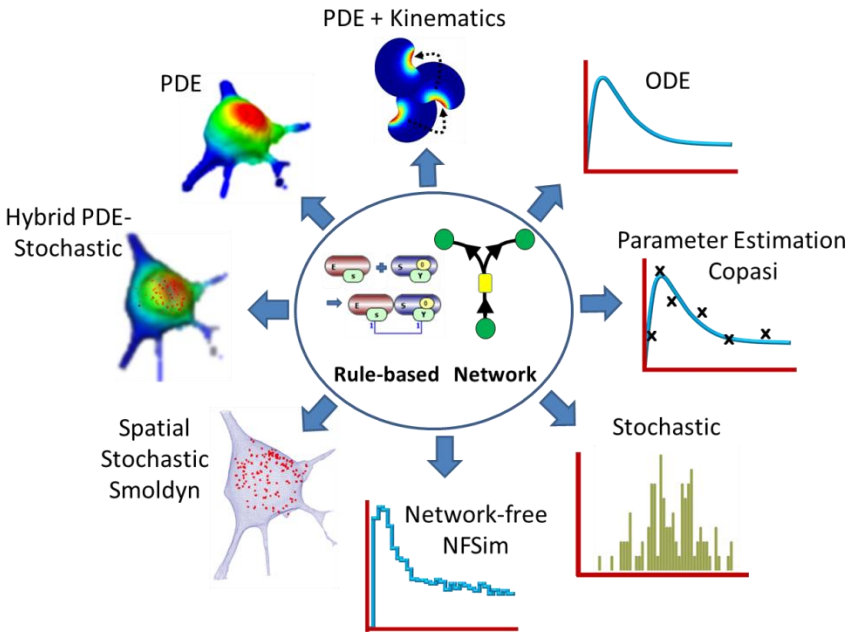
VCell

modeling environment for mathematical simulation of cellular events.

To run VCell go to:

vcell.org



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

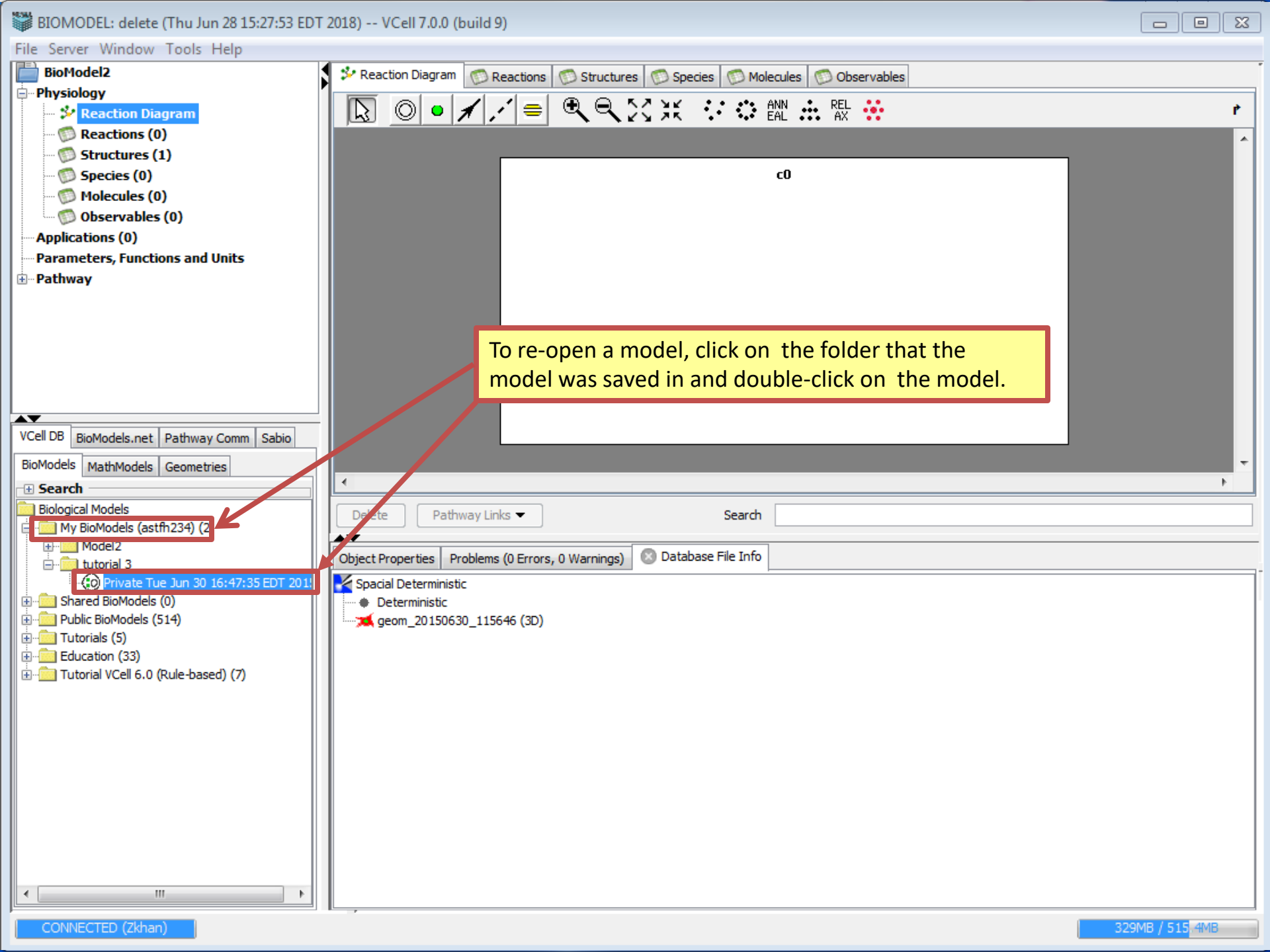
VCell Tutorial

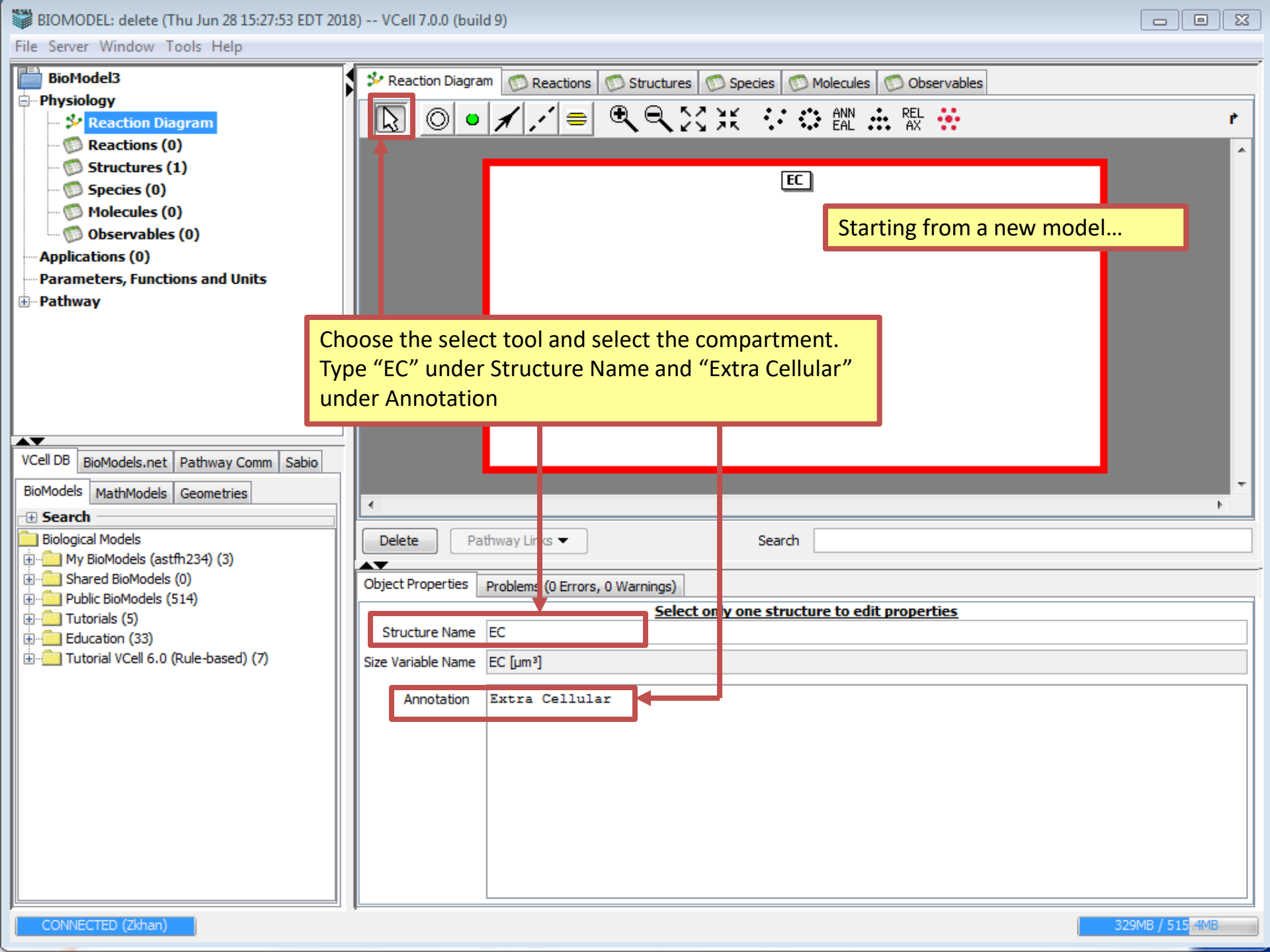
FRAP: Fluorescence Redistribution After Photo bleaching

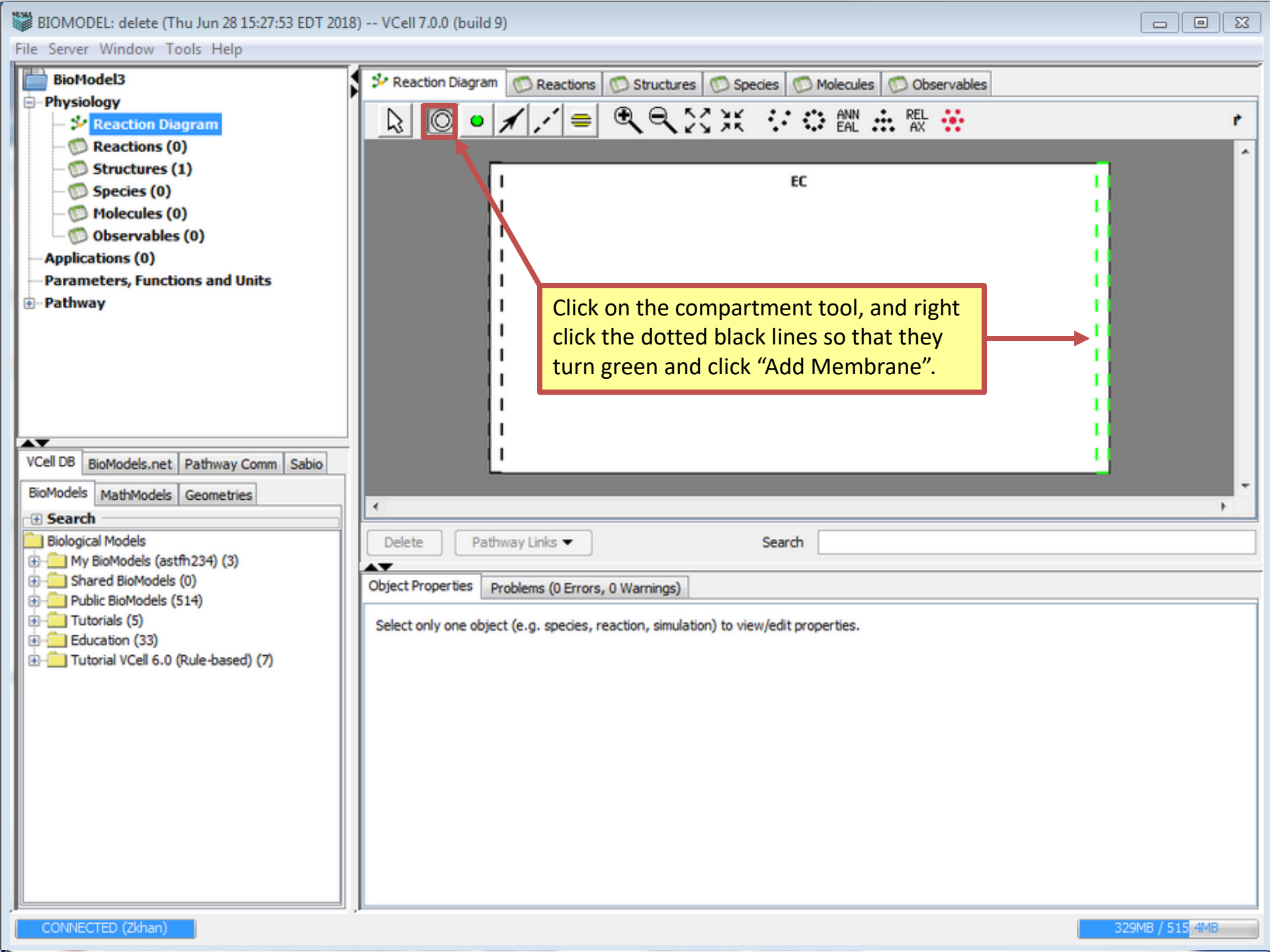
Create a simple biomodel and spatial (PDE) application to simulate a photobleaching experiment and view the results.

