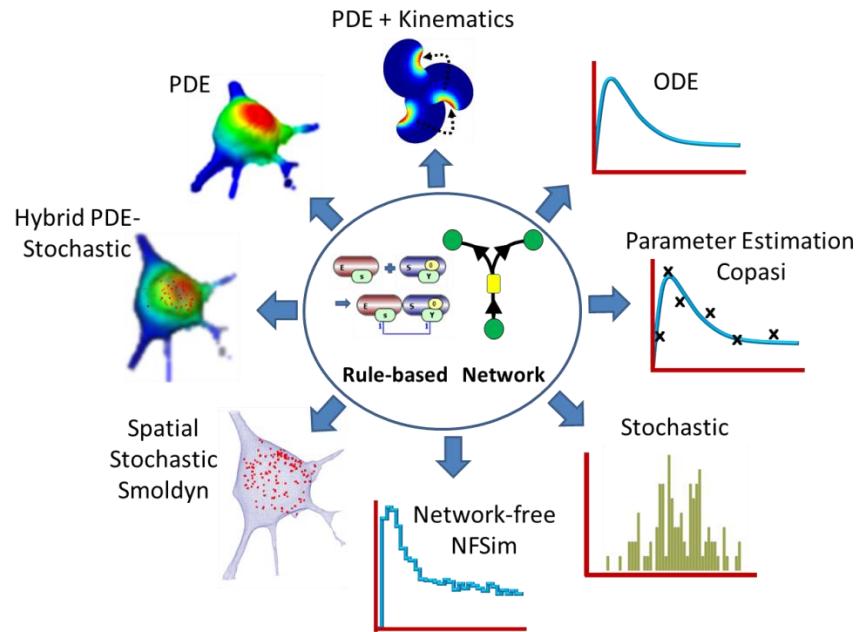


# VCell

A modeling environment for the simulation of cellular events, where you can download at [vcell.org](http://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

## PH-GFP binding to PIP2 and IP3

*Objective: Create a biomodel and 3D spatial (PDE) application to simulate pleckstrin homology domain (PH-GFP) reporter for conversion of  $PIP_2$  to  $IP_3$ .*

# In this tutorial you will:

- Create a BioModel with reactions involving membrane and volume species.
- Create a compartmental (ODE) application that uses events to include time-dependent triggers.
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a 3D geometry
- Define initial concentrations that are non-uniform in space and create timed events in spatial models using Boolean expressions
- Create output functions for more complex analysis of simulation results, e.g. to sum all fluorescent species in a compartment.

BioModel1

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (1)
- Species (0)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

+ Pathway  
Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

+ My BioModels

- + multiapp tutorial
- + PH-GFP

Private Fri May 03 13:54:20 EDT 2019

+ Public BioModels (688)  
+ Tutorials (9)  
+ Education (33)  
+ Published BioModels (171)

Reaction Diagram Reactions Structures Species Molecules Observables



c0

You can start with an empty BioModel, or you can re-open a saved model. Click on the folder that the model was saved in and double-click on the model.

Delete Pathway Links ▾

Search

Pathway Links ▾

Search

Select Properties Annotations Problems (0 Errors, 0 Warnings)

Database File Info

Application Provenance

BioModel1  
Physiology  
Reaction Diagram  
Reactions (0)  
Structures (1)  
Species (0)  
Molecules (0)  
Observables (0)  
Applications (0)  
Parameters, Functions and Units  
Pathway  
Scripting

VCell DB BMDB Pathway Comm Sabio  
BioModels MathModels Geometries  
Search  
Biological Models  
My BioModels  
multiapp tutorial  
PH-GFP  
Private Fri May 03 13:54:20 EDT 2019  
Shared BioModels (0)  
Public BioModels (688)  
Tutorials (9)  
Education (33)  
Published BioModels (171)

## Creating a new BioModel

Select the compartment tool.  
Click the dotted black lines so they turn green and select “Add Membrane” from the dropdown menu.

Add Compartment  
Add Membrane

**BioModel1**  
Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

- Applications (0)
- Parameters, Functions and Units
- Pathway
- Scripting

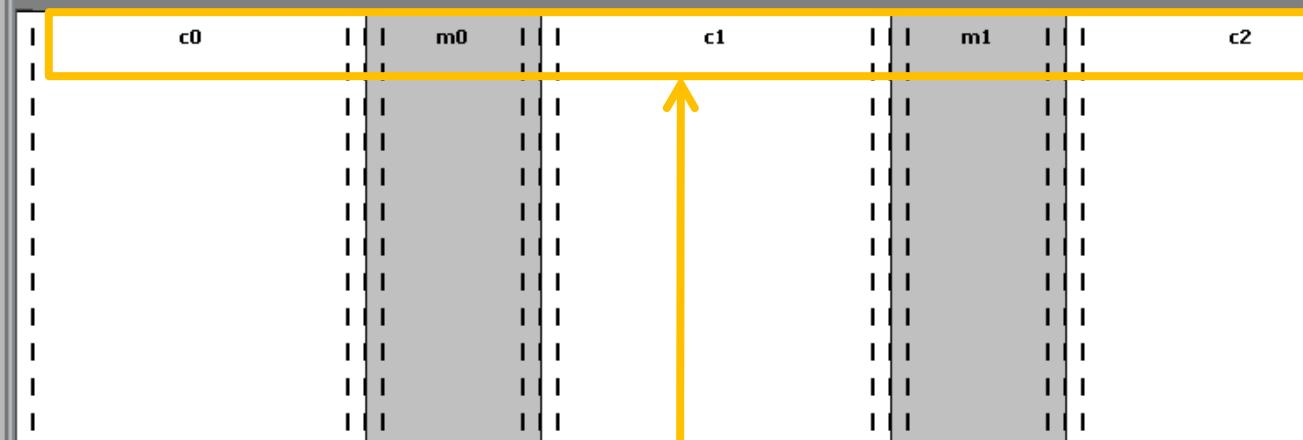
VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

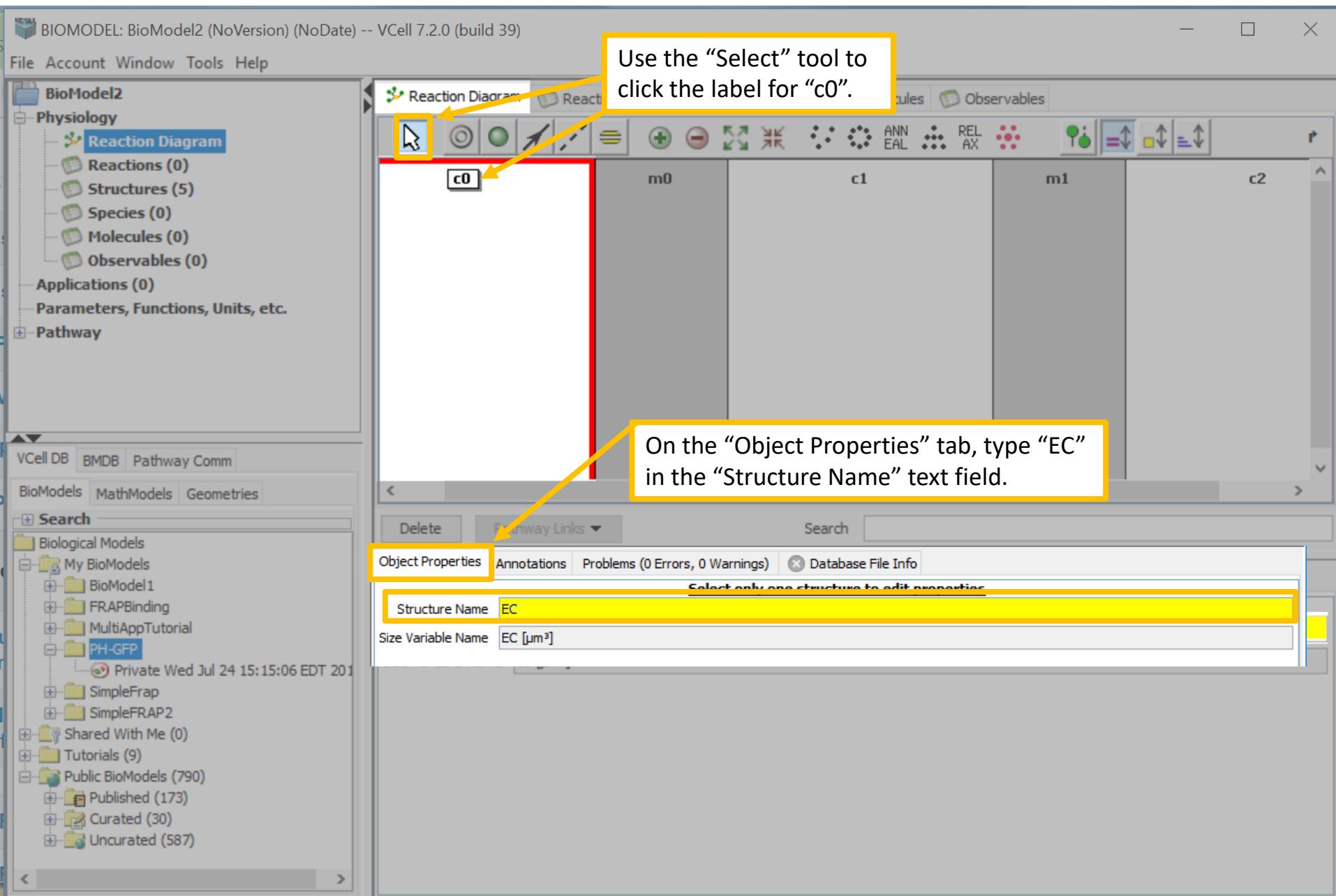
## + Search

- Biological Models
- + My BioModels
  - + multiapp tutorial
  - + PH-GFP
    - Private Fri May 03 13:54:20 EDT 2019
- + Shared BioModels (0)
- + Public BioModels (688)
- + Tutorials (9)
- + Education (33)
- + Published BioModels (171)

Reaction Diagram Reactions Structures Species Molecules Observables



Continue creating compartments and membranes until from left to right your diagram reads "c0", "m0", "c1", "m1" and "c2".  
The structures will be renamed in the next slides.



BioModel1

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- multiapp tutorial
- PH-GFP

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Public BioModels (688)

Tutorials (9)

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Reaction Diagram Reactions Structures Species Molecules Observables

EC m0 c1 m1 c2

Select the Annotations tab, and enter "Extracellular" under the "Text Annotations" heading.

Annotations Problems (0 Errors, 0 Warnings) Database File Info

User defined cross-references.

Provider PubMed Add...

Text Annotations

Extracellular

CONNECTED 134.7MB / 278.4MB

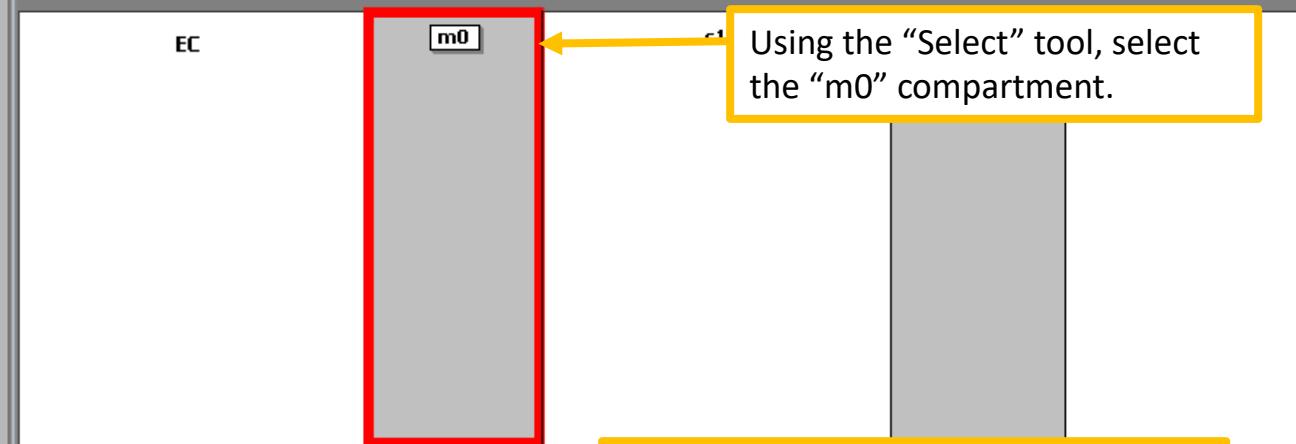
The screenshot shows the VCell 7.1.0 software interface. On the left, there's a navigation tree with sections like Physiology, Applications, and Pathway. Below that is a search bar and a list of shared and public bio models. The main workspace shows a reaction diagram with species EC, m0, c1, m1, and c2. A red box highlights the reaction row for EC. On the right, there's an 'Annotations' tab in the object properties panel, which is highlighted with a yellow box. A callout bubble with a yellow border points to this tab with the instruction: 'Select the Annotations tab, and enter "Extracellular" under the "Text Annotations" heading.' Below the tab, there's a 'Text Annotations' section containing the word 'Extracellular'. The bottom status bar indicates the system is connected and shows memory usage.

**BioModel1****Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

Applications (0)  
Parameters, Functions and Units

+ Pathway  
Scripting

**Reaction Diagram**   **Reactions**   **Structures**   **Species**   **Molecules**   **Observables**

Using the “Select” tool, select the “m0” compartment.

Select the Object Properties tab.  
Type “PM” (Plasma Membrane) in the “Structure Name” text field.

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

Select only one structure to edit properties

Structure Name	PM
Size Variable Name	PM [ $\mu\text{m}^2$ ]
Voltage Variable Name	Voltage_PM [mV]
Positive (inside feature)	
Negative (outside feature)	

**Electrophysiology**

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

PH-GFP

## ... Physiology

-  Reaction Diagram
  -  Reactions (0)
  -  Structures (5)
  -  Species (0)
  -  Molecules (0)
  -  Observables (0)

## Applications (0)

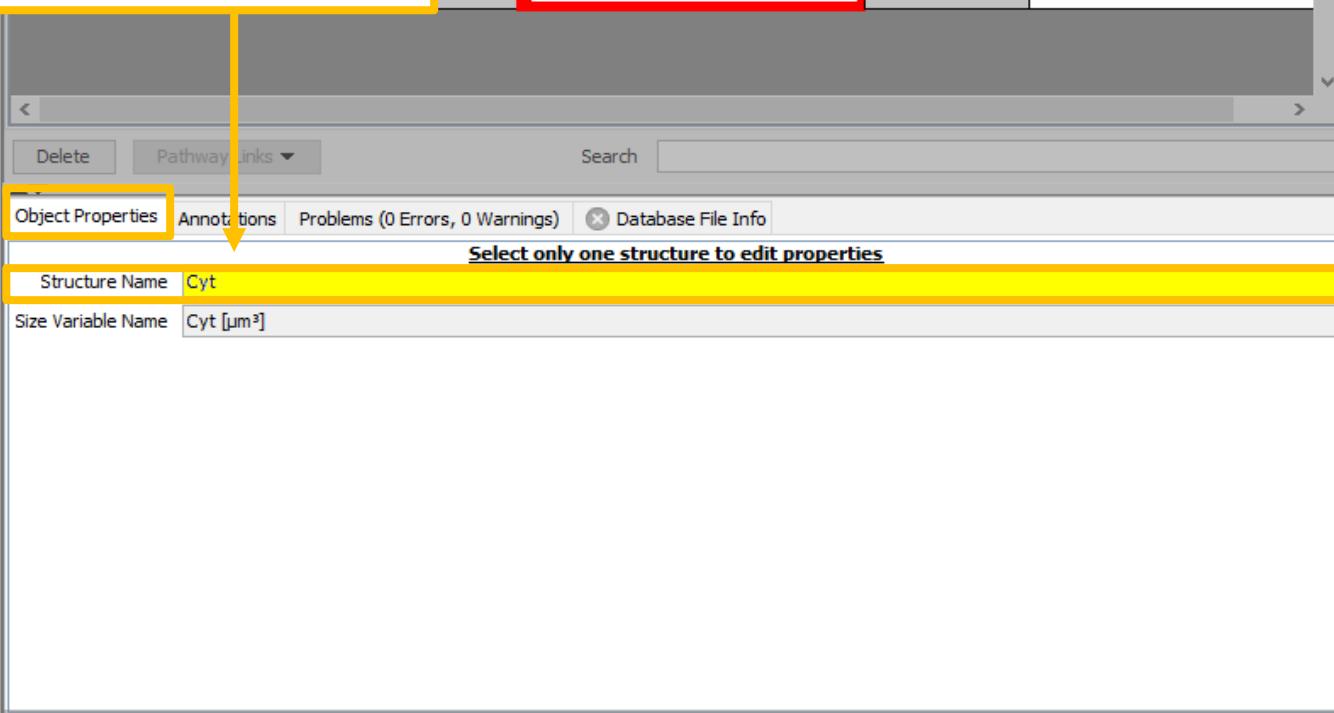
## Parameters, Functions and Units

Pathway

## ..... Scripting

Select the “c1” compartment

On the “Object Properties” tab, type “Cyt” (Cytosol) in the “Structure Name” text field.



**PH-GFP****Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

- Applications (0)

- Parameters, Functions and Units

- Pathway

- Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
  - My BioModels
    - BioModelPH-GFP
    - multiapp tutorial
    - PH-GFP
      - Private Tue May 07 19:33:01 EDT 2019
  - Shared BioModels (0)
  - Public BioModels (689)
  - Tutorials (9)
  - Education (33)
  - Published BioModels (171)

Reaction Diagram    Reactions    Structures    Species    Molecules    Observables

EC    PM    Cyt    m1    c2

Select the “Annotations” tab and type “Cytosol”, in the “Text Annotations” text field.

Annotations

User defined cross-references.

Provider PubMed Add...

Text Annotations

Cytosol

PH-GFP

Physiology

- Reaction Diagram (selected)
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
  - BioModelPH-GFP
  - multiapp tutorial
  - PH-GFP
    - Private Tue May 07 19:33:01 EDT 2019
- Shared BioModels (0)
- Public BioModels (689)
- Tutorials (9)
- Education (33)
- Published BioModels (171)

Reaction Diagram Reactions Structures Species Molecules Observables

EC PM Cyt m1 c2

Select the “m1” compartment.

On the “Object Properties” tab, type type “NM” (Nuclear Membrane), in the “Structure Name” text field.

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

Select only one structure to edit properties

Structure Name NM

Size Variable Name NM [ $\mu\text{m}^2$ ]

Electrophysiology

Voltage Variable Name Voltage\_NM [mV]

Positive (inside feature)

Negative (outside feature)

membrane voltage: "Voltage\_NM" = voltage(inside (+) compartment) - voltage(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 -).

CONNECTED

118.1 MB / 335.5 MB

**PH-GFP**  
**Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

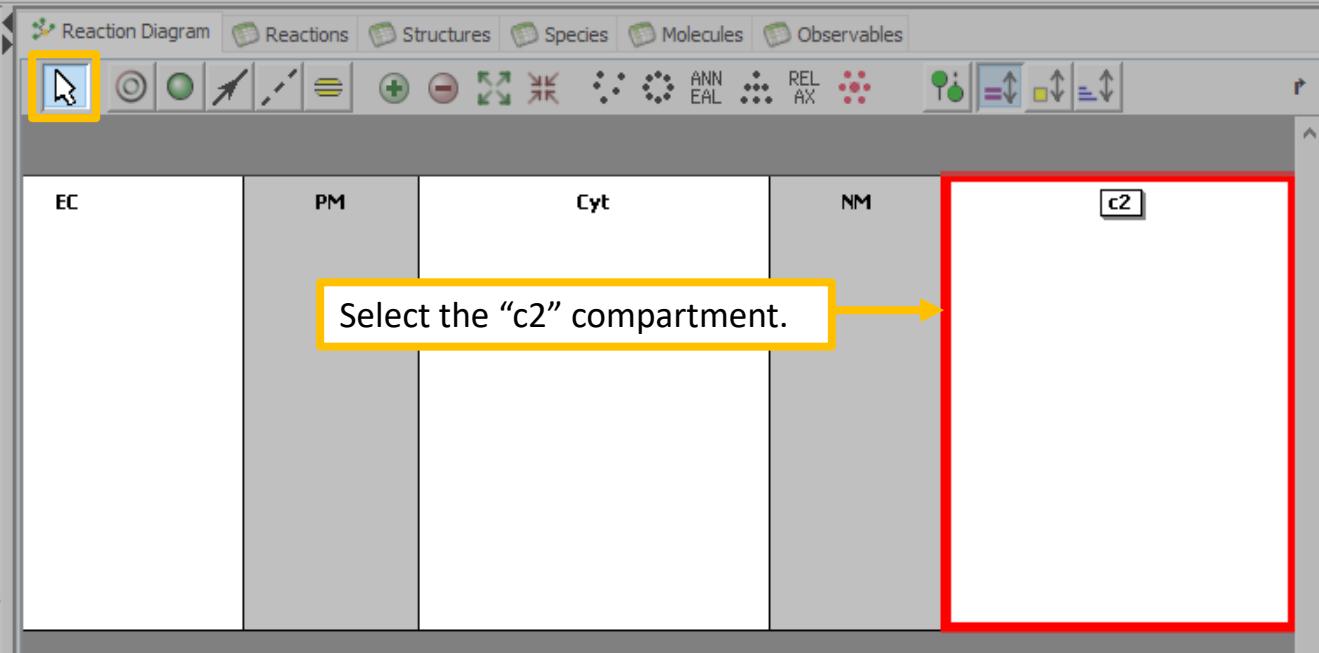
Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

## + Search

- Biological Models
- + My BioModels
  - + BioModelPH-GFP
  - + multiapp tutorial
  - + PH-GFP
    - Private Tue May 07 19:33:01 EDT 2019
- + Shared BioModels (0)
- + Public BioModels (689)
- + Tutorials (9)
- + Education (33)
- + Published BioModels (171)



On the Object Properties tab, type “Nuc” (Nucleus) in the “Structure Name” text field.

