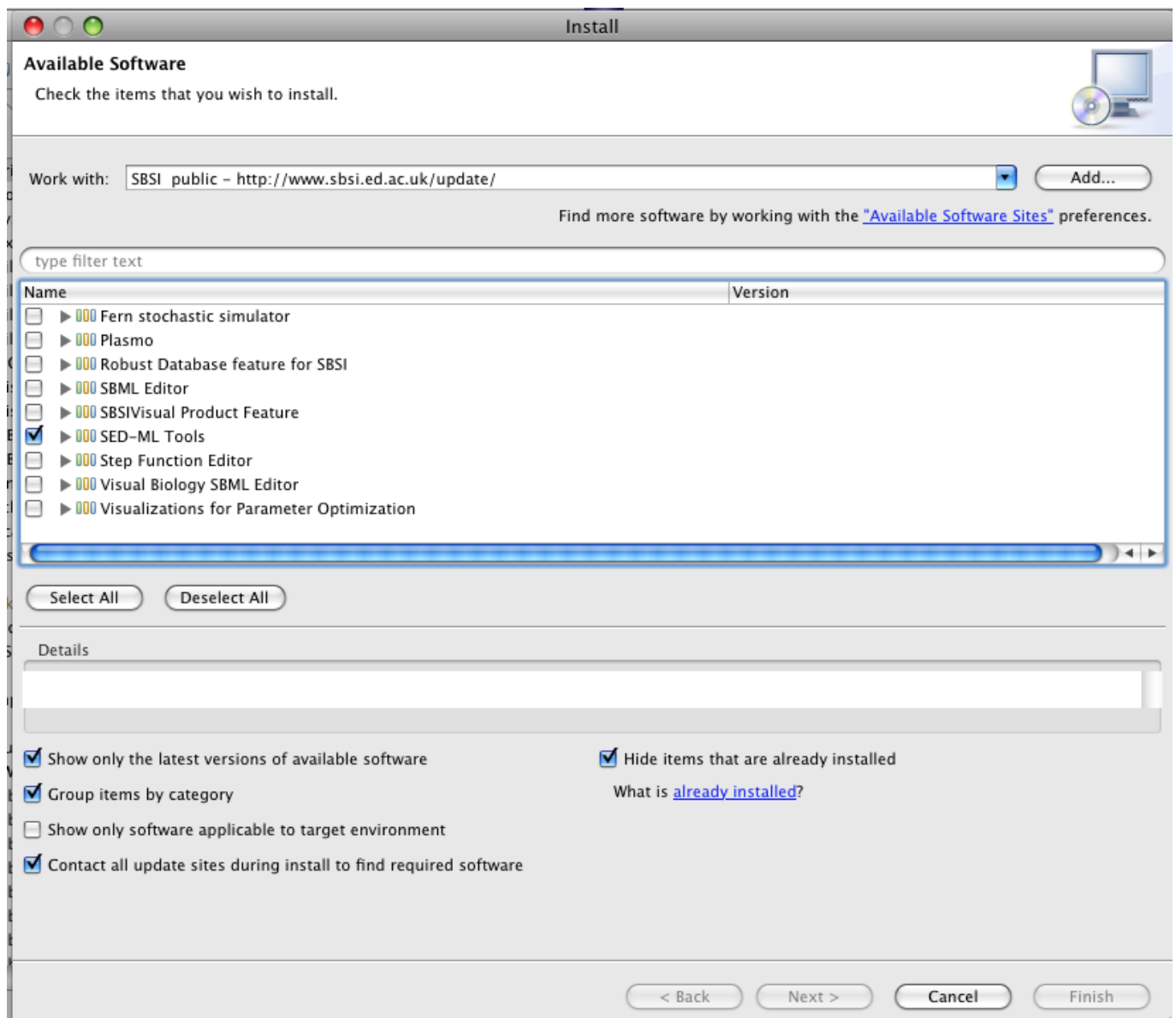
This installation will take a little longer, but once performed, you will also be able to run simulations encoded in SED-ML by accessing SBSI's simulation capability.

Installing SBSIVisual

1. Go to the “SBSI download site”: at <http://sourceforge.net/projects/sbsi> and download SBSI for your platform.
2. Unzip and launch by either clicking on the launch icon (Windows users) or on the ‘Launch.command’ script (MacOSX and Linux users). Please review the README file in the SBSI downloaded folder for more precise instructions.
3. The first time you run the application, you will be invited to choose a *workspace*. This should be a new folder on your filesystem that SBSI will use to manage the files and resources you create.
4. The application will now open to produce a rather empty-looking window.
5. Now, create a new project (**File->New->Other->SBSISystem**) and give it a name.

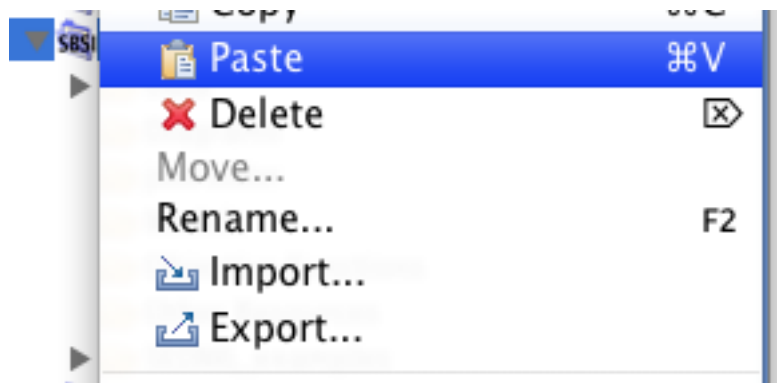
Installing the SED-ED plugin for SBSIVisual

Install the SED-ED by clicking on **Help->Install New Software**, and then in the “Work With” drop-down list, choose the “SBSI Public” plugin repository. Now, choose the **SEDML tools** project:



Follow the installation wizard and agree to all prompts for license agreements, and to restart the application. If you need more help to install the plugin, there is a brief video illustrating how to install a plugin.

Finally, copy the folder 'SEDML_examples' that has appeared in your SBSI installation folder and paste it into the project you created. To perform the paste operation, select the project, right-click and then paste.



Alternatively, you can just drag-and-drop the folder into your project.

Installation as an Eclipse plugin

You may prefer this installation mechanism if you already use Eclipse and want to install SED-ED as a plugin, without installing a new application.

The instructions are largely similar to the section 'Installing the SED-ED plugin for SBSIVisual' described above. Before performing these steps though, you'll need to tell Eclipse where the SBSI update site is located.

To do this, choose **Help->Install New Software**, and in the ensuing dialog, click 'Add' and add this URL: <http://www.sbsi.ed.ac.uk/update/>.