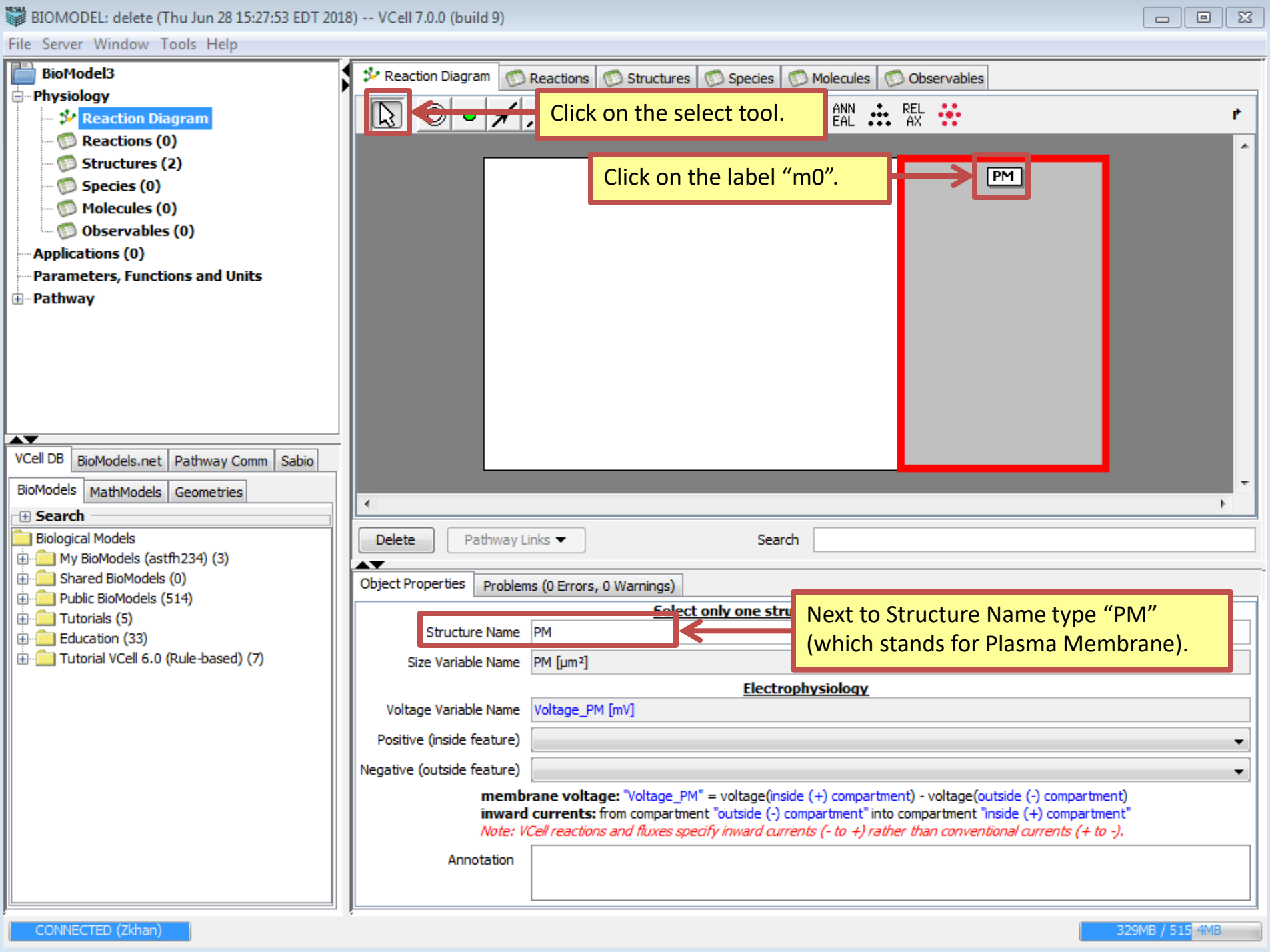
In this tutorial…

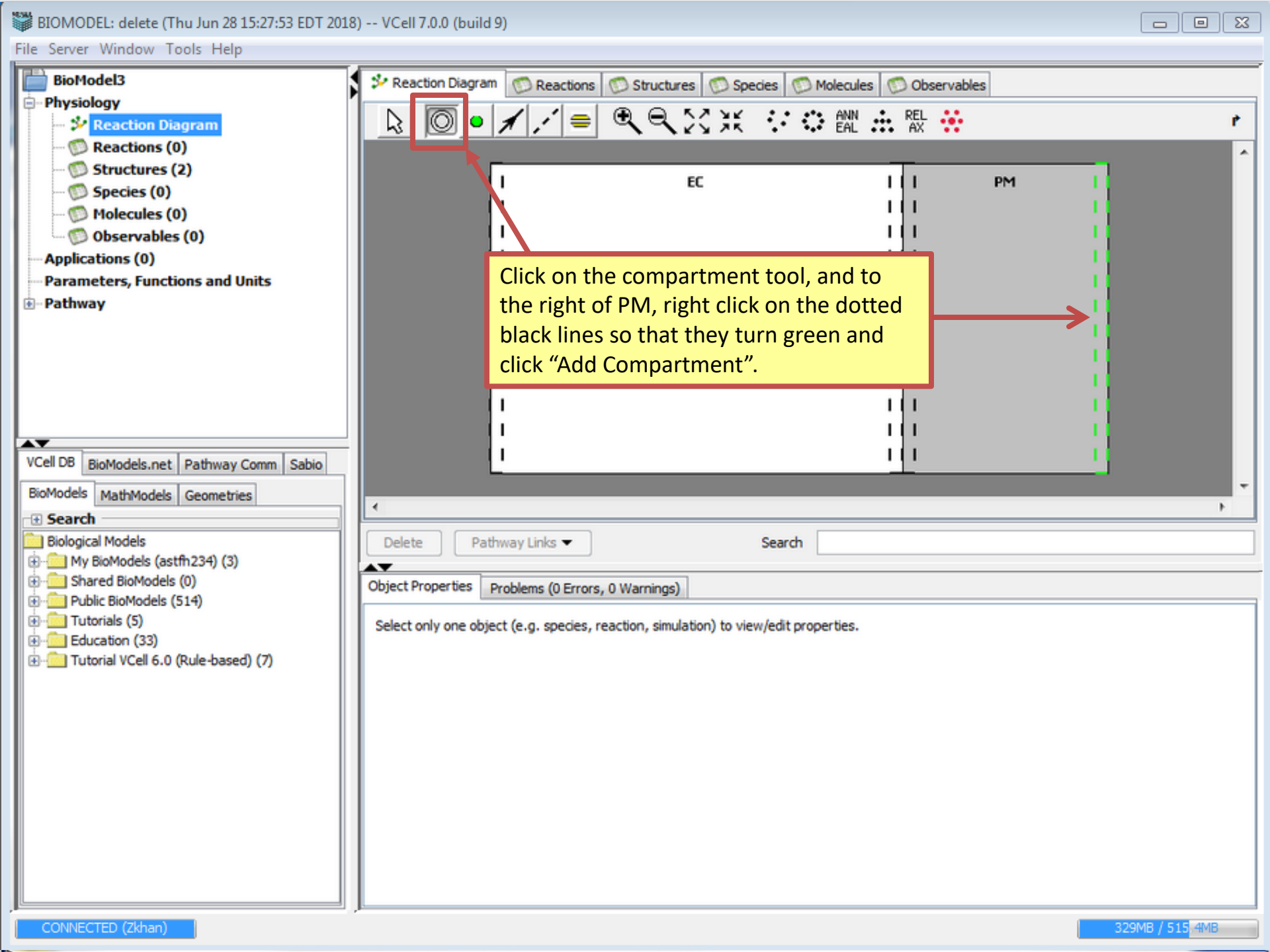
- Gain a basic introduction to the Virtual Cell interface
- Create a very simple biomodel with species but no reactions
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a simple geometry
- Define initial concentrations that are non-uniform using Boolean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

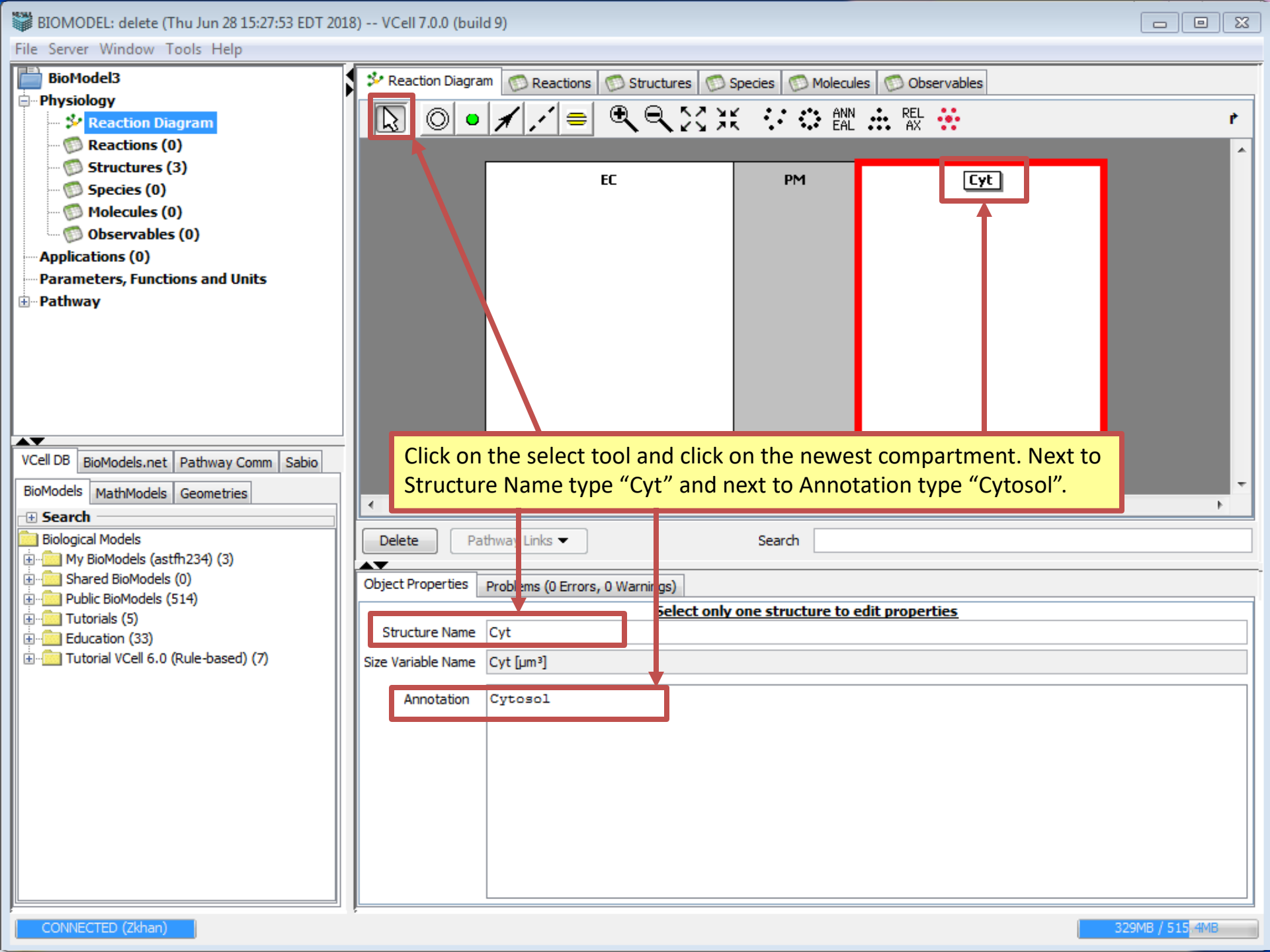

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel2
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
c0
To re-open a model, click on the folder that the model was saved in and double-click on the model.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2
Model2
tutorial 3
Private Tue Jun 30 16:47:35 EDT 201
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Spacial Deterministic
Deterministic
geom_20150630_115646 (3D)
CONNECTED (Zkhan)
329MB / 515.4MB

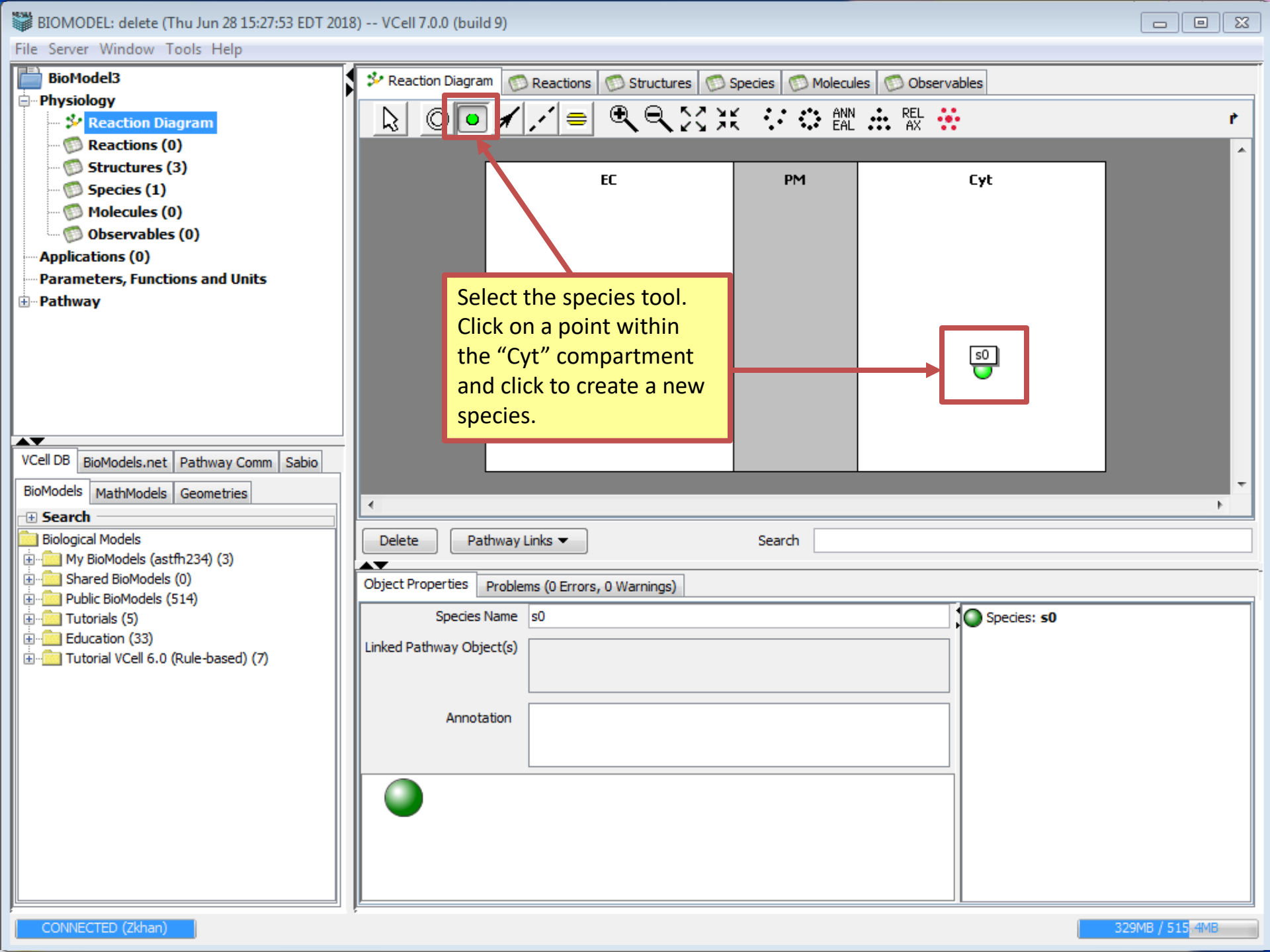

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
Starting from a new model…
Choose the select tool and select the compartment.
Type “EC” under Structure Name and “Extra Cellular”
under Annotation
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name EC
Size Variable Name EC [µm³]
Annotation Extra Cellular
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
CONNECTED (Zkhan)
329MB / 515.4MB

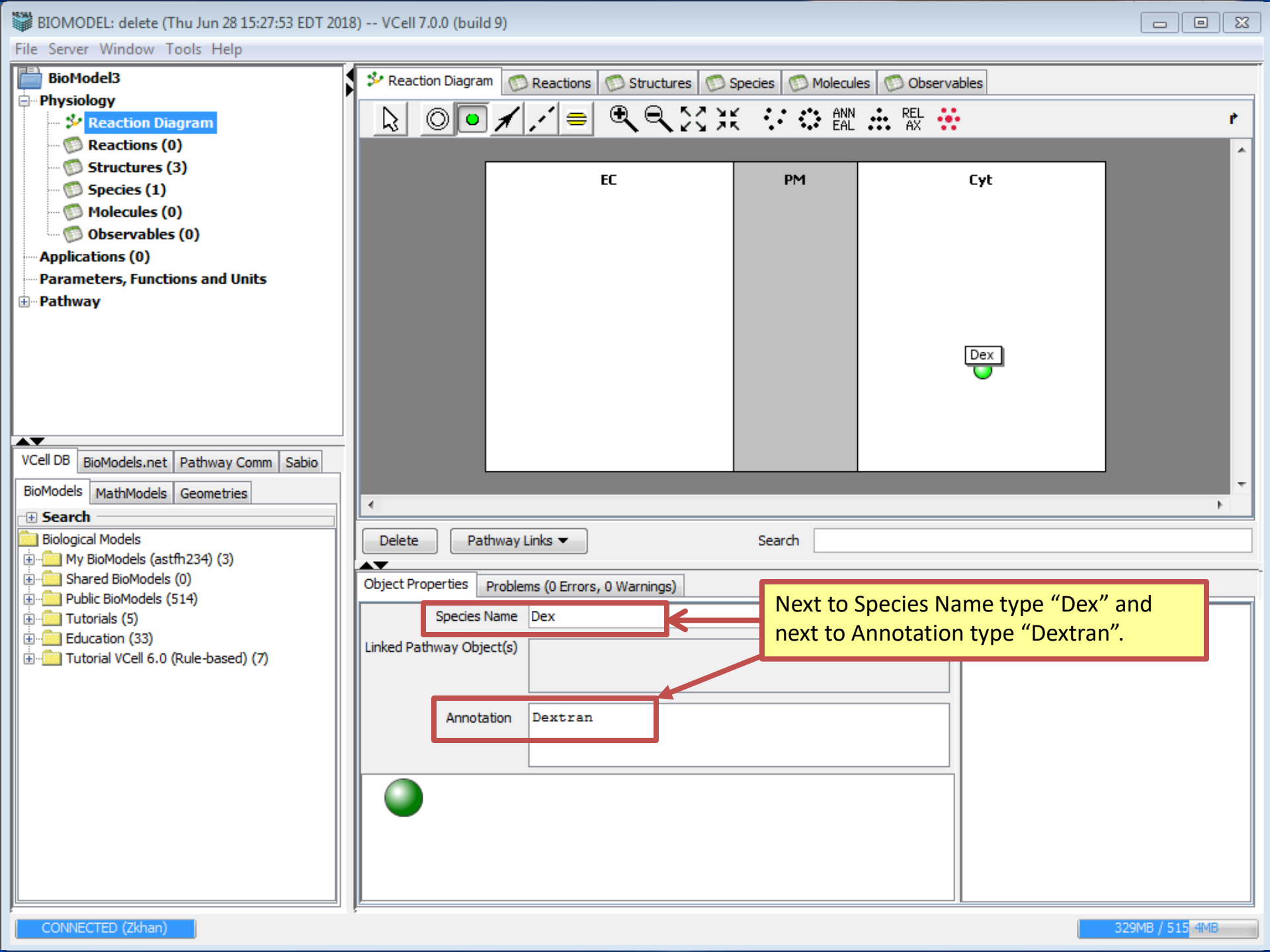

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
Click on the compartment tool, and right click the dotted black lines so that they turn green and click “Add Membrane”.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Zkhan)
329MB / 515.4MB

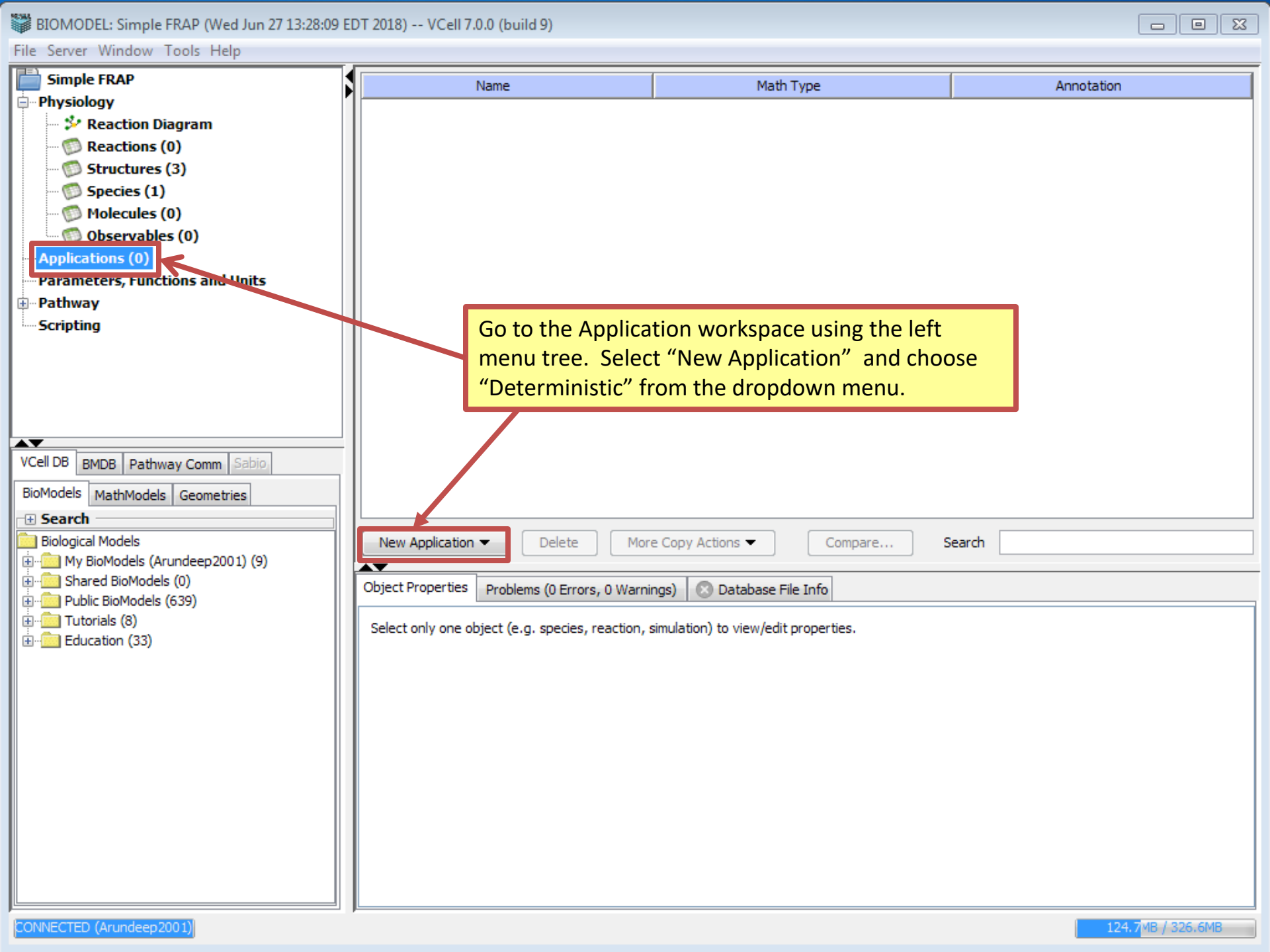

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (2)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Click on the select tool.
Click on the label “m0”.
PM
Delete
Pathway Links
Search
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Structure Name
PM
Next to Structure Name type “PM”
(which stands for Plasma Membrane).
Size Variable Name
PM [µm²]
Electrophysiology
Voltage Variable Name
Voltage_PM [mV]
Positive (inside feature)
Negative (outside feature)
membrane voltage: "Voltage_PM" = 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 -).
Annotation
CONNECTED (Zkhan)
329MB / 515.4MB

