

# 1. Model Select – Model Source

The screenshot shows the EASY MODEL application interface. The top navigation bar includes the EASY MODEL logo, a hamburger menu, and the text "Model Select". The left sidebar contains four navigation buttons: "1. Model Select", "2. Model Builder", "3. Simulation Launcher", and "4. Simulation Results". The main content area displays the "Model Source" section, which includes buttons for "Create New Model", "Public Repository", "Private Repository", and "Import SBML Model File". A "Drop file here" area is also present. The right sidebar contains two buttons: "Tutorial" and "Login & Register".

**Navigation buttons: from Model Select to Simulation Results.**

**Information buttons can be found across the application.**

**Model Source**

- Create New Model
- Public Repository
- Private Repository
- Import SBML Model File
- Drop file here

**Tutorial**

**Login & Register**


Create New Model  
Create blank model. Changes will not be saved unless logged in.

Public Repository  
Load and modify public models. Changes won't be saved.

Private Repository  
Create and modify your personal models. Changes will be saved every time model is validated.

Import SBML Model File  
Upload a SBML model file. Changes will not be saved unless logged in.

# 1. Model Select – Model Repository



- 1. Model Select
- 2. Model Builder
- 3. Simulation Launcher
- 4. Simulation Results

## Model Select

Back to Model Source

Public Models

BIOMD001 Edelstein1996 - EPSP ACh event

BIOMD002 Edelstein1996 - EPSP ACh species

BIOMD003 Goldbeter1991 - Min Mit Oscil

BIOMD004 Goldbeter1991 - Min Mit Oscil, Expl Inact

BIOMD005 Tyson1991 - Cell Cycle 6 var

BIOMD006 Tyson1991 - Cell Cycle 2 var

BIOMD007 Novak1997 - Cell Cycle

Goldbeter1991 - Min Mit Oscil


Minimal cascade model for the mitotic oscillator involving cyclin and cdc2 kinase.  
This model has been generated by MathSBML 2.4.6 (14-January-2005) 14-January-2005 18:33:39.806932.  
This model is described in the article:  
[A minimal cascade model for the mitotic oscillator involving cyclin and cdc2 kinase.](#)  
Goldbeter A.  
Proc. Natl. Acad. Sci. U.S.A. 1991; 88(20):9107-11

Copy to Private Models

Load the model to edit.

Load Model

## 2. Model Builder – Define Reactions



- 1. Model Select
- 2. Model Builder**
- 3. Simulation Launcher
- 4. Simulation Results

### Model Builder

BIOMD003 Goldbeter1991 - Min Mit Osc

**1. Start by naming your model. Description is optional.**






**2. Define reactions (see below note)**

**3. Set initial concentrations and variable types (see next slide)**











**4. Create or import rates (see next slide)**

**5. Select a rate for each reaction (see next slide)**

**6. Validate model to advance to the Simulation Launcher step.**

Name	Rate Law	Reaction
R		-> C
R2		C ->
R3		C -> ;X
R4		
R5		M ->
R6		-> X;M X
R7		X ->

**How to write reactions using Substrates, Products and Modifiers:**  
 $n1*S1 + n2*S2 + \dots \rightarrow m1*P1 + m2*P2 + \dots ; M1; M2; \dots$   
 $n_i, m_i$ : Stoichiometric coefficient.  
 $S_i, P_i$ : Substrates and Products.  
 $M_i$ : Modifiers that can activate or inhibit the reaction rate.

Name	Rate Definition	Edit	Remove
BIOMD003_K1	cell*vi		
BIOMD003_K2	C*cell*kd		
BIOMD003_K3	X*(C...		
BIOMD003_K4	cell*(1+-1*M)...		
BIOMD003_K5	cell*M*V2*(K2...		

**Adjustable Split Bar**

**Model editor**

**Rate editor**

## 2. Model Builder – Species, Define rates, Select a rate for each reaction

The screenshot displays the EAM Model Builder interface with several windows and annotations:

- Species Settings** window: A table with columns 'Name', 'Initial Concentration', and 'Variable Type'. It lists species C, M, and X, each with an initial concentration of 0.01 and a 'Time Deper' variable type.
- Rate Law Selection for R2 Reaction** window: Shows 'BIOMD003\_K2' selected. The 'Parameters values' table lists parameters C, cell, and kd with their respective values and dropdown menus.
- Edit Rate** window: Shows the rate definition  $C \cdot \text{cell} \cdot v_d \cdot X \cdot (C + K_d)^{-1}$  and 'Rate Options' (One substrate only, No products, One modifier only).
- Import Predefined Rates** window: A table with columns 'Name' and 'Rate Definition', listing various predefined rate laws like Power Laws, Saturating Cooperative, etc.
- Main Interface**: Shows a list of reactions (Mit Osc, C ->, C -> ;X, -> M;C M) and a 'Validate' button.