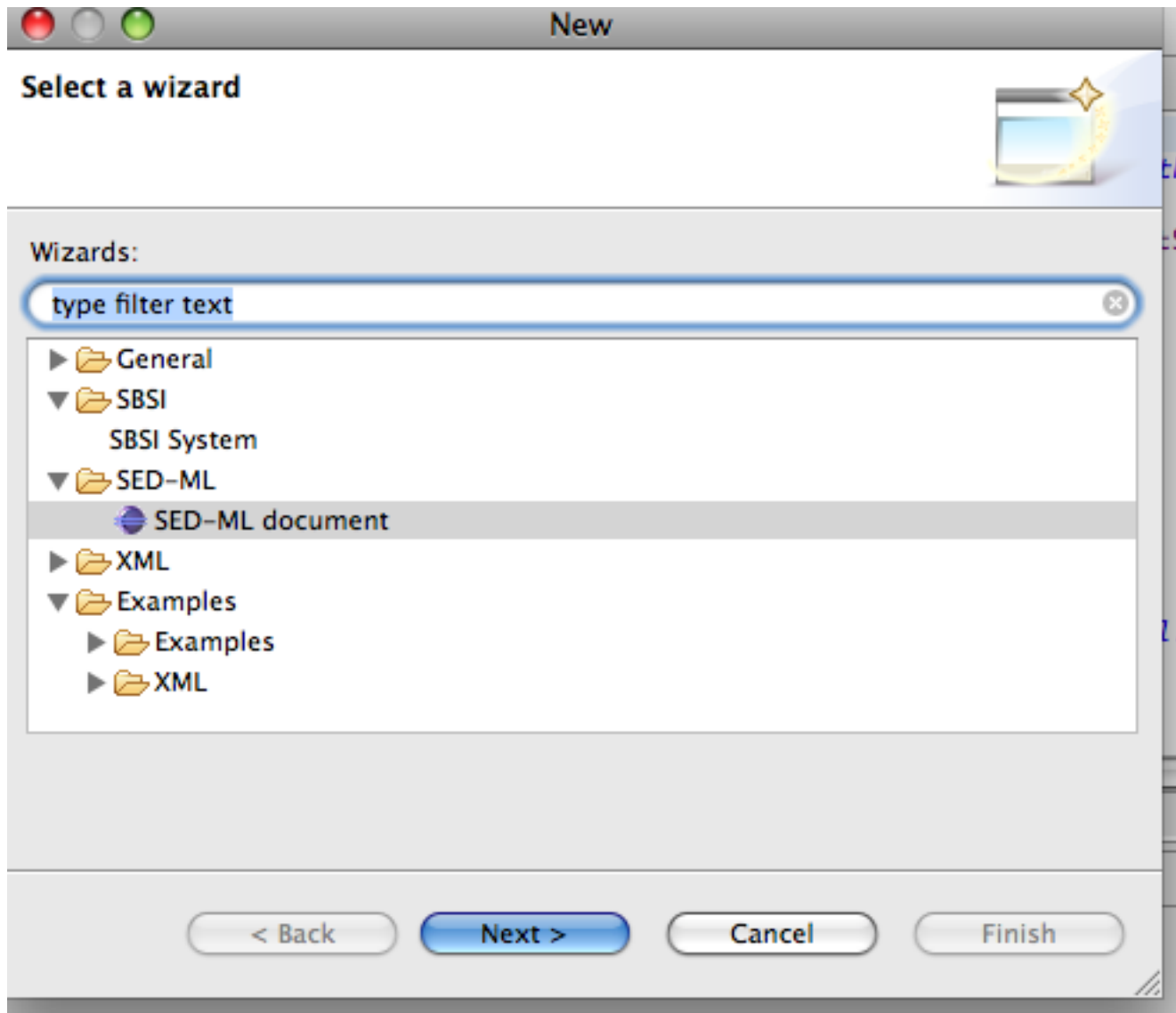
Now, proceed with installing the plugin, as described in 'Installing the SED-ED plugin for SBSIVisual' above.

Creating SED-ML files de novo

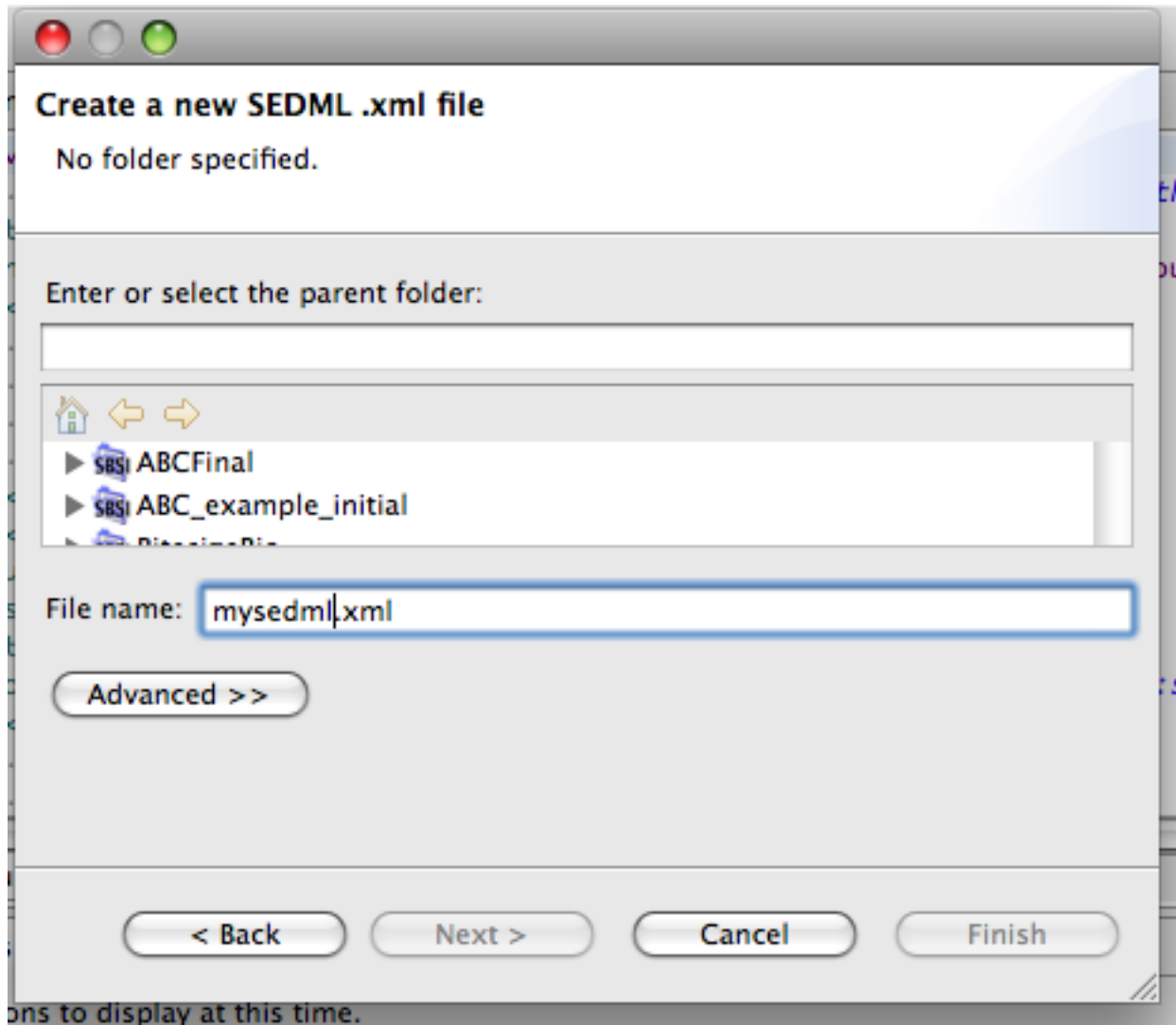
Creating a new SED-ML file

Using any of the installation mechanisms described above, we should now be in a position to create new SED-ML files. In this tutorial we'll reconstruct part of a SED-ML file used to describe simulations run on a Circadian clock model available from the BioModels database.