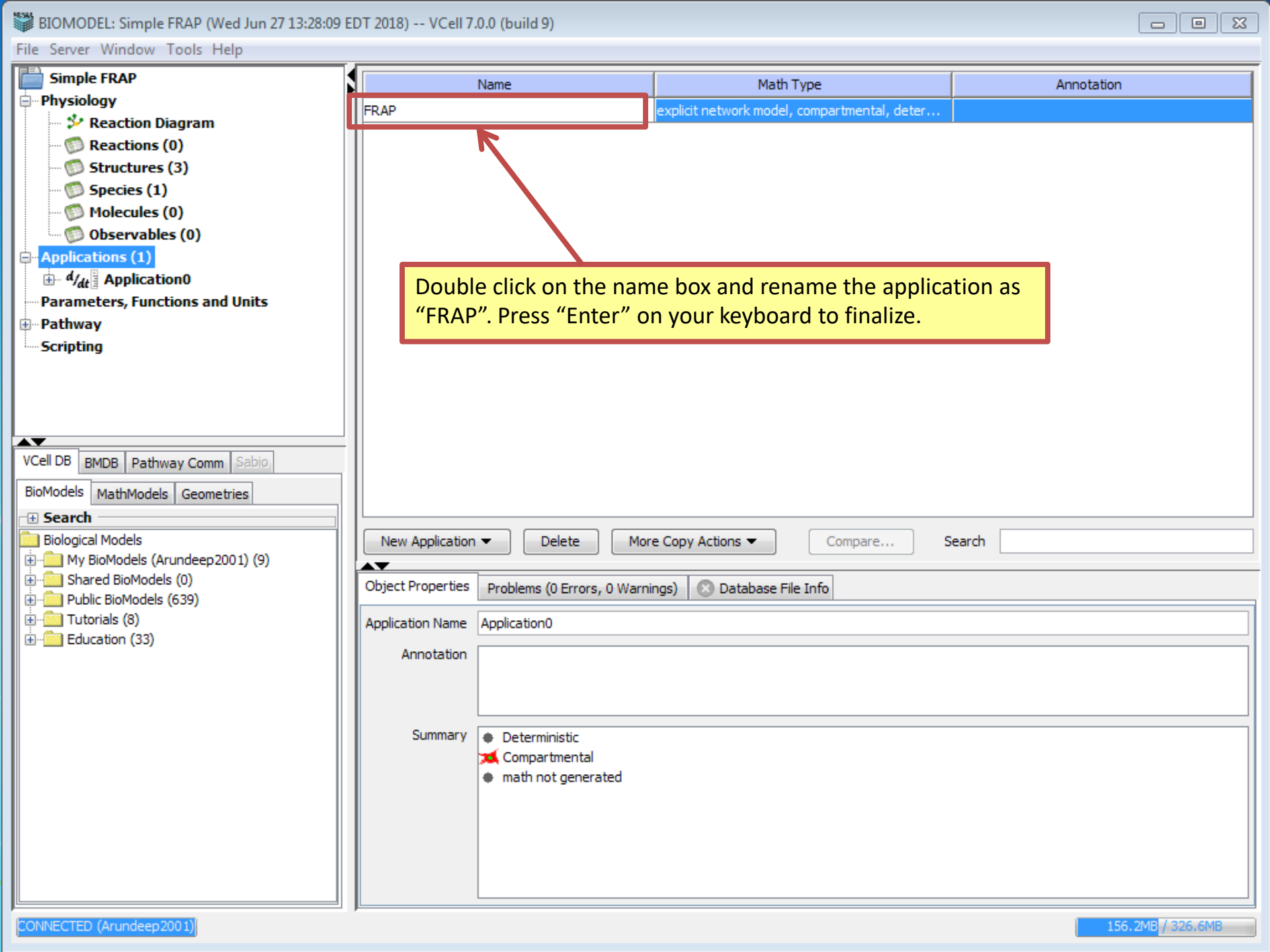

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (2)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
Click on the compartment tool, and to the right of PM, right click on the dotted black lines so that they turn green and click “Add Compartment”.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
CONNECTED (Zkhan)
329MB / 515.4MB

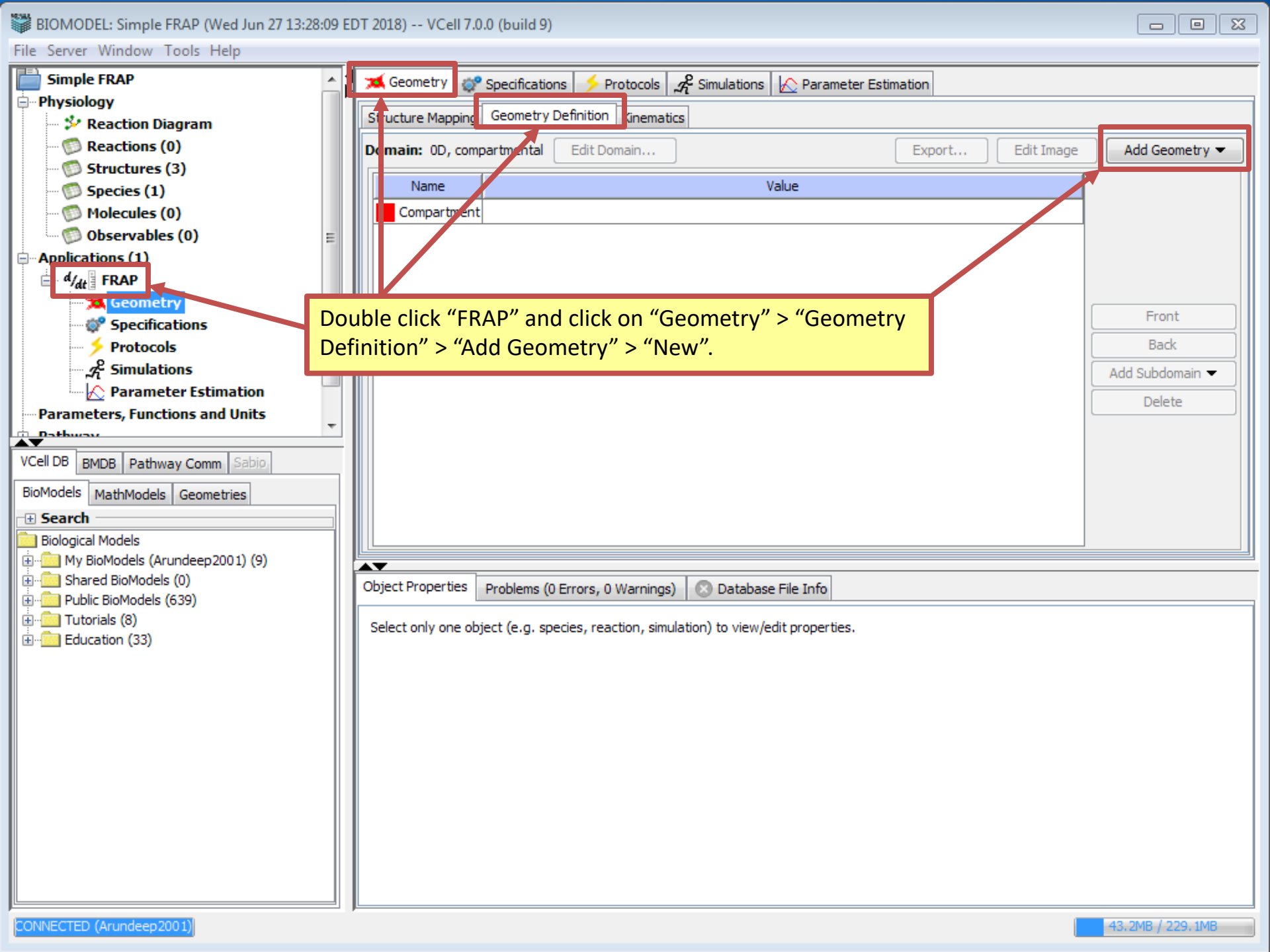

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
Cyt
Click on the select tool and click on the newest compartment. Next to Structure Name type “Cyt” and next to Annotation type “Cytosol”.
Delete
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name
Cyt
Size Variable Name
Cyt [µm³]
Annotation
Cytosol
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
CONNECTED (Zkhan)
329MB / 515.4MB

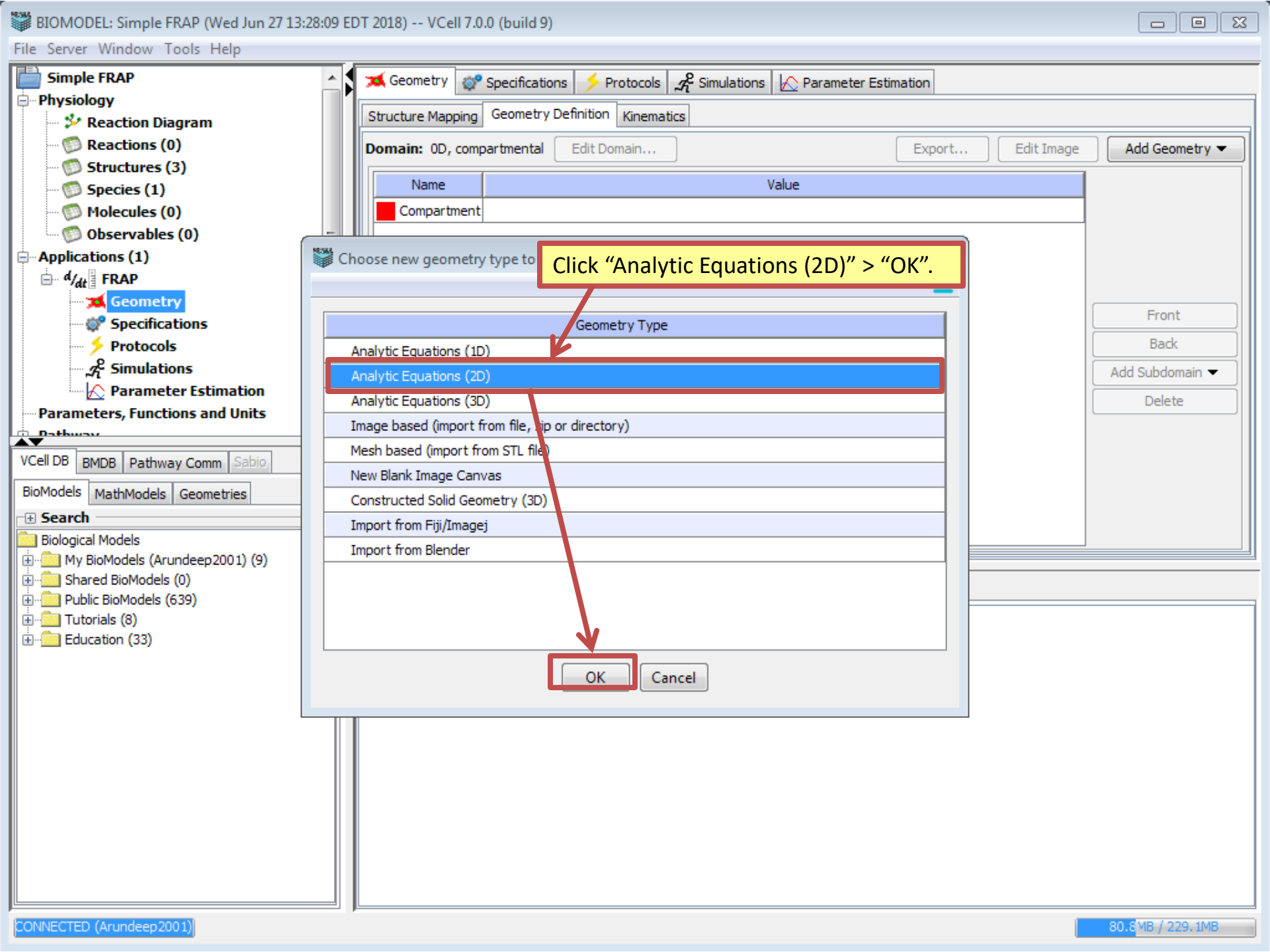

BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
Cyt
s0
Select the species tool. Click on a point within the "Cyt" compartment and click to create a new species.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Species Name
s0
Linked Pathway Object(s)
Annotation
Species: s0
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
Cyt
Dex
Delete
Pathway Links
Search
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Species Name
Dex
Linked Pathway Object(s)
Annotation
Dextran
Next to Species Name type “Dex” and next to Annotation type “Dextran”.
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Scripting
Name
Math Type
Annotation
Go to the Application workspace using the left menu tree. Select "New Application" and choose "Deterministic" from the dropdown menu.
New Application
Delete
More Copy Actions
Compare...
Search
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
124.7MB / 326.6MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
Application0
Parameters, Functions and Units
Pathway
Scripting
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Name
Math Type
Annotation
FRAP
explicit network model, compartmental, deter...
Double click on the name box and rename the application as "FRAP". Press "Enter" on your keyboard to finalize.
New Application
Delete
More Copy Actions
Compare...
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Application Name
Application0
Annotation
Summary
Deterministic
Compartmental
math not generated
CONNECTED (Arundeep2001)
156.2MB / 326.6MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
FRAP
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions and Units
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Kinematics
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
43.2MB / 229.1MB
Double click “FRAP” and click on “Geometry” > “Geometry Definition” > “Add Geometry” > “New”.