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

select only one structure to edit properties

Structure Name	Nuc
Size Variable Name	Nuc [ $\mu\text{m}^3$ ]

**PH-GFP**  
**Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (0)
- Molecules (0)
- Observables (0)

## Applications (0)

Parameters, Functions and Units

Pathway

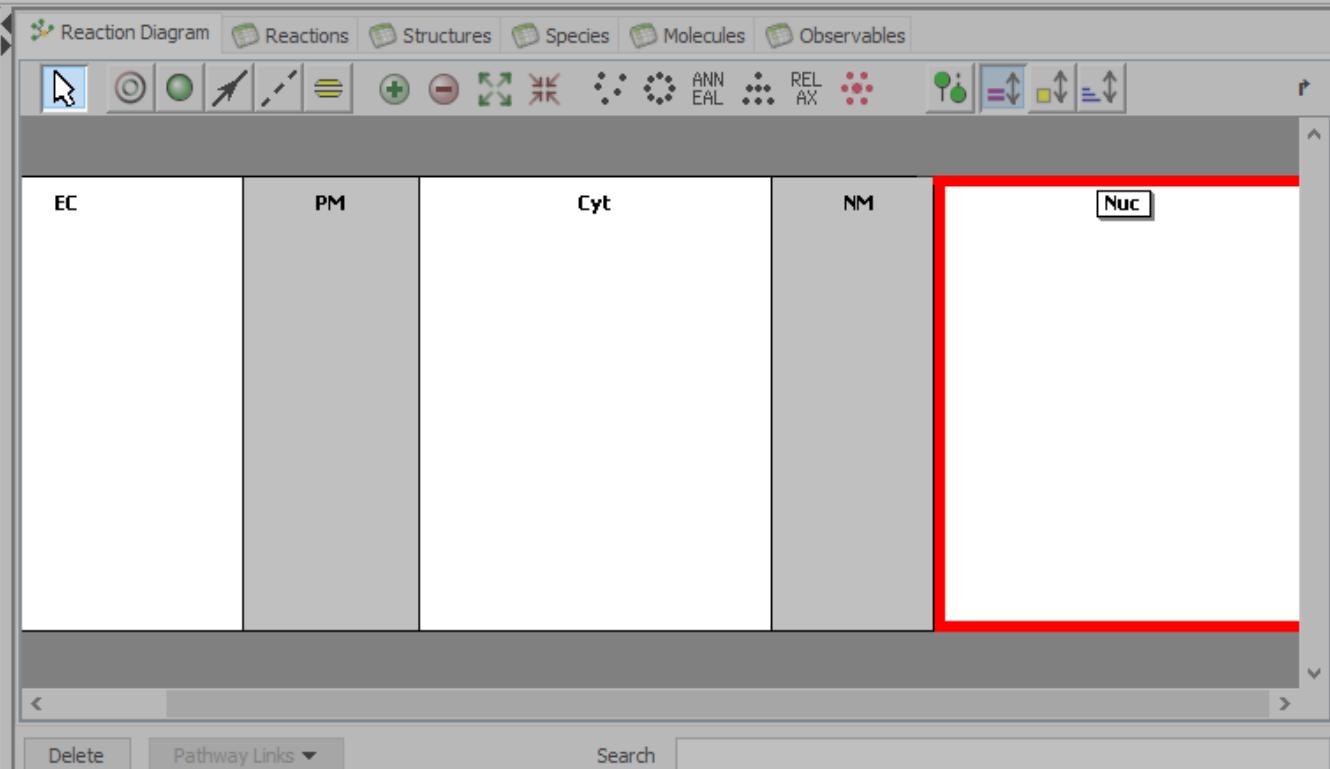
Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**+ Search**

- Biological Models
- My BioModels
  - + BioModelPH-GFP
  - + multiapp tutorial
  - + PH-GFP
    - Private Tue May 07 19:33:01 EDT 2019
- + Shared BioModels (0)
- + Public BioModels (689)
- + Tutorials (9)
- + Education (33)
- + Published BioModels (171)



Select the “Annotations” tab and type “Nucleus” in the “Text Annotations” text box.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (2)
- Molecules (0)
- Observables (0)

Click twice within the “PM” compartment to create two species.

Select the “Species” tool.

Reaction Diagram    Reactions    Structures    Species    Molecules    Observables

EC    PM    Cyt    NM    Nu

s0  
s1

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Tue May 07 17:17:33 EDT 2020
- Shared BioModels (0)
- Public BioModels (689)
- Tutorials (9)
- Education (33)
- Published BioModels (171)

Delete Pathway Links Search

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

Species Name: s1    Sbml Name:

Linked Pathway Object(s):

CONNECTED 114.5MB 227.5MB

The screenshot shows the VCell software interface for a model named "PH-GFP". The main workspace displays a reaction diagram with five compartments: EC, PM, Cyt, NM, and Nu. The PM compartment contains two green circular species labeled s0 and s1. A yellow box highlights the "Species" tool icon in the toolbar. Another yellow box highlights the "PM" compartment. A third yellow box highlights the "Species" section of the "Object Properties" panel, which shows the species name "s1". The left sidebar shows the model structure with "Species (2)" selected. The bottom status bar indicates "CONNECTED" and memory usage of "114.5MB / 227.5MB".

PH-GFP

Physiology

- Reaction Diagram (selected)
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway Scripting

Reaction Diagram

EC PM Cyt NM NL

s0 s1 s2 s3 s4 s5

Click four points within the “Cyt” compartment to create four species.

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

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

Species Name: s5 Sbml Name:

Linked Pathway Object(s):

CONNECTED 176.1MB / 227.5MB

The screenshot shows a VCell 7.1.0 interface with a central workspace for creating and editing biological models. On the left, a tree view displays the model structure under 'PH-GFP' in the 'Physiology' section. The main workspace shows a reaction diagram with five compartments: EC, PM, Cyt, NM, and NL. The Cyt compartment is highlighted with a yellow border and contains five green circular species labeled s0, s1, s2, s3, and s4. A sixth green circular species labeled s5 is located outside the Cyt compartment. A callout box with a yellow border and an arrow points from the text 'Click four points within the “Cyt” compartment to create four species.' to the Cyt compartment. The top menu bar includes File, Server, Window, Tools, and Help. The bottom status bar indicates 'CONNECTED' and memory usage of '176.1MB / 227.5MB'.

## PH-GFP

## Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

## Applications (0)

## Parameters, Functions and Units

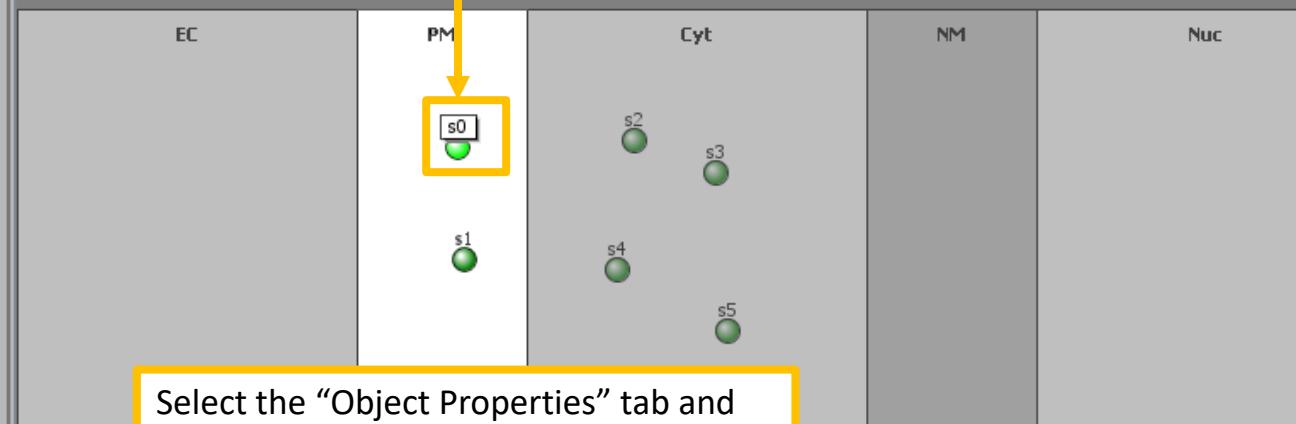
## Pathway

## Scripting

Reaction Diagram    Reactions    Structures    Species    Molecules    Observables



Use the “Select” tool to click “s0”.



Select the “Object Properties” tab and type “PIP2\_PM” in the “Species Name” text field.

Delete

Pathway Links ▾

Search

Object Properties

Annotations

Problems (0 Errors, 0 Warnings)

Database File Info

Species Name PIP2\_PM

Sbml Name

Linked Pathway Object(s)



PH-GFP

Physiology

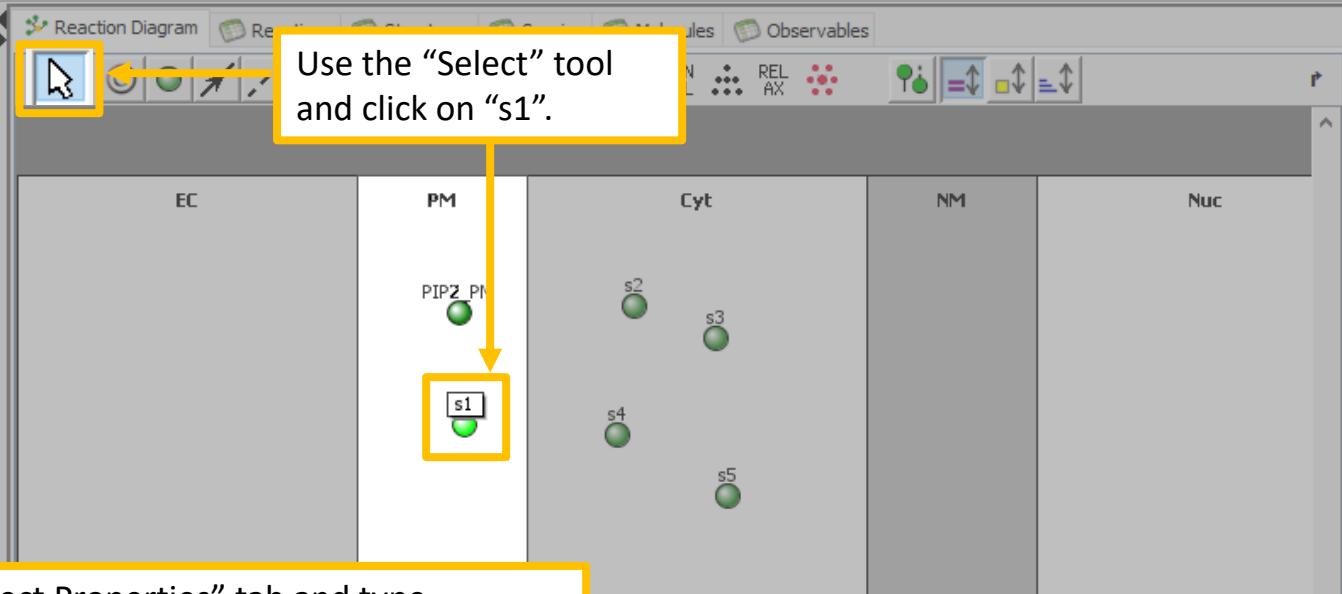
- Reaction Diagram (selected)
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

+ Pathway

Scripting



Select the “Object Properties” tab and type  
“PIP2\_PHGFP\_PM” in the “Species Name” text field.

Object Properties

Species Name PIP2\_PHGFP\_PM

Linked Pathway Object(s)



PH-GFP

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

Reaction Diagram

Molecules Observables

ANN EAL REL AX

EC PM Cyt NM NL

PIP2\_PM PIP2\_PHGFP\_PM s2 s3 s4 s5

VCell DB BMDB Pathway Comm Sabin

BioModels MathModels Geomet

Search

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

Species Name IP3\_Cyt Sbml Name

Linked Pathway Object(s)

Private Wed May 08 16:42:38 EDT 2019

Shared BioModels (0)

Public BioModels (690)

Tutorials (9)

Education (33)

Published BioModels (171)

CONNECTED

128.9MB / 27.1MB

Use the “Select” tool and click on “s2”.

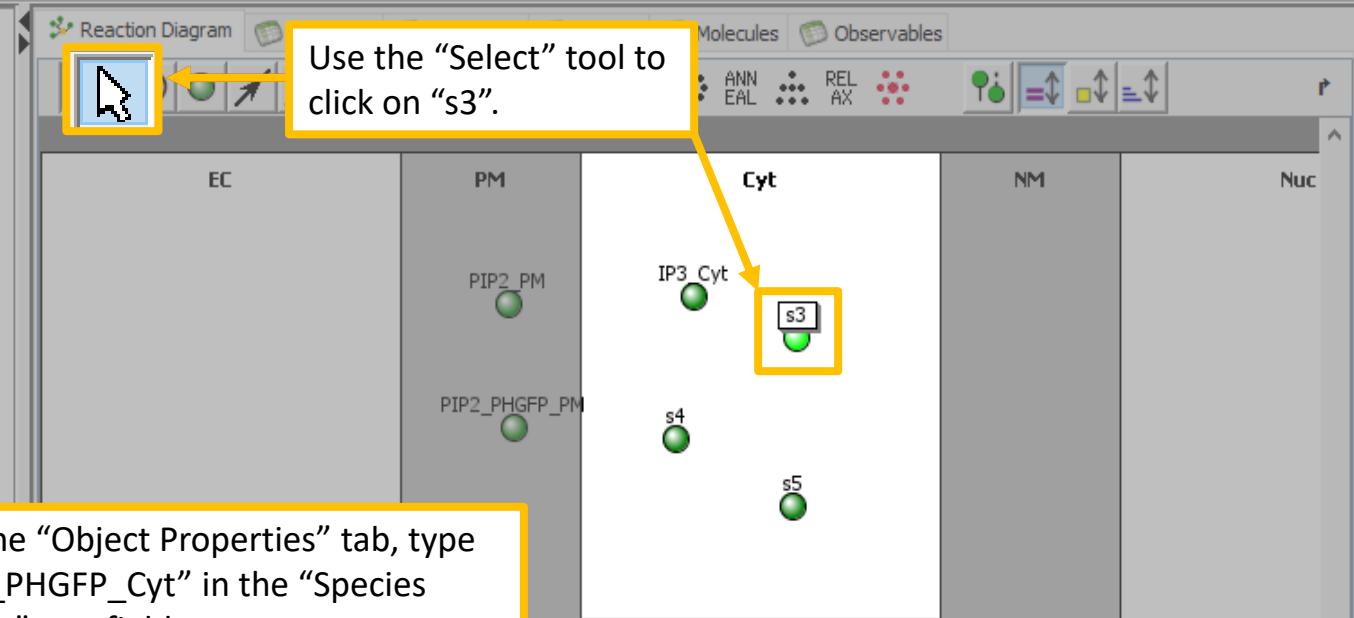
On the “Object Properties” tab, type “IP3\_Cyt” in the “Species Name” text field.

The screenshot shows the VCell 7.1.0 software interface. On the left, there's a navigation tree for the 'PH-GFP' model under 'Physiology'. The 'Reaction Diagram' node is selected. The main workspace shows a reaction diagram with compartments: EC, PM, Cyt, NM, and NL. In the Cyt compartment, a species labeled 's2' is highlighted with a yellow box and arrow. Below the workspace is a toolbar with various icons. At the bottom, there's a search bar and a list of public biomodels. A large yellow box highlights the 'Object Properties' tab in the bottom navigation bar, and another yellow box highlights the 'Species Name' input field, which contains 'IP3\_Cyt'. The status bar at the bottom indicates 'CONNECTED' and memory usage '128.9MB / 27.1MB'.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway
- Scripting



VCell DB BMDB Pathway Comm Sabid

BioModels MathModels Geometries

Search

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

Species Name IP3\_PHGFP\_Cyt Sbml Name

Linked Pathway Object(s)

Delete Pathway Links Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Thu May 09 17:08:47 EDT 2019
- Shared BioModels (0)
- Public BioModels (689)
- Tutorials (9)
- Education (33)
- Published BioModels (171)

CONNECTED 126.3MB / 123.9MB

PH-GFP

Physiology

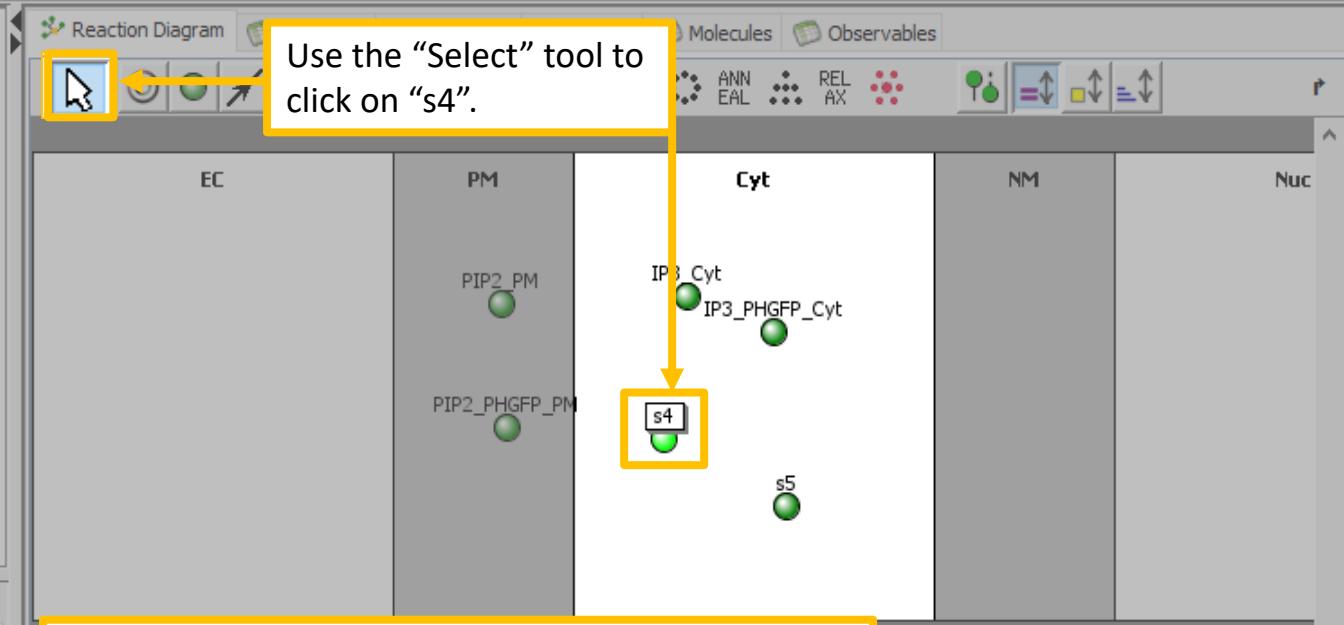
- Reaction Diagram (selected)
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting



VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Thu May 09 17:08:47 EDT 2020
- Shared BioModels (0)
- Public BioModels (689)
- Tutorials (9)
- Education (33)
- Published BioModels (171)

On the “Object Properties” tab, type “PH\_GFP\_Cyt” in the “Species Name” text field.

