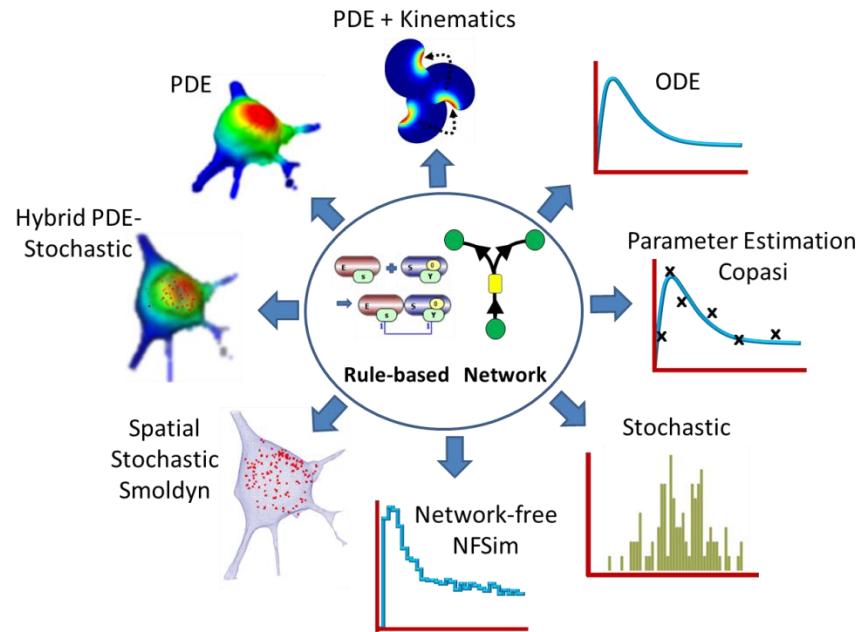


VCell

A modeling environment for the simulation of cellular events. Download at vcell.org.



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

VCell Tutorial

FRAP: Fluorescence Redistribution After Photobleaching

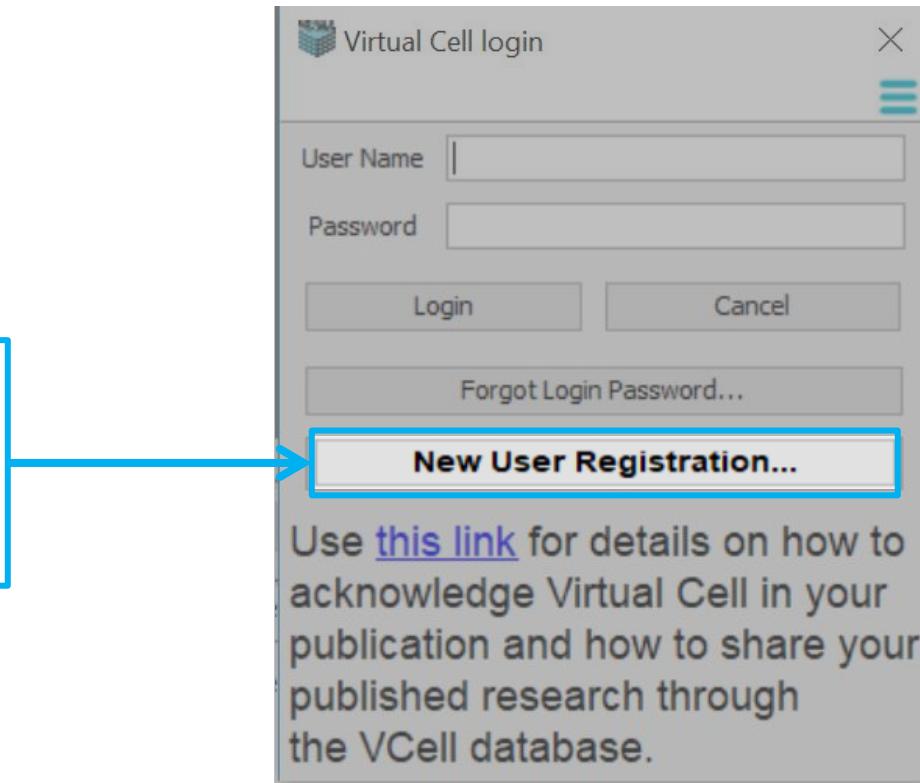
Objective: Create a simple biomodel and spatial (PDE) application to simulate a photobleaching experiment and view the results.

In this tutorial you will:

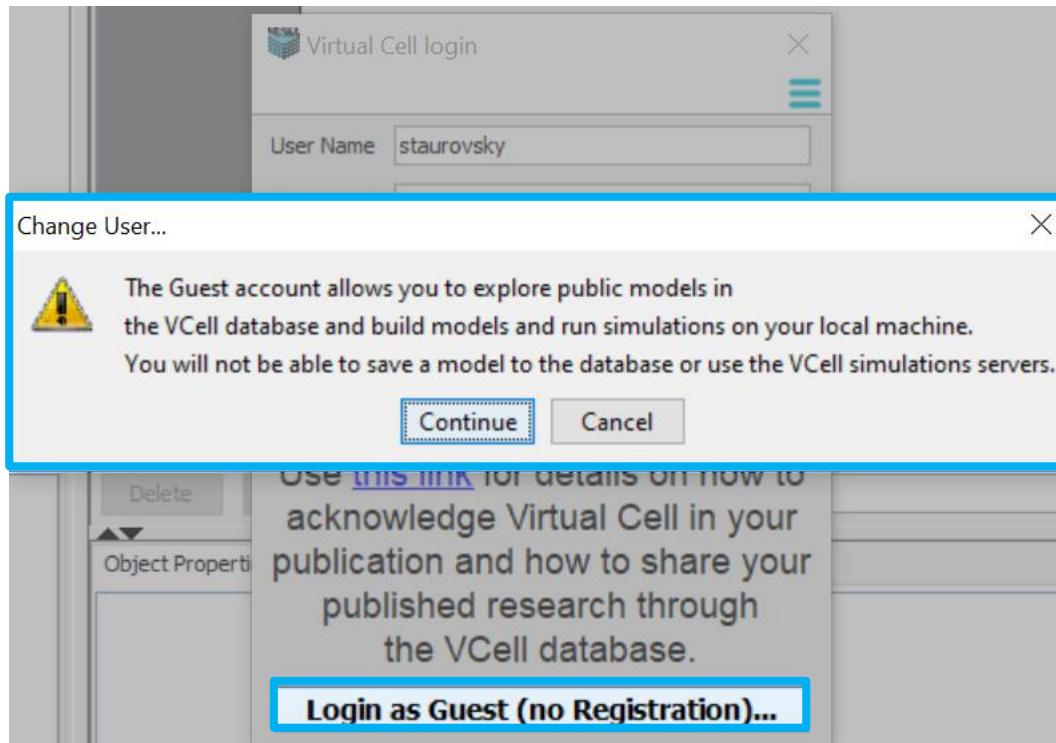
- Gain a basic introduction to the Virtual Cell interface
- Create a very simple biomodel with species but no reactions
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a simple geometry
- Use Boolean expressions to define initial concentrations that are non-uniform
- View and analyze results of a spatial simulation

Your first time opening VCell

You need to register as a New User if you want to run simulations on the VCell compute resources, or use the VCell database to store models that can be shared with collaborators.



Your first time opening VCell Guest Login Option



To re-open a model, click on the folder that the model was saved in and double-click on the model.

The screenshot shows the VCell software interface. On the left, the 'BioModels' search results are displayed under the 'My BioModels' folder. A blue arrow points from the 'SimpleFrap' model entry to the main workspace area. The main workspace contains a reaction diagram with various components like 'c0', a toolbar with icons for selection, zoom, and annotations, and a large empty canvas. At the bottom, there are tabs for 'Object Properties', 'Annotations', 'Problems (0 Errors, 0 Warnings)', and 'Database File Info'. The status bar at the bottom indicates 'CONNECTED' and memory usage '241.5MB / 288.4MB'.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

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

Reaction Diagram Read Tables

EC

Choose the “Select” tool and select the compartment. On the “Object Properties” tab, type “EC” in the “Structure Name” text field and press Enter to accept the entry.

