

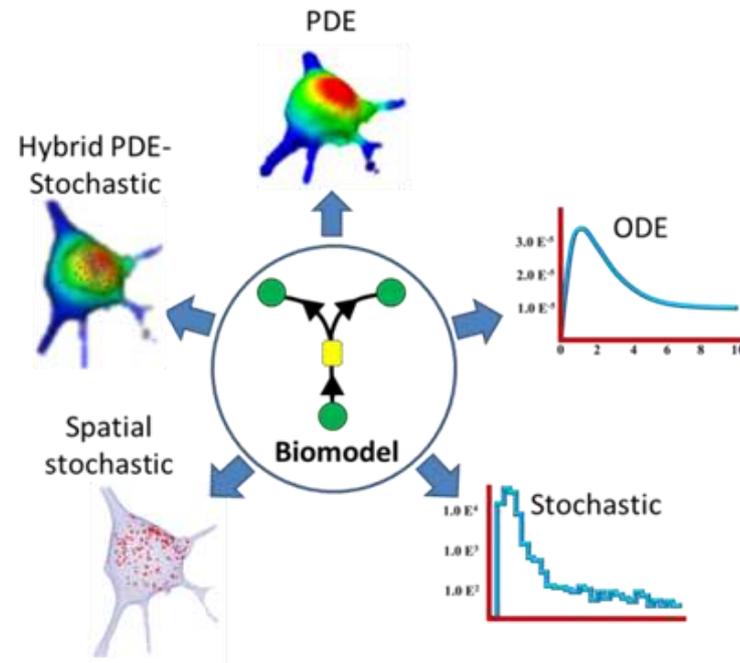
Virtual Cell Tutorials

VCell

modeling environment for
mathematical simulation of
cellular events.

To run VCell go to:

vcell.org



Virtual Cell is developed by the Center for Cell Analysis and Modeling at the University of Connecticut Health Center. It is funded as a Biomedical Technology Research Resource by the National Institute of General Medical Sciences (NIGMS)

VCell Tutorial

FRAP with binding

Create a simple biomodel and spatial (PDE) application to simulate a photobleaching experiment with both diffusion and binding .

In this tutorial...

- Gain a basic introduction to the Virtual Cell interface
- Create a simple biomodel with species and reactions
- Create a compartmental (ODE) application of the model to determine steady state binding conditions.
- Create a spatial deterministic (PDE) application using analytic equations to create a simple geometry
- Define initial concentrations that are non-uniform using Boolean expressions
- Created a timed event in a spatial simulation.
- View and analyze results of a spatial simulation.

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BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

New BioModel Diagram Reactions Structures Species

Open Math Model

Close Ctrl+W Geometry

Save

Save New Version

Save As...

Revert to Saved

Compare with Saved

Permissions...

Model Annotation ...

Edit Annotation...

Field Data...

Import...

Export...

Exit

- my biomodels (tanyamiller1221) (3)
 - BioModel2
 - Private Thu Jun 25 16:03:1...
 - Tutorial
 - Tutorial_MultiApp
- Shared BioModels (0)
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- Tutorials (5)
- Education (33)

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Database File Info

- DetSpatial
 - Deterministic
 - geom_20150625_105028 (3D)
 - Simulation0
- NonSpatialStoch
 - Stochastic
 - (copied from Application spatial deterministic)
 - Compartmental
 - Simulation1
- NonSpatialDet
 - Deterministic
 - (copied from DetSpatial)
 - Compartmental
- SpaStoch

CONNECTED (tanyamiller1221) 65.2MB / 130.5MB

To start a new BioModel, click "File" > "New" > "BioModel."

The screenshot shows the BIOMODEL software interface. The main window displays a compartment labeled 'c0' with two vertical dashed black lines representing membranes. One of these lines is highlighted with a green dashed line, indicating it has been selected. The toolbar at the top contains various tools, with the 'Add Membrane' tool (represented by a circle with a crosshair) highlighted by a red box and an arrow. A yellow callout box points to this tool with the text: "Click the structure tool." Another yellow callout box points to the green dashed line with the text: "Hover over dashed black lines so they turn green. Left click 'Add Membrane'." The left sidebar shows a tree view of the model structure, including 'BioModel1', 'Reactions (0)', 'Structures (1)', 'Species (0)', 'Applications (0)', 'Parameters and Functions', and 'Pathway'. The bottom status bar shows the user is connected as 'tanyamiller1221' and has 59.6MB of memory used out of 122.0MB.

Click the structure tool.

Hover over dashed black lines so they turn green. Left click "Add Membrane".

CONNECTED (tanyamiller1221) 59.6MB 122.0MB

The screenshot displays the VCell software interface for a BioModel. The main window is titled "BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the model structure under "BioModel1". The "Physiology" folder is expanded, showing "Reaction Diagram" (selected), "Reactions (0)", "Structures (2)", and "Species (0)". Other folders include "Applications (0)", "Parameters and Functions", and "Pathway".
- Top Panel:** A toolbar with icons for "Reaction Diagram", "Reactions", "Structures", and "Species". Below the icons are buttons for "ANN EAL" and "REL AX".
- Center Panel:** A compartment diagram showing two compartments, "c0" and "m0", separated by vertical dashed black lines. A red arrow points to one of these lines, which is highlighted with a green dashed border. A yellow callout box with a red border contains the text: "Hover over dashed black lines so they turn green. Right click 'Add Compartment'".
- Bottom Panel:** A search bar with a "Delete" button and a "Pathway Links" dropdown. Below it is an "Object Properties" section with a "Problems (0 Errors, 0 Warnings)" tab and a text area containing the instruction: "Select only one object (e.g. species, reaction, simulation) to view/edit properties."

At the bottom of the window, there is a status bar showing "CONNECTED (tanyamiller1221)" on the left and "61.8MB / 122.3MB" on the right.

The screenshot displays the VCell 5.3 (build 4) interface. The main window is titled "BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the model structure under "BioModel1", including "Physiology", "Structures (3)", "Species (0)", "Applications (0)", "Parameters and Functions", and "Pathway".
- Top Panel:** A toolbar with various icons for editing and viewing. A red box highlights the select tool (a mouse cursor icon) with the instruction "Click the select tool.".
- Center Panel:** A workspace showing a compartment labeled "Cyt". A red box highlights this label with the instruction "Click on the label of the first compartment.".
- Bottom Panel:** The "Object Properties" panel, which is currently selected. It shows the following fields:
 - Structure Name:** "Cyt" (highlighted with a red box and the instruction "Next to Structure Name type 'Cyt'").
 - Size Variable Name:** "Cyt [μm^3 "]
 - Annotation:** "Cytosol" (highlighted with a red box and the instruction "Next to Annotation type 'Cytosol'").

At the bottom of the window, there is a status bar showing "CONNECTED (tanyamiller1221)" on the left and "66.6MB / 22.3MB" on the right.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

Physiology

Reaction Diagram

Reactions (0)

Structures (3)

Species (0)

Applications (0)

Parameters and Functions

Pathway

Reaction Diagram

Reactions

Structures

Species

Click on the membrane label.

NM

c1

Delete

Pathway Links

Search

Object Properties

Problems (0 Errors, 0 Warnings)

Select only one structure to edit properties

Structure Name NM

Size Variable Name NM [μm^2]

Electrophysiology

Next to Structure Name type "NM" (which stands for "Nuclear Membrane").

Negative (outside feature)

membrane voltage: $\text{Voltage_NM} = \text{voltage}(\text{inside (+) compartment}) - \text{voltage}(\text{outside (-) compartment})$
 inward currents: from compartment "outside (-) compartment" into compartment "inside (+) compartment"
Note: VCell reactions and fluxes specify inward currents (- to +) rather than conventional currents (+ to -).

Annotation

CONNECTED (tanyamiller1221)

70.2MB / 122.2MB

The screenshot shows the VCell software interface. The main window displays a compartment labeled "Nuc" in a diagram. A yellow callout box with a red border points to the "Nuc" label with the text "Click on the label of the second compartment." Below the diagram, the "Object Properties" panel is visible, showing the following fields:

Structure Name	Nuc
Size Variable Name	Nuc [μm^3]
Annotation	Nucleus

Two yellow callout boxes with red borders point to the "Nuc" and "Nucleus" text in the Object Properties panel. The first callout says "Next to Structure Name type 'Nuc'." and the second callout says "Next to Annotation type 'Nucleus'." The bottom status bar shows "CONNECTED (tanyamiller1221)" and "77.8MB / 123.2MB".

The screenshot displays the VCell software interface for a model named "BioModel1". The main workspace is divided into three compartments: "Cyt", "NM", and "Nuc". The "Nuc" compartment is highlighted with a red box and contains six green circular species objects labeled s0, s1, s2, s3, s4, and s5. A red arrow points from a yellow text box to the "Species" tool icon in the top toolbar, which is also highlighted with a red box. Another red arrow points from a yellow text box to the "Nuc" compartment. The bottom panel shows the "Object Properties" for the selected species s5, with fields for "Species Name" (s5), "Linked Pathway Object(s)", and "Annotation".

Click the species tool.

Click on six different points within the "Nuc" compartment to create six species.

Species Name: s5

Linked Pathway Object(s):

Annotation:

CONNECTED (tanyamiller1221) 82.9MB / 122.2MB

The screenshot displays the VCell software interface for editing a reaction diagram. The main workspace is divided into three compartments: Cyt, NM, and Nuc. Several species are represented by colored circles: s0, s1, s2, s3, s4, and s5. Species s1 is a red circle located in the Nuc compartment and is highlighted with a red box. A red arrow points from a yellow callout box to the select tool icon in the top toolbar, and another red arrow points from the callout box to species s1. The callout box contains the text: "To move a species, click the select tool and click a drag a species to a point." The left sidebar shows a tree view of the model structure, including Physiology, Reaction Diagram, Reactions (0), Structures (3), and Species (6). The bottom panel shows the Object Properties for the selected species s1, with fields for Species Name, Linked Pathway Object(s), and Annotation.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

s0 s1 s2 s3 s4 s5

To move a species, click the select tool and click a drag a species to a point.

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name s1

Linked Pathway Object(s)

Annotation

CONNECTED (tanyamiller1221) 56.9MB / 123.7MB

The screenshot displays the VCell software interface for editing a reaction diagram. The main workspace is divided into three compartments: Cyt (Cytosol), NM (Nucleus Membrane), and Nuc (Nucleus). A reaction diagram is shown with a red circle labeled 'r' in the Cyt compartment, and several green circles labeled 's1' through 's5' in the Nuc compartment. A yellow callout box with a red border points to the 'r' circle, containing the text "Click on 's0'".

Below the workspace, the "Object Properties" panel is visible. It has two tabs: "Object Properties" and "Problems (0 Errors, 0 Warnings)". The "Object Properties" tab is active, showing a "Species Name" field with the value "r" and an "Annotation" field with the value "RAN". Yellow callout boxes with red borders point to these fields, containing the text "Next to Species Name type 'r'." and "Next to Annotation type 'RAN'." respectively.

The interface also includes a left sidebar with a tree view showing the model structure: BioModel1 > Physiology > Reaction Diagram (selected), Reactions (0), Structures (3), and Species (6). Below this is a search bar and a list of biological models. The bottom status bar shows "CONNECTED (tanyamiller1221)" and memory usage "60.3MB / 123.7MB".

The screenshot displays the VCell 5.3 (build 4) interface. The main window shows a reaction diagram with three compartments: Cyt, NM, and Nuc. A reaction 'r' is shown in the Cyt compartment, and a species 'rf' is shown in the Nuc compartment. A yellow callout box with a red arrow points to the 'rf' species icon, containing the text "Click on 's1'".

Below the reaction diagram, the Object Properties panel is visible. It shows the following fields:

- Species Name: rf (with a yellow callout box containing "Next to Species Name type 'rf'")
- Linked Pathway Object(s):
- Annotation: RAN_FITC (with a yellow callout box containing "Next to Annotation type 'RAN_FITC'")

The bottom status bar shows "CONNECTED (tanyamiller1221)" and "63.4MB / 123.7MB".

The screenshot displays the VCell software interface for a model named "BioModel1". The main workspace shows a reaction diagram with three compartments: Cyt, NM, and Nuc. In the Nuc compartment, several species are represented by green circles: 'r', 'rf', 's3', 's4', and 's5'. A red box highlights a species labeled 'rB', with a yellow callout box containing the text "Click on 's2'." and an arrow pointing to it.

Below the diagram, the "Object Properties" panel is visible. It contains a "Species Name" field with the value "rB" and an "Annotation" field with the value "RAN_Bound". Red boxes highlight these fields, with yellow callout boxes containing the text "Next to Species Name type 'rB'." and "Next to Annotation type 'RAN_Bound'." respectively, with arrows pointing to the input fields.

The interface also includes a left-hand navigation pane with a tree view showing "Physiology" and "Reaction Diagram" selected. At the bottom, a status bar indicates "CONNECTED (tanyamiller1221)" and "72.7MB / 13.7MB".

