Simmune and Its Support to SBML and SBML packages

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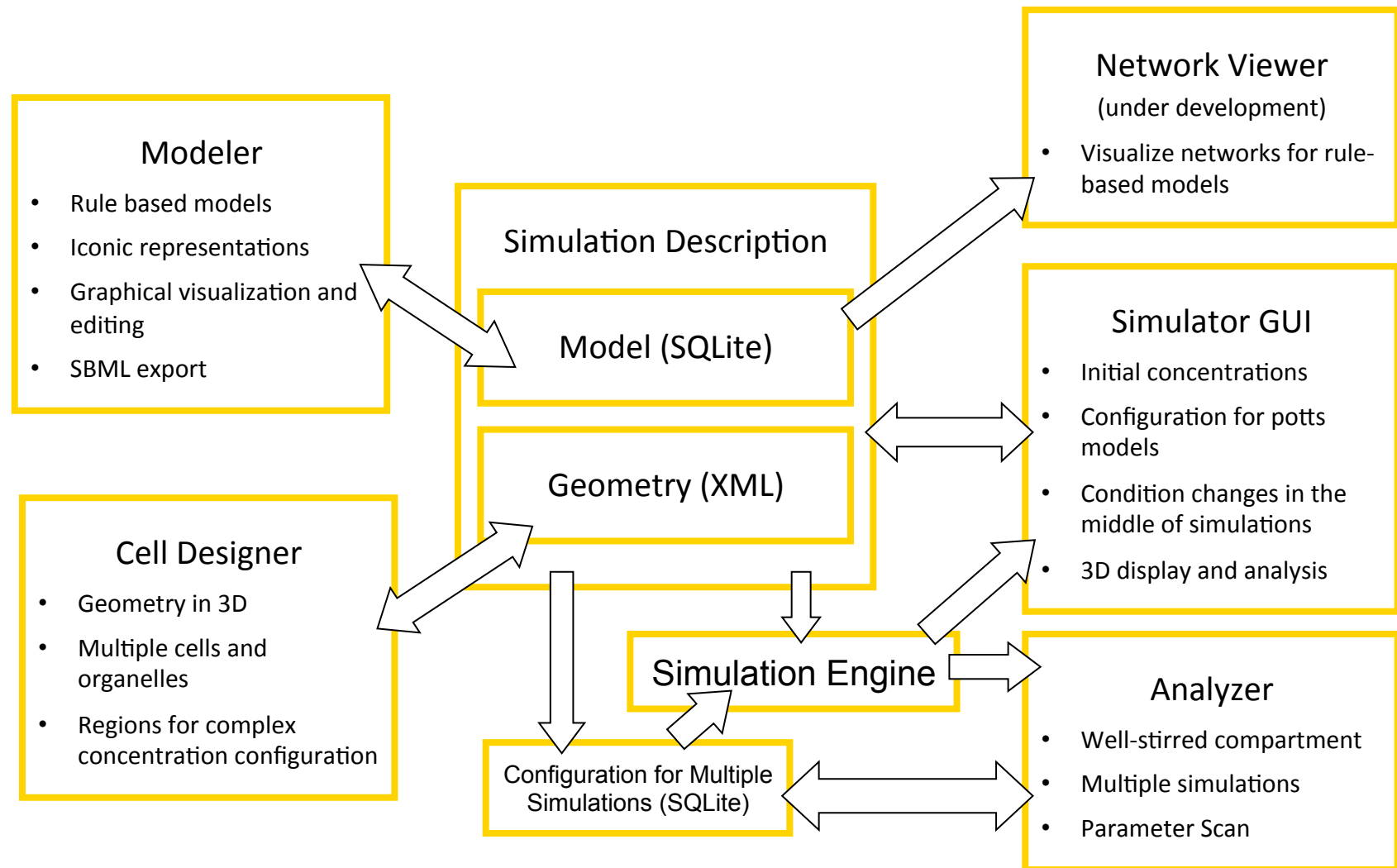*National Institutes of Health, USA*
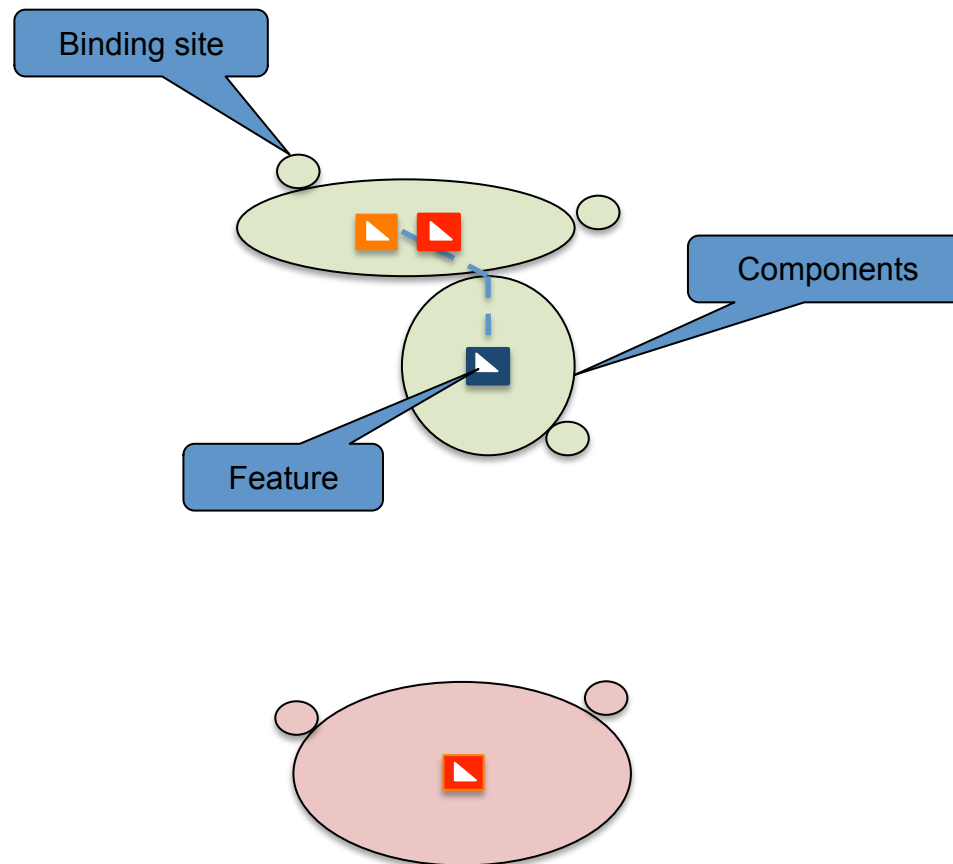
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Outline