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
FRAP
Geometry
Specifications
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Parameters, Functions and Units
VCell DB
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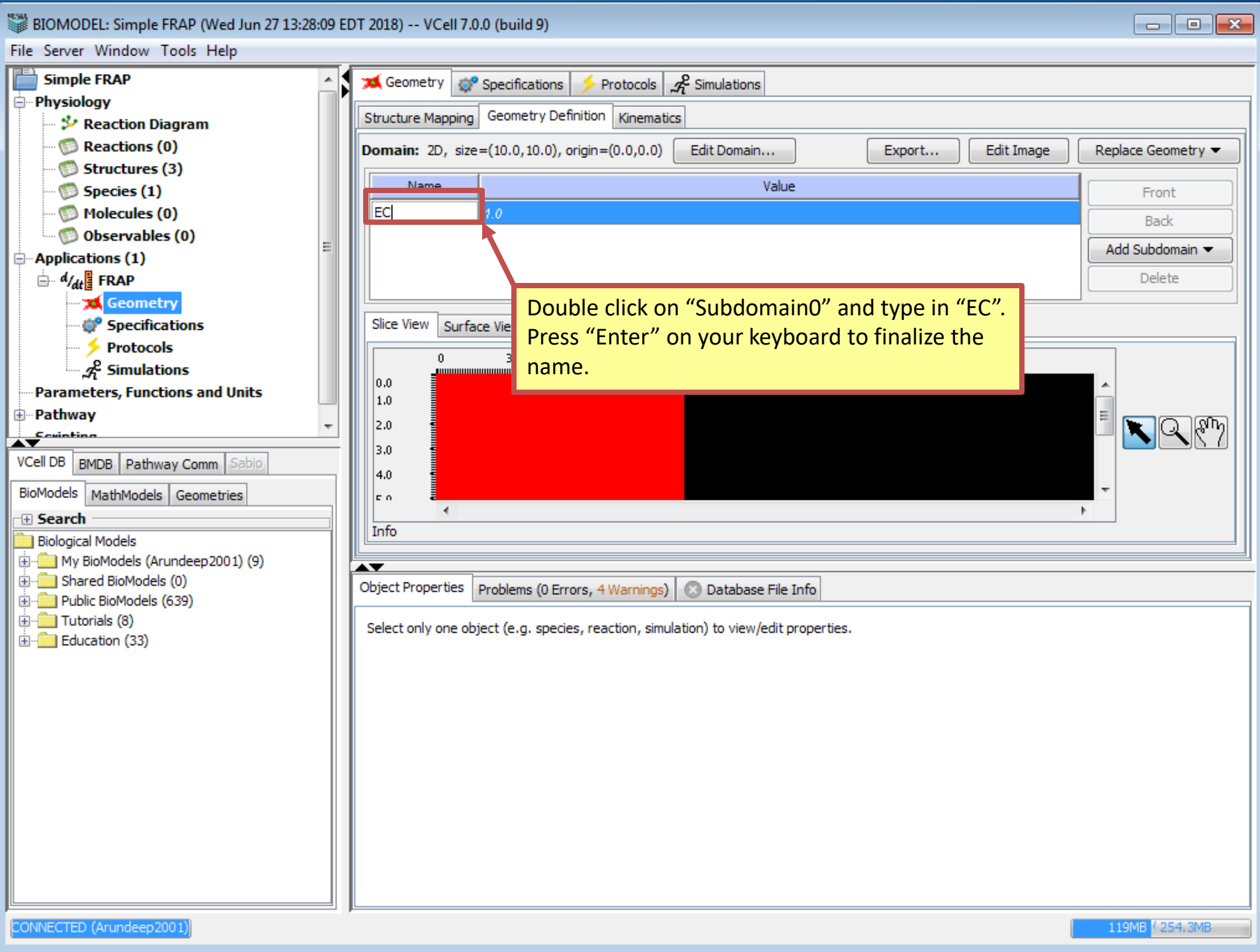
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Kinematics
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
Choose new geometry type to
Click “Analytic Equations (2D)” > “OK”.
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)
Import from Fiji/Imagej
Import from Blender
OK
Cancel
CONNECTED (Arundeep2001)
80.8MB / 229.1MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
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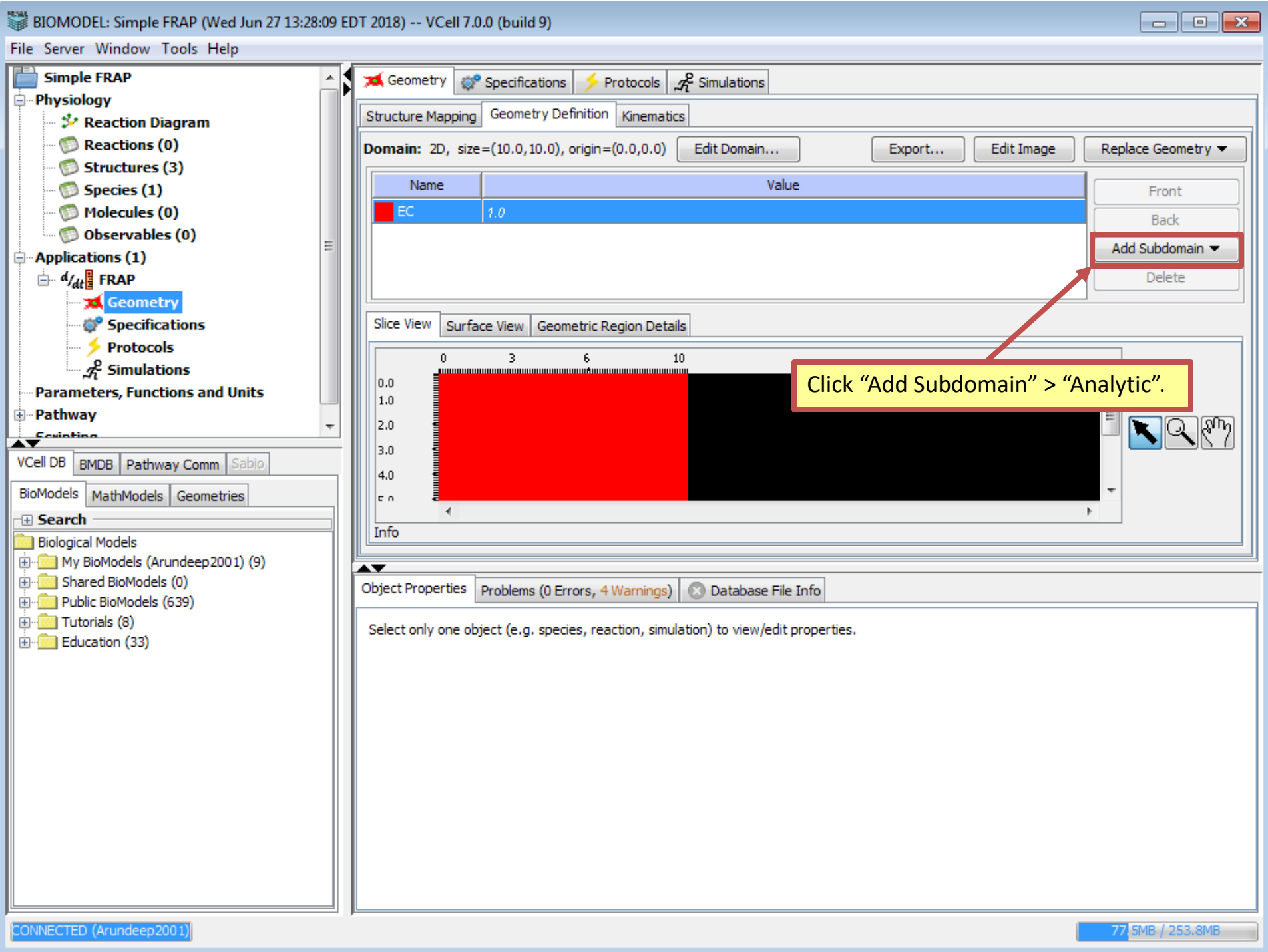
Protocols
Simulations
Parameters, Functions and Units
Pathway
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Geometry
Specifications
Protocols
Simulations
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
Delete
Slice View
Surface Vie
0.0
1.0
2.0
3.0
4.0
Info
Double click on “Subdomain0” and type in “EC”. Press “Enter” on your keyboard to finalize the name.
Object Properties
Problems (0 Errors, 4 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
119MB / 254.3MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
FRAP
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Parameters, Functions and Units
Pathway
VCell DB
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Pathway Comm
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BioModels
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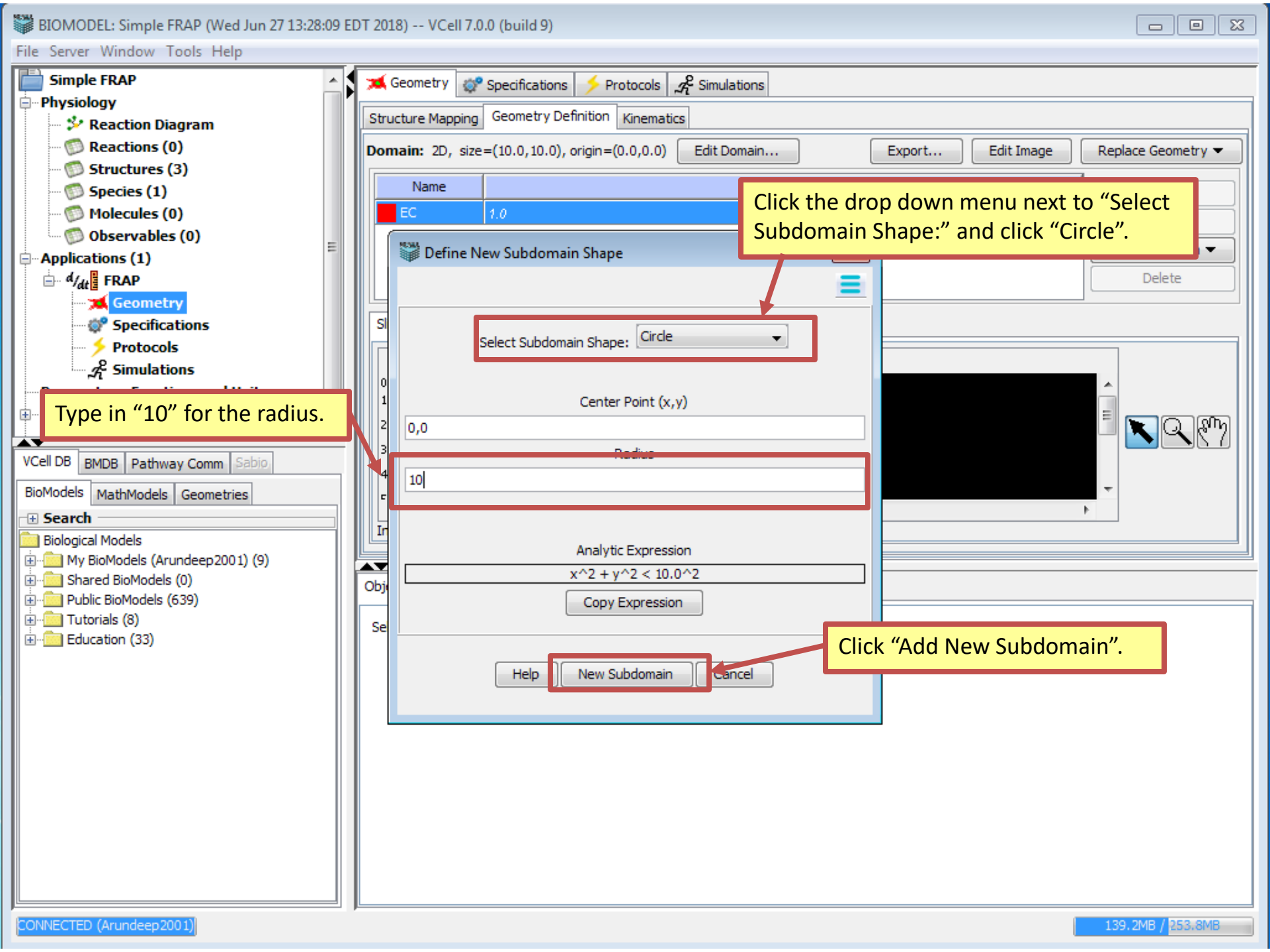
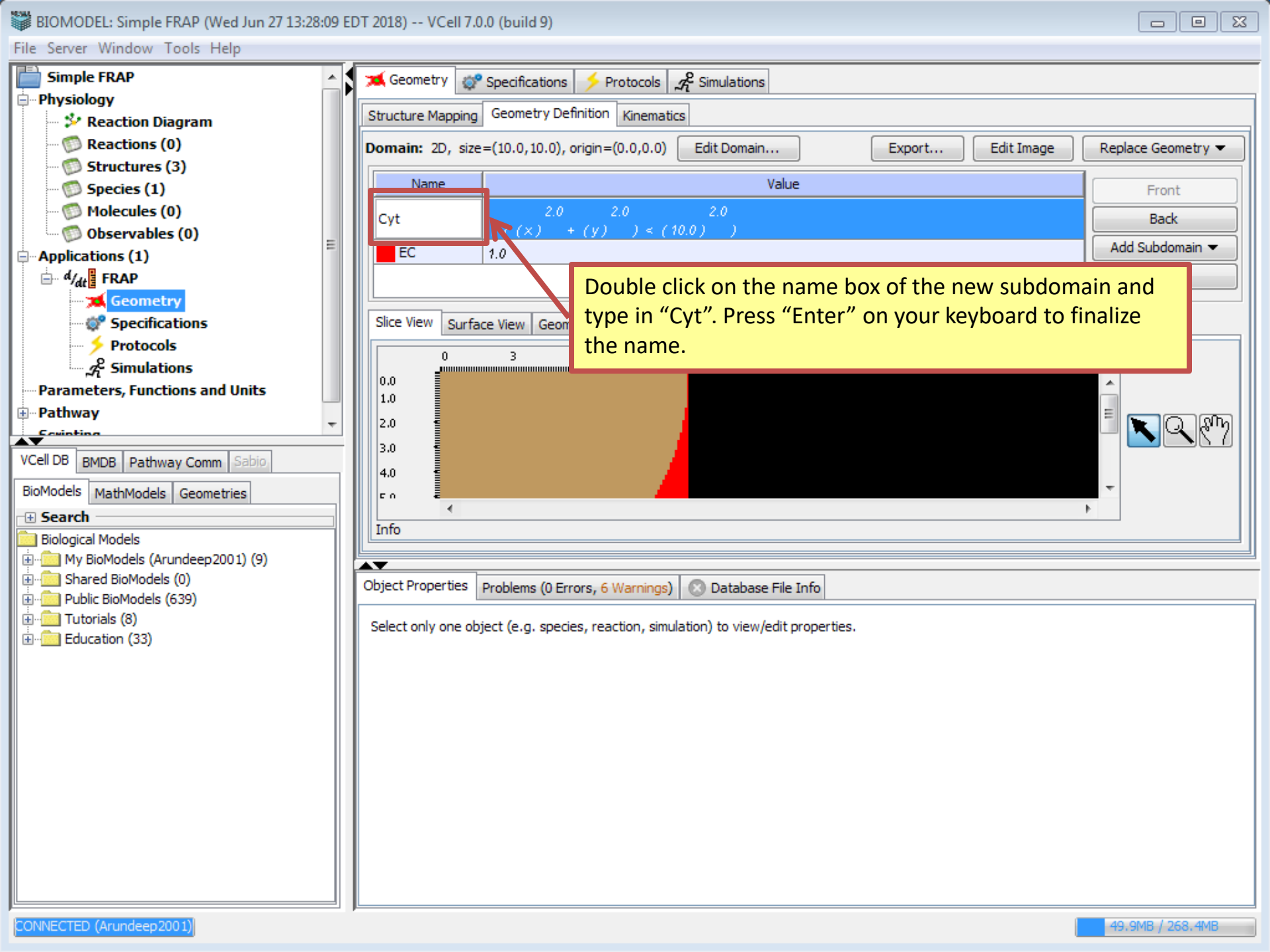
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
Info
Click “Add Subdomain” > “Analytic”.
Object Properties
Problems (0 Errors, 4 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
77.5MB / 253.8MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
FRAP
Geometry
Specifications
Protocols
Simulations
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
EC
1.0
Delete
Define New Subdomain Shape
Select Subdomain Shape:
Circle
Center Point (x,y)
0,0
Radius
10
Analytic Expression
x^2 + y^2 < 10.0^2
Copy Expression
Help
New Subdomain
Cancel
Click the drop down menu next to “Select Subdomain Shape:” and click “Circle”.
Type in “10” for the radius.
Click “Add New Subdomain”.
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
CONNECTED (Arundeep2001)
139.2MB / 253.8MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
Simple FRAP
Physiology
Reaction Diagram
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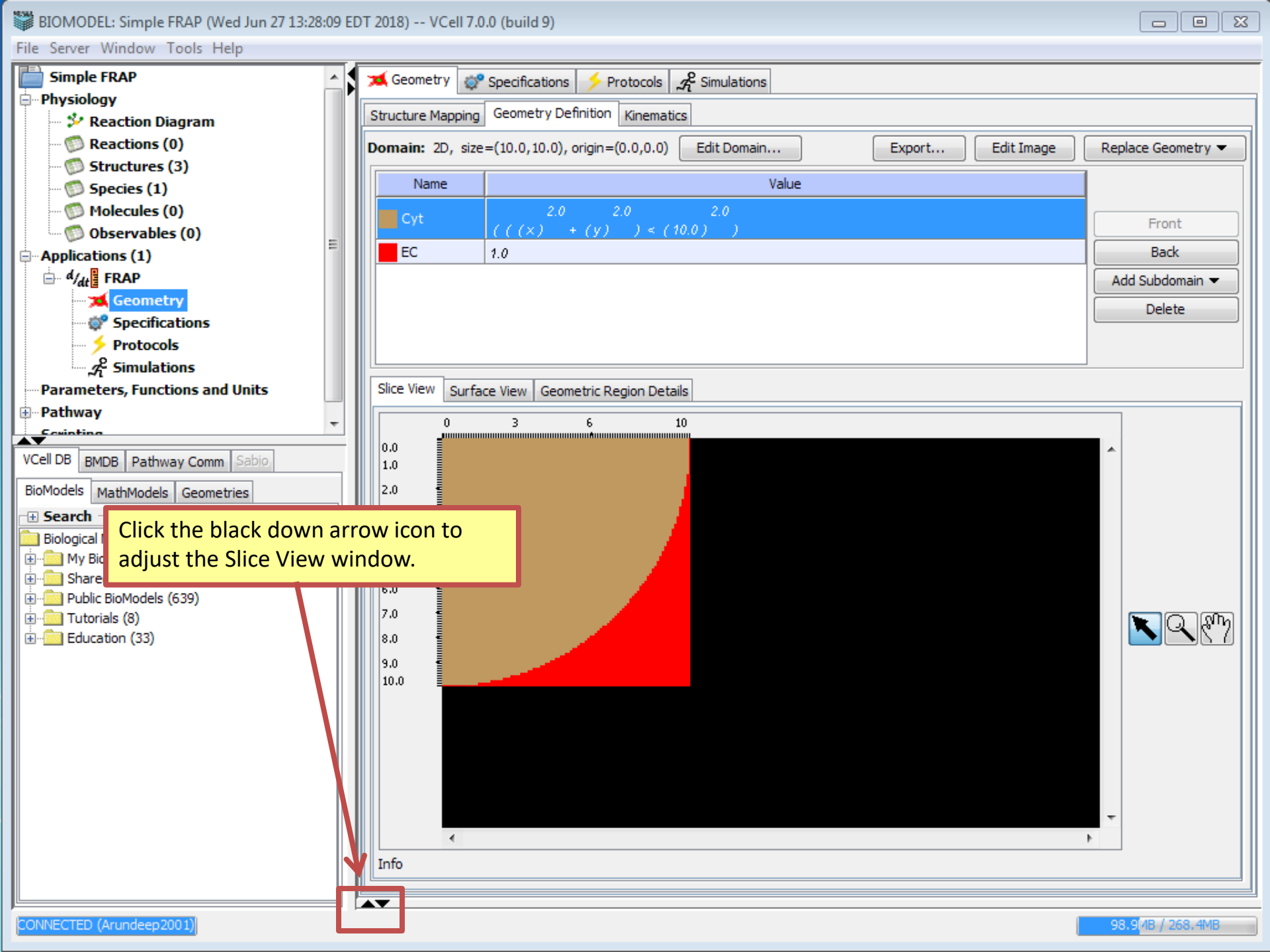
Geometry Definition
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
2.0 2.0 2.0
(x) + (y)) < (10.0)
EC
1.0
Front
Back
Add Subdomain
Double click on the name box of the new subdomain and type in “Cyt”. Press “Enter” on your keyboard to finalize the name.
Slice View
Surface View
Info
Object Properties
Problems (0 Errors, 6 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
49.9MB / 268.4MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
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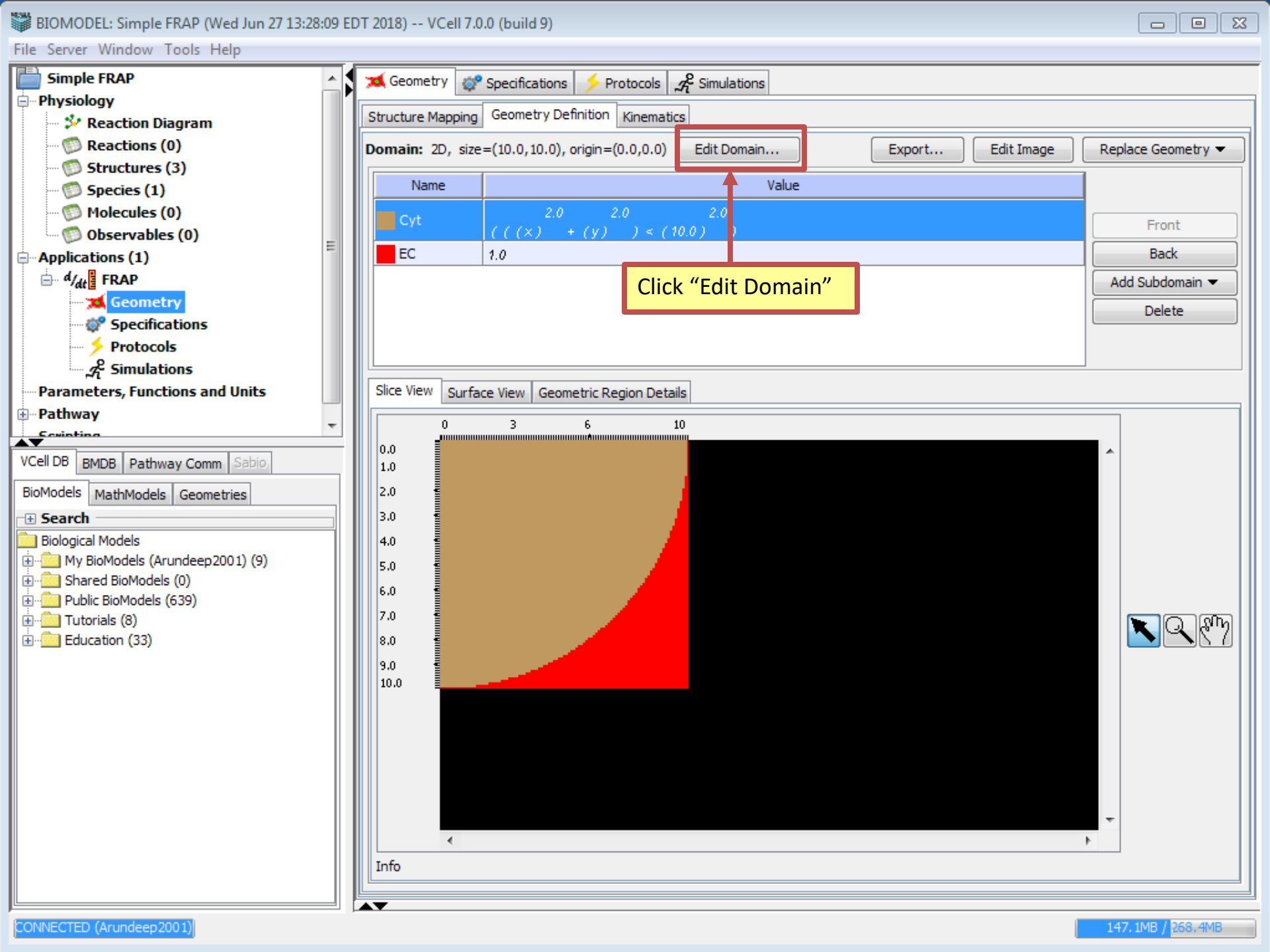
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
2.0 2.0 2.0
(((x) + (y)) < (10.0))
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
7.0
8.0
9.0
10.0
Info
Click the black down arrow icon to adjust the Slice View window.
CONNECTED (Arundeep2001)
98.9 MB / 268.4MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
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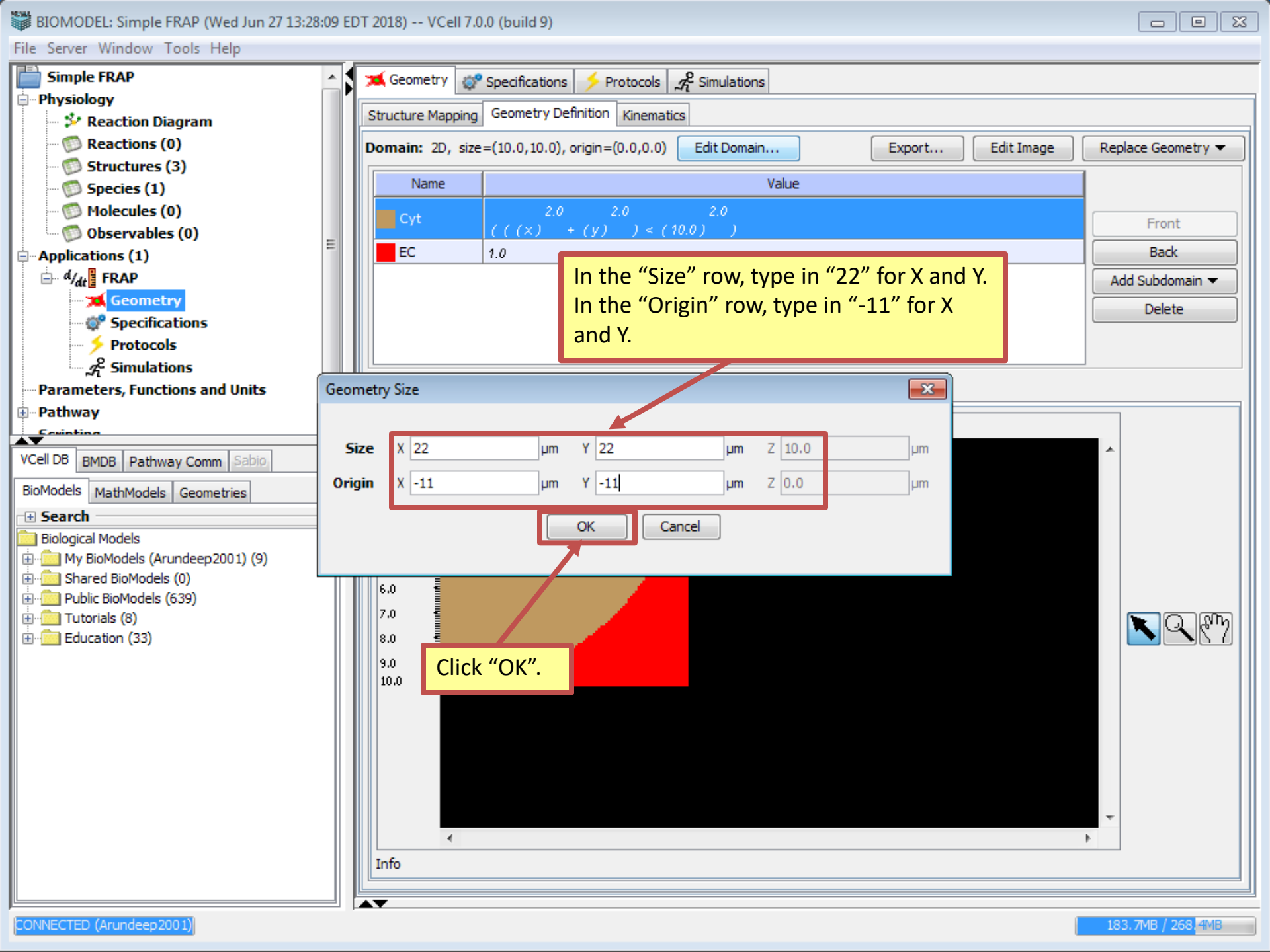
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
2.0 2.0 2.0
(((x) + (y)) < (10.0))
EC
1.0
Front
Back
Add Subdomain
Delete
Click “Edit Domain”
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Info
CONNECTED (Arundeep2001)
147.1MB / 268.4MB


