LetItB User's Manual

Okinawa Institute of Science and Technology
Neural Computation Unit

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Contents

1 Introduction

LetItB is developed as a support tool to identify parameters for biochemical reactions. In the current version, LetItB accepts SBML (Systems Biology Markup Language) files as inputs to visually perform the following operations to the SBML models (SBML is the standard format for describing biochemical reaction models in systems biology):

- Create block diagrams to illustrate biochemical reaction networks
- Run simulations
- Identify reaction parameters and estimate their confidence intervals to provide the best recreation for given experimental data (concentration time series of each molecule)
- Assess quantitative model validity from data recreation and model complexity for given experimental data

You can save these results as text files or image files such as jpeg or png via easy-to-use GUI.

LetItB’s internal calculation engine is programmed in C language and its Graphic User Interface is developed with the Qt toolkit. Therefore, you can run and recompile LetItB on any platforms including Windows, Mac OS X, and Linux operation systems if you install an appropriate set of libraries in advance.

2 Getting Started

This chapter briefly describes how to use LetItB by using sample data. Try to use LetItB with sample data by following the instructions in this section. Also, refer to Chapter 3 and later for detailed information about each function.

2.1 Activating Program

Run the LetItB execution file contained in the installation directory.

Start with GUI operation: Double-click LetItB contained in the installation directory.

Start with CUI operation: Use a terminal to run LetItB contained in the installation directory.

Example: Start with CUI operation

From a terminal or like, move to the installation directory, and then execute the following command:

```
> LetItB &
```

2.2 Loading SBML Sample File

From the LetItB's menu, select **File** > **Open SBML**.
In the file dialog, select a SBML file.

Example: Loading a SBML file

Load the SBML sample file contained in the following folder:
"installation directory" > **sampledata** > **Model01** > **model.xml**

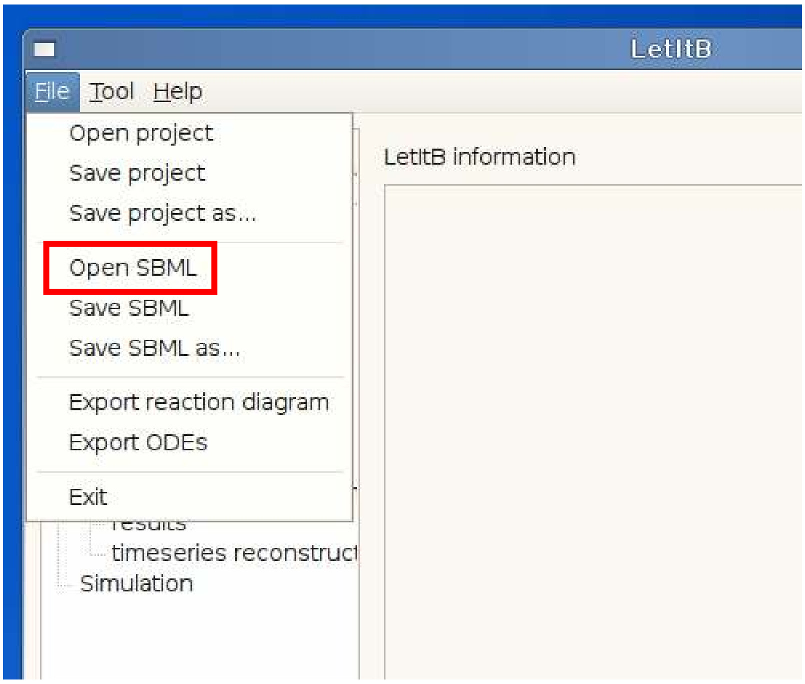


Figure 1 SBML File Loading

2.3 Displaying Diagram

From the LetItB's menu, select **Tool** > **Show reaction diagram**.

Then, you can see a diagram export window.

* The right figure in Figure 2 shows the resultant diagram when you load model.xml.

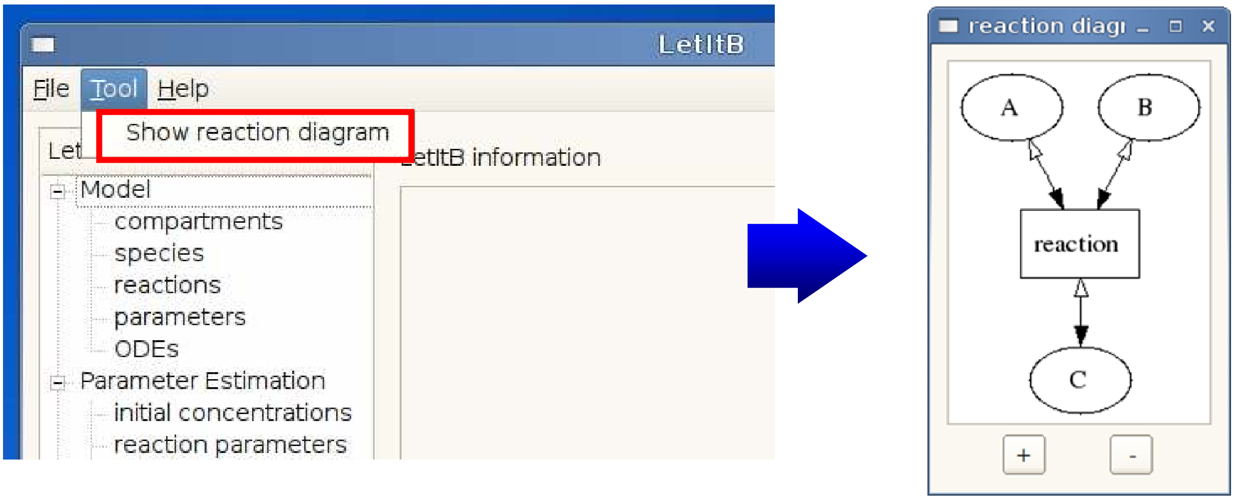


Figure 2: Reaction Diagram Operation Screen (Display)

2.4 Running Simulation

From the tree menu in the left pane, click **Simulation**.

Next, specify options in the **ODE solver option** pane on the right side of the screen.

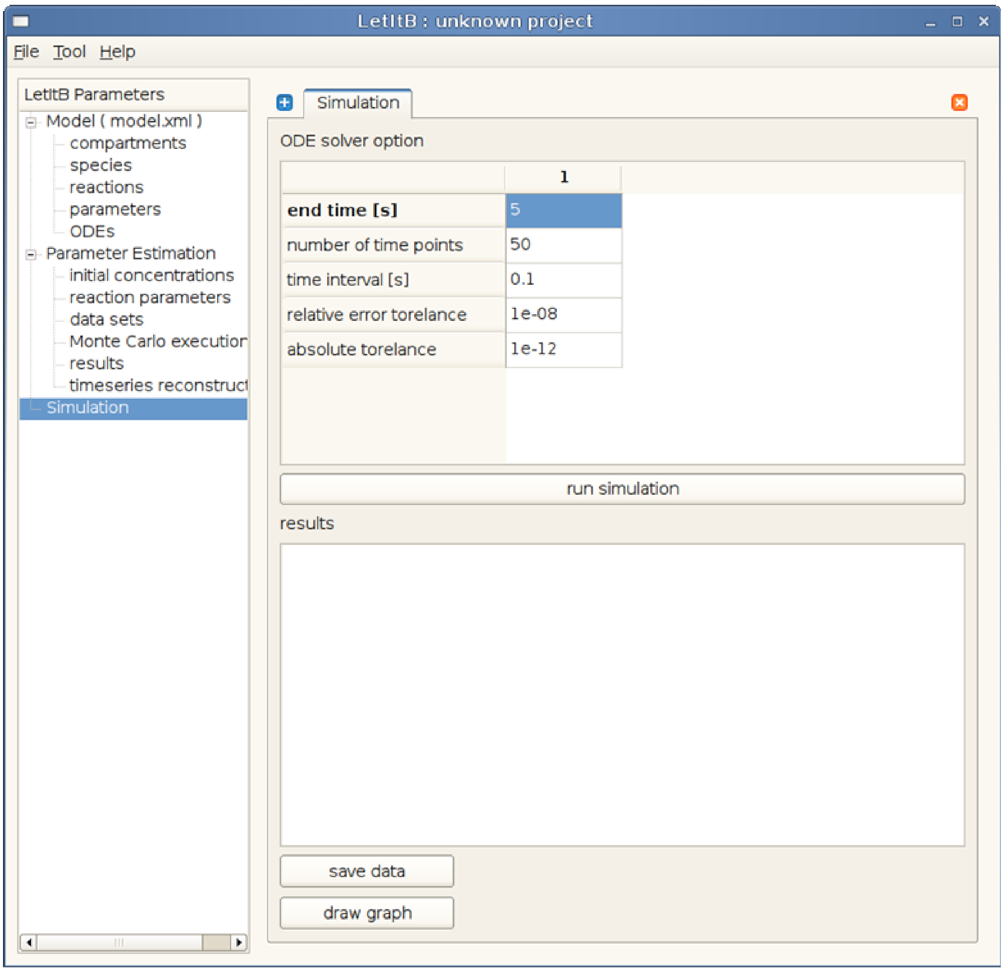
Example: Setting **ODE solver option**

end time: 5 (Time to terminate the simulation)

number of time points: 50 (Number of simulation steps)

* Any options other than above are set by default

Finally, click the **run simulation** button to start the simulation.



	1
end time [s]	5
number of time points	50
time interval [s]	0.1
relative error torelance	1e-08
absolute torelance	1e-12

Figure 3: Simulation Run Screen

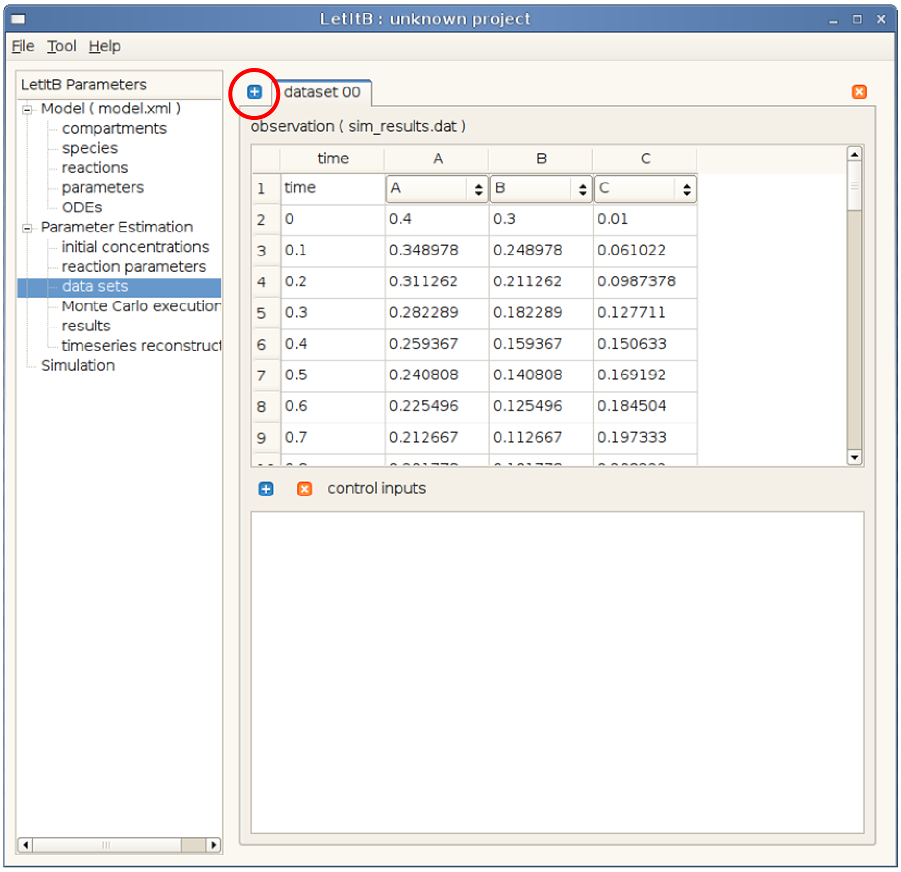
2.5 Saving Simulation Results File

After simulation results are displayed in the **results** pane on the **Simulation** screen, click the **save data** button and save the file with any name.

Example: File name: sim_results.dat

2.6 Defining Simulation Results File Loading

From the tree menu on the left, select **data sets**. On the right side of the **data sets** screen, click the “**+**” on the upper left corner of the screen, and load the previously saved results file (e.g. sim_results.dat).



observation (sim_results.dat)

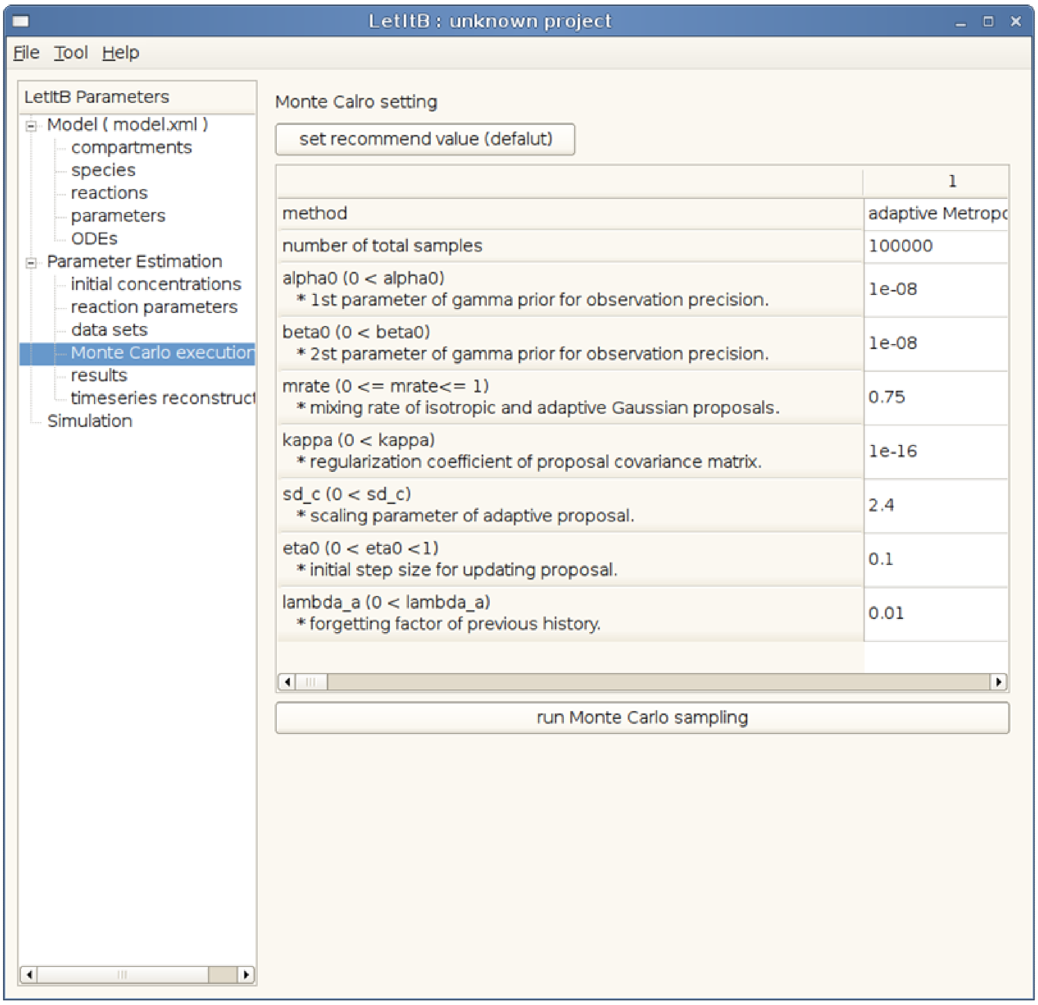
	time	A	B	C
1	time	A	B	C
2	0	0.4	0.3	0.01
3	0.1	0.348978	0.248978	0.061022
4	0.2	0.311262	0.211262	0.0987378
5	0.3	0.282289	0.182289	0.127711
6	0.4	0.259367	0.159367	0.150633
7	0.5	0.240808	0.140808	0.169192
8	0.6	0.225496	0.125496	0.184504
9	0.7	0.212667	0.112667	0.197333

Figure 4 : Results File Loading Screen

2.7 Performing Parameter Estimation

From the tree menu on the left, select **Monte Carlo execution** and click the **run Monte Carlo sampling** button on the right side of the screen. Then, LetItB starts parameter estimation.

NOTE: The run time required for each parameter estimation depends on your machine environment and other environment factors.



	1
method	adaptive Metropc
number of total samples	100000
alpha0 (0 < alpha0) * 1st parameter of gamma prior for observation precision.	1e-08
beta0 (0 < beta0) * 2st parameter of gamma prior for observation precision.	1e-08
mrate (0 <= mrate<= 1) * mixing rate of isotropic and adaptive Gaussian proposals.	0.75
kappa (0 < kappa) * regularization coefficient of proposal covariance matrix.	1e-16
sd_c (0 < sd_c) * scaling parameter of adaptive proposal.	2.4
eta0 (0 < eta0 <1) * initial step size for updating proposal.	0.1
lambda_a (0 < lambda_a) * forgetting factor of previous history.	0.01

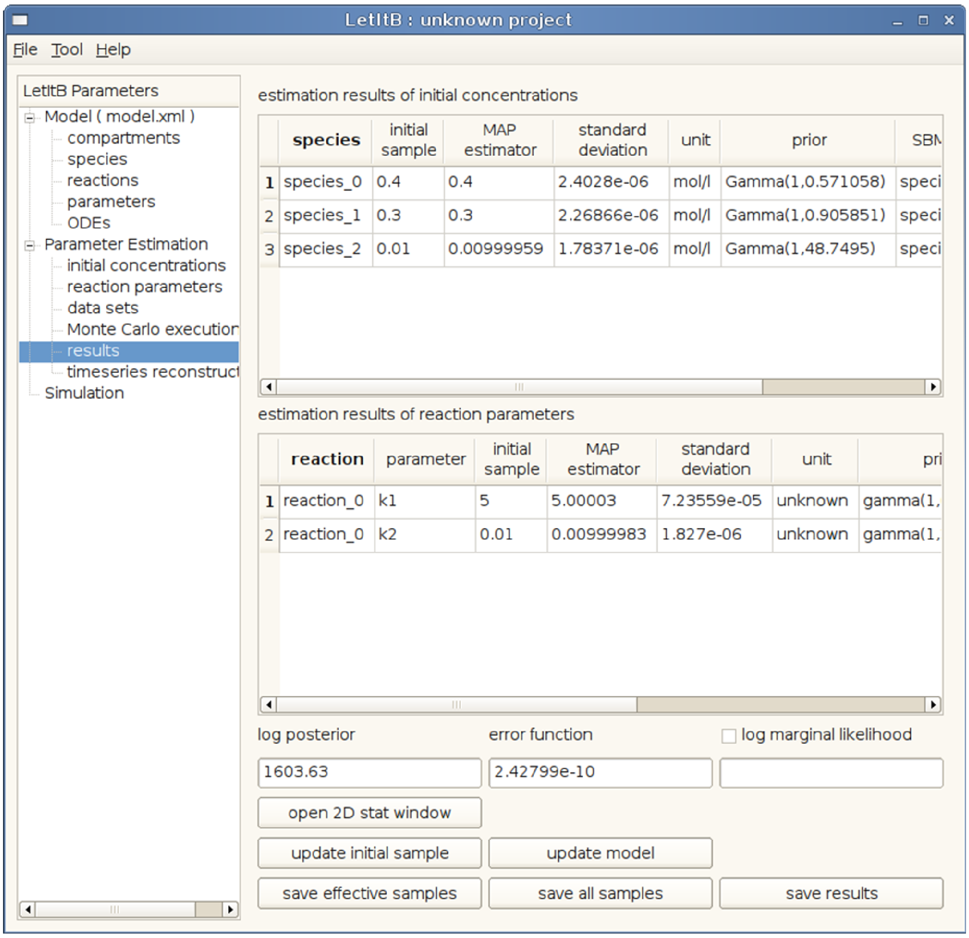
Figure 5 : Parameter Estimation Execution Screen

2.8 Displaying Parameter Estimation Results

After parameter estimation completes, select **results** from the tree menu on the left. Then, a list of the estimation results is displayed on the right side of the screen.

You can view more detailed information about the results by using the **open 2D stat window** button or the **log marginal likelihood** checkbox on the same screen.

NOTE: For more information, see Section 6.5 “results”.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SB
1	species_0	0.4	0.4	2.4028e-06	mol/l	Gamma(1,0.571058)	speci
2	species_1	0.3	0.3	2.26866e-06	mol/l	Gamma(1,0.905851)	speci
3	species_2	0.01	0.00999959	1.78371e-06	mol/l	Gamma(1,48.7495)	speci

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	pri
1	reaction_0	k1	5	5.00003	7.23559e-05	unknown	gamma(1,
2	reaction_0	k2	0.01	0.00999983	1.827e-06	unknown	gamma(1,

log posterior: 1603.63

error function: 2.42799e-10

☐ log marginal likelihood:

Figure 6 : Estimation Results Display Screen

2.9 Storing Project File

To save the current project status, select **File** > **Save project as…** from the LetItB’s menu. When a file dialog appears, specify a desirable file name and save the file.