- Simmune infrastructure and work flow

- Simmune graphical representations

- Simmune: (Yeast Model)

  – Simmune Modeler

  – Simmune CellDesigner

  – Simmune Simulator

- SBML support

Simmune Structure and Workflow

Modeler

- Rule based models
- Iconic representations
- Graphical visualization and editing
- SBML export

Simulation Description

Model (SQLite)

Geometry (XML)

Network Viewer

(under development)

- Visualize networks for rule-based models

Simulator GUI

- Initial concentrations
- Configuration for potts models
- Condition changes in the middle of simulations
- 3D display and analysis

Cell Designer

- Geometry in 3D
- Multiple cells and organelles
- Regions for complex concentration configuration

Simulation Engine

Configuration for Multiple Simulations (SQLite)

Analyzer

- Well-stirred compartment
- Multiple simulations
- Parameter Scan

Graphical Representation of Simmune Models
Molecule: Component, binding sites, features

Graphical Representation of Simmune Models
Complex Species

Bond in species
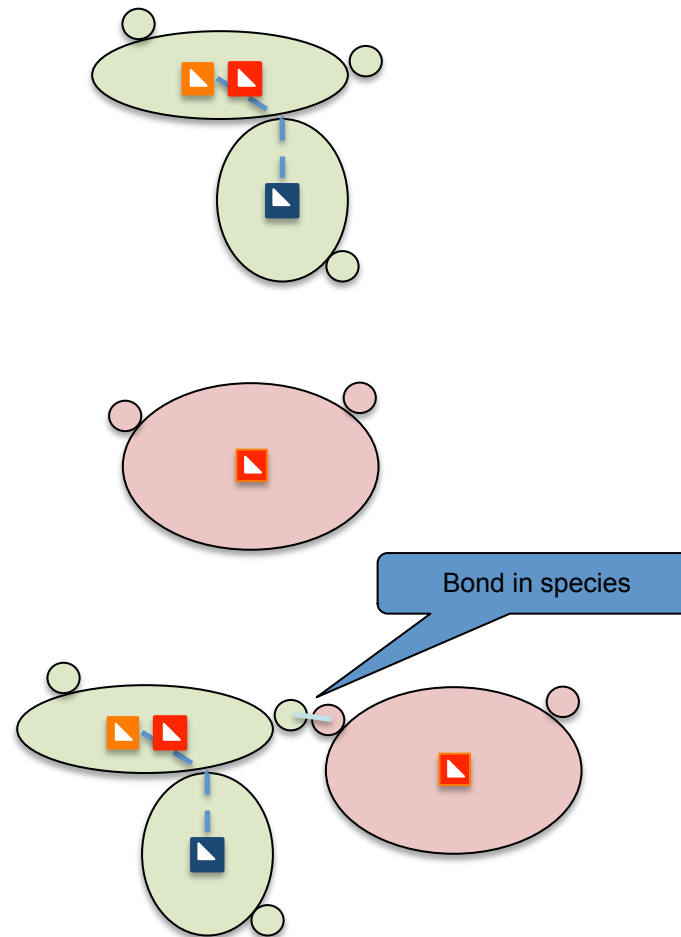
Graphical Representation of Simmune Models
Complex
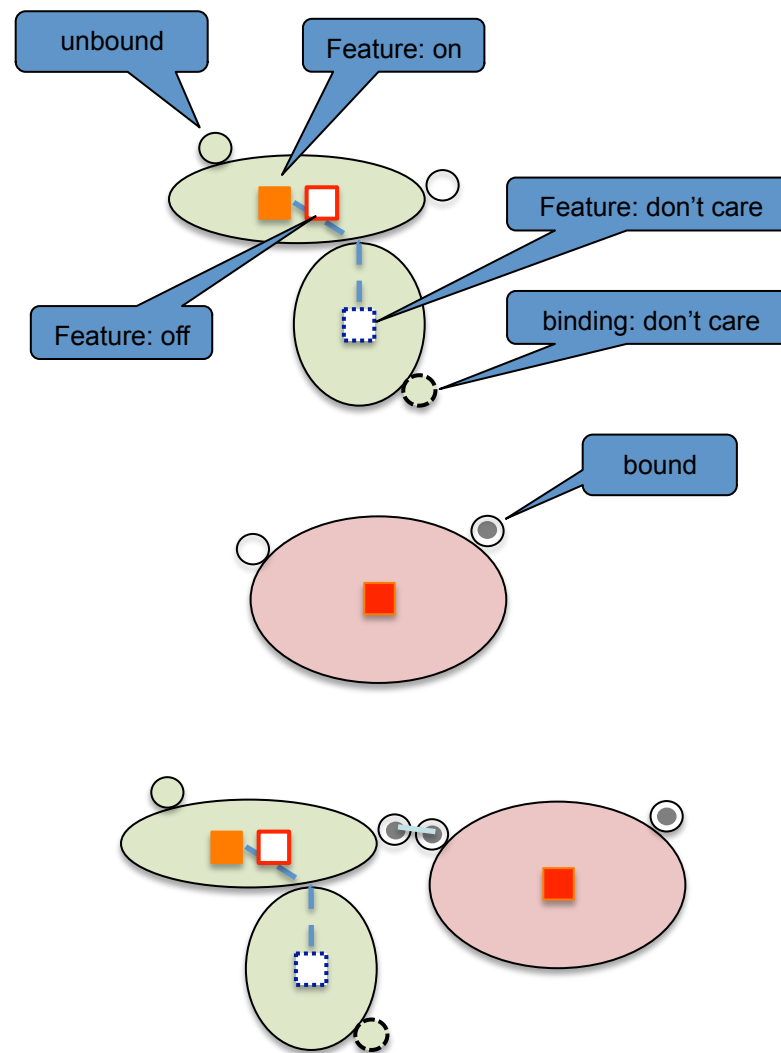
Graphical Representation of Simmune Models
Reaction
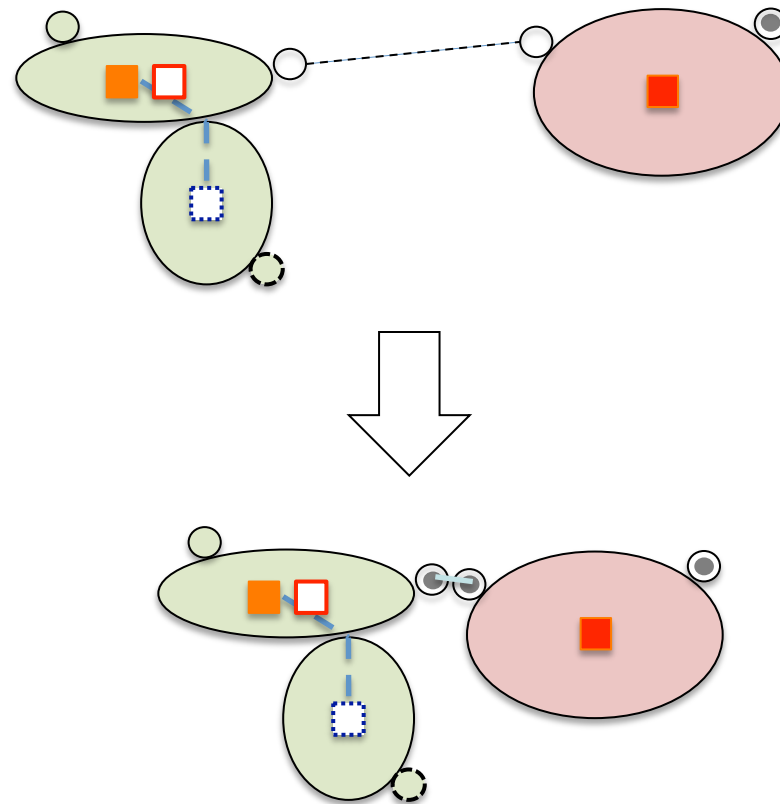
Simmune Modeler: Yeast Model: **Molecules**

