Simmune and Its Support to SBML and SBML packages

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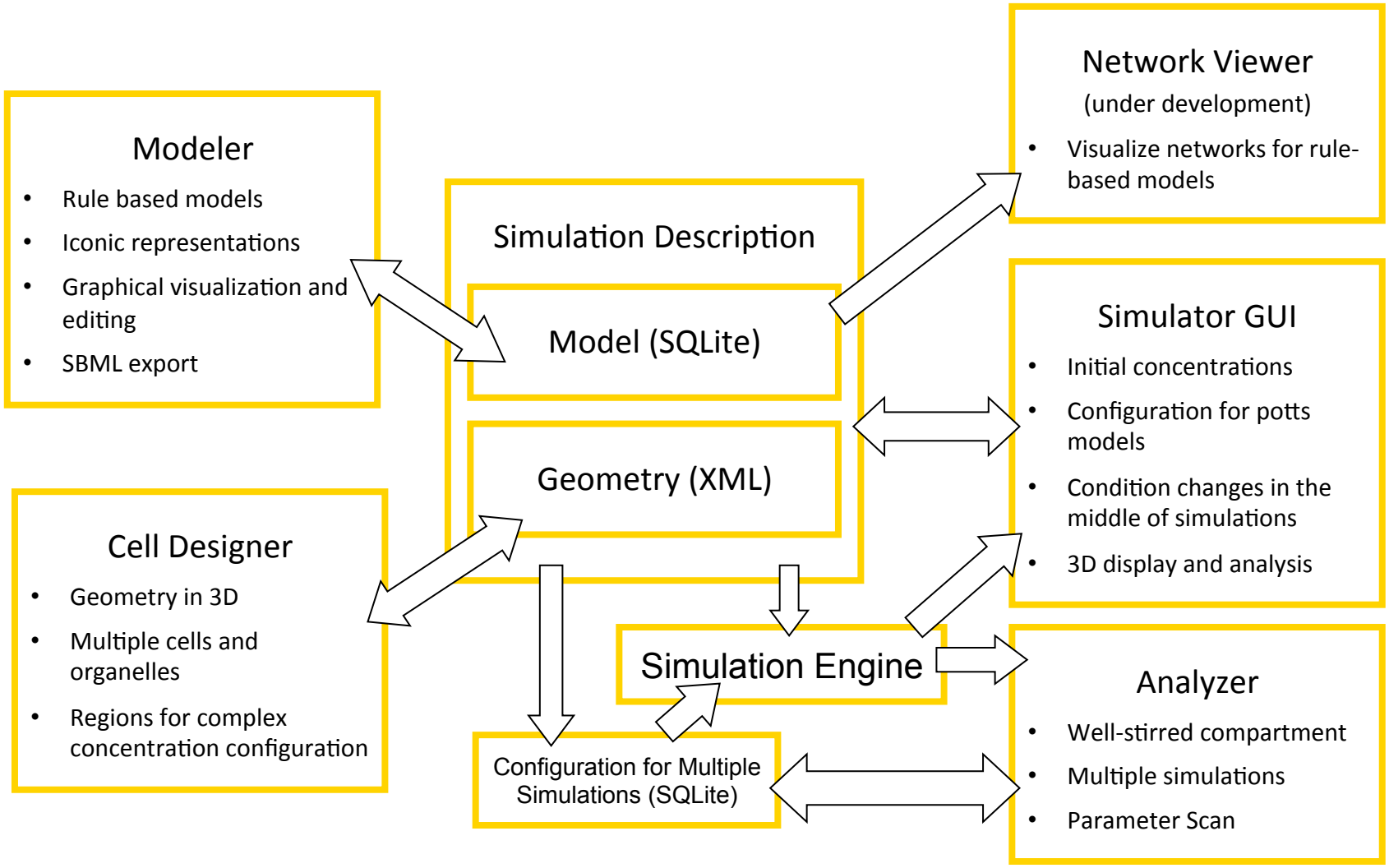
Outline

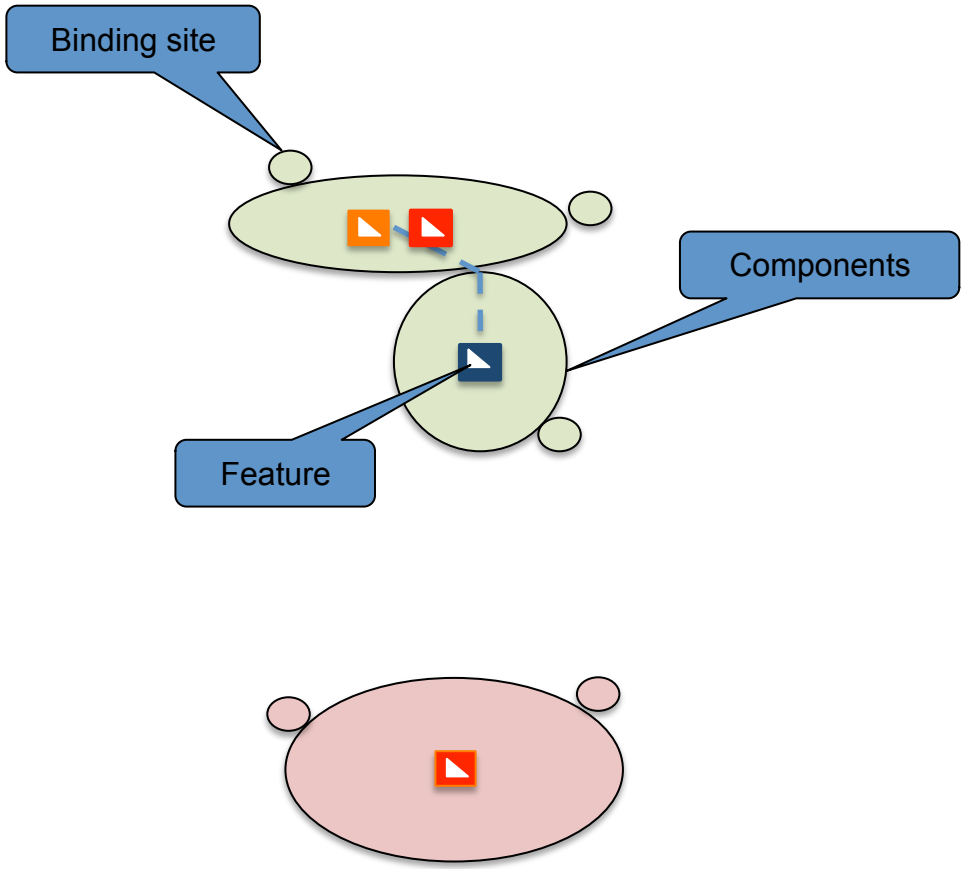
- Simmune infrastructure and work flow
- Simmune graphical representations
- Simmune: (Yeast Model)
  - Simmune Modeler
  - Simmune CellDesigner
  - Simmune Simulator
- SBML support

Simmune Structure and Workflow



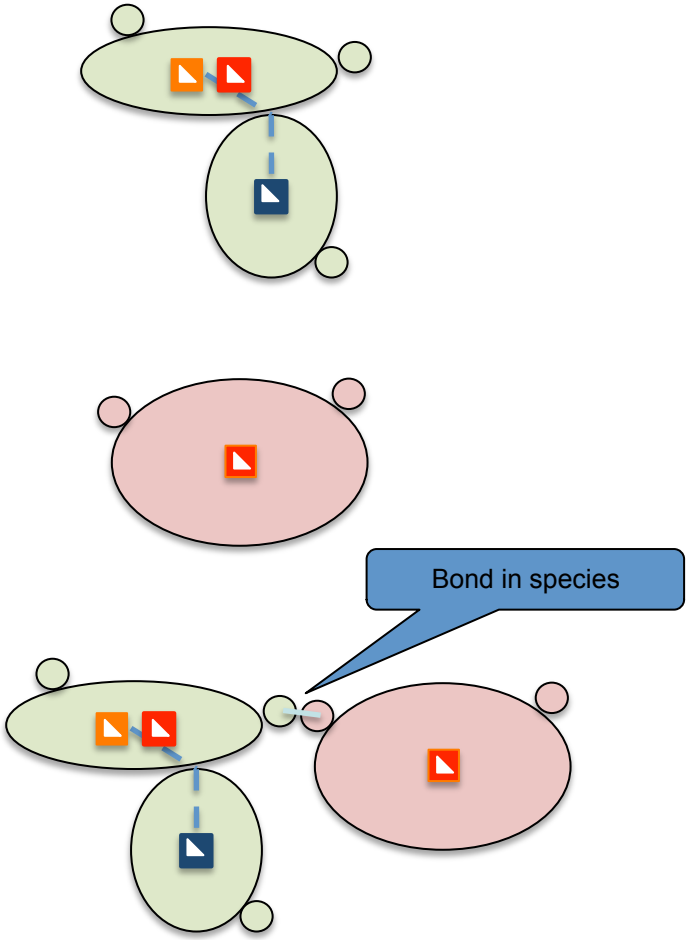
Graphical Representation of Simmune Models