Object Properties (highlighted)
Annotations Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name EC (highlighted)
Size Variable Name EC [μm^3]

VCell DB BMDB Pathway Comm Sabio
BioModels MathModels Geometries
Search
Delete Pathway Links Search
Biological Models
My BioModels
multiapp tutorial
PH-GFP
Shared BioModels (0)
Public BioModels (699)
Tutorials (9)
Education (31)
Published BioModels (164)

CONNECTED 60.7MB / 214.4MB

BIOMODEL: SimpleFrap (Thu Aug 01 16:45:41 EDT 2019) -- VCell 7.1.0 (build 6)

File Server Window Tools Help

SimpleFrap

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
 - SimpleFrap
 - multiapp tutorial
 - PH-GFP
- Shared BioModels (0)
- Public BioModels (699)
- Tutorials (9)
- Education (31)
- Published BioModels (164)

Reaction Diagram Reactions Structures Species Molecules Observables

EC

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

Annotations

User defined cross-references.

Provider PubMed Add...

Text Annotations

Extracellular

CONNECTED 714B / 213.4MB

The screenshot shows the VCell software interface for a model named "SimpleFrap". On the left, there's a tree view of the model components under "Physiology". The main workspace shows a reaction diagram with a node labeled "EC". A large red box highlights this node. Below it, the "Object Properties" panel is open, showing tabs for "Annotations" (which is highlighted with a blue box) and "Problems (0 Errors, 0 Warnings)". A callout bubble with a blue border points to the "Annotations" tab with the instruction: "Select the ‘Annotations’ tab and type ‘Extracellular’ in the ‘Text Annotations’ text field." To the right of the properties panel, a "Text Annotations" field contains the text "Extracellular". At the bottom, there's a status bar indicating "CONNECTED" and memory usage "714B / 213.4MB".

BioModel3

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (1)
- Species (0)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions, Units, etc.
- + Pathway

Reaction Diagram

Reactions Structures Species Molecules Observables

ANN EAL REL AX

c0

Select the compartment tool, and hover over the dotted black lines so that they turn green. Click on the lines to access the “Add Membrane” menu, select “Add Membrane”.

Add Compartment
Add Membrane

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

My BioModels

- MultiAppTutorial
- PH-GFP
- SimpleTrap

Private Thu Aug 01 16:51:27 EDT 2013

Shared With Me (0)

Tutorials (9)

Public BioModels (787)

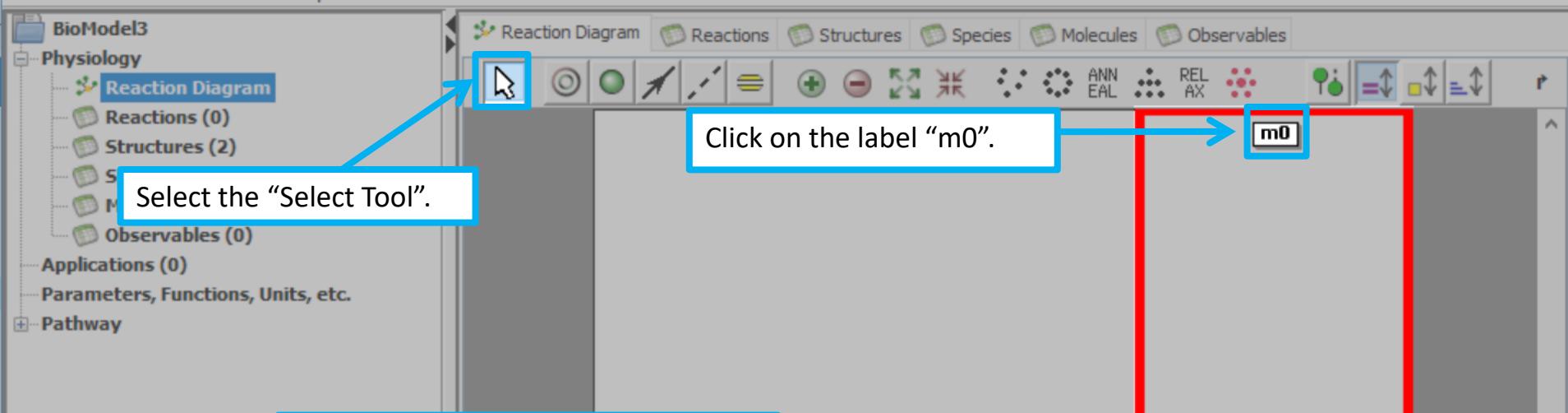
- Published (172)
- Curated (30)
- Uncurated (585)

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

Application Provenance

CONNECTED 112.6MB / 267.4MB

The screenshot shows the VCell 7.2.0 software interface. On the left, there's a navigation pane with a tree view of a model named 'BioModel3'. Under 'Physiology', 'Reaction Diagram' is selected. The main workspace shows a reaction diagram with a compartment labeled 'c0'. A blue callout box with a dashed border contains the instruction: 'Select the compartment tool, and hover over the dotted black lines so that they turn green. Click on the lines to access the “Add Membrane” menu, select “Add Membrane”.' An arrow points from this box to a context menu that appears on the right side of the workspace. This menu has two items: 'Add Compartment' (disabled, greyed out) and 'Add Membrane' (highlighted with a blue background). The top menu bar includes 'File', 'Account', 'Window', 'Tools', and 'Help'. The bottom status bar shows 'CONNECTED' and memory usage '112.6MB / 267.4MB'.



On the Object Properties tab, type
“PM”, for Plasma Membrane,
in the Structure Name text field.

This part of the screenshot shows the 'Object Properties' tab of the VCell interface. At the top, there is a search bar and a 'Delete' button. Below that, the 'Object Properties' tab is active, indicated by a blue border. A blue arrow points from the previous step's callout box to this tab. The 'Structure Name' field is highlighted with a yellow background and contains the text 'PM'. Other fields visible include 'Size Variable Name' (set to 'PM [μm²]'), 'Voltage Variable Name' (set to 'Voltage_PM [mV]'), and sections for 'Electrophysiology', 'Positive (inside feature)', and 'Negative (outside feature)'. A note at the bottom explains membrane voltage calculations and inward currents.

Select only one structure to edit properties

Structure Name PM

Size Variable Name PM [μm^2]

Voltage Variable Name Voltage_PM [mV]

Electrophysiology

Positive (inside feature)

Negative (outside feature)

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 -).

BioModel3

Physiology

Reaction Diagram

Reactions (0)

Structures (2)

Species (0)

Molecules (0)

Observables (0)

Applications (0)

Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

Biological Models

My BioModels

MultiAppTutorial

PH-GFP

SimpleFrap

Private Thu Aug 01 16:51:27 EDT 2013

Shared With Me (0)

Tutorials (9)