The screenshot displays the VCell 5.3 (build 4) interface. The main window shows a reaction diagram with three compartments: Cyt, NM, and Nuc. Several species are represented by colored circles: 'r', 'rf', 'rB' (green) and 's3', 's4', 's5' (red). A red box highlights the 's3' species, with a yellow callout box containing the text "Click on 's3'.". Below the diagram, the 'Object Properties' panel is visible. The 'Species Name' field contains 'BS', highlighted by a red box with a yellow callout box containing the text "Next to Species Name type 'BS'.". The 'Annotation' field contains 'Binding Sites', also highlighted by a red box with a yellow callout box containing the text "Next to Annotation type 'Binding Sites'.". The left sidebar shows a tree view of the model structure, including 'Physiology', 'Reaction Diagram', 'Reactions (0)', 'Structures (3)', and 'Species (6)'. The bottom status bar shows "CONNECTED (tanyamiller1221)" and "74.7MB / 128.7MB".

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

r rf rB

s3 s4 s5

Click on "s3".

BS

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name BS

Next to Species Name type "BS".

Linked Pathway Object(s)

Annotation Binding Sites

Next to Annotation type "Binding Sites".

CONNECTED (tanyamiller1221) 74.7MB / 128.7MB

The screenshot displays the VCell software interface for a model named "BioModel1". The main window is titled "Reaction Diagram" and shows a compartmental model with three compartments: "Cyt", "NM", and "Nuc". Several species are represented by colored circles: "rf" (green), "rB" (green), "B5" (green), "s5" (green), and "rfB" (red). A red box highlights the "rfB" species, with a yellow callout box pointing to it that says "Click on 's4'".

Below the reaction diagram, the "Object Properties" panel is visible. It shows the "Species Name" field containing "rfB", with a yellow callout box pointing to it that says "Next to Species Name type 'rfB'". The "Annotation" field contains "RAN_FITC_Bound", with a yellow callout box pointing to it that says "Next to Annotation type 'RAN_FITC_Bound'".

The left sidebar shows a tree view of the model structure, including "Physiology", "Reaction Diagram", "Reactions (0)", "Structures (3)", and "Species (6)". The bottom status bar indicates the user is "CONNECTED (tanyamiller1221)" and the memory usage is "78.4MB / 123.7MB".

The screenshot displays the VCell 5.3 (build 4) interface. The main window is titled "BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the model structure under "BioModel1". The "Physiology" folder is expanded, showing "Reaction Diagram" (selected), "Reactions (0)", "Structures (3)", and "Species (6)". Below this is a "VCell DB" section with tabs for "BioModels", "MathModels", and "Geometries". A "Search" section lists various model categories like "Biological Models", "My BioModels", "Shared BioModels", "Public BioModels", "Tutorials", and "Education".
- Top Panel:** A toolbar with icons for navigation and editing. Below the toolbar are tabs for "Reaction Diagram", "Reactions", "Structures", and "Species".
- Center Panel:** A reaction diagram showing three compartments: "Cyt", "NM", and "Nuc". A red box highlights a "Laser" object in the "Nuc" compartment, with a callout box saying "Click on 's5'".
- Bottom Panel:** An "Object Properties" window. The "Species Name" field is set to "Laser", with a callout box saying "Next to Species Name type 'Laser'". The "Annotation" field is set to "Light Source", with a callout box saying "Next to Annotation type 'Light Source'".

At the bottom left, the status bar shows "CONNECTED (tanyamiller1221)". At the bottom right, it shows "81.6MB / 123.7MB".

The screenshot shows the VCell software interface. The main window displays a reaction diagram with three compartments: Cyt, NM, and Nuc. The Nuc compartment contains several species represented by colored circles: 'r' (green), 'Laser' (green), 'rB' (green), 'rf' (green), 'BS' (red), and 'rfB' (green). A red box highlights the select tool (a mouse cursor icon) in the top toolbar, with a yellow callout box containing the text "Click the select tool." Another red box highlights the arrangement of species in the Nuc compartment, with a yellow callout box containing the text "Click and drag the species so that the order is from left to right 'r', 'Laser', 'rB', 'rf', 'BS', 'rfB'." The interface also shows a left sidebar with a tree view of the model structure, a bottom toolbar with buttons like 'Delete' and 'Pathway Links', and a bottom status bar showing 'CONNECTED (tanyamiller1221)' and '37.5MB / 135.8MB'.

Click the select tool.

Click and drag the species so that the order is from left to right "r", "Laser", "rB", "rf", "BS", "rfB".

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameterized Functions
- Pathway

Reaction Diagram | Reactions | Structures | Species

Cyt | NM | Nuc

Laser | rB | r0 | rf

<<REACTANT>>

BS

Delete | Pathway Links | Search

Object Properties | Problems (0 Errors, 0 Warnings)

Species Name: BS

Linked Pathway Object(s):

Annotation: Binding

CONNECTED (tanyamiller1221) | 50.71B / 135.8MB

Click the RX connection tool.

Click on "BS" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on a point inside the "Nuc" compartment which will create a reaction node called "r0".

Click the select tool and click and drag "r0" to move its position within the compartment. Drop your cursor to finalize the position of "r0".

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [$\mu\text{M/s}$] (recommended for stochastic application) Convert to [molecules.s^{-1}]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 68MB / 135.8MB

The screenshot displays the VCell software interface for editing a reaction diagram. The main window is titled "BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface includes a menu bar (File, View, Server, Tools, Help), a toolbar with various icons, and a central workspace divided into compartments labeled "Cyt", "NM", and "Nuc".

In the "Nuc" compartment, a reaction diagram is shown. A red box highlights a species icon labeled "r" (a red circle with a white square containing "r"). A red arrow points from this icon to another red box highlighting a species icon labeled "r0" (a yellow square with a red circle containing "r0"). A line connects the two boxes, representing a reaction. Other species icons in the diagram include "rf", "BS", "Laser", "rB", and "rfB".

A yellow callout box with a red border is overlaid on the diagram, containing the text: "Click on 'r' and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on 'r0'." Below the diagram, the "Object Properties" panel shows the following information:

Species Name	r
Linked Pathway Object(s)	
Annotation	RAN

At the bottom of the window, the status bar shows "CONNECTED (tanyamiller1221)" on the left and "74.7MB / 35.8MB" on the right.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (1)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

rf Laser r0 BS rB rFB

Click on "r0" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "rB".

Delete

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot rB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 82.4MB / 135.8MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

r rB

rf rB

BS

r1

Click on "BS" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on a point inside the "Nuc" compartment which will create a reaction node called "r1".

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r1

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M}\cdot\text{s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 95.1MB / 135.6MB

The screenshot displays the VCell software interface for editing a biological model. The main window shows a reaction diagram with three compartments: Cyt, NM, and Nuc. A callout box with a red border and yellow background contains the following text:

Click on "rf" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "r1".

The diagram shows a reaction network with species represented by green circles. A red circle labeled "rf" is highlighted with a red box. A yellow square is also highlighted with a red box. Red arrows point from the callout box to these elements. The "Object Properties" panel at the bottom shows the following details for the selected species:

Property	Value
Species Name	rf
Linked Pathway Object(s)	
Annotation	RAN_FITC

The interface includes a menu bar (File, View, Server, Tools, Help), a toolbar with various icons, and a search bar. The status bar at the bottom indicates the user is connected as "tanyamiller1221" and shows memory usage of 39.5MB / 124.8MB.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram

Reactions Structures Species

Cyt NM Nuc

Laser

r rB

rf BS

r1 rfB

Click on "r1" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "rfB".

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r1

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot rf - K_r \cdot rfB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rfB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 46.31 MB / 124.3 MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (3)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram

Reactions Structures Species

Cyt NM Nuc

Laser

rfB

rf

rfB

BS

Click on "rf" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "r". A reaction node "r2" will be created.

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r2

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot rf - K_r \cdot r)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221)

104.2MB / 124.8MB

The screenshot shows the VCell software interface. On the left is a tree view of the model structure. The main window displays a reaction diagram with compartments Cyt, NM, and Nuc. A reaction node 'r2' is being created between 'rf' and 'r' in the Cyt compartment. A yellow callout box with a red border provides instructions on how to create this reaction. The bottom right panel shows the 'Object Properties' for 'r2', including its name, kinetic type, and a table of parameters and species.

The screenshot shows the VCell software interface. On the left is a navigation tree for 'BioModel1' with categories like Physiology, Reactions (4), Structures (3), and Species (6). The main window displays a reaction diagram with compartments Cyt, NM, and Nuc. A reaction node 'r3' is highlighted in a red box, with arrows pointing to its reactants 'rB' and 'rB', which are also highlighted in red boxes. A yellow callout box contains the instruction: 'Click on "rB" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "rB". A reaction node "r3" will be created.'

Below the diagram is the 'Object Properties' panel for reaction 'r3'. It shows the kinetic type as 'Mass Action' and the expression as $(K_f \cdot rB - K_r \cdot rB)$. Below this is a table of parameters:

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot rB - K_r \cdot rB)$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

At the bottom of the interface, there is a status bar showing 'CONNECTED (tanyamiller1221)' and a memory usage indicator '36.4MB / 121.6MB'.

The screenshot shows the VCell software interface. The main window displays a reaction diagram with three compartments: Cyt, NM, and Nuc. A species named 'Laser' is shown in the Nuc compartment, represented by a red dot. A yellow callout box with a red border contains the following text: "Click on 'r2' and drag your cursor, which will create a line marked <<CATALYST>>. Drop your cursor on 'Laser'". A red arrow points from the callout box to a yellow square node labeled 'r2' in the reaction diagram. Another red arrow points from the 'r2' node to the 'Laser' species. The interface includes a menu bar (File, View, Server, Tools, Help), a toolbar with various icons, and a search bar at the bottom. The status bar at the bottom indicates the user is connected as 'tanyamiller1221' and shows memory usage of 58.2MB / 121.6MB.

Click on the catalyst tool.

Click on "r2" and drag your cursor, which will create a line marked <<CATALYST>>. Drop your cursor on "Laser".

Species Name: Laser

Linked Pathway Object(s):

Annotation: Light Source

CONNECTED (tanyamiller1221) 58.2MB / 121.6MB

The screenshot shows the VCell software interface. The main window displays a reaction diagram with three compartments: Cyt, NM, and Nuc. A red box highlights the 'Laser' species in the Nuc compartment. A yellow callout box with a red border contains the text: "Click on 'Laser' and drag your cursor, which will create a line marked <<CATALYST>>. Drop your cursor on 'r3'." A red arrow points from the callout box to the 'Laser' species, and another red arrow points from the 'Laser' species to a yellow square node labeled 'r3' in the Nuc compartment. The 'Object Properties' panel at the bottom shows the following information:

Object Properties	
Species Name	Laser
Linked Pathway Object(s)	
Annotation	Light Source

At the bottom of the window, the status bar shows "CONNECTED (tanyamiller1221)" on the left and "64.9MB / 121.6MB" on the right.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

Reactions (4)
Structures (3)
Species (6)
Applications (0)
Parameters and Functions
Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Click the select tool.

Click on "r0".

Click on "RAN binding".

Next to Reaction Name type "RAN binding".

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name RAN binding

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot rB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 40.5MB / 122.7MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram

Reactions Structures Species

Cyt NM Nuc

Laser

RAN binding

BS

r

rB

rB

1

Delete Pathway Links Search

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
1	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot rB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.02	$\text{s}^{-1}\cdot\text{M}^{-1}$
Kr	reverse rate constant	<input checked="" type="checkbox"/>	.1	s^{-1}
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

CONNECTED (tanyamiller1221)

122.7MB

In the forward rate constant row, type ".02" under the Expression column. Press "Enter" on your keyboard to finalize.

In the reverse rate constant row, type ".1" under the Expression column. Press "Enter" on your keyboard to finalize.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

Click "r1".

RAN_FITC binding

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name RAN_FITC binding

Kinetic Type Mass Action [m³] (recommended for stochastic application) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>		M ⁻¹ s ⁻¹
Kf	forward	<input type="checkbox"/>		M ⁻¹ s ⁻¹
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s ⁻¹
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rfB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 67.5MB / 22.7MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

r rB

BS

RAN_FITC binding

Delete Pathway Links Search

In the forward rate constant row, type ".02" under the Expression column. Press "Enter" on your keyboard to finalize.

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r_f - K_r \cdot r_fB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.02	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.1	s^{-1}
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r _f	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r _{fB}	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

In the reverse rate constant row, type ".1" under the Expression column. Press "Enter" on your keyboard to finalize.

CONNECTED (tanyamiller1221) 122.7MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

r2

Click "r2".

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r2

Kinetic Type General [$\mu\text{M/s}$]

Convert to [molecules.s^{-1}]

Name	Description	Global	Expression	Units
r2	reaction rate	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$

Click the drop down menu next to Kinetic Type. Click "General [$\mu\text{M/s}$ "].