Molecule: Component, binding sites, features



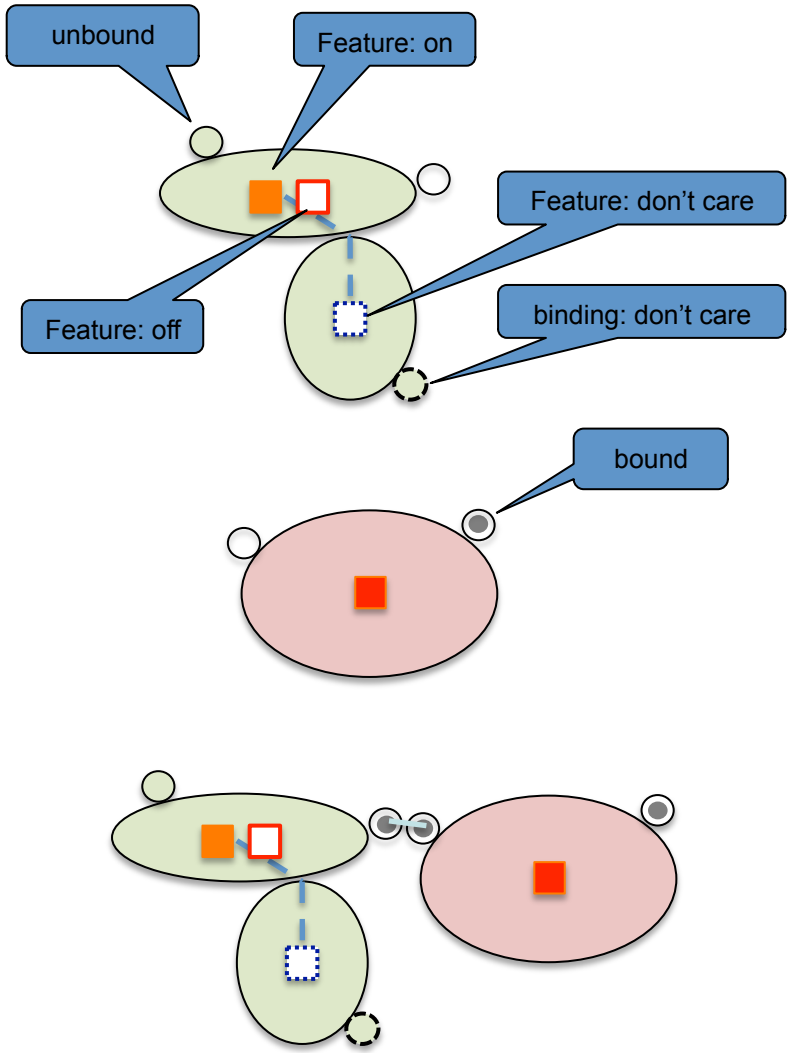
Graphical Representation of Simmune Models

Complex Species



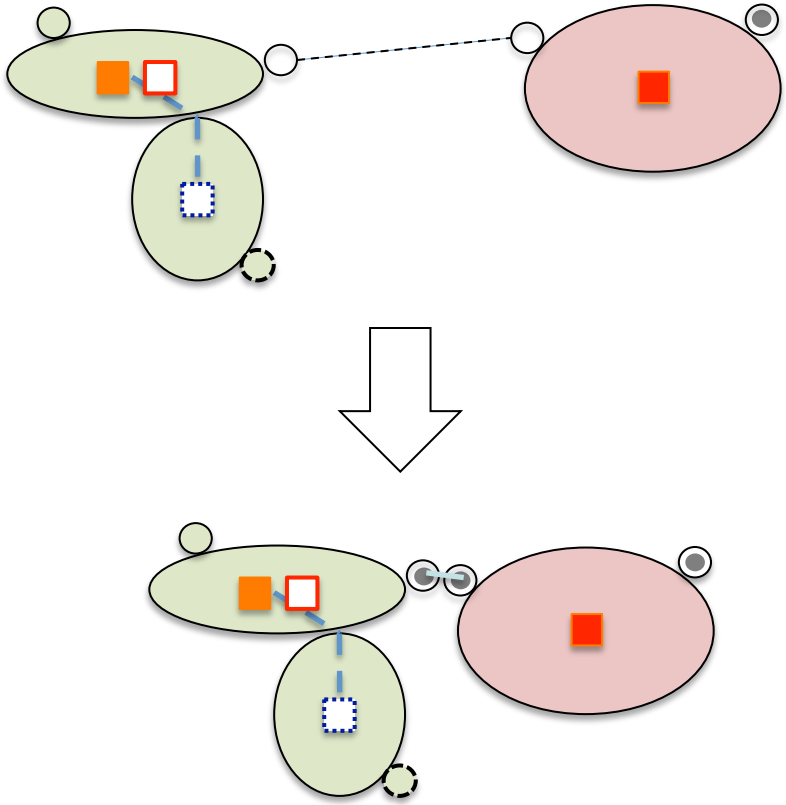
Graphical Representation of Simmune Models

