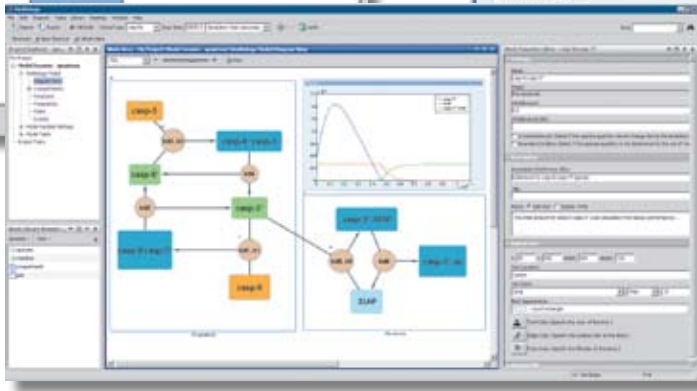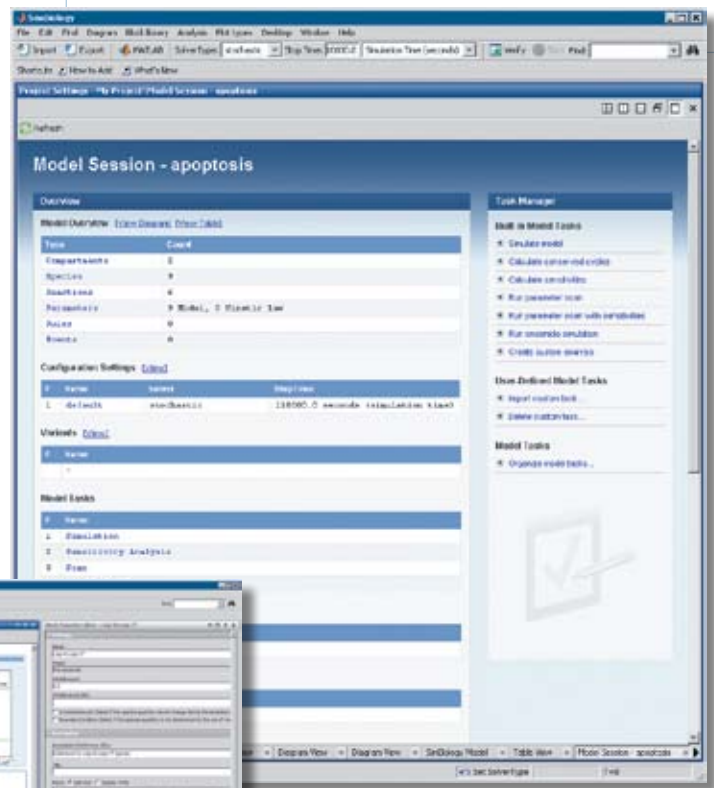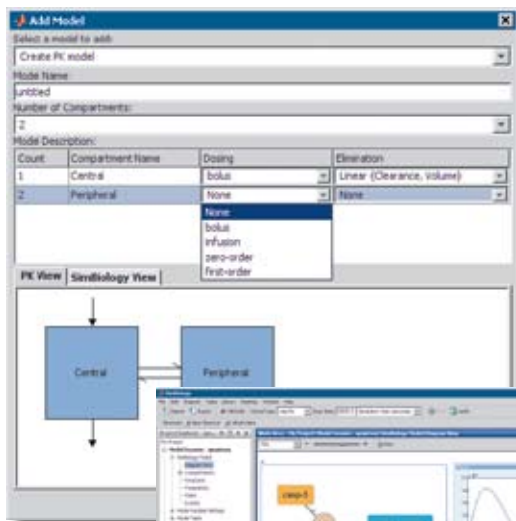# SimBiology 3

Model, simulate, and analyze biological systems

SimBiology® provides graphical and programmatic tools for modeling, simulating, and analyzing biological systems. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB® programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

KEY FEATURES

- Graphical and programmatic interfaces

- Functionality for fitting data and estimating parameters using nonlinear mixed effects

- Tools for sensitivity analysis and parameter scans

- Stochastic, stiff deterministic, and nonstiff deterministic solvers

- Pharmacokinetics (PK) wizard for automatically generating PK models

- Diagnostic plots of individual and population fits

The integrated environment available in SimBiology. Graphical and programmatic tools provide functionality for modeling, simulation, and analysis.