Simmune Modeler: Yeast Model: **Complex Species**

Simmune Modeler: Yeast Model: **Complex**

Simmune Modeler: Yeast Model: **Reaction**

Simmune CellDesigner: Yeast Geometry: Cell

Simmune CellDesigner: Yeast Geometry:
Flexible Cell Shape Configuration
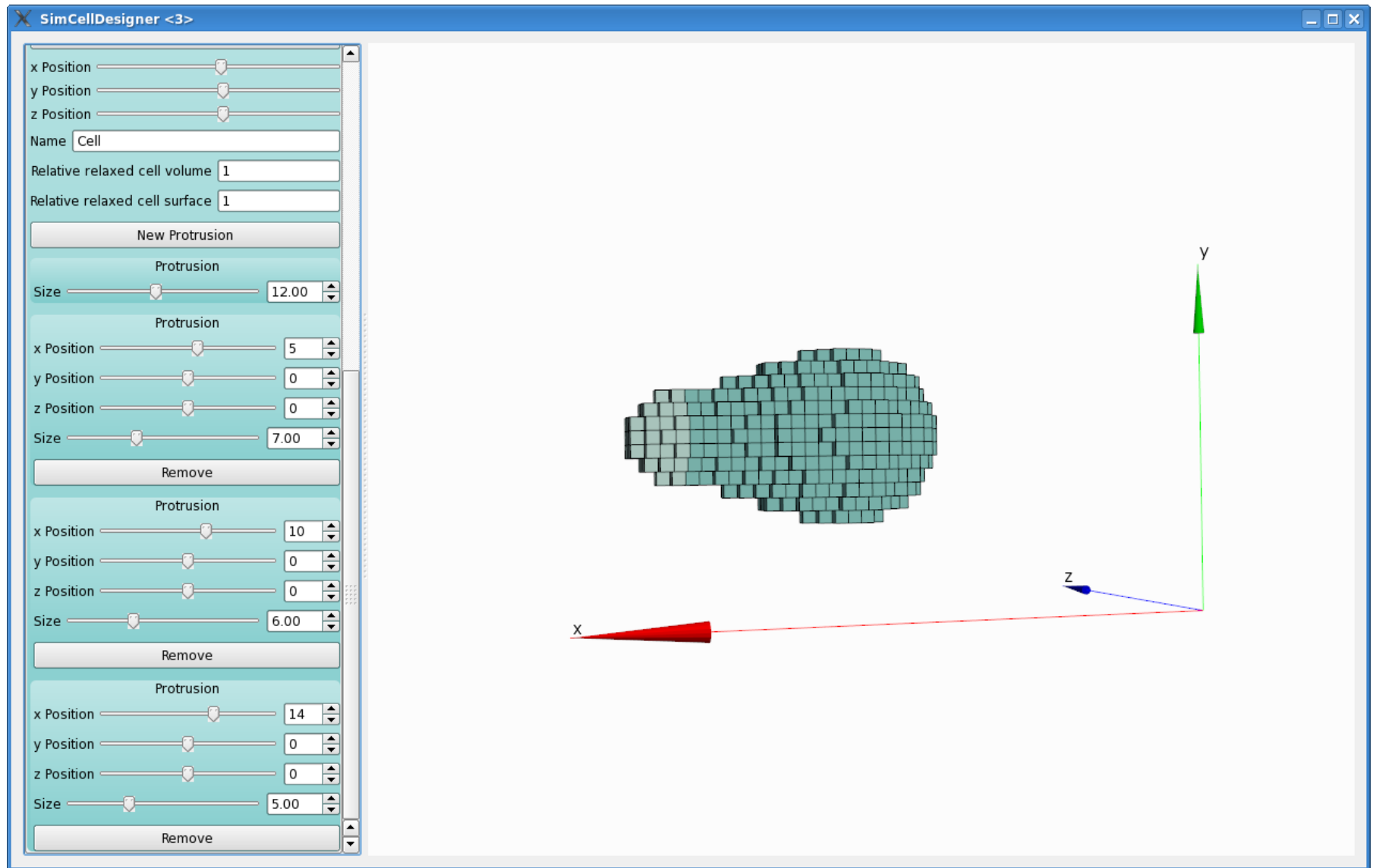
Simmune CellDesigner: Yeast Geometry: **Oganelle**