Complex

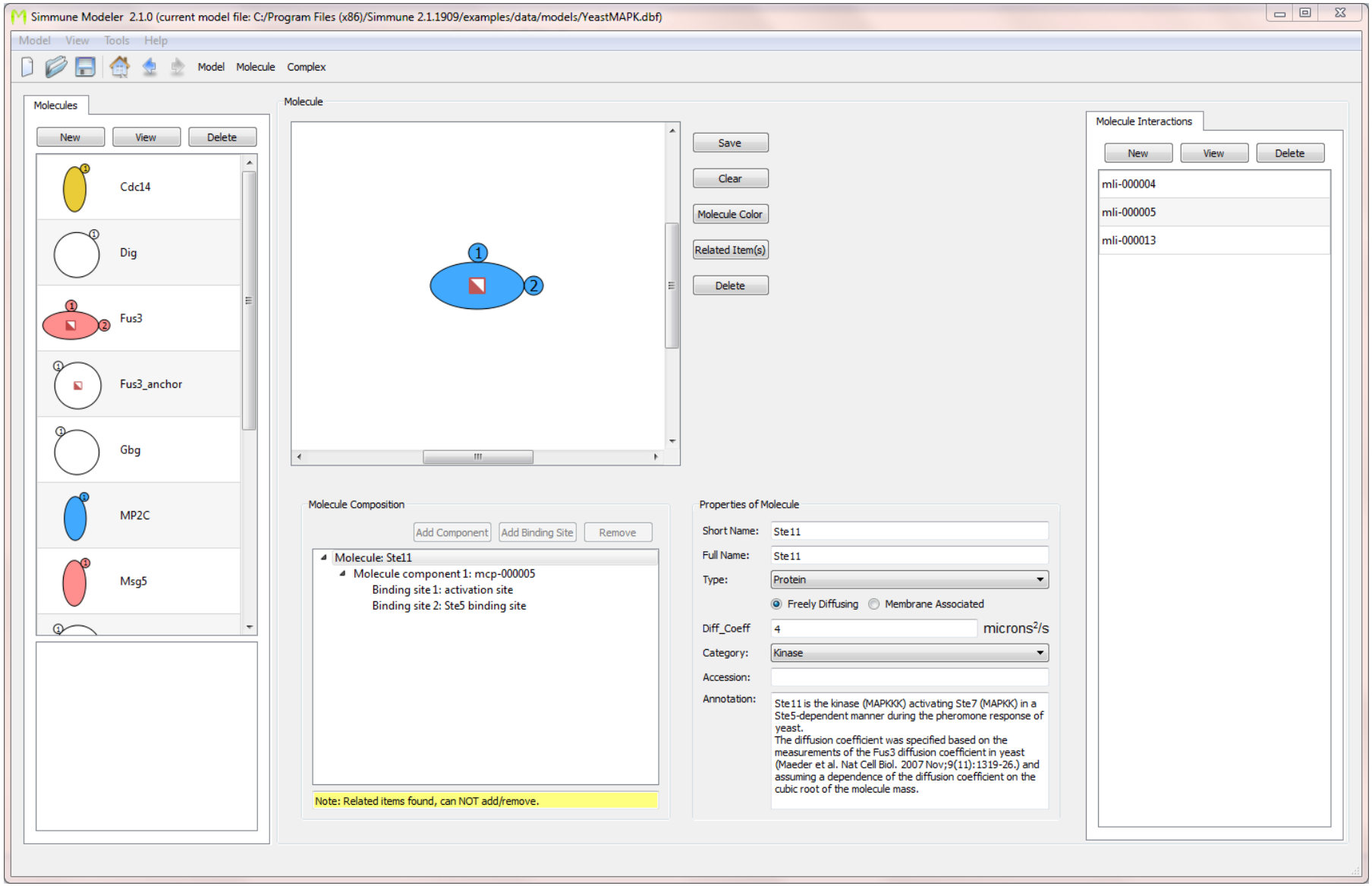


Graphical Representation of Simmune Models

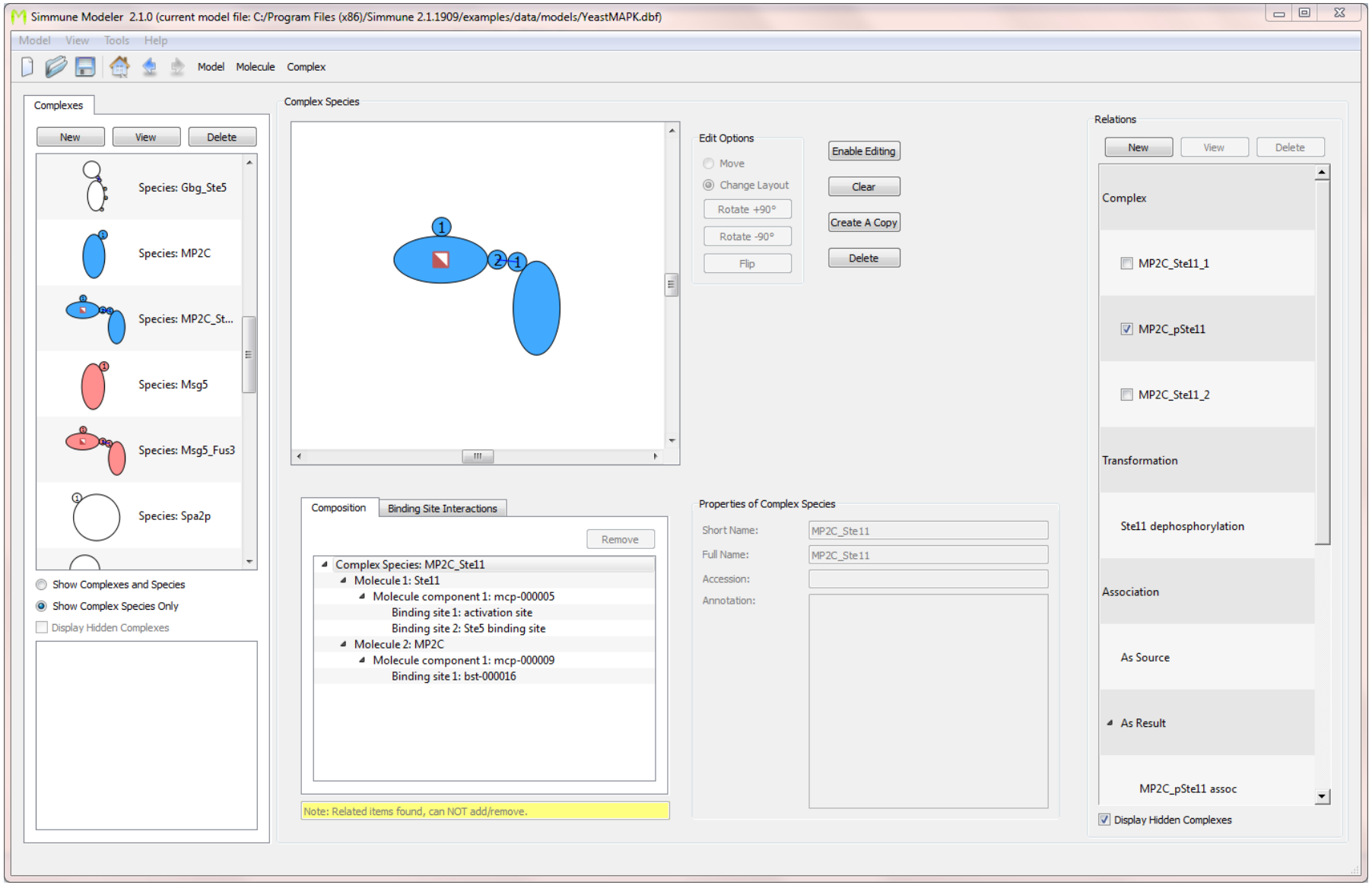
Reaction



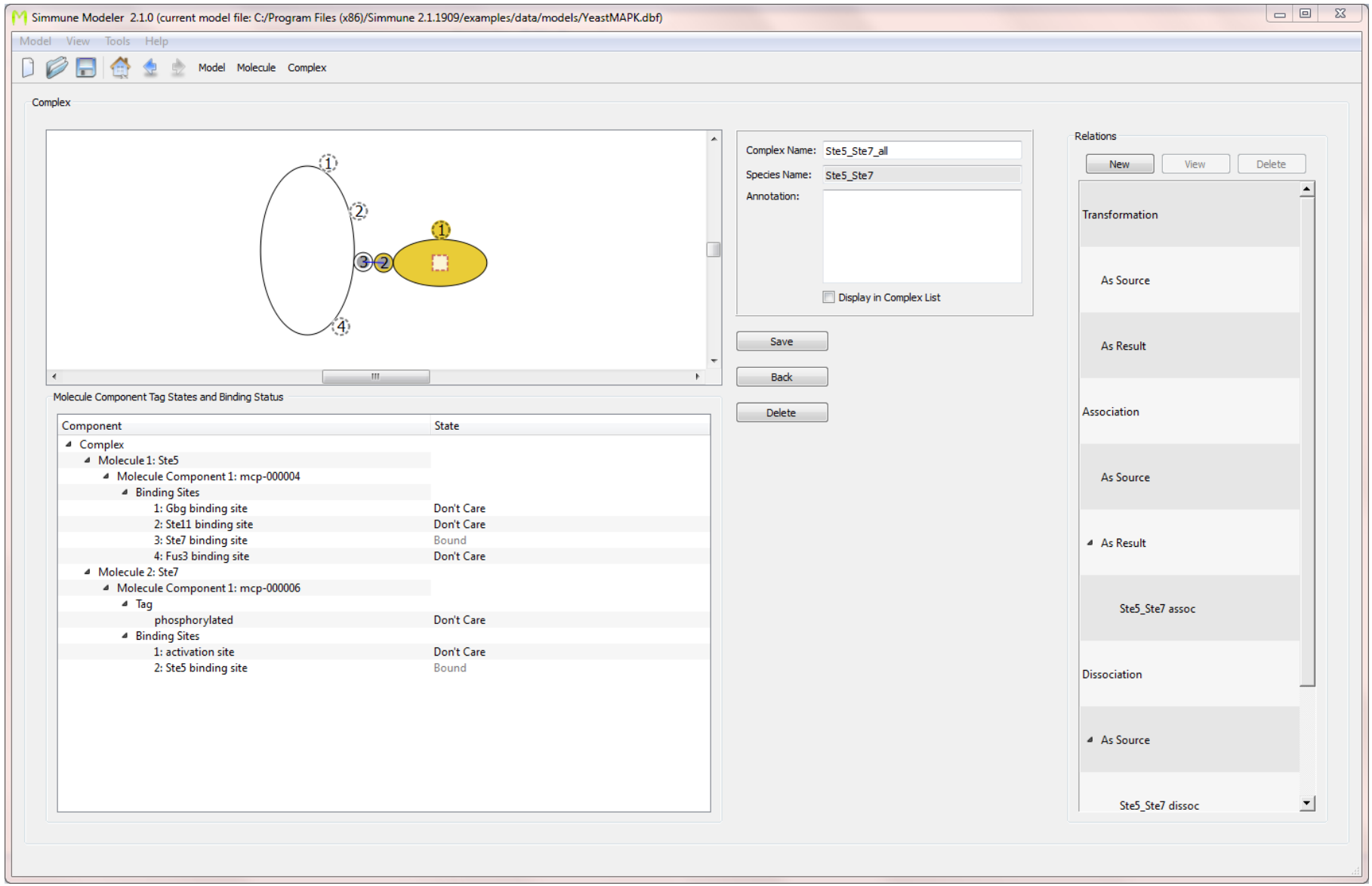
Simmune Modeler: Yeast Model: **Molecules**