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

Species Name PH\_GFP\_Cyt Sbml Name

Linked Pathway Object(s)

+

-

Use the “Select” tool to click on “s4”.

On the “Object Properties” tab, type “PH\_GFP\_Cyt” in the “Species Name” text field.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

Reaction Diagram

Molecules Observables

EC PM Cyt NM Nuc

PIP2\_PM  
PIP2\_PHGFP\_PM  
IP3\_Cyt  
P3\_PHGFP\_Cyt  
PH\_GFP\_Cyt  
s5

Use the “Select” tool to click on “s5”.

On the “Object Properties” tab, type “Stim” in the “Species Name” text field.

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- multiapp tutorial
- PH-GFP
  - Private Thu May 09 17:08:47 EDT 2020

Shared BioModels (0)

Public BioModels (689)

Tutorials (9)

Education (33)

Published BioModels (171)

Delete Pathway Links Search

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

Species Name Stim Sbml Name

Linked Pathway Object(s)

CONNECTED 112.6MB 220.7MB

The screenshot shows the VCell 7.1.0 software interface for a model named 'PH-GFP'. The left sidebar contains a tree view of the model's components under 'Physiology' and 'Pathway'. The main workspace displays a reaction diagram with compartments EC, PM, Cyt, NM, and Nuc. Species are represented by green spheres: PIP2\_PM, PIP2\_PHGFP\_PM, IP3\_Cyt, P3\_PHGFP\_Cyt, PH\_GFP\_Cyt, and s5. A yellow box highlights the 'Reaction Diagram' button in the toolbar at the top. A callout bubble with a yellow border and arrow points to the 's5' species in the Cyt compartment, with the text 'Use the “Select” tool to click on “s5”.' Another callout bubble with a yellow border and arrow points to the 'Species Name' field in the 'Object Properties' tab, with the text 'On the “Object Properties” tab, type “Stim” in the “Species Name” text field.' The bottom right corner shows memory usage: 112.6MB / 220.7MB.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

Reaction Diagram    Reactions    Structures    Species    Molecules    Observables

ANN EAL    REL AX

EC    PM    Cyt    NM    Nuc

PIP2\_PM  
PIP2\_PHGFP\_PM  
IP3\_PHGFP\_Cyt  
IP3\_Cyt  
Stim  
PH\_GFP\_Cyt

Click the “Select” tool.

Arrange each species in membrane “PM” and compartment “Cyt”, such that they appear as seen above.

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Object Properties

Delete Pathway Links Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Thu May 09 17:08:47 EDT 20
- Shared BioModels (0)
- Public BioModels (689)
- Tutorials (9)
- Education (33)
- Published BioModels (171)

CONNECTED

142.5MB / 207 1MB

The screenshot shows the VCell 7.1.0 software interface with the following details:

- Toolbar:** Includes tools for Reaction Diagram, Reactions, Structures, Species, Molecules, Observables, ANN EAL, REL AX, and selection tools.
- Compartments:** EC, PM, Cyt, NM, and Nuc.
- Species in PM:** PIP2\_PM, PIP2\_PHGFP\_PM.
- Species in Cyt:** Stim, IP3\_PHGFP\_Cyt, IP3\_Cyt, PH\_GFP\_Cyt.
- Annotations:**
  - A yellow box surrounds the PM and Cyt compartments with the text "Click the ‘Select’ tool." and an arrow pointing to the select tool icon.
  - A yellow box surrounds the PM and Cyt compartments with the text "Arrange each species in membrane ‘PM’ and compartment ‘Cyt’, such that they appear as seen above." and an arrow pointing to the species in the compartments.
- Bottom Left:** Shows a file tree under "Biological Models" with sections like My BioModels, Shared BioModels, Public BioModels, Tutorials, Education, and Published BioModels.
- Bottom Right:** Shows memory usage: 142.5MB / 207 1MB.

**PH-GFP**

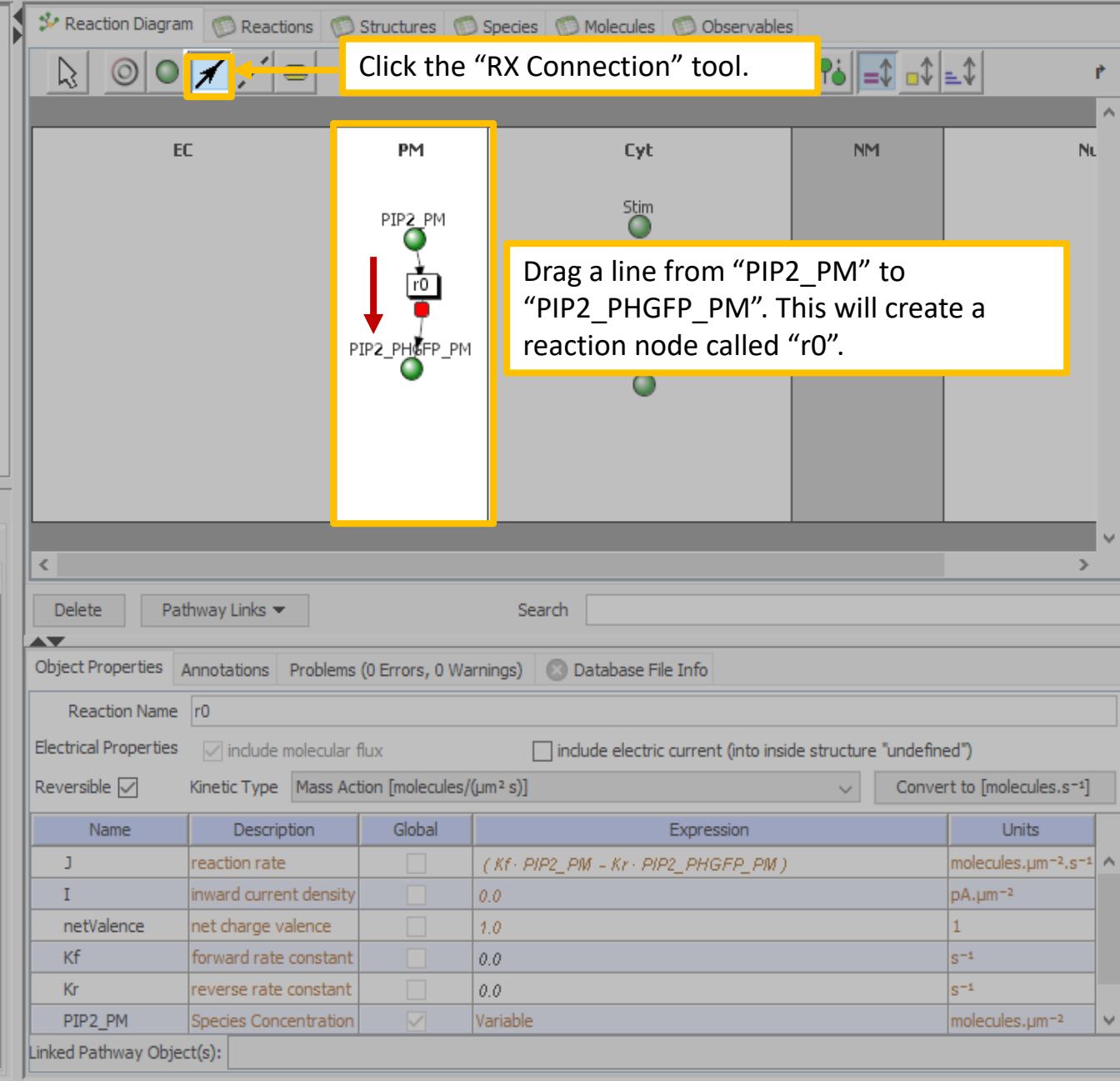
- Physiology**
  - Reaction Diagram** (selected)
  - Reactions (1)
  - Structures (5)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway
- Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
  - My BioModels
    - multiapp tutorial
  - PH-GFP
    - Private Fri May 10 17:14:27 EDT 2019
- Shared BioModels (0)
- Public BioModels (687)
- Tutorials (9)
- Education (33)
- Published BioModels (171)



**PH-GFP**

**Physiology**

- Reaction Diagram (1)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Pathway
- Scripting

Use the "RX Connection" tool to drag a line from "PH\_GFP\_Cyt" to "r0".

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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

Reaction Name: r0

Electrical Properties:  include molecular flux  include electric current (into inside structure "undefined")

Reversible  Kinetic Type: Mass Action [molecules/(μm² s)]  Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	(Kf · PIP2_PM · PH_GFP_Cyt - Kr · PIP2_PHGFP_PM)	molecules.μm⁻².s⁻¹
I	inward current density	<input type="checkbox"/>	0.0	pA.μm⁻²
netValence	net charge valence	<input type="checkbox"/>	1.0	1
Kf	forward rate constant	<input type="checkbox"/>	0.0	s⁻¹.μM⁻¹
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s⁻¹
PIP2_PM	Species Concentration	<input checked="" type="checkbox"/>	Variable	molecules.μm⁻²

Linked Pathway Object(s):

## PH-GFP

## Physiology

- Reaction Diagram
- Reactions (2)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

## Applications (0)

## Parameters, Functions and Units

## Pathway

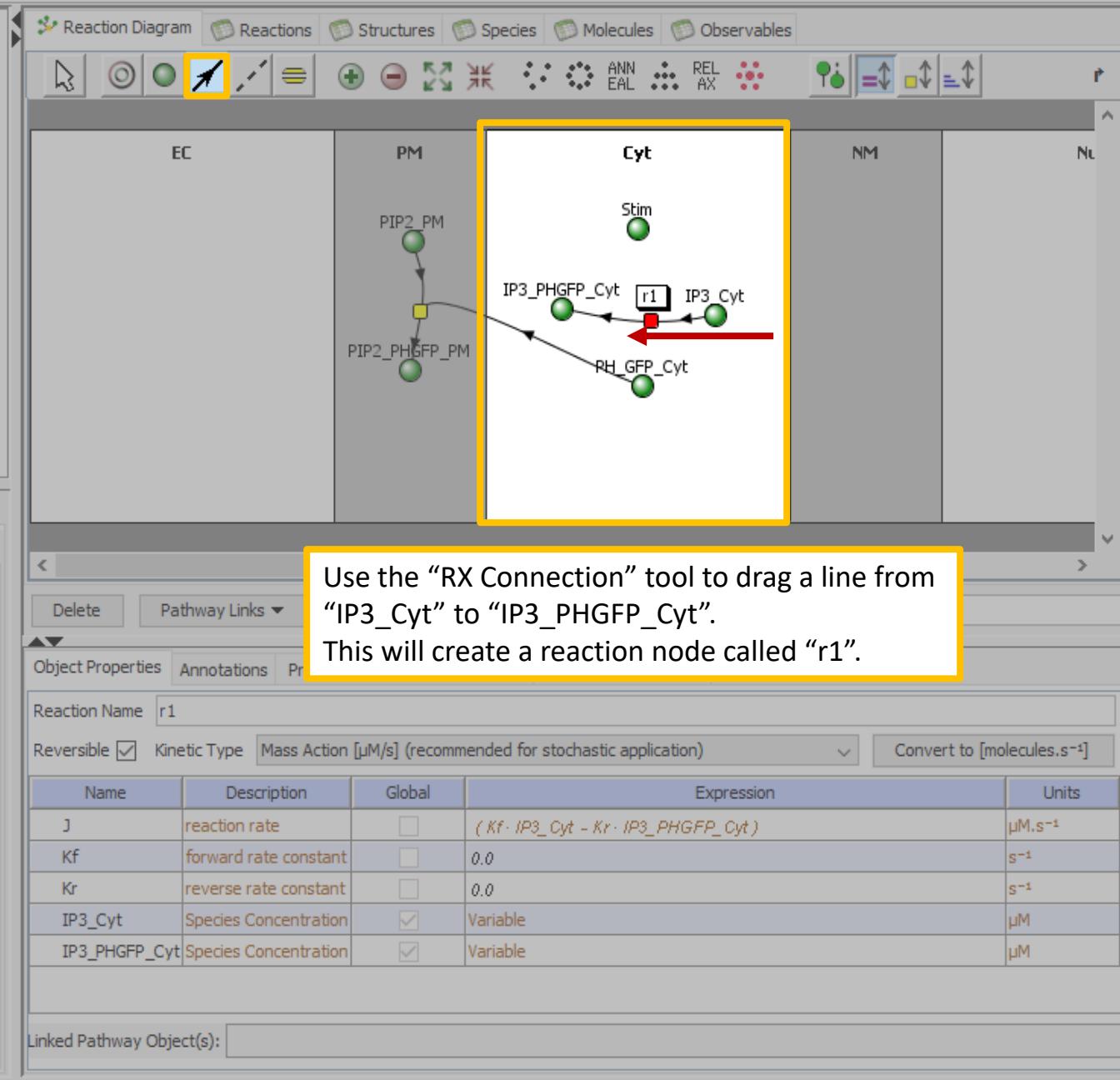
## Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

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    - multiapp tutorial
  - PH-GFP
    - Private Wed May 29 17:23:29 EDT 2019
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- Public BioModels (686)
- Tutorials (9)
- Education (33)
- Published BioModels (171)



**PH-GFP**

**Physiology**

- Reaction Diagram** (selected)
- Reactions (2)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway
- Scripting

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- Education (33)
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**Reaction Diagram**

EC PM Cyt NM

**Object Properties**

Reaction Name: r1

Reversible  Kinetic Type: Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application) | Name | Description | Global | Expression | Units |
| --- | --- | --- | --- | --- |
| J | reaction rate |  | $(Kf \cdot IP3\_Cyt \cdot PH\_GFP\_Cyt - Kr \cdot IP3\_PHGFP\_Cyt)$ | $\mu\text{M} \cdot \text{s}^{-1}$ |
| Kf | forward rate constant |  | 0.0 | $\text{s}^{-1}, \mu\text{M}^{-1}$ |
| Kr | reverse rate constant |  | 0.0 | $\text{s}^{-1}$ |
| IP3\_Cyt | Species Concentration |  | Variable | $\mu\text{M}$ |
| IP3\_PHGFP\_Cyt | Species Concentration |  | Variable | $\mu\text{M}$ |
| PH\_GFP\_Cyt | Species Concentration |  | Variable | $\mu\text{M}$ |

Linked Pathway Object(s):

Use the “RX Connection” tool to drag a line from “PH\_GFP\_Cyt” to “r1”.

CONNECTED

67 8MB / 227.5MB

**PH-GFP****Physiology****Reaction Diagram**

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observables (0)

Applications (0)

Parameters, Functions and Units

**Pathway****Scripting**

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## BioModels

## MathModels

## Geometries

**Search**

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## My BioModels

## multiapp tutorial

## PH-GFP

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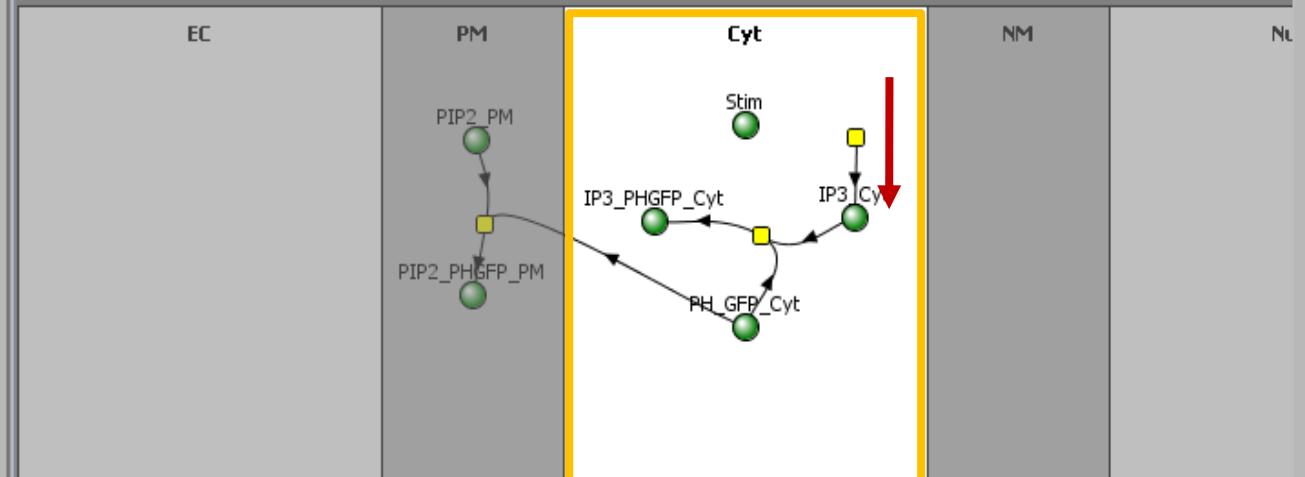
## Shared BioModels (0)

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## Tutorials (9)

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**Reaction Diagram**   **Reactions**   **Structures**   **Species**   **Molecules**   **Observables**

Click on any point within the “Cyt” compartment and use the “RX Connection” tool to connect to “IP3\_Cyt”. This will create a reaction node called “r2”.

Use the “Selection” tool to adjust the position of “r2”.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions and Units

Pathway

Scripting

Reaction Diagram    Reactions    Structures    Species    Molecules    Observables

Click the “Catalyst” tool.

Drag a line from “Stim” to “r2”.

Note that the catalyst tool creates a dotted line for visual reference. When you specify the flux for that reaction, you must include that species concentration in the reaction explicitly.

EC    PM    Cyt    NM    NL

Stim → r2

r2 → IP3\_PHGFP\_Cyt

IP3\_PHGFP\_Cyt → PIP2\_PHGFP\_PM

PIP2\_PHGFP\_PM → PH\_GFP\_Cyt

PH\_GFP\_Cyt → IP3\_Cyt

IP3\_Cyt → r2

VCell DB BMDB Pathway Comm Sabio

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Object Pr

Delete

CONNECTED

167.9MB / 238MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- d/dt Steady State

Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

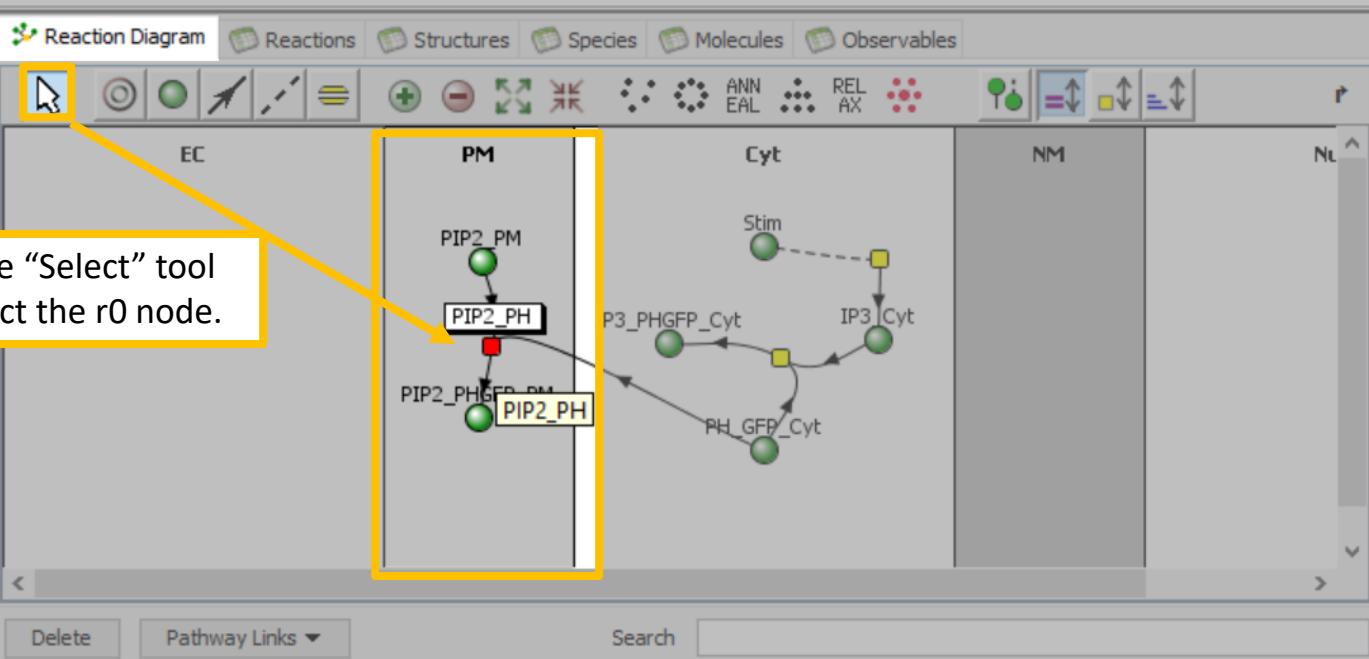
Biological Models

- My BioModels (staurovsky) (7)
- BioModel1
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- Published (173)
- Curated (30)

- Uncurated (587)



Object Properties

Reaction Name PIP2\_PH

Sbml Name

Electrical Properties

include molecular flux

include electric current (into inside structure "undefined")

Reversible

Kinetic Type Mass Action [molecules/(μm² s)]

Convert to [molecules.s⁻¹]

On the “Object Properties” tab, type “PIP2\_PH” in the “Reaction Name” text field.