Annotations (red boxes and arrows) highlight key steps:

- 3. Set initial concentrations and variable types**: Points to the Species Settings window.
- 4. Create or import rates**: Points to the '+ New Rate' and 'Import Rates' buttons.
- 5. Select a rate for each reaction and set a value for all the rate's parameters. Each parameter must have either a numeric value, a reference to a substrate, or a reference to a modifier.**: Points to the Rate Law Selection and Edit Rate windows.

### 3. Simulation Launcher – Dynamic and Steady State simulation

The screenshot displays the EASY MODEL Simulation Launcher interface. On the left, a sidebar lists four steps: 1. Model Select, 2. Model Builder, 3. Simulation Launcher (highlighted), and 4. Simulation Results. The main panel is titled 'Sim' and features a 'Select Simulation Types' section with three checked options: 'Dynamic (Deterministic)', 'Steady State', and 'Dynamic (Stochastic)'. Below this are buttons for 'Plot Settings' (enclosed in a dashed red box), 'Mathematica Notebook', 'Export SBML Model', and a prominent blue 'Launch Simulation' button. The right panel shows 'Dynamic (Deterministic) Simulation Settings' with fields for 'Initial time' (0), 'Final time' (100), and 'Time step' (0.1). It also includes expandable sections for 'Analysis', 'Plot Views', and 'Parameter Scan'. At the bottom, 'Steady State Simulation Settings' is partially visible. Several red callout boxes provide detailed explanations: one for 'Dynamic simulation' (time evolution), one for 'Steady state simulation' (non-trivial equilibriums), one for 'Plot settings' (configuration parameters), one for the 'Launch Simulation' button (adding jobs to the queue), and one for 'Steady State Analysis options' (describing Gains, Sensitivities, and Stability analysis).

**EASY MODEL**

1. Model Select  
2. Model Builder  
3. Simulation Launcher  
4. Simulation Results

Sim

*Dynamic simulation: time evolution of the species in the model.*

Select Simulation Types

- ✓ Dynamic (Deterministic)
- ✓ Steady State
- ✓ Dynamic (Stochastic)

*Steady state simulation: calculates the steady states (non-trivial equilibriums) of the biological system. These steady states remain constant over the time.*

Plot Settings

Mathematica Notebook

Export SBML Model

Launch Simulation

*Plot settings: contains several configuration parameters for the graphical plots that will be performed.*

*Launching the simulation will add the simulation job to the job queue. You can check the progress of the job inside of the queue in the next step.*

**Dynamic (Deterministic) Simulation Settings**

- Main Settings
  - Initial time: 0 (Min=0)
  - Final time: 100 (Min=0)
  - Time step: 0.1 (Min=0.000001 ; Max=0.1)
- Analysis
- Plot Views
- Parameter Scan