3 Starting and Exiting LetItB Software

3.1 Starting LetItB

To start LetItB, run the LetItB execution file contained in the installation directory.

Depending on your OS (Operating System), select an appropriate operation method from the below:

Start with GUI operation: Double-click LetItB contained in the installation directory

Start with CUI operation: Use a terminal to run LetItB contained in the installation directory

After starting LetItB, a LetItB Start screen shown in the figure below (Figure 7) appears.

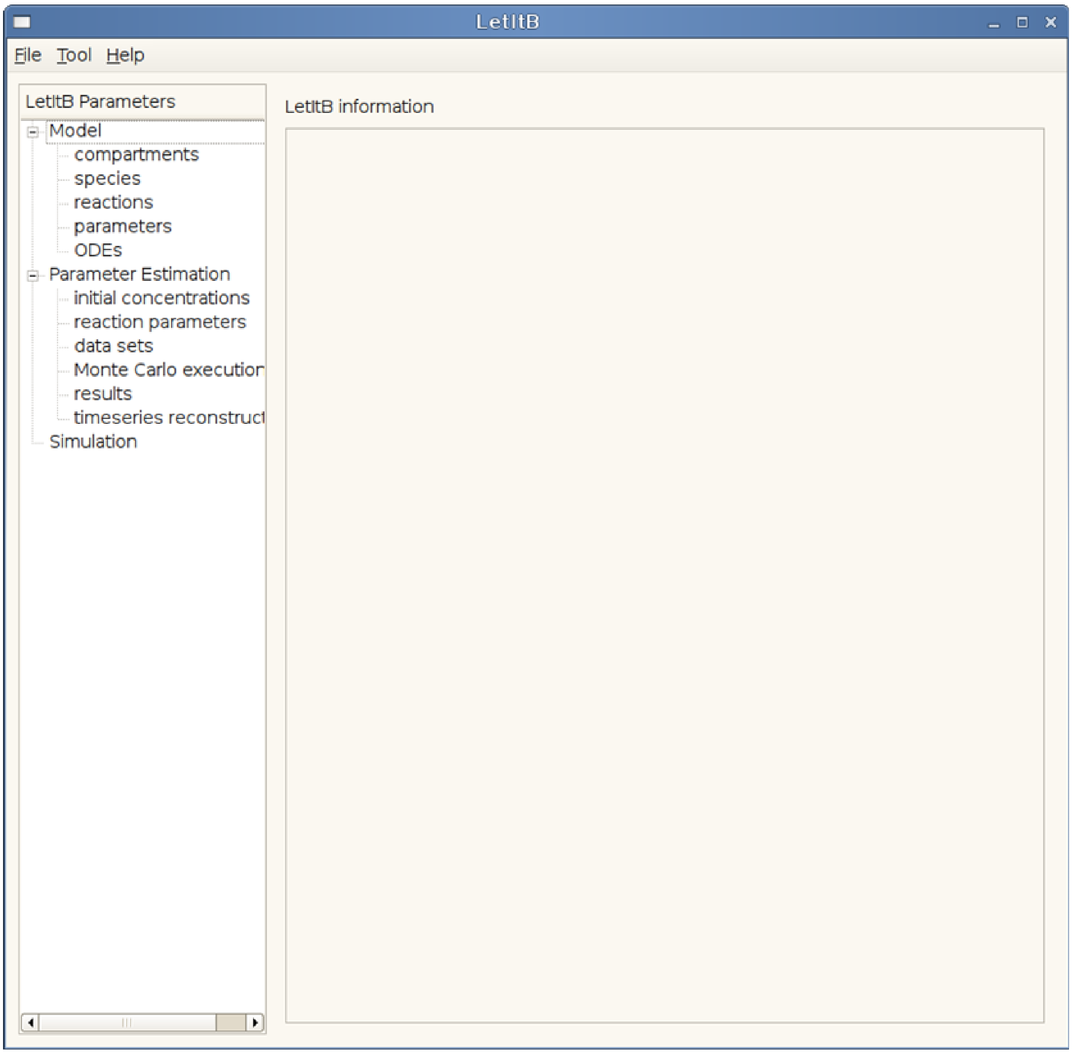


Figure 7: LetItB Start Screen

3.2 Exiting LetItB

To exit LetItB, select **File** > **Exit** from the LetItB's menu or click the "**×**" button on the upper right corner of the screen.

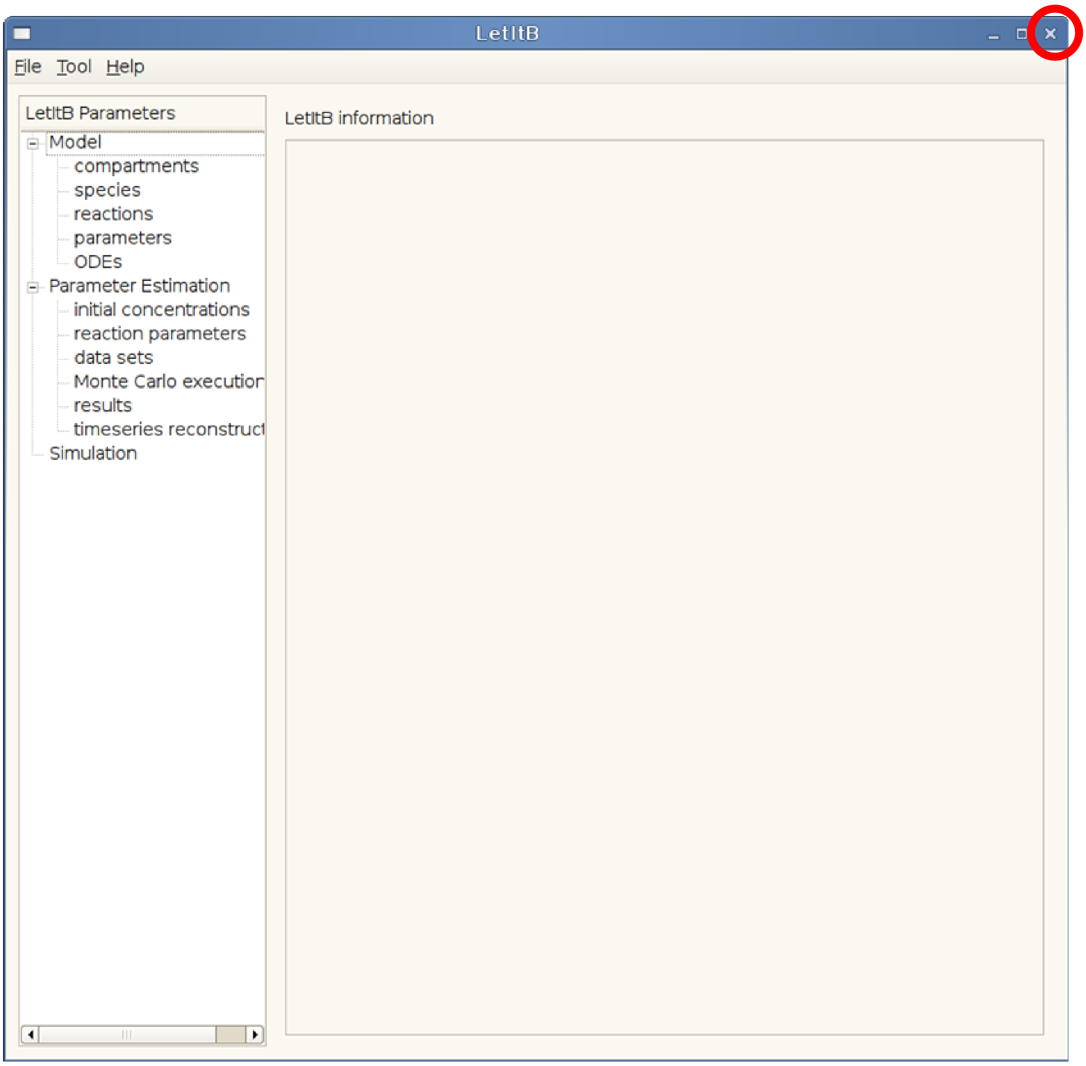


Figure 8: LetItB Exit Screen (Sample)

4 Loading, Writing, and Exporting Files

4.1 Loading Project File

From the LetItB's menu, select **File** > **Open project**, and in the file dialog, select a project file (.lbp file). After you select a .lbp file, the existing project data is automatically loaded into LetItB.

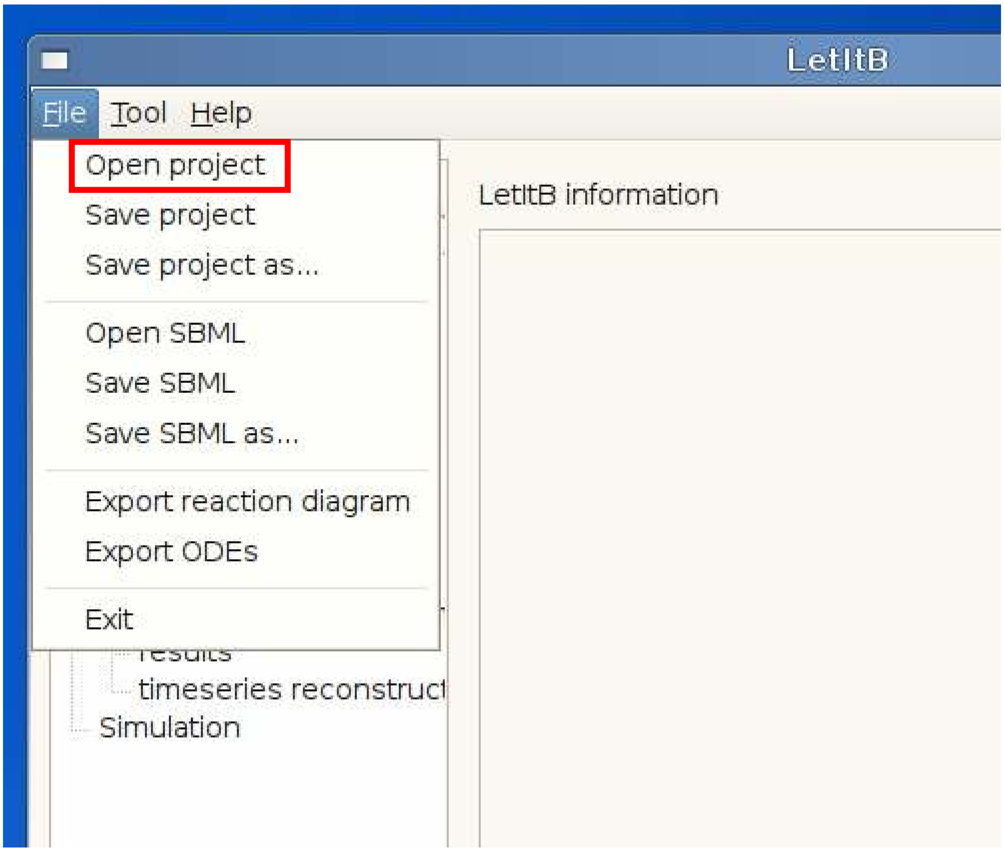


Figure 9: Project File Loading

4.2 Writing Project File

From the LetItB's menu, select **File** > **Save project** or **Save project as…**. As a file dialog appears when you select **Save project as…**, specify where the file will be saved and a name of the file in the file dialog displayed.

Save project (overwrite saving): Automatically overwrite the existing project file
Save project as... (saving under a new file name): Create a new project file

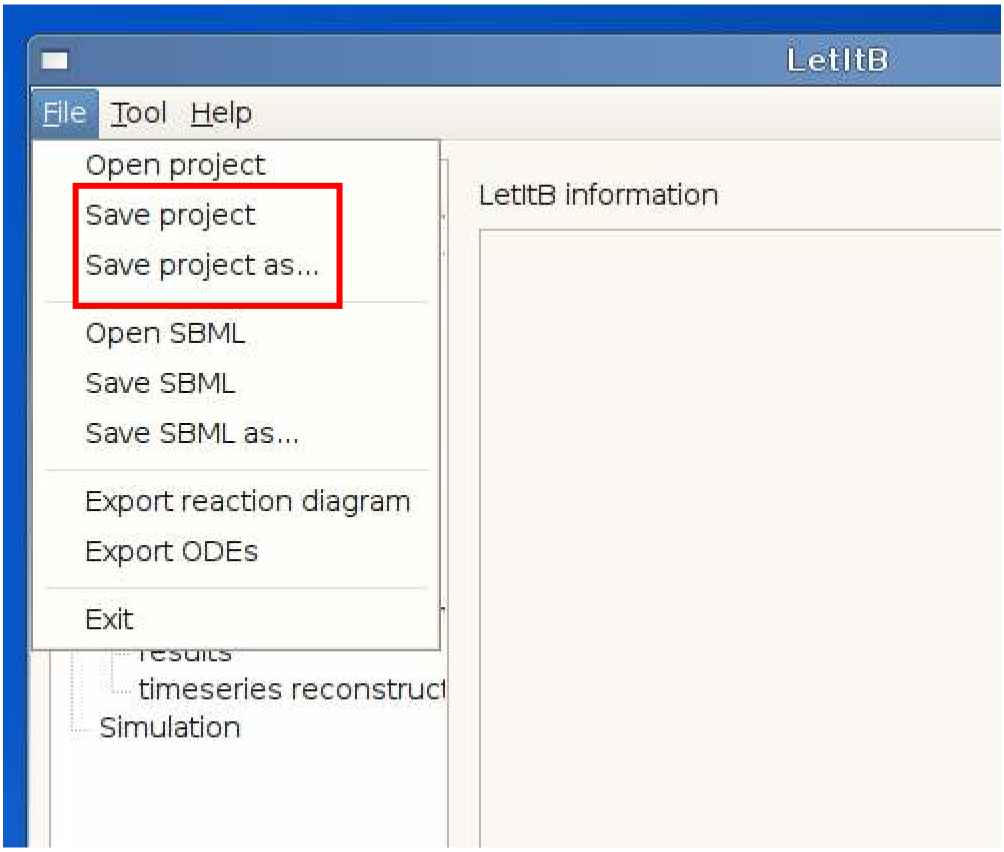


Figure 10: Project File Writing

This LetItB software allows you to load/write project files both in the SBML (System Biology Markup Language) Level 1 and Level 2 formats.

For the units to be used in LetItB, liter (l), Mol (mol) and second (s) are used, unless expressly defined in the **compartment**, **species** and **parameter** tags in SBML files.

(For **parameter**, however, LetItB displays “**unknown**” by default if no **unit** definition is found in the **parameter** tag.)

4.3 Loading SBML File

From the LetItB’s menu, select **File** > **Open SBML** and select a SBML file in the file dialog. After selecting a file, the SBML file data is automatically loaded into LetItB.

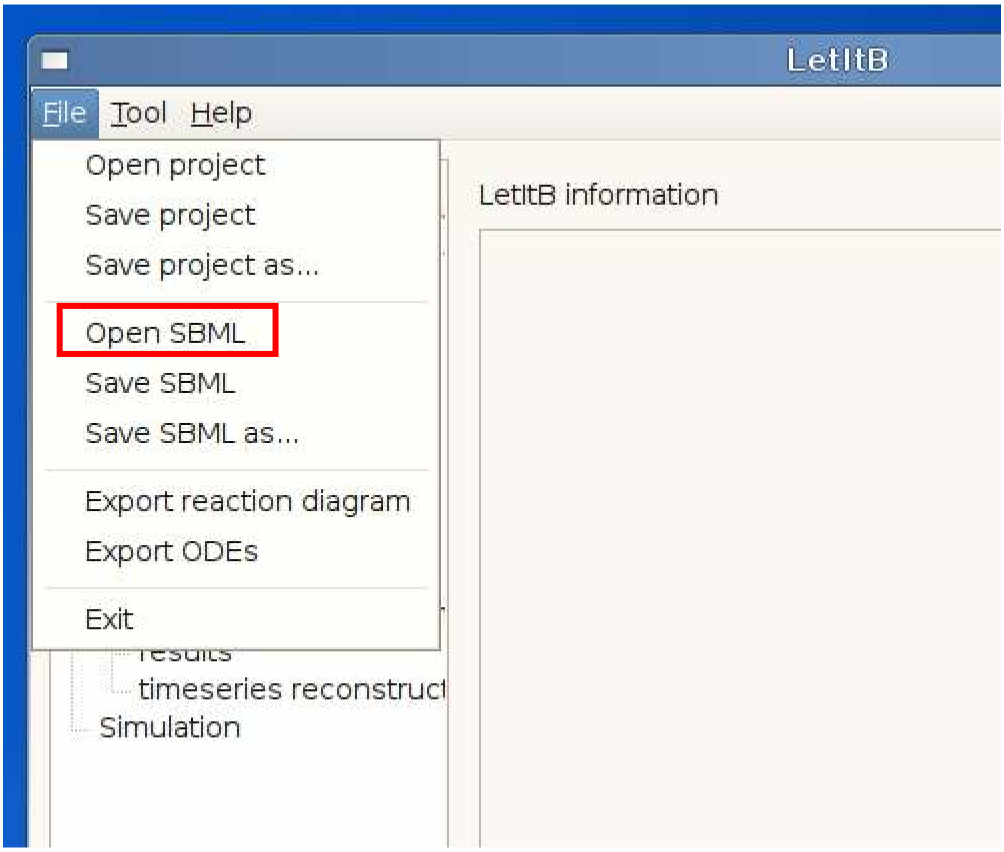


Figure 11: SBML File Loading

4.4 Writing SBML File

From the LetItB’s menu, select **File** > **Save SBML** or **Save SBML as…**. As a file dialog appears when you select **Save SBML as…**, specify where the file will be saved and a name of the SBML file in the file dialog.

Save SBML (overwrite saving): Automatically overwrite the existing SBML file
Save SBML as... (saving under a new file name): Create a new SBML file

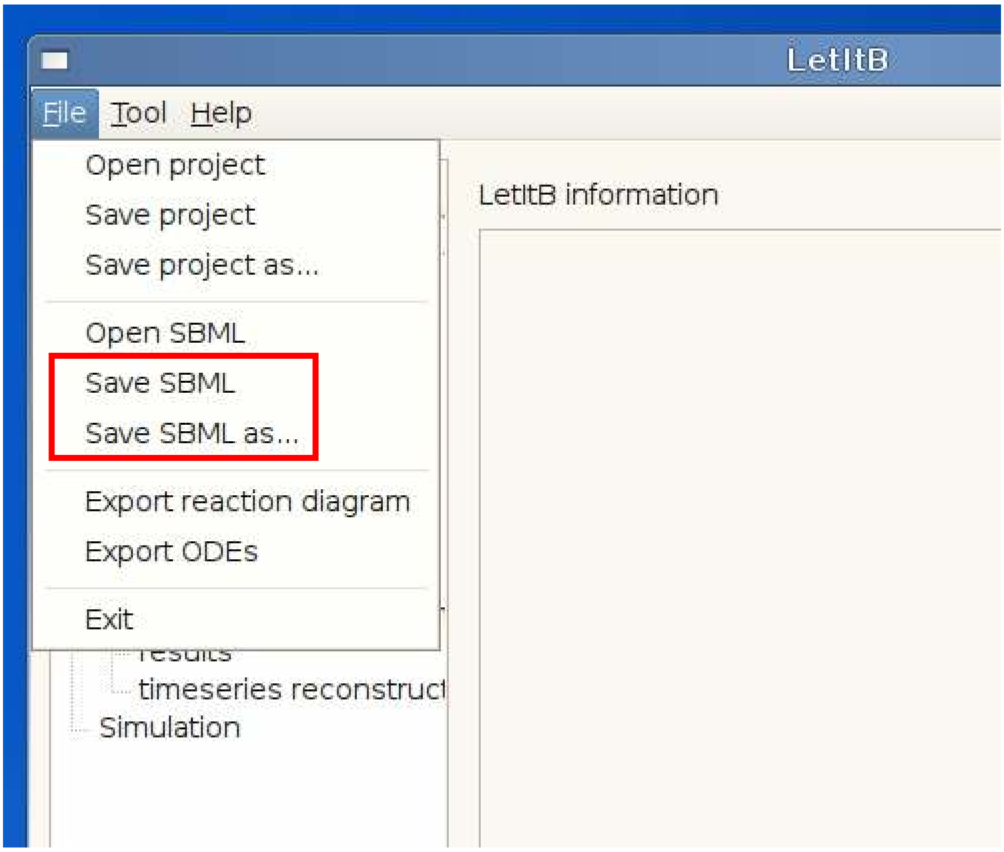


Figure 12: SBML File Writing

4.5 Exporting Reaction Diagram

You can export a diagram of the simulation model defined in SBML files.

[To display Reaction Diagram]

After loading the SBML file (See Section 4.3), select **Tool** > **Show reaction diagram** from the LetItB's menu. Then, a reaction diagram export window will be displayed (Figure 13).