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Building a Model

SimBiology lets you create models that include compartments, species, parameters, reactions, events, rules, kinetic laws, and units.

You can create a model by:

- Dragging and dropping predefined blocks in the block diagram editor
- Entering equations and relevant parameters into a tabular interface
- Using SimBiology command-line functions
- Using the model wizard to create pharma-cokinetic models

You can configure the appearance of any pre-defined compartment, species, or reaction block. Customized blocks can be stored in libraries or used to create standardized blocks or elements. All model components can have URLs, tags, or notes added to their description.

Variants are collections of alternate values for parameters that you can apply to a model during simulation. This enables you to study various values for model compo-nents without creating new models.

SimBiology lets you work with built-in kinetic laws and units or create your own. Both built-in and user-defined kinetic laws are stored in libraries for easy reuse and distribution.

Data from external sources can be associated and saved with a SimBiology project. You can import, visualize, and use the external data for fitting parameters. Data can be imported from a Microsoft® Excel® file, text file, MAT-file, or the MATLAB workspace.

Running a Simulation

Together, SimBiology and MATLAB provide a wide range of solvers for simulating sto-chastic and deterministic systems.

Solvers

SimBiology provides three types of stochastic solvers: a stochastic simulation algorithm (SSA), explicit tau-leaping, and implicit tau-leaping.

SimBiology also provides determinis-tic solvers for stiff and nonstiff systems. In addition to the traditional MATLAB solvers, SimBiology adds CVODE from the SUNDIALS suite of solvers.

Simulation Events

Simulation events let you define a sudden change in model behavior. You can specify that an event occurs at a specific simulation time or in response to a change within the system, such as the value of a species.

Ensemble Runs

Ensemble runs let you analyze model output over multiple simulations—helpful when you are dealing with stochastic simulations or need to perform parameter scans on your model. You specify the model and number of iterations as inputs. You can calculate the mean and variance of the ensemble data, and visualize your ensemble results with distribu-tion and mountain plots.