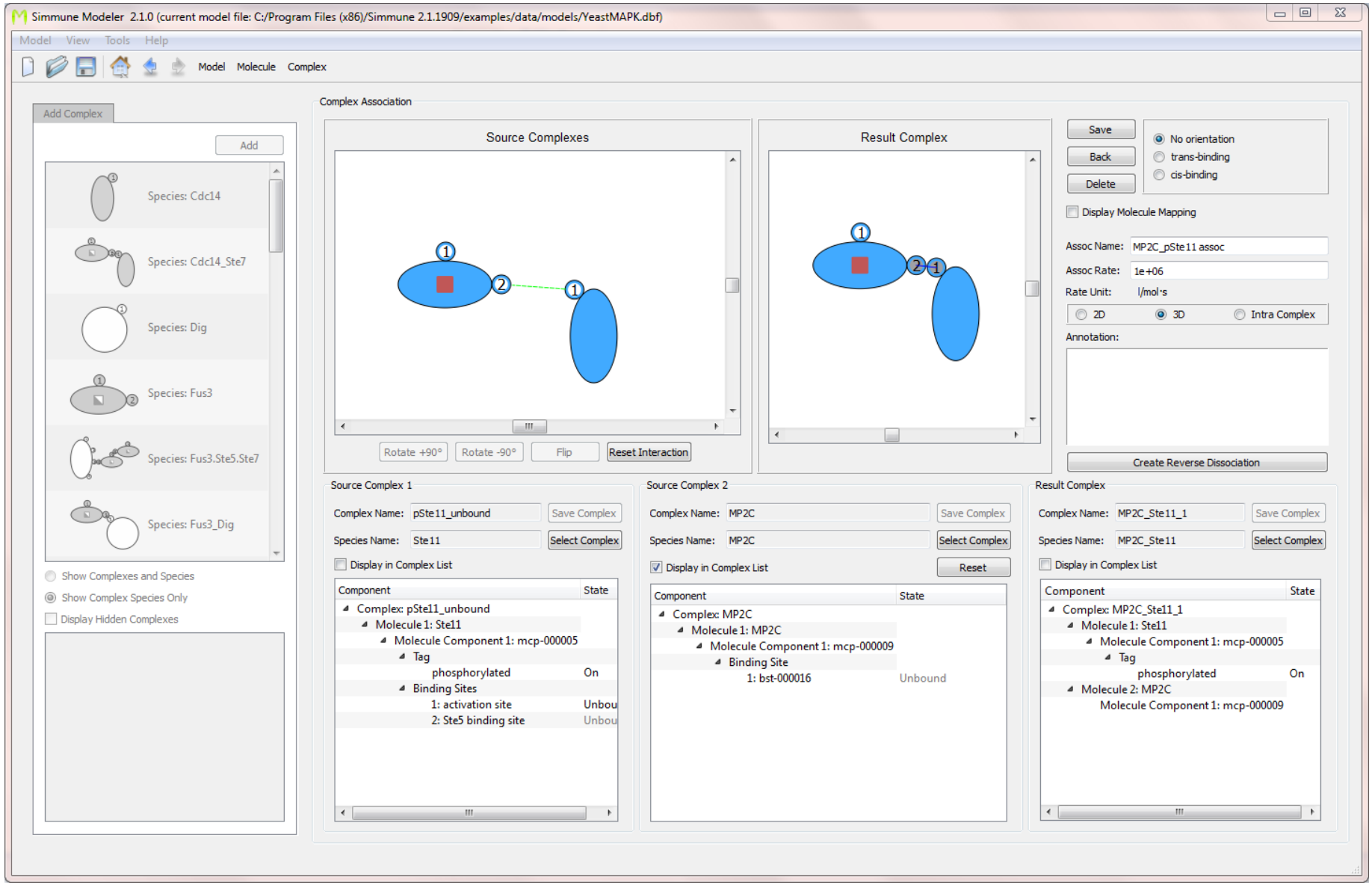
Simmune Modeler: Yeast Model: **Complex Species**



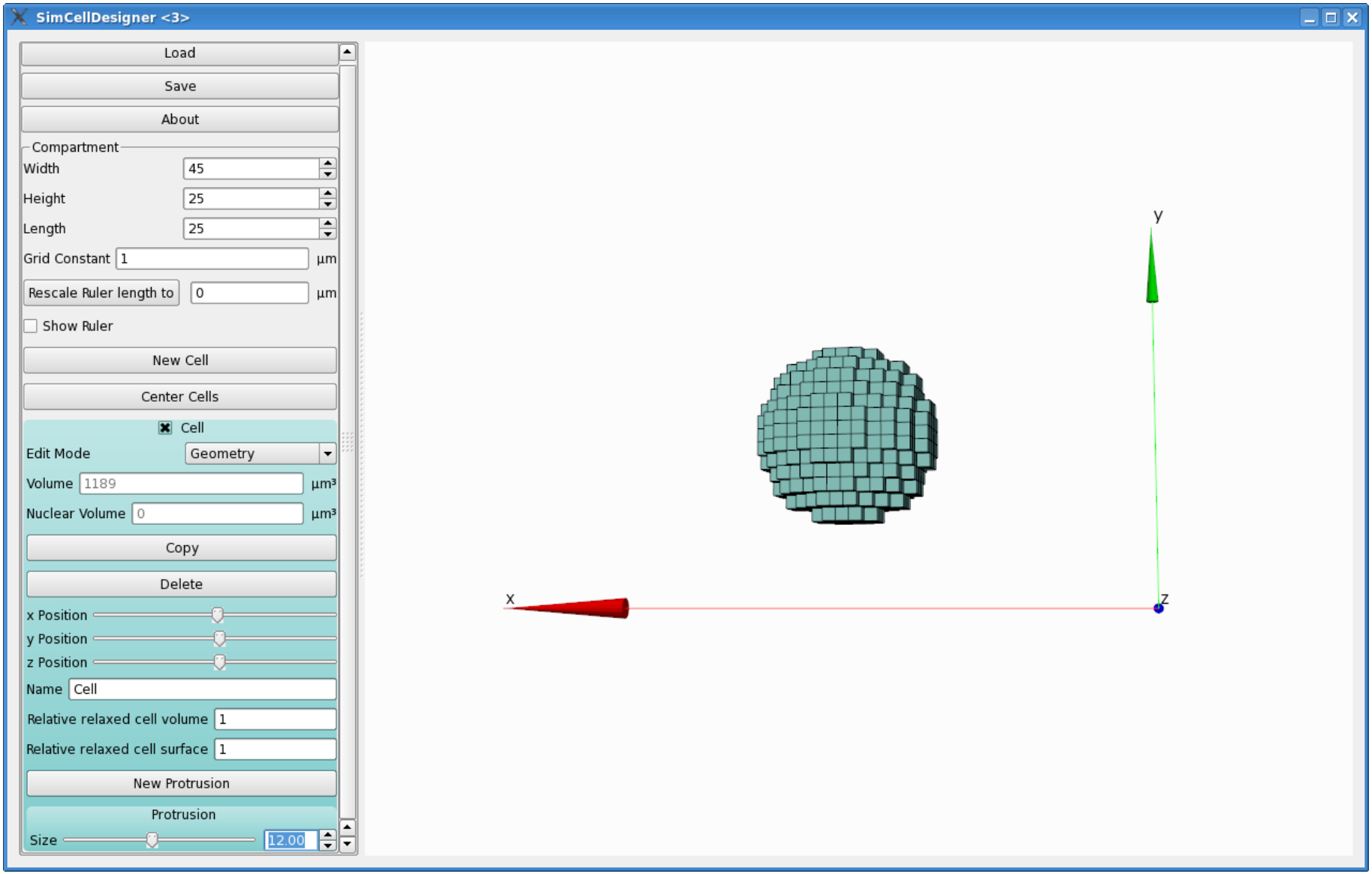
Simmune Modeler: Yeast Model: **Complex**



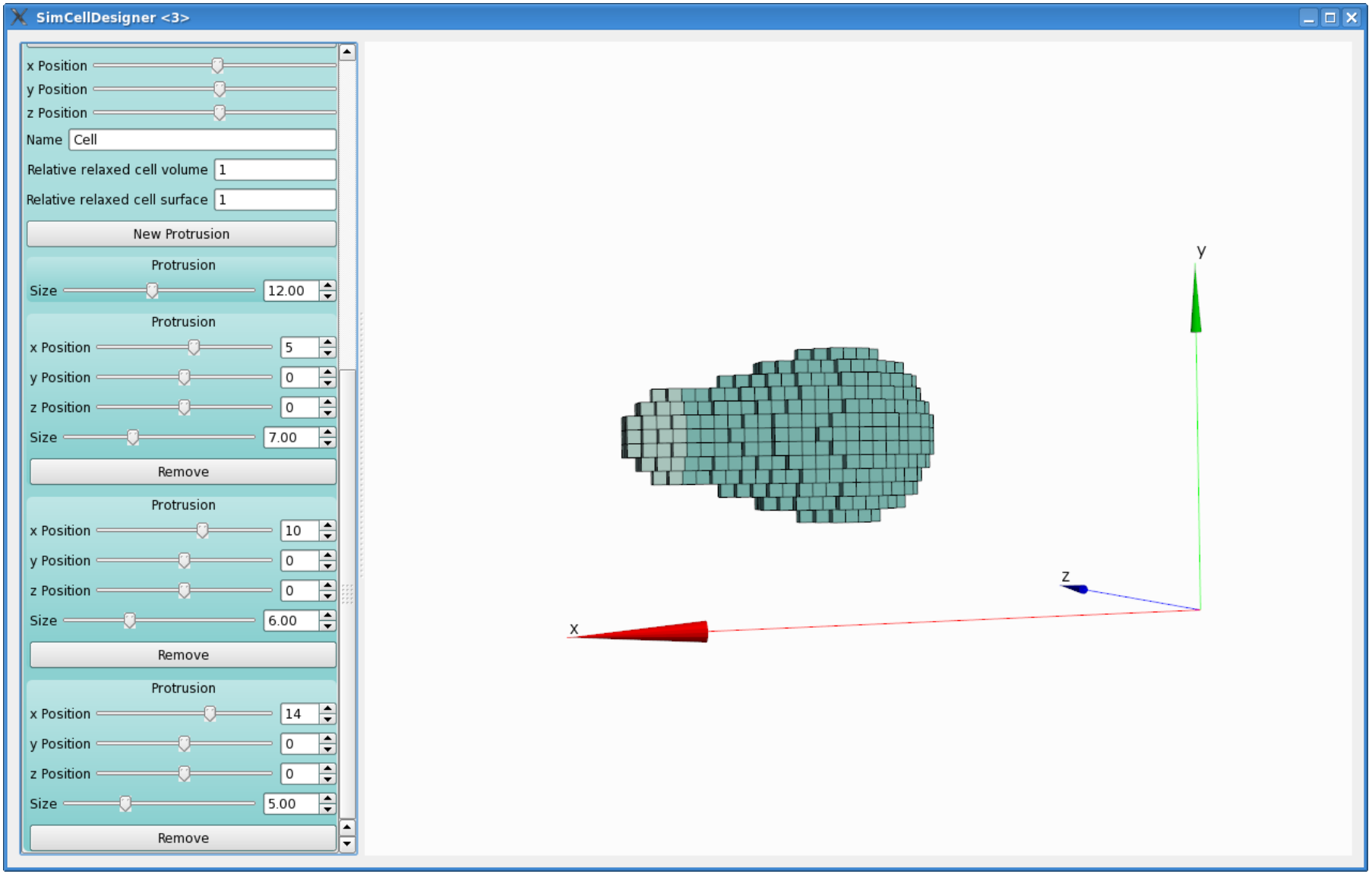
Simmune Modeler: Yeast Model: **Reaction**