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 47.6MB / 118.5MB

The screenshot shows the VCell software interface. The main window displays a reaction diagram with three compartments: Cyt, NM, and Nuc. The Nuc compartment contains a network of reactions involving species Laser, r, rB, and r1B. A reaction labeled 'r2' is highlighted in a red box. Below the diagram, the Object Properties panel shows the reaction name 'r2' and its kinetic type 'General [μM/s]'. A table below the properties panel shows the reaction rate parameters:

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(V_{max} * r_f * Laser * ((t > 1.0) \& \& (t < 1.5)))$	μM.s ⁻¹

An arrow points from the text box below to the expression column of the table.

In the reaction rate row, type “(Vmax*rf*Laser*((t>1.0)&&(t<1.5)))” under the Expression column. Press “Enter” on your keyboard to finalize. The Boolean expression evaluates to 1 during the time interval from 1.0 to 1.5 secs; at other times, the expression evaluates to 0 so the bleaching reactions only occur during the specified time interval.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (0)
 - Tutorials (0)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

r r2 rB rB

BS

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Kinetic Type General [$\mu\text{M}/\text{s}$] Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$V_{\text{max}} \cdot r_f \cdot \text{Laser} \cdot ((t > 1.0) \&\& (t < 1.5))$	$\mu\text{M}\cdot\text{s}^{-1}$
Vmax	user defined	<input type="checkbox"/>	50	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
r _f	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
t	time	<input checked="" type="checkbox"/>	Variable	s

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 61.6MB / 120.6MB

In the Vmax row, type "50" under the Expression column. Press "Enter" on your keyboard to finalize.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

bleaching 1

rf

rfB

BS

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name **bleaching 1**

Kinetic Type General [$\mu\text{M}/\text{s}$] Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$v_{\text{max}} \cdot r_f \cdot \text{Laser} \cdot ((t > 1.0) \ \&\& \ (t < 1.5))$	$\mu\text{M}\cdot\text{s}^{-1}$
vmax	user defined	<input type="checkbox"/>	50.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
t	time	<input checked="" type="checkbox"/>	Variable	s

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 85.5MB / 120.6MB

Next to Reaction Name type "bleaching 1".

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

Click "r3".

bleaching 2

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 2

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot rB - K_r \cdot rB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s^{-1}
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

CONNECTED (tanyamiller1221)

44.418 / 114.8MB

The screenshot displays the VCell software interface. On the left, a tree view shows the model structure: BioModel1 > Physiology > Reaction Diagram. The main window shows a reaction diagram with compartments Cyt, NM, and Nuc. A reaction named 'bleaching 2' is highlighted. Below the diagram, the 'Object Properties' panel shows the reaction name 'bleaching 2' and its kinetic type set to 'General [μM/s]'. A red box highlights the 'Kinetic Type' dropdown menu, and a red arrow points to it from a yellow callout box. The callout box contains the text: 'Click the drop down menu next to Kinetic Type. Click "General [μM/s]"'. Below the properties panel, a table lists the reaction details:

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	0.0	μM.s ⁻¹

At the bottom of the interface, the status bar shows 'CONNECTED (tanyamiller1221)' and '48.2M3 / 114.8MB'.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram

Reactions Structures Species

Cyt NM Nuc

Laser

r

rB

bleaching 2

rFB

BS

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 2

Kinetic Type General [$\mu\text{M}/\text{s}$] Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(Vmax2*rFB*Laser*((t>1.0)\&\&(t<1.5)))$	$\mu\text{M}\cdot\text{s}^{-1}$

CONNECTED (tanyamiller1221) 75.9MB / 114.8MB

In the reaction rate row, type “(Vmax2*rFB*Laser*((t>1.0)&&(t<1.5)))” under the Expression column. Press “Enter” on your keyboard to finalize.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (0)
 - Tutorials (0)
 - Education (33)

Reaction Diagram Reactions Structures Species

Cyt NM Nuc

Laser

rB

bleaching 2

rB

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

kinetic type General $\mu\text{M}/\text{s}$ Convert to [molecules $\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$v_{\text{max}2} \cdot rB \cdot \text{Laser} \cdot ((t > 1.0) \ \&\& \ (t < 1.5))$	$\mu\text{M}\cdot\text{s}^{-1}$
vmax2	user defined	<input type="checkbox"/>	50	$\text{s}^{-1} \cdot \text{M}^{-1}$
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
t	time	<input checked="" type="checkbox"/>	Variable	s

Annotation and Pathway Links

CONNECTED (tanyamiller1221) 85.4MB / 114.8MB

In the Vmax row, type "50" under the Expression column. Press "Enter" on your keyboard to finalize.

The screenshot displays the VCell software interface. The main window title is "BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel (BioModel1):** A tree view showing the model structure. Under "Physiology", the "Applications (0)" folder is highlighted with a red box and a red arrow pointing to it.
- Bottom-Left Panel (VCell DB):** Shows a search interface with tabs for "BioModels", "MathModels", and "Geometries". The "BioModels" tab is active, showing a search results list with folders like "My BioModels", "Shared BioModels", "Public BioModels", "Tutorials", and "Education".
- Main Panel:** A table with columns "Name", "Math Type", and "Annotation". Below the table is a toolbar with buttons for "Add New", "Delete", and "More Copy Actions". The "Add New" button is highlighted with a red box, and its dropdown menu is open, showing "Deterministic" and "Stochastic" options. The "Deterministic" option is also highlighted with a red box. A red arrow points from a yellow text box to the "Add New" button.

A yellow text box with a red border contains the instruction: "Click 'Applications' > 'Add New' > 'Deterministic'." A red arrow points from this box to the "Add New" button in the toolbar.

At the bottom of the window, the status bar shows "CONNECTED (tanyamiller1221)" on the left and "62.3MB / 118MB" on the right.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Application0
- Parameters and Functions
- Pathway

Name	Math Type	Annotation
Compartmental	compartmental deterministic	

Double click "Application0" under the Name column. Type in "Compartmental". Press "Enter" on your keyboard to finalize. This compartmental application will be used to determine the steady-state concentrations for the binding reaction.

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Object Properties Problems (0 Errors, 0 Warnings)

Application Name: Application0

Annotation:

Summary

- Deterministic
- Compartmental
- math not generated

CONNECTED (tanyamiller1221) 51.1MB / 118.5MB

The screenshot shows the VCell software interface. The left sidebar contains a tree view with 'BioModel1' expanded to 'Geometry'. The main window displays 'Physiology (structures)' with three ovals labeled 'Cyt', 'NM', and 'Nuc' connected to a red square labeled 'Compartment' in the 'Geometry (subd...' panel. A yellow callout box points to the 'Geometry' tab in the sidebar and the 'Structure Mapping' sub-tab, with the text: "Click 'Geometry' > 'Structure Mapping'". Another yellow callout box points to the 'Size' column in the table below, with the text: "In the Size column for 'Cyt', 'NM' and 'Nuc', type in '523.33', '130.8325' and '26.1665' respectively. Press 'Enter' on your keyboard to finalize." The table below has the following data:

Structure	Size
Cyt	523.33 [μm^3]
NM	130.8325 [μm^2]
Nuc	26.1665

At the bottom of the window, it shows 'CONNECTED (tanyamiller1221)' and '49.4MB / 113.2MB'.

Click "Specifications" > "Species".

Species	Structure	Clamped	Initial Condition
r	Nuc	<input type="checkbox"/>	5.0
rf	Nuc	<input type="checkbox"/>	5.0
rB	Nuc	<input type="checkbox"/>	0.0
BS	Nuc	<input checked="" type="checkbox"/>	20
rfB	Nuc	<input type="checkbox"/>	0.0
Laser	Nuc	<input type="checkbox"/>	0.0

In the Initial Condition column for "r", "rf" and "BS", type in "5", "5" and "20" respectively. Press "Enter" on your keyboard to finalize.

CONNECTED (tanyamiller1221) 80.4MB / 113.2MB

The screenshot shows the VCell software interface. The 'File' menu is highlighted with a red box. A red arrow points from the 'File' menu to a yellow callout box containing the text: "To save your model, click 'File' > 'Save As'".

The main window displays the 'Species' tab of a table with the following data:

Species	Structure	Clamped	Initial Condition
r	Nuc	<input type="checkbox"/>	5.0
rf	Nuc	<input type="checkbox"/>	5.0
rB	Nuc	<input type="checkbox"/>	0.0
pc	Nuc	<input checked="" type="checkbox"/>	20.0
pc	Nuc	<input type="checkbox"/>	0.0
Laser	NUC	<input type="checkbox"/>	0.0

The interface also shows a 'Pathway' browser on the left with a search bar and a list of folders: Biological Models, My BioModels (tanyamiller1221) (4), Shared BioModels (0), Public BioModels (519), Tutorials (5), and Education (33). The status bar at the bottom indicates 'CONNECTED (tanyamiller1221)' and '45.5MB / 115.3MB'.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

Geometry Specifications Protocols Simulations Parameter Estimation

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
 - Geometry**
 - Specifications
 - Protocols
 - Simulations
 - Parameter Estimation
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller 1221) (4)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Save document:

Search

Advanced >>

Search Show All

- Biological Models
 - My BioModels (tanyamiller 1221) (4)**
 - BioModel2
 - FRAPTutorial
 - Tutorial
 - Tutorial_MultiApp
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)

Selected BioModel Summary

Please type a new name:

FRAPBindingTutorial

Save Cancel

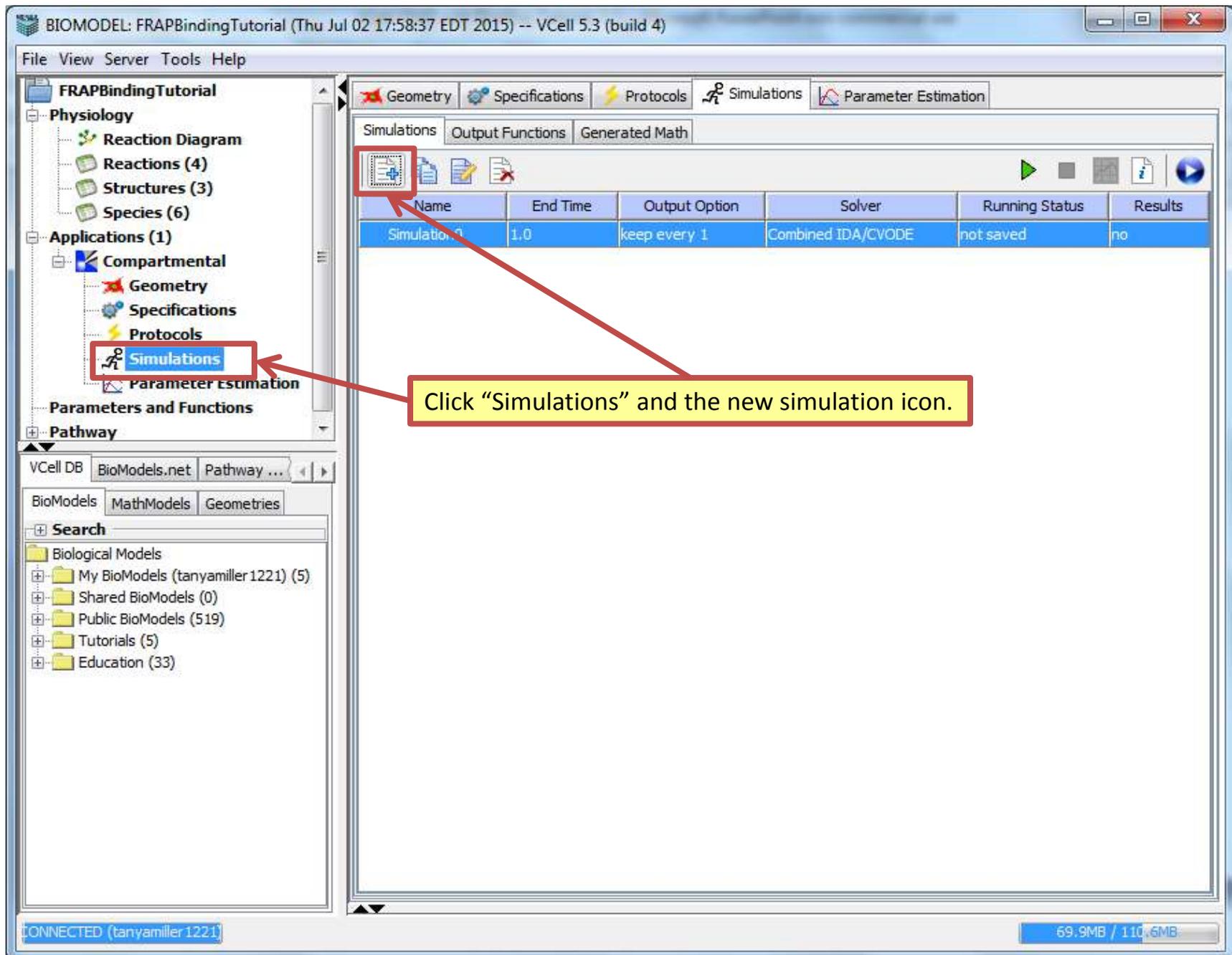
Click on a folder to select the location for your model to be saved.