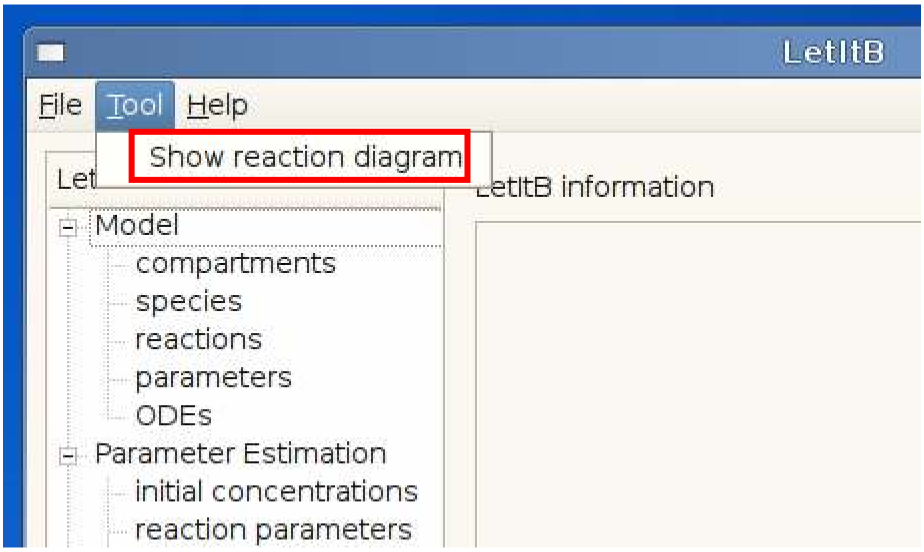


Figure 13: Reaction Diagram Export Operation Screen (Display)

Diagram Export Window

+ button: Zoom in the diagram

- button: Zoom out the diagram

* The right figure shows the resultant diagram when loading sample data.

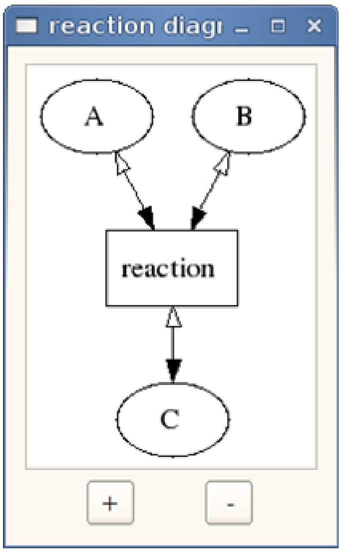


Figure 14: Resultant Reaction Diagram Export

[To save the reaction diagram]

You can save the reaction diagram as image data. After loading the SBML file (See Section 4.3), select **File** > **Export reaction diagram** from the LetItB's menu. When a file dialog appears, select where the file will be exported, a name of the file and an image format you want to save, and then save the data.

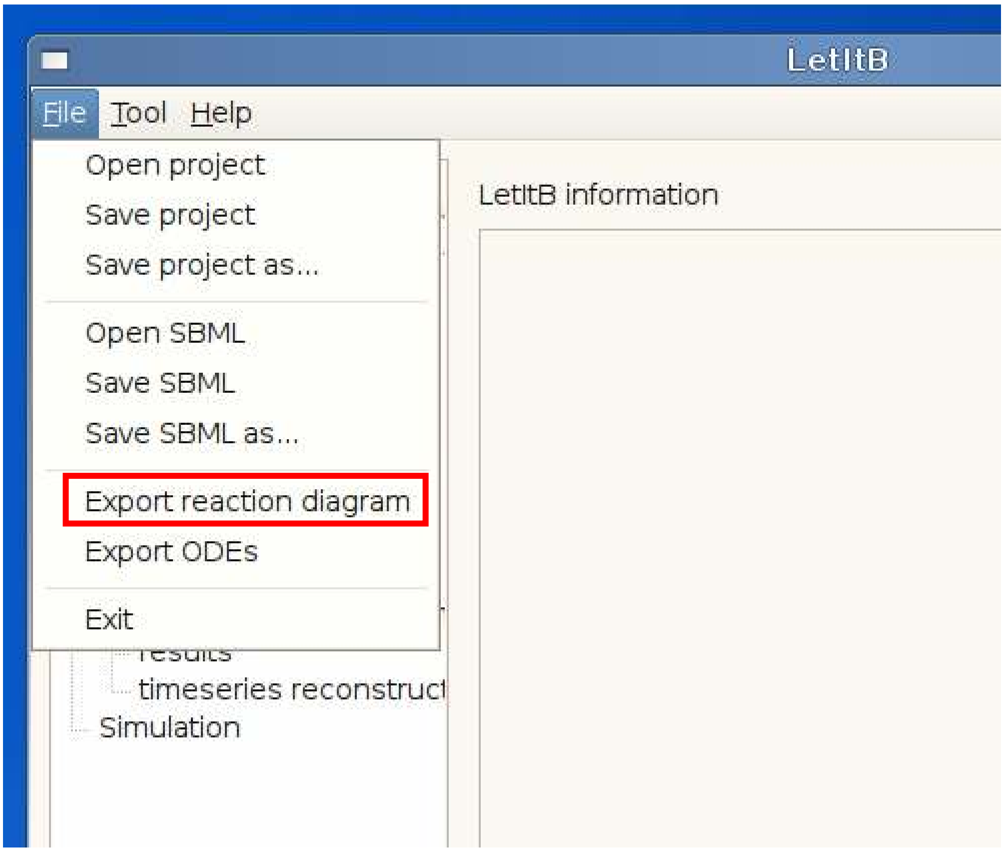


Figure 15: Reaction Diagram Export Operation Screen (File Store)

4.6 Exporting ODEs

You can export Ordinary Differential Equations (ODEs) of the simulation model defined in the SBML file. For more information on how to display ODEs, see Section 5.5.

[To save ODEs]

You can save ODEs as text data. After loading the SBML file (See Section 4.3), select **File** > **Export ODEs** from the LetItB's menu. When a file dialog appears, select where the file will be exported and a name of the file, and then save the data.

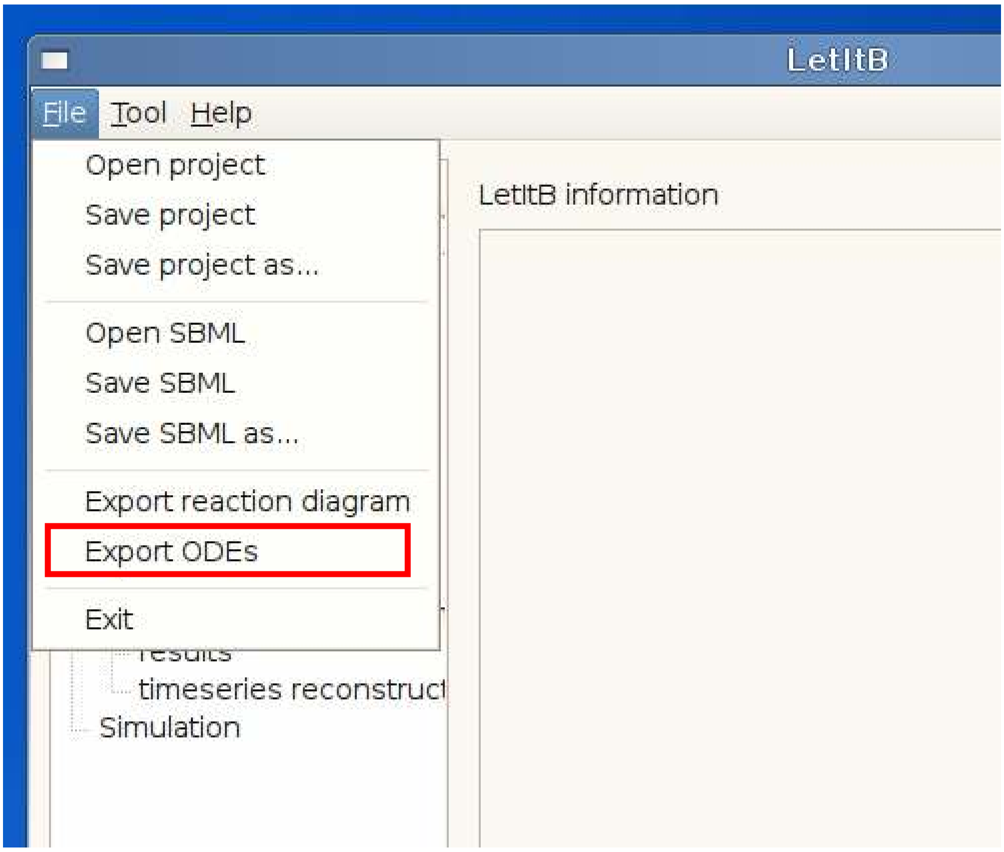


Figure 16: ODEs Export (File Store)

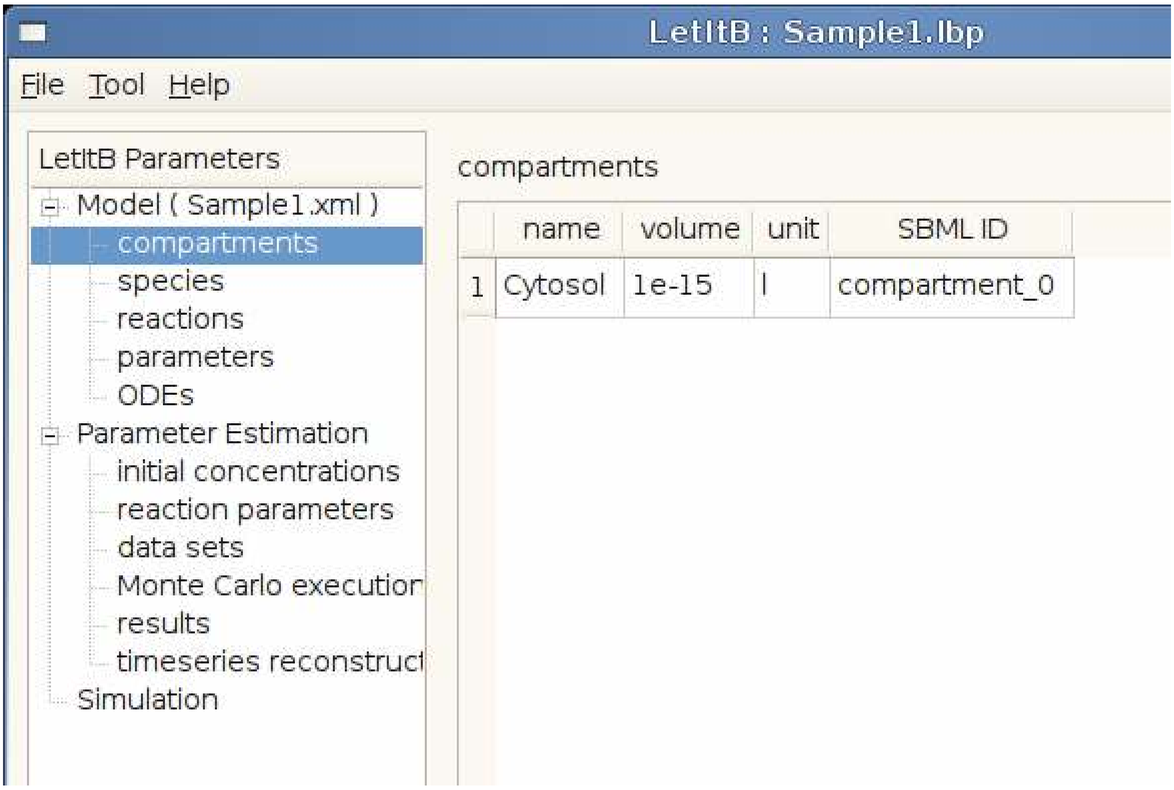
5 Model

The **Model** part is divided into 5 subparts: **compartments**, **species**, **reactions**, **parameters** and **ODEs**. With the Model part, you can display a list of relevant items of the loaded SBML file and edit their numeric data.

By selecting one of the subparts (**compartments**, **species**, **reactions**, **parameters** or **ODEs**) under **Model** in **LetItB Parameters** in the left pane, you can list corresponding information of the selected subpart in the right pane.

5.1 compartments

The **compartments** subpart displays the information about **compartment** in the SBML file.



	name	volume	unit	SBML ID
1	Cytosol	1e-15	l	compartment_0

Figure 17: compartments Screen

[About **compartments** screen]

name: Display **name** information in the **compartment** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

volume: Display **volume** or **size** information in the **compartment** tag

* If there is no information about **volume** or **size** in the tag, set (l) as default.

unit: Display the unit used in **compartment** (Default : liter (l))

SBML ID: Display **ID** information in the **compartment** tag

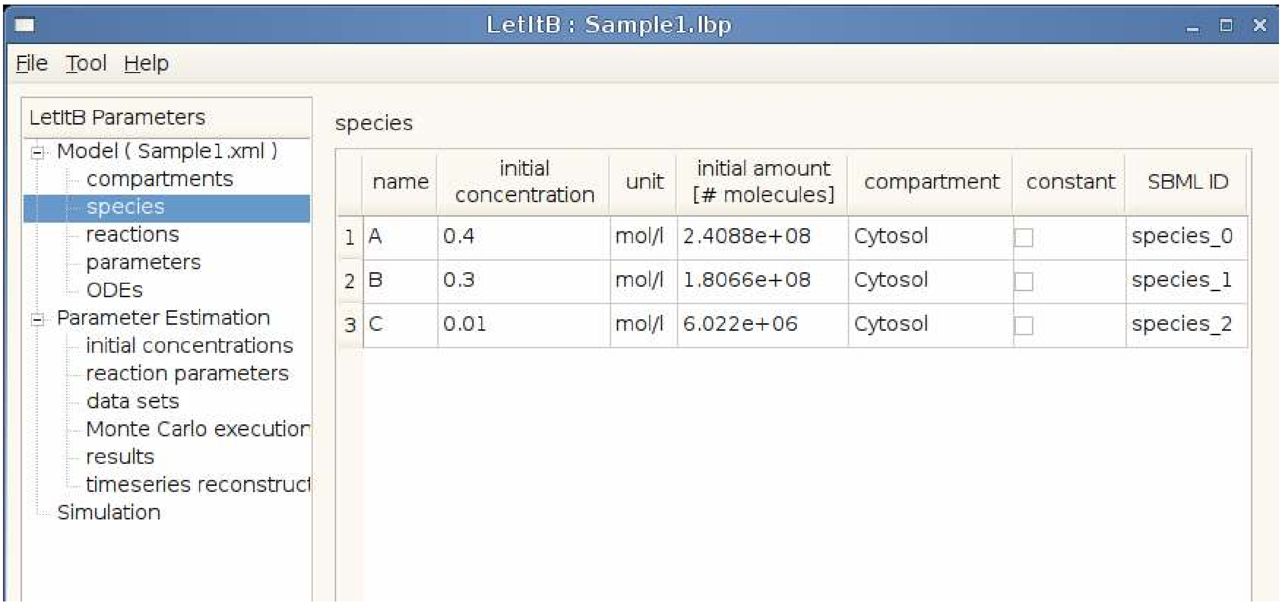
[To edit data]

You can edit numeric data in the **volume** item. Select any cells you want to edit, and then enter values.

NOTE: You cannot select and edit any cells other than those in the volume item.

5.2 species

The **species** subpart displays the information about **species** in the SBML file.



	name	initial concentration	unit	initial amount [# molecules]	compartment	constant	SBML ID
1	A	0.4	mol/l	2.4088e+08	Cytosol	☐	species_0
2	B	0.3	mol/l	1.8066e+08	Cytosol	☐	species_1
3	C	0.01	mol/l	6.022e+06	Cytosol	☐	species_2

Figure 18: species Screen

[About **species** screen]

name: Display **name** information in the **species** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

initial concentration: Display **initialConcentration** information in the **species** tag

* If there is no **initialConcentration** information in the tag, define (1) as default.

unit: Display the unit used in **species** (Default: mol/l)

initial amount: Display the **initial amount** defined as **initial concentration** information

* The **initial amount** is calculated by the calculation formula:

volume item in the **compartments** subpart × **initial concentration** item in the **compartments** subpart × 6.022e+23

compartment: Display **compartment** information in the **species** tag

constant: Display **constant** information in the **species** tag

* If there is no information about **constant** in the tag, “false” (constant = false) is set by default.

SBML ID: Display **ID** information in the **species** tag

[To edit data]

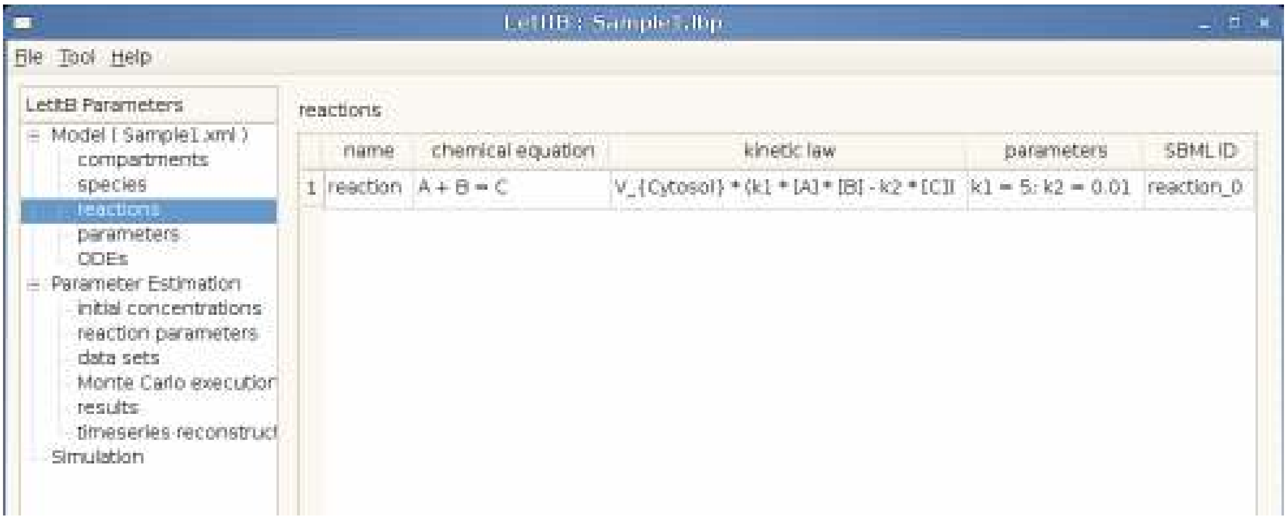
You can edit numeric data in the **initial concentration** item and the check box in the **constant** item. If you edit the **initial concentration** item, select any cells you want to edit, and then enter values.

With the check box in the **constant** item, you can enable/disable the check box by clicking appropriate cells.

NOTE: You cannot select and edit any cells other than those in the initial concentration and constant items.

5.3 reactions

The **reactions** subpart displays the information about **reaction** in the SBML file.



reactions

	name	chemical equation	kinetic law	parameters	SBML ID
1	reaction	A + B = C	V_{Cytosol} * (k1 * [A] * [B] - k2 * [C]	k1 = 5; k2 = 0.01	reaction_0

Figure 19: reactions Screen

[About **reactions** screen]

name: Display **name** information in the **reaction** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

chemical equation: Display chemical equations for **reaction**

kinetic law: Display the kinetic law for **reaction**

parameters: Display **ID** or **name** of **parameter** and corresponding numeric data

SBML ID: Display **ID** information in the **reaction** tag

NOTE: You cannot edit the data on the reactions screen.