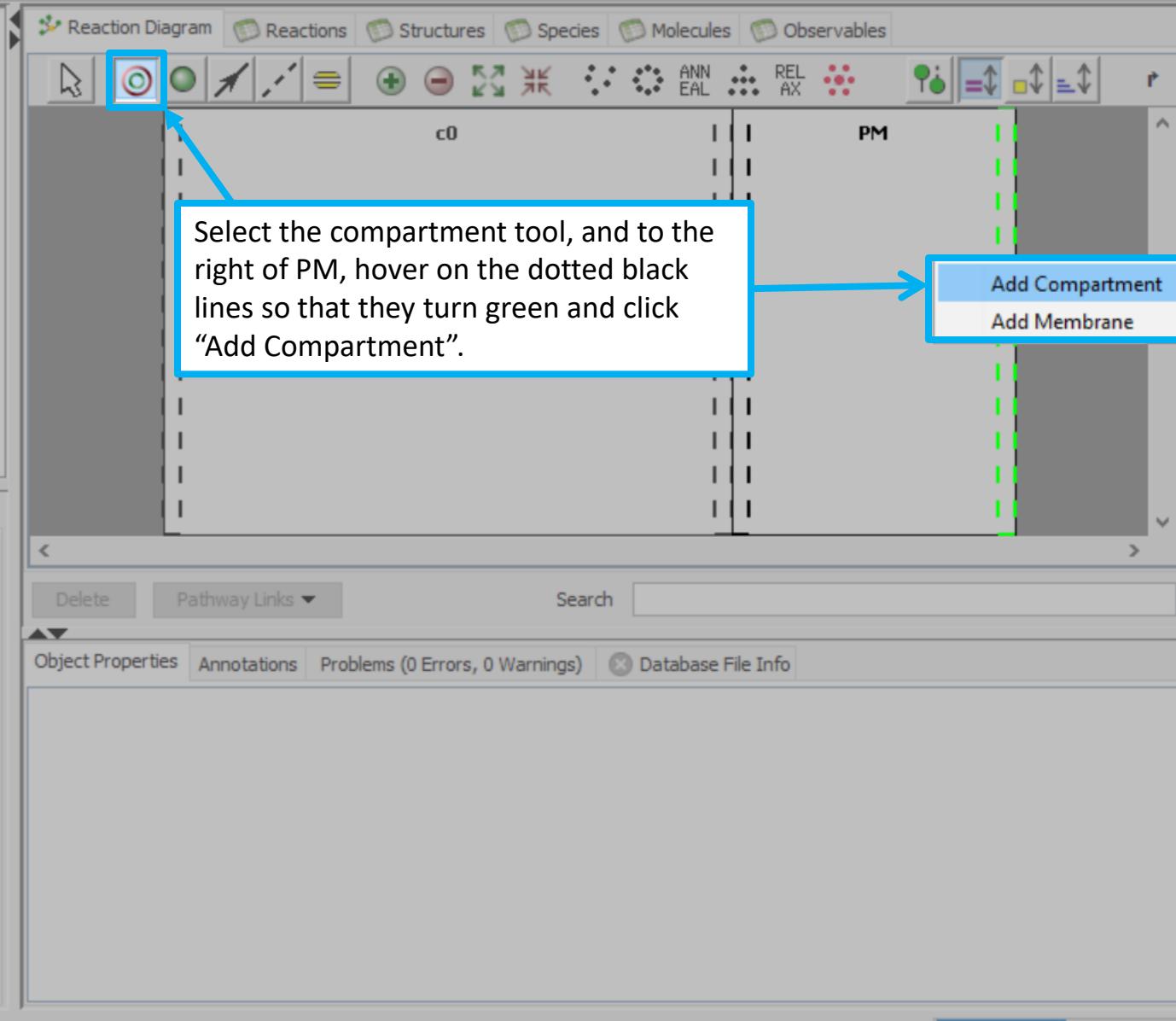
Public BioModels (787)

Published (172)

Curated (30)

Uncurated (585)

CONNECTED





SimpleFRAP2

Physiology

Reaction Diagram

Reactions (0)

Structures (3)

Species (0)

Molecules (0)

Observables (0)

Applications (0)

Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

Biological Models

My BioModels

SimpleFRAP2

MultiAppTutorial

PH-GFP

SimpleFrapp

Private Thu Aug 01 16:51:27 EDT 201

Shared With Me (0)

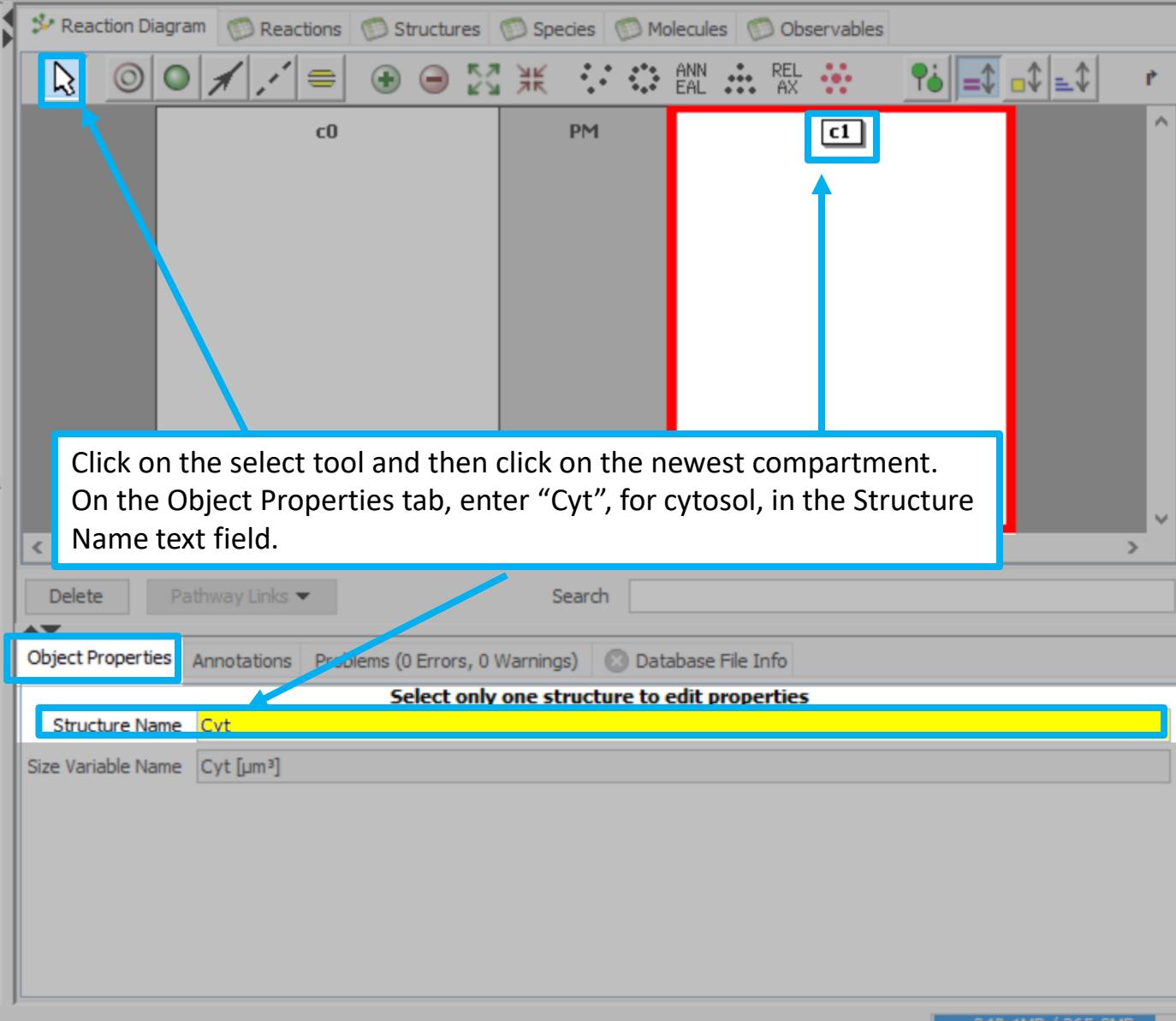
Tutorials (9)

Public BioModels (787)

Published (172)

Curated (30)

Uncurated (585)



SimpleFRAP2

Physiology

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

Applications (0)

Parameters, Functions, Units, etc.

Pathway

Reaction Diagram

Reactions Structures Species Molecules Observables

EC PM Cyt

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

Annotations

User defined cross-references.

Provider PubMed Add...