Type in a name under "Please type in a new name:" and click "Save".

	Initial Condition
	5.0
	5.0
	0.0
	20.0
	0.0
	0.0

CONNECTED (tanyamiller 1221)

57.9MB / 110.1MB



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 17:58:37 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
 - Geometry
 - Specifications
 - Protocols
 - Simulations**
 - Parameter Estimation
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

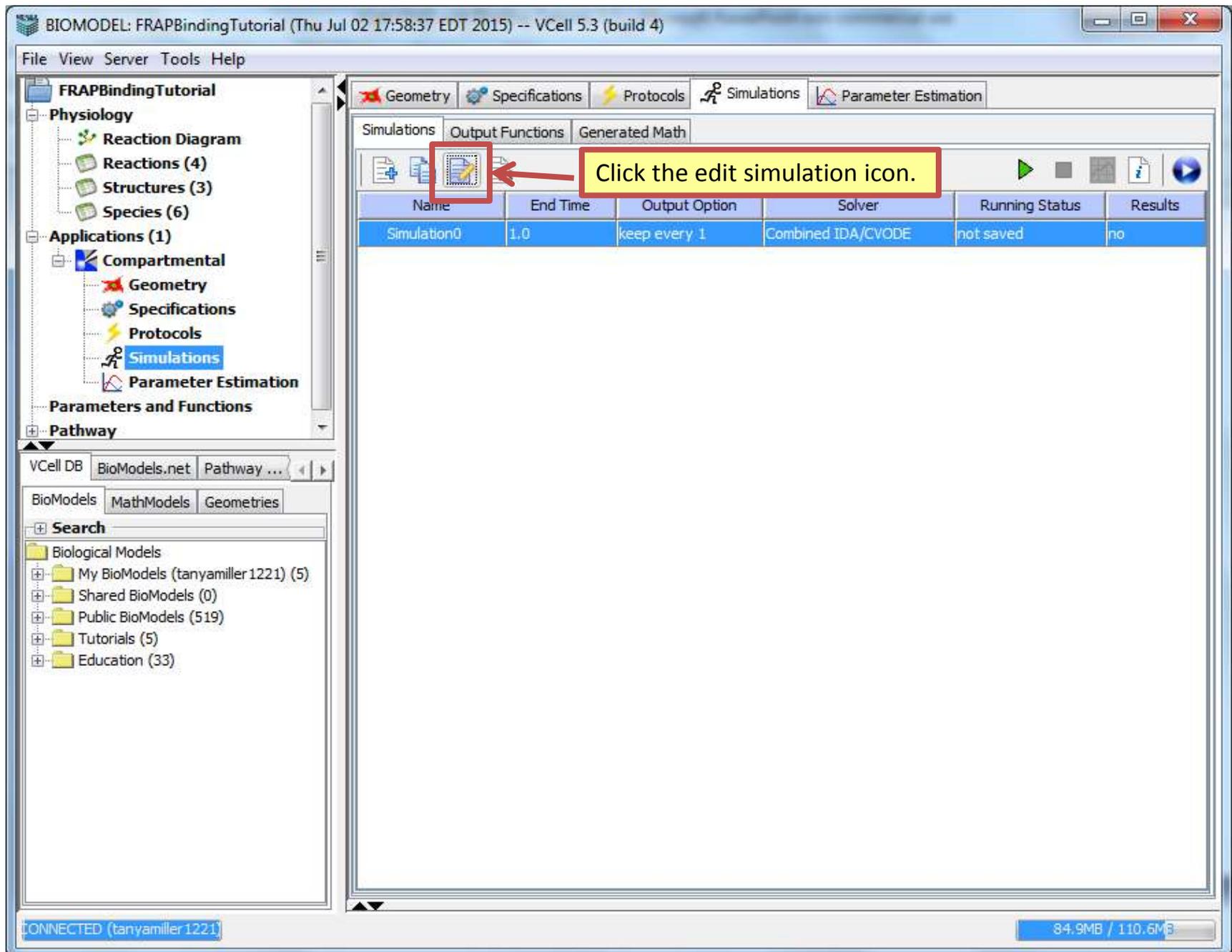
Geometry Specifications Protocols **Simulations** Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation_0	1.0	keep every 1	Combined IDA/CVODE	not saved	no

CONNECTED (tanyamiller1221) 69.9MB / 110.6MB

Click "Simulations" and the new simulation icon.



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 17:58:37 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
 - Geometry
 - Specifications
 - Protocols
 - Simulations
 - Parameter Estimation
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
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 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Click the edit simulation icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Combined IDA/CVODE	not saved	no

CONNECTED (tanyamiller1221) 84.9MB / 110.6MB

BIOMODEL: Tutorial_FRAPbinding (Wed Aug 12 09:40:56 EDT 2015) -- VCell 5.3 (build 9)

File View Server Tools Help

Tutorial_FRAPbinding

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
 - Compartmental
 - Geometry
 - Specifications
 - Protocols
 - Simulations
 - Parameter Estimation
- Spatial

Parameters and Functions

VCell DB BioModels.net Pathway Co...

BioModels MathModels Geometries

Search

- TIR_FRAP 1
- TIR_FRAP 2
- Tutorial_FRAP
- Tutorial_FRAPbinding
 - Access[tanyamiller 1221,thor]
- Tutorial_MultiApp
- Tutorial_MultiApp_sims
- Tutorial_PH-GFP
- Utrophin_01
- vFRAPtest1_APCcell_laser
- vFRAPtest1_APCcell_nonuc_lase
- vFRAPtest1_APCcell_Nuc&ER
- VICE FRAP 3-09 VICE2 FRAP
- VICE FRAP Nuc only
- VirtualSensor_globals_fixed

Edit: Simulation0

Parameters **Solver** ← Click "Solver".

Choose solver algorithm and fine-tune time conditions:

Integrator Combined Stiff Solver (IDA/CVODE) ?

General

Time Bounds		Time Step		Error Tolerance	
Starting	0.0	Minimum		Absolute	1.0E-9
Ending	30.0	Default		Relative	1.0E-9
		Maximum	1.0		

Local Sensitivity Analysis

time samples and at most 1000 time samples

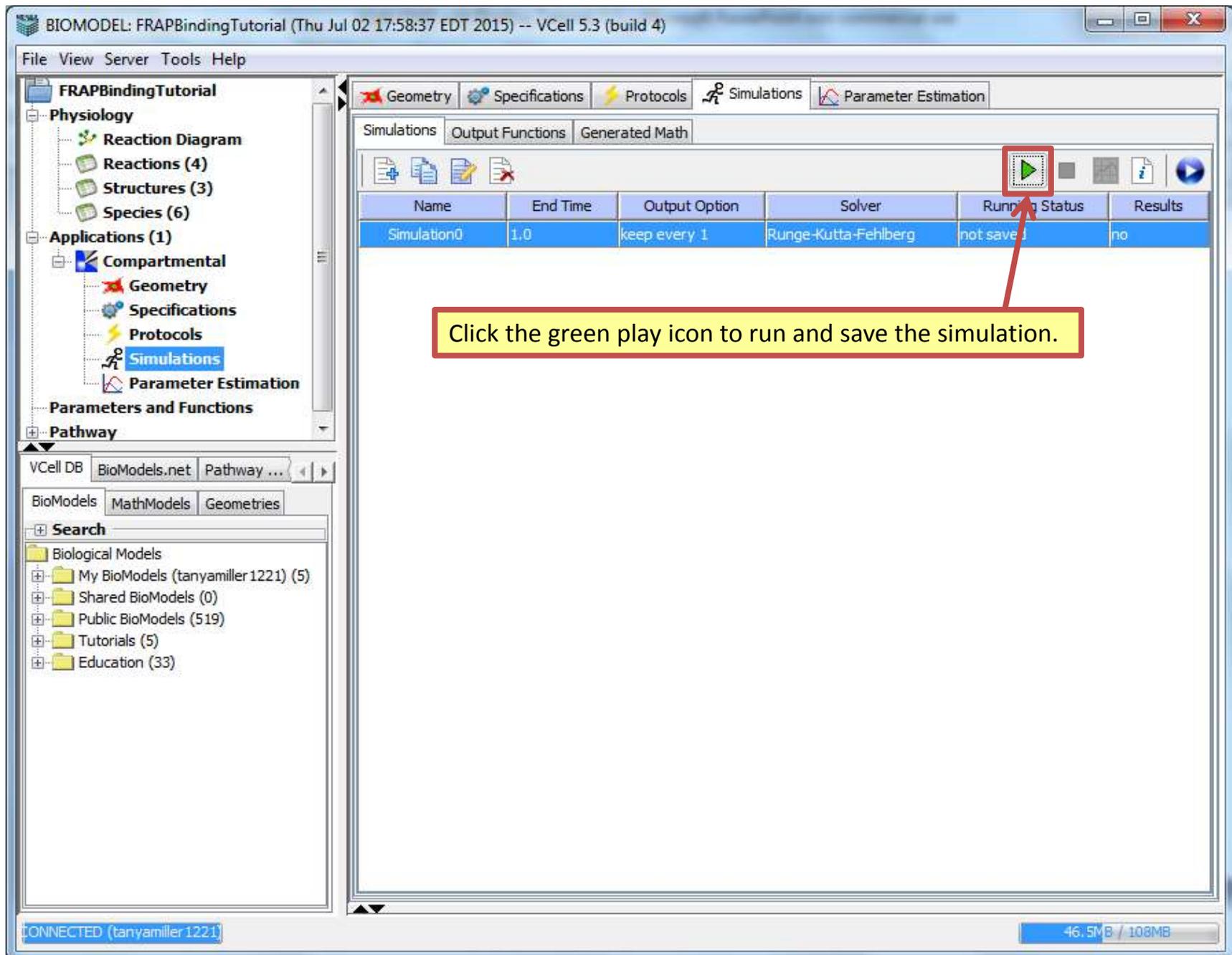
Output Interval [] secs

Output Times []

(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)

OK Cancel

CONNECTED (ACowan) 115.5MB / 244.8MB



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 17:58:37 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
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 - Parameter Estimation
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

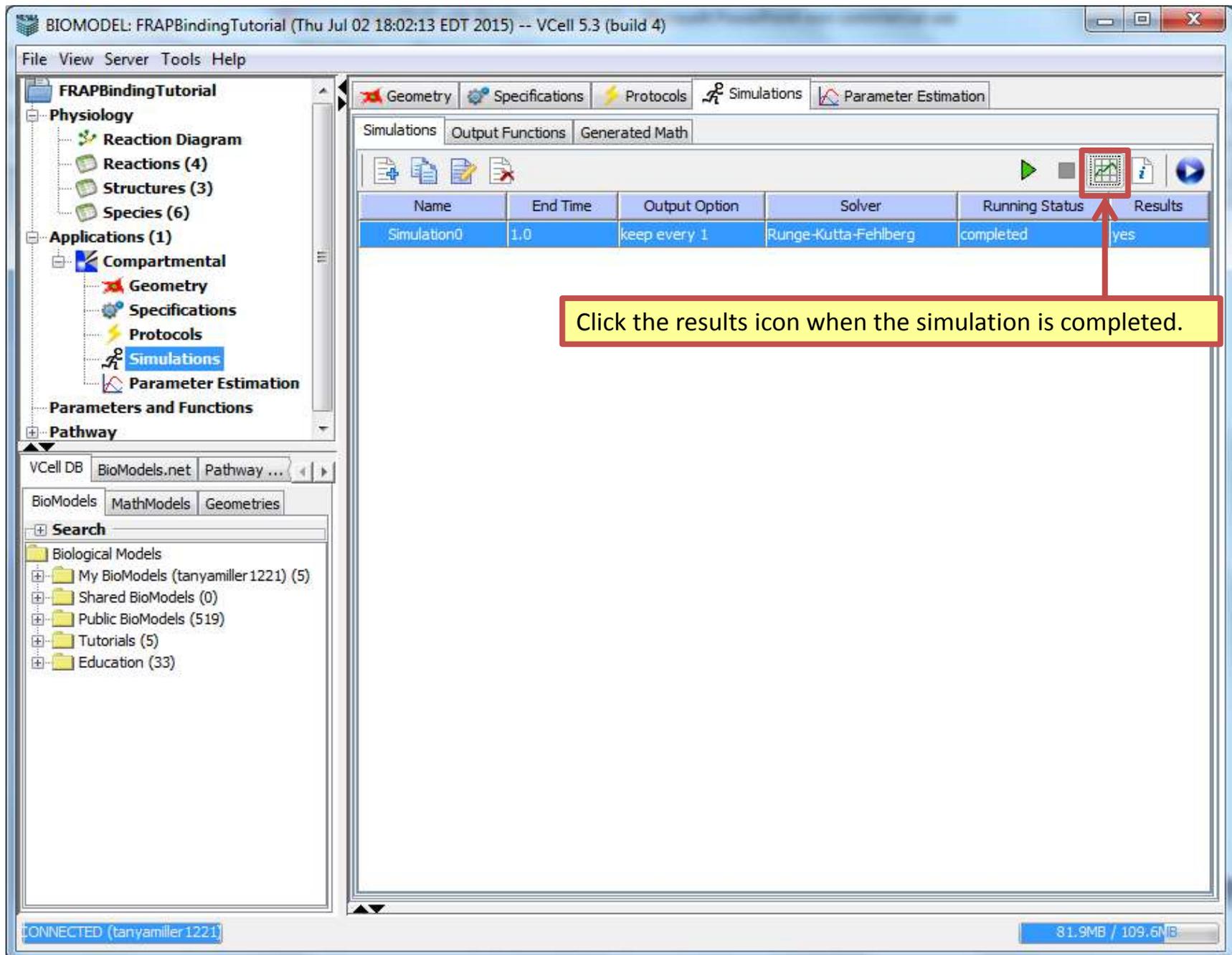
Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Runge-Kutta-Fehlberg	not saved	no

Click the green play icon to run and save the simulation.