5.4 parameters

The **parameters** subpart displays the information about **parameter** in the SBML file.

parameters

	reaction	parameter	value	unit	kinetic law	chemical equation	SBML ID
1	reaction	k1	5	unknown	V_{Cytosol} * (k1 * [A] * [B] - k2 * [C])	A + B = C	reaction_0
2	reaction	k2	0.01	unknown	V_{Cytosol} * (k1 * [A] * [B] - k2 * [C])	A + B = C	reaction_0

Figure 20: parameters Screen

[About **parameters** screen]

reaction: Display **name** information in the **reaction** tag (See the **name** item in Section 5.3)

*If there is no **name** information in the tag, LetItB displays **ID** information.

parameter: Display **ID** information in the **parameter** tag

value: Display **value** information in the **parameter** tag

unit: Display the unit used in **parameter**

* If there is no **unit** information in the tag, LetItB displays “unknown” by default.

kinetic law: Display the kinetic law for **parameter**

chemical equation: Display the chemical equation for **parameter**

reaction ID: Display **ID** information in the **reaction** tag

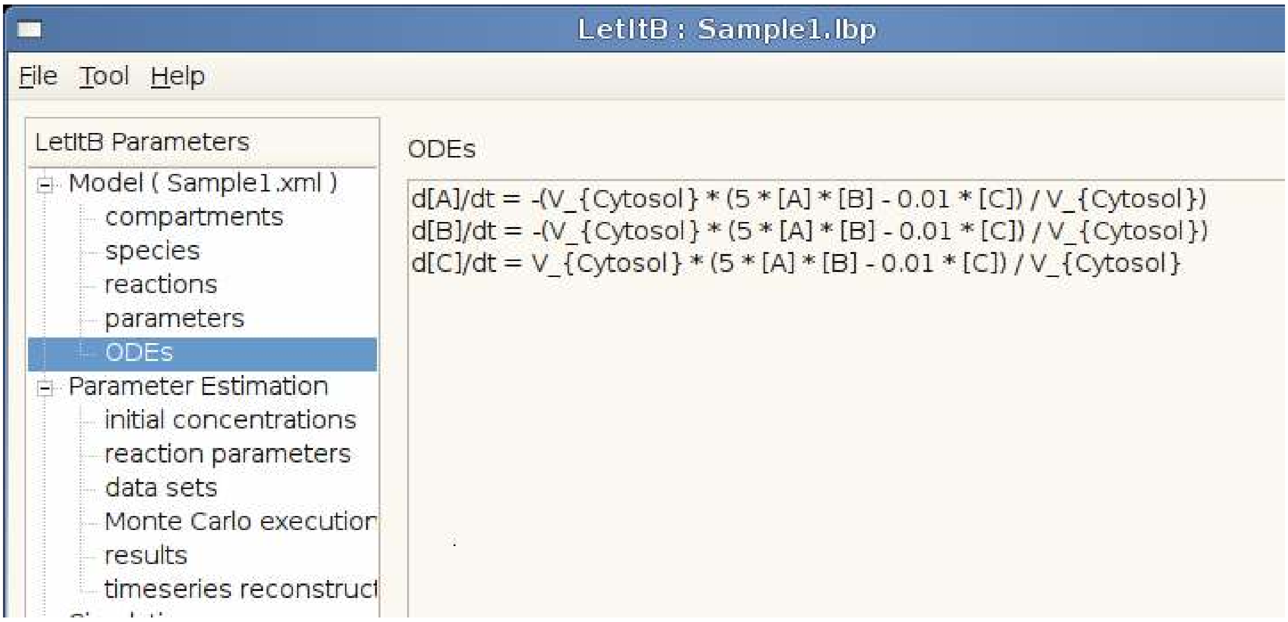
[To edit data]

You can edit numeric data in the **value** item. Select any cells you want to edit, and then enter values.

NOTE: You cannot select and edit any cells other than those in the value item.

5.5 ODEs

The **ODEs** subpart displays Ordinary Differential Equations (ODEs) of the simulation model defined in the SBML file.



```
d[A]/dt = -(V_{Cytosol} * (5 * [A] * [B] - 0.01 * [C]) / V_{Cytosol})
d[B]/dt = -(V_{Cytosol} * (5 * [A] * [B] - 0.01 * [C]) / V_{Cytosol})
d[C]/dt = V_{Cytosol} * (5 * [A] * [B] - 0.01 * [C]) / V_{Cytosol}
```

Figure 21: ODEs Screen

If you want to save the exported ODEs data, see Section 4.6.

NOTE 1: You cannot edit the data on the ODEs screen.

NOTE 2: ODEs are represented in the formats used in the SBML ODE Solver.

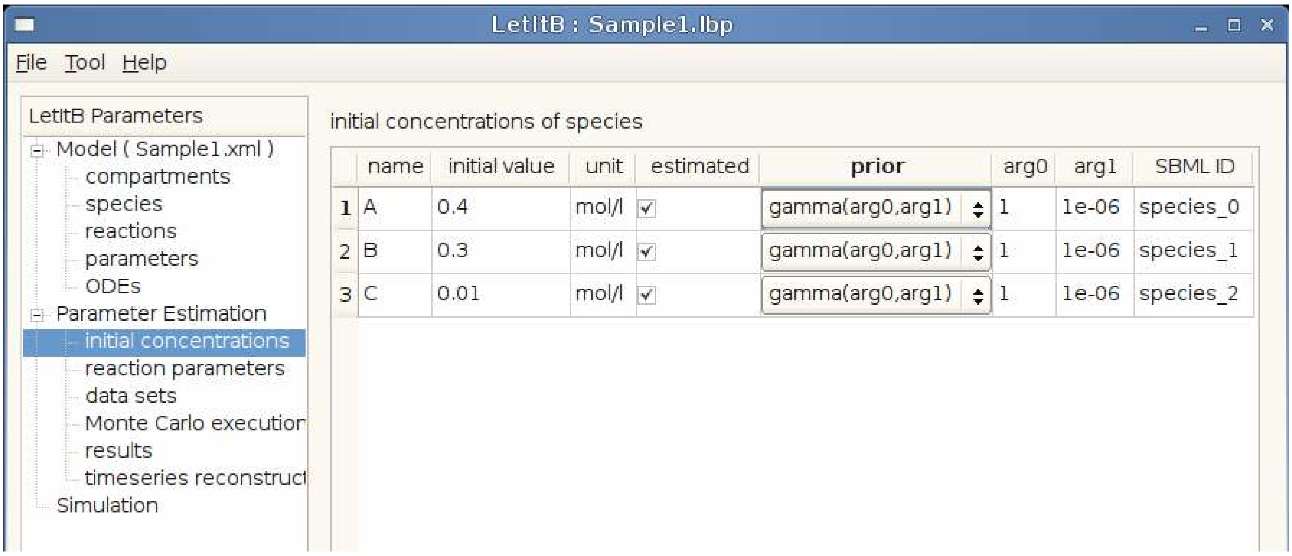
6 Parameter Estimation

The **Parameter Estimation** part is divided into 6 subparts: **initial concentrations**, **reaction parameters**, **data sets**, **Monte Carlo execution**, **results** and **timeseries reconstruction**. Using the simulation model defined in the loaded SBML file, you can list relevant items, edit numeric data, perform the parameter estimation, display results and save the estimation results data.

By selecting one of the subparts (**initial concentrations**, **reaction parameters**, **data sets**, **Monte Carlo execution**, **results** or **timeseries reconstruction**) under **Parameter Estimation** in **LetItB Parameters** in the left pane, you can list corresponding information of the selected subpart in the right pane.

6.1 initial concentrations

The **initial concentrations** subpart displays the information on estimating initial concentrations.



initial concentrations of species

	name	initial value	unit	estimated	prior	arg0	arg1	SBML ID
1	A	0.4	mol/l	☑	gamma(arg0,arg1)	1	1e-06	species_0
2	B	0.3	mol/l	☑	gamma(arg0,arg1)	1	1e-06	species_1
3	C	0.01	mol/l	☑	gamma(arg0,arg1)	1	1e-06	species_2

Figure 22: initial concentrations Screen

[About **initial concentrations** screen]

name: Display **name** information in the **species** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

initial value: Display **initialConcentration** information in the **species** tag

* If there is no **initialConcentration** information in the tag, LetItB sets (1) as default.

unit: Display the unit used in **species** (Default: mol/l)

estimated: Display the factors enabled for parameter estimation (Default: All factors are defined for parameter estimation targets)

prior: Display applicable probability distribution functions used as **prior**

arg0: Display the first argument of **prior**

arg1: Display the second argument of **prior**

SBML ID: Display **ID** information in the **species** tag

[To edit data]

You can edit numeric data in **initial value**, **arg0** and **arg1** items. Select any cells you want to edit, and then enter values.

With the check boxes in the **estimated** item, you can enable/disable any factors you want for parameter estimation targets by clicking appropriate cells.

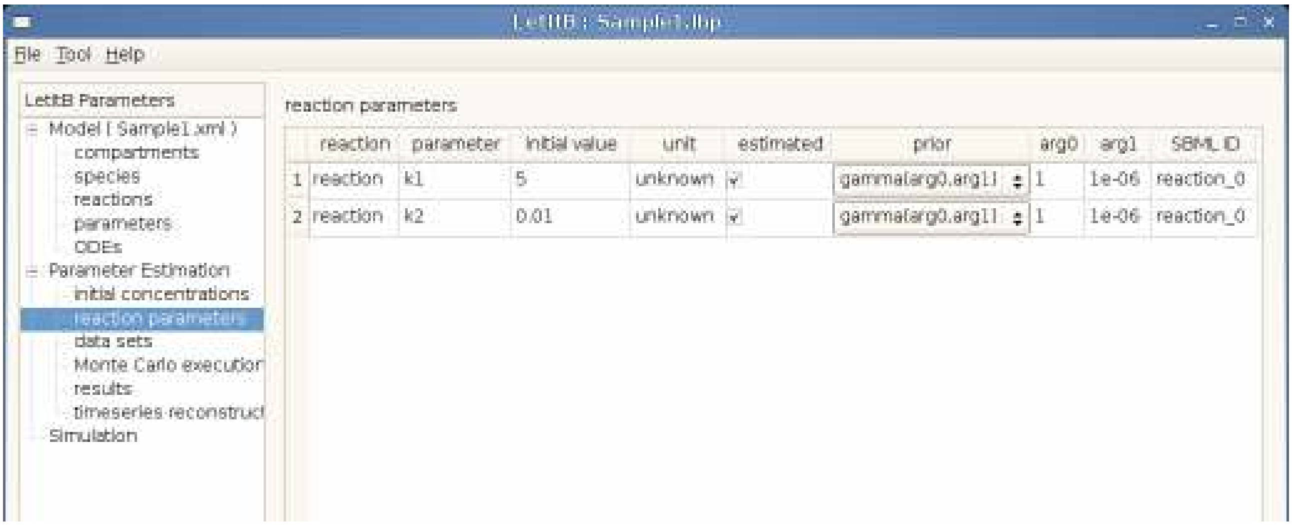
NOTE 1: You cannot select and edit any cells other than above.

NOTE 2: No values you edit in the **initial value** item on the **initial concentrations** screen will be reflected in those on the **species** screen.

NOTE 3: With the estimated item, parameter estimation will be performed for only the factors selected with enabled check boxes.

6.2 reaction parameters

The **reaction parameters** subpart displays the information on estimating reaction parameters.



reaction parameters

	reaction	parameter	initial value	unit	estimated	prior	arg0	arg1	SBML ID
1	reaction	k1	5	unknown	☑	gamma(arg0,arg1)	1	1e-06	reaction_0
2	reaction	k2	0.01	unknown	☑	gamma(arg0,arg1)	1	1e-06	reaction_0

Figure 23: reaction parameters Screen

[About **reaction parameters** screen]

reaction: Display **name** information in the **reactions** tag (See the **name** item in Section 5.3)

* If there is no **name** information in the tag, LetItB displays **ID** information.

parameter: Display **ID** information in the **parameter** tag

* If there is no **initialConcentration** information in the tag, LetItB sets the default value (1).

initial value: Display **volume** information in the **parameter** tag

unit: Display the unit used in **parameter**

* If there is no **unit** information in the **parameter** tag, LetItB displays “unknown” by default.

estimated: Display the factors enabled for parameter estimation (Default: All factors are defined for parameter estimation targets)

prior: Display applicable probability distribution functions used as **prior**

arg0: Display the first argument of **prior**

arg1: Display the argument of **prior**

SBML ID: Display **ID** information in the **reactions** tag

[To edit data]
You can edit numeric data in the **initial value**, **arg0** and **arg1** items. Select any cells you want to edit, and then enter values.
With check boxes in the **estimated** item, you can enable/disable any factors you want for parameter estimation targets by clicking appropriate cells.

NOTE 1: You cannot select and edit any cells other than above.
NOTE 2: No values you edit in the **initial** value item on the **reaction parameters** screen will be reflected in those on the **species** screen.
NOTE 3: With the estimated item, parameter estimation will be performed for only the factors selected with enabled check boxes.

6.3 data sets

Any observation data and control data to be used for parameter estimation can be loaded into LetItB from external files (or deleted from LetItB). If no observation data is loaded into LetItB, you cannot perform any estimate simulation for parameter estimation.

LetItB supports the following five text file formats for external files:

- Comma Separated Values
- Tab Separated Values
- Space Separated Values
- Semicolon Separated Values

* For your reference, see SampleData contained in the installation folder.

6.3.1 Loading and Deleting Observation Data

[To load observation data]

Click the "**+**" button on the upper left corner of the **data sets** screen. When a file dialog appears, select any observation data. Then, the selected data will be automatically displayed in the **observation** pane.

* With **Files of type** in the file dialog, select an appropriate file format and a separation type.

* If you load multiple observation data files into LetItB, click the "**+**" button each time.

Once loaded, observation data is separated with tab windows to allow you to switch your observation data tab window.

[To delete observation data]

Select the dataset tab window you want to delete and click the "**×**" button on the upper right corner of the **data sets** screen. * You can delete observation data only when multiple tab windows are loaded.

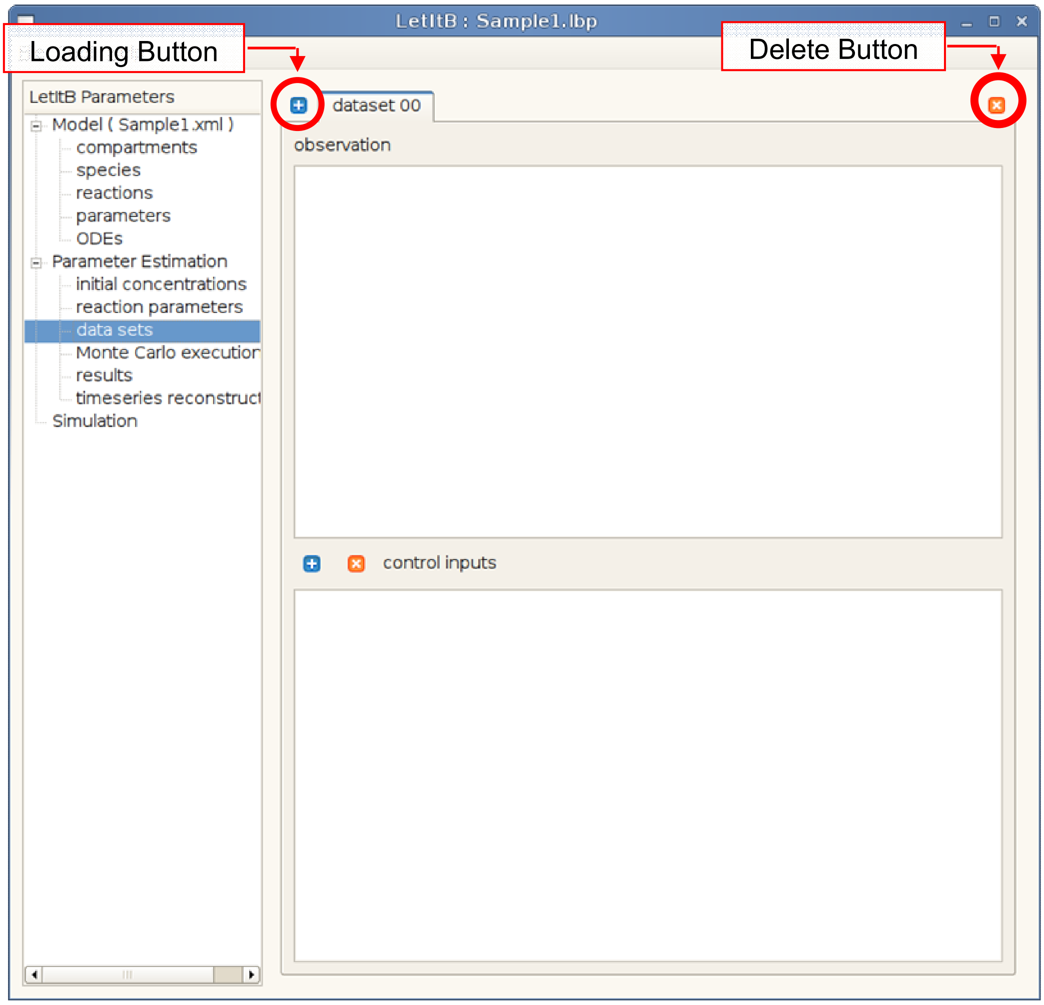


Figure 24 : data sets Screen (Observation Data Loading/Deleting)

6.3.2 Loading and Deleting Control Data

[To load control data]

As a file dialog appears by clicking the “**+**” button in the center left of the dataset tab window, you can select any control data in the file dialog. Once selected, the selected data will be automatically displayed in the **control inputs** pane.

* With **Files of type** in the file dialog, select an appropriate file format and a separation type.

[To delete control data]

Select the **dataset** window (tab) you want to delete, and then click the “**×**” button in the center left of the **dataset** tab window.

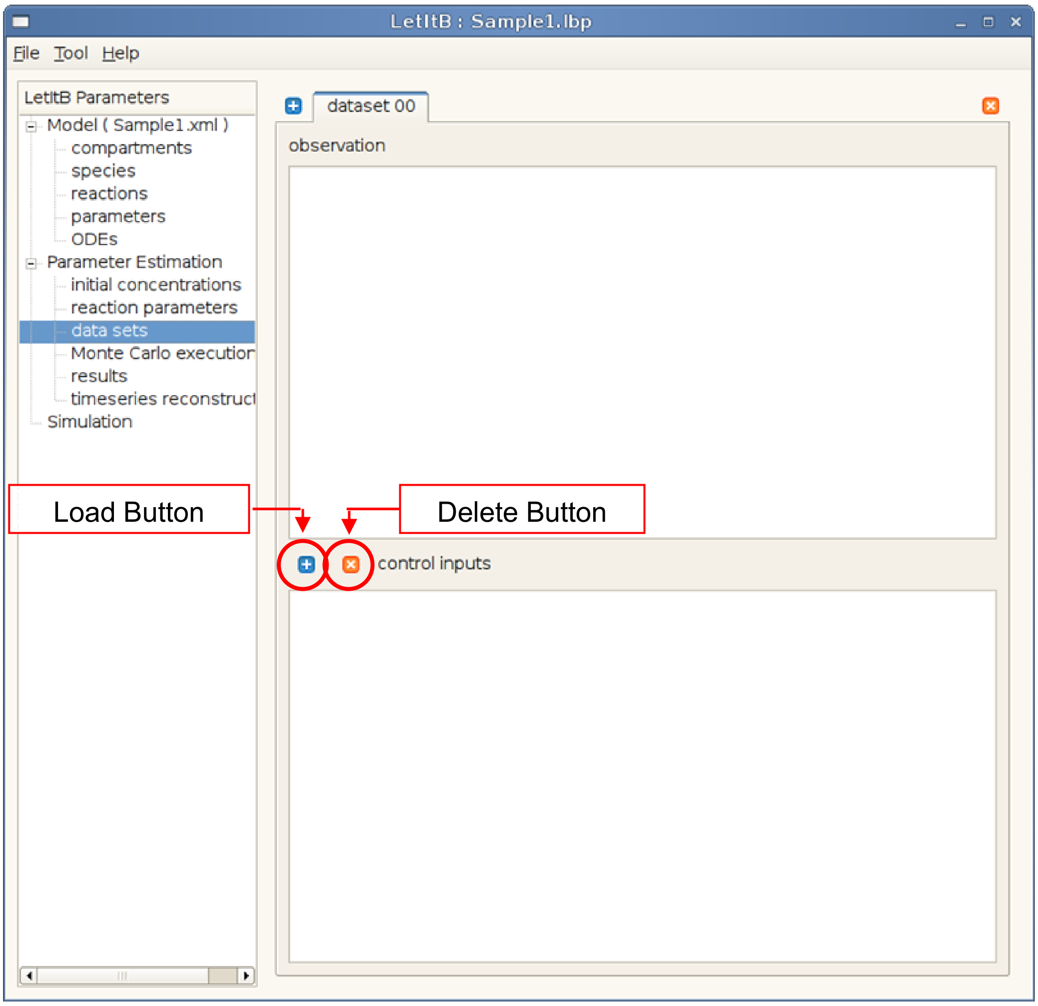


Figure 25: data sets Screen (Control Data Loading/Deleting)

6.3.3 Mapping External Input Data

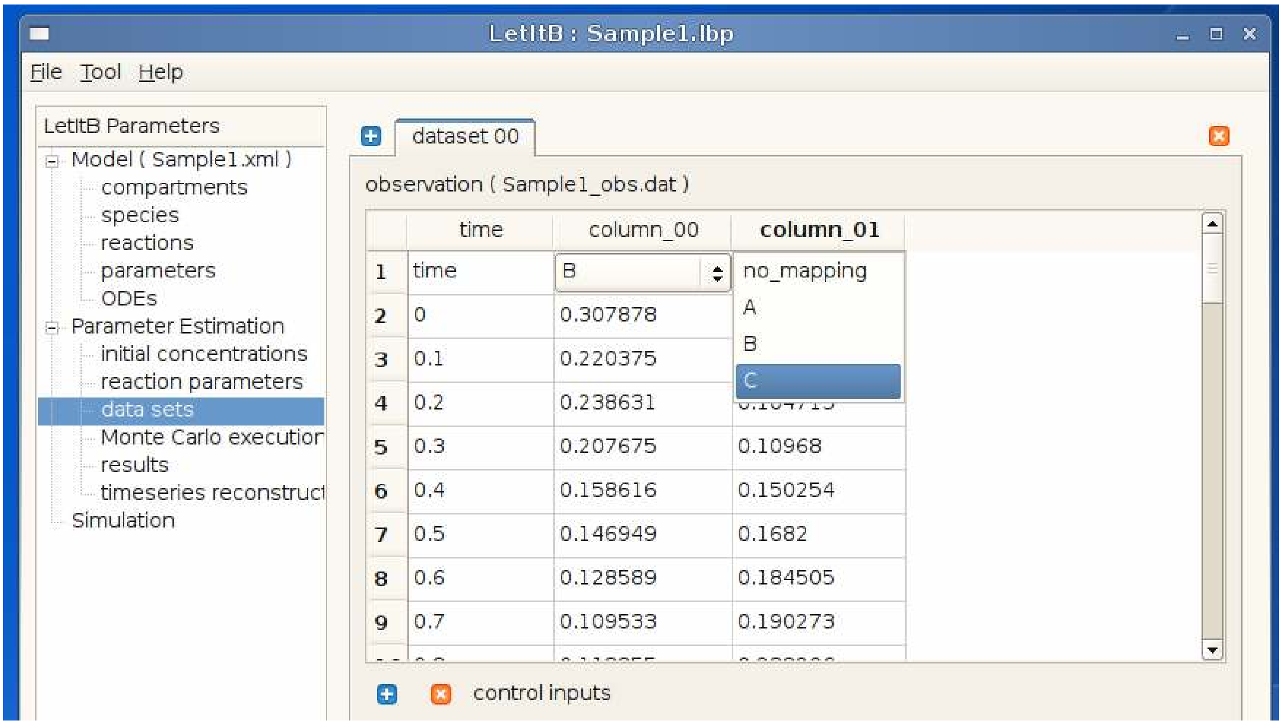
After loading observation data or control data into LetItB, select all the factors you need for mapping.
NOTE: If your required factors (**SBML ID** or **name**) are contained as header information in line 1 of the external input file, you don't need to perform this step.
(For your reference, see SampleData contained in the installation folder.)