			Units
I	inward current density	<input type="checkbox"/>	0.0 pA.μm⁻²
netValence	net charge valence	<input type="checkbox"/>	1.0
Kf	forward rate constant	<input type="checkbox"/>	s⁻¹.μM⁻¹

Linked Pathway Object(s):

The figure shows the VCell software interface. The left sidebar displays the project structure under 'PH-GFP' and 'Physiology'. The main workspace shows a reaction diagram with compartments EC, Cyt, and NM. A reaction in the EC compartment, involving species PIP2\_PM, PIP2\_PH, and PIP2\_PHGFP\_PM, is highlighted with a yellow box. In the Cyt compartment, species Stim, IP3\_PHGFP\_Cyt, IP3\_Cyt, and PH\_GFP\_Cyt are shown with interactions. Below the diagram is an 'Object Properties' panel for the reaction 'PIP2\_PH'. A yellow box highlights the 'Kf' row in the table, with the instruction: 'Type "0.12" for "Kf", the forward rate constant. Press "Enter" on your keyboard to accept the value.' Another yellow box at the bottom highlights the 'Kr' row, with the instruction: 'Type in "(Kf\*KdPIP2PH)" for "Kr", the reverse rate constant expression. Press "Enter" to accept the value.' The table rows are as follows:

Name	Description	Value	Units	
J	reaction rate	<input type="text"/>	( $Kf \cdot PIP2\_PM \cdot PH\_GFP\_Cyt - Kr \cdot PIP2\_PHGFP\_PM$ )	molecules. $\mu\text{m}^{-2}.\text{s}^{-1}$
I	inward current density	<input type="text"/>	.0	pA. $\mu\text{m}^{-2}$
netValence	net charge valence	<input type="text"/>	.0	1
Kf	forward rate constant	<input type="text"/>	0.12	$\text{s}^{-1}.\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="text"/>	$k_f \cdot K_dPIP2PH$	$\text{s}^{-1}$
PIP2_PM	Species Concentration	<input checked="" type="checkbox"/>	Variable	molecules. $\mu\text{m}^{-2}$

## PH-GFP New

## Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

## Applications (2)

- $d/dt$  Spatial
- $d/dt$  Steady State

Parameters, Functions, Units, etc.

## Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

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SimpleFrap

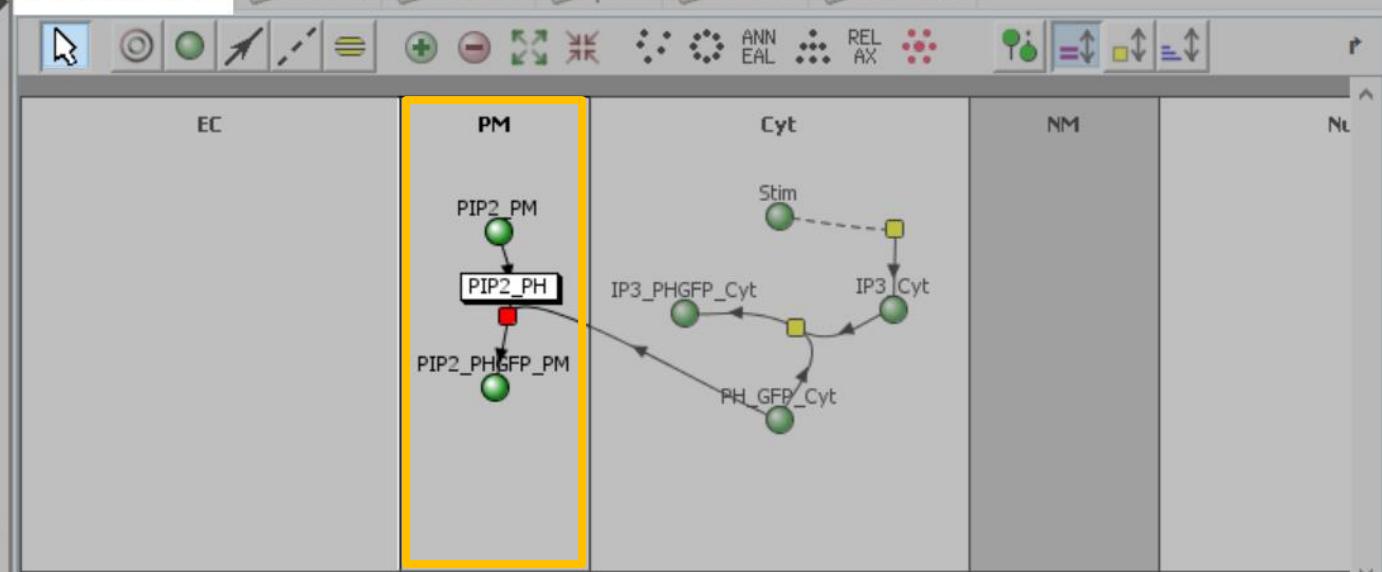
SimpleFRAP2

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Tutorials (9)

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## Reaction Diagram



Delete Pathway Links ▾

Search

## Object Properties

## Annotations

Reaction Name Electrical Properties Reversible Kinetic Type Convert to 

Type in “2.0” for the expression value for “KdPIP2PH”,  
and  $\mu\text{M}$  for the defined units.  
Press “Enter” to accept the changes.

Name	Description	Global	Expression	Units
Kf	forward rate constant	<input type="checkbox"/>	0.12	$\text{s}^{-1}, \mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	$k_f / K_dPIP2PH$	$\text{s}^{-1}$
KdPIP2PH	user defined	<input type="checkbox"/>	2.0	$\mu\text{M}$

Linked Pathway Object(s):

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- $d/dt$  Steady State

Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

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Reaction Diagram

EC PM Cyt NM N

Stim

PIP<sub>2</sub>\_PM

PIP<sub>2</sub>\_PHGFP\_PM

IP<sub>3</sub>\_PHGFP\_Cyt

r1

IP<sub>3</sub>\_Cyt

PH\_GFP\_Cyt

Use the “Select” tool to select the r1 node.

Object Properties

Annotations Problems (0 Errors, 1 Warnings) Database File Info

Reaction Name IP3PH Sbml Name

Reversible  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"/>	$(K_f \cdot IP_3\_Cyt \cdot PH\_GFP\_Cyt - K_r \cdot IP_3\_PHGFP\_Cyt)$	$\mu\text{M} \cdot \text{s}^{-1}$
				$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
				$\text{s}^{-1}$
				$\mu\text{M}$
				$\mu\text{M}$

On the “Object Properties” tab, type “IP3PH” in the “Reaction Name” text field; press Enter to accept the change.

PH-GFP New

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observables (0)

Applications (2)

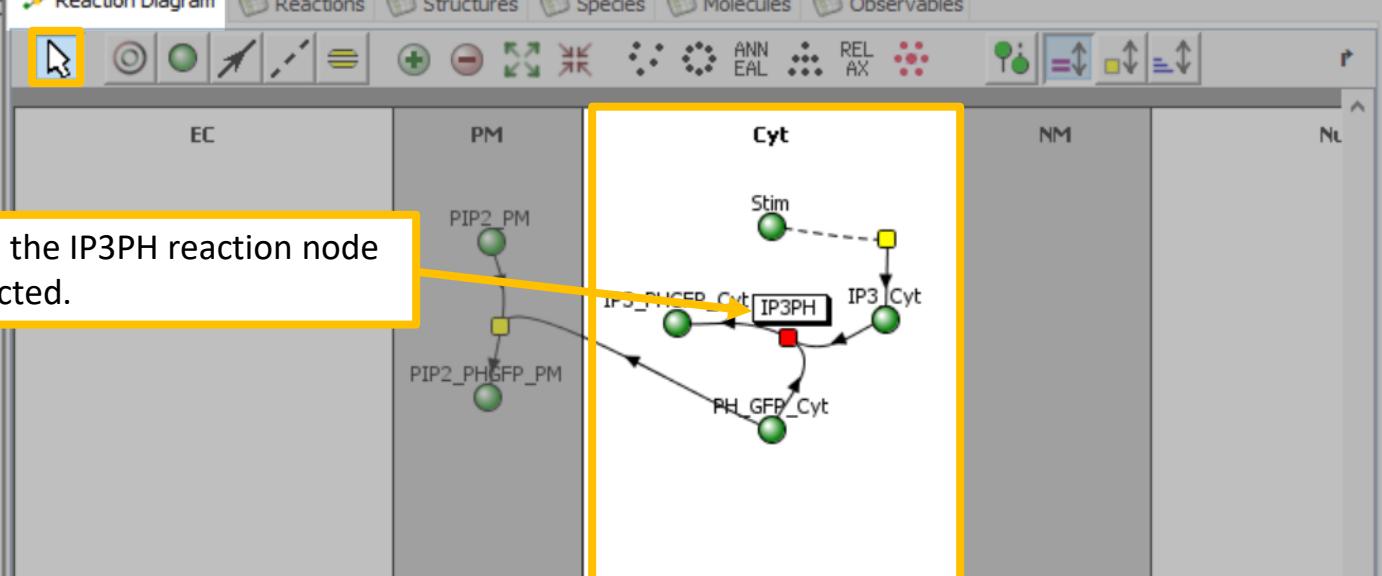
 $d/dt$  Spatial $d/dt$  Steady State

Parameters, Functions, Units, etc.

Pathway

Reaction Diagram

Reactions



Make sure the IP3PH reaction node is still selected.

On the “Object Properties” tab, type “10” for the “forward rate constant” expression.

Press “Enter” on your keyboard to accept the entry.

Object Properties

Name	Description	Global	Expression	Units
J	reaction rate		$(Kf \cdot IP3_Cyt \cdot PH_GFP_Cyt - Kr \cdot IP3_PHGFP_Cyt)$	$\mu M \cdot s^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	10.0	$s^{-1} \cdot \mu M^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	$Kf \cdot KdIP3PH$	$s^{-1}$
KdIP3PH	user defined	<input type="checkbox"/>	0.1	$\mu M$
IP3_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$

Type “(Kf\*KdIP3PH)” for the “reverse rate constant” expression. Press “Enter” on your keyboard to accept the entry.

BIOMODEL: PH-GFP New (Thu May 28 19:33:12 EDT 2020) -- VCell 7.2.0 (build 39)

File Account Window Tools Help

PH-GFP New

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observables (0)

Applications (2)

d/dt Spatial

d/dt Steady State

Parameters, Functions, Units, etc.

Pathway

Reaction Diagram

EC PM Cyt NM

PIP2\_PM PIP2\_PHGFP\_PM IP3\_Cyt Stim IP3PH IP3\_Cyt PH\_GFP\_Cyt

Make sure the IP3PH reaction node is selected.

Object Properties Annotat

Reaction Name IP3PH

Reversible  Kinetic Type Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application)

Type in "0.1" for the expression "KdIP3PH".  
Press "Enter" on your keyboard to accept the change.

Name	Description	Global	Expression	Units
Kf	forward rate constant	<input type="checkbox"/>	10.0	$\text{s}^{-1}, \mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	$KdIP3PH$	$\text{s}^{-1}$
KdIP3PH	user defined	<input type="checkbox"/>	0.1	$\mu\text{M}$
IP3_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
PH_GFP_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Linked Pathway Object(s):

PH-GFP New

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observables (0)

Applications (2)

d/dt Spatial

d/dt Steady State

Parameters, Functions, Units, etc.

Pathway

Reaction Diagram

EC

PM

Cyt

NM

Stim

r2

PIP2\_PHGFP\_PM

IP3\_PHGFP\_Cyt

IP3\_Cyt

PH\_GFP\_Cyt

Use the “Select” tool to select “r2”

On the “Object Properties” tab, click the “Kinetic Type” drop down menu and select “General [μM/s]”.

Object Properties

Annotations Problems (0 Errors, 1 Warnings)

Reaction Name r2

Kinetic Type General [μM/s]

Name J reaction

Mass Action [μM/s] (recommended for stochastic application)

General [μM/s]

General [molecules/s]

Henri-Michaelis-Menten (Irreversible) [μM/s]

Henri-Michaelis-Menten (Reversible) [μM/s]

Sbml Name

Convert to [molecules.s<sup>-1</sup>]

Units

μM.s<sup>-1</sup>

s<sup>-1</sup>

μM

Linked Pathway Object(s):

PH-GFP New

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observables (0)

Applications (2)

d/dt Spatial

d/dt Steady State

Parameters, Functions, Units, etc.

Pathway

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Reaction Diagram

Reactions

Structures

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Molecules

Observables

EC

PM

Cyt

NM

Stim

r2

PIP2\_PM

PIP2\_PHGFP\_PM

IP3\_PHGFP\_Cyt

IP3\_Cyt

PH\_GFP\_Cyt

Make sure "r2" is still selected.

On the "Object Properties" tab, type "Ksynth\*Stim" in the "reaction rate" text field.  
Please note the reaction is case-sensitive.  
Press "Enter" on your keyboard to accept the entry.

Name	Description	Global	Expression	Units
r2	reaction rate	<input type="checkbox"/>	Ksynth · Stim	$\mu\text{M}\cdot\text{s}^{-1}$
Ksynth	user defined	<input type="checkbox"/>	1.0	$\text{s}^{-1}$
Stim	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Linked Pathway Object(s):

PH-GFP New

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

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Molecules (0)

Observables (0)

Applications (2)

$d/dt$  Spatial

$d/dt$  Steady State

Parameters, Functions, Units, etc.

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Reaction Diagram

Reactions

Structures

Species

Molecules

Observables

EC

PM

Cyt

NM

Make sure "r2" is still selected.

PIP<sub>2</sub>\_PM

PIP<sub>2</sub>\_PHGFP\_PM

IP<sub>3</sub>\_PHGFP\_Cyt

IP<sub>3</sub>\_Cyt

PH\_GFP\_Cyt

r2

On the "Object Properties" tab, type "1.0" for the expression for "Ksynth".  
Press "Enter" on your keyboard to accept the entry.

Object Properties

Reaction Name: r2

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"/>	Ksynth * Stim	$\mu\text{M} \cdot \text{s}^{-1}$
Ksynth	user defined	<input type="checkbox"/>	1.0	$\text{s}^{-1}$
Stim	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Linked Pathway Object(s):

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
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- Observables (0)

**Applications (0)**

Parameters, Functions and Units

Pathway

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Name Math Type Annotation

Click "Applications">> "New Application" > "Deterministic".

New Application ▾

Deterministic

Stochastic

Network-Free

Name	Math Type	Annotation

80MB / 242.2MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- $\frac{d}{dt}$  Steady State

Parameters, Functions and Units

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Scripting

Name	Math Type	Annotation
Steady State	explicit network model, compartmental, deter...	

Double click “Application0” under the “Name” column. Type “Steady State”, and press “Enter” on your keyboard to accept the entry.

VCell DB BMDB Path

BioModels MathMode

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Application Name Application0

Annotation

Summary

- Deterministic
- Compartimental
- math generated

CONNECTED

145.5MB / 230.7MB

Make sure “Steady State” is selected, and then expand the menu tree:  
“Applications”>“Steady State”>  
“Specifications”.

The screenshot shows the VCell interface with the left sidebar expanded. Under the Applications section, "Steady State" is selected, and its sub-menu "Specifications" is also highlighted with a yellow box. Other options like "Geometry" and "Protocols" are visible but not selected.

Species	Structure	Depiction	Clamped	Initial Condition
IP3_Cyt	Cyt	●	<input type="checkbox"/>	0.1 [μM]
IP3_PHGFP_Cyt	Cyt	●	<input type="checkbox"/>	0.0 [μM]
PH_GFP_Cyt	Cyt	●	<input checked="" type="checkbox"/>	1.0 [μM]
Stim	Cyt	●	<input type="checkbox"/>	0.0 [μM]
PIP2_PM	PM	●	<input type="checkbox"/>	120000.0 [molecules, μm⁻²]
PIP2_PHGFP_PM	PM	●	<input type="checkbox"/>	0.0 [molecules, μm⁻²]

Enter the following “Initial Condition” values for the following species, according to the table below.  
Press “Enter” to accept each value.

Species	Initial Condition
IP3_Cyt	0.1
PH_GFP_Cyt	1.0
PIP2_PM	120000

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
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- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

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Geometry Specifications **Protocols** Simulations Parameter Estimation

Events Rate Rules Assignment Rules Microscope Measurements

Search Event Name Actions

New Delete Selected

Select the “Protocols” tab, “Events”>“New”.

You can use protocols in compartmental applications to create timed events.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

The screenshot shows the VCell 7.1.0 interface for a model named "PH-GFP". The left sidebar displays the model's structure under "PH-GFP" and "Physiology". The main workspace is titled "Protocols" and contains an "Events" tab. A modal dialog box is open, titled "Pre-Defined Trigger conditions". It contains four radio button options: "at a single time" (selected), "variable exceeds upper limit", "variable below lower limit", and "list of times". The "at a single time" field has the value "5.0" highlighted with a yellow box. To the right of the trigger conditions are dropdown menus for "IP3\_Cyt" and "IP3\_Cyt" with a value of "0.0". Below the trigger conditions is a section for "log time range" with fields for "Min" (1.0), "Max" (100.0), and "# values" (3). At the bottom of the dialog are "OK" and "Cancel" buttons, with "OK" highlighted with a yellow box. A large yellow callout box points from the text "For the event time, enter 5.0 in the ‘at a single time’ text field." to the "5.0" input field. Another arrow points from the text "Click ‘OK’, to accept the value." to the "OK" button.

For the event time, enter 5.0 in the “at a single time” text field.  
Click “OK”, to accept the value.

File Account Window Tools Help

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Reactions (3)
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Geometry Specifications Protocols Simulations Parameter Estimation

Events Rate Rules Assignment Rules Microscope Measurements

Event Name Trigger Condition Actions

Activation at time of 5.0 s No actions defined

Double click “event0” and type in “Activation” in the “Event Name” text field.  
Press “Enter” on your keyboard to accept your entry.

The caution sign by the “Event Name” signifies that an action has not yet been defined for this event. You will define that event next.

Object Properties Annotations Problems (0 Errors, 2 Warnings) Database File Info

Trigger: SingleTriggerTime Edit Trigger... Plot Trigger...

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
--------------------	--	-------

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
  - BioModel1
  - BioModel2
  - FRAPBinding
  - MultiAppTutorial
  - PH-GFP
  - PH-GFP New**
    - Private Mon Jun 01 15:30:07 EDT 2020
    - SimpleFrap
    - SimpleFRAP2
  - Shared With Me (0)
  - Tutorials (9)
  - Public BioModels (790)
  - Published (173)

Geometry Specifications **Protocols** Simulations Parameter Estimation

Electrical Events Rate Rules Assignment Rules Microscope Measurements

Search  New Delete Selected

Event Name	Trigger Condition	Actions
Activation	at time of 5.0 s	No actions defined

Make sure "Activation" is selected.  
Click "Add Action" on the "Object Properties" tab.

Object Properties Annotations Problems (0 Errors, 2 Warnings) Database File Info

Trigger: SingleTriggerTime

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
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  - BioModel2
  - FRAPBinding
  - MultiAppTutorial
  - PH-GFP
  - PH-GFP New
    - Private Mon Jun 01 15:30:07 EDT 2020
  - SimpleFrap
  - SimpleFRAP2
  - Shared With Me (0)
  - Tutorials (9)
  - Public BioModels (790)
  - Published (173)

Geometry Specifications Protocols Simulations Parameter Estimation

Events Rate Rules Assignment Rules Microscope Measurements

Search Event Name Trigger Condition Actions

Activation	at time of 5.0 s	No actions defined
------------	------------------	--------------------

Select "Stim" from the drop down menu.

Trigger: SingleTriggerTime

Action Delay (sec): 0.0

New Action Event

Event Actions:

Variable to modify

Variable to modify when action triggered IP3\_Cyt

Stim

Voltage\_NM

Voltage\_PM

IP3\_Cyt

Click "OK".