Text Annotations

Cytosol

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

CONNECTED 230.3MB / 259.5MB

The screenshot shows the VCell 7.2.0 software interface. On the left, there's a navigation pane with sections like 'SimpleFRAP2', 'Physiology', and 'Pathway'. Below it are tabs for 'VCell DB', 'BMDB', and 'Pathway Comm', and buttons for 'BioModels', 'MathModels', and 'Geometries'. A 'Search' section lists various BioModels categories. The main workspace shows a 'Reaction Diagram' with compartments 'EC', 'PM', and 'Cyt' (which is highlighted with a red border). At the bottom, there are tabs for 'Object Properties', 'Annotations' (which is selected and highlighted with a blue border), and 'Problems (0 Errors, 0 Warnings)'. The 'Annotations' tab contains sections for 'User defined cross-references.' and 'Text Annotations'. The 'Text Annotations' section has a text input field containing 'Cytosol' and a 'Delete' button. A large callout box with a blue border and arrow points from the text 'Select the “Annotations” tab and type “Cytosol” in the “Text Annotations” text field.' to the 'Text Annotations' section. The status bar at the bottom right indicates 'CONNECTED' and memory usage '230.3MB / 259.5MB'.

SimpleFRAP2

Physiology

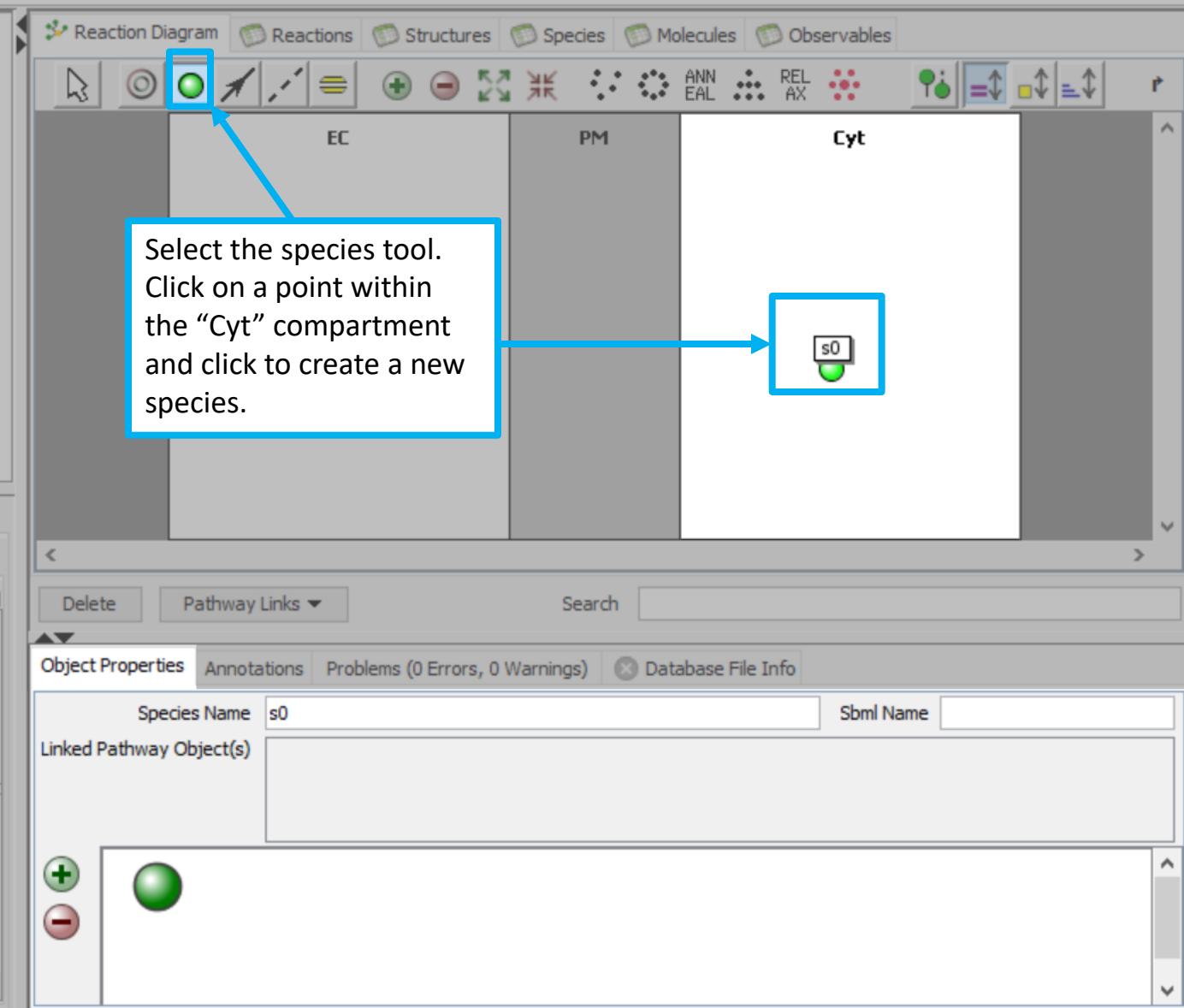
- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions, Units, etc.
- Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

- Biological Models
- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrap
 - Private Thu Aug 01 16:51:27 EDT 20
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)



SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions, Units, etc.

+ Pathway

Reaction Diagram

EC PM Cyt

Dex

On the Object Properties tab, enter "Dex" in the Species Name text field.

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

Species Name Dex Sbml Name

Linked Pathway Object(s)

CONNECTED 134MB / 153.2MB

The screenshot shows the VCell 7.2.0 software interface. On the left, there's a navigation panel with a tree view of the model structure. The 'Reaction Diagram' node is selected. The main workspace shows a grid representing compartments: EC, PM, and Cyt. In the Cyt compartment, there is a green sphere labeled 'Dex'. Below the workspace is a toolbar with various icons. In the bottom right corner, there's a status bar showing memory usage. A callout box with a blue border points from the text above to the 'Species Name' input field in the 'Object Properties' tab of a dialog window. The 'Species Name' field contains the text 'Dex'.

SimpleFRAP2

Physiology

- Reaction Diagram (selected)
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (0)

Parameters, Functions, Units, etc.

Pathway

Reaction Diagram

EC PM Cyt

Dex

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

Annotations

User defined cross-references.

Provider PubMed Add...

Text Annotations

Dextran

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

CONNECTED 147.1MB / 253.2MB

The screenshot shows the VCell 7.2.0 software interface. On the left, there's a navigation pane with sections like 'SimpleFRAP2', 'Physiology', and 'Pathway'. Below it is a search bar and a list of BioModels. The main workspace shows a 'Reaction Diagram' with compartments 'EC', 'PM', and 'Cyt'. A green sphere labeled 'Dex' is present in the Cyt compartment. At the bottom, there's an 'Annotations' tab highlighted with a blue box, and a text field containing 'Dextran' which is also highlighted with a blue box. A callout bubble points to this text field with the instruction: 'Select the “Annotations” tab and type “Dextran” in the “Text Annotations” text field.' The status bar at the bottom right indicates 'CONNECTED' and memory usage '147.1MB / 253.2MB'.

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (0) Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrap
 - Private Thu Aug 01 16:51:27 EDT 2020
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

New Application ▾

- Deterministic
- Stochastic
- Network-Free

Name Math Type Annotation

Go to the Application workspace using the left menu tree. Select “New Application” and choose “Deterministic” from the dropdown menu.

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt Application0

Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

- Biological Models
- My BioModels
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 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
 - Private Thu Aug 01 16:51:27 EDT 2019
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

Name Math Type Annotation

FRAP explicit network model, compartmental, det...

Double click on the Name text field and rename the application as "FRAP". Press "Enter" on your keyboard to accept the entry.

New Application Delete More Copy Actions Compare... Search

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

Application Name Application0

Annotation

Summary

- Deterministic
- Compartmental
- math not generated

The screenshot shows the VCell 7.2.0 interface for editing a model named "SimpleFRAP2". The left sidebar displays the model structure under "SimpleFRAP2" and "Physiology". A callout box highlights the "Applications (1)" section, specifically the "FRAP" application, which is expanded to show "Geometry". The main workspace is titled "Geometry" and contains tabs for "Structure Mapping", "Geometry Definition", and "Kinematics". The "Geometry Definition" tab is selected. It shows a table with one row for "Compartment", which is currently set to "0D, compartmental". A blue box highlights the "Add Geometry" dropdown menu, which has "New..." and "Open from..." options. The bottom right corner of the workspace shows memory usage: "199.4MB / 253.2MB".