CONNECTED (tanyamiller1221) 46.5MB / 108MB



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
 - Geometry
 - Specifications
 - Protocols
 - Simulations
 - Parameter Estimation
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

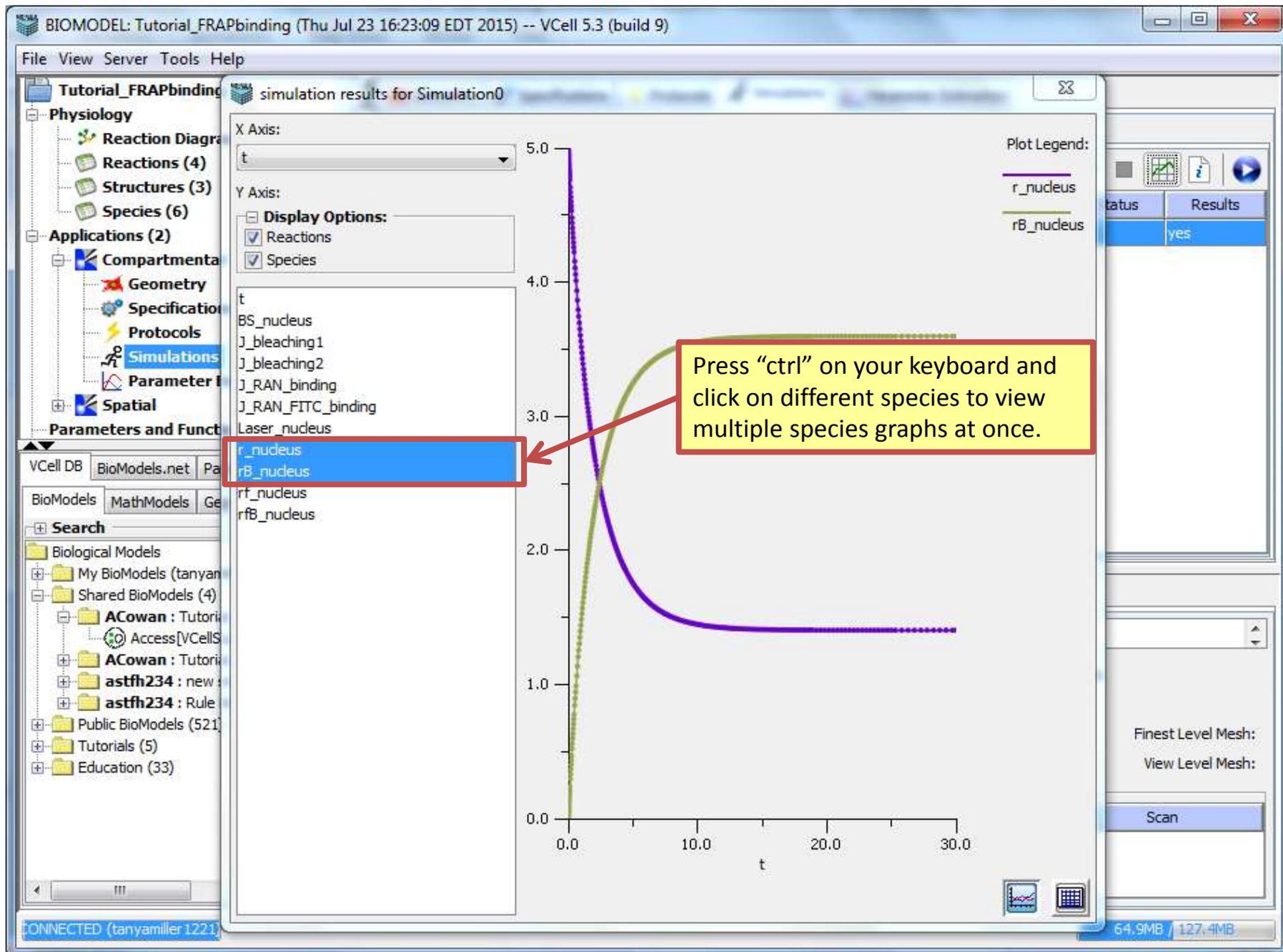
Geometry Specifications Protocols Simulations Parameter Estimation

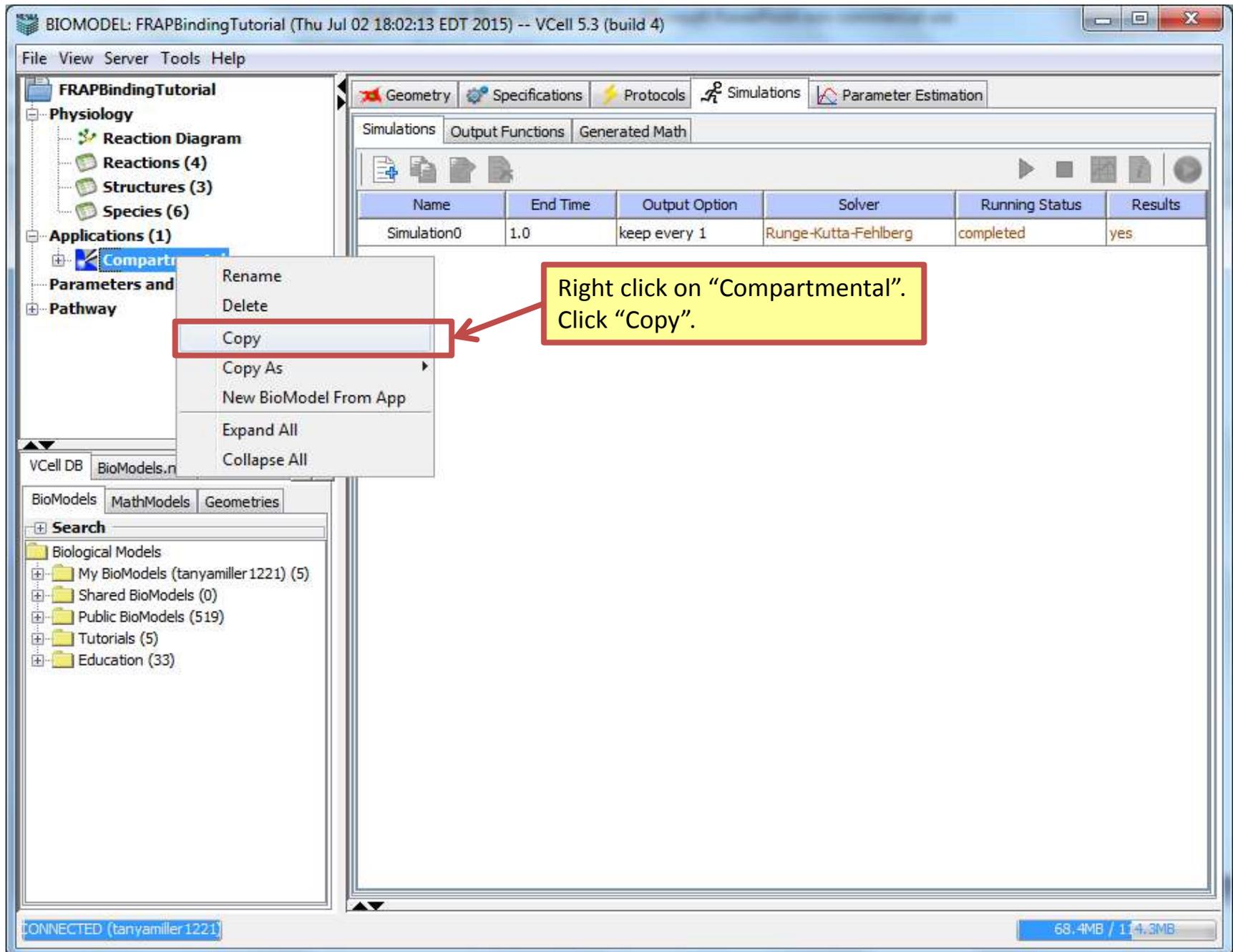
Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Runge-Kutta-Fehlberg	completed	yes

Click the results icon when the simulation is completed.

CONNECTED (tanyamiller1221) 81.9MB / 109.6MB





BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (1)
 - Compartmental
- Parameters and
- Pathway

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Runge-Kutta-Fehlberg	completed	yes

Right click on "Compartmental".
Click "Copy".

Copy

Expand All Collapse All

VCeLl DB BioModels.n

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

CONNECTED (tanyamiller1221) 68.4MB / 1.4.3MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
 - Compartmental
 - Copy of C
- Parameters and
- Pathway

VCell DB BioModels.n

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	1.0	keep every 1	Runge-Kutta-Fehlberg	not saved	no

CONNECTED (tanyamiller1221) 53.2MB 112.7MB

Click "Geometry" > "Geometry Definition".

Click "Add Geometry" > "New".

Domain: OD, compartmental

Name	Value
Compartment	

CONNECTED (tanyamiller1221) 74.7MB / 112.7MB

The screenshot shows the VCell software interface. The main window is titled "BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)". The "Geometry" tab is active, and the "Geometry Definition" sub-tab is selected. The "Domain" is set to "0D, compartmental". A table with columns "Name" and "Value" is visible. A dialog box titled "Select Geometry Type" is open, showing a list of geometry types. The "Analytic Equations (2D)" option is highlighted with a red box. A yellow callout box with a red arrow points to this option, containing the text "Click 'Analytic Equations (2D)'". Another yellow callout box with a red arrow points to the "OK" button at the bottom of the dialog box, containing the text "Click 'OK'".

File View Server Tools Help

FRAPBindingTutorial

Physiology

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)

Application

- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters and Functions

VCell DB BioModels.net Pathway

BioModels MathModels Geomet

Search

- Biological Models
 - My BioModels (tanyamiller1221)
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 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition

Domain: 0D, compartmental Edit Domain... Export... Edit Image Add Geometry

Name	Value

Select Geometry Type

- Analytic Equations (1D)
- Analytic Equations (2D)**
- Analytic Equations (3D)
- Image based (import from file, zip or directory)
- Mesh based (import from STL file)
- New Blank Image Canvas
- Constructed Solid Geometry (3D)

Front Back Add Subdomain Delete

OK Cancel

CONNECTED (tanyamiller1221) 87.2MB / 112.7MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
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 - Compartmental
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- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) Ed... Export... Edit Image Replace Geometry ▾

Name	Value
Cyt	0

Front
Back
Add Subdomain ▾
Delete

Slice

0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0

Info

CONNECTED (tanyamiller1221) 82.4MB / 104.3MB

Double click "subdomain0" and type "Cyt". Press "Enter" on your keyboard to finalize.

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
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 - Specifications
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- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) Ed... Export... Edit Image Replace Geometry ▾

Name	Value
Cyt	1.0

Front
Back
Add Subdomain ▾
Delete

Click "Add Subdomain" > "Analytic".

Slice View Surface View Geometric Region Details

Info

CONNECTED (tanyamiller1221) 55.2MB / 111.1MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
 - Compartment
 - Spatial
- Geometry
- Specification
- Protocols
- Simulation

Parameters and Functions

Pathway

VCell DB BioModels.net P

BioModels MathModels G

Search

- Biological Models
 - My BioModels (tanya)
 - Shared BioModels (0)
 - Public BioModels (51)
 - Tutorials (5)
 - Education (33)

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)

Export... Edit Image Replace Geometry

Front Back Add Subdomain Delete

Define New Subdomain Shape

Select Subdomain Shape: Circle

Center Point (x,y)
0,0

Radius
10

Analytic Expression
 $x^2 + y^2 < 10.0^2$
Copy Expression

Add New Subdomain Cancel

CONNECTED (tanyamiller1221) 62.7MB / 111.1MB

Click the drop down menu next to "Select Subdomain Shape:".
Click "Circle".