BIOMODEL: Simple FRAP (Wed Jun 27 13:28:09 EDT 2018) -- VCell 7.0.0 (build 9)
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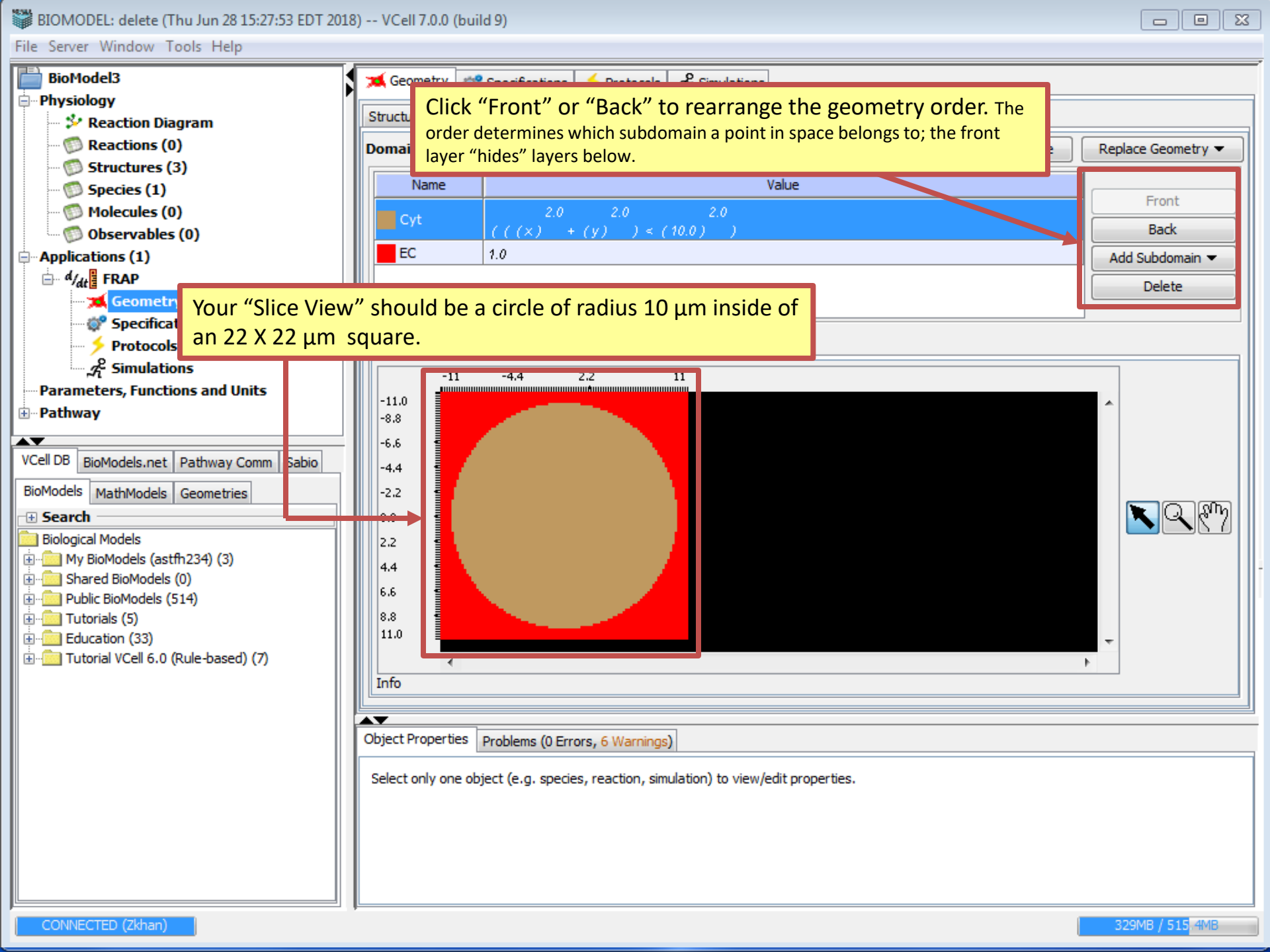
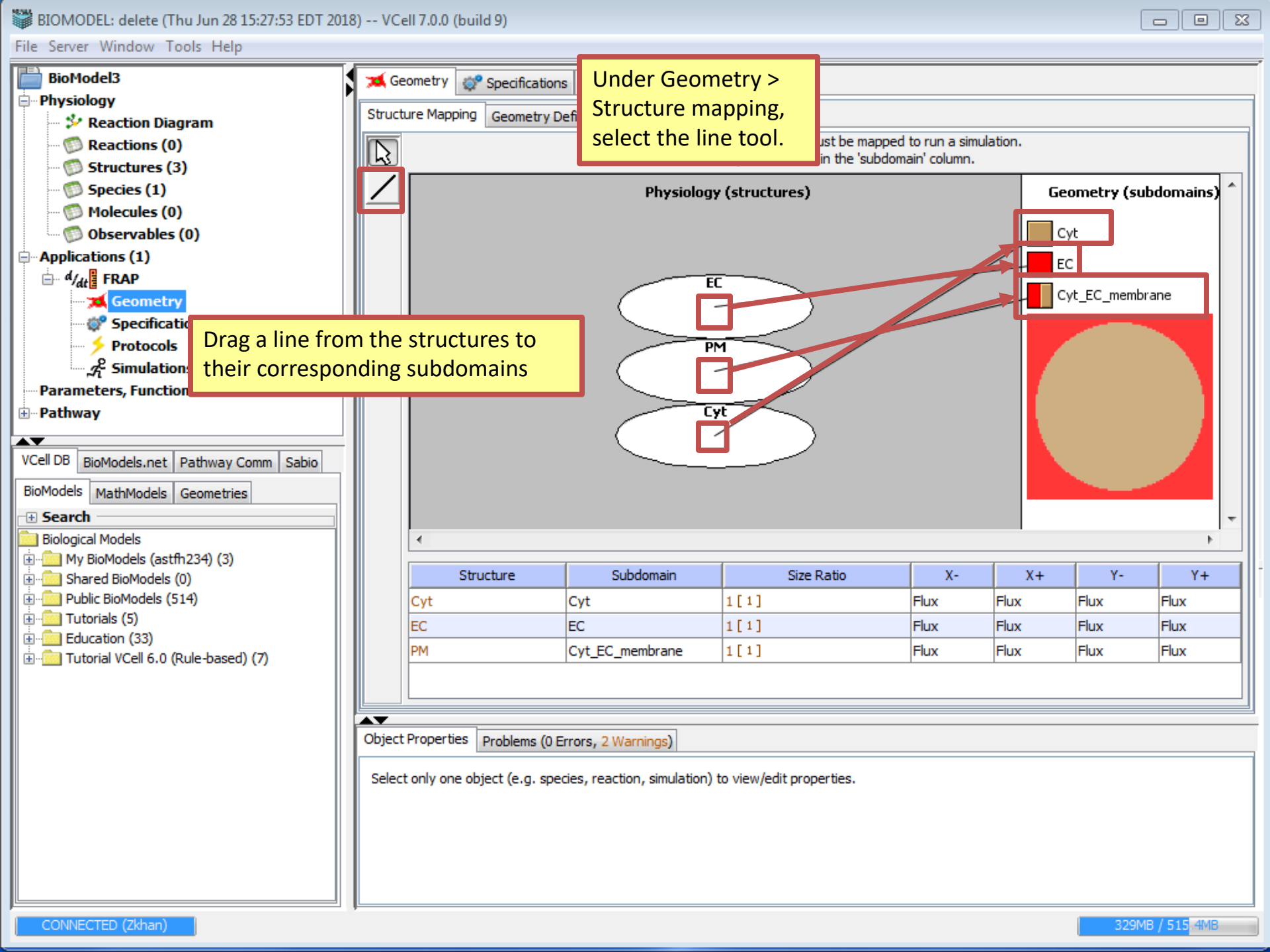
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
EC
1.0
Front
Back
Add Subdomain
Delete
In the “Size” row, type in “22” for X and Y.
In the “Origin” row, type in “-11” for X and Y.
Geometry Size
Size
Origin
X 22 µm Y 22 µm Z 10.0 µm
X -11 µm Y -11 µm Z 0.0 µm
OK
Cancel
Click “OK”.
6.0
7.0
8.0
9.0
10.0
Info
CONNECTED (Arundeep2001)
183.7MB / 268.4MB



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.

Your “Slice View” should be a circle of radius 10 µm inside of an 22 X 22 µm square.