Simmune CellDesigner: Yeast Geometry: **Regions**

Simmune Simulation : Yeast : **Initial Condition**

Simmune Simulation : Yeast : **Simulation Setup**

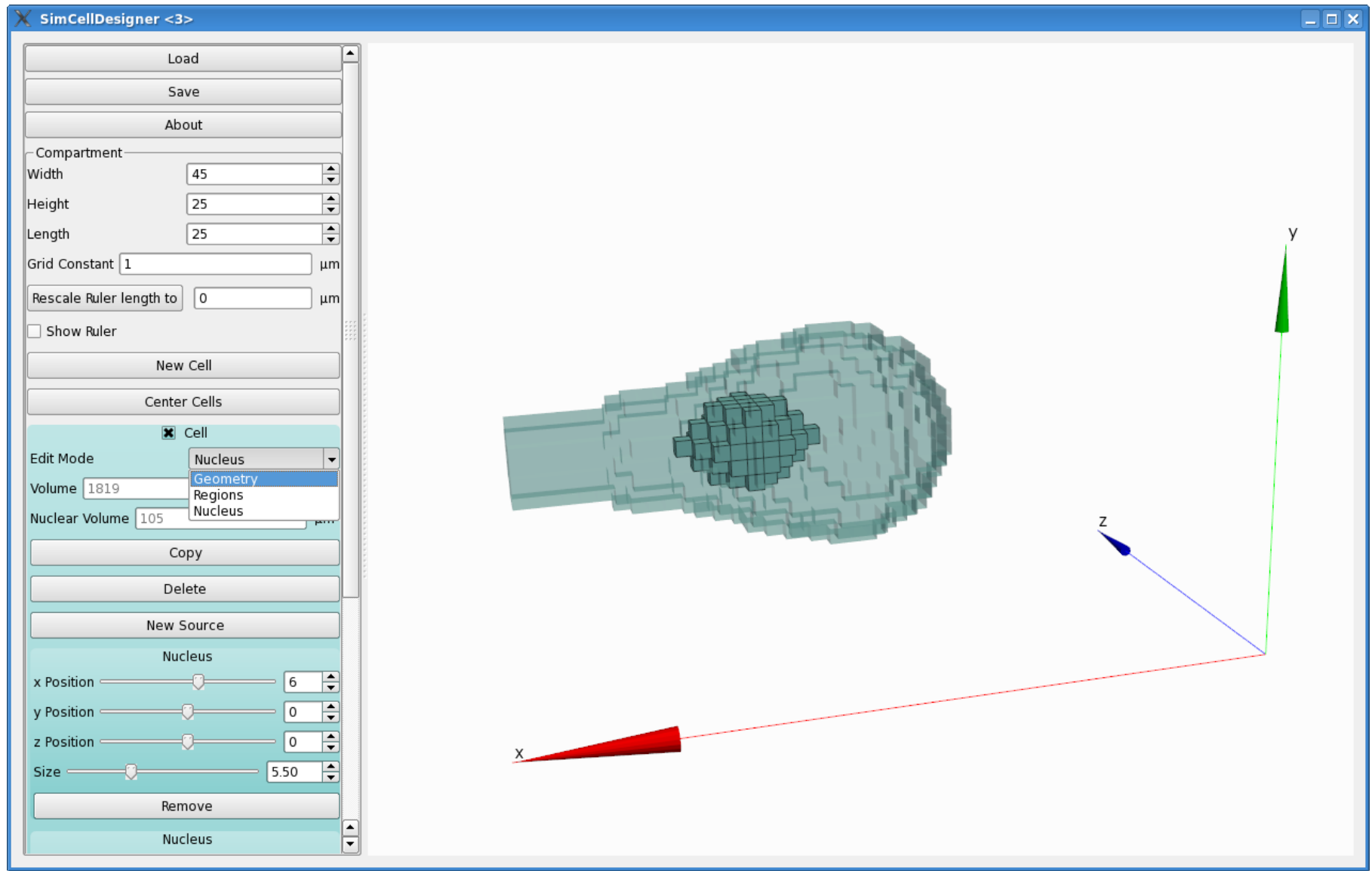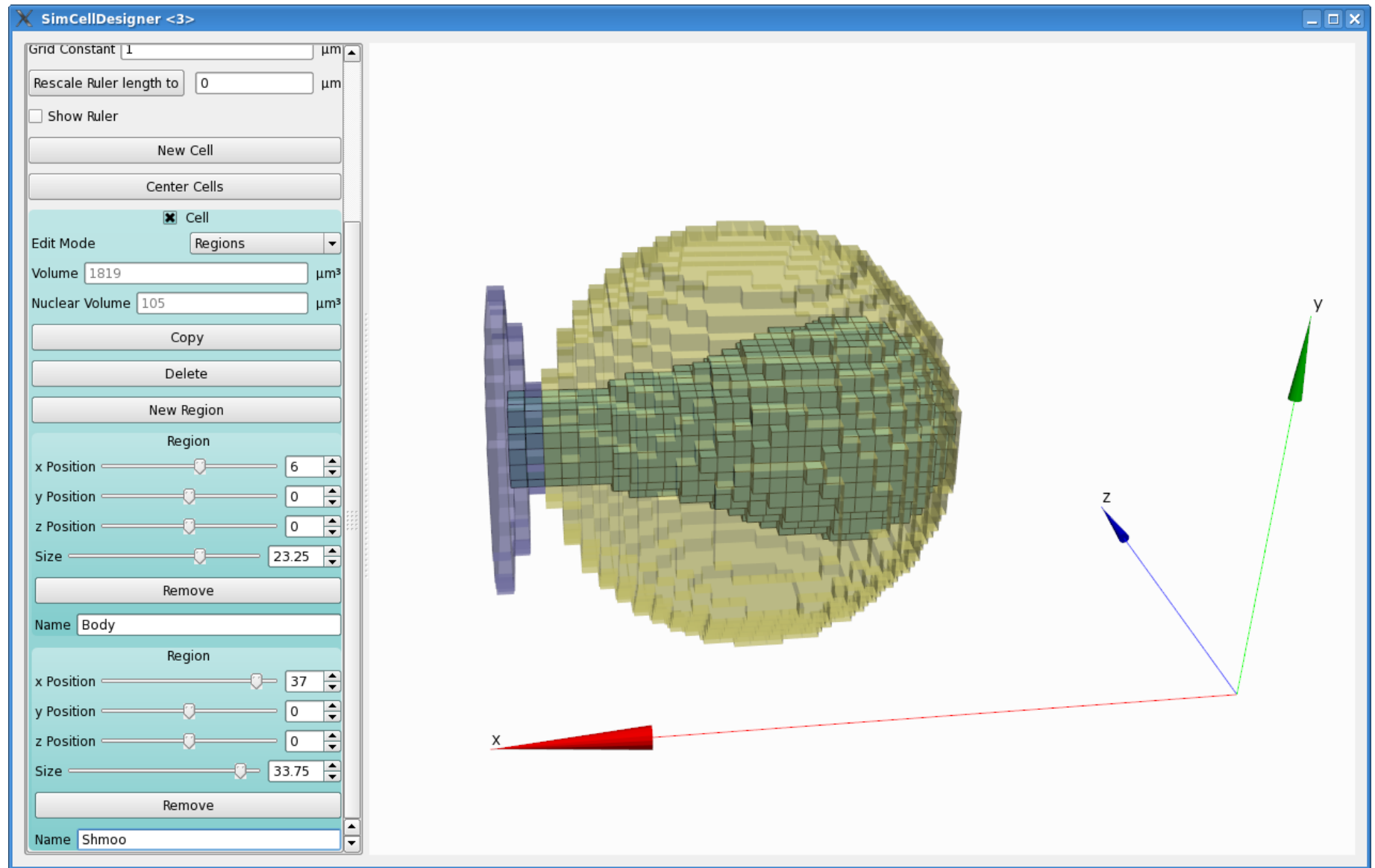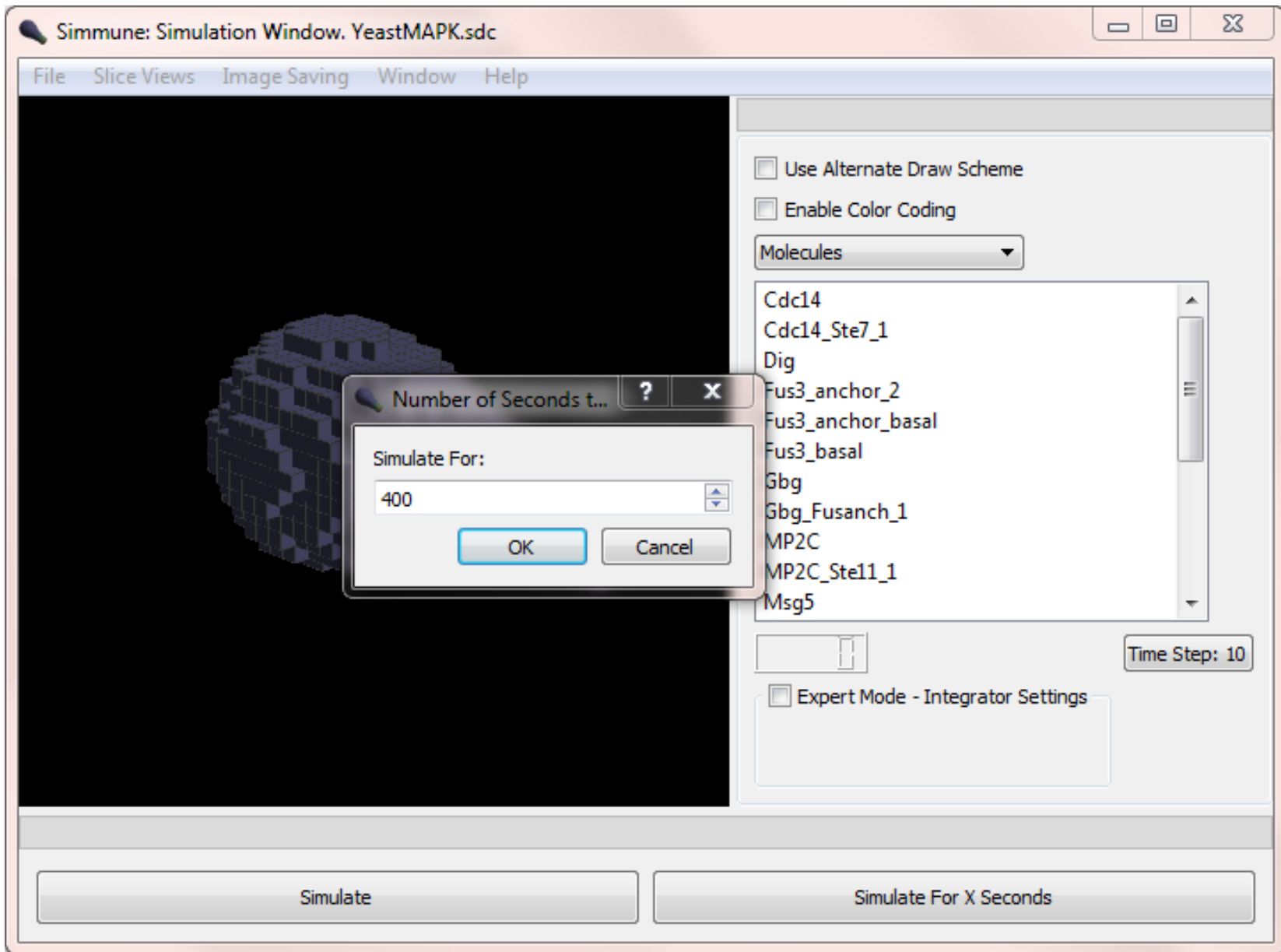# Simmune Simulation : Yeast : **Time Plot**