Under "Radius" type "10".

Click "Add New Subdomain".

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
 - Compartmental
 - Spatial
- Geometry
- Specifications
- Protocols
- Simulations

Parameters and Functions

Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) Ed... Export... Edit Image Replace Geometry ▾

Name	Value
Nuc	2.0 $(((x - 2.0)^2 + (y - 2.0)^2) < (10.0)^2)$
Cyt	1.0

Front Back Add Subdomain ▾ Delete

Slice View Sur

0 3 6 10

0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0

Info

CONNECTED (tanyamiller1221) 69.2MB / 101.7MB

Double click "subdomain0" and type "Nuc". Press "Enter" on your keyboard to finalize.

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
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VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
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 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) **Ed...** Export... Edit Image Replace Geometry ▾

Name	Value
Nuc	$2.0 \quad 2.0 \quad 2.0$ $((x) + (y)) < (10.0)$
Cyt	1.0

Front
Back
Add Subdomain ▾
Delete

Slice View Surfa **Click "Edit Domain".**

Info

CONNECTED (tanyamiller1221) 47.5MB / 107.5MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 19:03:55 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- App
- Spatial
 - Geometry
 - Specifications
 - Protocols
 - Simulations
- Parameters
- Pathway

VCell DB BioModel

BioModels Math

Search

disconnected

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(22.0,22.0), origin=(-11.0,-11.0) ... Export... Edit Image Replace Geometry ▾

Name	Value
	2.0 2.0 2.0
	$(x) + (y) < (10.0)$
Cyt	7.0

Front

Back

Add Subdomain ▾

Delete

Geometry Size

Size X 22.0 μm Y 22.0 μm Z 10.0 μm

Origin X -11.0 μm Y -11.0 μm Z 0.0 μm

OK Cancel

Click "OK".

Next to "Size", type "22" for X and Y.

Next to "Origin", type "-11" for X and Y.

DISCONNECTED

62.3MB / 134.2MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
 - Compartmental
 - Spatial
- Geometry
- Specifications
- Protocols
- Simulations

Parameters and Functions

Pathway

VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
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 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(22.0,22.0), origin=(-11.0,-11.0) ... Export... Edit Image Replace Geometry

Name	Value
Nuc	$((x)^2 + (y)^2) < (10.0)$
Cyt	1.0

Front

Slice View Surface View Geometric Region Details

Info

CONNECTED (tanyamiller1221)

67.2MB / 99.1MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

Physiol

Click the line tool.

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.

Physiology (structures)

Geometry (subdomains)

Cyt Nuc NM

Nuc Cyt Cyt_Nuc_membrane

Drag your cursor from a point inside the "Cyt" physiology and drop your cursor on the "Cyt" geometry.

Drag your cursor from a point inside the "Nuc" physiology and drop your cursor on the "Nuc" geometry.

Drag your cursor from a point inside the "NM" physiology and drop your cursor on the "Cyt_Nuc_membrane" geometry.

Structure	Subdomain				
Cyt	Cyt				
Nuc	Nuc				
NM	Cyt_Nuc_membrane	1 [1]	Flux	Flux	Flux Flux

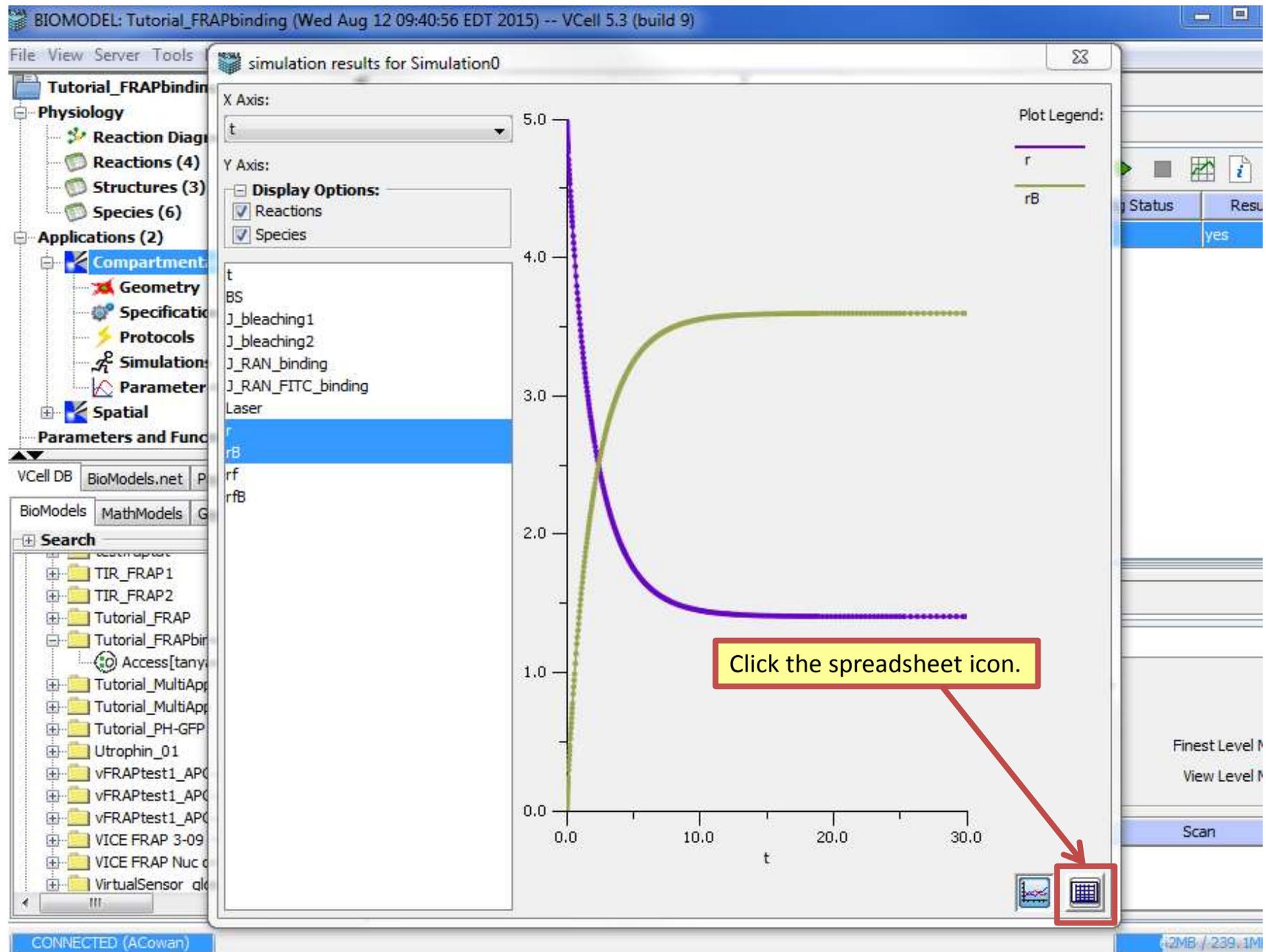
CONNECTED (tanyamiller1221) 59.4MB / 09.6MB

The screenshot shows the VCell software interface for the FRAPBindingTutorial project. The left sidebar displays the project hierarchy, with 'Compartmental' and 'Simulations' highlighted. The main window shows the 'Simulations' tab with a table of simulation results. A red box highlights the 'Results' icon in the toolbar, and a yellow callout box provides instructions on how to access the results.

Click "Compartmental" > " Simulations" > results icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Runge-Kutta-Fehlberg	completed	yes

CONNECTED (tanyamiller1221) 42.71B / 110.1MB



BIOMODEL: Tutorial_FRAPbinding (Wed Aug 12 09:40:56 EDT 2015) -- VCell 5.3 (build 9)

simulation results for Simulation0

X Axis: t

Y Axis: BS

Display Options:
 Reactions
 Species

t	BS	r	rB	rf	rfB
0	20	5	0	5	0
4.776259...	20	5	9.552535...	5	9.552518...
4.776736...	19.999998	4.999999	9.553470...	4.999999	9.553470...
5.253932...	19.999979	4.9999895	1.050784...	4.9999895	1.050784...
2.332024...	19.999907	4.9999534	4.664007...	4.9999534	4.664007...
6.424071...	19.999743	4.9998715	1.284784...	4.9998715	1.284784...
1.423373...	19.999431	4.9997153	2.846604...	4.9997153	2.846604...
2.825687...	19.99887	4.9994349	5.650814...	4.9994349	5.650814...
5.293824...	19.997883	4.9989414	1.058568...	4.9989414	1.058568...
9.658910...	19.996138	4.9980689	1.931129...	4.9980689	1.931129...
1.801728...	19.992798	4.9963988	3.601186...	4.9963988	3.601186...
3.409863...	19.986377	4.9931884	6.811598...	4.9931884	6.811598...
6.017998...	19.979963	4.9899816	1.001840...	4.9899816	1.001840...
6.626133...	19.973557	4.9867784	0.0132216	4.9867784	0.0132216
8.234268...	19.967158	4.9835788	1.642120...	4.9835788	1.642120...
9.842403...	19.960766	4.9803828	0.01961721	4.9803828	0.01961721
1.165139...	19.953584	4.9767919	2.320810...	4.9767919	2.320810...
1.346037...	19.946411	4.9732055	2.679446...	4.9732055	2.679446...
1.526936...	19.939247	4.9696237	3.037630...	4.9696237	3.037630...
0.01817295	19.927768	4.963884	3.611602...	4.963884	3.611602...
2.107653...	19.916312	4.9581559	4.184413...	4.9581559	4.184413...
2.398011...	19.904879	4.9524393	4.756067...	4.9524393	4.756067...
2.688369...	19.893469	4.9467343	5.326566...	4.9467343	5.326566...
3.199124...	19.873454	4.9367269	6.327312...	4.9367269	6.327312...
3.709879...	19.85351	4.9267549	7.324511...	4.9267549	7.324511...
4.220634...	19.833636	4.9168182	8.318182...	4.9168182	8.318182...
5.175343...	19.796677	4.8983384	0.10166156	4.8983384	0.10166156

Press "Ctrl" on your keyboard and click "BS", "rB", "rf" and "rfB".

CONNECTED (ACowan) 151.8MB / 238

BIOMODEL: Tutorial_FRAPbinding (Wed Aug 12 09:40:56 EDT 2015) -- VCell 5.3 (build 9)

File View Server Tools

simulation results for Simulation0

X Axis: t

Y Axis: Display Options: Reactions Species

t	BS	rB	rf	rfB
20.147306	12.80908	3.59546	1.40454	3.59546
20.469109	12.808917	3.5955417	1.4044583	3.5955417
20.790912	12.808773	3.5956133	1.4043867	3.5956133
21.112716	12.808648	3.595676	1.404324	3.595676
21.434519	12.808538	3.595731	1.404269	3.595731
21.756322	12.808442	3.595779	1.404221	3.595779
22.078125	12.808358	3.5958212	1.4041788	3.5958212
22.399928	12.808284	3.595858	1.404142	3.595858
22.721731	12.808219	3.5958903	1.4041097	3.5958903
23.043534	12.808163	3.5959186	1.4040814	3.5959186
23.365337	12.808113	3.5959434	1.4040566	3.5959434
23.68714	12.80807	3.5959651	1.4040349	3.5959651
24.008943	12.808032	3.5959841	1.4040159	3.5959841
24.330746	12.807999	3.5960007	1.4039993	3.5960007
24.652549	12.807969	3.5960153	1.4039847	3.5960153
24.974352	12.807944	3.596028	1.403972	3.596028
25.296156	12.807922	3.5960392	1.4039608	3.5960392
25.78				
26.27				
26.76				
27.26				
27.75				
28.242627	12.807811	3.5960946	1.4039054	3.5960946
28.733706	12.807802	3.5960989	1.4039011	3.5960989
29.224785	12.807795	3.5961024	1.4038976	3.5961024
29.715863	12.80779	3.5961052	1.4038948	3.5961052
30	12.807787	3.5961066	1.4038934	3.5961066

Press "Ctrl" on your keyboard and click the final concentrations for "BS", "rB", "rf" and "rfB". Right click "Copy".

CONNECTED (ACowan) 118.5MB 229.1MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
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Geometry Specifications Protocols Simulations

Species Reactions

Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant
r	Nuc	<input type="checkbox"/>	5.0	<input type="checkbox"/>	10.0
rf	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	
rB	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	
BS	Nuc	<input type="checkbox"/>	20.0	<input type="checkbox"/>	
rfB	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	
Laser	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	

Copy
Copy All
Paste
Paste All
Specify Column Value for Selected Row(s)
Clamped
Initial Condition
Well Mixed
Diffusion Constant

Click "Spatial" > "Specifications" > "Species".

Click on the first cell in the Initial Condition column. Right click "Paste All".