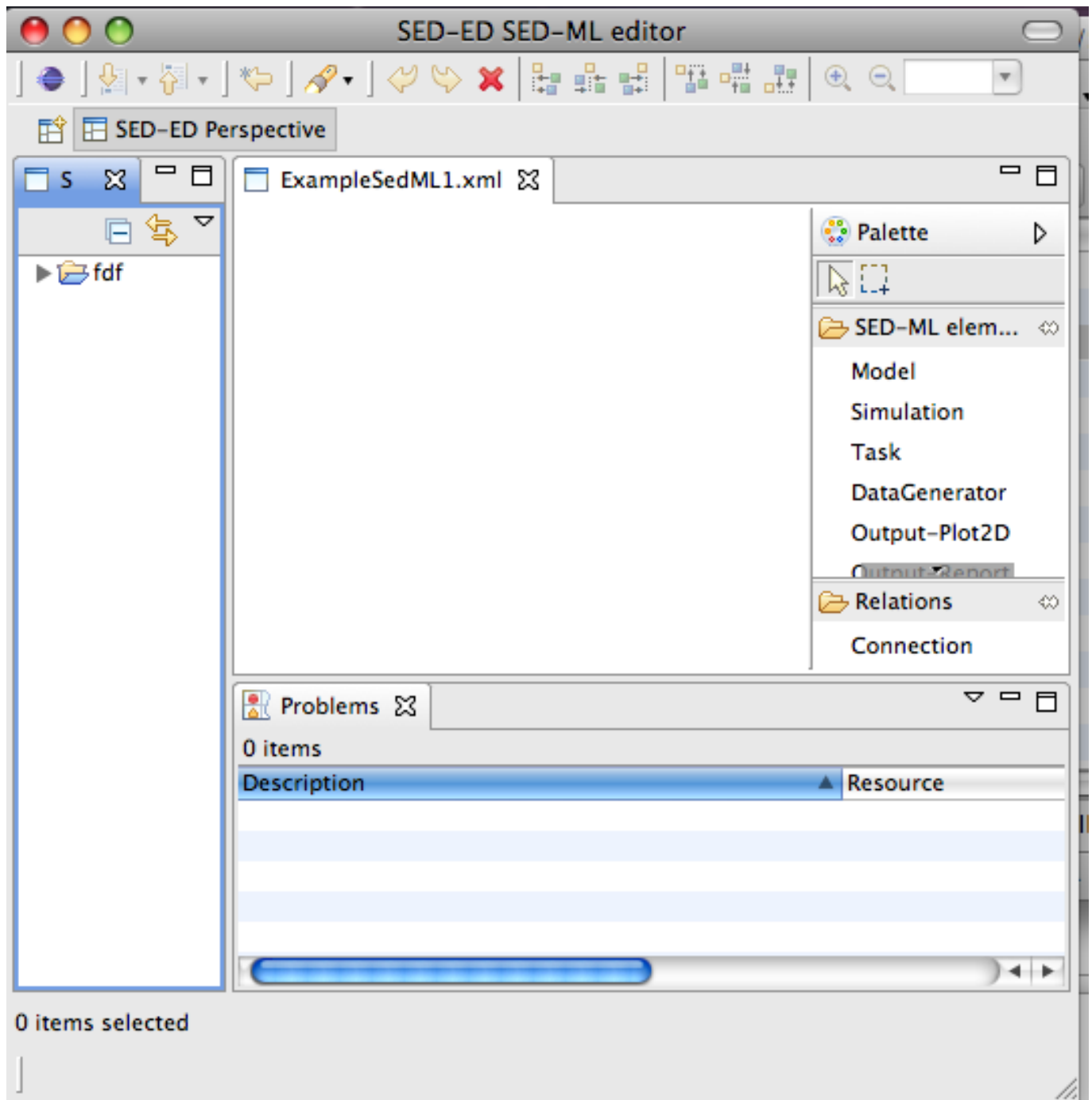
To do this, click **File->New->Other** and select the SED-ML Document option:



Give the file a name, and a project to which it will belong. **Make sure the file name ends with the suffix .xml .**



Once you click **OK** an empty editor will open:



(Note: It's possible, depending on how your application is set up, that a simple text editor displaying some XML might open, rather than a graphical editor.
 If this is the case, just select the file in the workspace, right-click and choose 'Open With->SED-ML editor').

Building the SED-ML document

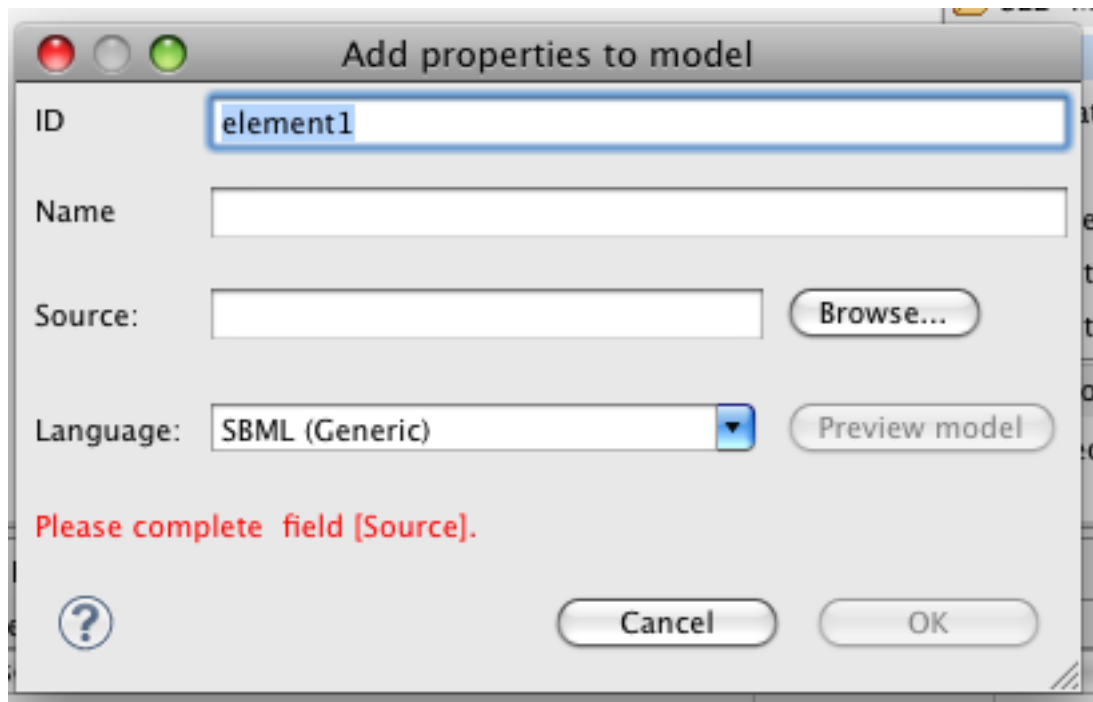
There are five main elements of a SED-ML document, and we'll create these one by one:

1. **Models**, which specify where models to be simulated can be found.
2. **Simulations**, describing the algorithm and time period of simulation.
3. **Tasks** These match a model to a simulation, and define an experiment.
4. **DataGenerators** are used to prepare the raw simulation output for presentation (for example, normalisation).

5. **Outputs** describe the presentation of the results: 2D /3D plot, or report.

Creating a Model

Click on the 'Model' tab of the palette menu in the editor, then click again somewhere on the editor canvas. A configuration dialog will pop up:

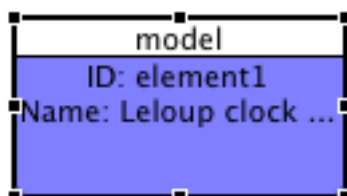


Initially, the 'OK' button is disabled, because some essential information is needed – where to locate the model. In the 'Source' text-box, type in the following URN:

```
urn:miriam:biomodels.db:BIOMD0000000021
```

and give the model a name (optional).