Expand the menu tree under Applications>FRAP>Geometry. Select the “Geometry” application and then “Geometry Definition” on the Geometry tab. Go to “Add Geometry” and select “New”.

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt FRAP
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

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

Geometry type

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

OK Cancel

Front Back Add Subdomain Delete

Click “Analytic Equations (2D)”, then press “OK”.

OK

Cancel

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

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

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrap
 - Private Thu Aug 01 16:51:27 EDT 2019
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Name	Value
subdomain0	1.0

Slice View Surface View C

Front Back Add Subdomain ▾ Delete

Double click on “Subdomain0” and type in “EC”. Press “Enter” on your keyboard to accept the entry.

Object Properties Annotations Problems (0 Errors, 4 Warnings) Database File Info

File Account Window Tools Help

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

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

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

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 - Private Thu Aug 01 16:51:27 EDT 2019
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

CONNECTED

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Name	Value
EC	1.0

Front Back Add Subdomain ▾

Click "Add Subdomain", select "Analytic".

Analytic ... Constructed Solid Geometry

Slice View Surface View Geometric Region Details

0 3 6 10
0.0 1.0 2.0 3.0

Info

Object Properties Annotations * Problems (0 Errors, 4 Warnings) * Database File Info

129.8MB / 247.5MB

File Account Window Tools Help

SimpleFRAP2**Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt FRAP
- Geometry

Type in "0,0" for the Center Point.

Type in "10" for the radius.

CONNECTED

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Select "Circle" from the drop down menu.

Define New Subdomain Shape

Select Subdomain Shape: Circle

Center Point (x,y)
0,0

Radius
10.00

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

Copy Expression

Help New Subdomain Cancel

Click "Add New Subdomain".

169MB / 247.4 MB

SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

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

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

Biological Models

- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
 - Private Thu Aug 01 16:51:27 EDT 2020
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Name	Value
subdomain0	2.0 $(x < 10.0) \wedge (y < 10.0) \wedge (x + y < 10.0)$
EC	1.0

Front Back

Slice View Surface View Geometric Region Details

0 3 6 10

0.0 1.0 2.0 3.0

Info

Object Properties Annotations Problems (0 Errors, 6 Warnings) Database File Info

CONNECTED 207.1MB / 247.5MB

Double click on the name box of the new subdomain and type in "Cyt", press "Enter".

File Account Window Tools Help

SimpleFRAP2

Physiology

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

Applications (1)

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

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

Search

- Biological Models
- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
 - Private Thu Aug 01 16:51:27 EDT 2020
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Name	Value
chain0	2.0 2.0 2.0 $((x) + (y)) < (10.0)$
LC	1.0

Front Back Add Subdomain ▾ Delete

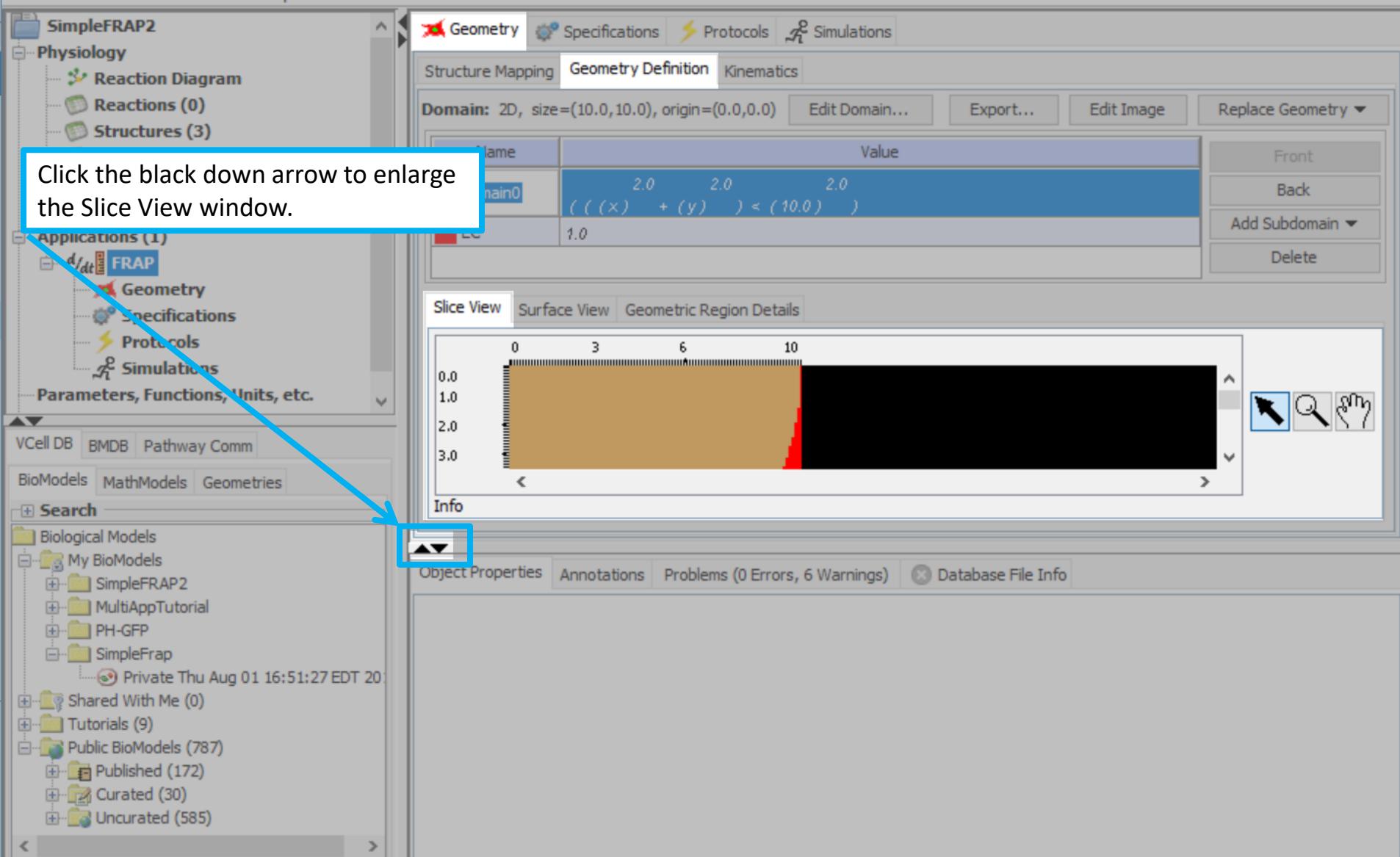
Slice View Surface View Geometric Region Details

0 3 6 10

0.0 1.0 2.0 3.0

Info

Object Properties Annotations Problems (0 Errors, 6 Warnings) Database File Info



SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt FRAP
- Geometry
- Specifications
- Protocols

Geometry

Structure Mapping Geometry Definition Kinematics

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

Name	Value
subdomain0	2.0 2.0 2.0 $((x) + (y)) < (10.0)$
EC	1.0

Front

Back

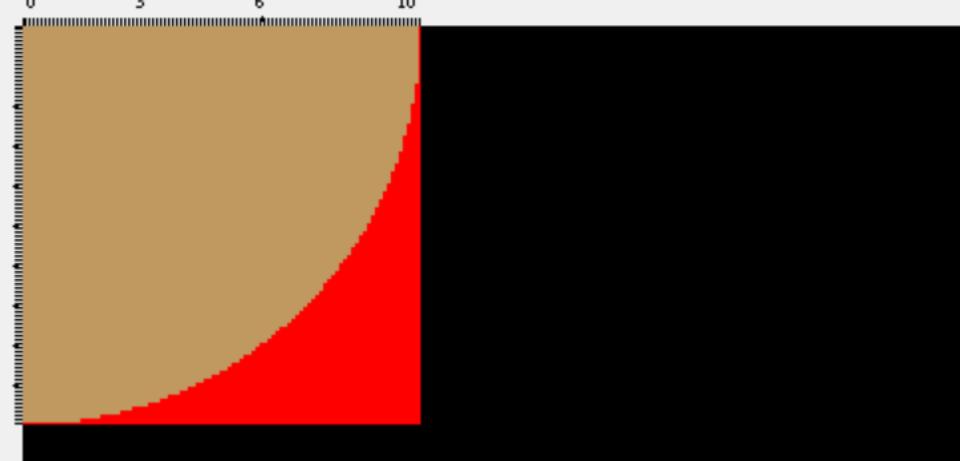
Add Subdomain ▾

Delete

Slice View Surface View Geometric Region Details

0 3 6 10

3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0



Info

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
 - Uncurated (585)

CONNECTED

207.1MB / 247.5MB

Click the black up arrow to minimize the Slice View window.



SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

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

Parameters, Functions, Units, etc.

VCell DB BMDB Pathway Comm

BioModels MathModels Geometries

+ Search

- Biological Models
- My BioModels
 - SimpleFRAP2
 - MultiAppTutorial
 - PH-GFP
 - SimpleFrapp
 - Private Thu Aug 01 16:51:27 EDT 20
- Shared With Me (0)
- Tutorials (9)
- Public BioModels (787)
 - Published (172)
 - Curated (30)
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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Edit Domain...

Export...

Edit Image

Replace Geometry ▾

Select "Edit Domain"

Geometry Size

Size X 22 μm Y 22 μm Z 10.0 μm

Origin X -11 μm Y -11 μm Z 0.0 μm

OK

Cancel

Enter the following values for:

"Size": 22 for X and Y

"Origin": -11 for X and Y.

Press "OK" to accept your entries.

SimpleFRAP2

Physiology

- Reaction Diagram
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Click "Front" or "Back" to rearrange the geometry order.
The order determines which subdomain a point in space belongs to; the front layer "hides" layers below.

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

Name	Value
Cyt	2.0 2.0 2.0 $((x) + (y)) < (10.0)$
EC	1.0

Front

Back

Add Subdomain ▾

Delete

Your geometry in the "Slice View" option should be a circle of radius 10 μm , inside a 22 X 22 μm square.

Slice View Surface View Geometric Region Details

-11 -4.4 2.2 11

-11.0 -8.8 -6.6 -4.4 -2.2 0.0 2.2 4.4 6.6 8.8 11.0

Info

2020-04-15 10:57:52 EDT 2020 -- VCell 7.2.0 (build 39)

Select the "Structure Mapping" tab, on the "Geometry" tab.

Use the Line tool to drag a line from the structures to their corresponding subdomains. You must select the line tool each time you create a new mapping.

Be sure your mapping says "Resolved" to complete the mapping.

Structure Mapping

Geometry Definition Kinematics

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Structure Subdomain Size Ratio X- X+ Y- Y+

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

Geometry (subdomains)

- Cyt
- EC
- Cyt_EC_membrane

RESOLVED>>

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106.7MB / 304.6MB

Click the “Specifications” tab, and then the “Species” tab.

Species Reaction Network

Species	Structure	Depiction	Clamped	Rules	Initial Co...	Well Mixed	Diffusion...
Dex	Cyt	<input checked="" type="radio"/>	<input type="checkbox"/>		<input type="text" value="(10.0 * ((x < -5.0) (x > 5.0) (y < -5.0) (y > 5.0)))"/>	<input type="checkbox"/>	<input type="text" value="10.0 [μM]"/>

Double click on the “Initial Condition” box for Dex and type in:
“(10.0*((x<-5.0)|| (x>5.0)|| (y<-5.0)|| (y>5.0)))”.
Press “Enter” on your keyboard to accept your entry.

This Boolean expression for the initial concentration evaluates to 10 μM everywhere except from x = -5 to 5 and from y = -5 to 5, where the expression evaluates to 0.

Geometry Specifications Protocols Simulations

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Search

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SimpleFRAP2

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

Description	Parameter	Expression	Units
initial concentration for Dex	initConc	$10.0 \cdot ((x < -5.0) \parallel (x > 5.0) \parallel (y < -5.0) \parallel (y > 5.0))$	μM
diffusion constant for Dex	diff	20.0	μm ² .s ⁻¹
Boundary Condition X- for Dex	BC_Xm	<zero flux>	μM.μm.s ⁻¹

241.3MB / 304.6MB

Type “20” in the “Diffusion Constant” text field.
Press “Enter” to accept your entry.

Click "Simulations" and the New Simulation icon.

The screenshot shows the VCell software interface. On the left, there is a navigation pane with sections like 'SimpleFRAP2', 'Physiology', 'Applications (1)', 'Parameters, Functions, Units, etc.', and 'Pathway'. Below this are tabs for 'VCell DB', 'BMDB', and 'Pathway Comm'. A 'Search' section lists 'Biological Models', 'Shared With Me (0)', 'Tutorials (9)', and 'Public BioModels (787)'. A status bar at the bottom left says 'CONNECTED'.

The main workspace has tabs for 'Geometry', 'Specifications', 'Protocols', and 'Simulations'. The 'Simulations' tab is active, showing a table with one row:

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	every 0.05 s	Fully-Implicit	not saved	no

A blue box highlights the 'Simulations' tab, and another blue box highlights the 'New Simulation' icon (a plus sign inside a document icon) in the toolbar above the table. A callout box with a blue border points to the 'Simulation0' row with the text: "Double click on 'Simulation0' and type in 'FRAP'. Press 'Enter' to accept your entry."

At the bottom, there are tabs for 'Object Properties', 'Annotations', 'Problems (0 Errors, 0 Warnings)', and 'Database File Info'. The 'Annotations' tab is selected, showing an empty input field. Below it, a 'Settings' table shows values for 'Max timestep' (0.1s), 'Output' (every 0.05 sec), 'Rel tol' (1.0E-7), and 'Abs tol' (1.0E-9). The 'Mesh' is listed as '101x101 = 10201 elements' and the 'Geometry size' is '(22.0,22.0) microns'.

SimpleFRAP2

Physiology

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Parameters, Functions, Units, etc.

Pathway

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name End Time Edit Simulation Output Option Solver Running Status Results

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

Click the “Edit Simulation” icon.

Object Properties Annotations Problems (0 Errors, 0 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: 101x101 = 10201 elements Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

CONNECTED 64.7MB / 347.6MB

Select the “Mesh” tab.

Leave “Lock aspect ratio” option checked.
Type in “51” for X “Mesh Size”.

Next, select the “Solver” tab.

OK Cancel

SimpleFRAP2

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Parameters, Functions, Units, etc.