Simmune Simulation : Yeast : **Concentration Distribution**
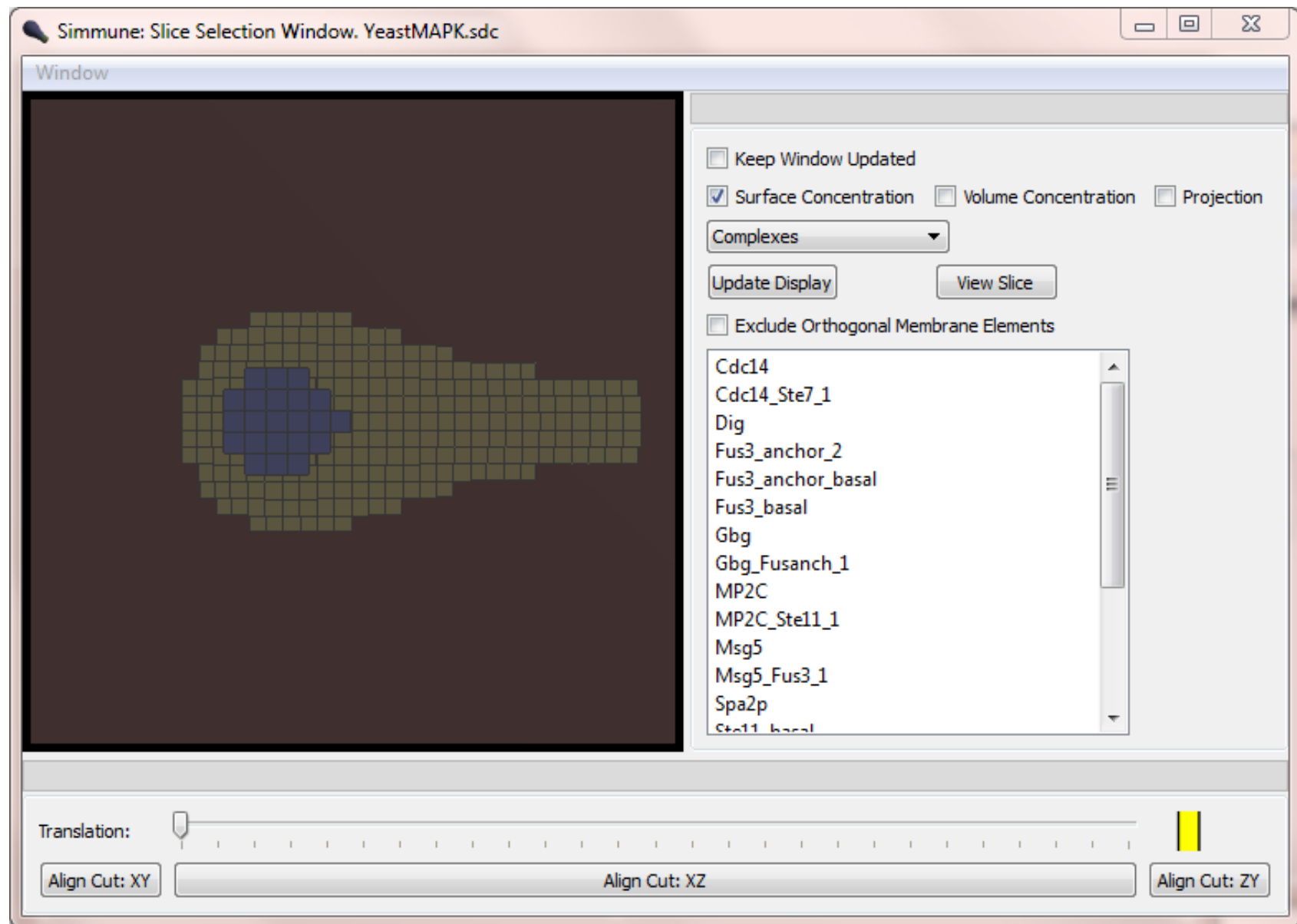
Simmune Simulation : Yeast : **Line Configuration**
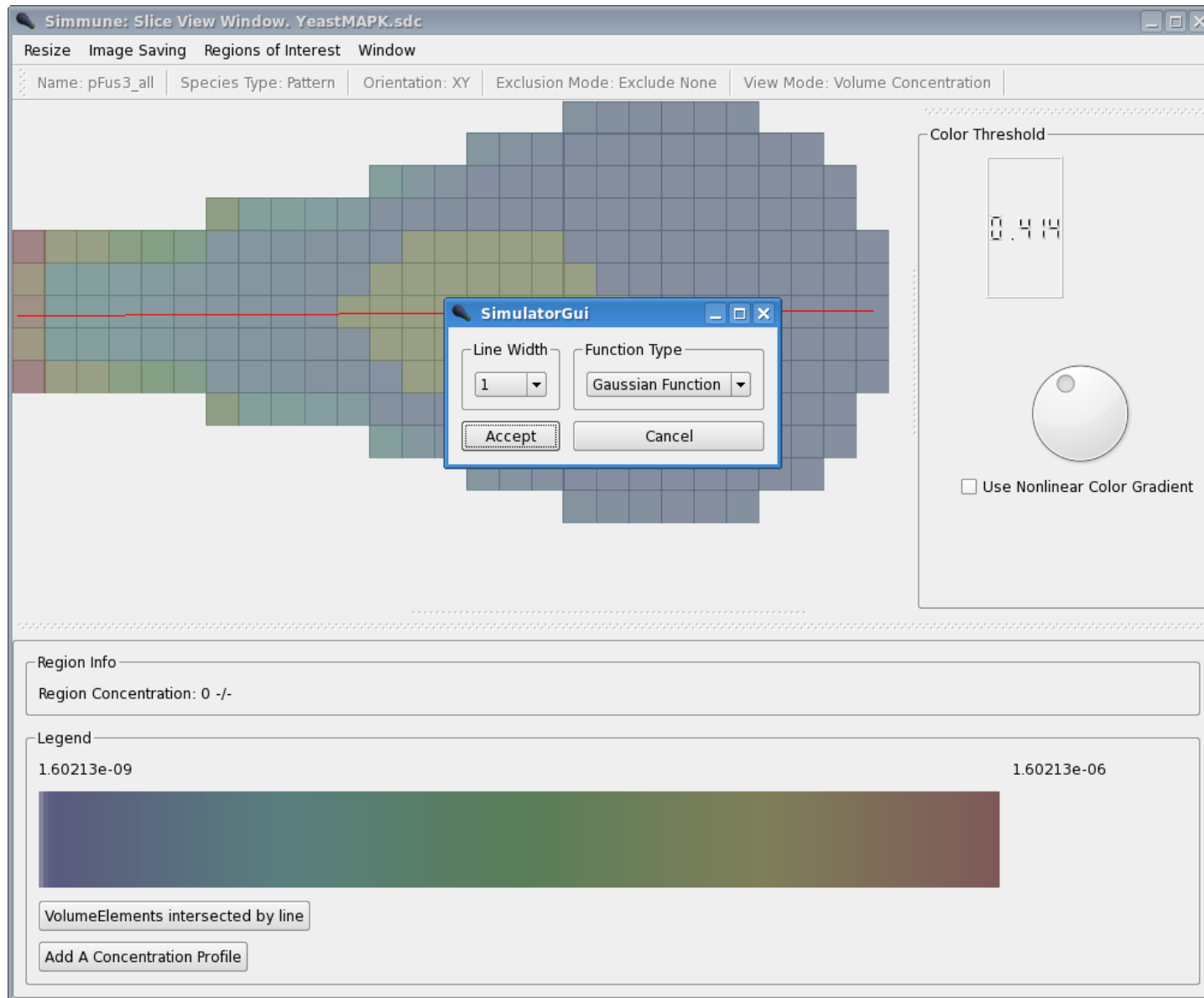
Simmune Simulation : Yeast : **Concentration Line Profile**