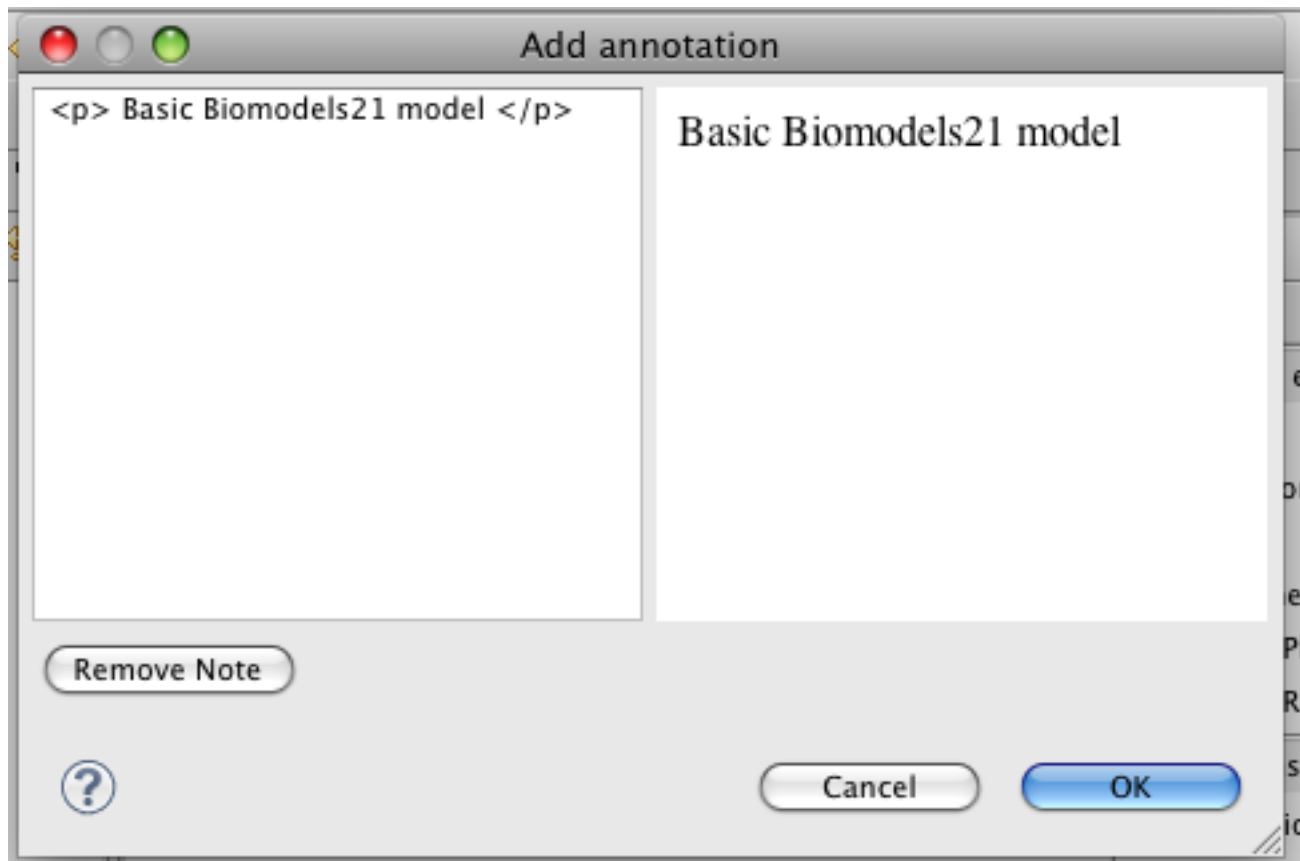
If you are networked, the 'OK' button will now be enabled, and so will the 'Preview model' button which gives a generic view of the model. Investigate this if you like, then click **OK** to dismiss the model configuration dialog. You'll see a shape on the canvas displaying the model's ID and name (if set):



While we're editing the model, we'll add a note for annotation. Click on the model shape to select it, then right-click and choose **Add/View/Edit note** from the context menu. Add a simple piece of well-formed HTML into the left-hand text-box. E.g.,

```
<p> Basic Biomodels21 model </p>
```

A browser preview will appear in the right-hand panel:



Now, click **OK** to dismiss the dialog. You'll see an icon displayed on the model shape now, indicating that it is annotated.

You can add Notes to any SED-ML element, not just Model elements.

Simulations

Now, we'll configure a simulation. Click on the 'Simulations' tab of the palette, and click again on the editor canvas.

Add properties to time course

ID:

Name:


Simulation start:

Output start:

Simulation end:

Number of timepoints:

Algorithm:



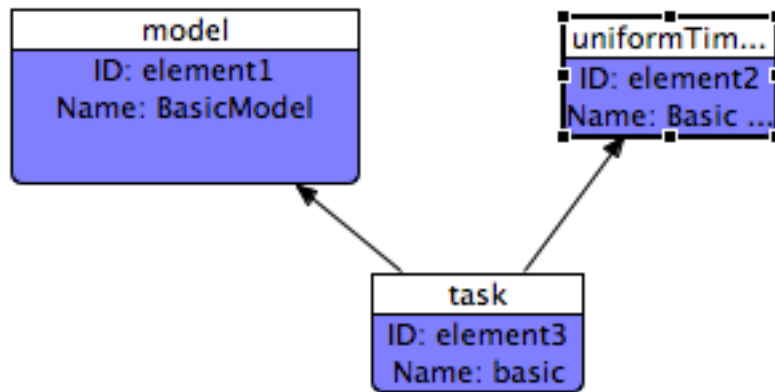
In this case, there are default settings which we can use- just edit the 'Simulation End' to be 100, then click OK. A simulation shape will be added to the canvas. By default a generic ODE solver algorithm is selected, this is fine for our purpose.

Task

Now we'll create a task which will link the model to the simulation. Click on the 'Tasks' tab of the palette, and click again on the editor canvas. This dialog is much simpler – optionally give the task a name.

You'll notice that the task shape is highlighted in red, indicating there is a problem.

In SED-ML, tasks need to refer to a model and to a simulation. To resolve this, click on the 'Connection' tab in the palette and then connect the task to the model by first clicking on the task, then on the model. Repeat, this time connecting the task to the simulation:



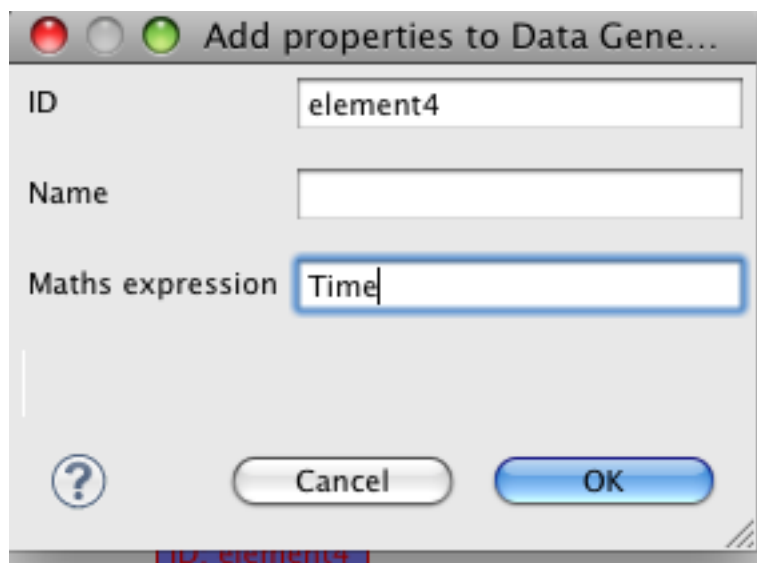
Once you've connected the Task properly, it will cease to be coloured red.

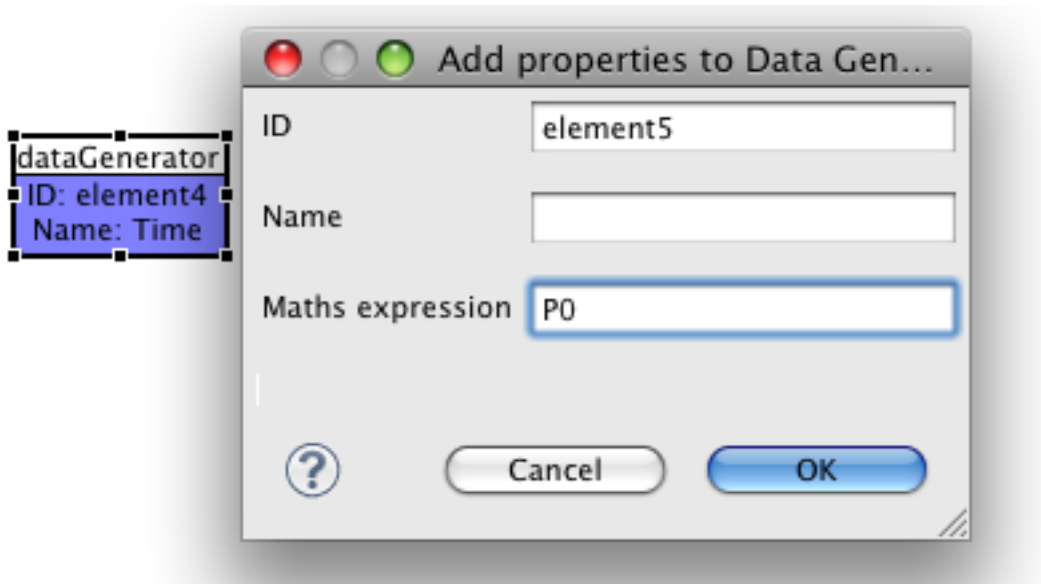
Now is a good time to save the file, by **File->Save**.