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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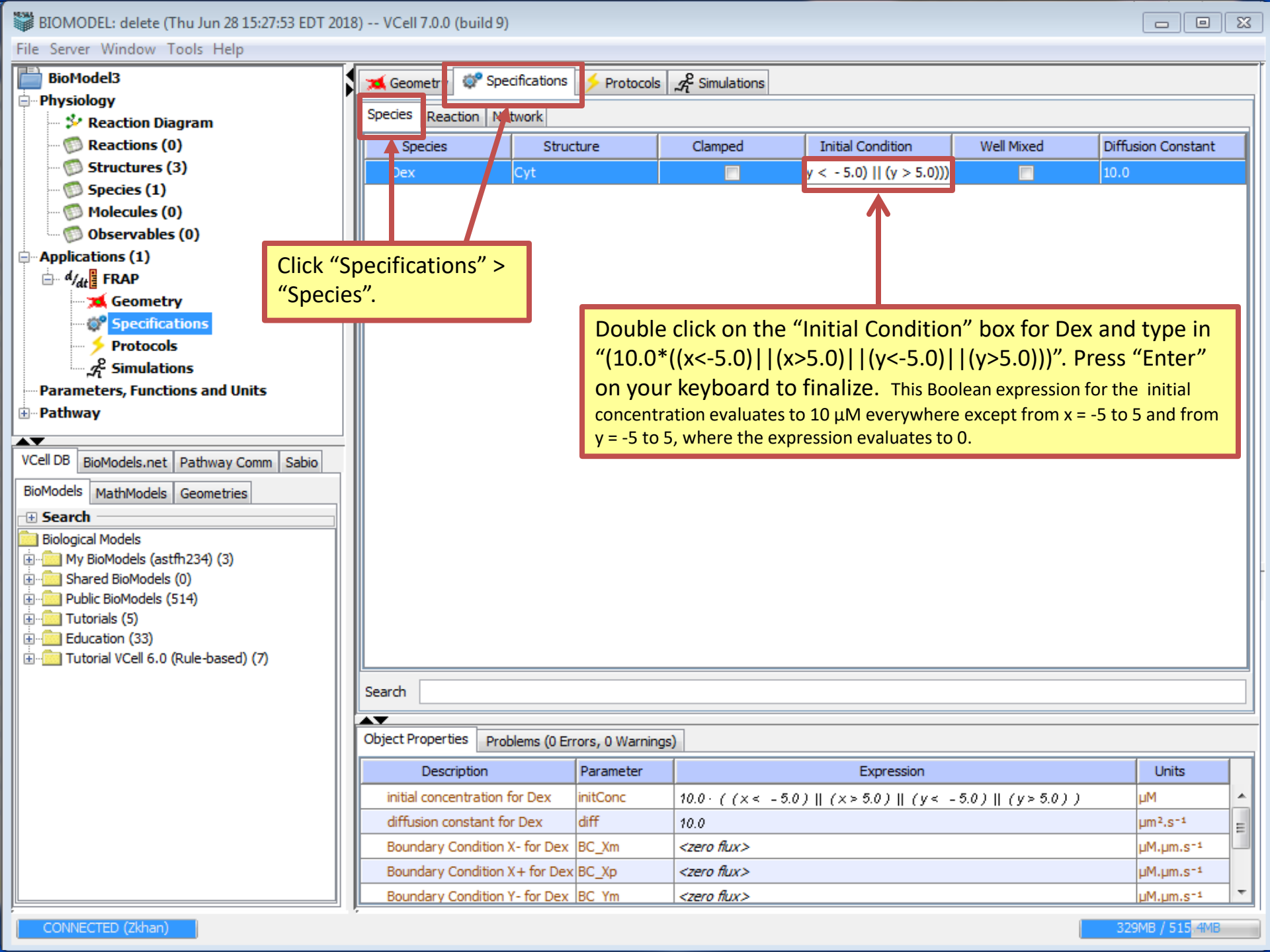
Specifications
Structure Mapping
Geometry Defi
Under Geometry > Structure mapping, select the line tool.
ust be mapped to run a simulation.
in the 'subdomain' column.
Physiology (structures)
Geometry (subdomains)
EC
PM
Cyt
Cyt
EC
Cyt_EC_membrane
Drag a line from the structures to their corresponding subdomains
Structure
Subdomain
Size Ratio
X-
X+
Y-
Y+
Cyt
Cyt
1 [1]
Flux
Flux
Flux
Flux
EC
EC
1 [1]
Flux
Flux
Flux
Flux
PM
Cyt_EC_membrane
1 [1]
Flux
Flux
Flux
Flux
Object Properties
Problems (0 Errors, 2 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Network
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Dex
Cyt
y < - 5.0) || (y > 5.0)))
10.0
Click “Specifications” > “Species”.
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 finalize. 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.
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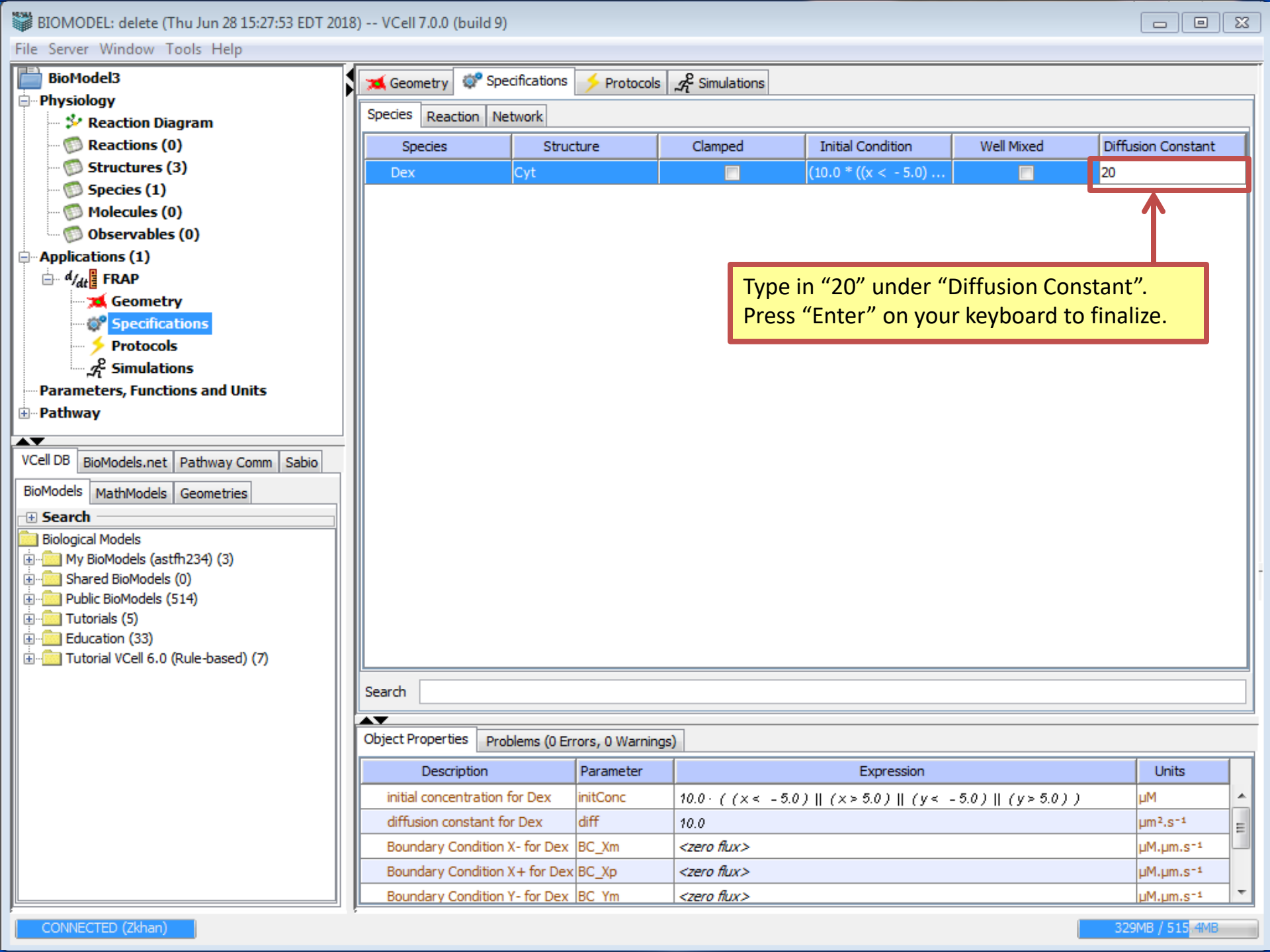
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Description
Parameter
Expression
Units
initial concentration for Dex
initConc
10.0 · ((x < - 5.0) || (x > 5.0) || (y < - 5.0) || (y > 5.0))
µM
diffusion constant for Dex
diff
10.0
µm².s⁻¹
Boundary Condition X- for Dex
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for Dex
BC_Xp
<zero flux>
µM.µm.s⁻¹
Boundary Condition Y- for Dex
BC_Ym
<zero flux>
µM.µm.s⁻¹
CONNECTED (Zkhan)
329MB / 515 4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Initial Condition
Well Mixed
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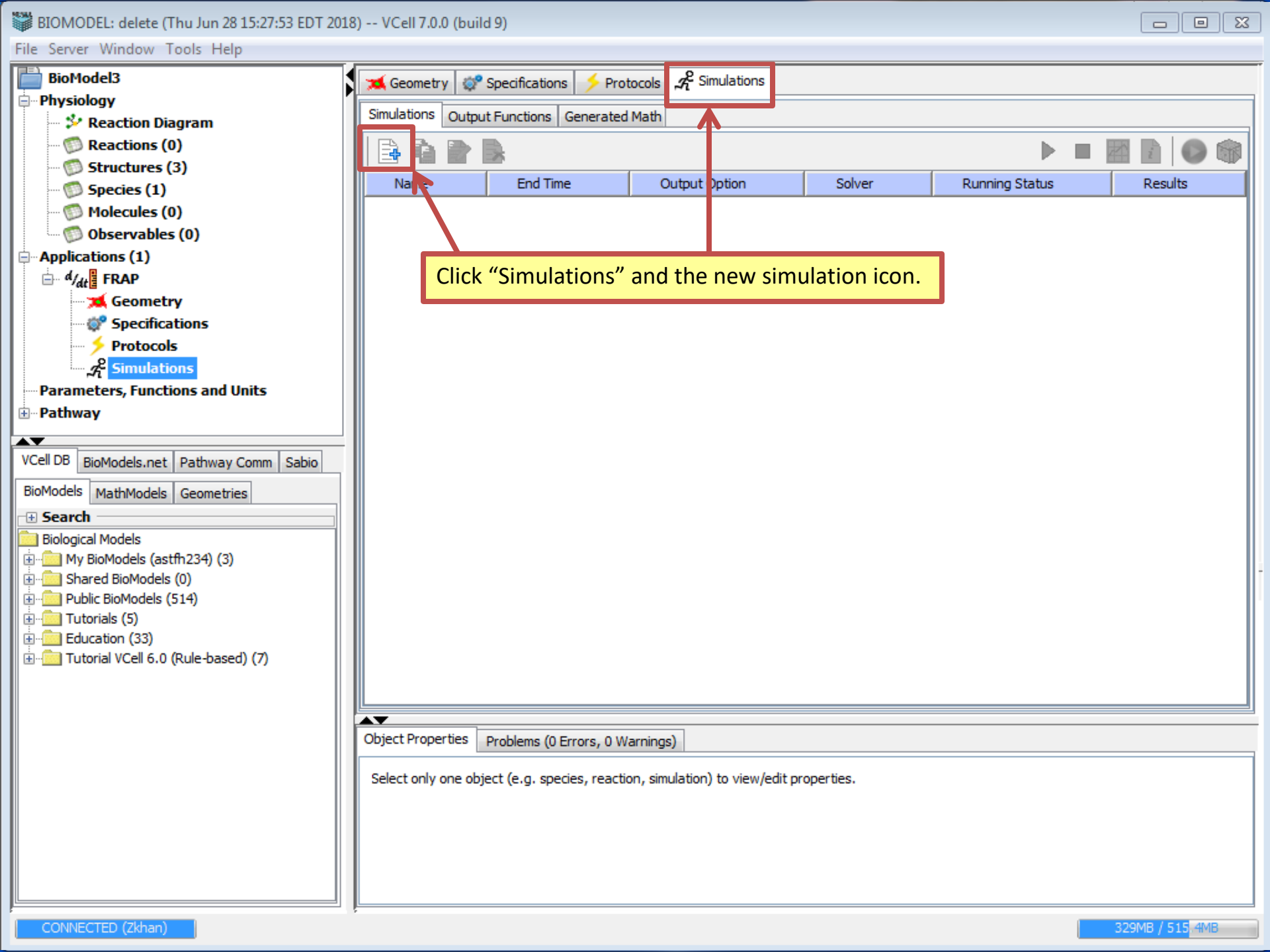
Dex
Cyt
(10.0 * ((x < - 5.0) ...
20
Type in “20” under “Diffusion Constant”.
Press “Enter” on your keyboard to finalize.
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Description
Parameter
Expression
Units
initial concentration for Dex
initConc
10.0 · ((x < - 5.0) || (x > 5.0) || (y < - 5.0) || (y > 5.0))
µM
diffusion constant for Dex
diff
10.0
µm².s⁻¹
Boundary Condition X- for Dex
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for Dex
BC_Xp
<zero flux>
µM.µm.s⁻¹
Boundary Condition Y- for Dex
BC_Ym
<zero flux>
µM.µm.s⁻¹
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Output Functions
Generated Math
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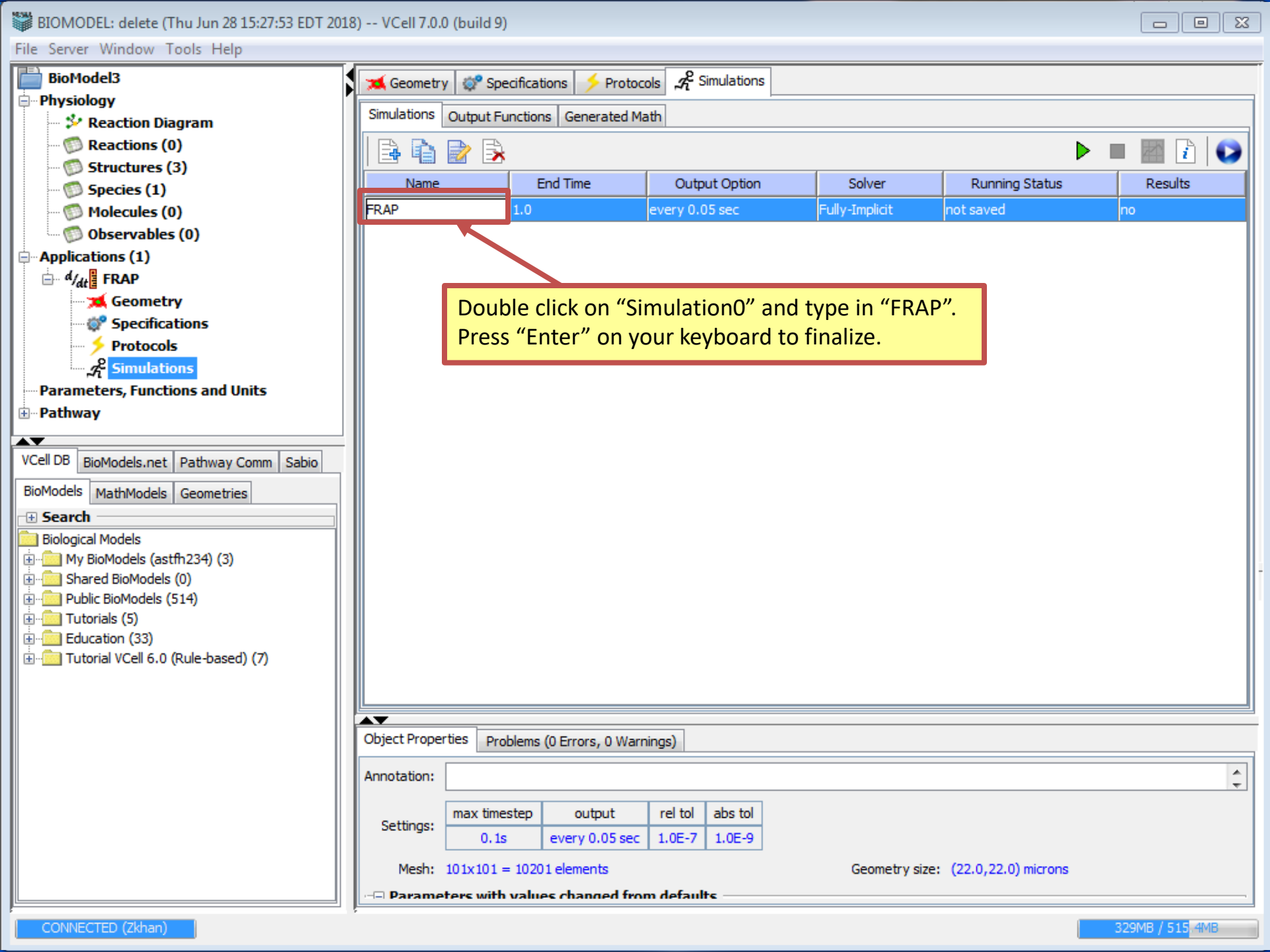
Output Option
Solver
Running Status
Results
Click “Simulations” and the new simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Output Option
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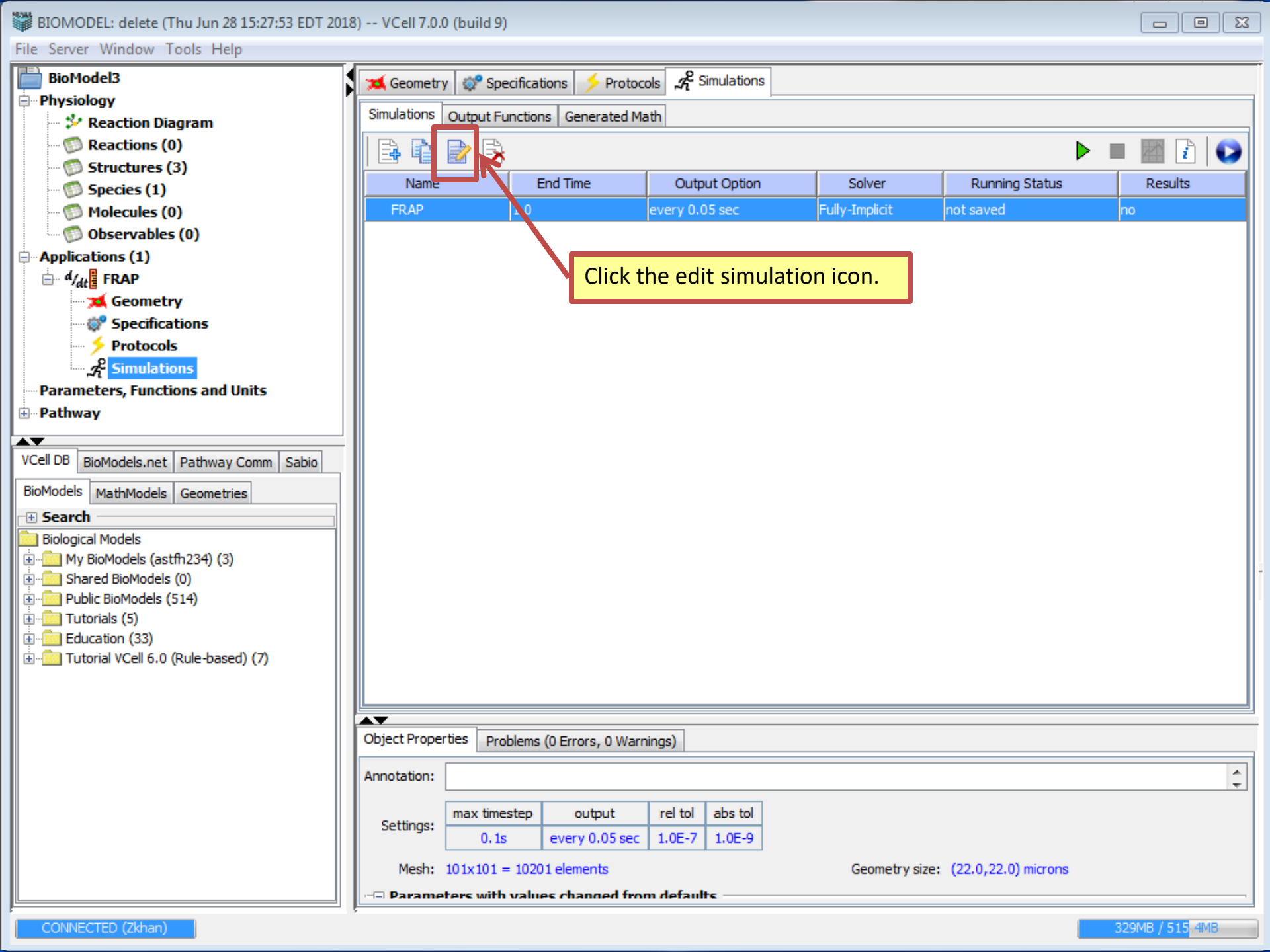
FRAP
1.0
every 0.05 sec
Fully-Implicit
not saved
no
Double click on “Simulation0” and type in “FRAP”.
Press “Enter” on your keyboard to finalize.
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 101x101 = 10201 elements
Geometry size: (22.0,22.0) microns
Parameters with values changed from defaults
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Generated Math
Name
End Time
Output Option
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Running Status
Results
FRAP
1.0
every 0.05 sec
Fully-Implicit
not saved
no
Click the edit simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
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 (Zkhan)
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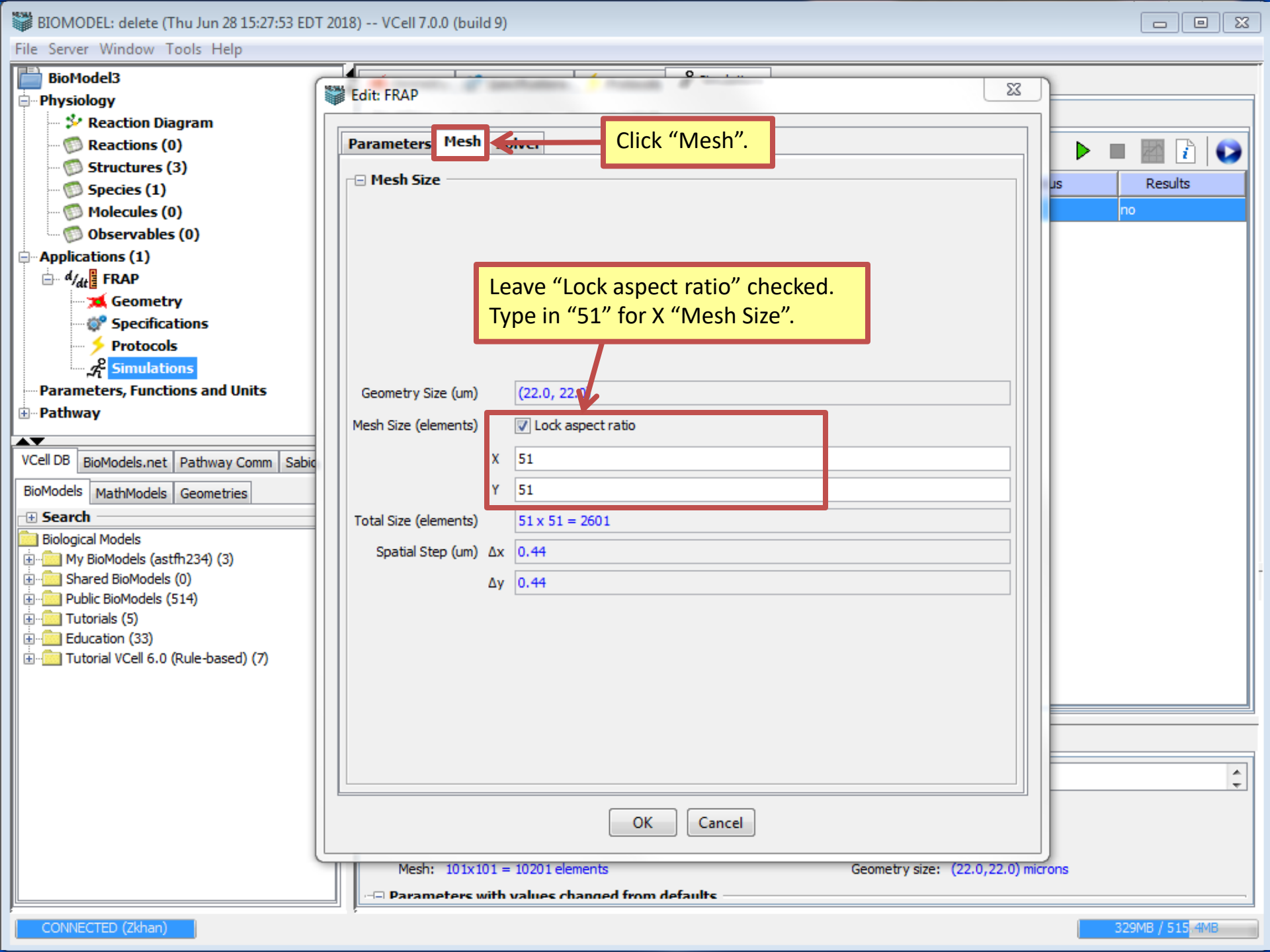
BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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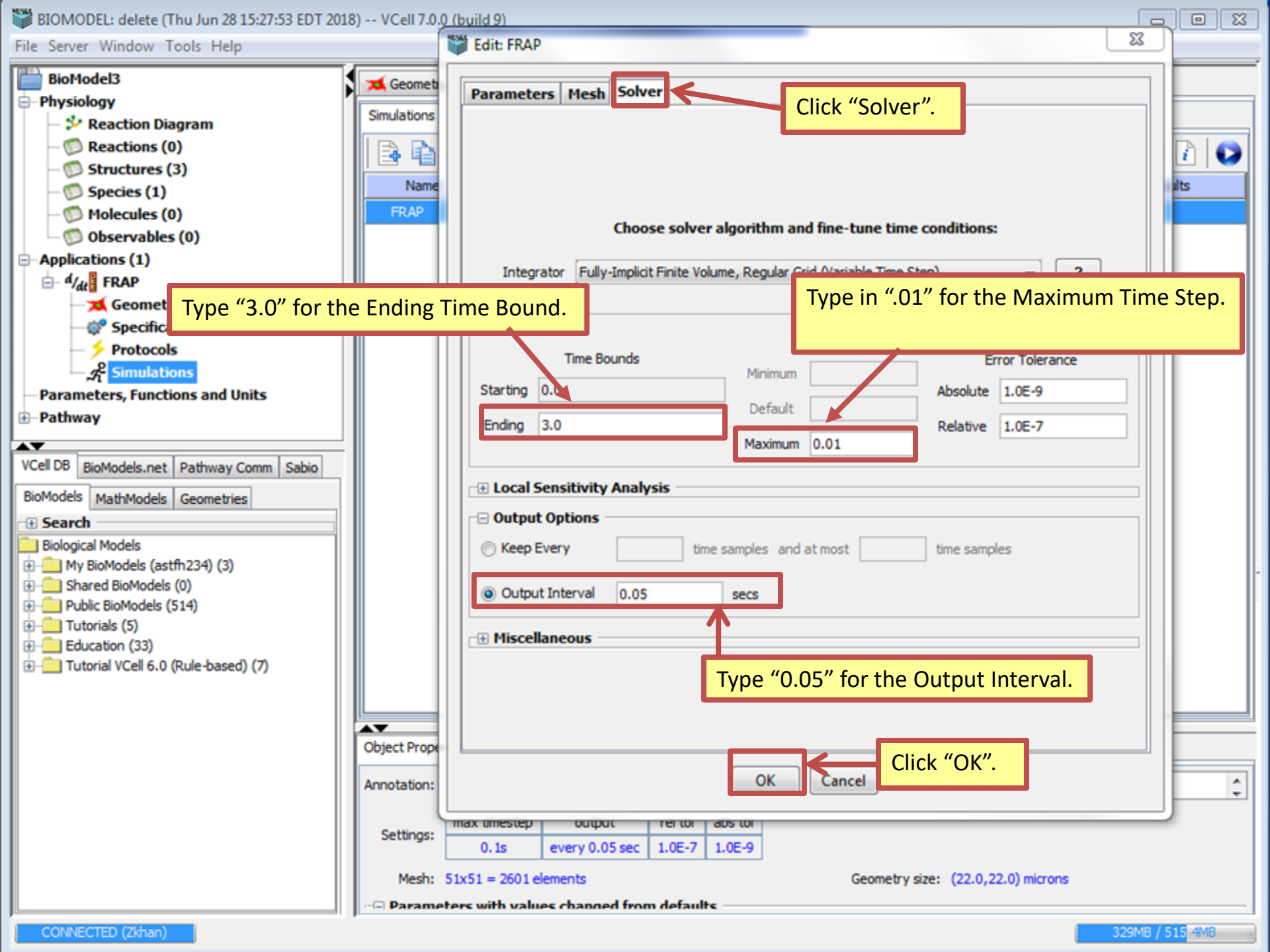
Edit: FRAP
Parameters
Mesh
Click “Mesh”.
Mesh Size
Leave “Lock aspect ratio” checked.
Type in “51” for X “Mesh Size”.
Geometry Size (um)
(22.0, 22.0)
Mesh Size (elements)
Lock aspect ratio
X
51
Y
51
Total Size (elements)
51 x 51 = 2601
Spatial Step (um) Δx
0.44
Δy
0.44
OK
Cancel
Results
no
Mesh: 101x101 = 10201 elements
Geometry size: (22.0,22.0) microns
Parameters with values changed from defaults
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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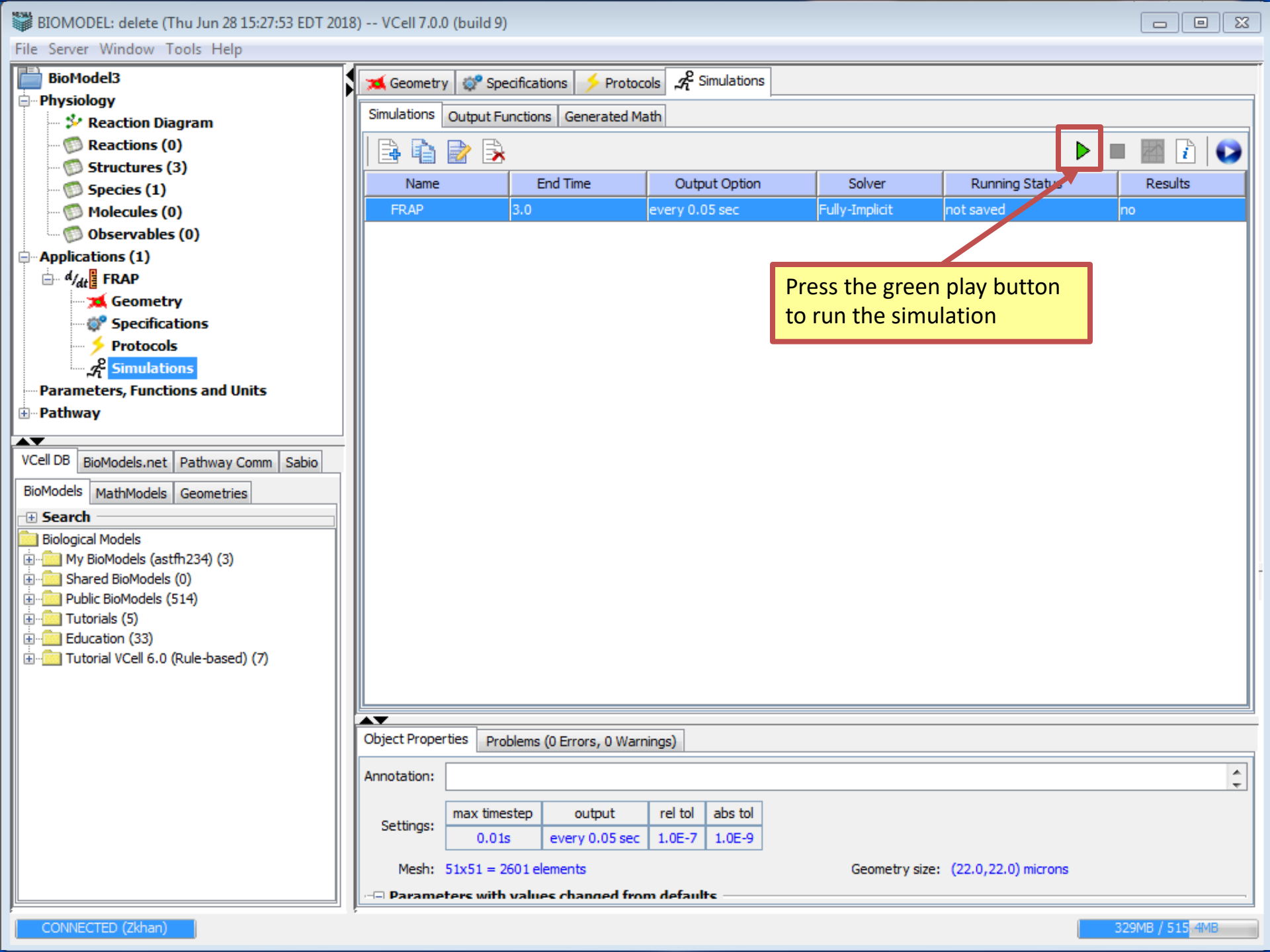
Simulations
Name
FRAP
Object Prope
Annotation:
Settings:
0.1s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 51x51 = 2601 elements
Geometry size: (22.0,22.0) microns
Edit: FRAP
Parameters
Mesh
Solver
Click “Solver”.
Choose solver algorithm and fine-tune time conditions:
Integrator
Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)
Type “3.0” for the Ending Time Bound.
Type in “.01” for the Maximum Time Step.
Time Bounds
Starting
Ending
3.0
Minimum
Default
Maximum
0.01
Error Tolerance
Absolute
1.0E-9
Relative
1.0E-7
Local Sensitivity Analysis
Output Options
Keep Every
time samples and at most
time samples
Output Interval
0.05
secs
Miscellaneous
Type “0.05” for the Output Interval.
OK
Cancel
Click “OK”.
CONNECTED (Zkhan)
329MB / 515 4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Generated Math
Name
End Time
Output Option
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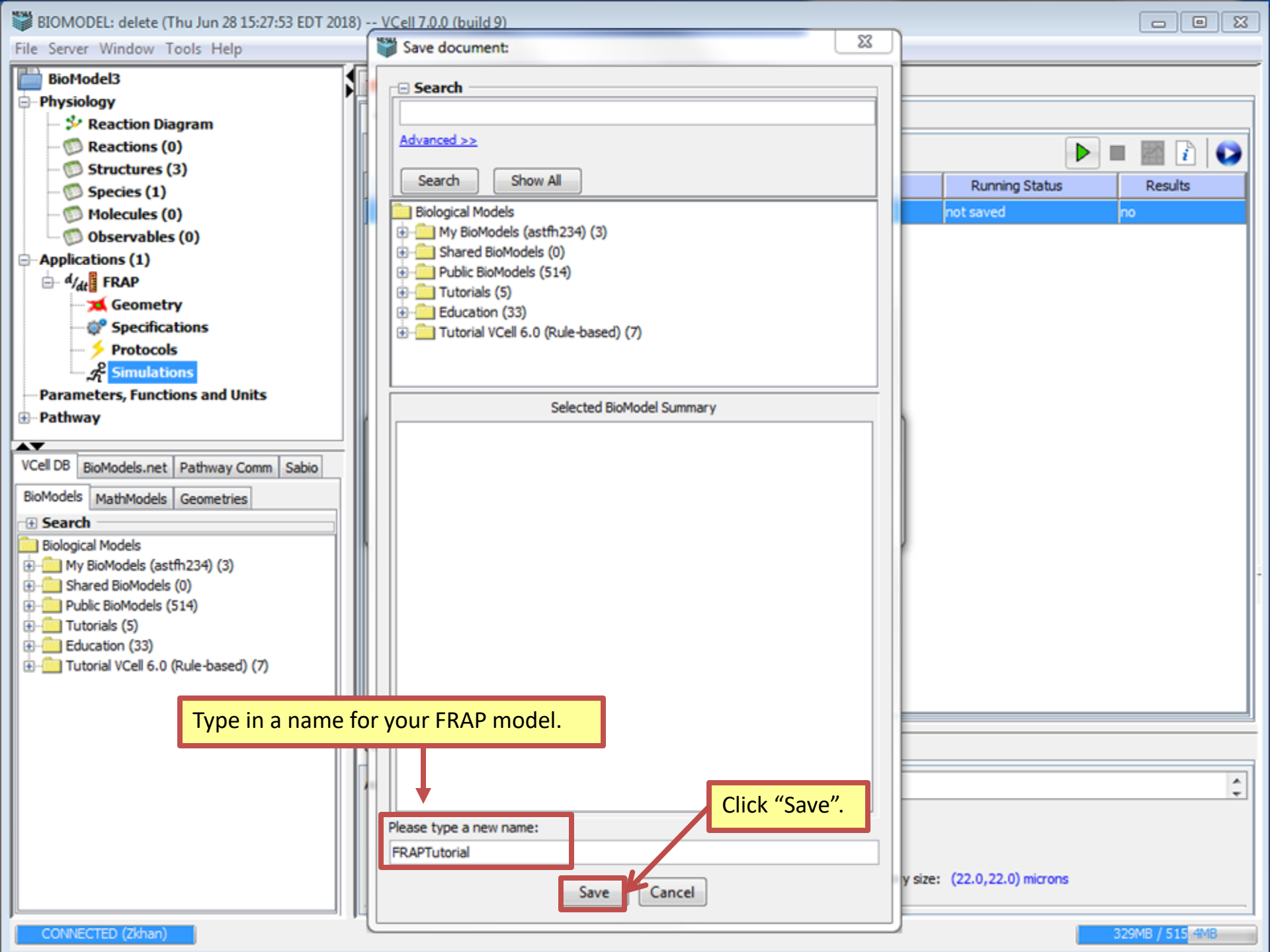
FRAP
3.0
every 0.05 sec
Fully-Implicit
not saved
no
Press the green play button to run the simulation
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.01s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 51x51 = 2601 elements
Geometry size: (22.0,22.0) microns
Parameters with values changed from defaults
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
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Tutorial VCell 6.0 (Rule-based) (7)
Save document:
Search
Advanced >>
Search
Show All
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
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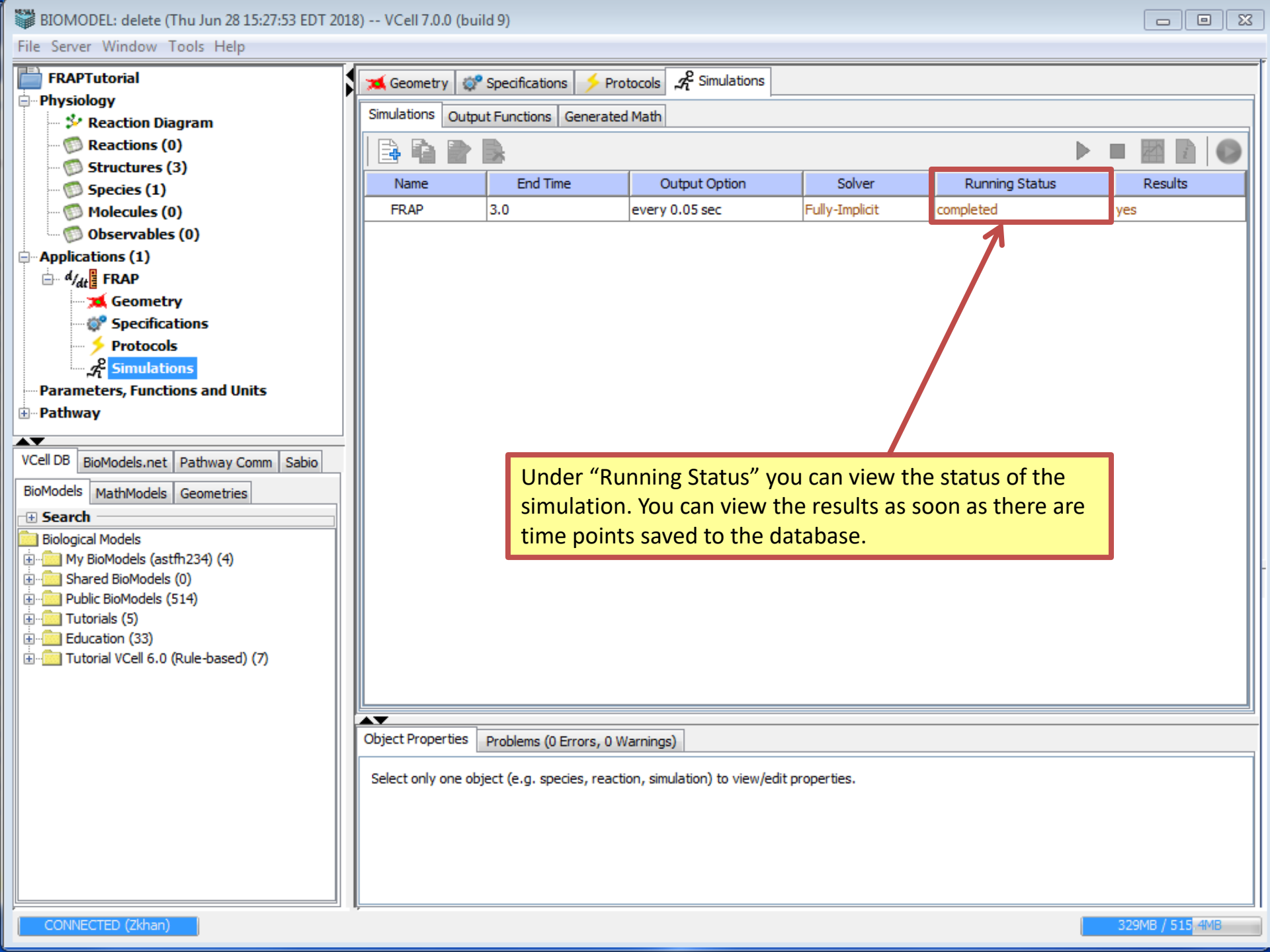
Tutorial VCell 6.0 (Rule-based) (7)
Selected BioModel Summary
Running Status
Results
not saved
no
Please type a new name:
FRAPTutorial
Save
Cancel
Type in a name for your FRAP model.
Click “Save”.
y size: (22.0,22.0) microns
CONNECTED (Zkhan)
329MB / 515MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
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Physiology
Reaction Diagram
Reactions (0)
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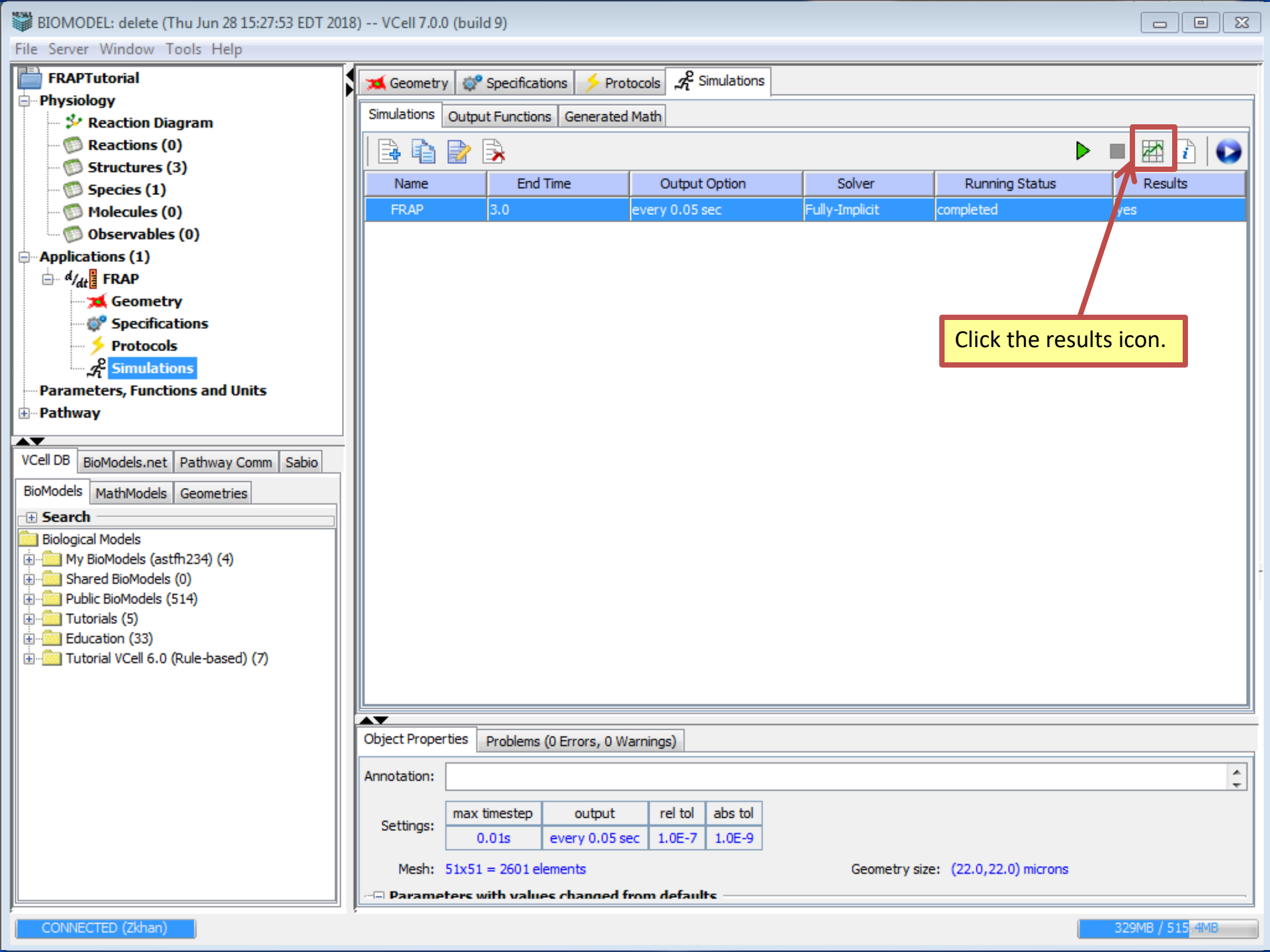
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
FRAP
3.0
every 0.05 sec
Fully-Implicit
completed
yes
Under “Running Status” you can view the status of the simulation. You can view the results as soon as there are time points saved to the database.
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Zkhan)
329MB / 515 4MB