Simmune SBML Support

Support SBML Packages:

- SBML-Multi: Rule – based models
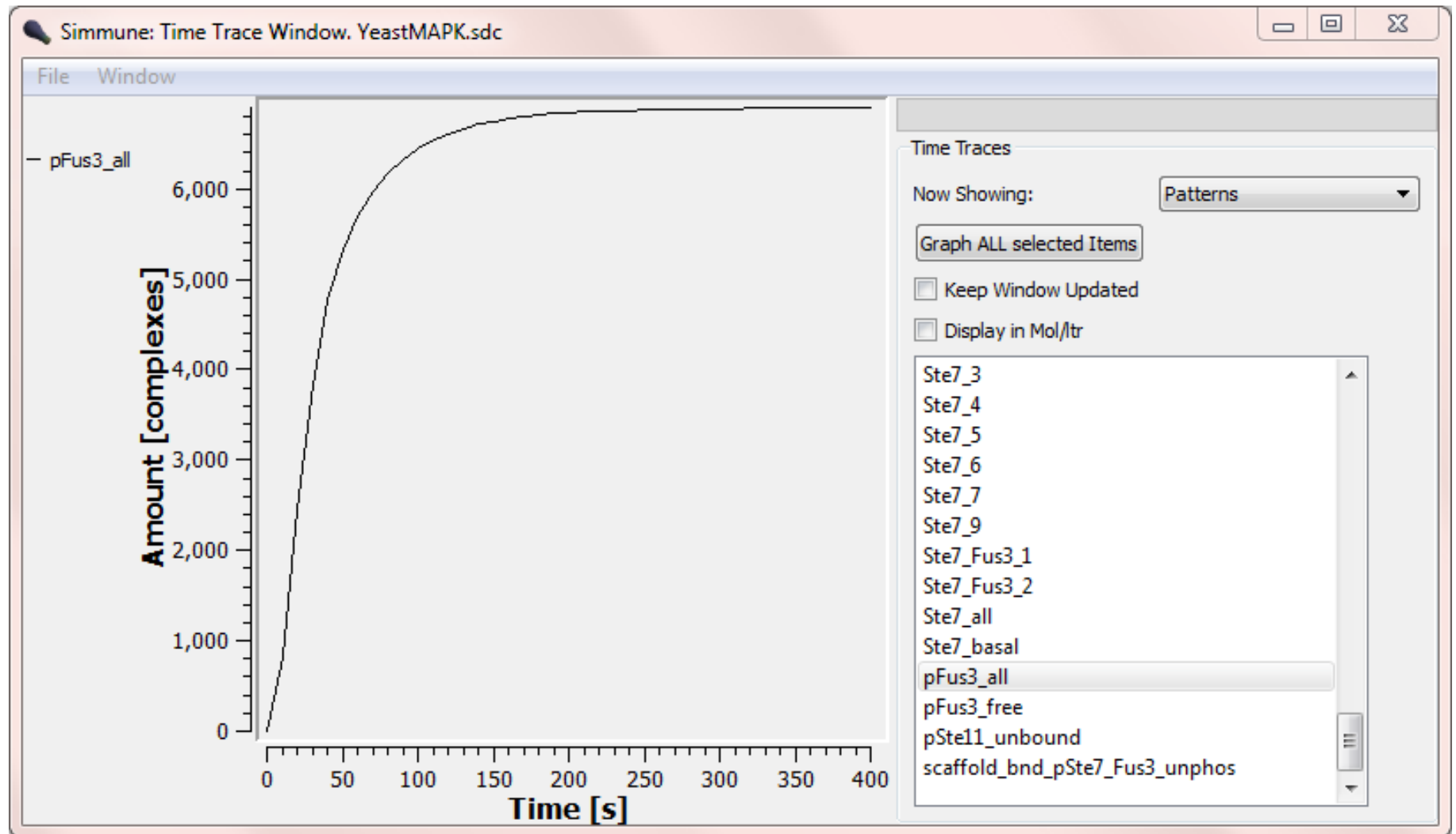 (under development)

- SBML-Spatial: Geometry
  (We are working on determining how the
  'Spatial' package can be combined with multi.)

Other:

- SED-ML (under consideration)

Simmune

- Rule-based spatially resolved models of cellular signaling networks

- Implemented with Qt, boost, fortran, OpenGL, VTK, libSBML

- Runs on Linux, Mac and Windows

- Standalone and distributed (in progress)

- Free for non-commercila use and available for download at:
  http://go.usa.gov/QeH

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  National Institute of Allergy and Infectious Disease (NIAID)

  National Institutes of Health (NIH) , USA

- Simmune Users

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