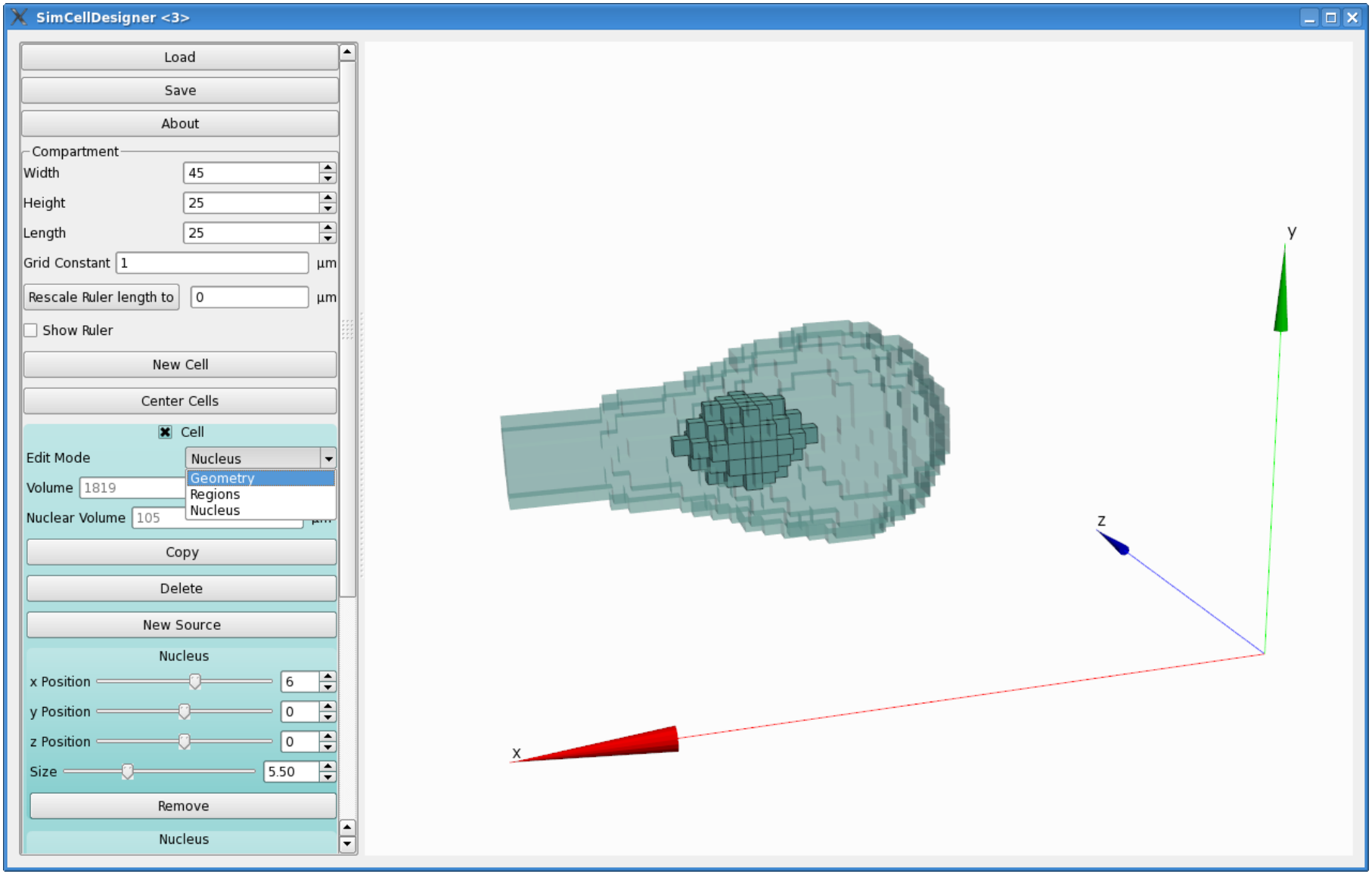
Simmune CellDesigner: Yeast Geometry: **Cell**



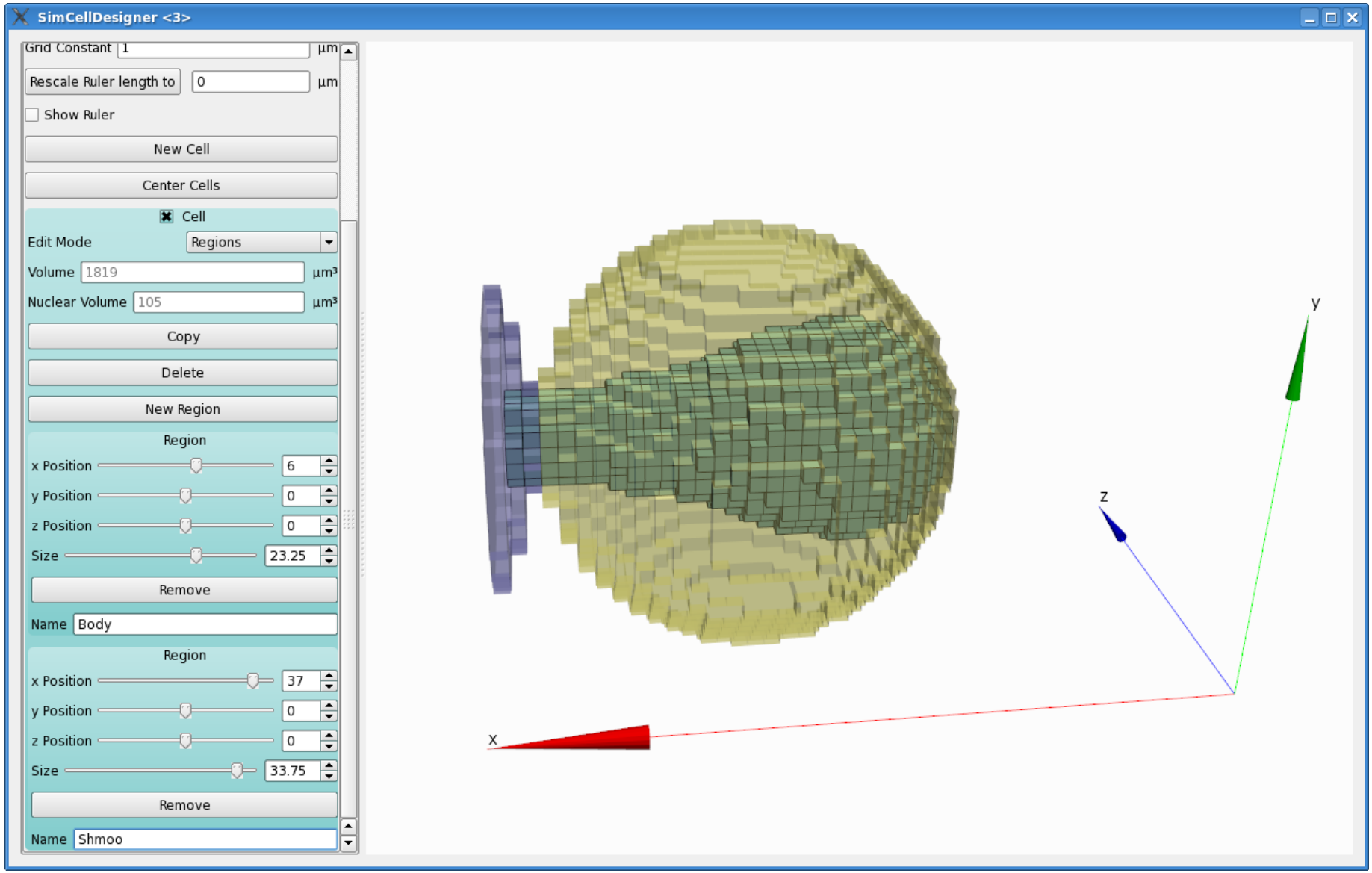
Simmune CellDesigner: Yeast Geometry:
Flexible Cell Shape Configuration