BIOMODEL: delete (Thu Jun 28 15:27:53 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
FRAPTutorial
Physiology
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Reactions (0)
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Simulations
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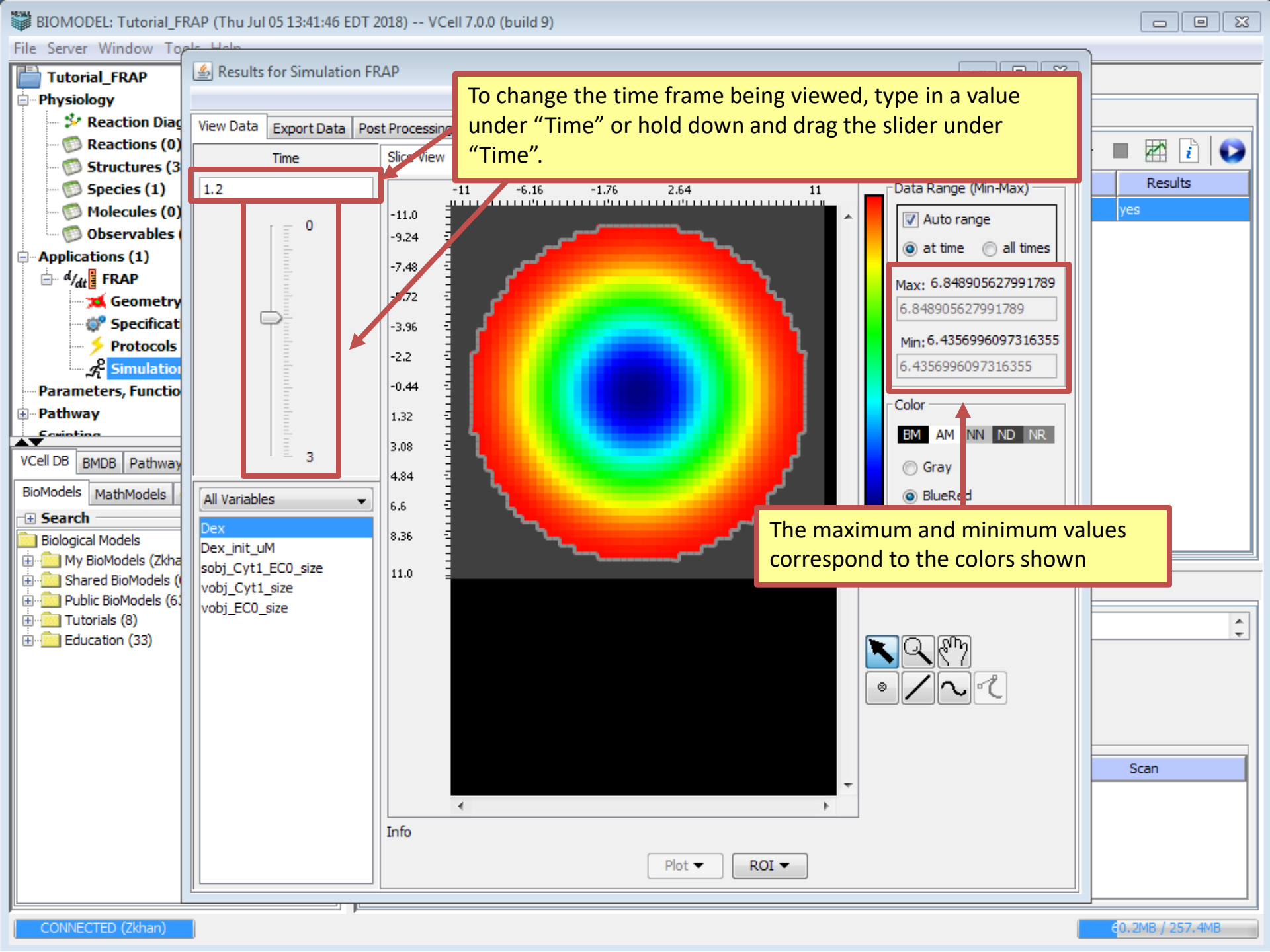
Name
End Time
Output Option
Solver
Running Status
Results
FRAP
3.0
every 0.05 sec
Fully-Implicit
completed
yes
Click the results icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.01s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 51x51 = 2601 elements
Geometry size: (22.0,22.0) microns
Parameters with values changed from defaults
CONNECTED (Zkhan)
329MB / 515.4MB