OK Cancel

BIOMODEL: PH-GFP New (Mon Jun 01 19:30:07 EDT 2020) -- VCell 7.2.0 (build 39)

File Account Window Tools Help

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

Parameters, Functions, Units, etc.

VCel DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Trigger: SingleTriggerTime

Action Delay (sec): 0.0

evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify Expression to evaluate when action triggered Units

Stim 1.0  $\mu\text{M}$

On the “Object Properties” tab, type in “1.0” in the “Expression to evaluate when action triggered” text field.

The species “Stim” will be set to a value of 1.0 when the event is triggered.

BIOMODEL: PH-GFP (Wed Jun 26 21:44:48 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Wed Jun 26 17:44:48 EDT 2019
- Shared BioModels (0)
- Public BioModels (694)
- Tutorials (9)
- Education (31)
- Published BioModels (171)

Geometry Specifications Protocols Simulations Parameter Estimation

Events Electrical Rate Rules

Search

Event Name Activation

Actions on trigger reset Stim

Click "New" to define a second event that will turn off the stimulus.

New Delete Selected

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Trigger: SingleTriggerTime Edit Trigger... Plot Trigger...

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
Stim	1.0	μM

CONNECTED 107MB / 275.8MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
- multiapp tutorial
- PH-GFP

Private Wed Jun 26 17:44:48 EDT 2019

Shared BioModels (0)

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Education (31)

Published BioModels (171)

Geometry Specifications Protocols Simulations Parameter Estimation

Events Electrical Rate Rules

Search New Delete Selected

event trigger

Pre-Defined Trigger conditions

at a single time 6.0

variable exceeds upper limit IP3\_Cyt

variable below lower limit IP3\_Cyt

list of times 0.0

Min 1.0  
Max 100.0  
# values 3

log time range

when condition becomes true

OK Cancel

Enter 6.0 in the “at a single time” text field; click “OK”.

The second event at 6.0 s will be used to set the value of “stim” back to 0.

New Delete Selected

on trigger reset Stim

Add Action Delete Action

evaluate at trigger time  evaluate after delay

ed Units  $\mu\text{M}$

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

## Applications (1)

- $d/dt$  Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

## Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

## Search

Biological Models

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  - MultiAppTutorial
  - PH-GFP
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- Shared With Me (0)
- Tutorials (9)
- Public BioModels (790)
- Published (173)

Events		
Event Name	Trigger Condition	Actions
Activation	at time of 5.0 s	on trigger reset Stim
Inactivation	at time of 6.0 s	No actions defined

Double click “event0” and type in “Inactivation”.  
Press “Enter” on your keyboard to accept the entry.

Object Properties Annotations Problems (0 Errors, 2 Warnings) Database File Info

Trigger: SingleTriggerTime

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
--------------------	--	-------

**PH-GFP New****Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- $d/dt$  Steady State
- Geometry
- Specifications
- Protocols**
- Simulations
- Parameter Estimation

**Parameters, Functions, Units, etc.**

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

**Search**

- Biological Models
- My BioModels
  - BioModel1
  - BioModel2
  - FRAPBinding
  - MultiAppTutorial
  - PH-GFP
- PH-GFP New
  - Private Mon Jun 01 15:30:07 EDT 2020
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (790)
- Published (173)

Geometry Specifications **Protocols** Simulations Parameter Estimation

Electrical Events Rate Rules Assignment Rules Microscope Measurements

Search  New Delete Selected

Event Name	Trigger Condition	Actions
Activation	at time of 5.0 s	on trigger reset Stim
Inactivation	at time of 6.0 s	No actions defined

With “Inactivation” selected, press “Add Action”.

Object Properties Annotations Problems (0 Errors, 2 Warnings) Database File Info

Trigger: SingleTriggerTime

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Add Action

Variable to modify	Expression to evaluate when action triggered	Units

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

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Biological Models

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  - BioModel2
  - FRAPBinding
  - MultiAppTutorial
  - PH-GFP
  - PH-GFP New
    - Private Mon Jun 01 15:30:07 EDT 2020
  - SimpleFrap
- Tutorials (9)
- Public BioModels (790)
- Published (173)

Geometry Specifications Protocols Simulations Parameter Estimation

Events Rate Rules Assignment Rules Microscope Measurements

Event Name Trigger Condition Actions

Activation	at time of 5.0 s	on trigger reset Stim
Inactivation	at time of 6.0 s	No actions defined

From the “New Action Event” drop down menu, select “Stim”.

Trigger: SingleTriggerTime

Action Delay (sec): 0.0

New Action Event

Variable to modify when action triggered

OK Cancel

[P3\_Cyt  
[P3\_PHGFP\_Cyt  
PH\_GFP\_Cyt  
PIP2\_PHGFP\_PM  
PIP2\_PM  
Stim  
Voltage\_NM  
Voltage\_PM  
TP3\_Cyt]

Press “OK” to accept your selection.

BIOMODEL: PH-GFP (Mon Jul 08 20:59:36 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions and Units

Pathways

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
  - multiapp tutorial
- PH-GFP
  - Private Mon Jul 08 16:59:36 EDT 2019
- Shared BioModels (0)
- Public BioModels (694)
- Tutorials (9)
- Education (31)
- Published BioModels (176)

Geometry Specifications Protocols Simulations Parameter Estimation

Events Electrical Rate Rules

Search New Delete Selected

Event Name	Trigger Condition	Actions
Activation	at time of 5.0 s	on trigger reset Stim
Inactivation	at time of 6.0 s	on trigger reset Stim

Keep the default value of 0 for “Stim”.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Trigger: SingleTriggerTime Edit Trigger... Plot Trigger...

Action Delay (sec): 0.0  evaluate at trigger time  evaluate after delay

Event Actions:

Variable to modify Expression to evaluate when action triggered Units

Stim 0.0  $\mu\text{M}$

CONNECTED 109.4MB / 212.3MB

BIOMODEL: PH-GFP (Mon Jul 08 20:59:36 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Mon Jul 08 16:59:36 EDT 2019
- Shared BioModels
- Public BioModels
- Tutorials
- Education
- Published

Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition Kinematics

Physiology (structures)

- Nuc
- EC
- Cyt
- PM
- NM

Geometry (subdc)

Compartment

Select “Geometry”, which will bring you to the “Geometry” > “Structure Mapping” tab.

Enter the following values for the “Size” of each “Structure” as listed in the table. Press “Enter” to accept your entry.

Structure	Size
Nuc	50000 [ μm <sup>3</sup> ]
EC	50000 [ μm <sup>3</sup> ]
Cyt	50000 [ μm <sup>3</sup> ]

Structure	Size
Nuc	33.389
Cyt	489.794
NM	49.8
EC	476.817
PM	501.804

Tip: If you have already created a spatial application with geometry (as you will do next), if you copy the spatial application as a non-spatial deterministic application, the exact sizes will automatically be copied into the new non-spatial application.

CONNECTED

38.5MB / 212.3MB

The screenshot shows the VCell 7.1.0 interface for a model named "PH-GFP". The left sidebar contains a tree view of the model components: "PH-GFP", "Physiology" (with "Reaction Diagram", "Reactions (3)", "Structures (5)", "Species (6)", "Molecules (0)", "Observables (0)" listed), "Applications (1)" (with "Steady State", "Geometry", "Specifications", "Protocols", "Simulations" selected), and "Parameters, Functions and Units". The main workspace has tabs at the top: "Geometry", "Specifications", "Protocols", "Simulations" (which is highlighted with a yellow box and an arrow pointing to it from the text below), and "Parameter Estimation". Below these tabs is a toolbar with icons for "Simulations", "Output Functions", and "Generated Math". A large yellow box encloses the "Simulations" tab and the "New Simulation" icon (a blue square with a white plus sign). A callout bubble with the text "Go to the ‘Simulations’ tab and click the ‘New Simulation’ icon." is positioned over the "Simulations" tab. At the bottom of the workspace, there are tabs for "Object Properties", "Annotations", "Problems (0 Errors, 1 Warnings)", and "Database File Info". The bottom status bar shows "CONNECTED" and "108.3MB / 209.7MB".

Go to the “Simulations” tab and click the “New Simulation” icon.

BIOMODEL: PH-GFP (Mon Jul 08 20:59:36 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

**PH-GFP**

**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Mon Jul 08 16:59:36 EDT 2019
- Shared BioModels (0)
- Public BioModels (694)
- Tutorials (9)
- Education (31)
- Published BioModels (176)

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 sample	Combined IDA/CVODE	not saved	no

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
1.0s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

CONNECTED 75.7MB / 210.8MB

File Account Window Tools Help

**PH-GFP New**

**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

Parameters, Functions, Units, etc

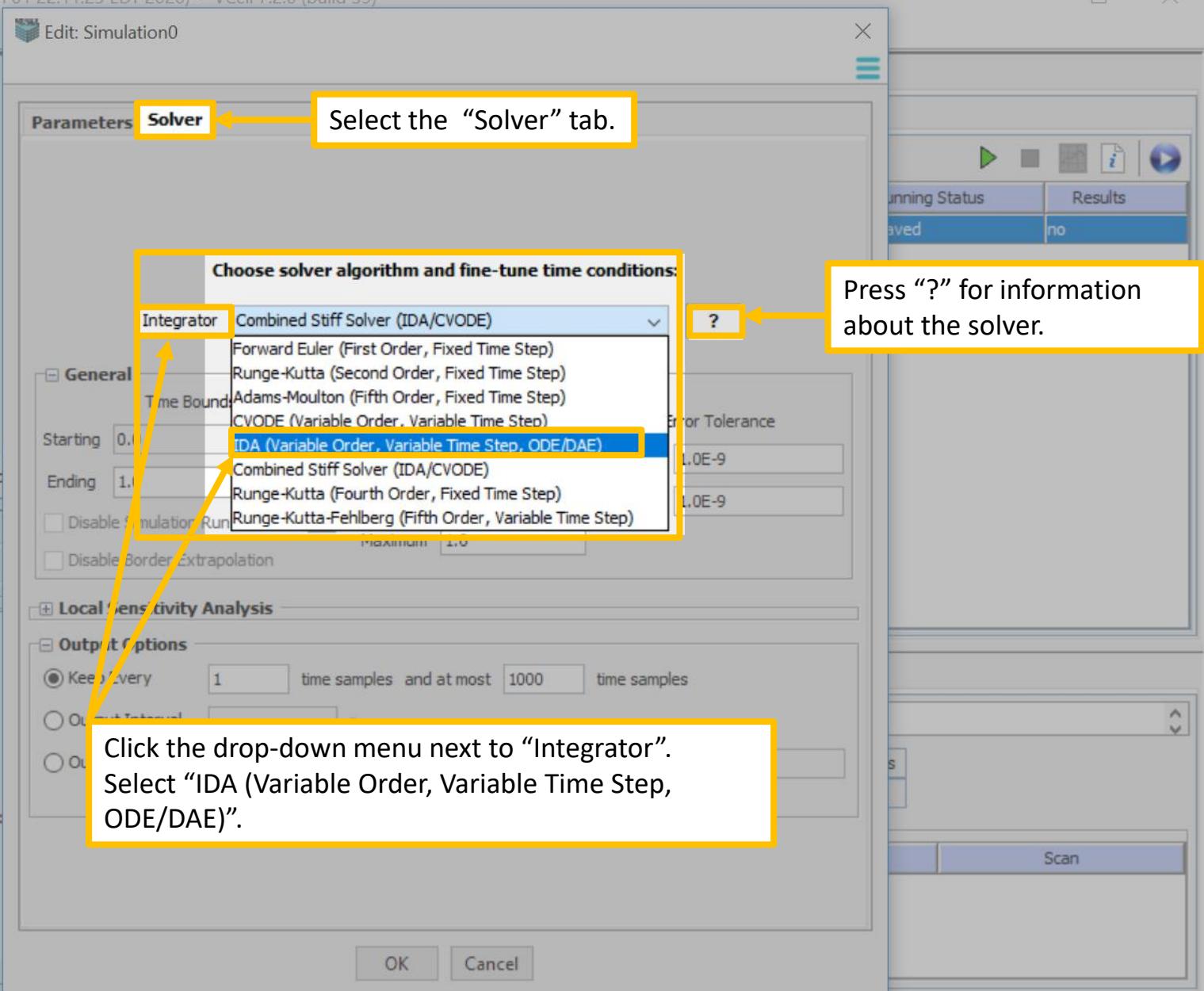
Cell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
  - BioModel1
  - BioModel2
- FRAPBinding
- MultiAppTutorial
- PH-GFP
- PH-GFP New**
  - Private Mon Jun 01 18:11:25 EDT 2020
- SimpleFrap
- SimpleFRAP2
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (790)



BIOMODEL: PH-GFP New (Mon Jun 01 22:11:25 EDT 2020) -- VCell 7.2.0 (build 39)

File Account Window Tools Help

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

Parameters, Functions, Units, etc

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- BioModel1
- BioModel2
- FRAPBinding
- MultiAppTutorial
- PH-GFP
- PH-GFP New**
- Private Mon Jun 01 18:11:25 EDT 2020
- SimpleFrap
- SimpleFRAP2
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (790)

Edit: Simulation0

Parameters Solver

Type “30.0” for the “Ending Time Bounds”.

Starting 0.0

Ending 30.0

Time Step

Minimum

Absolute 1.0E-9

Default

Relative

Maximum .01

Disable Simulation Run Timeout

Disable Border Extrapolation

Local Sensitivity Analysis

Output Options

Keep Every 1 time samples and at most 1000 time samples

Output Interval s

Output Times

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

OK Cancel

Running Status Results

Saved no

Scan

BIMODEL: PH-GFP New (Mon Jun 01 22:11:25 EDT 2020) -- VCell 7.2.0 (build 39)

File Account Window Tools Help

PH-GFP New

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- $d/dt$  Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

Parameters, Functions, Units, etc

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- BioModel1
- BioModel2
- FRAPBinding
- MultiAppTutorial
- PH-GFP

PH-GFP New

Private Mon Jun 01 18:11:25 EDT 2020

- SimpleFrap
- SimpleFRAP2

Shared With Me (0)

Tutorials (9)

Public BioModels (790)

Edit: Simulation0

Solver

Choose solver algorithm and fine-tune time conditions:

Integrator IDA (Variable Order, Variable Time Step, ODE/DAE) ?

General

Time Bounds

Starting 0.0 Ending 30.0

Time Step

Minimum Default Maximum 0.01

Error Tolerance

Absolute 1.0E-9 Relative 1.0E-9

Local Sensitivity Analysis

Output Options

Keep Every 10  Output Interval \_\_\_\_\_ s  Output Times \_\_\_\_\_

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

Type "10" for "Keep Every" time sample.  
Press enter to accept your entry.

Click "OK".

OK Cancel

Running Status Results

Saved no

Scan

BIOMODEL: PH-GFP (Tue Jul 09 21:40:27 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

**PH-GFP**

**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- $d/dt$  Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

Biological Models

- My BioModels (staurovsky) (2)
  - multiapp tutorial
  - PH-GFP
    - Private Tue Jul 09 17:40:27 EDT 2019
- Shared BioModels (0)
- Public BioModels (699)
- Tutorials (9)
- Education (31)
- Published BioModels (176)

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	not saved	Run and Save Simulation

Select the simulation and click the green play button.

Pressing the green button will first save the BioModel to the database, and then dispatch the simulation job to the VCell servers.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Annotation:

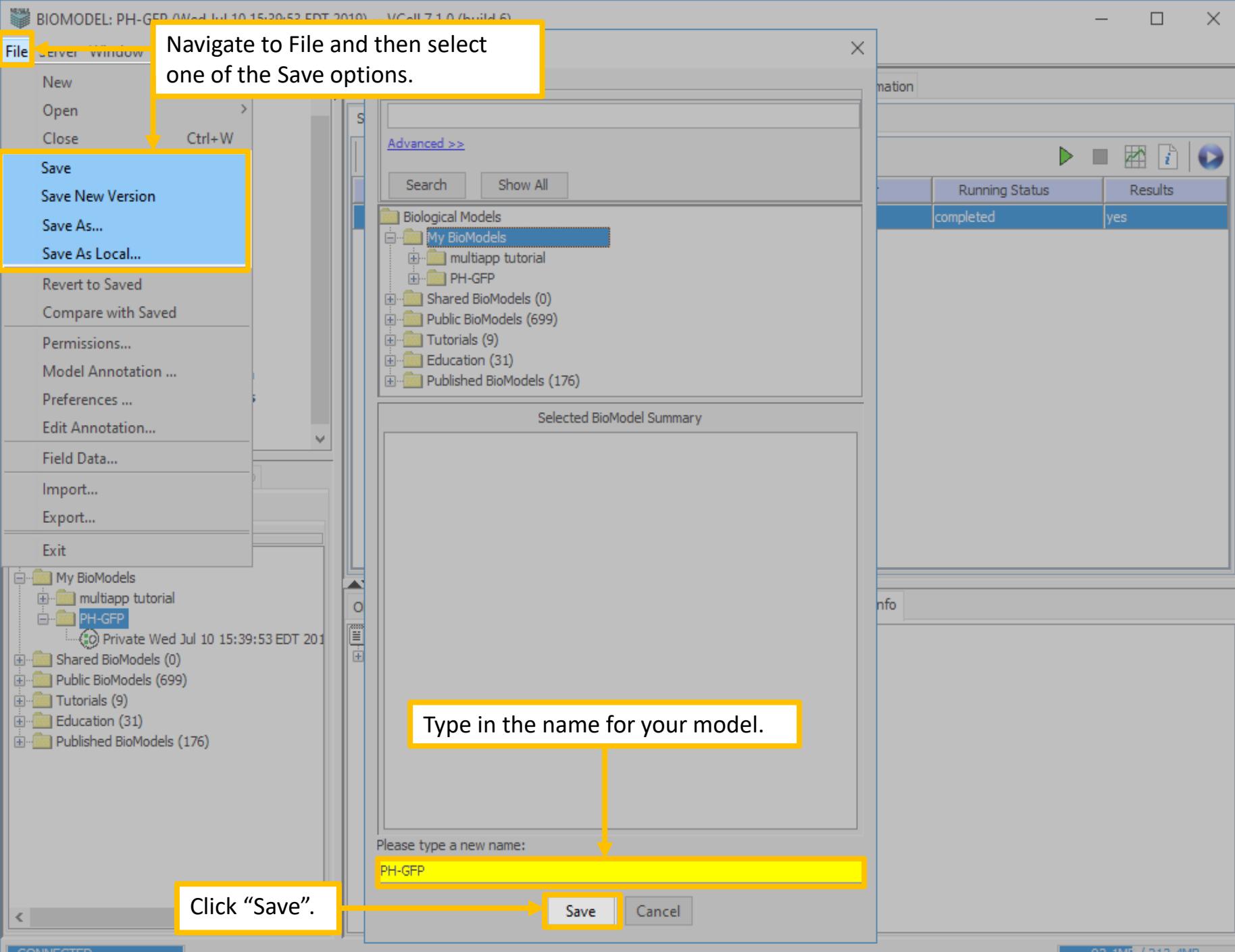
Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

CONNECTED (staurovsky) 133.4MB / 130.7MB



**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- d/dt Steady State
- Geometry
- Specifications
- Protocols
- Simulations**
- Parameter Estimation

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
- + My BioModels
- + Shared BioModels (0)
- + Public BioModels (698)
- + Tutorials (9)
- + Education (31)
- + Published BioModels (176)

Geometry Specifications Protocols **Simulations** Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	completed	yes

Click the “Results” icon once “Simulation0” is completed.