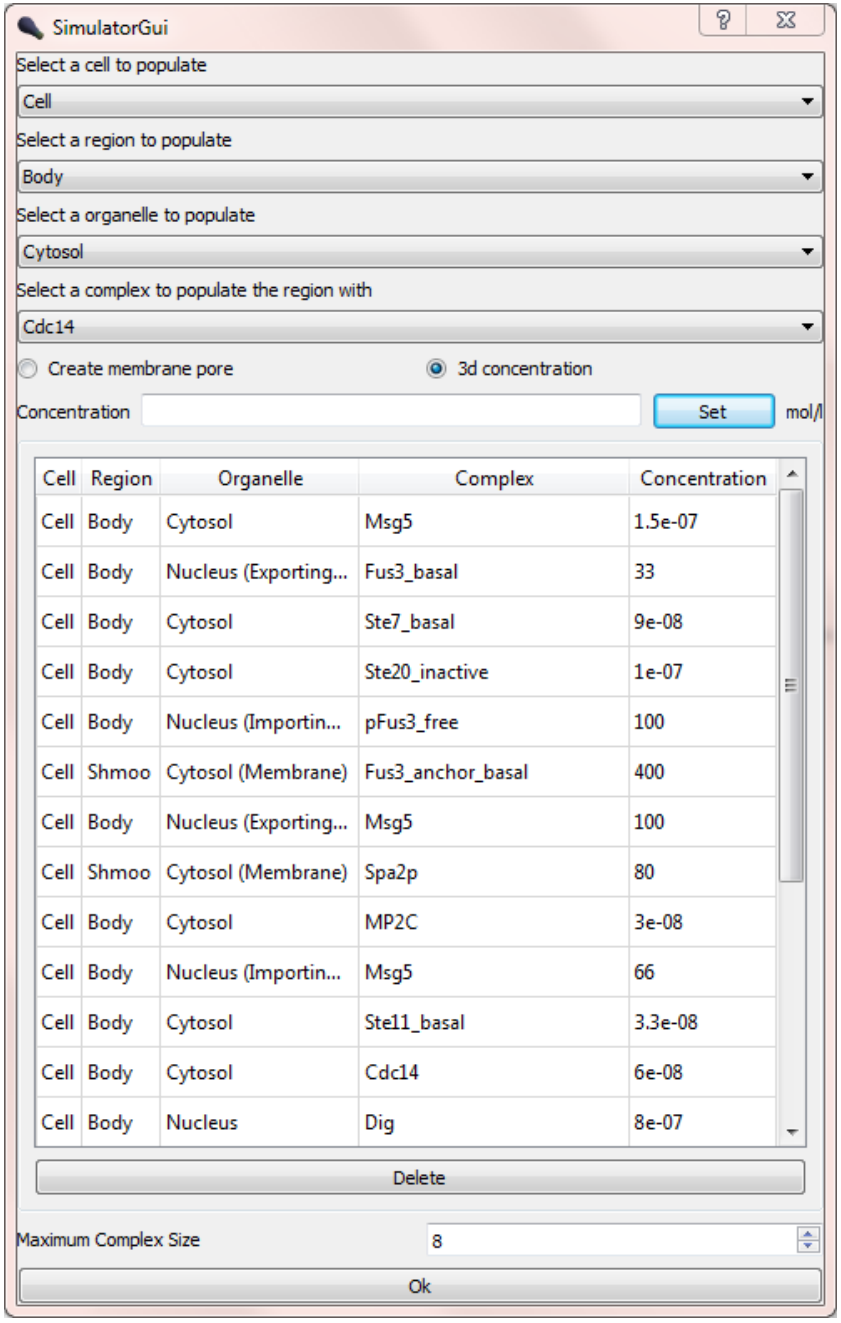
Simmune CellDesigner: Yeast Geometry: **Oganelle**



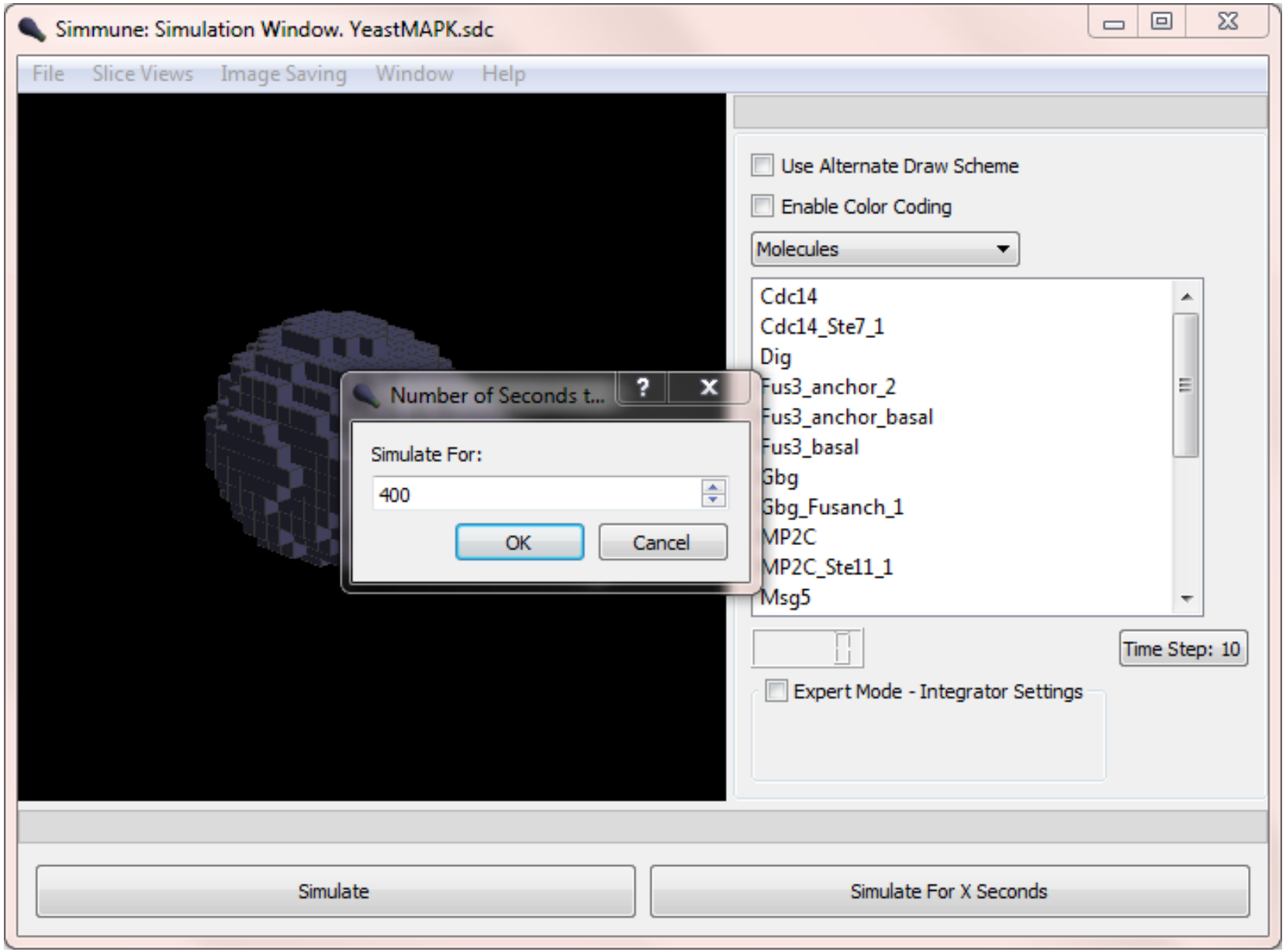
Simmune CellDesigner: Yeast Geometry: **Regions**



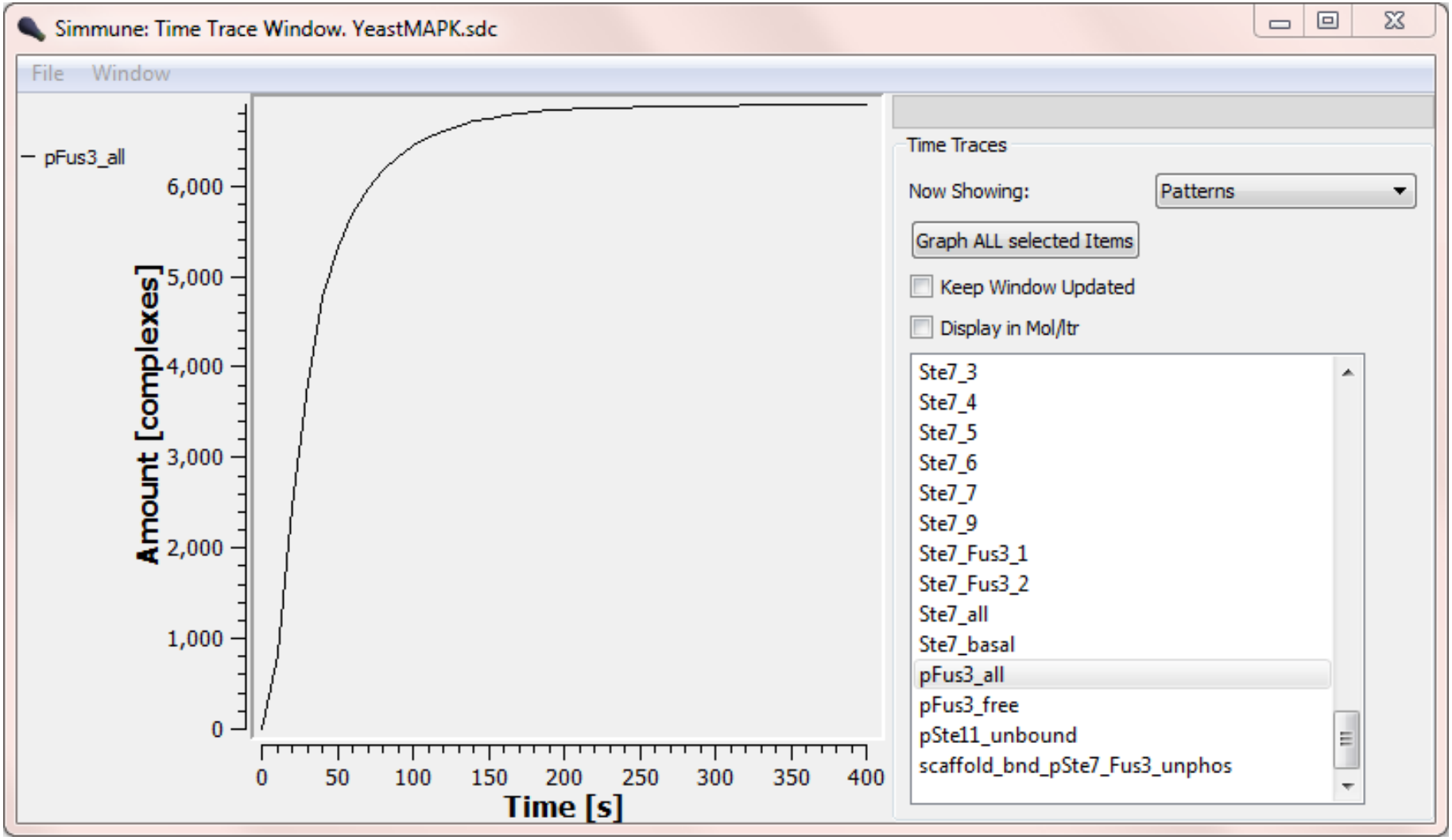
Simmune Simulation : Yeast : **Initial Condition**