Simulation Settings

You can specify the solver type, simulation stop time, and other simulation options. You can also specify whether dimensional analy-sis should be performed on the model as a verification step. Dimensional analysis checks that all mathematical expressions in the model are in consistent dimensions and then performs unit conversions automatically.
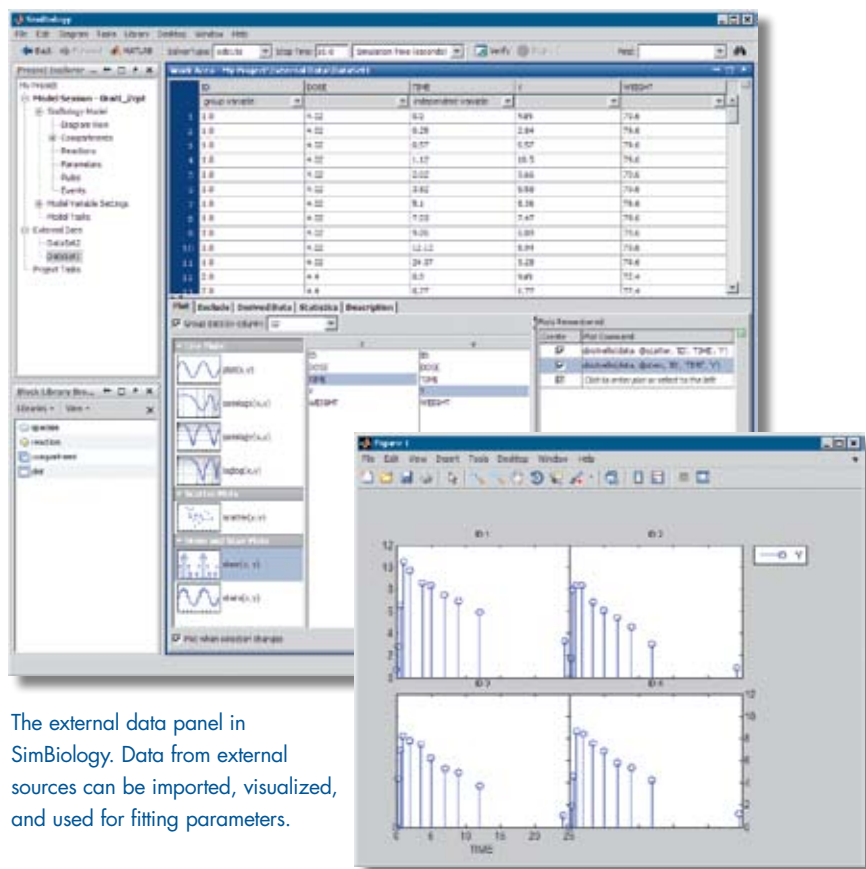
The external data panel in SimBiology. Data from external sources can be imported, visualized, and used for fitting parameters.
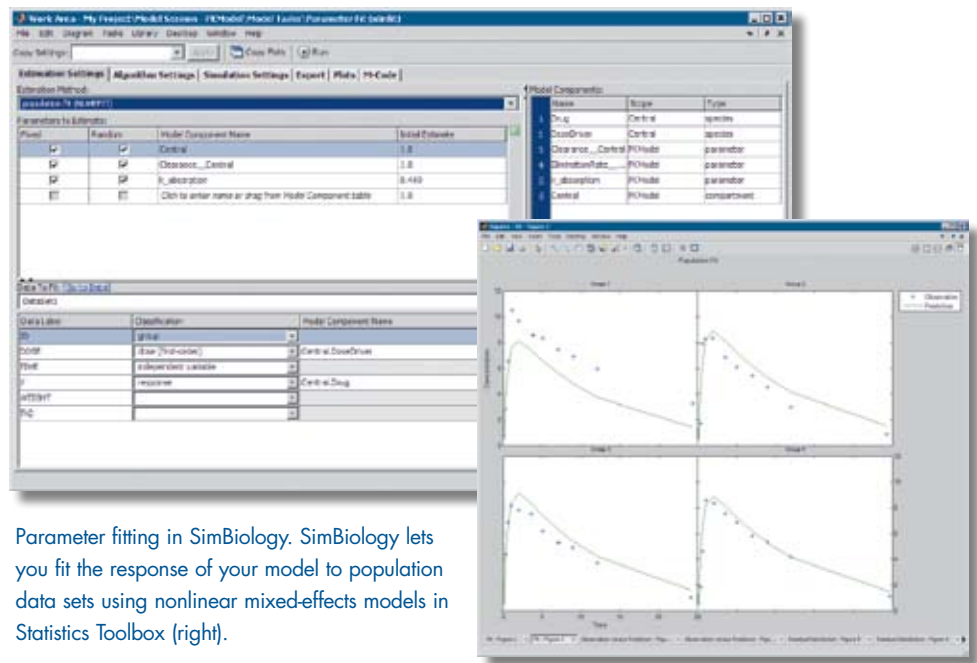
Parameter fitting in SimBiology. SimBiology lets you fit the response of your model to population data sets using nonlinear mixed-effects models in Statistics Toolbox (right).

Analyzing a Model

SimBiology provides functionality that lets you gain insight into your model via parameter estimation, sensitivity analysis, and parameter scans.

Parameter Estimation

With SimBiology you can fit the response of your model to experimental data. You can fit parameters with MATLAB or by using optimization algorithms in Optimization Toolbox™. SimBiology also lets you fit parameters to population data sets using nonlinear mixed-effects models in Statistics Toolbox™.

Sensitivity Analysis

SimBiology lets you calculate the sensitivities of all system species relative to the specified parameters and species' initial conditions. This analysis helps you better understand the behavior of the network and lets you determine parameters of highest importance.

Sensitivities to various initial conditions enable investigation into the behavior of the network across populations.

SimBiology provides several options for analyzing sensitivities. For example:

- Computed sensitivities can be normalized or presented without normalization.
- Sensitivities can be computed relative to a user-specified set of parameters, species' initial conditions, or both.

Parameter Scans

SimBiology allows you to perform parameter scans to visualize the dynamic behavior of the model over a range of parameter values. You can also perform scans on species and compartment values.

Visualizing and Reporting Results

SimBiology provides multiple tools for visualizing, storing, and sharing your results.

Diagnostic plots are automatically generated after parameter fitting. They display results such as predicted time courses and observations, residuals, and observed versus predicted values. SimBiology also provides plots for viewing simulation and analysis results.

Project files store all information related to the project, including models, simulation settings, and simulation results. Models can also be exported to the SBML format.