After loading the external file into LetItB with the **observation** and **control inputs** panes, select all **SBML ID** or **Name** targets from the combo boxes in all the columns other than the **time** column.

NOTE 1: Before mapping with the combo boxes, be sure to select all columns for the factors you need to map.

NOTE 2: Do not select the same **SBML ID** or **Name** for different factors.

NOTE 3: If you define no correct mapping, you cannot perform parameter estimation properly.



	time	column_00	column_01
1	time	B	no_mapping
2	0	0.307878	
3	0.1	0.220375	
4	0.2	0.238631	
5	0.3	0.207675	0.10968
6	0.4	0.158616	0.150254
7	0.5	0.146949	0.1682
8	0.6	0.128589	0.184505
9	0.7	0.109533	0.190273

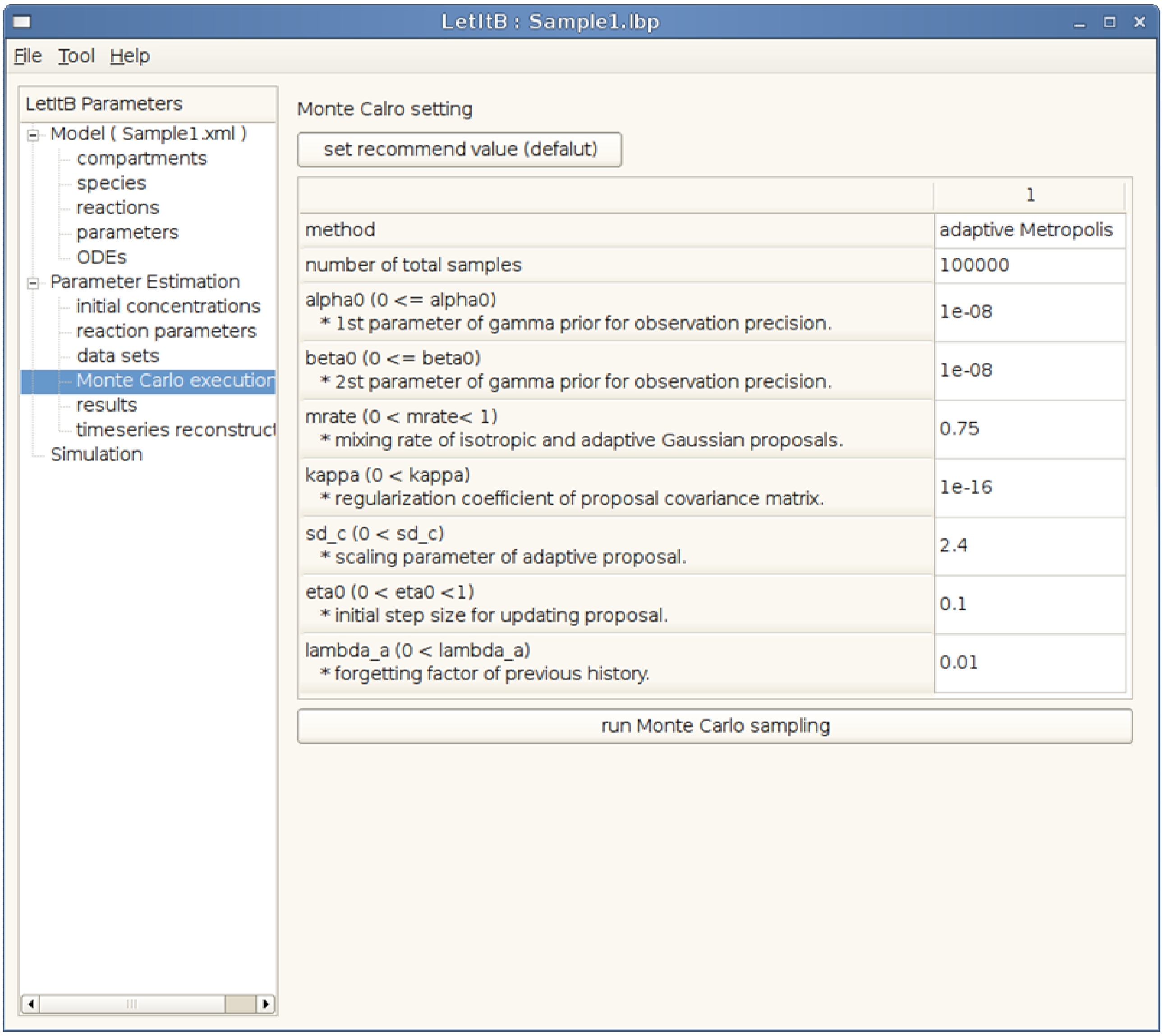
Figure 26: data sets Screen (Input Data Mapping)

6.4 Monte Carlo execution

The **Monte Carlo execution** subpart allows you to change LetItB settings for parameter estimation and to perform parameter estimation by using the Monte Carlo method.

Then, the LetItB software uses the Monte Carlo method for parameter estimation. With software enhancements or new versions, new methods will be added.

* For the current version, you can select only the “adaptive Metropolis”.



Monte Calro setting

	1
method	adaptive Metropolis
number of total samples	100000
alpha0 (0 <= alpha0) * 1st parameter of gamma prior for observation precision.	1e-08
beta0 (0 <= beta0) * 2st parameter of gamma prior for observation precision.	1e-08
mrate (0 < mrate< 1) * mixing rate of isotropic and adaptive Gaussian proposals.	0.75
kappa (0 < kappa) * regularization coefficient of proposal covariance matrix.	1e-16
sd_c (0 < sd_c) * scaling parameter of adaptive proposal.	2.4
eta0 (0 < eta0 <1) * initial step size for updating proposal.	0.1
lambda_a (0 < lambda_a) * forgetting factor of previous history.	0.01

Figure 27: Monte Carlo execution Screen

6.4.1 Setting Monte Carlo

The **Monte Carlo execution** subpart displays settings information for parameter estimation.

method: Display the Monte Carlo method you use (adaptive Metropolis)
[About adaptive metropolis settings]
- **number of total samples**: Display the number of samples
- **alpha0**: Display the first argument of **prior**
- **beta0**: Display the second argument of **prior**
- **mrate**: Display the information on the mixing rate
- **kappa**: Display regularization parameters for the covariance matrix
- **sd_c**: Display parameter information for scaling
- **eta0**: Display the information about default values for update interval
- **lambda_a**: Display the information about forgetting factors

* The default values displayed on the adaptive metropolis settings screen are recommended to use as simulation run-time effective values.

[To edit data]
You can edit numeric data in all the items (**number of total samples**, **alpha0**, **beta0**, **mrate**, **kappa**, **sd_c**, **eta0**, **lambda_a**) except for **method** in the **Monte Carlo setting** pane. Select any cells you want to edit, and then enter values.
To change the data to the recommended values, click the **set recommend value (default)** button in the top of the pane.
NOTE 1: You cannot enter any values out of the range.

6.4.2 Estimating Parameters by the Monte Carlo method

To estimate parameters, click the **run Monte Carlo sampling** button on the **Monte Carlo execution** screen.
NOTE: The run time required for each parameter estimation depends on your machine environment and other environment factors such as SBML models and the number of total samples.

6.4.3 Displaying a Progress Graph during Parameter Estimation

During parameter estimation, a progress window showing how parameter estimation is proceeding will be displayed. An error graph and a log posterior graph for parameter estimation will be displayed in real-time if you select their check boxes in the window.

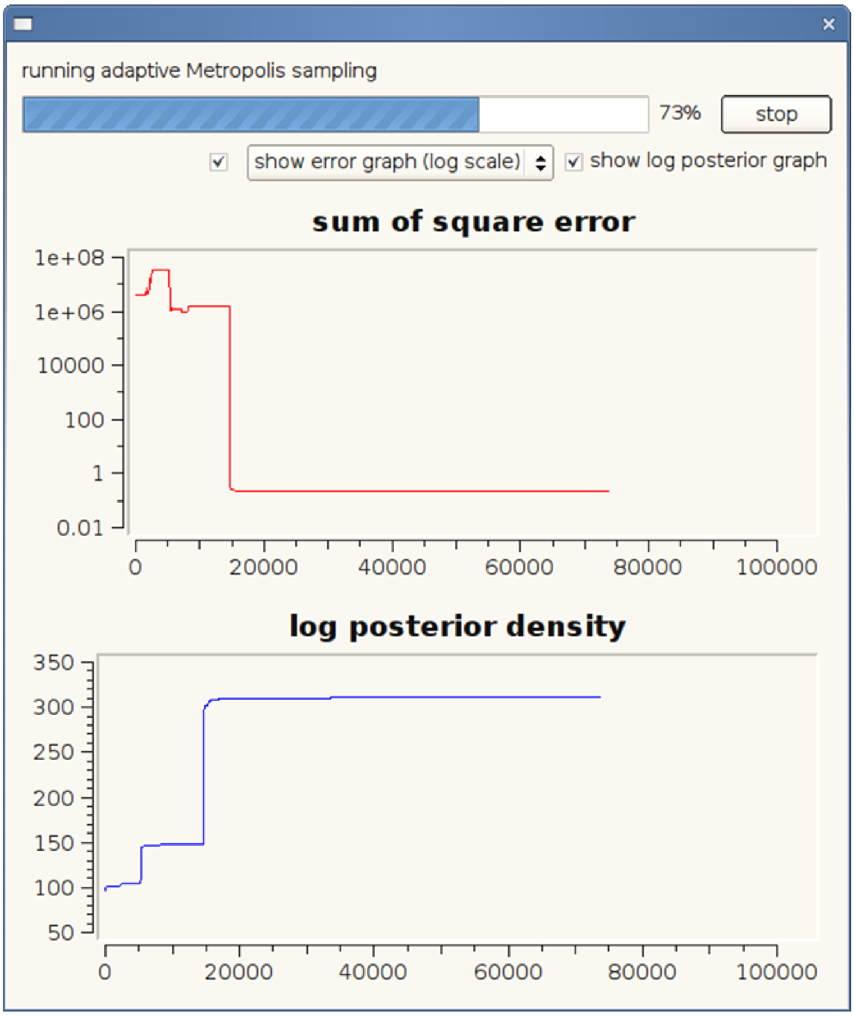
show error graph / show error graph (log scale):

Display the **sum of square error** graph

* From the combo box, you can change the vertical scale of a graph.

log posterior graph:

Display the log posterior density graph



running adaptive Metropolis sampling

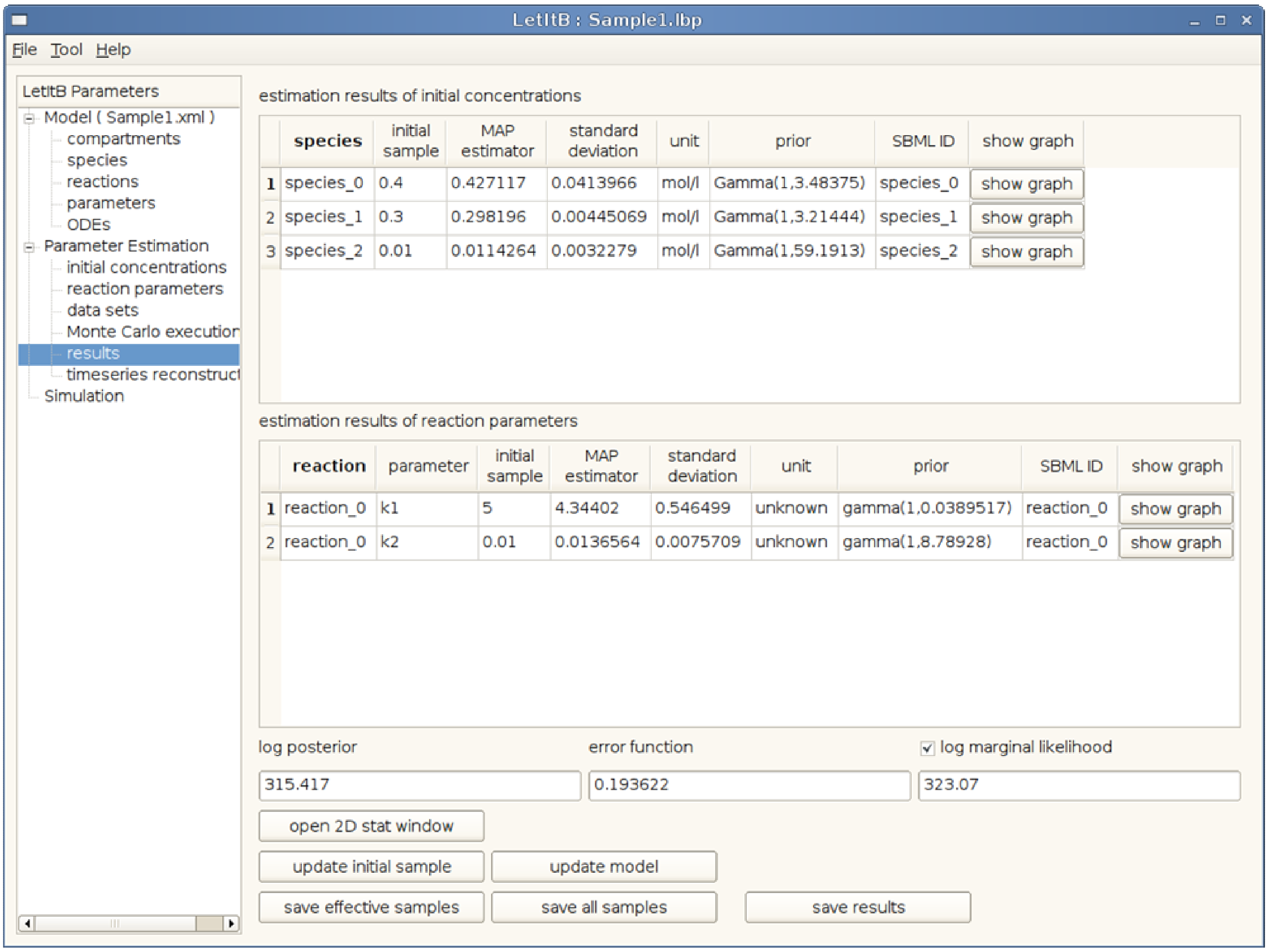
73%

☑ show error graph (log scale) ☑ show log posterior graph

Figure 28: Run time Progress Window displayed during Parameter Estimation

6.5 results

The **results** subpart allows you to list the results after parameter estimation, draw graphs, reflect estimated values, and save data.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

error function: 0.193622

☑ log marginal likelihood: 323.07

Figure 29: results Screen

6.5.1 List Parameter Estimation Results

The **results** subpart lists estimation results for each factor and any corresponding information.

[**estimation results of initial concentrations** (top table on the **results** screen)]

species: Display **name** information in the **species** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

initial sample: Display default values before parameter estimation

MAP estimator: Display results after parameter estimation

standard deviation: Display the standard deviation

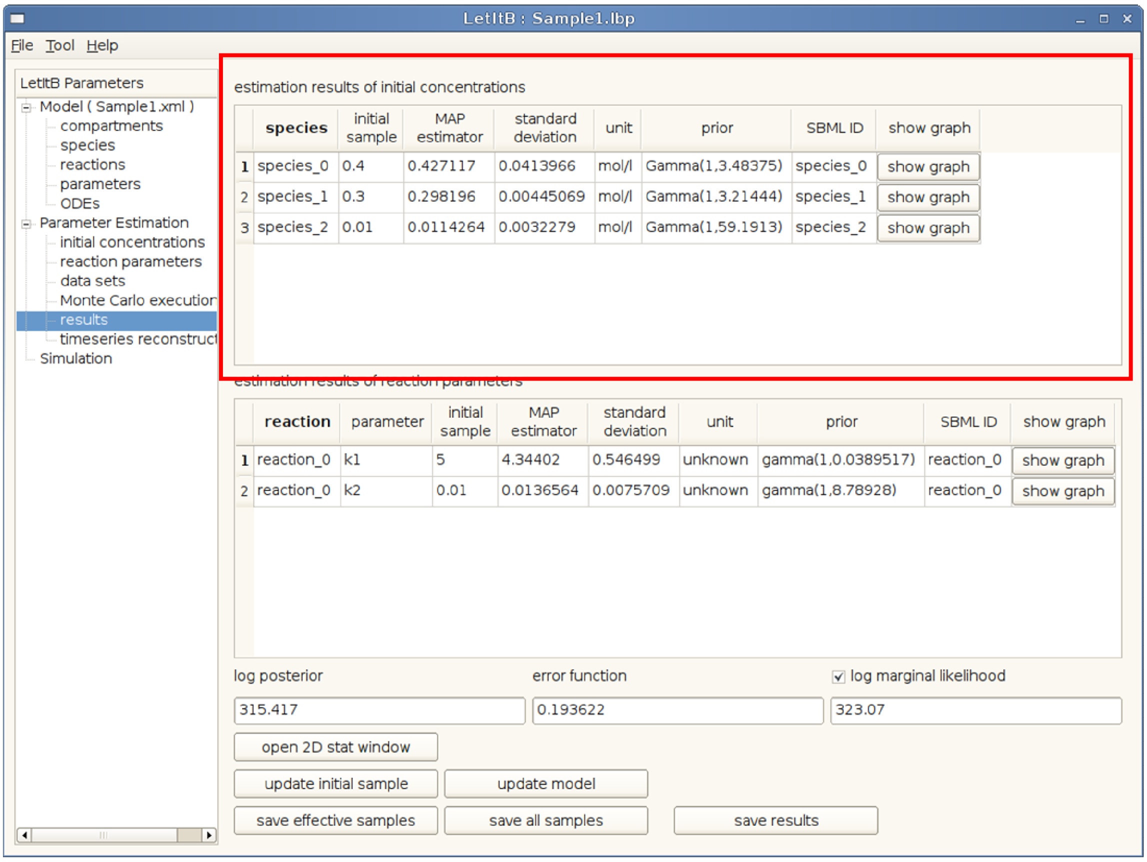
unit: Display the unit (the same **unit** as displayed on the **initial concentration** screen)

prior: Display **prior** information used for the parameter estimation simulation

SBML ID: Display **ID** information of SBML files, for each corresponding factor

show graph: The button to display a 1D histogram

NOTE: For 1D histograms, see Section 6.5.4.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

error function: 0.193622

☑ log marginal likelihood: 323.07

Figure 30: results Screen (estimation results of initial concentrations)

[**estimation results of reaction parameters** (middle table on the **results** screen)]

reaction: Display **name** information in the **reaction** tag

* If there is no **name** information in the tag, LetItB displays **ID** information.