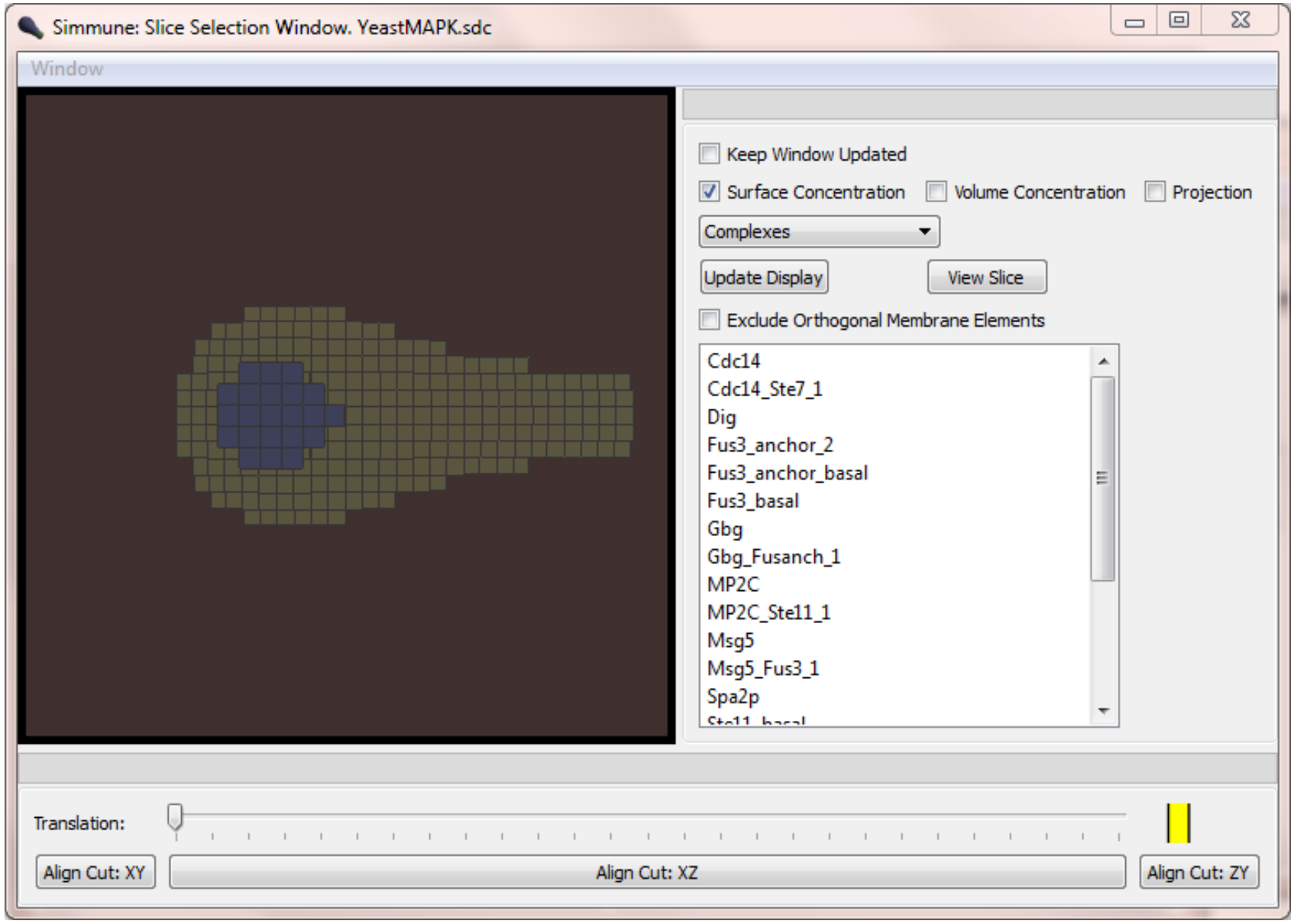
Simmune Simulation : Yeast : **Simulation Setup**



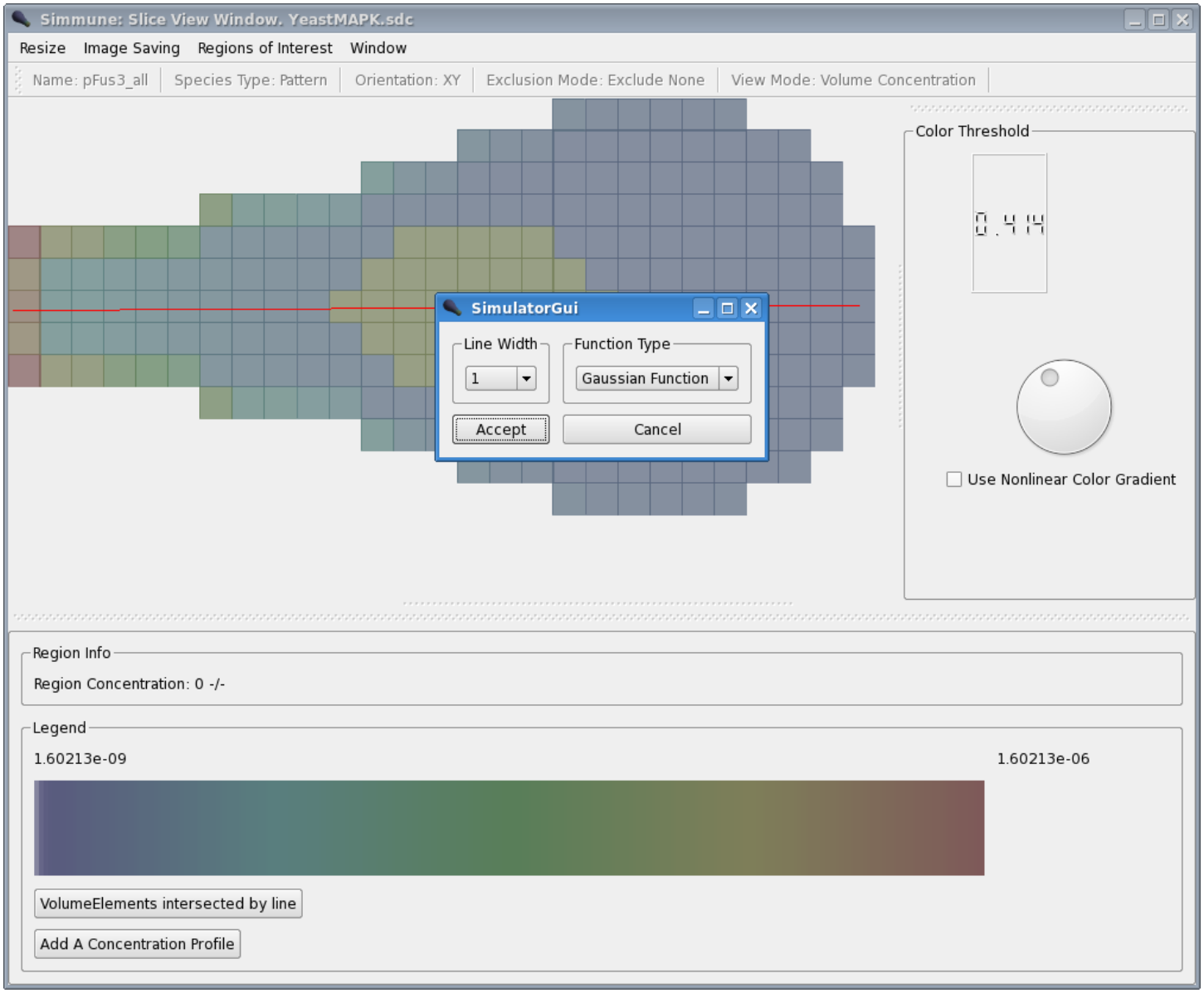
Simmune Simulation : Yeast : **Time Plot**