As soon as results are available they can be viewed. If the simulation has not completed, the results will be updated as they are saved to the database.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

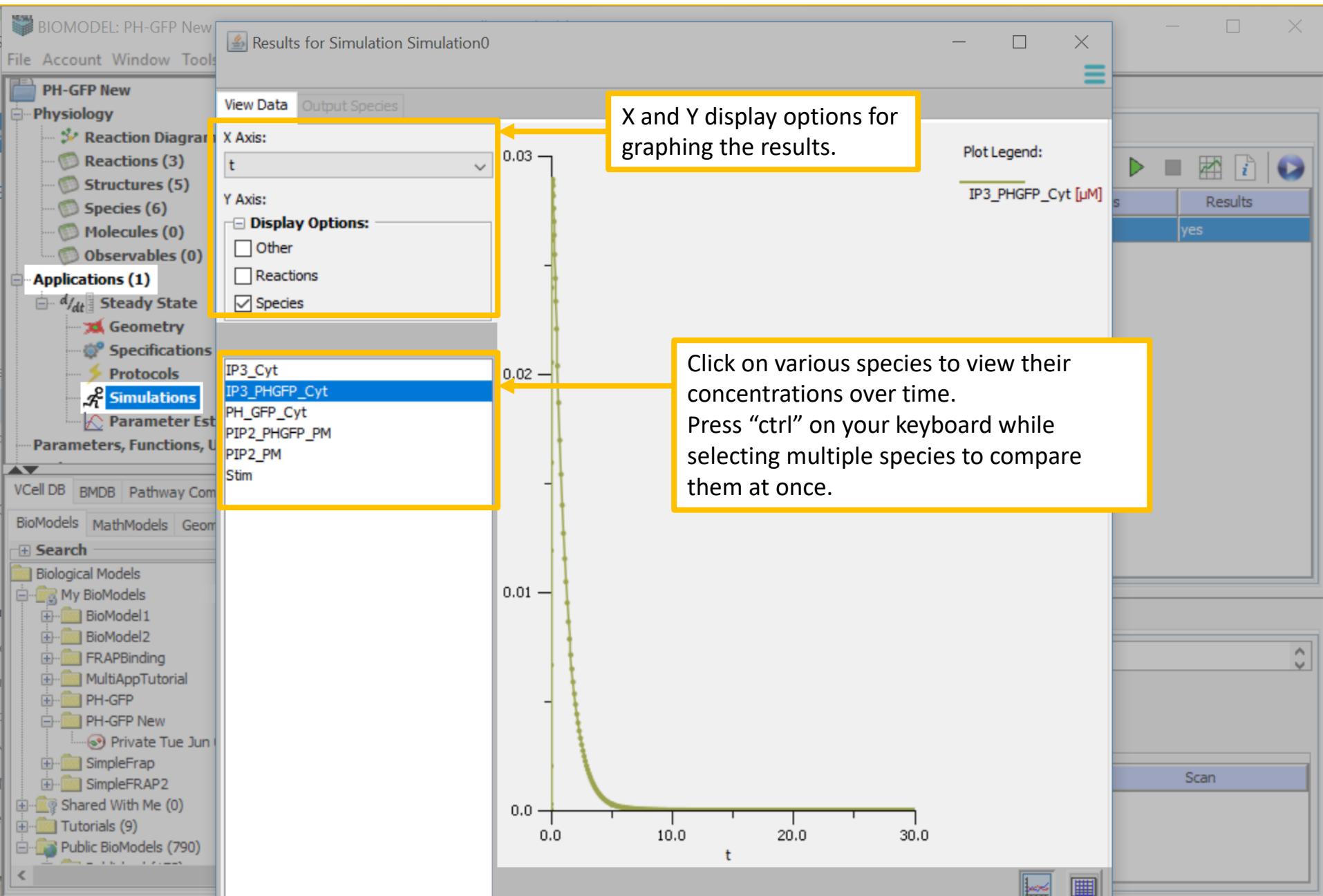
Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan



PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Application

- New Application > Deterministic
- Remove Apps...
- Expand All
- Collapse All

Parameter:

Pathway Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- multiapp tutorial
- PH-GFP

Private Wed Jul 10 11:39:53 EDT 201

Shared BioModels (0)

Public BioModels (698)

Tutorials (9)

Education (31)

Published BioModels (176)

Name Math Type Annotation

$d/dt$  Steady State explicit network model, compartmental, deter...

Select “Applications” then click your right mouse button to access “New Application” >“Deterministic”.

New Application Delete More Copy Actions Compare... Search

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

CONNECTED 137.7MB / 236.5MB

**PH-GFP**  
**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- $\frac{d}{dt}$  Application0
- $\frac{d}{dt}$  Steady State

**Parameters, Functions and Units****Pathway****Scripting**[VCell DB](#) [BMDB](#) [Pathway Comm](#) [Sabio](#)[BioModels](#) [MathModels](#) [Geometries](#)**Search**

- Biological Models
  - My BioModels
    - multiapp tutorial
    - PH-GFP
      - Private Wed Jul 10 11:39:53 EDT 2019
  - Shared BioModels (0)
  - Public BioModels (698)
  - Tutorials (9)
  - Education (31)
  - Published BioModels (176)

Name	Math Type	Annotation
$\frac{d}{dt}$ Steady State	explicit network model, compartmental, deter...	
Application0	explicit network model, compartmental, deter...	

Double click "Application0" and type in "Spatial".  
Press "Enter" on your keyboard to accept your entry.

[New Application](#) [Delete](#) [More Copy Actions](#) [Compare...](#) [Search](#)[Object Properties](#) [Annotations](#) [Problems \(0 Errors, 1 Warnings\)](#) [Database File Info](#)Application Name 

## Annotation

- Deterministic
- Compartmental
- math not generated

The screenshot shows the VCell 7.1.0 interface for a model named "PH-GFP". The left sidebar lists model components like "Reaction Diagram", "Reactions (3)", "Structures (5)", etc., and "Applications (2)" which includes "Spatial" and "Geometry". The "Geometry" tab is highlighted with a yellow box. The main workspace has tabs for "Structure Mapping", "Geometry Definition", and "Kinematics". The "Geometry Definition" tab is active, showing a table with one row: "Compartment" under "Name" and "0D, compartmental" under "Value". A button "Edit Domain..." is available. On the right, there's a "Add Geometry" dropdown menu with options "New...", "Open from...", and "Delete". A large yellow callout box points to the "New..." option in the dropdown.

Expand the menu under “Spatial” and click “Geometry” to open the “Geometry” tab. Go to the “Geometry Definition” tab to gain access to “Add Geometry”.

Click “Add Geometry” > “New”.

BIOMODEL: PH-GFP (Wed Jul 10 15:39:53 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- Geometry

Specifications

Protocols

Simulations

Parameter Estimation

d/dt Steady State

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

Biological Models

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  - PH-GFP
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- Published BioModels (176)

Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition Kinematics

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

Choose new geometry type to create

Select “Analytic Equations (3D)”.

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

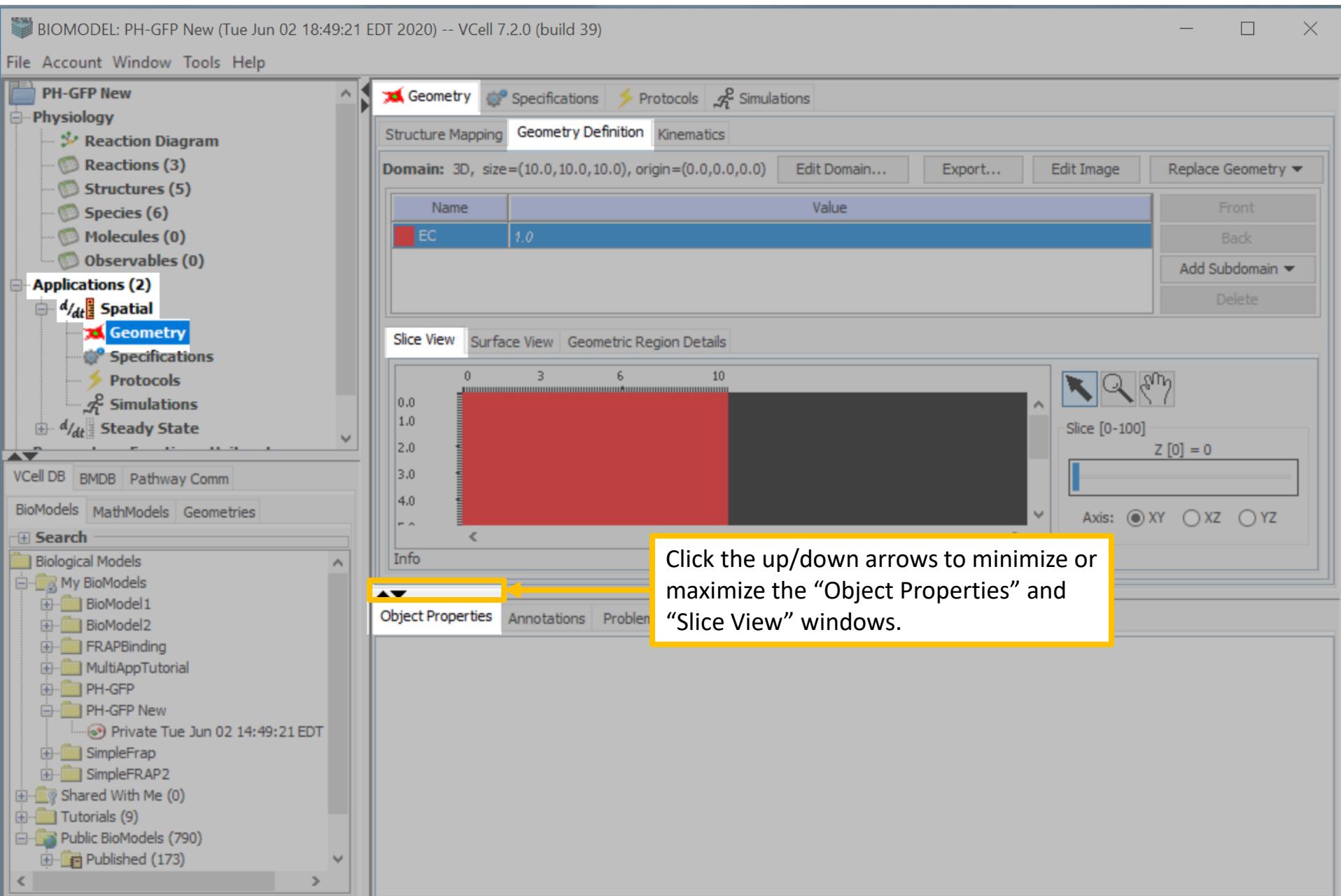
Constructed Solid Geometry (3D)

Click “OK”.

OK Cancel

Front Back Add Subdomain Delete

CONNECTED 191.2MB / 243.3MB



BIOMODEL: PH-GFP (Wed Jul 10 15:39:53 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- Geometry

- Specifications
- Protocols
- Simulations

d/dt Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Name Value

subdomain0 1.0

Front Back Add Subdomain ▾ Delete

Double click "subdomain0" and type "EC".  
Press "Enter" on your keyboard to accept your entry.

Slice View Surface View Geometric Region Details

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

slice [0-100] Z [0] = 0 Axis: XY XZ YZ

Info

CONNECTED 167.8MB / 274.7MB

BIOMODEL: PH-GFP (Wed Jul 10 15:39:53 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- Geometry

Specifications

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d/dt Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

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- Published BioModels (176)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Name EC 1.0

You will create a sphere to represent the cell for the Geometry.

Click “Add Subdomain” > “Analytic”.

Add Subdomain ▾

Analytic ...

Constructed Solid G

Slice View Surface View Geometric Region Details

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

Slice [0-100] Z [0] = 0

Axis:  XY  XZ  YZ

Info

CONNECTED 141.4MB / 271.6MB

The screenshot shows the VCell 7.1.0 software interface with the 'Geometry' tab selected. In the 'Geometry Definition' tab, there is a message box stating 'You will create a sphere to represent the cell for the Geometry.' A second message box contains the instruction 'Click “Add Subdomain” > “Analytic”.'. A third message box highlights the 'Analytic ...' option under the 'Add Subdomain' dropdown menu. The main workspace displays a 3D slice view of a red rectangular region, representing a subdomain. The bottom right corner of the screen shows memory usage information: 141.4MB / 271.6MB.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
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Parameters, Functions and Units

VCell DB BMDB Pathway Com

BioModels MathModels Geom

+ Search

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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Name Value

EC

Select Subdomain Shape: Sphere

Center Point (x,y,z)  
5.0,5.0,5.0

Radius  
5.0

Analytic Expression  
 $(x-5.0)^2 + (y-5.0)^2 + (z-5.0)^2 < 5.0^2$

Copy Expression

Help New Subdomain Cancel

Front Back Add Subdomain ▾ Delete

Slice View

Slice [0-100] Z [0] = 0

Axis: XY XZ YZ

Click the drop-down menu next to “Select Subdomain Shape” and click “Sphere”.

Type “5.0” for the radius.

Click “New Subdomain”.

CONNECTED 141.4MB / 271.6MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Application0
- Geometry

- Specifications
- Protocols
- Simulations

d/dt Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

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- Education (31)
- Published BioModels (164)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Edit Domain... Export... Edit Image Replace Geometry

Name	Value
subdomain0	$((((x - 5.0))^2 + ((y - 5.0))^2 + ((z - 5.0))^2) < (5.0)^2$
EC	1.0

Front Back Add Subdomain Delete

Slice view Surface View Geometric Region Details

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

Slice [0-100] Z [0] = 0

Axis: XY XZ YZ

Info

Double click “subdomain0” and type “Cyt”.  
Press “Enter” on your keyboard to accept your entry.

Name	Value
subdomain0	$((((x - 5.0))^2 + ((y - 5.0))^2 + ((z - 5.0))^2) < (5.0)^2$
EC	1.0

**PH-GFP**

**Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- d/dt Application0
  - Geometry
  - Specifications
  - Protocols
  - Simulations
- d/dt Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
Cyt	$( ( ( (x - 5.0) ) + ( (y - 5.0) ) + ( (z - 5.0) ) ) < (5.0) )$
EC	1.0

Edit Domain... Export... Edit Image Replace Geometry ▾

Front Back Add Subdomain ▾ Delete

Slice View Surface View Geometric Region Details

Click and drag the Z-Slicer so that the circle (Cytosol) almost touches the perimeter of the square (Extra Cellular). Alternatively, select the area and use your arrow keys to adjust the position.

Slice [0-100] Z [49] = 4.9

Axis:  XY  XZ  YZ

Info

147.7 MB / 363.3 MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Application0
- Geometry

Specifications

Protocols

Simulations

d/dt Steady State

Parameters, Functions and Units

Pathway

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

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- Published BioModels (164)

Geometry

Specifications

Protocols

Simulations

Structure Mapping

Geometry Definition

Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Edit Domain... Export... Edit Image Replace Geometry

Name Value

Cyt	$((((x - 5.0)^2) + ((y - 5.0)^2) + ((z - 5.0)^2)) \leq (5.0)^2$
EC	1.0

Front Back Add Subdomain

Click "Add Subdomain" > "Analytic".

Analytic ...

Constructed Solid Geometry

Slice View Surface View Geometric Region Details

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

slice [0-100] Z [49] = 4.9

Axis: XY XZ YZ

147.7 MB / 363.3 MB

BIOMODEL: PH-GFP (Wed Jul 10 15:39:53 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Application0
- Geometry

Specifications

Geometry

Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry

Select “Sphere” from the “Select Subdomain Shape” drop-down menu.

Select Subdomain Shape: Sphere

Center Point (x,y,z)  
3.5,3.5,3.5

Radius  
2.0

Analytic Expression  
 $(x-3.5)^2 + (y-3.5)^2 + (z-3.5)^2 < 2.0^2$

Copy Expression

Enter “3.5, 3.5, 3.5” for the center point.

Type “2.0” for the radius.

View

New Subdomain Cancel

Help

Front Back Add Subdomain Delete

VCell DB

BioModels MathModels Geometries

+ Search

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Published BioModels (164)

Slice [0-100]  
Z [49] = 4.9

Axis: XY XZ YZ

CONNECTED

147.7 MB / 363.3 MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Application0
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Specifications

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d/dt Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

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- Tutorials (9)
- Education (31)
- Published BioModels (164)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Edit Domain... Export... Edit Image Replace Geometry

Name	Value
subdomain0	$(((x - 3.5)^2 + (y - 3.5)^2 + (z - 3.5)^2) < (2.0^2))$
Cyt	$((((x - 5.0)^2 + (y - 5.0)^2 + (z - 5.0)^2) < (5.0^2))$

Front Back Add Subdomain Delete

Double click “subdomain0” and type “Nuc”.  
Press “Enter” on your keyboard to accept your entry.

Slice View Surface View Geometric Region Details

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

Slice [0-100] Z [49] = 4.9

Axis: XY XZ YZ

CONNECTED 227.5MB / 365.5MB

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- Geometry

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Name	Value
Nuc	$((((x - 3.5)^2 + (y - 3.5)^2 + (z - 3.5)^2) < (2.0)^2)$
Cyt	$((((x - 5.0)^2 + (y - 5.0)^2 + (z - 5.0)^2) < (5.0)^2)$
EC	1.0

Front Back Add Subdomain ▾ Delete

Click "Surface View" to view the 3-dimensional representation of your model.

Surface View Geometric Region Details

Reset View

Opacity: 75

Click and drag the slider to change the opacity, which will allow you to visualize the nucleus.

PH-GFP

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Go to the “Structure Mapping” tab.

Use the line tool to connect the structures to their corresponding subdomains. Do note, you have to reselect the line tool for each mapping.

Physiology (structures)

Nuc  
EC  
Cyt  
PM  
NM

Geometry (subdomains)

Nuc  
Cyt  
EC  
Cyt\_EC\_membrane  
Cyt\_Nuc\_membrane

SOLVE >>

Membrane boundary conditions are chosen alphabetically among the adjacent subdomains.

Structure	Subdomain	Size Ratio	X-	X+	Y-	Y+	Z-	Z+
Nuc	Nuc	1 [ 1 ]	Flux	Flux	Flux	Flux	Flux	Flux
EC	EC	1 [ 1 ]	Flux	Flux	Flux	Flux	Flux	Flux
Cyt	Cyt	1 [ 1 ]	Flux	Flux	Flux	Flux	Flux	Flux
PM	Unmapped		Flux	Flux	Flux	Flux	Flux	Flux
NM	Unmapped		Flux	Flux	Flux	Flux	Flux	Flux

CONNECTED

637.5MB / 725.6MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- d/dt Steady State

- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Simulations

Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	completed	yes

Double click the “Steady State” application and select “Simulations”.

Make sure “Simulation0” is selected and then click the results icon.

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

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- Education (31)
- Published BioModels (164)

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

CONNECTED 113.9MB / 230.2MB

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- $d/dt$  Steady State
  - Geometry
  - Specifications
  - Protocols
  - Simulations
  - Parameter Est

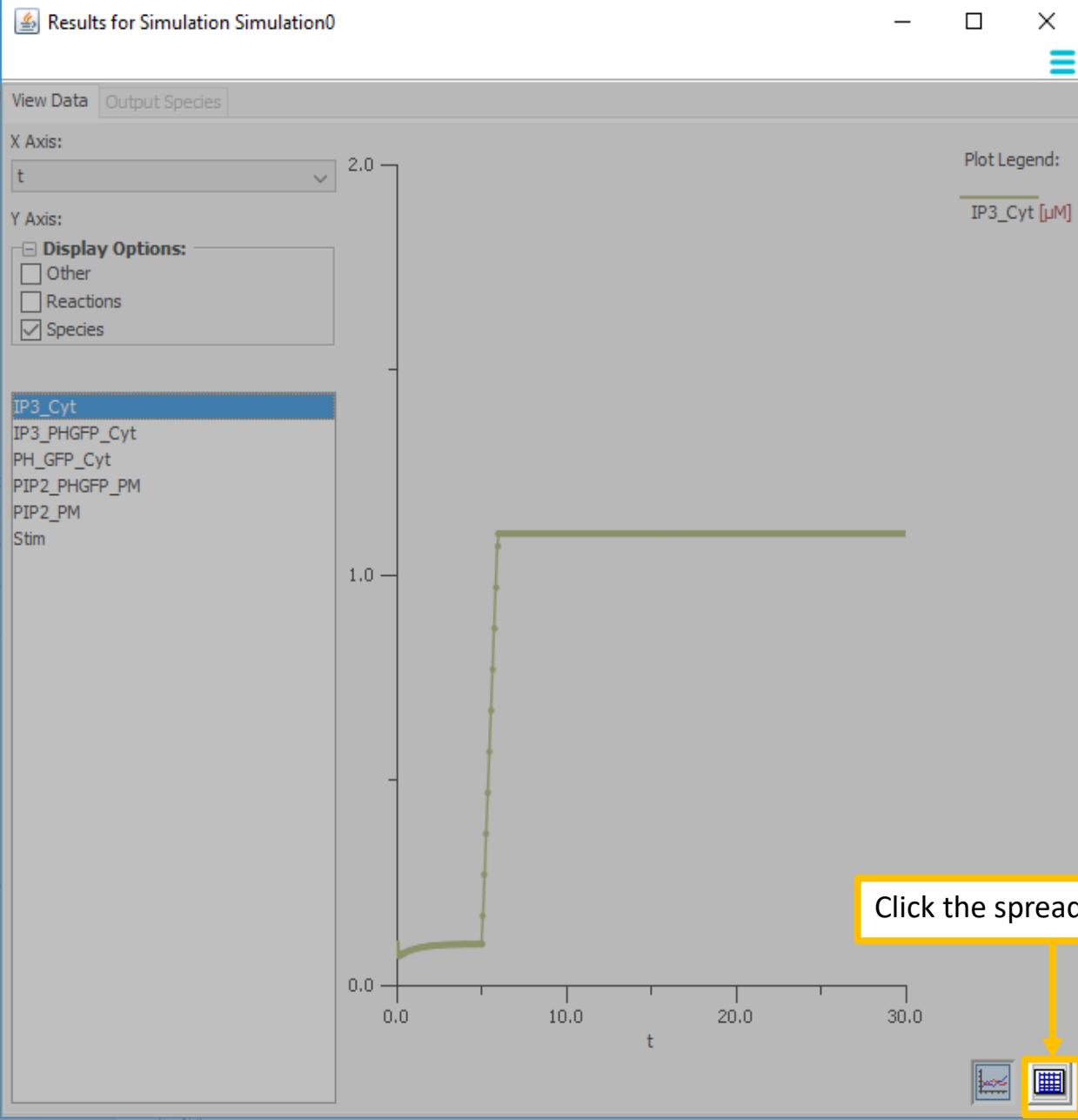
Parameters Functions

VCell DB BMDB Pathway Com

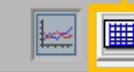
BioModels MathModels Geom

Search

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Click the spreadsheet icon.