parameter: Display **ID** information in the **parameter** tag

initial sample: Display default values before parameter estimation

MAP estimator: Display results after parameter estimation

standard deviation: Display the standard deviation

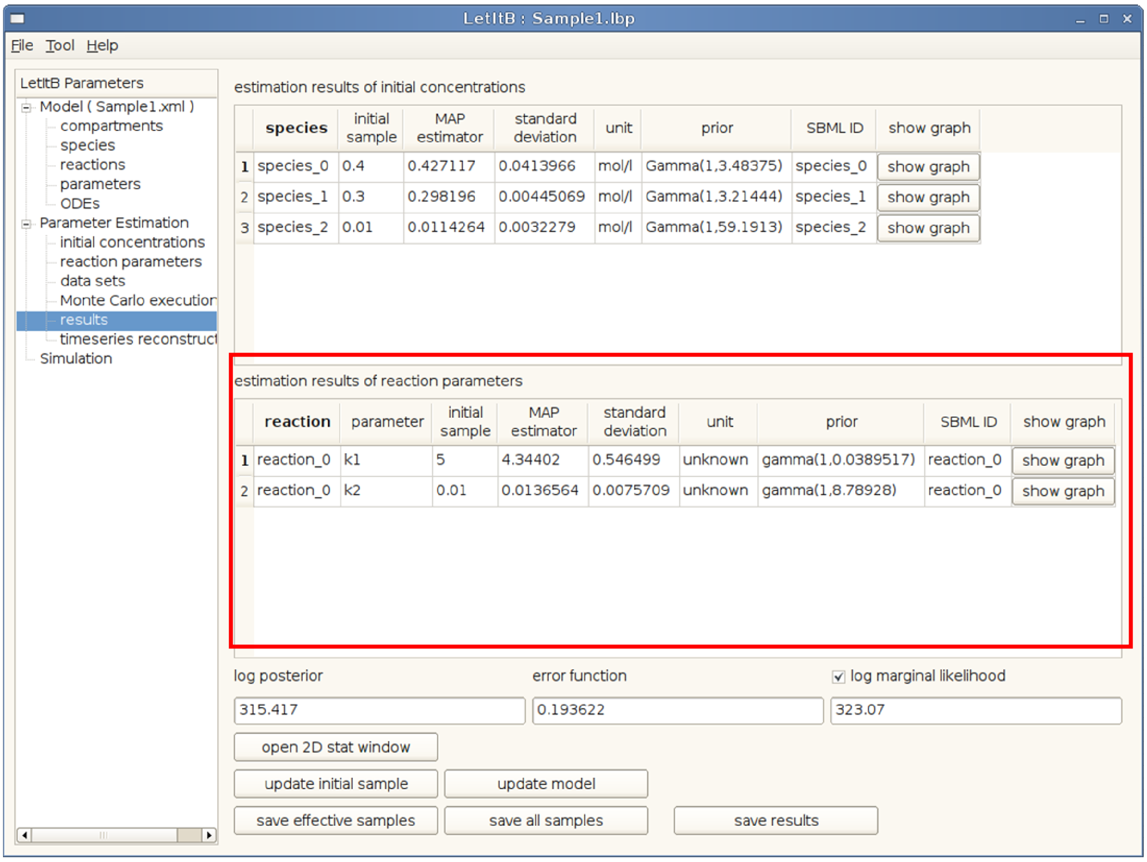
unit: Display the unit (the same **unit** as displayed on the **reaction parameters** screen)

prior: Display **prior** information used for the parameter estimation simulation

SBML ID: Display **ID** information of SBML files, for each corresponding factor

show graph: The button to a display 1D histogram

NOTE: For 1D histograms, see Section 6.5.4.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

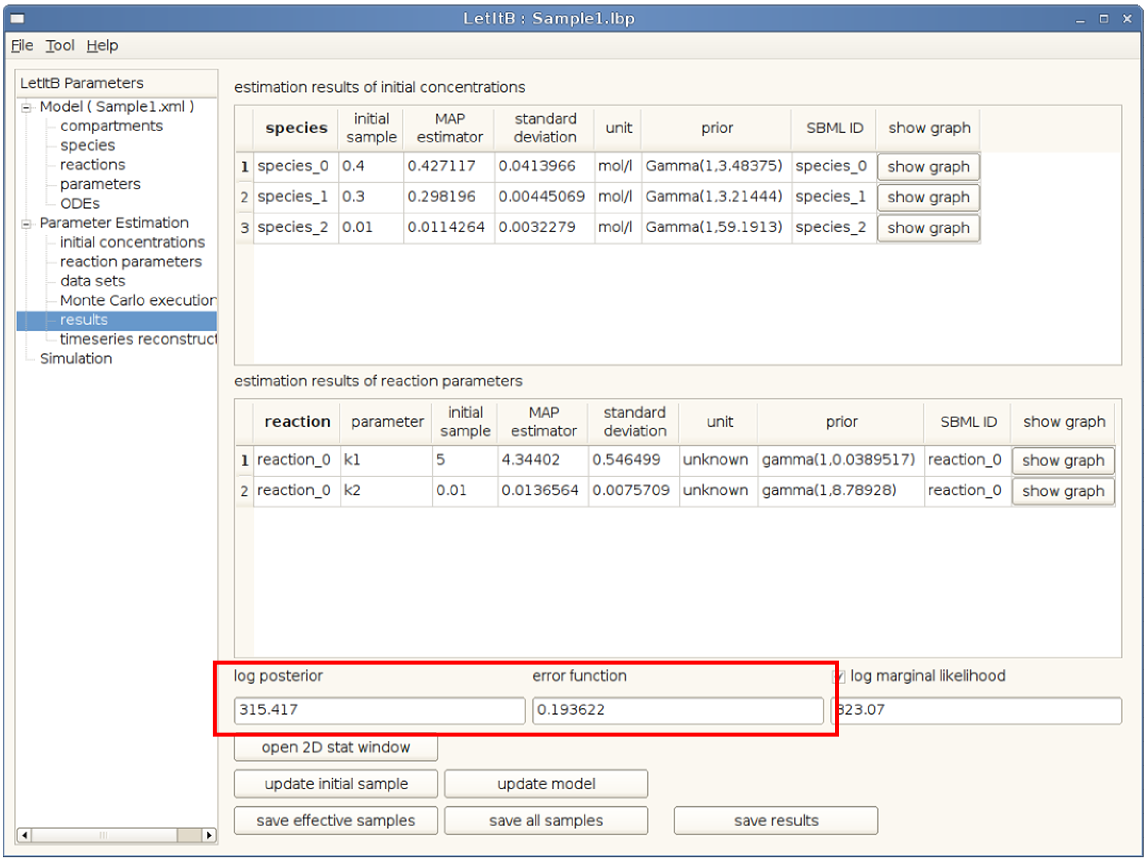
error function: 0.193622

☑ log marginal likelihood: 323.07

Figure 31: results Screen (estimation results of reaction parameters)

[**log posterior** and **error function** (Bottom part of the **results** screen)]

The **log posterior** and **error function** fields display final log posterior and error function numeric values after parameter estimation.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417
error function: 0.193622
☑ log marginal likelihood: 323.07

Figure 32: results Screen (“log posterior” and “error function”)

[To edit data]

You can edit numeric data in the **initial sample** items in **estimation results of initial concentrations** and **estimation results of reaction parameters**. Select any cells you want to edit, and then enter values.

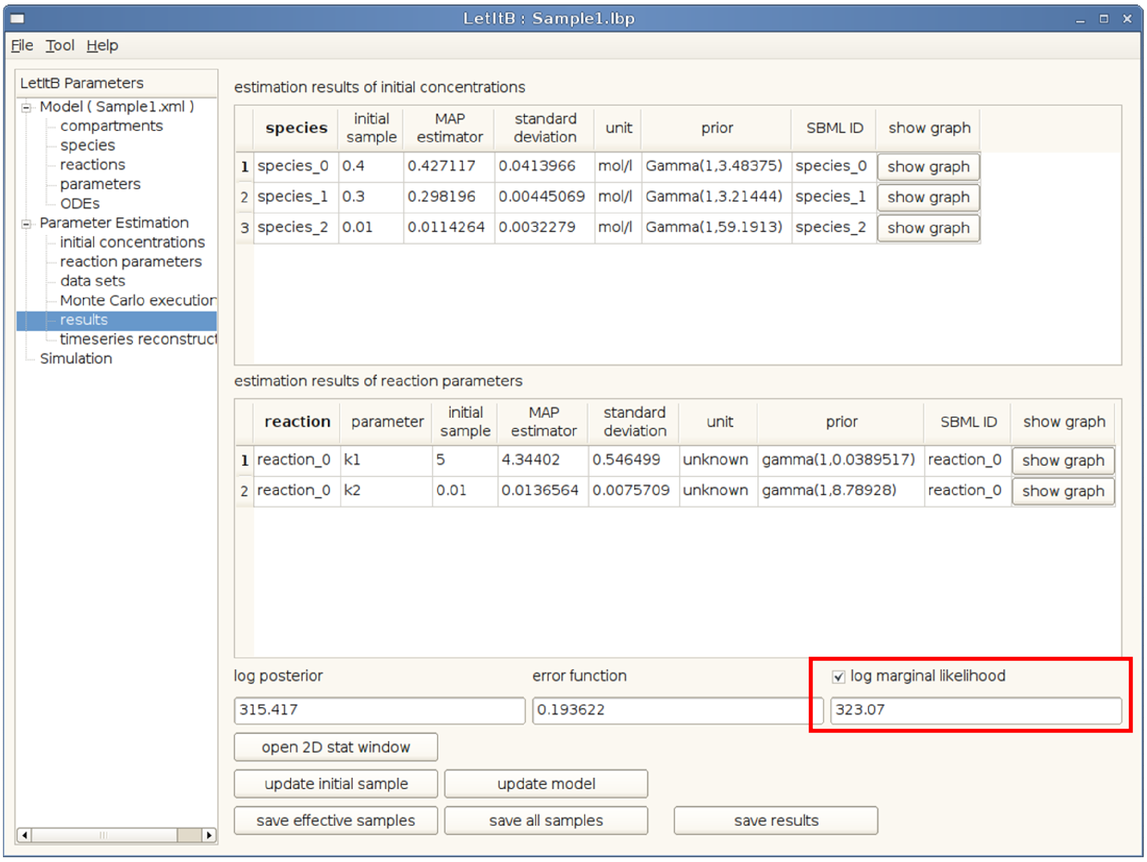
NOTE 1: You cannot select and edit any cells other than above.

NOTE 2: See Section 6.5.3 for how to reflect values of the **MAP estimator** item into those of the **initial sample** item collectively.

6.5.2 Estimating log marginal likelihood

You can estimate the marginal likelihood on log scale. To start estimation, select the **log marginal likelihood** check box highlighted in red below.

NOTE 1: By default, the log marginal likelihood check box is not selected.
NOTE 2: The run time required for each log marginal likelihood estimation depends on your machine environment and other environment factors such as SBML models and the number of total samples.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417
error function: 0.193622
☑ log marginal likelihood: 323.07

Figure 33: results Screen (log marginal likelihood)

6.5.3 Reflecting Estimated Values

You can collectively reflect the results of parameter estimation in the following two ways by clicking an appropriate button as needed:

update initial sample:

Reflect values of the **Map estimator** item into those of the **initial sample** item.

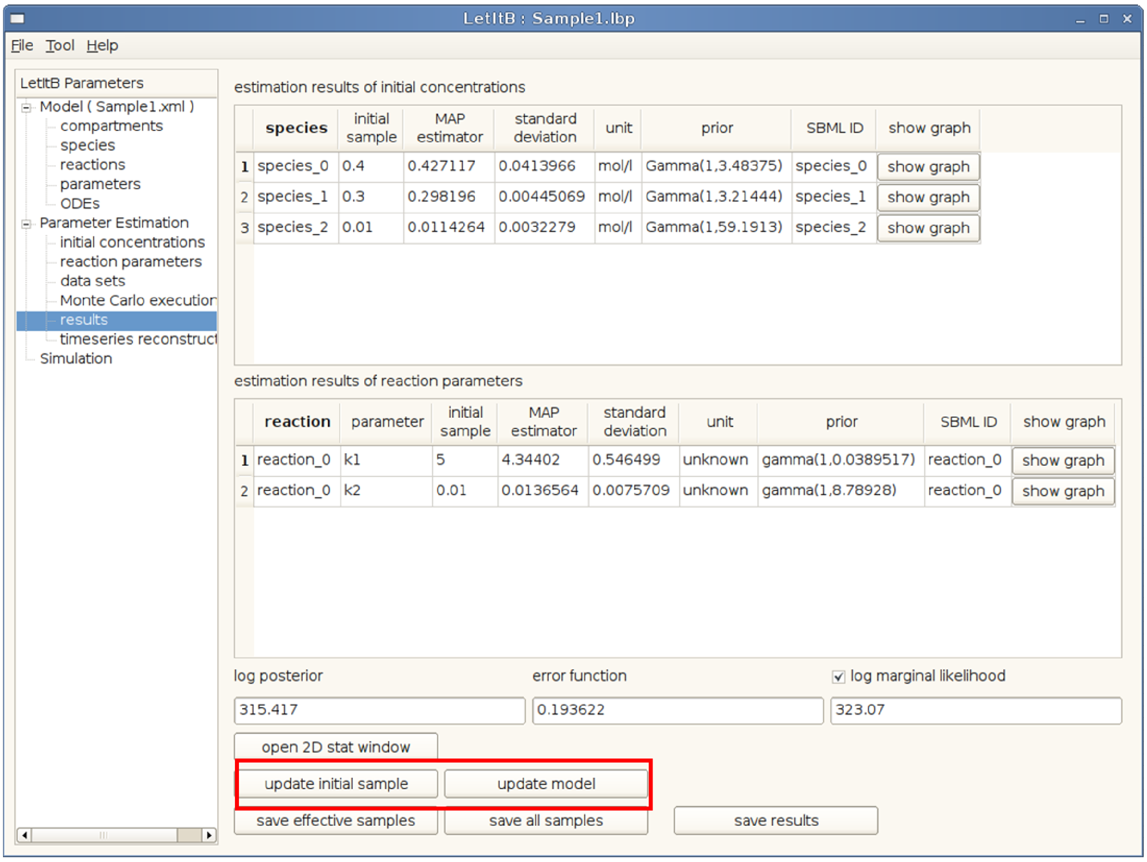
* The **initial concentrations** and **reaction parameters** information in the **Parameter Estimation** part will also be updated.

* No information of the SBML model (the **Model** part) will be updated.

update model:

Reflect values of the **Map estimator** item into those of the **volume** item in **species** and the **initial concentration** item of **parameters** in the **Model** part.

* No information of the **Parameter Estimation** part will be updated.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

error function: 0.193622

☑ log marginal likelihood: 323.07

Figure 34: results Screen (“update initial sample” and “update model”)

6.5.4 Display 1D and 2D Histograms

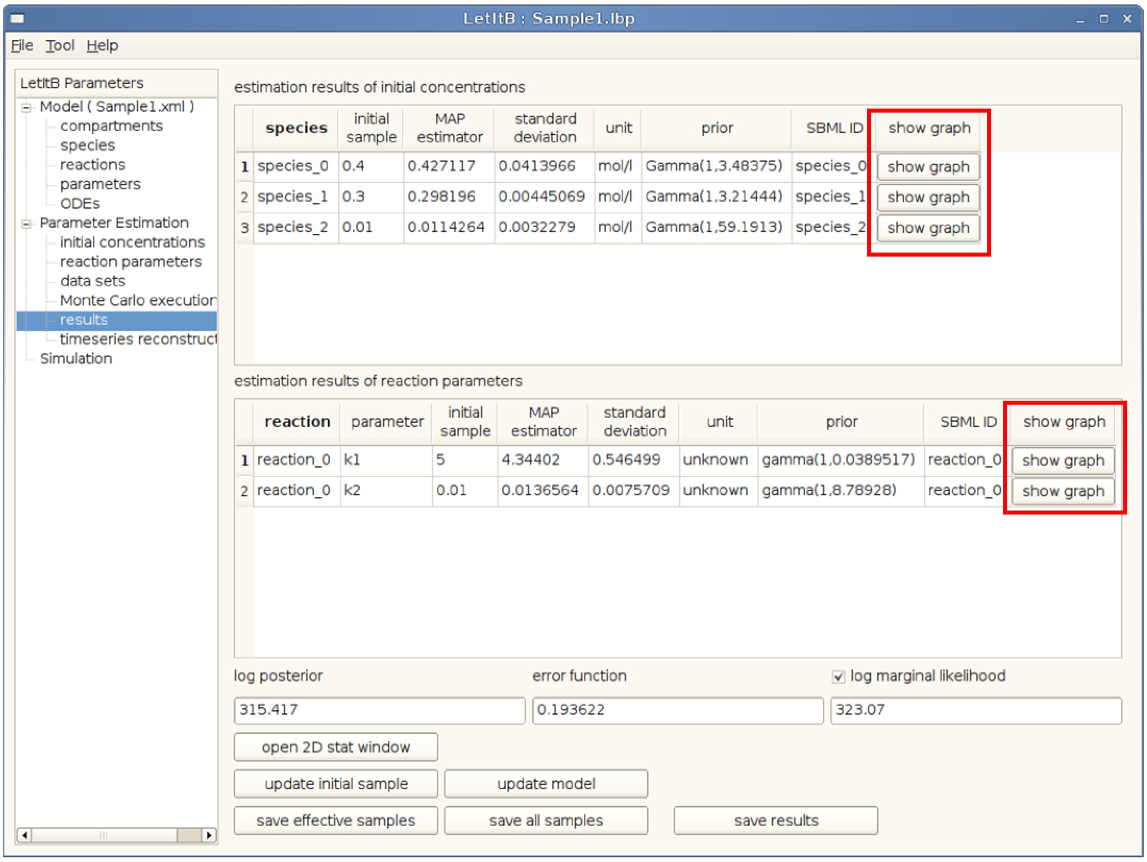
You can display the results of parameter estimation as 1D or 2D histograms.

[To display a 1D histogram]

How to Display:

When you click the button in the **show graph** items on the **results** screen, a 1D graph appears.

NOTE: Before clicking the **show graph** button, be sure to click the **SBML ID** cell of any factors you want to display.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

error function: 0.193622

☑ log marginal likelihood: 323.07

Figure 35: results Screen (show graph)

About 1D Graphs:

1D histograms are displayed to show probability density in vertical axis and histogram bins in horizontal axis. Both vertical axis and horizontal axis are automatically set by default when the 1D histogram is displayed first time.

About graph components

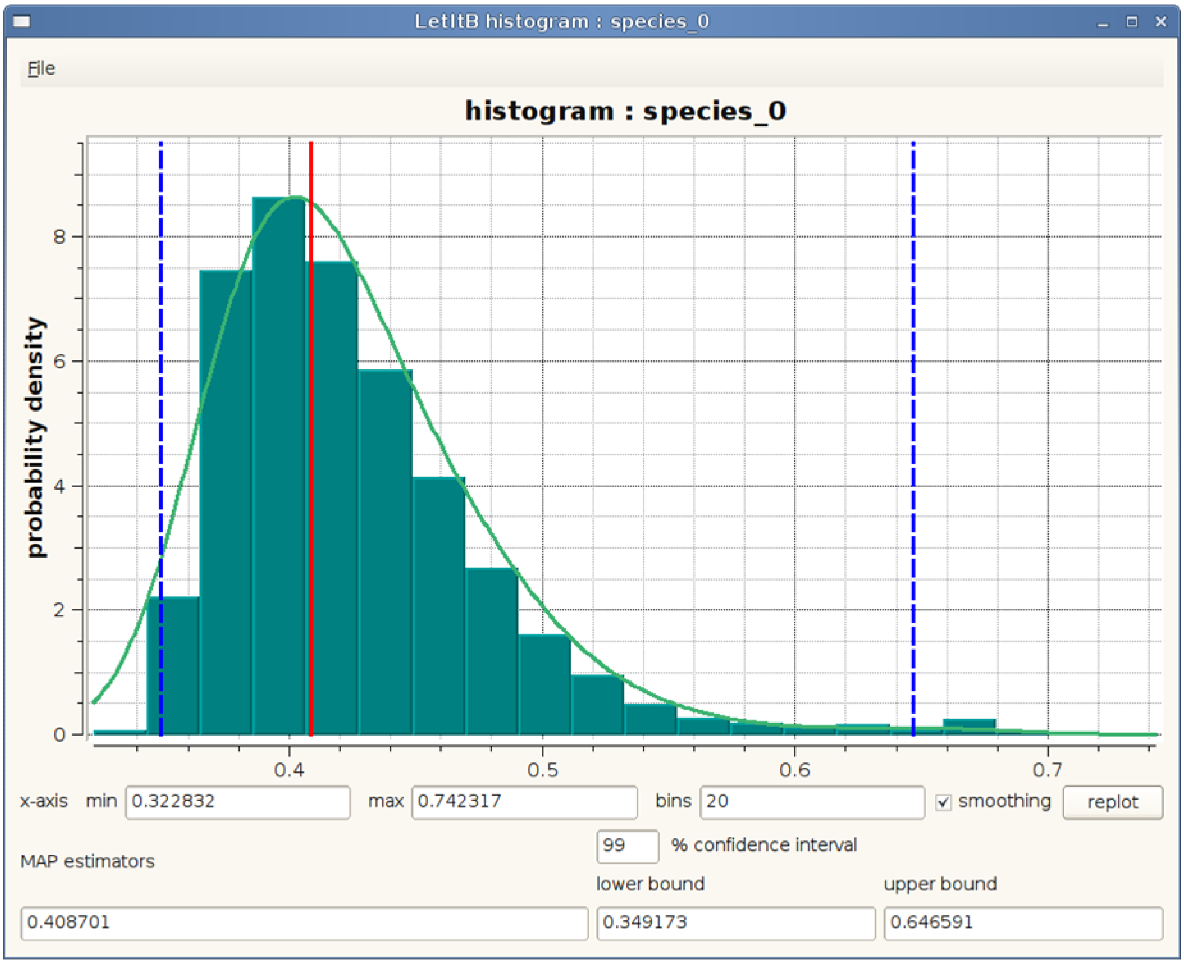
Green Bar Graph: Histogram

Red Solid Line: The **MAP estimator** values

Blue Dotted Line: The **lower bound** and **upper bound** values for confidence interval (99% by default)

Light Green Solid Line: Resultant graph after histogram smoothing (Disabled by default)

LetItB displays the 1D graph with the above settings. In addition, LetItB displays numeric values for the above items in the bottom part of the histogram window.



x-axis min 0.322832 max 0.742317 bins 20 ☑ smoothing

MAP estimators 0.408701

99 % confidence interval

lower bound 0.349173

upper bound 0.646591

Figure 36: 1D Histogram Window

How to Configure:

1 To save an image:

From the menu of the histogram window, select **File** > **Save graph**.