DataGenerators

Now, we'll start configuring the output we want from the simulation. To keep things easy, we want to get a simple 2D plot of Time vs Per(unphosphorylated) protein.

First of all we'll add two datagenerators from the palette. In the required 'Math expression' field, write 'Time' in one, and 'P0' in the other. E.g.,



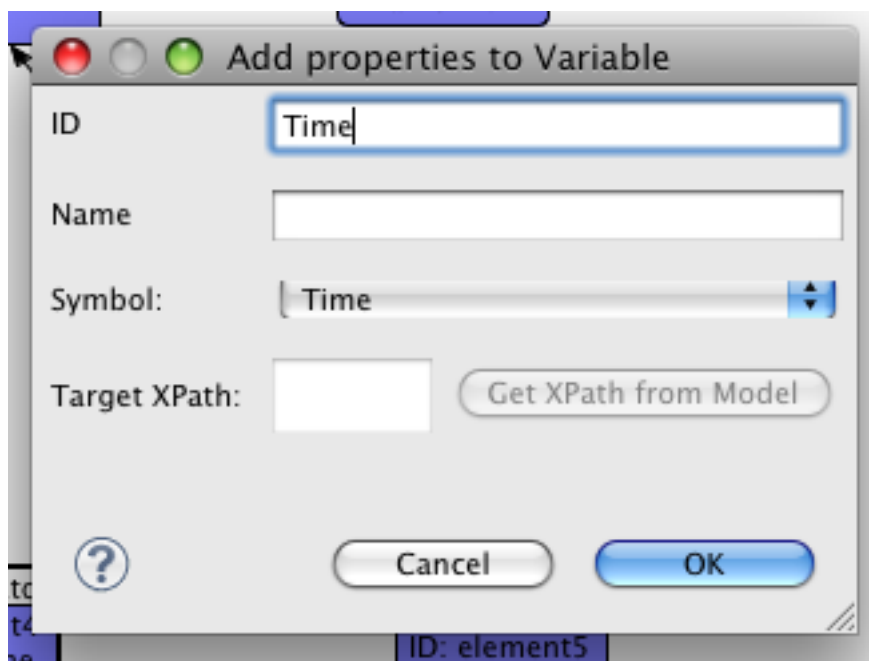


This math expression will use the IDs of **variables** that reference the model via the **task** we created earlier.

First of all, we'll create a variable for time.

To do this, select the 'Time' data generator, right-click and choose the 'Add Variable' option.

Variables can refer to either explicit variables in the model or implicit 'symbols'. In SED-ML there is only one implicit symbol, time. We'll choose this now:



Make sure that the value in the 'Id' field is 'Time' (i.e., corresponding to the identifier you used in the Maths expression in the DataGenerator).

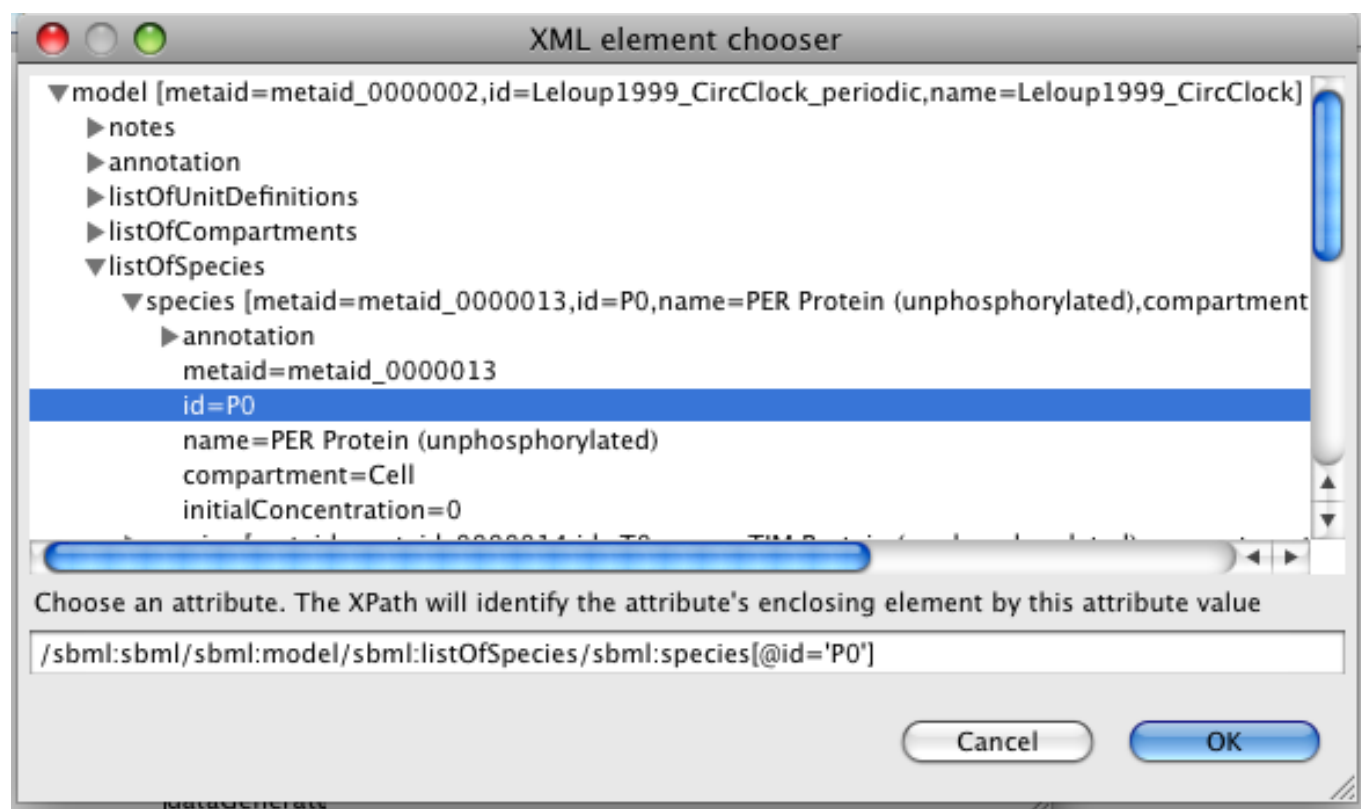
Click **OK**. Now, you'll notice that the Variable is still highlighted in red. This is because it is not yet connected to a **Task**. To resolve this, click on the **Connection** tab in the palette and draw a connection from the Variable to the Task. The Variable Shape will now turn black, indicating it is configured properly.

Now, create a variable that will refer to the model variable P0. As we did for time, select the DataGenerator for P0, right-click and choose the 'Add Variable' option.

- Set the Id to 'P0'.
- This time we want to keep the 'No Symbol' option as we're choosing a Variable

(Note, there is currently a bug which means you have to click 'Cancel' at this point – the variable is still created on the diagram, though).

- Now, connect the new variable to the task.
- The Variable still is displayed in red, though, as we haven't yet specified which model variable we want to refer to. To do this, double-click on the P0 Variable shape to re-open the configuration dialog, and click 'GetXPath From Model'.
- A dialog will open, showing a tree-view of the SBML model.
- Expand the tree. Choose an attribute that will uniquely identify the variable you want to choose. For SBML models, this will typically be the 'id' attribute:



SED-ML uses XPath to identify components of the model – this is displayed in the bottom of the model viewer.

Finally, click **OK** and the red highlights should disappear.

Configuring the data generators is probably the trickiest part of authoring a SED-ML file. The **Problems View** accessible via **Window->Other->General->Problems** is useful to show any inconsistencies or validation errors in the document.