**PH-GFP****Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- $\frac{d}{dt}$  Spatial
- $\frac{d}{dt}$  Steady State
  - Geometry
  - Specifications
  - Protocols
  - Simulations
  - Parameter Est.

**Parameter Functions**

VCell DB BMDB Pathway Com

BioModels MathModels Geom

**Search**

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  - Education (31)
  - Published BioModels (16)

Results for Simulation Simulation0

View Data Output Species

X Axis: t

Y Axis:

Display Options:  
 Other  
 Reactions  
 Species

t	IP3_Cyt	IP3_PHG...	PH_GFP_...	PIP2_PH...	PIP2_PM	Stim
0	0.1	0	1	0	120000	0
3.555554...	0.1	3.555540...	1	5.119998...	120000	0
3.640887...	9.999996...	3.640885...	0.99999907	5.242875...	120000	0
1.864134...	9.998136...	1.863500...	0.99952463	0.26837124	119999.73	0
2.563184...	9.974487...	2.551236...	0.99348391	3.6788909	119996.32	0
1.747626...	9.830675...	1.693247...	0.95642258	24.610803	119975.39	0
5.391199...	9.510091...	4.899084...	0.87169108	72.514624	119927.49	0
1.156721...						
2.203597...						
0.03436711						
4.569824...						
5.702937...	7.482350...	2.517649...	0.23697619	433.55314	119566.45	0
6.836051...	7.338522...	2.661477...	0.17845885	467.09233	119532.91	0
7.969164...	7.240900...	2.759099...	0.13449358	492.35235	119507.65	0
9.102277...	7.176842...	2.823157...	0.10144774	511.39342	119488.61	0
0.11164544	7.118729...	2.881270...	6.089878...	534.87819	119465.12	0
0.13204148	0.07108178	0.02891822	3.695457...	548.88562	119451.11	0
0.15243752	7.124698...	2.875301...	2.260610...	557.41374	119442.59	0
0.17283356	7.156915...	2.843084...	1.400310...	562.6581	119437.34	0
0.1932296	7.198097...	2.801902...	8.841236...	565.93315	119434.07	0
0.21362564	7.244238...	2.755761...	5.740675...	568.02614	119431.97	0
0.23769297	7.301858...	2.698141...	3.628369...	569.60588	119430.39	0
0.27440585	7.391884...	2.608115...	2.077015...	571.04643	119428.95	0
0.31111872	7.481316...	2.518683...	1.438359...	571.9472	119428.05	0
0.34783159	0.07568632	0.02431368	1.163109...	572.62199	119427.38	0
0.39115278	7.668224...	2.331775...	1.017166...	573.29294	119426.71	0
0.45723595	7.812586...	2.187413...	9.141058...	574.20176	119425.8	0

Select "IP3\_Cyt" then use the "Shift" key to select the remaining Species.

All of the Species should be selected except "Stim".

**PH-GFP****Physiology**

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- $\frac{d}{dt}$  Spatial
- $\frac{d}{dt}$  Steady State
  - Geometry
  - Specifications
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  - Parameter Est.

**Parameters Functions**

- VCell DB
- BMDB
- Pathway Com

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- MathModels
- Geom

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- + Published BioModels (16)

Results for Simulation Simulation0

View Data Output Species

X Axis: t

Y Axis:

Display Options:  
 Other  
 Reactions  
 Species

	t	IP3_Cyt	IP3_PHGFP...	PH_GFP_Cyt	PIP2_PHGFP...	PIP2_PM
IP3_Cyt	3.9233191	9.9219238E-2	7.8076209E-4	3.1973031E-5	587.11439	119412.89
IP3_PHGFP_Cyt	4.0233191	0.09929066	7.0934006E-4	2.9047312E-5	587.15807	119412.84
PH_GFP_Cyt						
PIP2_PHGFP_PM						
PIP2_PM						
Stim	5	9.9722045E-2	2.7795536E-4	1.1380060E-5	587.42193	119412.58
	5	9.9722045E-2	2.7795536E-4	1.1380060E-5	587.42193	119412.58
	5	9.9			2193	119412.58
	5.0000011	9.9			2193	119412.58
	5.0011528	0.1			2212	119412.58
	5.0691701	0.16890972	2.6036057E-4	1.0499529E-5	587.43279	119412.57
	5.1691701	0.26893245	2.3763063E-4	9.2181383E-6	587.4469	119412.55
	5.2691701	0.36895245	2.1763809E-4	8.1137532E-6	587.45929	119412.54
	5.3691701	0.46897012	1.9996534E-4	7.1749712E-6	587.47023	119412.53
	5.4691701	0.56898581	1.8427228E-4	6.3732961E-6	587.47992	119412.52
	5.5691701	0.66899981	1.7027876E-4	5.6847920E-6	587.48855	119412.51
	5.6691701	0.76901233	1.5775216E-4	5.0902951E-6	587.49626	119412.5
	5.7691701	0.86902359	1.4649810E-4	4.5744009E-6	587.50318	119412.5
	5.8691701	0.96903373	1.3635311E-4	4.1246325E-6	587.5094	119412.49
	5.9691701	1.0690429	1.2717893E-4	3.7308112E-6	587.51502	119412.48
	6	1.0998755	1.2452759E-4	3.6193405E-6	587.51665	119412.48

Scroll down the spreadsheet and find where t = 5.  
Select the cells for “IP3\_Cyt”, “IP3\_PHGFP\_Cyt”, “PH\_GFP\_Ct”,  
“PIP2\_PHGFP\_PM”, and “PIP2\_PM”.

Right click your mouse  
and select “Copy Cells”.

Copy Cells  
Copy Rows  
Copy All

**Reaction Diagram**

- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- Spatial**

  - Geometry
  - Specifications**
  - Protocols
  - Simulations

- Steady State**

  - Geometry
  - Specifications
  - Protocols
  - Simulations

**Geometry Specifications Protocols Simulations**

**Species Reaction Network**

Species	Structure	Depiction	Clamped	Initial Condition	Well Mixed	Diffusion Constant
IP3_Cyt	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	0.0 [μM]		10.0 [μM.s <sup>-1</sup> ]
IP3_PHGFP_Cyt	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	0.0 [μM]		10.0 [μM.s <sup>-1</sup> ]
PH_GFP_Cyt	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	0.0 [μM]		10.0 [μM.s <sup>-1</sup> ]
			<input type="checkbox"/>	0.0 [molecules]		
			<input type="checkbox"/>	0.0 [molecules]		
			<input type="checkbox"/>	0.0 [molecules]		
			<input type="checkbox"/>	0.0 [molecules]		
			<input type="checkbox"/>	0.0 [molecules]		

Go back to "Applications">>"Spatial" and select "Specifications"

Right click the first cell, in the "Initial Condition" column and select "Paste All".

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Description	Parameter	Expression	Units
initial concentration for IP3_Cyt	initConc	0.0	μM
diffusion constant for IP3_Cyt	diff	10.0	μM <sup>2</sup> .s <sup>-1</sup>
Boundary Condition X- for IP3_Cyt	BC_Xm	<zero flux>	μM.μm.s <sup>-1</sup>
Boundary Condition X+ for IP3_Cyt	BC_Xp	<zero flux>	μM.μm.s <sup>-1</sup>
Boundary Condition Y- for IP3_Cyt	BC_Ym	<zero flux>	μM.μm.s <sup>-1</sup>
Boundary Condition Y+ for IP3_Cyt	BC_Yp	<zero flux>	μM.μm.s <sup>-1</sup>
Boundary Condition Z- for IP3_Cyt	BC_Zm	<zero flux>	μM.μm.s <sup>-1</sup>
Boundary Condition Z+ for IP3_Cyt	BC_Zp	<zero flux>	μM.μm.s <sup>-1</sup>
Velocity Y for IP3_Cyt	Vel_Y	<0.0>	μm.s <sup>-1</sup>

CONNECTED 69.2MB / 252.2MB

Reaction Diagram    Geometry    Specifications    Protocols    Simulations

Species    Reaction    Network

Species	Structure	Depiction	Clamped	Initial Condition	Well Mixed	Diffusion Constant
IP3_Cyt						

Choose Parameters to Paste

Select All    Click "Select All".

IP3\_Cyt    initConc    '0.0' -> '0.0997220446381'

IP3\_PHGFP\_Cyt    initConc    '0.0' -> '2.7795536187427'

PH\_GFP\_Cyt    initConc    '0.0' -> '1.1380060296069'

PIP2\_PM    initConc    '0.0' -> '119412.57806689'

PIP2\_PHGFP\_PM    initConc    '0.0' -> '587.42193310183'

Click "OK".

OK    Cancel

Boundary Condition Z+ for IP3\_Cyt BC\_Zp    <zero flux>

Velocity V for IP3\_Cyt Vel\_V    <0.0>

VCell DB    BMDB    Pathway Comm    Sabio

BioModels    MathModels    Geometries

Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Wed Jul 17 17:12:11 EDT 2019
- Shared BioModels (0)
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- Tutorials (9)
- Education (31)
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CONNECTED    69.2MB / 252.2MB

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
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- Species (6)
- Molecules (0)
- Observables (0)

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Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

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Geometry Specifications Protocols Simulations

Species Reaction Network

Species	Structure			Initial Condition	Well Mixed	Diffusion Constant
IP3_Cyt	Cyt			463812545 [μM]	<input type="checkbox"/>	10.0 [μm².s⁻¹]
IP3_PHGFP_Cyt	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	2.779553618742748E-4 [μM]	<input type="checkbox"/>	10.0 [μm².s⁻¹]
PH_GFP_Cyt	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	1.1380060296069762E-5 [μM]	<input type="checkbox"/>	10.0 [μm².s⁻¹]
Stim	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>	$((t>5)&&(t<6.0))$	<input checked="" type="checkbox"/>	
PIP2_PM	PM	<input checked="" type="radio"/>	<input type="checkbox"/>	119412.5780668985 [molecules]	<input type="checkbox"/>	0.1 [μm².s⁻¹]
PIP2_PHGFP_...	PM	<input checked="" type="radio"/>	<input type="checkbox"/>	587.421933101833 [molecules.μm⁻²]	<input type="checkbox"/>	0.1 [μm².s⁻¹]

Check off “Clamped” for “Stim”.

Type “  $((t>5)&&(t<6))$  ” in the “Initial Condition” column for “Stim”.  
Press “Enter” to accept the condition.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Description	Parameter	Expression	Units
initial concentration for Stim	initConc	0.0	μM

CONNECTED 87.2MB / 222.8MB

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
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- Molecules (0)
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Applications (2)

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Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

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- Education (31)
- Published BioModels (164)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

New Simulation End Time Output Option Solver Running Status Results

Click the “Simulations” tab and click the “New Simulation” icon.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

CONNECTED 148.1MB / 222.8MB

The screenshot shows the VCell 7.1.0 software interface for a model named 'PH-GFP'. On the left, there's a tree view of the model components under 'Physiology' and 'Applications'. The 'Simulations' application is selected. In the center, the 'Simulations' tab is active, and the 'New Simulation' icon (a blue plus sign inside a white document icon) is highlighted with a yellow box and an arrow. A large yellow box also surrounds the 'Simulations' tab itself. At the bottom, there are tabs for 'Object Properties', 'Annotations', 'Problems (0 Errors, 1 Warnings)', and 'Database File Info'. The status bar at the bottom indicates 'CONNECTED' and '148.1MB / 222.8MB'.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- d/dt Spatial
- Geometry
- Specifications
- Protocols
- Simulations

d/dt Steady State

Parameters, Functions and Units

Pathway

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
  - multiapp tutorial
  - PH-GFP
    - Private Fri Jul 19 11:59:51 EDT 2019
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- Published BioModels (164)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name Edit Simulation Time Output Option Solver Running Status Results

Simulation1	1.0	every 0.05 s	Fully-Implicit	not saved	no
-------------	-----	--------------	----------------	-----------	----

Click the “Edit Simulation” icon.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol
0.1s	every 0.05 sec	1.0E-7	1.0E-9

Mesh: 51x51x51 = 132651 elements Geometry size: (10.0,10.0,10.0) microns

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

CONNECTED 181.4MB / 222.8MB

- PH-GFP
- Physiology
  - Reaction Diagram
  - Reactions (3)
  - Structures (5)
  - Species (6)
  - Molecules (0)
  - Observables (0)

- Applications (2)
  - Spatial
    - Geometry
    - Specifications
    - Protocols
  - Simulations
- Steady State

## Parameters, Functions and Units

- VCell DB
- BMDB
- Pathway Comm
- Sabio

## BioModels MathModels Geometries

## Search

- Biological Models
  - My BioModels
    - multiapp tutorial
    - PH-GFP
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  - Shared BioModels (0)
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  - Education (31)
  - Published BioModels (164)

Edit: Simulation1

Parameters Mesh Solver

Select the “Mesh” tab.

Leave “Lock aspect ratio” checked and enter “31” for X.  
The other fields should automatically update to 31.

Geometry Size (um) (10.0, 10.0, 10.0)

Mesh Size (elements)  
 Lock aspect ratio  
X 31  
Y 31  
Z 31

Total Size (elements)  $31 \times 31 \times 31 = 29791$

Spatial Step (um)  
 $\Delta x$  0.3333333333333333  
 $\Delta y$  0.3333333333333333  
 $\Delta z$  0.3333333333333333

OK Cancel

- PH-GFP
- Physiology
  - Reaction Diagram
  - Reactions (3)
  - Structures (5)
  - Species (6)
  - Molecules (0)
  - Observables (0)

- Applications (2)
  - Spatial
  - Geometry
  - Specifications
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- d/dt Steady State

## Parameters, Functions and Units

## Pathway

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

## Search

- Biological Models
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    - multiapp tutorial
    - PH-GFP
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  - Tutorials (9)
  - Education (31)
  - Published BioModels (164)

Edit: Simulation1

Parameters Mesh Solver

Select the “Solver” tab.

Choose solver algorithm and fine-tune time conditions:

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

General

Time Bounds

Starting 0.0 Minimum

Ending 20.0 Default

Enter “20.0” for the “Ending Time Bounds”.

Time Step Maximum 0.1

Disable Simulation Run Timeout

Error Tolerance

Output Options

Keep Every time samples and at most

Output Interval 0.2 s

Enter “0.2” for the “Output Interval”.

Miscellaneous

OK Cancel

Click “OK”.

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- Geometry
- Specifications
- Protocols
- Simulations

$d/dt$  Steady State

Parameters, Functions and Units

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

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  - PH-GFP
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Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name Expression Defined In

Add Function Delete Function

Select the “Output Functions” tab and then click “Add Function”.

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

CONNECTED 93.4MB / 227.5MB

The screenshot illustrates the VCell 7.1.0 software interface for editing a BioModel named "PH-GFP". The main workspace is divided into several tabs: Geometry, Specifications, Protocols, Simulations, Output Functions, and Generated Math. The "Output Functions" tab is currently active, indicated by a yellow box and an upward-pointing arrow. Below the tabs, a toolbar features "Add Function" and "Delete Function" buttons, also highlighted with a yellow box and an upward-pointing arrow. A large yellow callout box with the text "Select the ‘Output Functions’ tab and then click ‘Add Function’." is positioned over the central workspace area. On the left, a tree view shows the model's components under "Physiology" and "Applications". The bottom of the screen includes a search bar, a database navigation section with "VCell DB", "BMDB", "Pathway Comm", and "Sabio" tabs, and a "BioModels" section with "MathModels" and "Geometries" options. The bottom right corner shows disk usage information: "93.4MB / 227.5MB".

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- Geometry
- Specifications
- Protocols
- Simulations

$d/dt$  Steady State

VCell

BioModels

My BioModels

- multiapp tutorial
- PH-GFP
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Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Add Function Delete Function Defined In

Name Expression

Type “Fluorescence” for the “Function Name”.

Type, or select the “Species” to define the “Function Expression” as “IP3\_PHGFP\_Cyt+PH\_GFP\_Cyt”.  
\*\*Note that the species names are case sensitive.\*\*

Add Output Function

Function Name: Fluorescence

Function Expression: IP3\_PHGFP\_Cyt+  
↓  
J\_r2  
KFlux\_PM\_Cyt  
Kr\_IP3PH  
Kr\_PIP2\_PH  
PH\_GFP\_cyt  
PIP2\_PHGFP\_PM  
PIP2\_PM  
Size\_Cyt

↑↑ to move; 'Esc' to cancel; 'Enter' to accept;

Object Properties Annotations Problems (0 Errors)

Applications Provenance

$d/dt$  Steady State

$d/dt$  Spatial

Add Output Function

Function Name: Fluorescence

Function Expression: IP3\_PHGFP\_Cyt+PH\_GFP\_Cyt

Next >> Cancel

Click “Next >>”.

This function allows you to look at the sum of all the different species that contribute to the fluorescence signal.

CONNECTED

93.4MB / 227.5MB

File Server Window Tools Help

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- Geometry
- Specifications
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- $d/dt$  Steady State

Parameters, Functions and Units

Pathway

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

- Biological Models
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Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Add Function

Delete Function

Name

Expression

Defined In

Click the drop-down menu and choose "Cyt".

Add Output Function

Defined In: Cyt

&lt;&lt; Previous

Finish

Cancel

Click "Finish".

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

The function appears on the “Simulations”>“Output Functions” tab.  
It will also appear in the simulation results.

Name	Expression	Defined In
Fluorescence	(IP3_PHGFP_Cyt + PH_GFP_Cyt)	Cyt

BIOMODEL: PH-GFP (Tue Jul 23 17:25:02 EDT 2019)

File Server Window Tools Help

Structures (5)  
Species (6)  
Molecules (0)  
Observables (0)

Applications (2)  
d/dt Spatial  
Geometry  
Specifications  
Protocols  
Simulations  
d/dt Steady State

Parameters, Functions and Units

Pathway

Scripting

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models  
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multiapp tutorial  
PH-GFP  
Private Tue Jul 23 17:25:02 EDT 2019

Shared BioModels (0)  
Public BioModels (698)  
Tutorials (9)  
Education (31)  
Published BioModels (164)

Object Properties Annotations Problems (0 Errors, 1 Warnings) Database File Info

Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol
0.1s	every 0.2 sec	1.0E-7	1.0E-9

Mesh: 51x51x51 = 132651 elements

Geometry size: (10.0,10.0,10.0) microns

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

CONNECTED 81.8MB / 314MB

Go to the "Simulations" tab.

Simulations

Run and Save Simulation

Press the green "Run and Save Simulation" icon.

The screenshot shows the VCell 7.1.0 interface for a BIOMODEL named "PH-GFP".

**Left Panel:** A tree view of the model components.

- Structures (5):** Species (6), Molecules (0), Observables (0).
- Applications (2):**
  - Spatial:** Geometry, Specifications, Protocols, Simulations (selected).
  - Steady State:**
- Parameters, Functions and Units**
- Pathway**
- Scripting**

**Bottom Left:** VCell DB, BMDB, Pathway Comm, Sabio tabs; BioModels, MathModels, Geometries buttons; Search bar.

**Bottom Left Tree:** Biological Models, My BioModels, multiapp tutorial, PH-GFP (selected), Private Tue Jul 23 17:25:02 EDT 2019; Shared BioModels (0), Public BioModels (698), Tutorials (9), Education (31), Published BioModels (164).