When a file dialog appears, select where the file will be saved, a name of the file and the image format you want to save, and then save the data.

2 To modify the X axis:

Enter values in min as the minimum value, in max as the maximum value and in **bins** as the number of histogram bins. Then click the **replot** button.

3 To smooth the graph:

Enable/disable the **smoothing** check box, and then click the **replot** button.

4 To set confidence interval:

Enter any number between 0 and 100 in **XX % confidence interval**, and then click the **replot** button.

NOTE: You cannot edit any values in **MAP estimator**, **lower bound** and **upper bound**.

[To display 2D histograms]

How to Display:

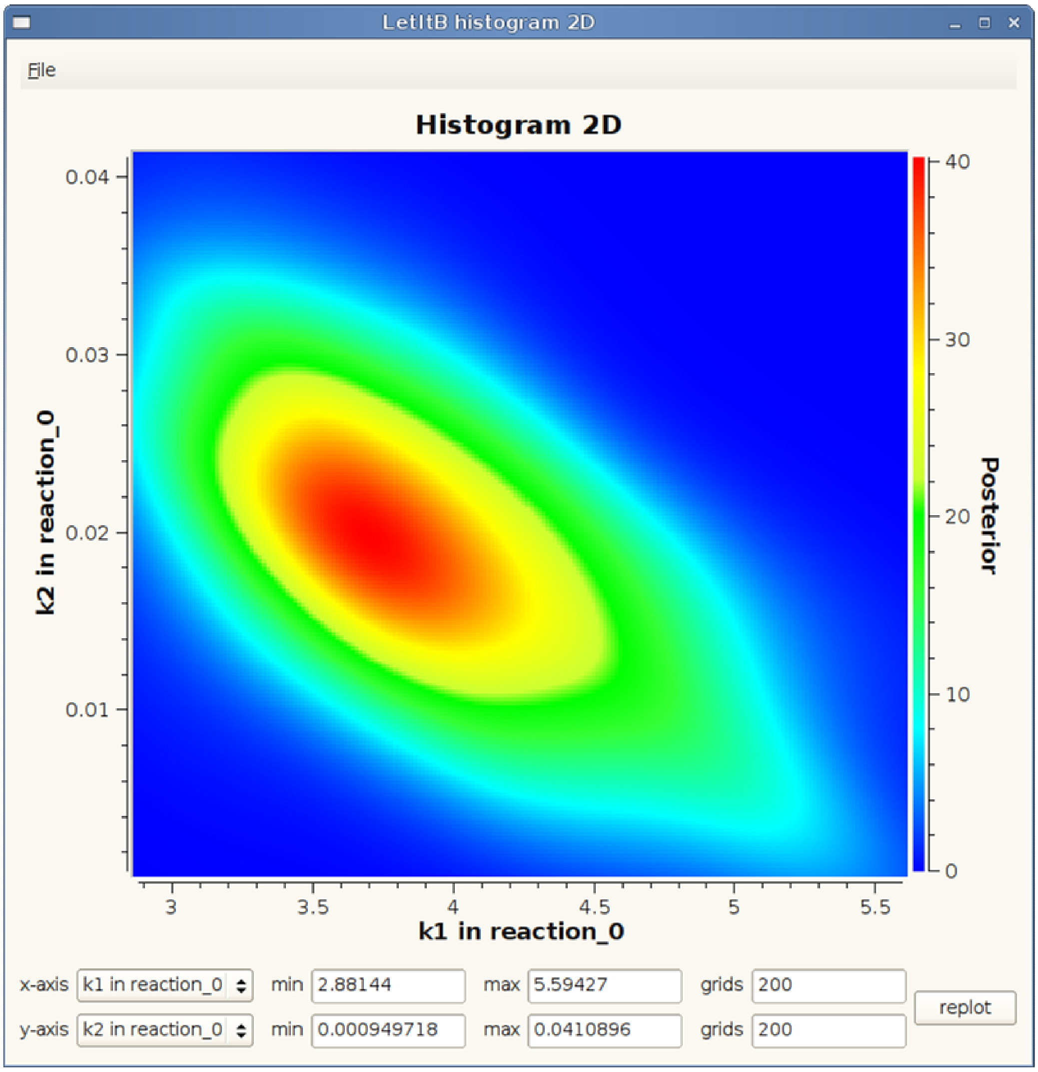
When you click the **open 2D stat window** button on the **results** screen, a 2D graph appears.

About 2D Graphs:

2D histograms are displayed to show any factors you specify for both vertical and horizontal axes. Each axis is automatically set by default when the 2D histogram is displayed at first time.

LetItB displays the 2D histogram by calculating two factors and indicates the number of histogram bins by color changes. The color for bins changes from blue (few bins) to red (many bins), according to the color bar on the right side of the graph.

In addition, numeric values for the above items are displayed at the bottom part of the histogram window.



x-axis k1 in reaction_0 min 2.88144 max 5.59427 grids 200

y-axis k2 in reaction_0 min 0.000949718 max 0.0410896 grids 200

Figure 37: 2D Histogram Window

How to Configure:

1 To save an image:

From the menu of the histogram window, select **File** > **Save graph**.

When a file dialog appears, select where the file will be saved, a name of the file and an image format you want to save, and then save the data.

2 To change the axes settings:

Select any factors you want to display for both of the X and Y axes.

* If you select factors for the axes, the minimum value and the maximum value for them are automatically set.

3 To edit the axes:

Enter values in **min** as the minimum value, in **max** as the maximum value and in **grids** as grid spacing for the axes. Then, click the **replot** button.

NOTE: The run time required to plot the 2D histogram depends your machine environment and other environment factors such as the estimated number of samples and the settings for the grid spacing specified in **grids**.

6.5.5 Saving Parameter Estimation Results

You can save the results of parameter estimation in the following three ways by clicking an appropriate button as needed:

save effective samples:

Display only effective results of parameter estimation by each occurrence of the number of simulation steps. When you click the button, a file dialog appears. Specify where the file will be saved and a name of the file.

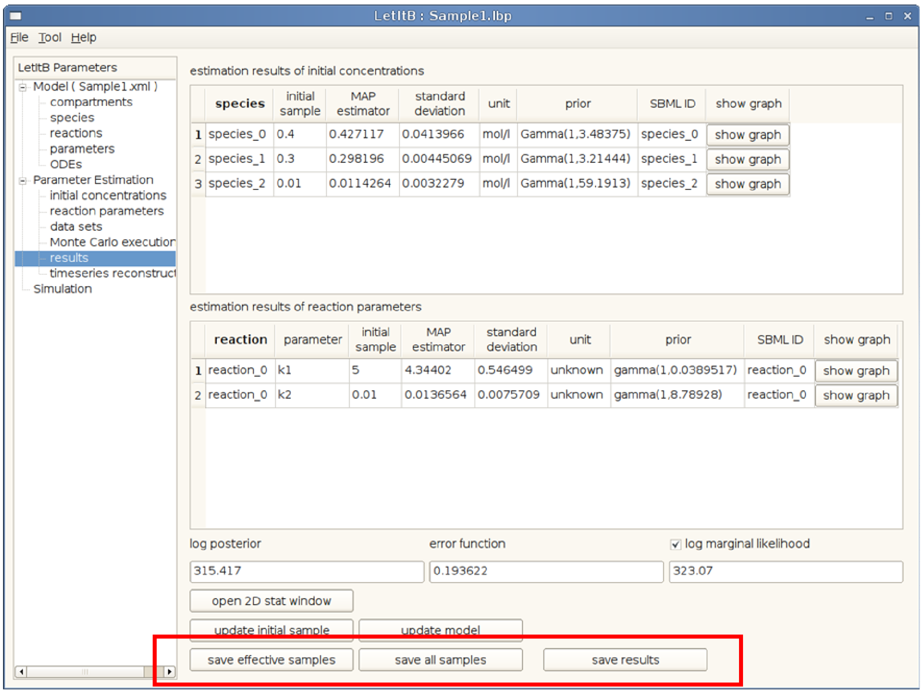
save all samples:

Display all results of parameter estimation by each occurrence of the number of simulation steps. When you click the button, a file dialog appears. Specify where the file will be saved and a name of the file.

save results:

Save the information on the **results** screen in the text format. When you click the **save results** button, a file dialog appears. Then, specify where the file will be saved and a name of the file.

NOTE: Only for **save effective samples** and **save all samples**, LetItB supports the same file save formats as specified in Section 6.3.



estimation results of initial concentrations

	species	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	species_0	0.4	0.427117	0.0413966	mol/l	Gamma(1,3.48375)	species_0	show graph
2	species_1	0.3	0.298196	0.00445069	mol/l	Gamma(1,3.21444)	species_1	show graph
3	species_2	0.01	0.0114264	0.0032279	mol/l	Gamma(1,59.1913)	species_2	show graph

estimation results of reaction parameters

	reaction	parameter	initial sample	MAP estimator	standard deviation	unit	prior	SBML ID	show graph
1	reaction_0	k1	5	4.34402	0.546499	unknown	gamma(1,0.0389517)	reaction_0	show graph
2	reaction_0	k2	0.01	0.0136564	0.0075709	unknown	gamma(1,8.78928)	reaction_0	show graph

log posterior: 315.417

error function: 0.193622

☑ log marginal likelihood: 323.07

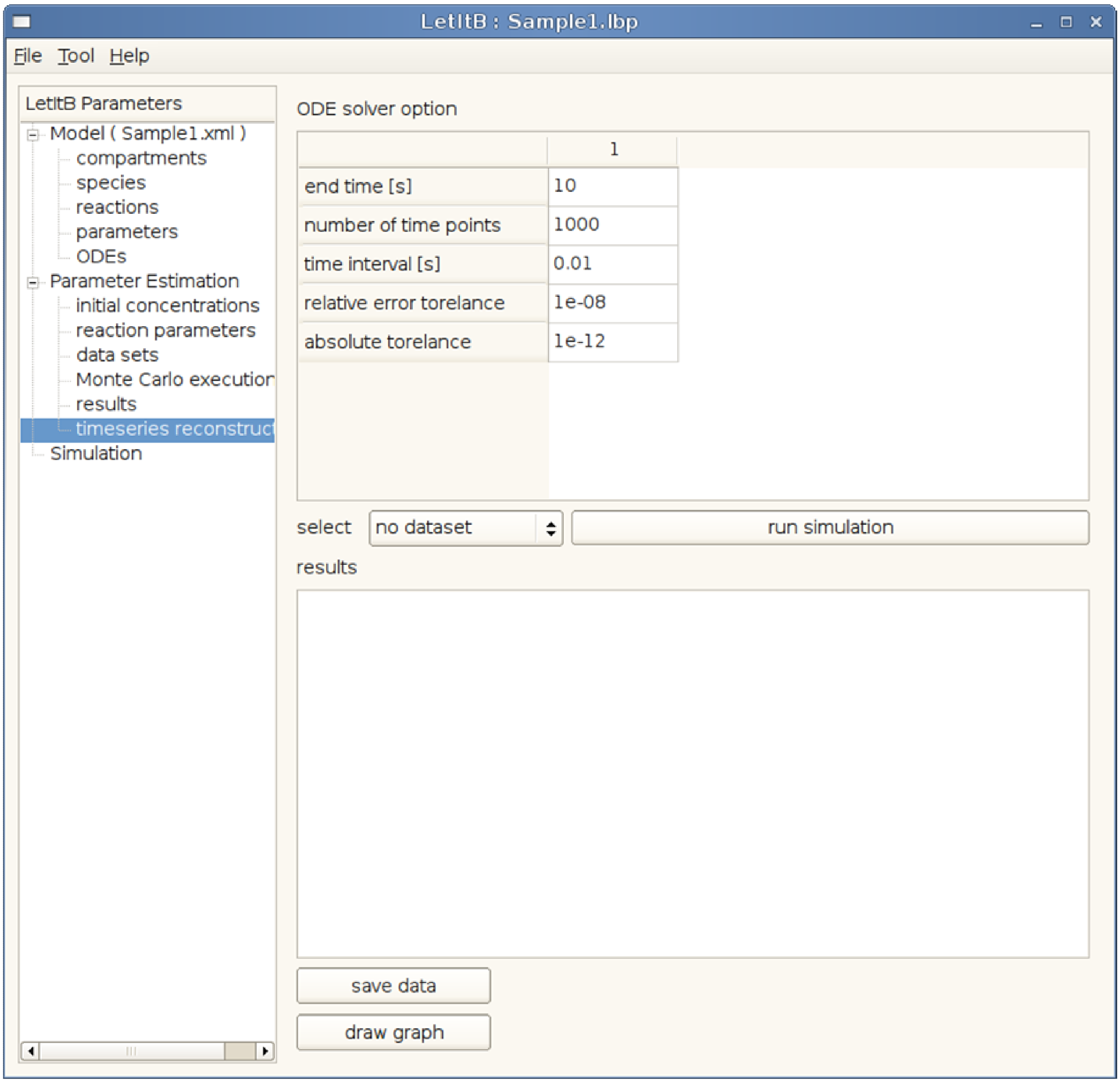
Figure 38: results Screen (Parameter Estimation Results Saving)

6.6 timeseries reconstruction

You can run timeseries simulation with **initial concentrations** and **reaction parameters** information in the **Parameter Estimation** part. This allows you to easily view the results of the timeseries simulation by using parameter estimation results.

* See Chapter 7 Simulation.

* Before running the timeseries simulation by using parameter estimation results, perform **update initial sample** in Section 6.5.3, and update information in **initial concentrations** and **reaction parameters**.



ODE solver option

	1
end time [s]	10
number of time points	1000
time interval [s]	0.01
relative error torelance	1e-08
absolute torelance	1e-12

select: no dataset

Figure 39: timeseries reconstruction Screen

[**ODE solver option**]

end time: The time to terminate the simulation (Default: 10)

* The start time is set to 0

number of time points: The number of simulation time steps (Default: 1000)

size of time intervals: The interval between simulation time steps

(end time ÷ number of time points = size of time intervals)

relative error tolerance: Tolerance error margin of simulation results - Relative unit (Default: 1×10^{-8})

absolute tolerance: Tolerance range of simulation results - Absolute unit (Default: 1×10^{-12})

* Unless expressly specified in SBML files, second (s) is used for a unit of time.

[To edit the data in **ODE solver option**]

You can edit numeric data in the **end time**, **number of time points**, **relative error tolerance**, and **absolute tolerance** items. Select any cells you want to edit, and then enter values.

[To run the timeseries simulation]

Select any data set from the **select** item on the middle of the **timeseries reconstruction** screen, and then click the **run simulation** button to start the simulation. The index, dataset XX, in the **select** item is linked to the tab index on the **data sets** screen described in Section 6.3.

NOTE 1: If you don’t select proper items from the **select** item, you cannot run the simulation.

NOTE 2: If you don’t load control data into LetItB on the **data sets** screen, you can run the simulation without control data. If you load control data into LetItB on the **data sets** screen, you can run the simulation with the control data.

[To display timeseries simulation results]

When the timeseries simulation completes, its results will be displayed in the **results** pane on the bottom of the **timeseries reconstruction** screen.

[To save timeseries simulation results data]

After the timeseries simulation completes, click the **save data** button on the bottom of the **timeseries reconstruction** screen. When a file dialog appears, specify where the file will be saved and a name of the file.

NOTE: LetItB supports the same file save formats as specified in Section 6.3.

[To display timeseries simulation results graphs]

From the **graph option** check box in the **results** pane, select any factors you want to display in the graph, and then click the **draw graph** button. The timeseries graph of simulation results will be displayed.

* For more information on how to display graphs, see Section 7.5.

A graph window displays a timeseries graph, with simulation results in Y axis and time in X axis, based on the factors you select in **graph option**. The simulation result for each factor is displayed in solid lines, and observation data from the selected dataset is displayed with “**×**” marks.

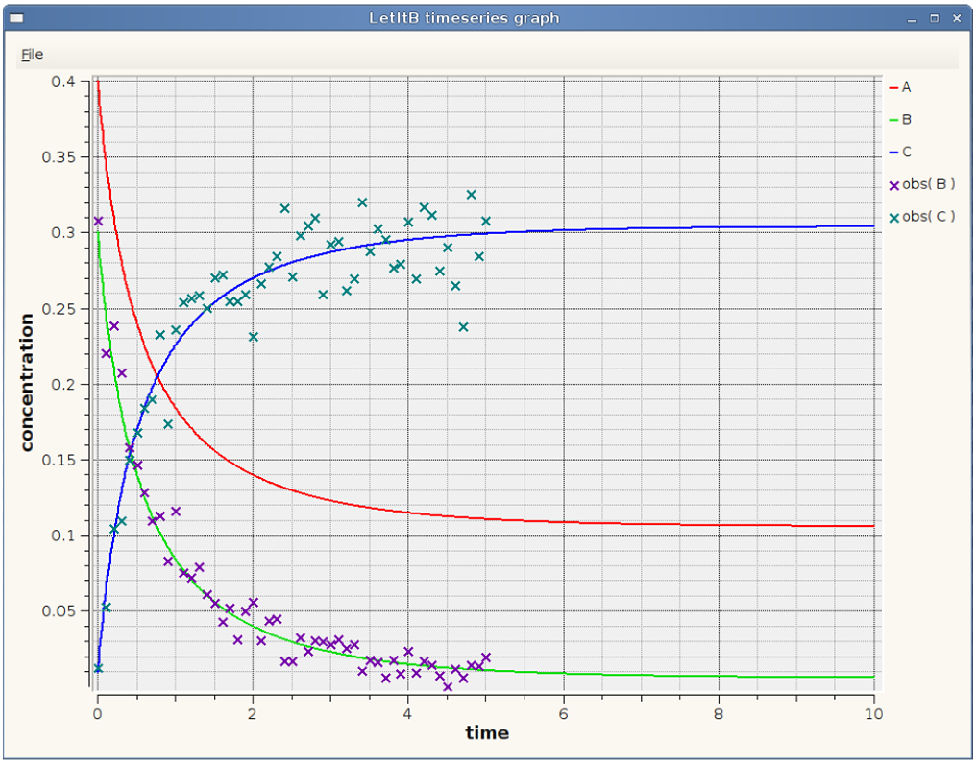


Figure 40: Graph Window for timeseries reconstruction

How to Configure:

1 To save an image:

From the menu of the graph window, select **File** > **Save graph**.

When a file dialog appears, select where the file will be saved, a name of the file, and an image format you want to save, and then save the data.

2 To display / hide the graph:

By clicking the captions in the upper right corner of the graph window, you can display/hide the graph.

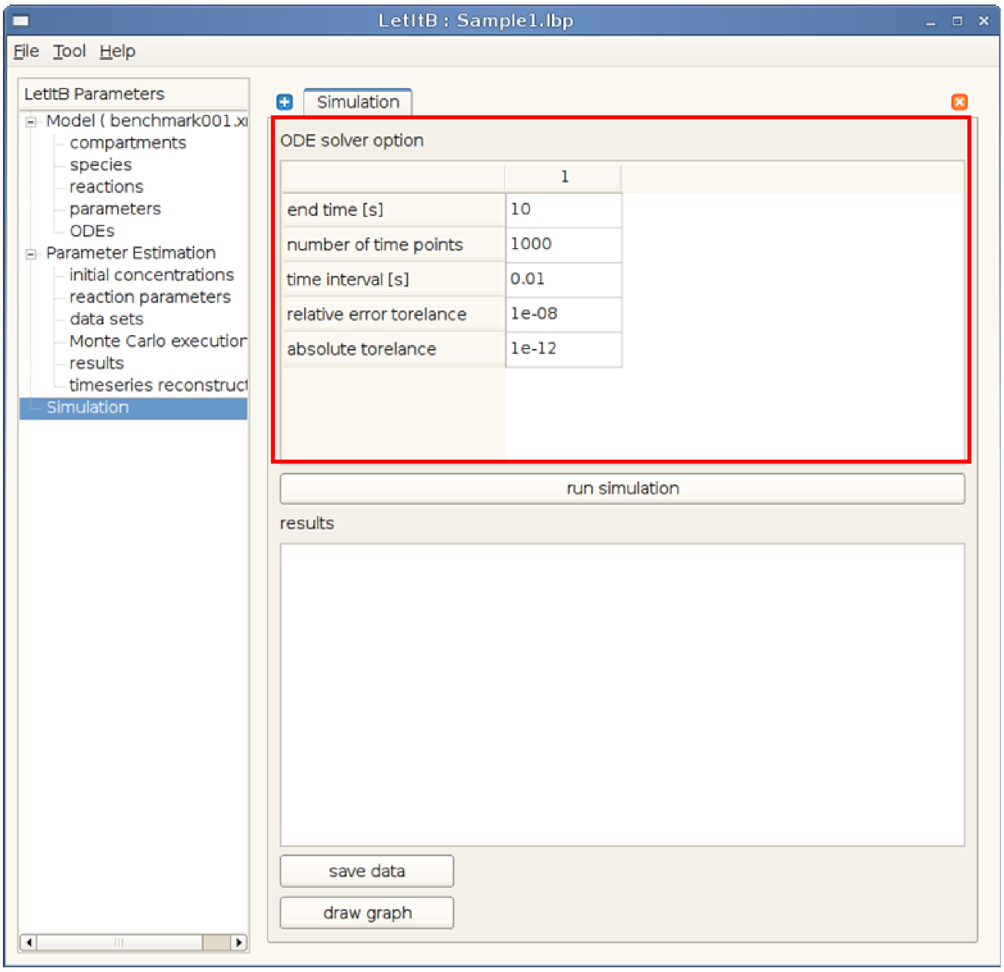
7 Simulation

The **Simulation** part allows you to run numeric simulation, display/save the results data, and display a results graph by using Ordinary Differential Equations (ODEs) of the simulation model defined in the SBML file.