Pathway

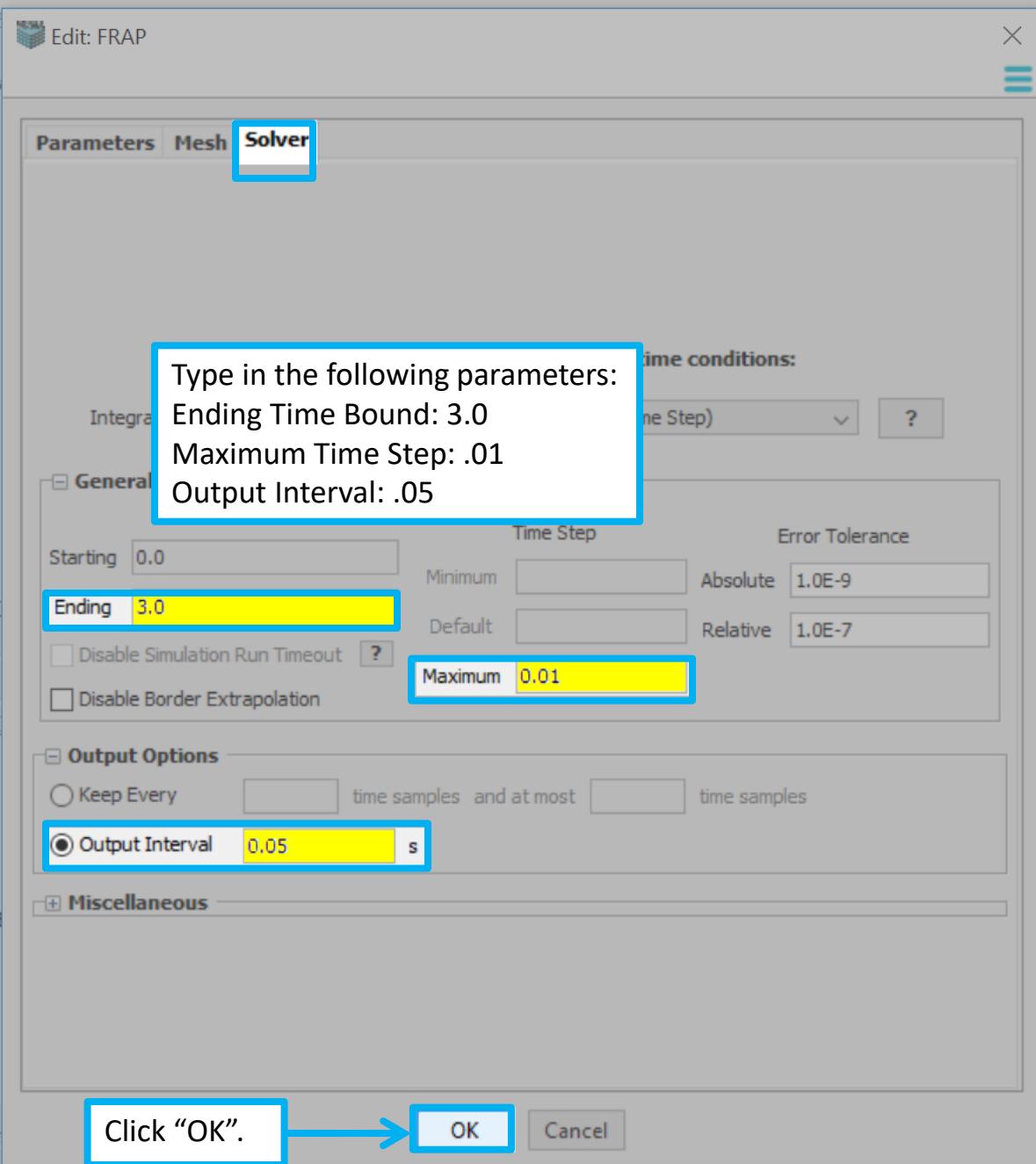
VCell DB BMDB Pathway Comm

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File

- New
- Open
- Close
- Ctrl+W
- Save**
- Save New Version
- Save As...
- Save As Local...
- Revert to Saved
- Compare with Saved
- Permissions...
- Field Data...
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- Export...
- Exit

BioModels MathModels Geometries

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Prior to running your simulation, first save your model.

Go to “File”, and then to one of the save options.

232.3MB / 347.6MB

SimpleFRAP2

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Parameters, Functions, Units, etc.

Pathway

VCell DB BMDB Pathway Comm

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Search

[Advanced >>](#)

Search

Show All

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Selected BioModel Summary

Type in a name for your FRAP model,
then click the “Save” button.

Please type a new name:

SimpleFrap

Save

Cancel

File Info

try size: (22.0,22.0) microns

163.3MB / 347.6MB

SimpleFRAP2

Physiology

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

Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol
0.01s	every 0.05 sec	1.0E-7	1.0E-9

Mesh: 51x51 = 2601 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

Simulations

Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
FRAP	3.0	every 0.05 s	Fully-Implicit	not saved	no

Press the green "Play" button to run the simulation.

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SimpleFRAP2

Physiology

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (1)
- Molecules (0)
- Observables (0)

Applications (1)

- d/dt FRAP
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Parameters, Functions, Units, etc

Pathway

VCel DB BMDB Pathway Comm

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+ Search

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Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

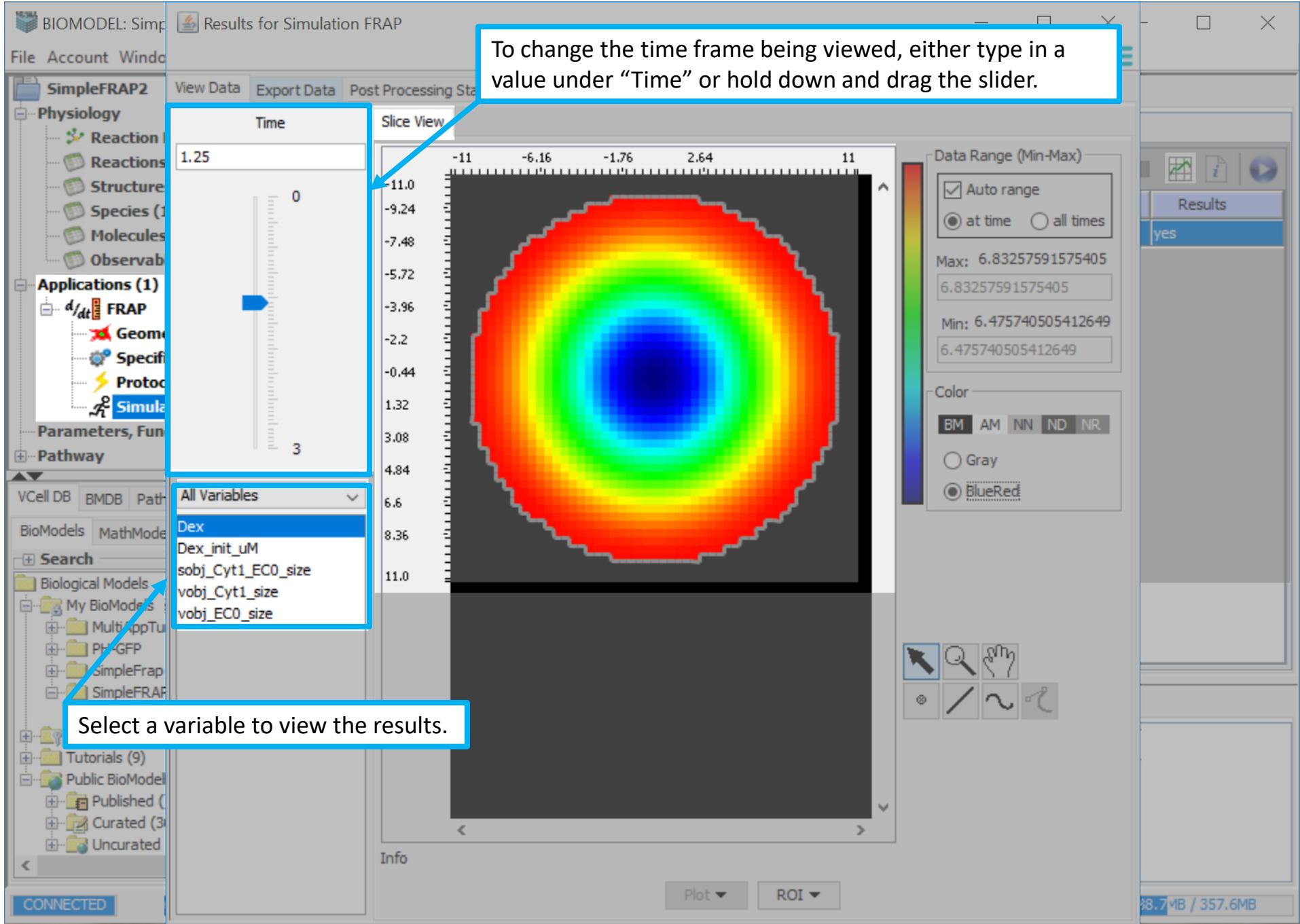
Name	End Time	Output Option	Solver	Running Status	Results
FRAP	3.0	every 0.05 s	Fully-Implicit	completed	yes