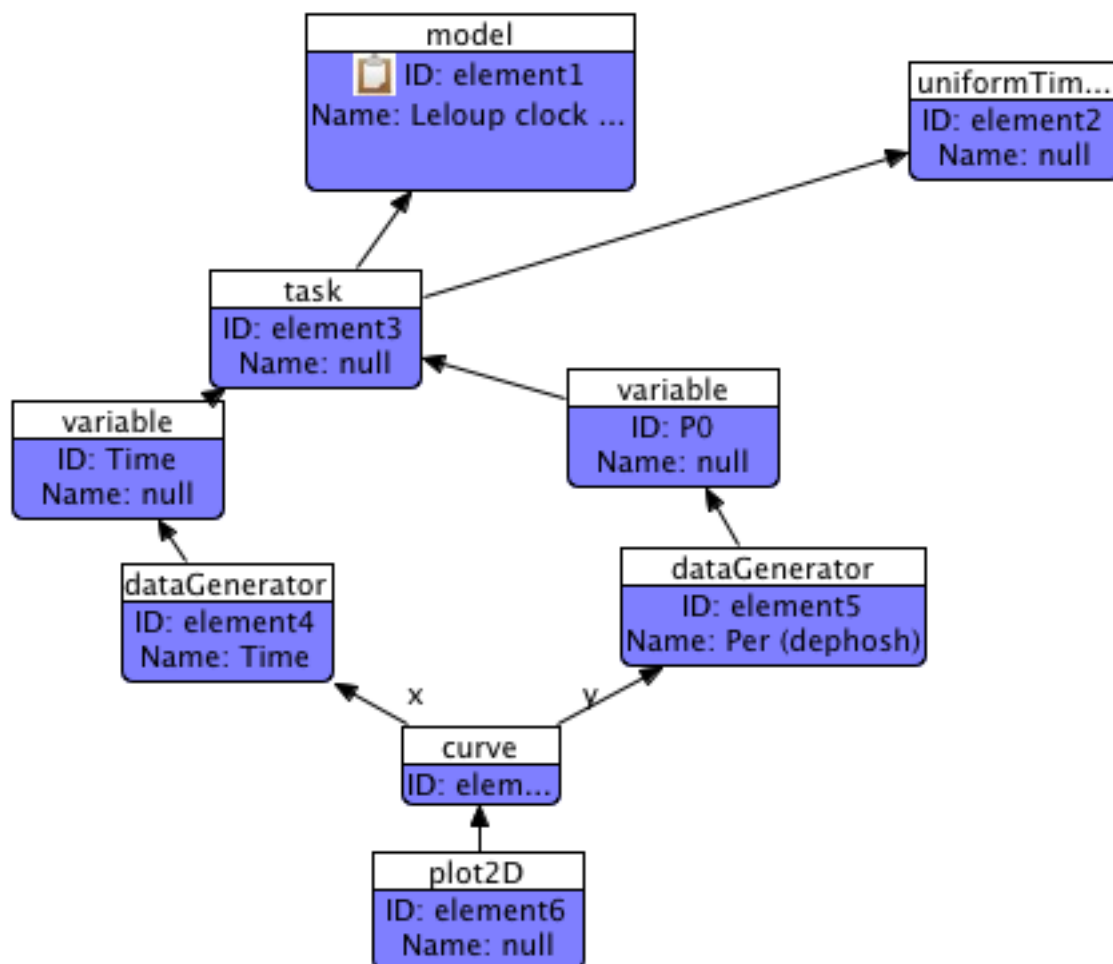
The outputs

We're almost done now – we just need to configure the presentation of the results.

For this example, add an 'Output - Plot2d' shape from the palette to the editor, adding an optional name if you like.

Now, select the Plot2D shape, right-click and choose 'Add Curve' from the menu. We'll just be adding one curve in this example. The curve will appear in red on the diagram. By now you know this means there is still work to be

done – in this case, we need to join the curve shape to the two data-generators that will produce the axes of the curve. Connect the curve to the Time(X) and P0(Y) data generators, ending up with something like this:

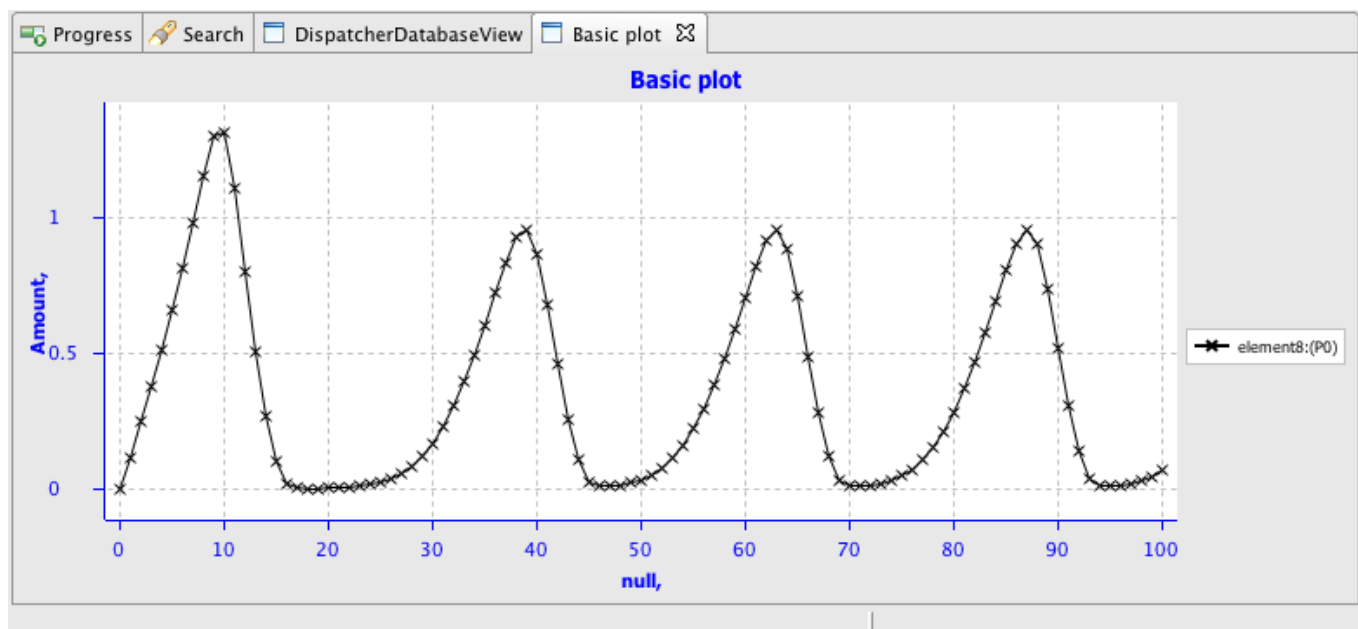


Working with your SED-ML file

We are now done! Check the **Problems View** at this stage if you've not already done so to ensure there are no errors.