**Steady State Simulation Settings**

- Main Settings

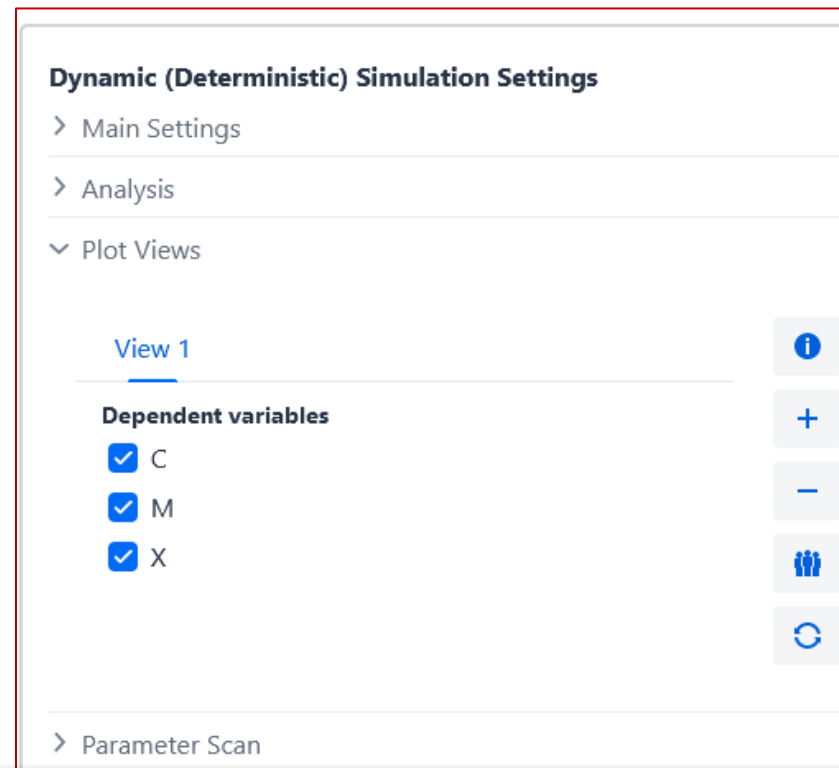
**Steady State Analysis options**

"Gains" option analyses how changes in the independent variables affect the values of the time-dependent variables.

"Sensitivities" option analyses how changes in the parameter values affect the values of the time-dependent variables.

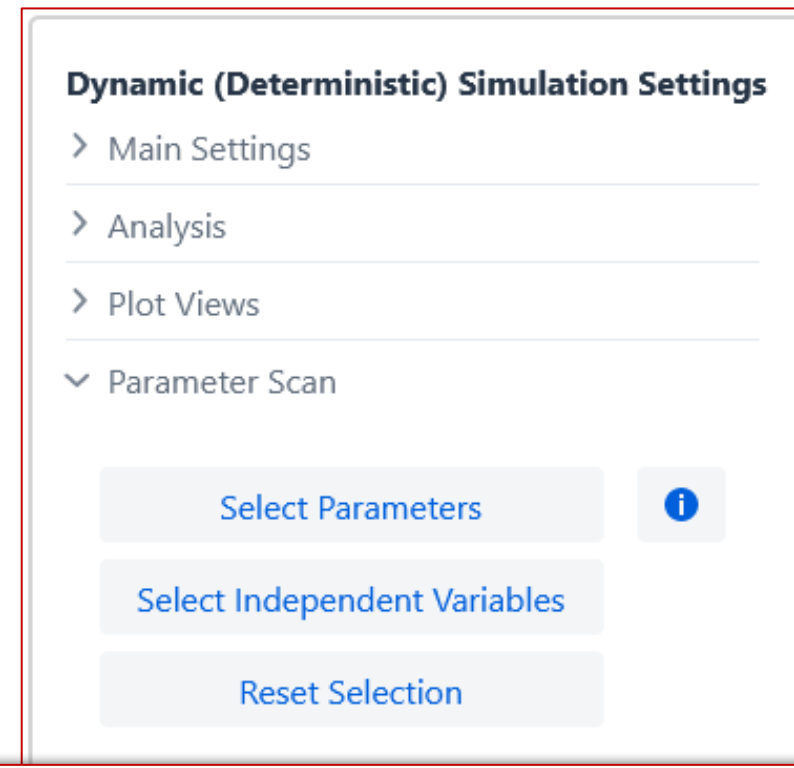
"Stability analysis" calculates if the steady state (homeostasis) is stable (negative real parts for all eigenvalues) or not (non-negative real part for at least one eigenvalue).