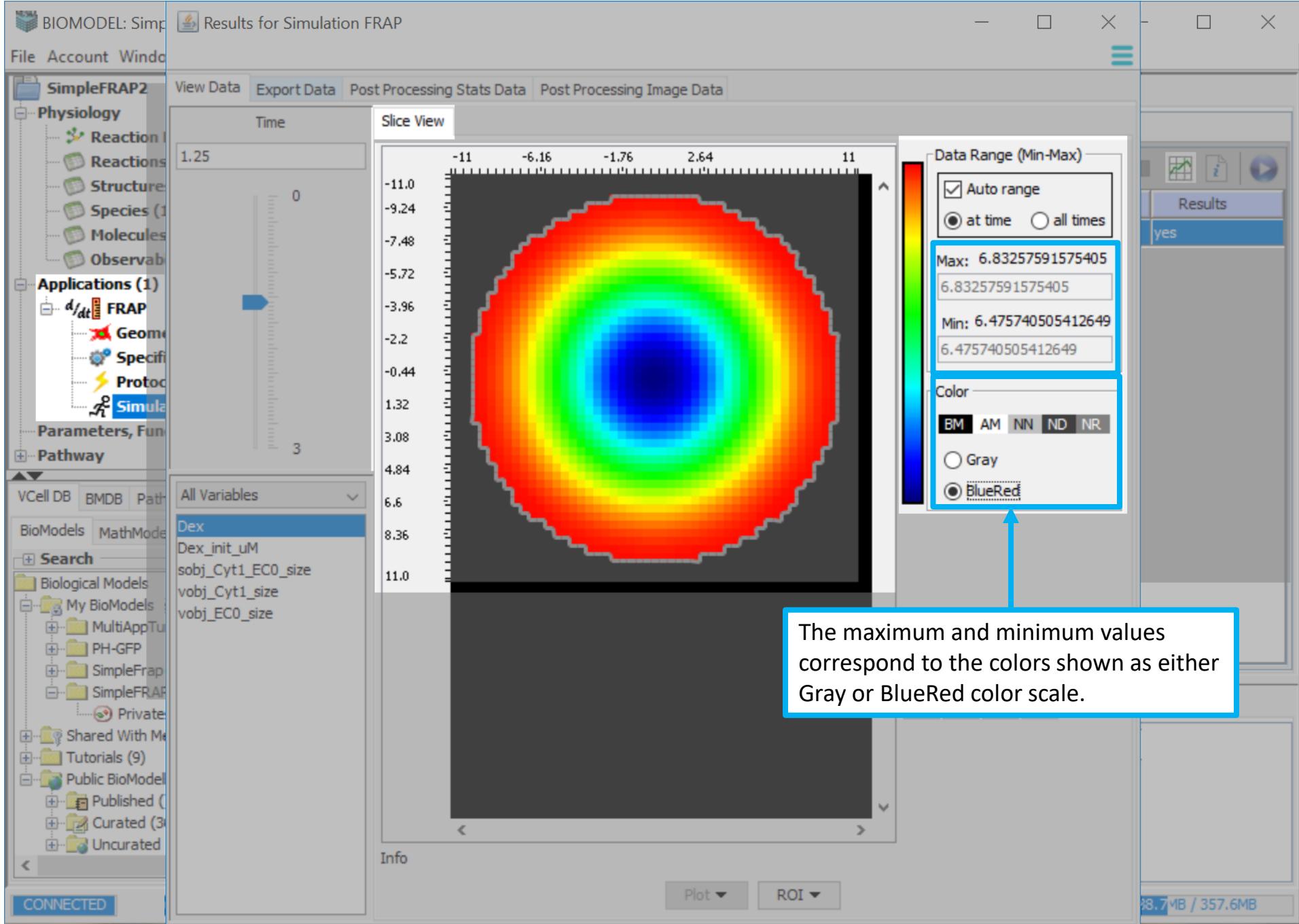
You can view the status of your simulation, under "Running Status". You can view the results as soon as there are time points saved to the database.

In order to see your results, make sure the simulation is selected, and then press the "Results" icon.

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

138.7 MB / 357.6 MB





File Account Window

SimpleFRAP2

Physiology

- Reaction
- Reactions
- Structure
- Species (1)
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- $\frac{df}{dt}$ FRAP
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Parameters, Fun

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VCell DB BMDB Path

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Search

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Public BioModel

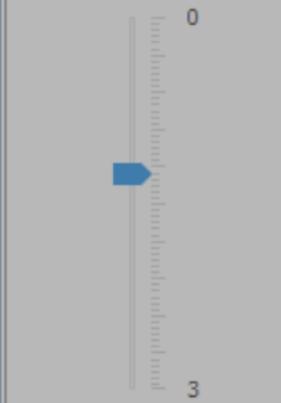
- Published (
- Curated (3)
- Uncurated

CONNECTED

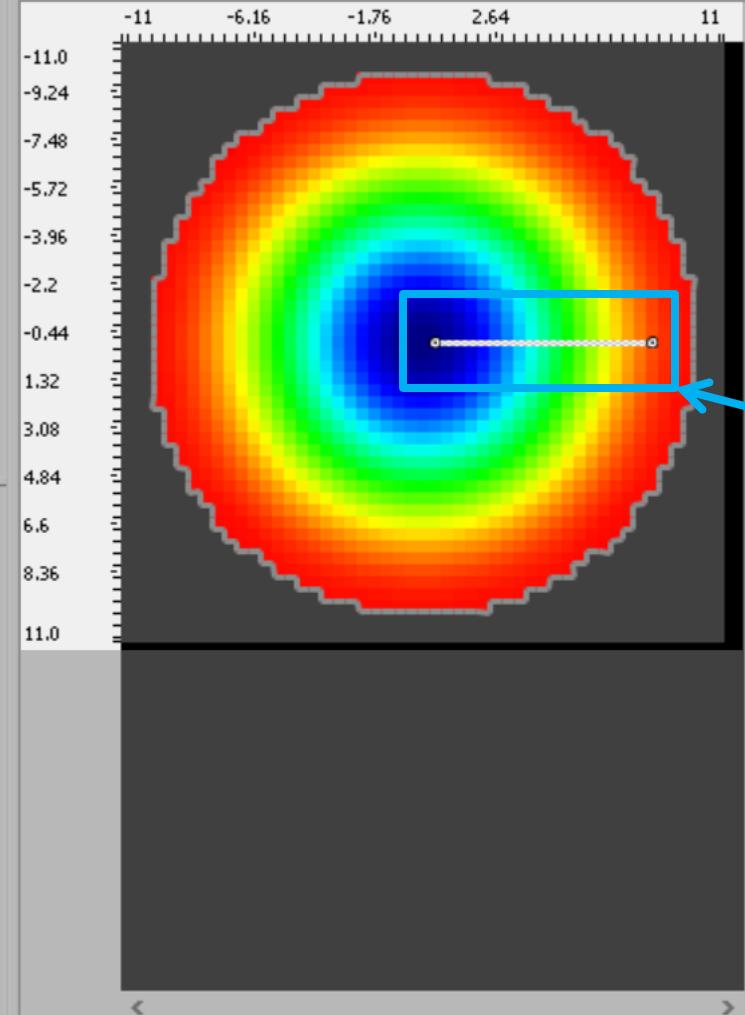
View Data Export Data Post Processing Stats Data Post Processing Image Data

Time

1.25



Slice View



Data Range (Min-Max)

- Auto range
- at time
- all times

Max: 6.83257591575405

6.83257591575405

Min: 6.475740505412649

6.475740505412649

Color

BM AM NN ND NR

All Variables

Dex

- Dex_init_uM
- sobj_Cyt1_EC0_size
- vobj_Cyt1_size
- vobj_EC0_size

To view the data, click
"Plot" > "Spatial".

Plot ▾

ROI ▾



Select the line tool, click on a point within the data and click on another point. A line will form and connect the two points.

38.7 MB / 357.6 MB