CONNECTED (tanyamiller1221) 71.3MB / 102.6MB

BIOMODEL: Tutorial_FRAPbinding (Thu Jul 23 16:23:09 EDT 2015) -- VCell 5.3 (build 9)

File View Server Tools Help

Applications (2)

- Compartmental
 - Geometry
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VCell DB BioModels.net Path...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (7)
 - Shared BioModels (4)
 - ACowan : Tutorial_FRAPbind
 - Access[VCellSupport, thom...
 - ACowan : Tutorial_MultiApp...
 - astfh234 : new stuff
 - astfh234 : Rule Based
 - Public BioModels (521)
 - Tutorials (5)
 - Education (33)

Species Reactions

Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant
r_nucleus	nucleus	<input type="checkbox"/>	5.0	<input type="checkbox"/>	10.0
rf_nucleus	nucleus	<input type="checkbox"/>	1.4038933566697134	<input type="checkbox"/>	10.0
rB_nucleus	nucleus	<input type="checkbox"/>	3.5961066433302924	<input type="checkbox"/>	0.0
BS_nucleus	nucleus	<input type="checkbox"/>	12.807786713339414	<input type="checkbox"/>	0.0
rfb_nucleus	nucleus	<input type="checkbox"/>	3.5961066433302924	<input type="checkbox"/>	0.0
Laser_nud...	nucleus	<input type="checkbox"/>	$(x > -2.0) \&\& (x < 2.0) \&\& (y > -2.0) \&\& (y < 2.0)$	<input type="checkbox"/>	0.0

Object Properties

Description	Parameter	Expression	Units
initial concentration for Laser_nucleus	initConc	$((x > -2.0) \&\& (x < 2.0) \&\& (y > -2.0) \&\& (y < 2.0))$	μM
diffusion constant for Laser_nucleus	diff	0.0	$\mu\text{m}^2 \cdot \text{s}^{-1}$

CONNECTED (tanyamiller1221)

78.4MB / 130.5MB

In the "Laser" row and "Initial Condition" column, type $((x > -2.0) \&\& (x < 2.0) \&\& (y > -2.0) \&\& (y < 2.0))$. Press "Enter" on your keyboard to finalize.

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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Geometry Specifications Protocols Simulations

Species Reactions

Name	Type	Enabled	Fast
RAN binding	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
RAN_FITC binding	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
bleaching 1	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
bleaching 2	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Click "Reactions".

Click on all boxes in the Enabled column so that they are checked off if they are not already.

VCCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

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CONNECTED (tanyamiller1221) 46.7MB / 88.1MB

Click "Simulations" > edit simulation icon.

Simulations

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	1.0	keep every 1	Runge-Kutta-Fehlberg	not saved	no

Error

Application geometry does not match Simulation geometry
Update Math before editing

OK

If an error message appears, click "OK".

CONNECTED (tanyamiller1221) 67.3MB / 88.1MB

The screenshot shows the VCell 5.3 software interface. On the left is a tree view with categories like Reaction Diagram, Applications, and Parameters. The 'Simulations' icon in the top toolbar is highlighted with a red box and a yellow callout box. Below it, the 'Simulations' tab is active, showing a table with one simulation entry. An error dialog box is overlaid on the main window, with its 'OK' button highlighted by a red box and a yellow callout box. The status bar at the bottom shows connection and memory usage information.

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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Geometry Specifications Protocols Simulations

Simulations Output Function **Generated Math**

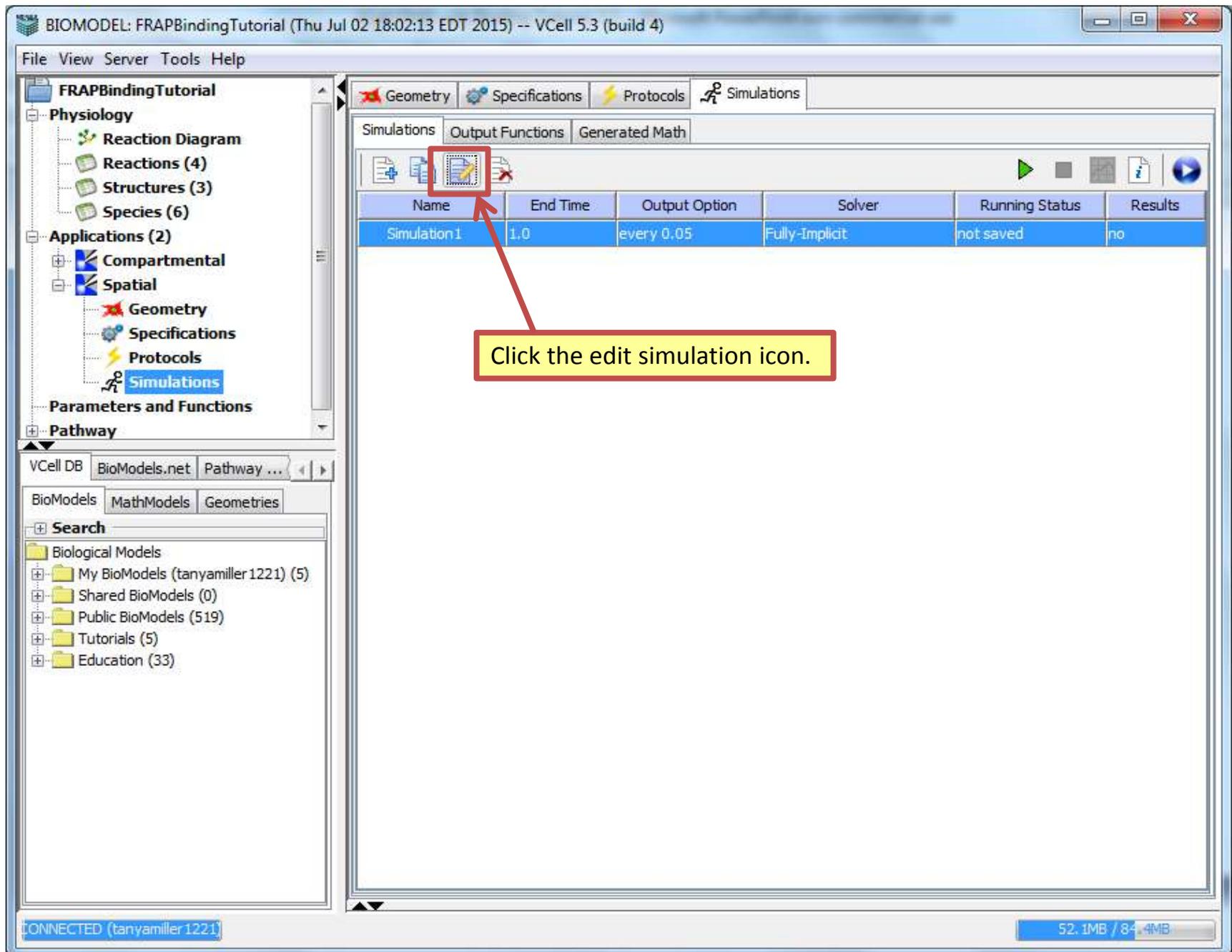
Choose View: Math Equations Math Description Language **Refresh Math** Create Math Model

- math description
 - constants
 - functions
 - volume domains

Show parameter: name value

CONNECTED (tanyamiller1221) 45.3MB 91.8MB

To fix the error message,
click "Generated Math" > "Refresh Math".



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	1.0	every 0.05	Fully-Implicit	not saved	no

CONNECTED (tanyamiller1221) 52.1MB / 84.4MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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Edit: Simulation1

Parameters Mesh

Click "Mesh".

Mesh Size

Geometry Size (um) (22.0, 22.0)

Mesh Size (elements) Lock aspect ratio

X 51

Y 51

Total Size (elements) 51 x 51 = 2601

Spatial Step (um) Δx 0.44

Δy 0.44

Click "Lock aspect ratio" if it is not checked off already. Type in "51" next to Mesh Size for X.

OK Cancel

CONNECTED (tanyamiller1221) 37.4M B / 89.7MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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Edit: Simulation1

Parameters Mesh **Solver**

Click "Solver".

Choose solver algorithm and fine-tune time conditions:

Integrator: Fully-Implicit Finite Volume, Regular Grid (Variable Time Step) ?

General

Time Bounds: Starting 0.0, Ending 50.0

Time Step: Minimum, Default, Maximum

Error Tolerance: Absolute 1.0E-9

Type "50.0" next to Ending, under Time Bounds.

Output Options

Keep Every [] time samples and at most [] time samples

Output Interval 0.5 secs

Type "0.5" next to Output Interval.

Miscellaneous

Click "OK".

OK Cancel

CONNECTED (tanyamiller1221) 65.8MB / 89.7MB

BIOMODEL: FRAPBindingTutorial (Thu Jul 02 18:02:13 EDT 2015) -- VCell 5.3 (build 4)

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VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

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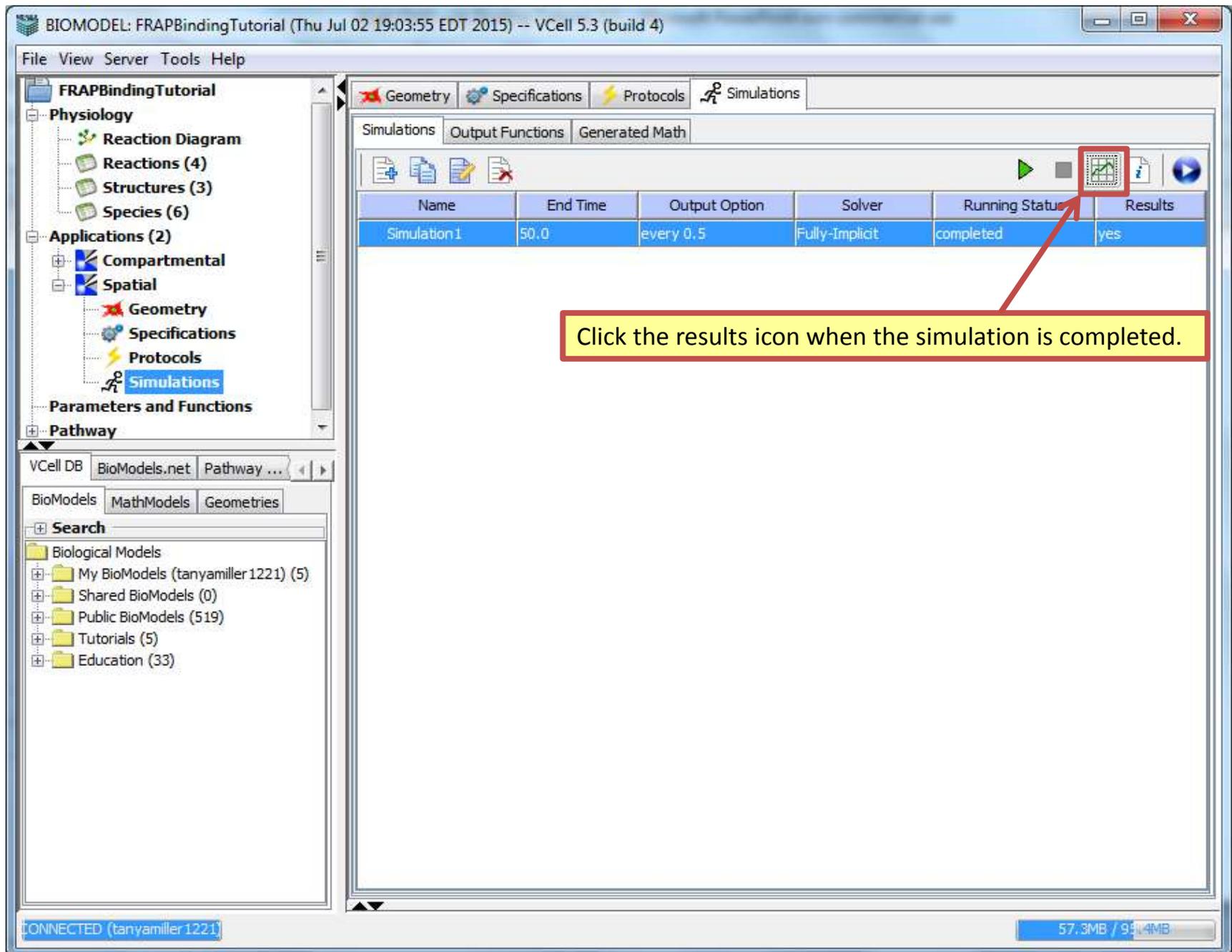
Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	50.0	every 0.5	Fully-Implicit	not saved	no

Click the green play icon to run and save the simulation.