### 3. Simulation Launcher – Plot Views, Parameter Scan, Stochastic simulation



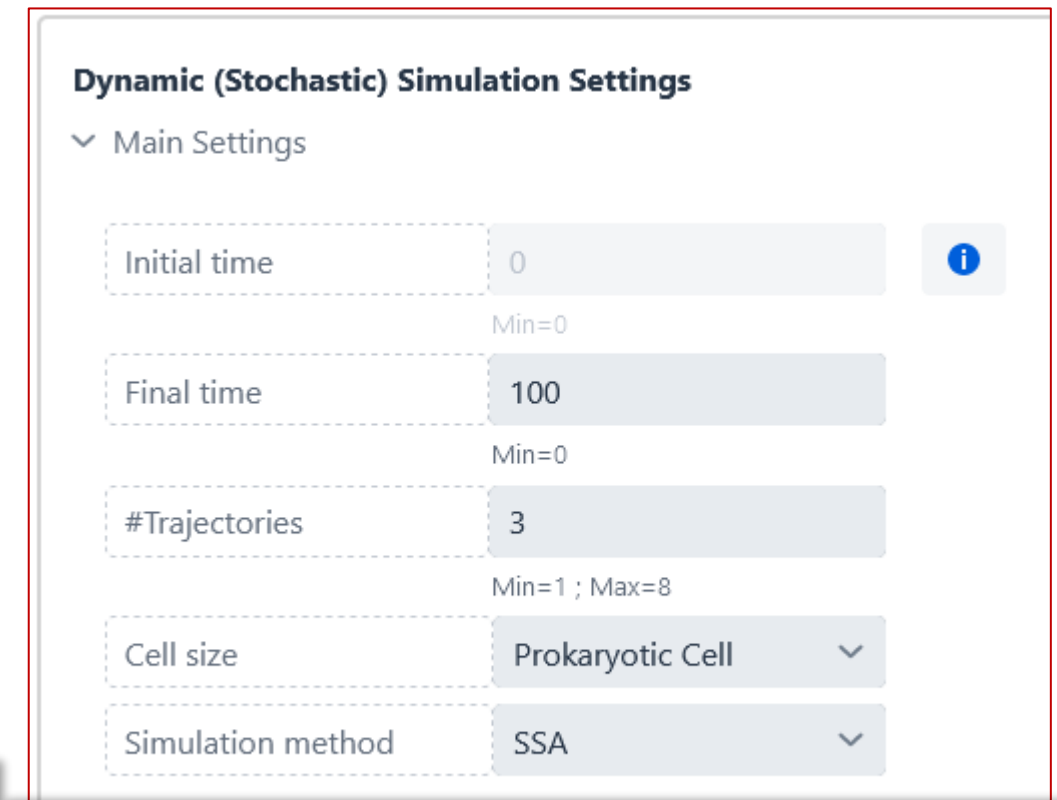
The image shows the 'Dynamic (Deterministic) Simulation Settings' interface, specifically the 'Plot Views' section. It features a sidebar with 'Main Settings', 'Analysis', 'Plot Views', and 'Parameter Scan'. The 'Plot Views' section is expanded, showing 'View 1' with a list of 'Dependent variables' (C, M, X) that are all checked. To the right of the list are icons for adding (+), removing (-), and refreshing (circular arrow) the variables. An information icon (i) is also present.

*Plot views: you can select which time-dependent species are to be plotted in the simulation graphics. Furthermore, you can define several plot views, each of them with its own selected time-dependent species.*



The image shows the 'Dynamic (Deterministic) Simulation Settings' interface, specifically the 'Parameter Scan' section. It features a sidebar with 'Main Settings', 'Analysis', 'Plot Views', and 'Parameter Scan'. The 'Parameter Scan' section is expanded, showing buttons for 'Select Parameters', 'Select Independent Variables', and 'Reset Selection'. An information icon (i) is present next to the 'Select Parameters' button.

*Parameter scan: perform the simulation for several values of the rate parameters or independent variables. Select a numerical range and the number of range intervals for the parameter you want to scan to observe how the system evolves with the values variation. Each parameter scan is simulated separated from the others.*