There are two types of the methods for running the simulation: “Simulation”, which solves ODEs without using any external input (control data), and “Simulation with Control Data”, which applies external data to ODEs and controls them.

7.1 Simulation Setting

You need to set each parameter for running numeric simulation by using ODEs.



	1
end time [s]	10
number of time points	1000
time interval [s]	0.01
relative error torelance	1e-08
absolute torelance	1e-12

Figure 41: Simulation Screen (Setting)

[**ODE solver option**]

end time: The time to terminate the simulation (Default: 10)

* The start time is set to 0

number of time points : The number of time steps in simulation (Default: 1000)

size of time intervals: The interval between simulation time steps

(end time ÷ number of time points = size of time intervals)

relative error tolerance: Tolerance error margin of simulation results - Relative unit (Default : 1×10^{-8})

absolute tolerance: Tolerance range of simulation results - Absolute unit (Default : 1×10^{-12})

* Unless expressly specified in SBML files, second (s) is used for a unit of time.

[To edit data in **ODE solver option**]

You can edit numeric data in the **end time**, **number of time points**, **relative error tolerance**, and **absolute tolerance** items. Select any cells you want to edit, and then enter values.

NOTE: The values you set in **ODE solver option** will be reflected in both Simulation and Simulation with Control Data ways.

7.2 Running Simulation

After setting properly as shown in Section 6.1, click the **run simulation** button on the middle of the **Simulation** screen (tab window) to start the simulation. After the simulation completes, its results will be displayed in the **results** pane on the bottom part of the screen.

NOTE: For Simulation (without Control Data), any factors where the check boxes in the **constant** item on the **species** screen are selected will be the values for **initial concentration** (the constant value).

7.3 Loading and Deleting Control Data

[To load control data]

Click the “**+**” button on the upper left corner of the **Simulation** screen. When a file dialog appears, select any control data file. Selecting a file automatically moves you to a new tab window, and displays the selected data in the **control inputs** pane in the new tab window.

* With **Files of type** in a file dialog, select an appropriate file format and separation type.

* If you load multiple control data files into LetItB, click the “**+**” button each time.

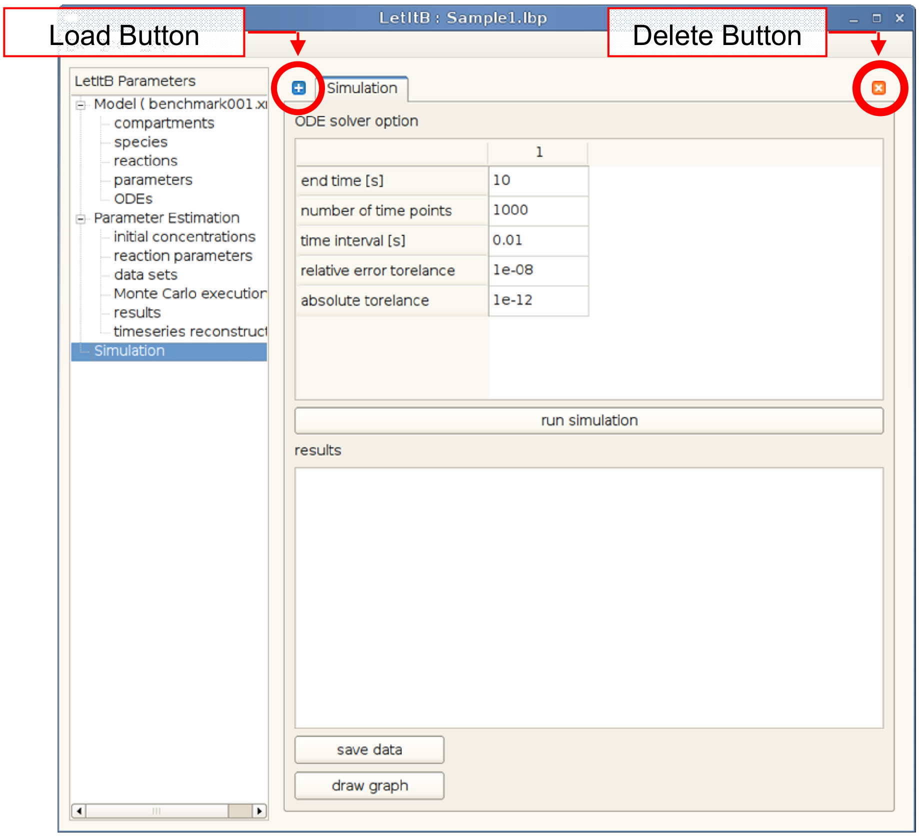
Once loaded, observation data is separated with tab windows to allow you to switch your data tab window.

* LetItB supports the same file formats for loading control data, as specified in Section 6.3.

[To delete control data]

Select the tab window you want to delete, and then click the “**×**” button on the upper right corner of the **Simulation** screen.

* You can delete observation data only when there are multiple tab windows.



	1
end time [s]	10
number of time points	1000
time interval [s]	0.01
relative error torelance	1e-08
absolute torelance	1e-12

Figure 42: Simulation Screen (Setting)

7.4 Mapping Control Data

After loading control data into LetItB, map them to an appropriate **SBML ID** or **name**.

NOTE: If **SBML ID** or **name** is contained as header information in line 1 of the external input file, you don't need to perform this step.

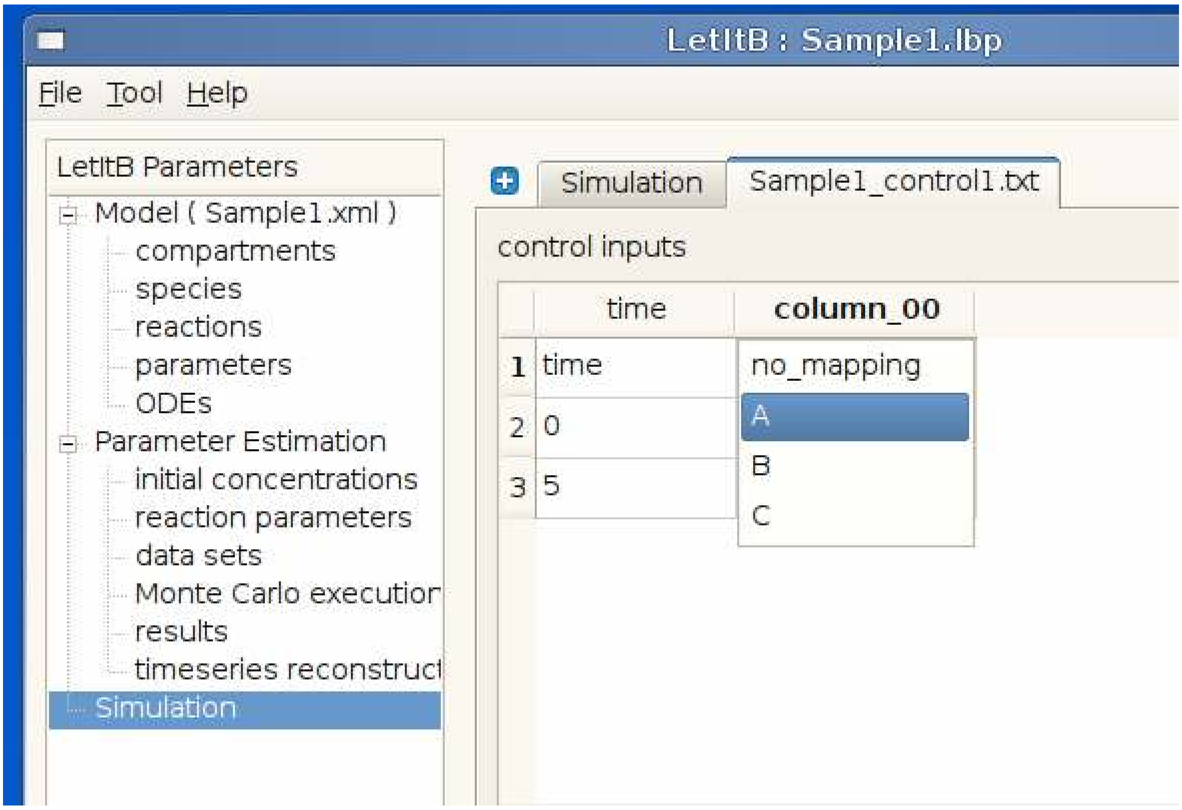
(For your information, see SampleData contained in the installation folder.)

In the **control inputs** pane where control data are loaded into, from the combo boxes in all the columns other than **time** column, select any **SBML ID** or **Name** you want to use as control data.

NOTE 1: Before mapping with the combo boxes, be sure to select all columns for the factors you need to map.

NOTE 2: Do not select the same **SBML ID** or **Name** for different factors.

NOTE 3: If you define no correct mapping, you cannot run Simulation with Control Data properly.



	time	column_00
1	time	no_mapping
2	0	
3	5	

Figure 43: Simulation Screen (Control Data Mapping)

7.5 Running Simulation with Control Data

After loading control data into LetItB in Section 7.3, run Simulation with Control Data.

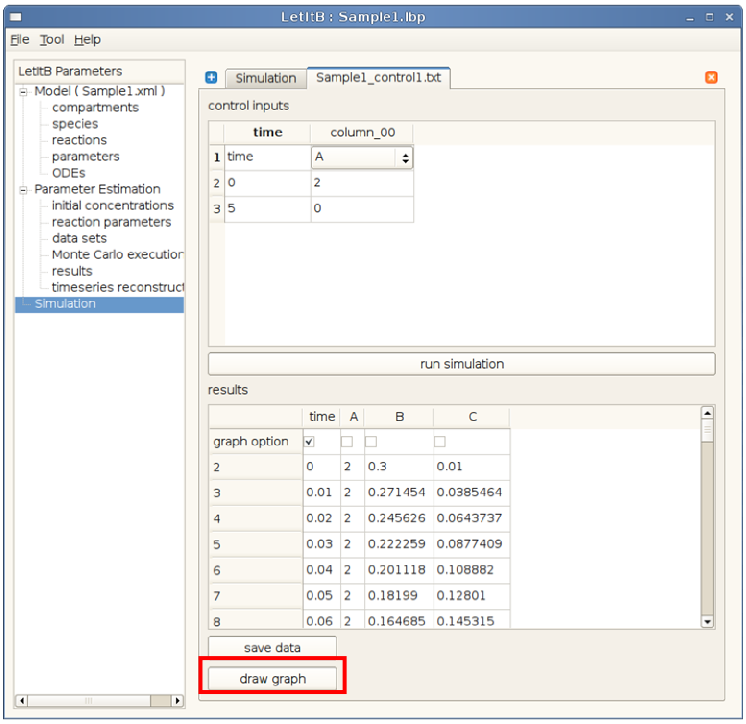
Move to the tab window where the control data you want to perform the simulation is loaded into, and then click the **run simulation** button on the middle of the screen to start the simulation. After the simulation completes, its results will be displayed in the **results** pane on the bottom of the screen.

NOTE: For Simulation with Control Data, **constant** item information on the **species** screen will be ignored.

7.6 Saving Results of Simulation with Control Data

To save the results data of Simulation and Simulation with Control Data, click the **save data** button on the bottom of the screen after their results data are displayed in the **results** pane. When a file dialog appears, specify where the file will be saved and a name of the file.

NOTE: LetItB supports the same file save formats as specified in Section 6.3.



control inputs

	time	column_00
1	time	A
2	0	2
3	5	0

results

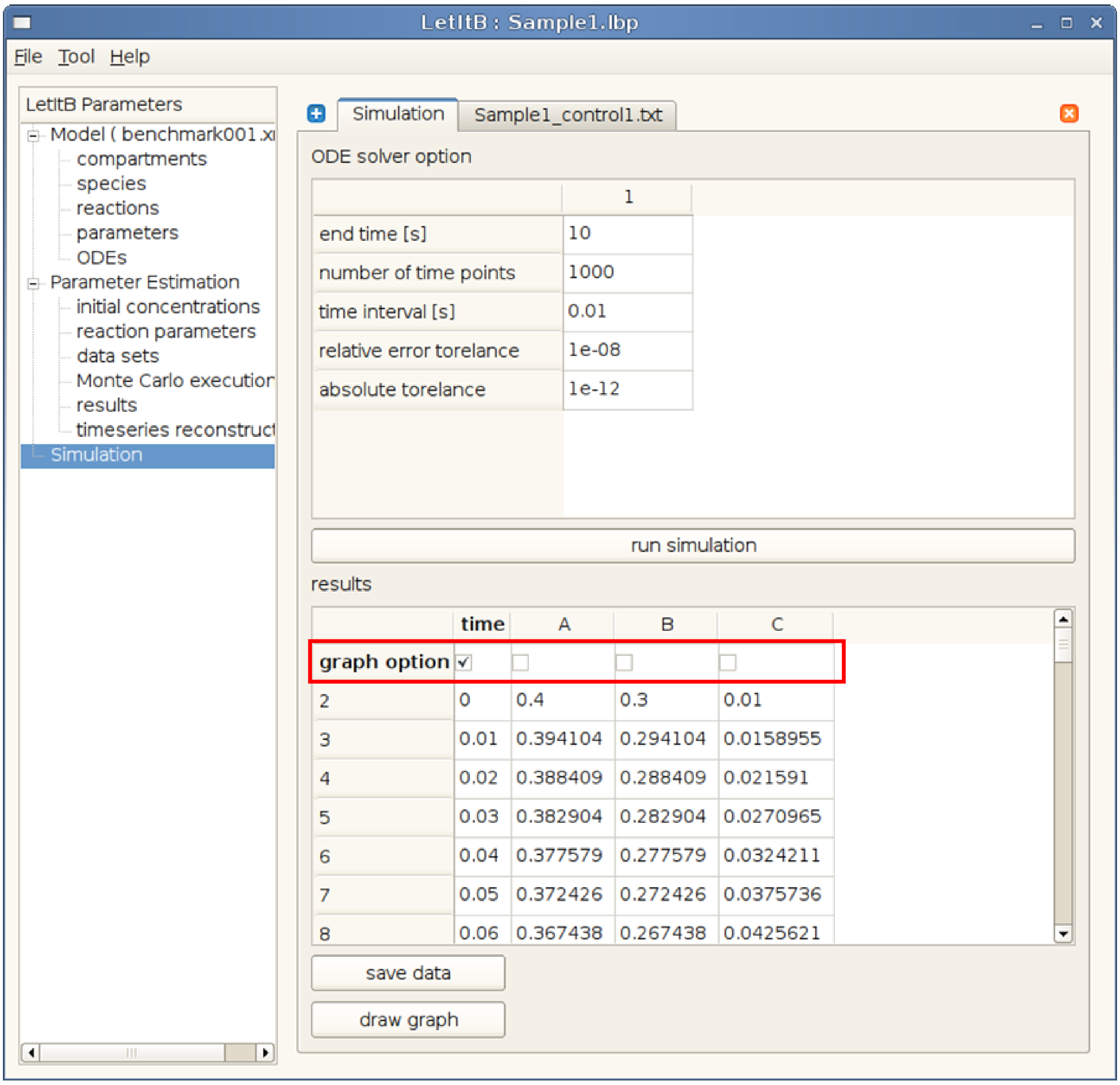
	time	A	B	C
graph option	☑	☐	☐	☐
2	0	2	0.3	0.01
3	0.01	2	0.271454	0.0385464
4	0.02	2	0.245626	0.0643737
5	0.03	2	0.222259	0.0877409
6	0.04	2	0.201118	0.108882
7	0.05	2	0.18199	0.12801
8	0.06	2	0.164685	0.145315

Figure 44: Simulation Screen (Results Data Saving)

7.7 Displaying Simulation Results Graph

To display a results graph of Simulation and Simulation with Control Data, select from the **graph option** check box in the **results** pane any factors you want to display in the graph, and then click the **draw graph** button. A timeseries graph of simulation results will be displayed.

* By default, not all the factors in **graph option** are selected. If no factors in **graph option** is selected, no graph can be displayed.



ODE solver option

	1
end time [s]	10
number of time points	1000
time interval [s]	0.01
relative error torelance	1e-08
absolute torelance	1e-12

results

	time	A	B	C
graph option	☑	☐	☐	☐
2	0	0.4	0.3	0.01
3	0.01	0.394104	0.294104	0.0158955
4	0.02	0.388409	0.288409	0.021591
5	0.03	0.382904	0.282904	0.0270965
6	0.04	0.377579	0.277579	0.0324211
7	0.05	0.372426	0.272426	0.0375736
8	0.06	0.367438	0.267438	0.0425621

Figure 45: Simulation Screen (Graph Displaying Operation Screen)

A graph window displays a timeseries graph, with simulation results in Y axis and time in X axis, based on the factors you select in **graph option**. The simulation result for each factor is displayed in solid lines.
NOTE: The colors of solid lines are automatically set.

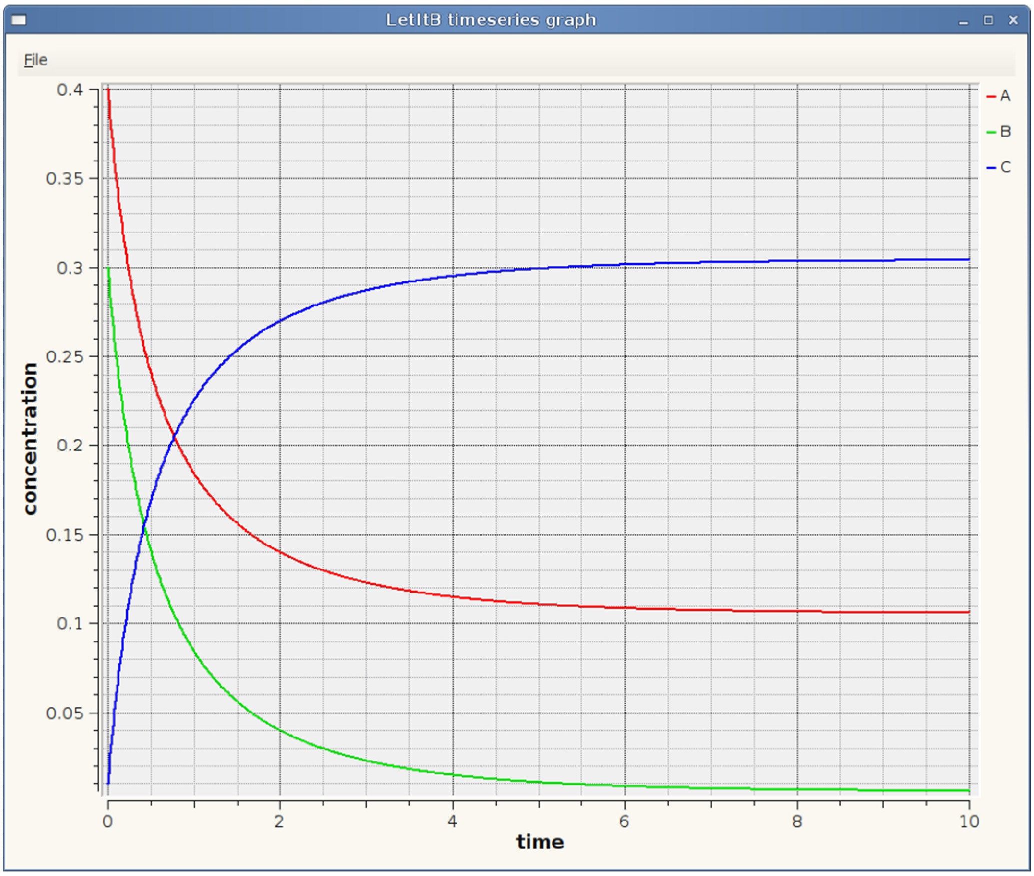


Figure 46: Timeseries Graph Screen

How to Configure:

1 To save an image:

From the menu of a graph window, select **File** > **Save graph**.

When a file dialog appears, select where the file will be saved, a name of the file and an image format you want to save, and then save the data.

2 To display/hide graph:

By clicking the captions in the upper right corner of a graph window, you can display/hide the graph.

End