**Top Center:** A tabbed panel with Geometry, Specifications, Protocols, and Simulations tabs. The Simulations tab is active.

**Simulations View:** A table showing simulation details.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	20.0	every 0.2 s	Fully-Implicit	completed	yes

**Bottom Center:** Object Properties, Annotations, Problems (0 Errors, 1 Warnings), Database File Info tabs.

**Annotation:** Text input field.

**Settings:** Table with Max timestep, Output, Rel tol, Abs tol.

Max timestep	Output	Rel tol	Abs tol
0.1s	every 0.2 sec	1.0E-7	1.0E-9

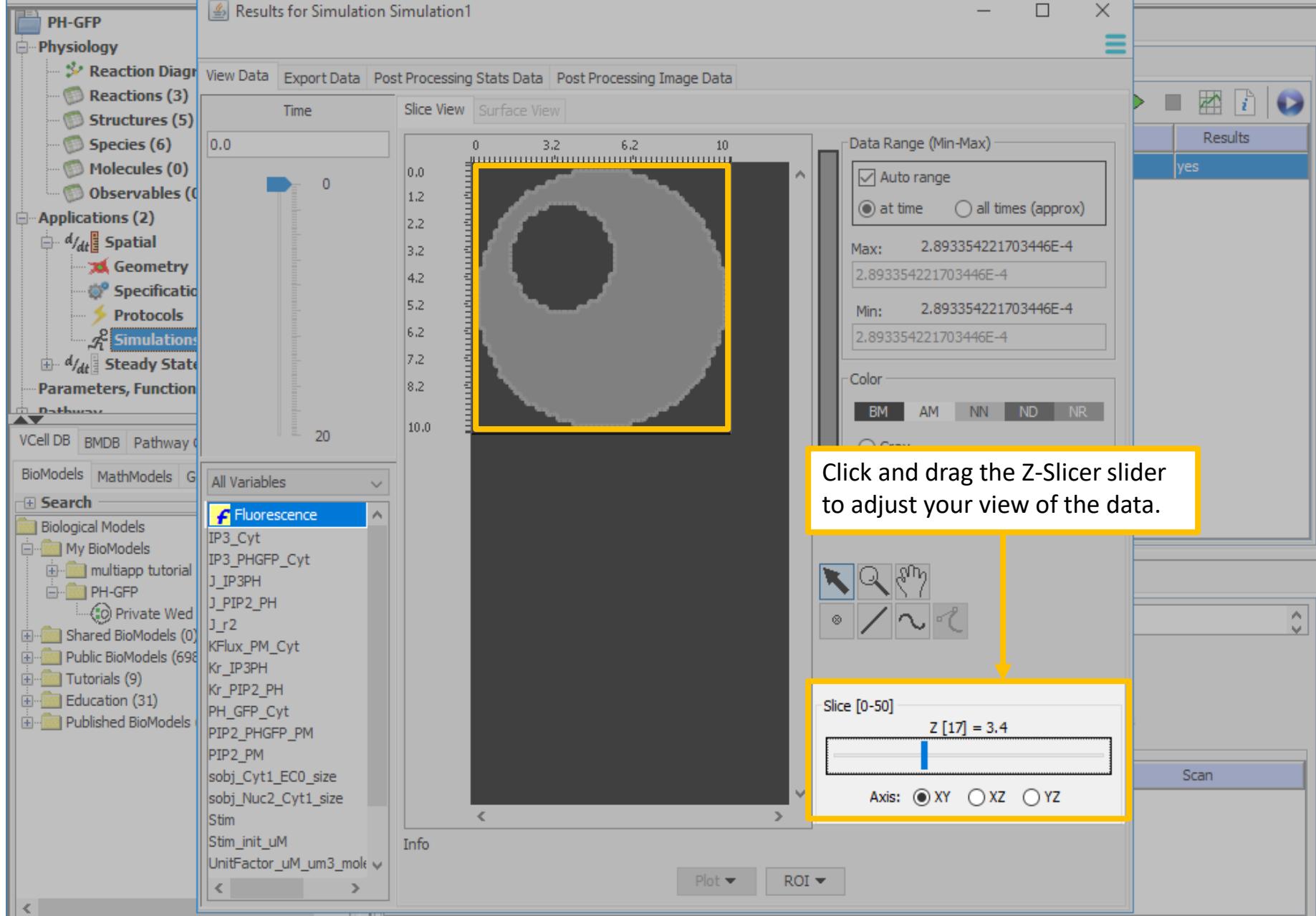
Mesh: 51x51x51 = 132651 elements      Geometry size: (10.0,10.0,10.0) microns

**Bottom Right:** Parameters with values changed from defaults table.

Parameter Name	Default	New Value/Expression	Scan

**Bottom Status Bar:** CONNECTED, 8.1.8MB / 314MB

**Callout:** A yellow box highlights the "Results" icon in the top right of the Simulations view, with the text: "Once your simulation is completed, click the 'Results' icon."



File Server Window Tools

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (2)

- $d/dt$  Spatial
- Geometry
- Specification
- Protocols
- $d/dt$  Simulations
- $d/dt$  Steady State
- Parameters, Functions

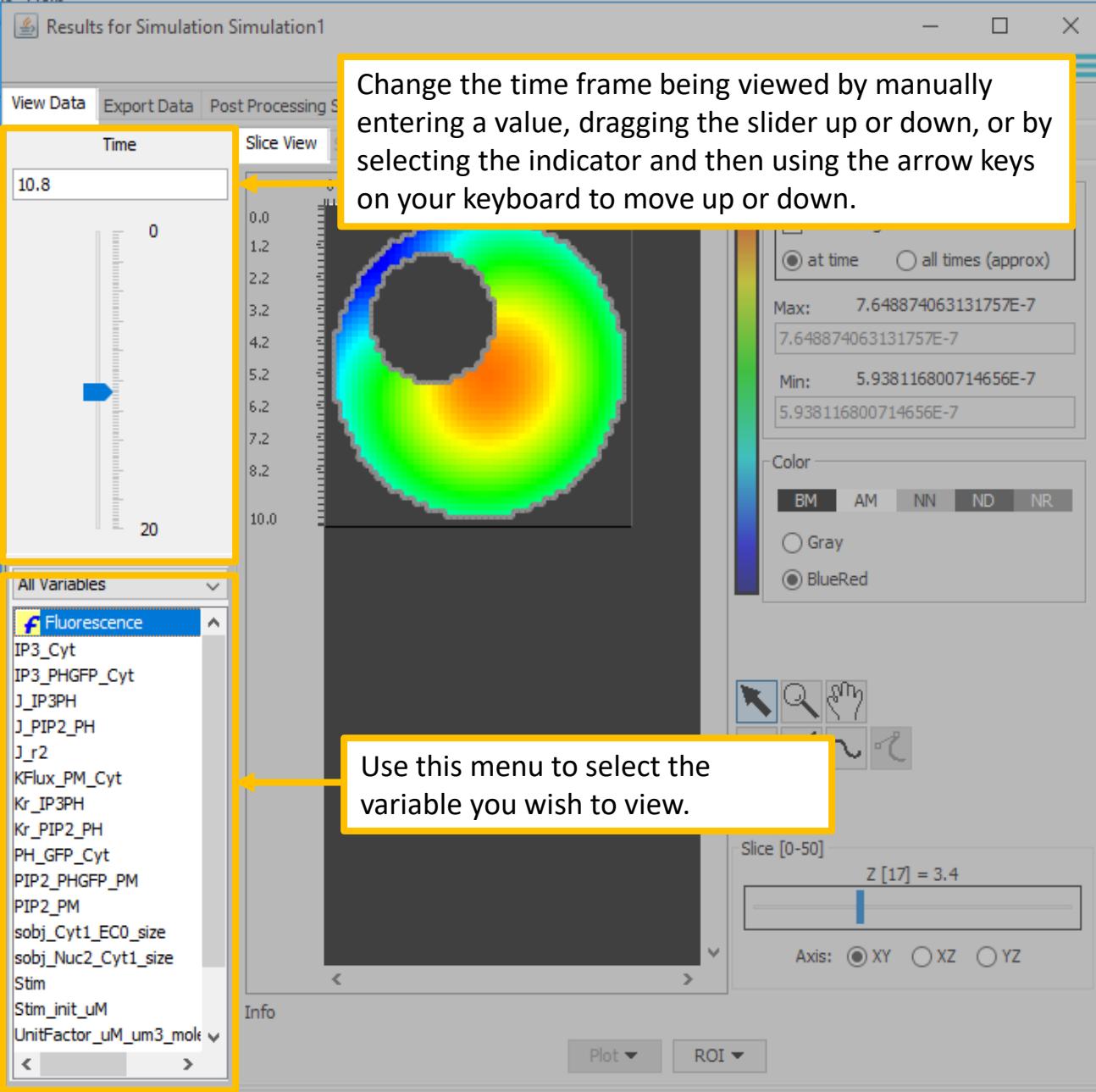
Pathway

VCell DB BMDB Pathway

BioModels MathModels G

Search

- Biological Models
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File Server Window Tools

PH-GFP

Physiology

- Reaction Diagram
- Reactions (3)
- Structures (5)
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- Observables (0)

- Applications (2)
  - d/dt Spatial
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  - Specification
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- d/dt Steady State
- Parameters, Functions

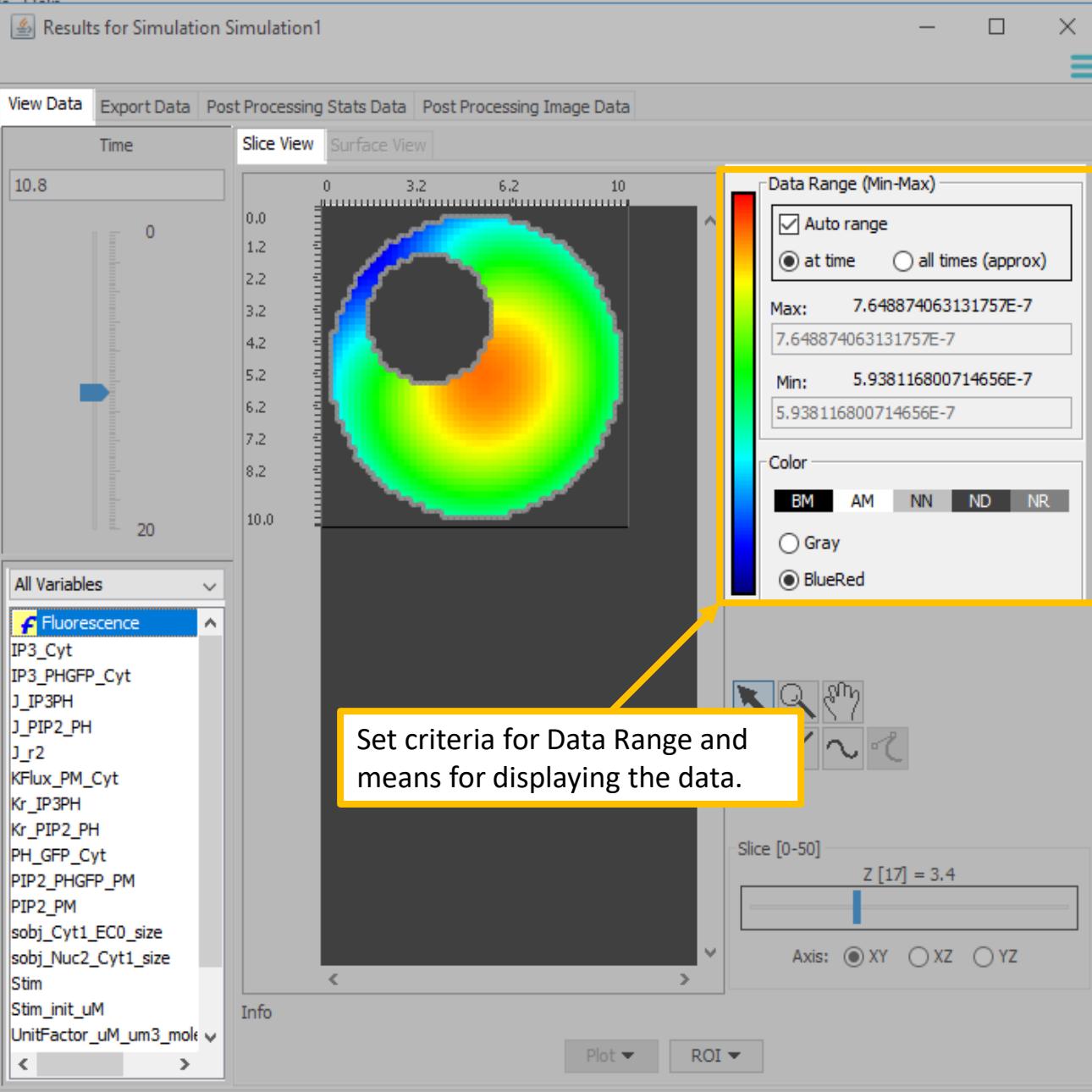
Pathway

VCell DB BMDB Pathway

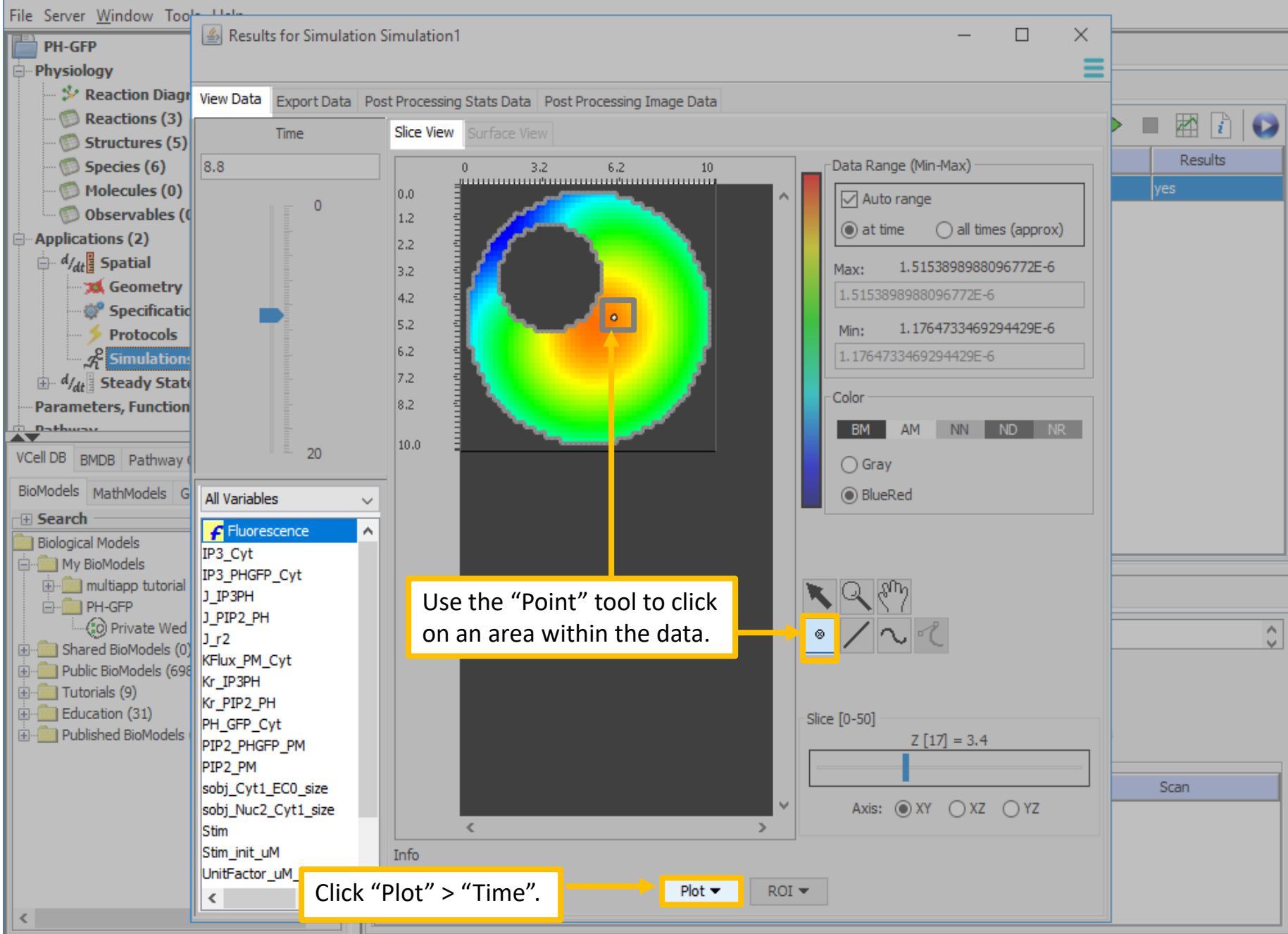
BioModels MathModels G

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- Published BioModels



Scan





File Server Window Tools

PH-GFP

Physiology

Reaction Diagram

Reactions (3)

Structures (5)

Species (6)

Molecules (0)

Observations

Results for Simulation Simulation1

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

Time

Slice View

Surface View

8.8

0

3.2

6.2

10

Data Range (Min-Max)

Time Plot (Volume) [PH-GFP::Spatial]:[Simulation1]:ps=0

Applications

d/dt

S

Selected Points

P[0] (6.0,5.0,3.4)

Time Plot

Plot Legend:

Fluorescence at P[0]

Click on any species to see its graph.

Y Axis

Fluorescence

IP3\_Cyt

IP3\_PHGFP\_Cyt

J\_IP3PH

J\_r2

Kr\_IP3PH

PH\_GFP\_Cyt

Stim

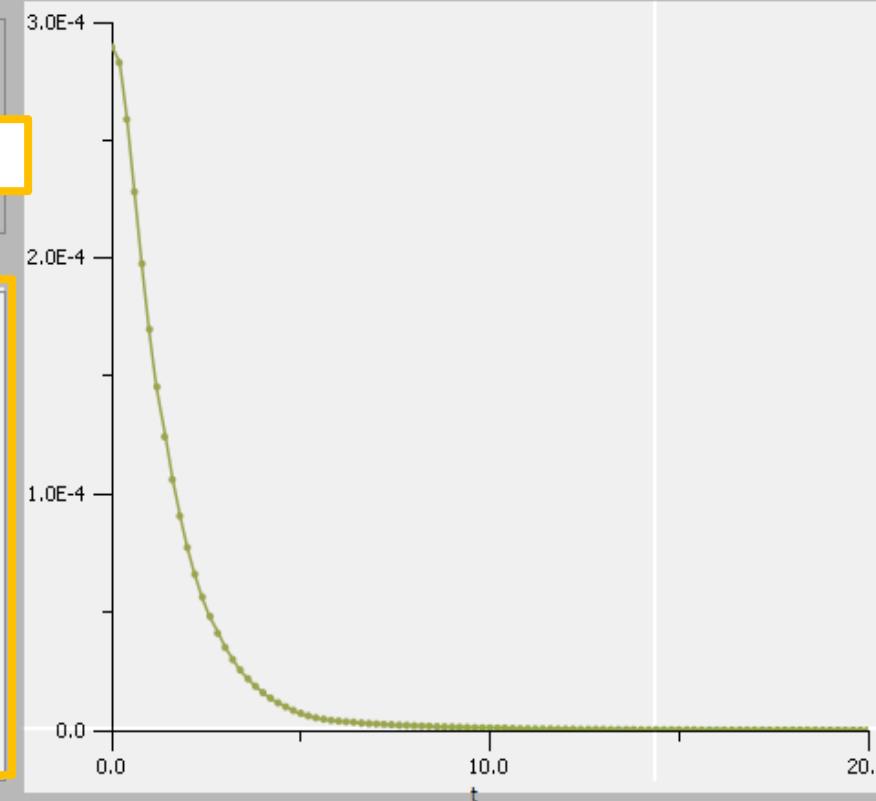
Stim\_init\_uM

UnitFactor\_uM\_um3\_molecules\_neg\_1

vobj\_Cyt1\_size

vobj\_EC0\_size

vobj\_Nuc2\_size

Click to view your  
data; Plot or Table  
view.

1.440E01, 2.181E-07



## Acknowledgements

The following students worked on this tutorial:

Arundeepr Singh (2018) – Sport and Medical Sciences Academy

Zaiba Khan (2018) – East Windsor High School

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