Report Generator

SimBiology lets you create customizable reports using template-specified model elements. You can automatically populate your report content with a single click. Reports can be generated in XML or HTML.

Diagnostic plots in SimBiology displaying results such as predicted time courses and observations, observed versus predicted values, and residuals.
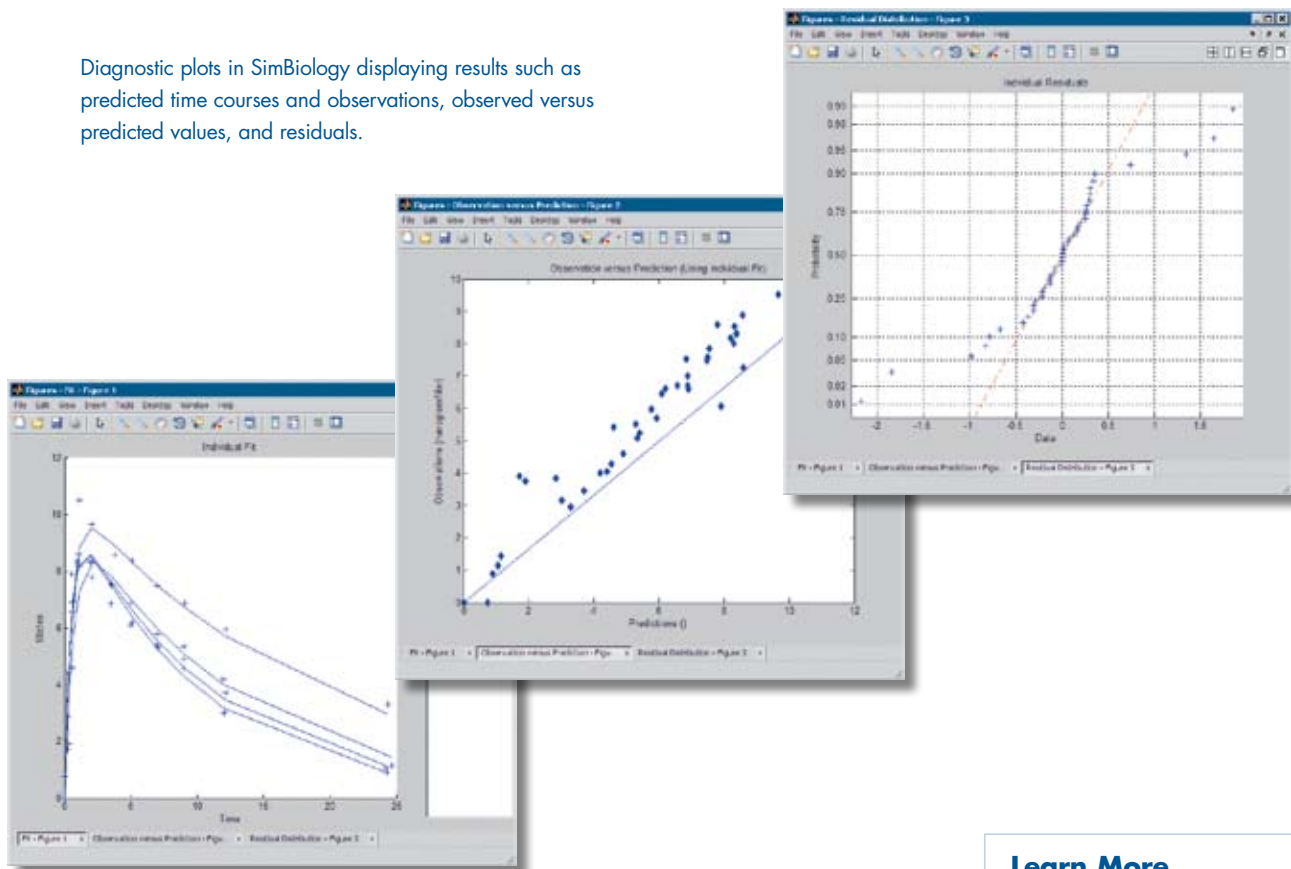
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MATLAB®

Related Products
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Read, analyze, and visualize genomic, proteomic, and microarray data

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Solve optimization problems using genetic algorithms, simulated annealing, and direct search

Optimization Toolbox™
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Statistics Toolbox™
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