Execution of the SED-ML file

If you're running SED-ED from within SBSIVisual, and are networked, you can now select the SED-ML file in the System View, right click and run the simulation via the 'Execute SED-ML' menu. You should see the your labours rewarded with a graph something like this:

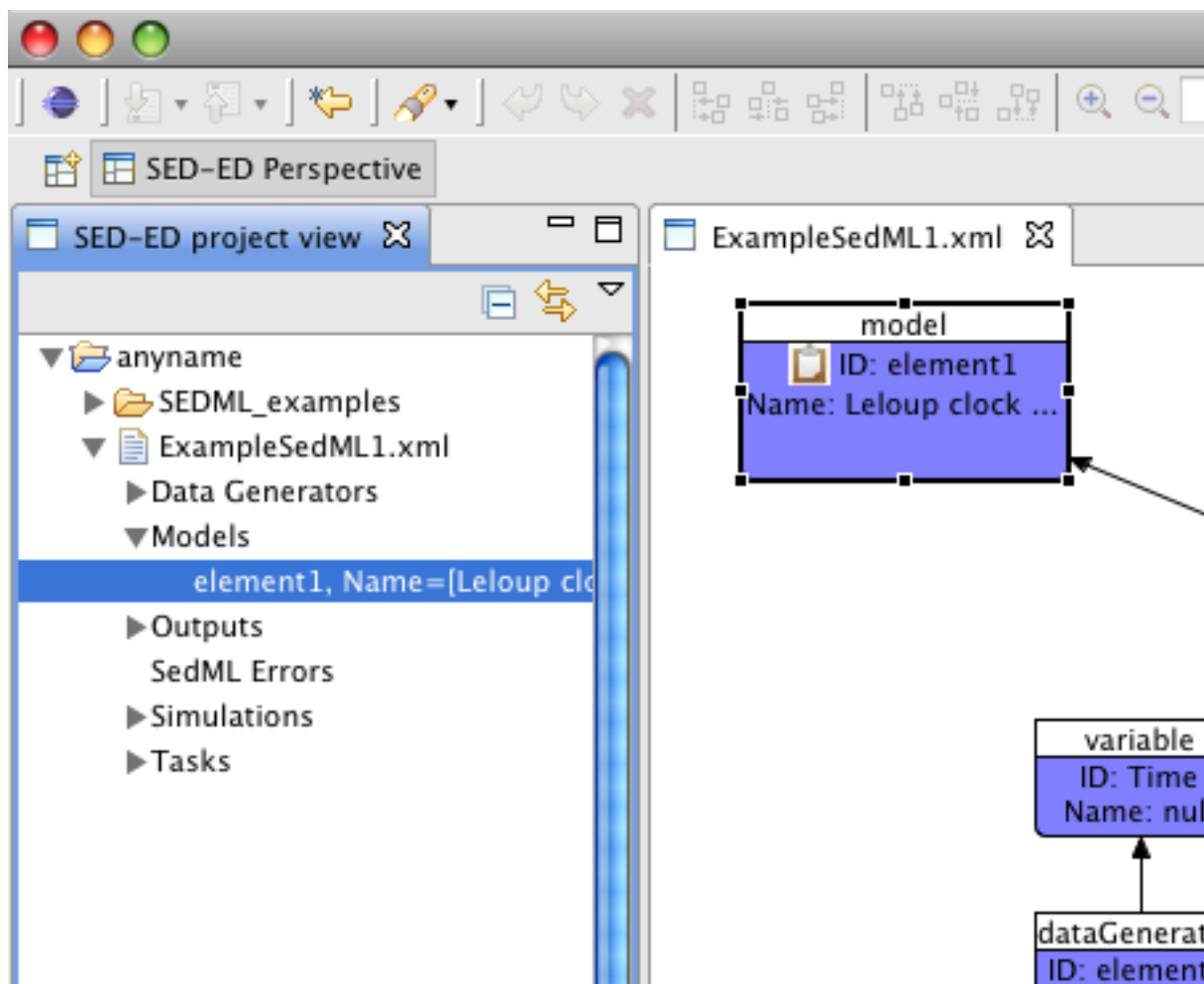


Improving the view

SED-ED contains standard alignment tools and zoom control to help you refine the appearance of the workflow diagram. These are available from the application toolbar.

Navigation

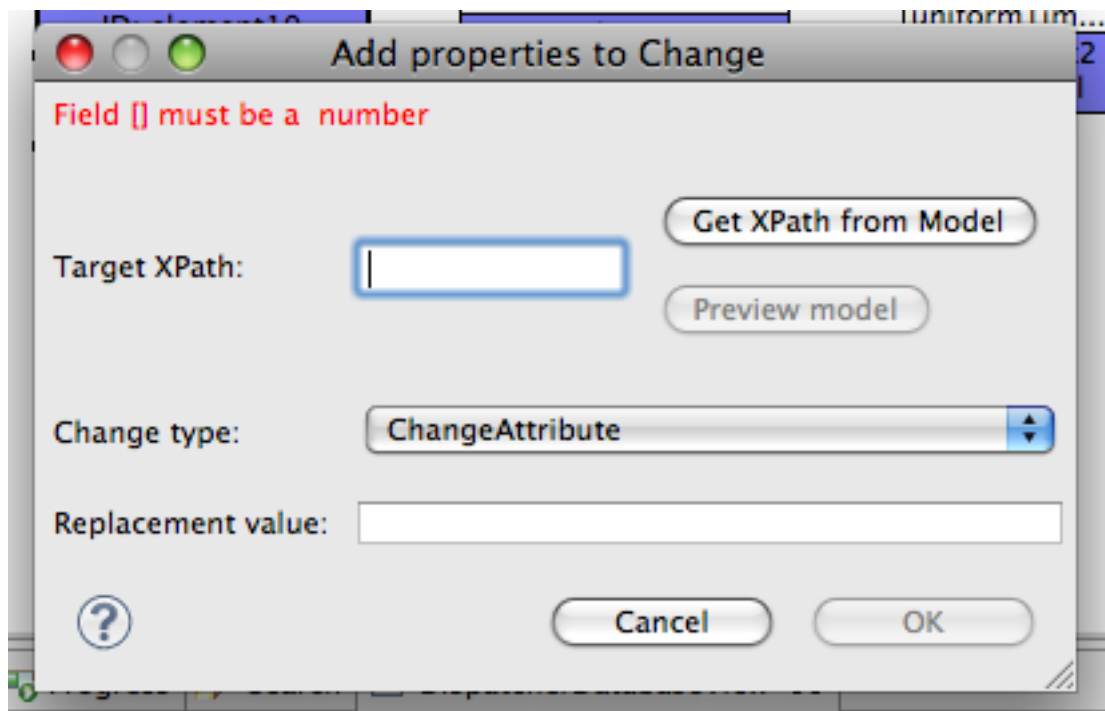
This example file is quite small so probably all the elements are visible in the editor view. However, as documents grow in size it's useful to be able to locate an individual element easily. To do this, use the Project/System view to expand the SED-ML file – clicking on an element in this expanded view will select it in the editor:



More complex editing

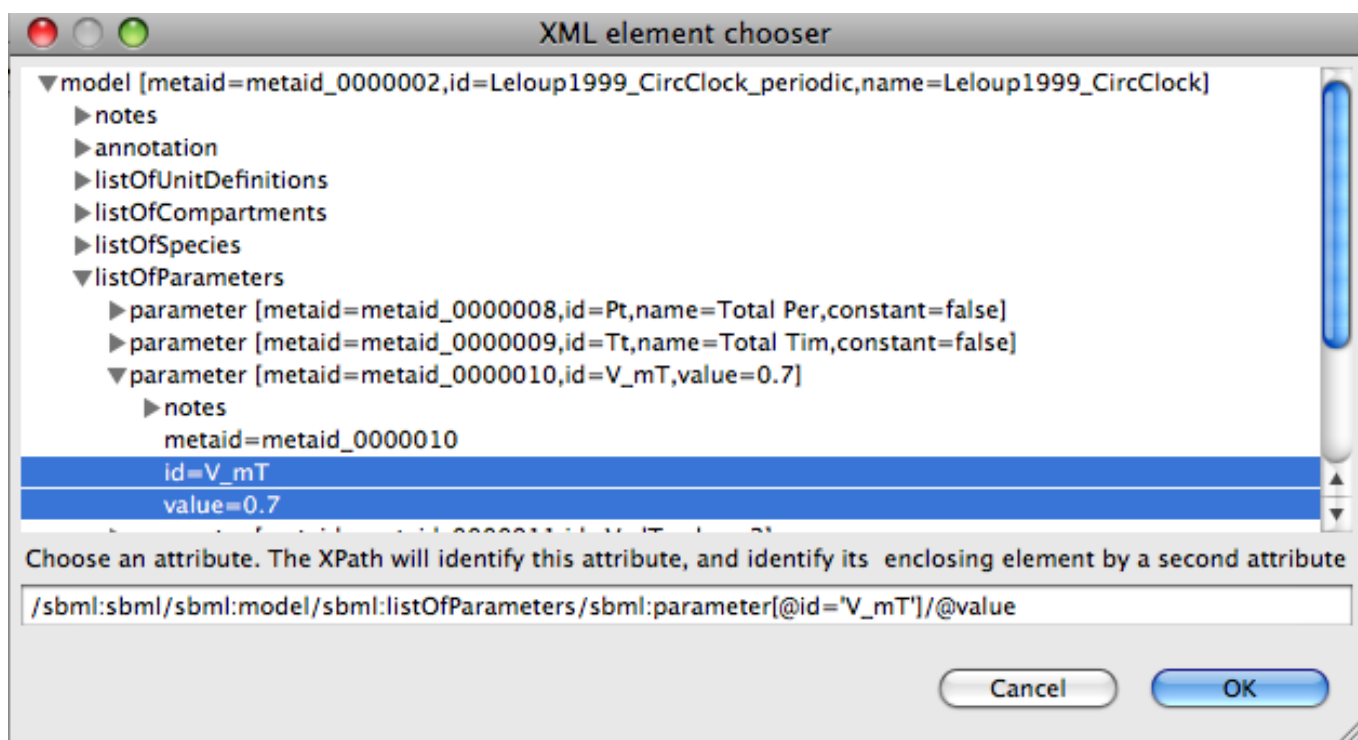
Now, we'll enhance our document to include a variant of the model that modifies two parameter values to alter the model's behaviour. We can do this quite easily by copying the existing model element and adding two changes to it.