CONNECTED (tanyamiller1221) 38.3MB / 85.5MB



BIOMODEL: FRAPBindingTutorial (Thu Jul 02 19:03:55 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

FRAPBindingTutorial

- Physiology
 - Reaction Diagram
 - Reactions (4)
 - Structures (3)
 - Species (6)
- Applications (2)
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VCell DB BioModels.net Pathway ...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (5)
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	50.0	every 0.5	Fully-Implicit	completed	yes

CONNECTED (tanyamiller1221) 57.3MB / 99.4MB

BIOMODEL: Tutorial_FRAPbinding (Wed Aug 12 09:40:56 EDT 2015) -- VCell 5.3 (build 9)

simulation results for FRAP binding

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data

Time: 39.5

Slice View

To change the time frame being viewed, type in a value under "Time" or hold down and drag the slider under "Time".

0

50

1.2892572668295028

Min: 1.284306269805525

1.284306269805525

Color

BM AM NN ND NR

Gray

BlueRed

All Variables

- BS
- J_bleaching1
- J_bleaching2
- J_RAN_binding
- J_RAN_FITC_binding
- Laser
- Laser_init_uM
- r
- rB
- rF
- rFB

Plot

ROI

CONNECTED (A)

233.6MB

BIOMODEL: Tutorial_FRAPbinding (Wed Aug 12 09:40:56 EDT 2015) -- VCell 5.3 (build 9)

simulation results for FRAP binding

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data

Time: 39.5

Slice View

Data Range (Min-Max):
 Auto (current time)
Max: 1.2892572668295028
Min: 1.284306269805525

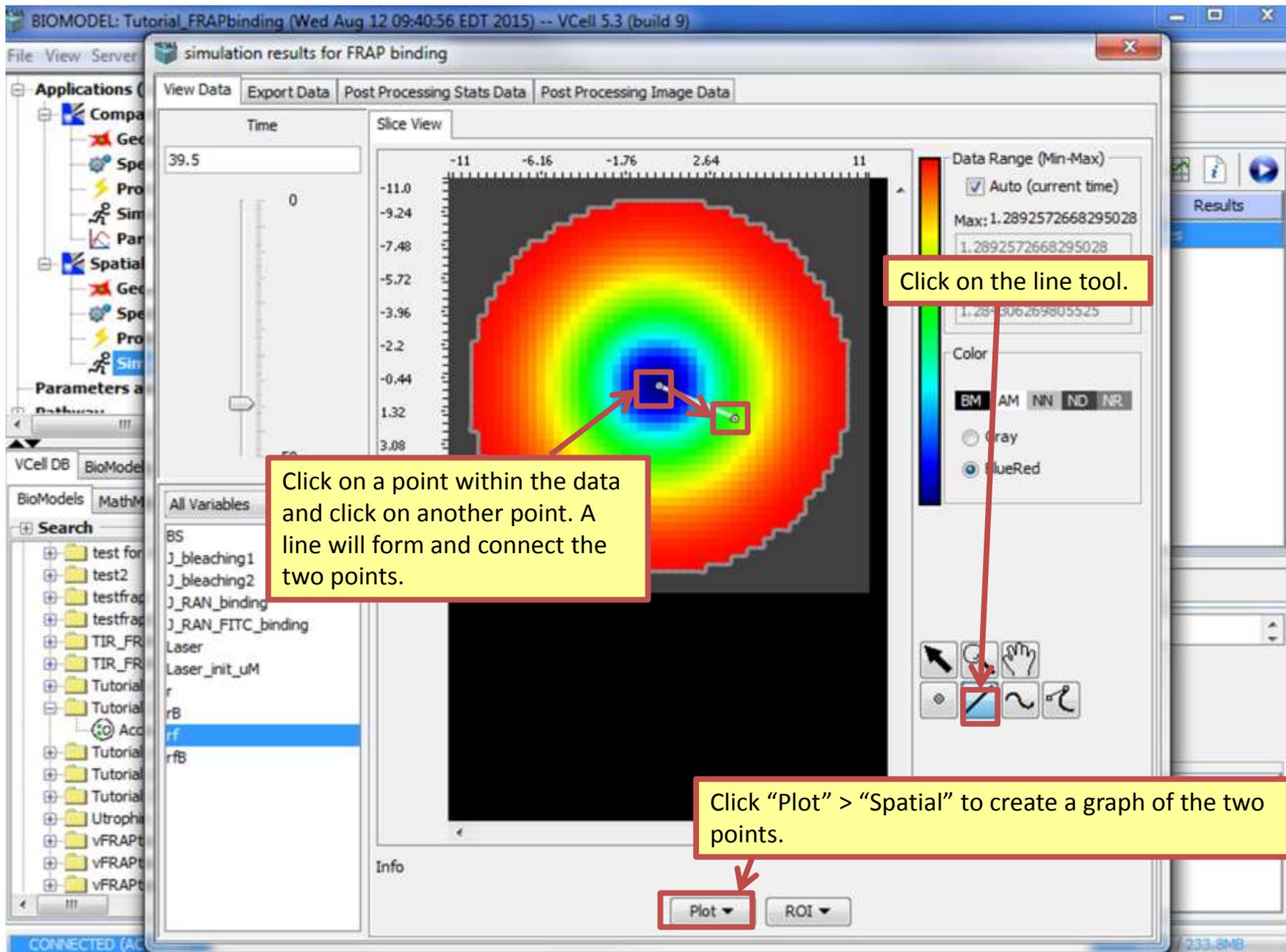
Color:
 Gray
 BlueRed

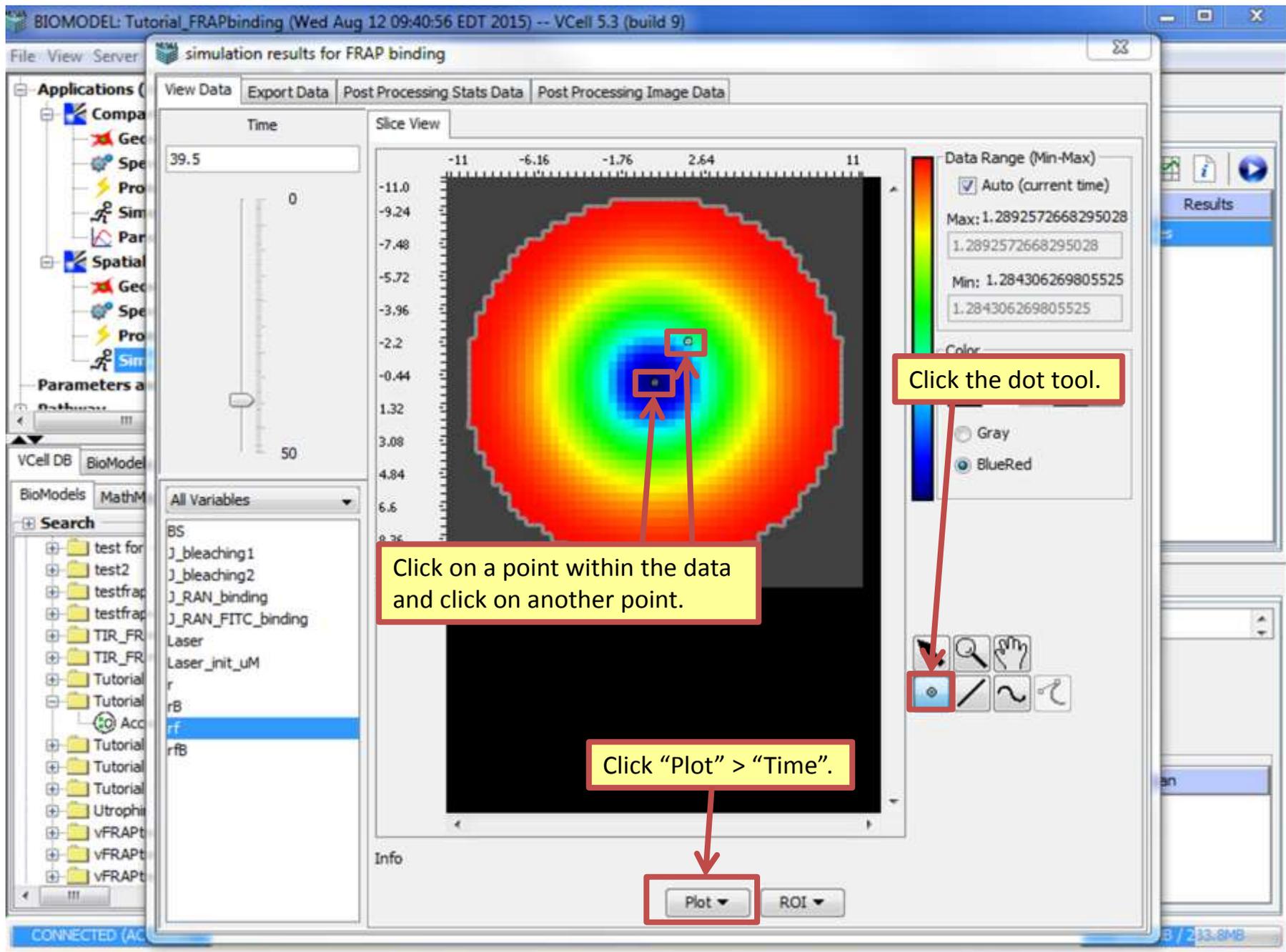
Click on either "Gray" or "BlueRed" to change the color gradient.

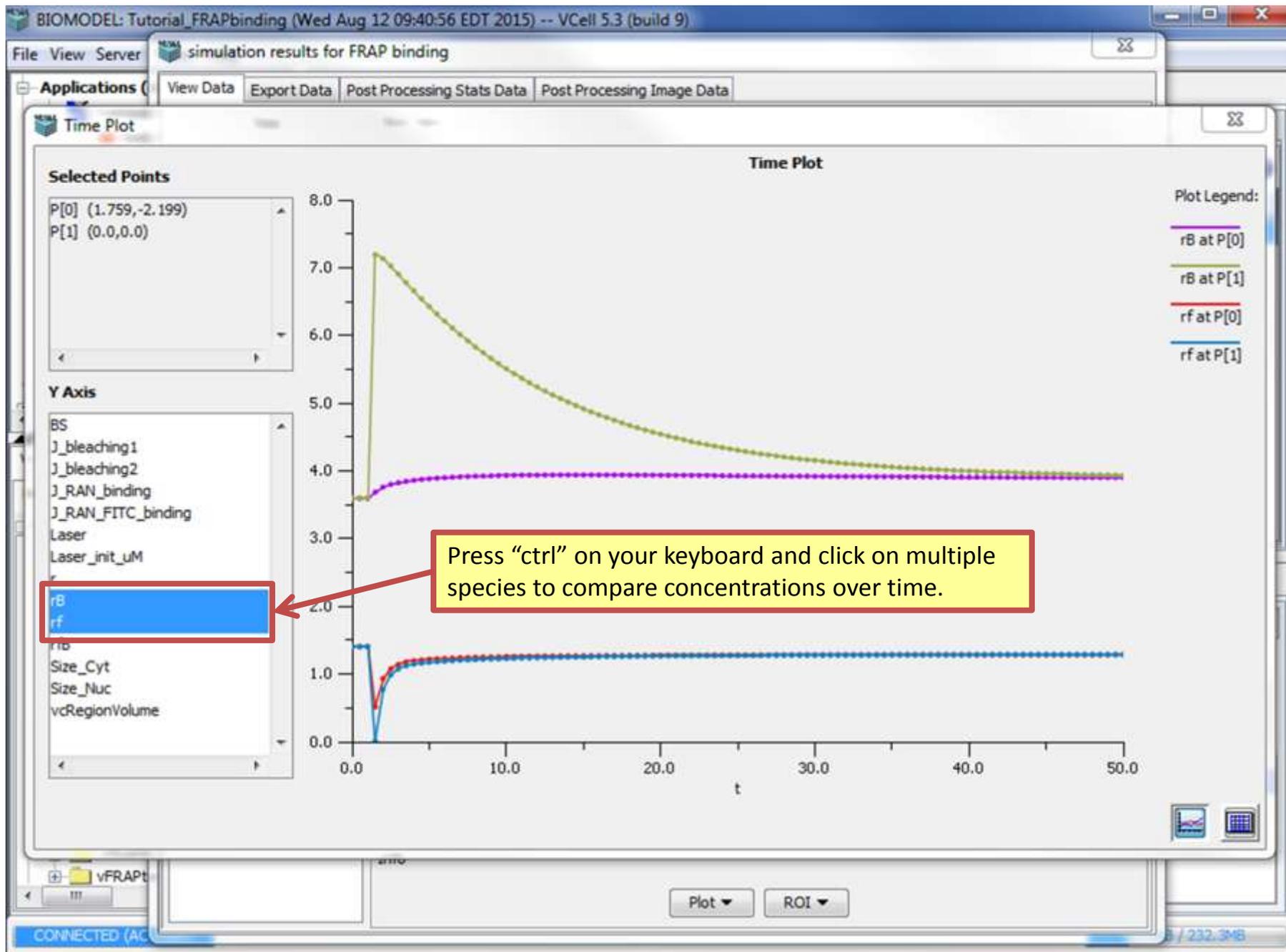
Info

Plot | ROI

CONNECTED (AC) / 233.8MB







Next VCell tutorial: PIP2 to IP3