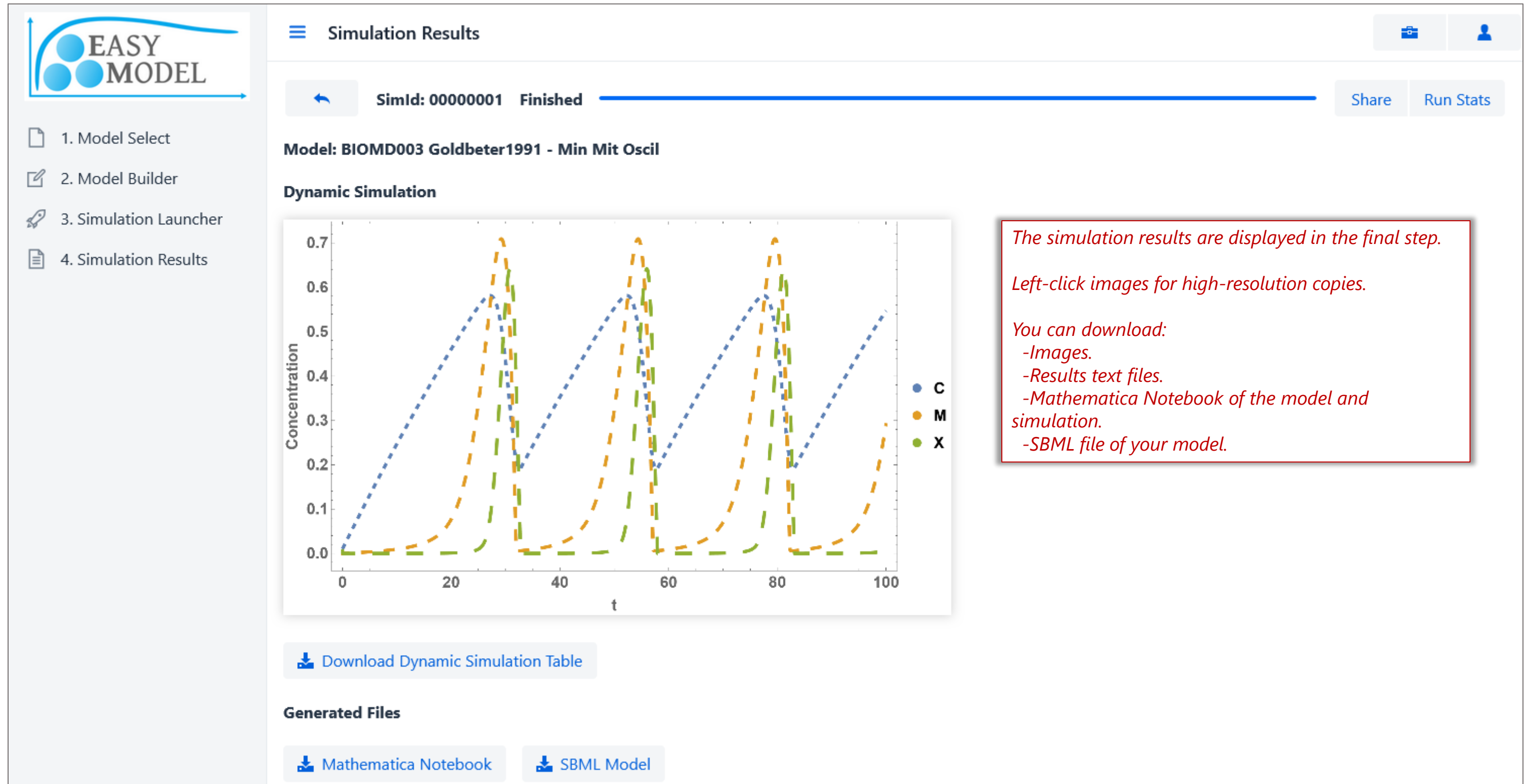


The image shows the 'Dynamic (Stochastic) Simulation Settings' interface, specifically the 'Main Settings' section. It features a sidebar with 'Main Settings' expanded. The settings include: 'Initial time' (0), 'Final time' (100), '#Trajectories' (3), 'Cell size' (Prokaryotic Cell), and 'Simulation method' (SSA). Each input field has a dashed border and an information icon (i) is present next to the 'Initial time' field. The 'Cell size' and 'Simulation method' fields are dropdown menus.


*Stochastic simulation: time evolution of the species using the Gillespie SSA stochastic simulation method. Compared to the deterministic simulation, it provides a more accurate simulation, specially when the model is composed of a small number of molecules and linear noise analysis is a more appropriate tool than the deterministic sensitivity analysis to understand the limitations and regulation of the system. All these benefits come at the expense of a longer simulation time. Tau-leaping method: useful to reduce the simulation time. Not all models can benefit from it.*



## 4. Simulation Results – Simulation Job Results





## 4. Simulation Results – Simulation Queue

















- 1. Model Select
- 2. Model Builder
- 3. Simulation Launcher
- 4. Simulation Results

### Simulation Results



#### Your Launched Simulations

Simulation Id	Status	Position in Queue	Copy URL	Cancel
00000001	Finished	-		
00000002	Finished	-		
00000003	Finished	-		
00000004	Finished	-		
00000005	Running	R		
00000006	Pending	1		
00000007	Pending	2		

When you launch a simulation, it is added into the processing queue. You can check the progress of your launched simulations in the queue view. You may also share and cancel unfinished simulations.