1. First of all, copy and paste the existing model.
2. Make a note of the original model's ID.
3. Double click the model copy to open the configuration dialog, and set the 'source' to be the value of the ID of the original model. If you do this correctly the 'Show Preview' button should be active. Click **OK**.
4. Now select the new model and choose 'Add Change' from the context menu.
5. This dialog configures the change you want to apply to the model. In SED-ML you can change specific attributes, add, remove or swap XML elements. In this example we'll change an attribute.



6. Click 'Get XPath from model'.

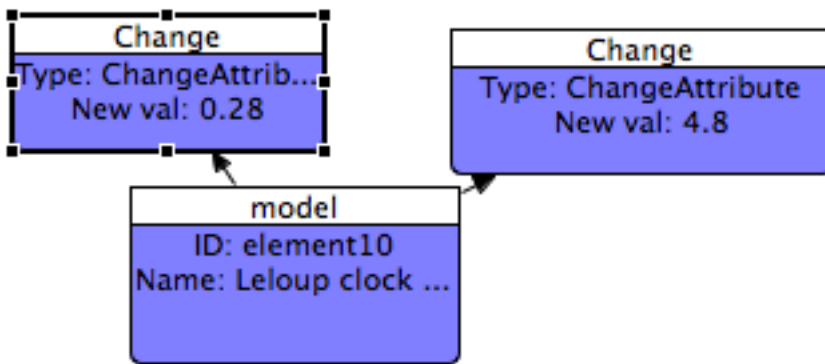
7. Now, we need to identify an element, and the attribute to change for the parameter V_mT. Expand the tree view of the model so that you can see the attributes for that parameter, then, with the shift key held down, click firstly on the **id** attribute, then on **value** so that the XPath expression is the same as in the screenshot below.



Now, set the replacement value to 0.28.

8. Now repeat from step 4, adding a second change where we alter the value of V_dT to be 4.8.

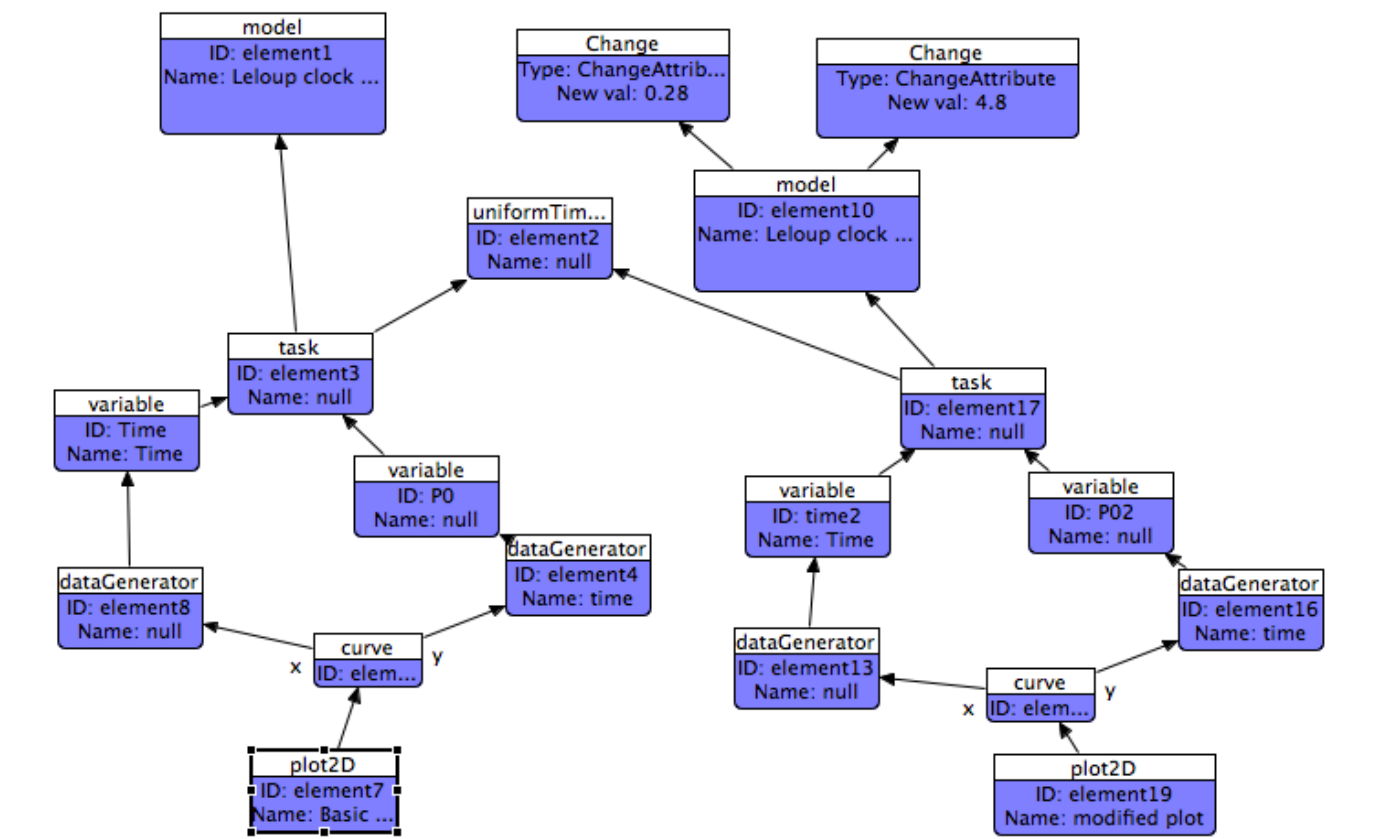
You should now see a new model element with two Change Shapes attached to it.



The changes we applied above have the effect of dampening oscillations in the model. If you're running SBSIVisual then you can see this by reconnecting the task shape to the new model and executing the SED-ML file. (To reconnect, click on the connection between the task and the original model to select it, then drag the connection target from the first model to the second).

To generate a new output showing the simulation output of the new model, make a copy of the existing tasks, dataGenerators, and outputs, and connect the new model to the new copy of the task. You may need to edit the new Variable Ids and Math expressions – every ID must be globally unique in SED-ML.

At the end, you should end up with a diagram something like:



Summary

This tutorial has given you an overview of some of the features of SED-ML and the SED-ED editor. The embedded Help pages for SED-ED contain further information about filtering the view based on output, and autolayout – please refer to them for more detailed explanations of the functionality described here.

We're certainly aware that SED-ED is not perfect yet – please get in touch with us if you have any bug reports or feature requests.

December 2011.