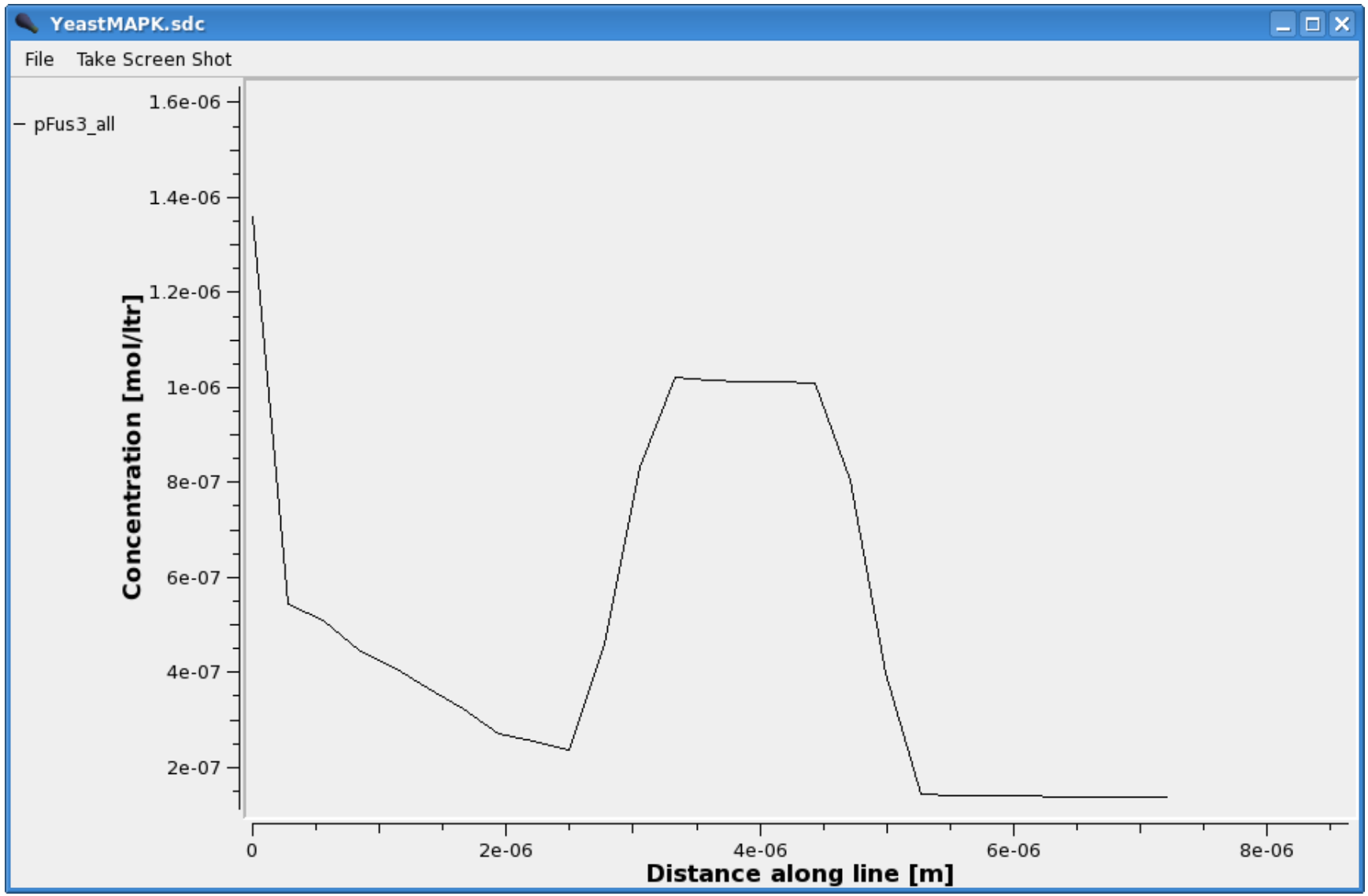
Simmune Simulation : Yeast : **Concentration Distribution**



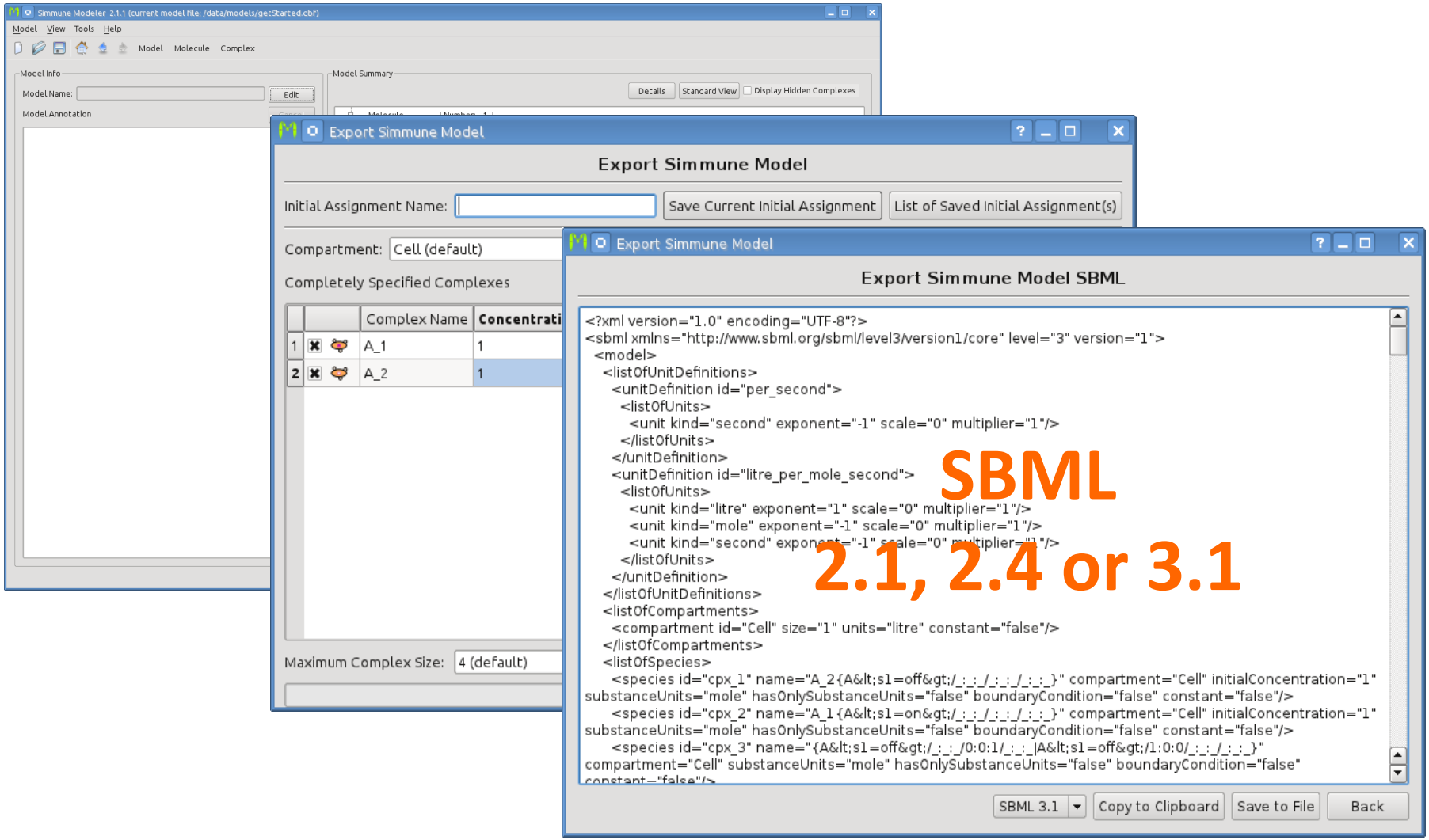
Simmune Simulation : Yeast : **Line Configuration**



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



Simmune SBML Support



Simmune SBML Support

Support SBML Packages:

- SBML-Multi: Rule – based models
  (Under development)
- SBML-Spatial: Geometry
  (Able to be supported with multi?)

Other:

- SED-ML (in consideration)

Simmune

- Rule-based spatially resolved models of cellular signaling networks
- Implemented with Qt, boost, fortran, OpenGL, VTK, libSBML
- Can run on Linux, Mac and Windows
- Standard alone and distributed (in progress)
- Free for academic use and available for download at: http://www.niaid.nih.gov/labsandresources/labs/aboutlabs/lsb/Pages/simmuneproject.aspx

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- Members of

  Laboratory of Systems Biology (LSB)

  National Institute of Allergy and Infectious Disease (NIAID)

  National Institutes of Health (NIH) , USA

- Simmune Users

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