BIOMODEL: Tutorial_FRAP (Thu Jul 05 13:41:46 EDT 2018) -- VCell 7.0.0 (build 9)
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1.2
0
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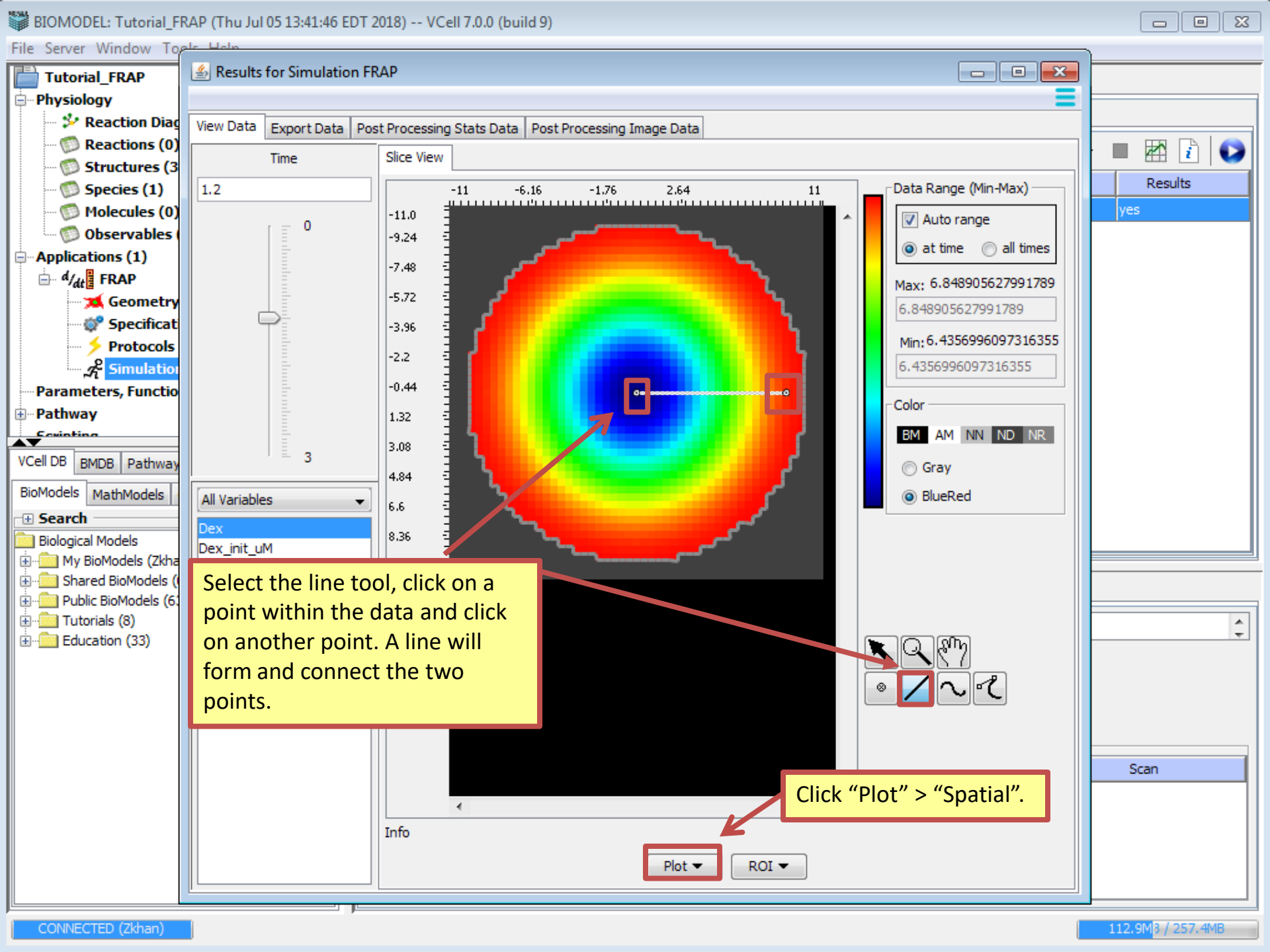
Slice View
-11
-6.16
-1.76
2.64
11
-11.0
-9.24
-7.48
-5.72
-3.96
-2.2
-0.44
1.32
3.08
4.84
6.6
8.36
11.0
All Variables
Dex
Dex_init_uM
sobj_Cyt1_EC0_size
vobj_Cyt1_size
vobj_EC0_size
Info
Plot
ROI
Data Range (Min-Max)
Auto range
at time
all times
Max: 6.848905627991789
6.848905627991789
Min: 6.4356996097316355
6.4356996097316355
Color
BM
AM
NN
ND
NR
Gray
BlueRed
Results
yes
Scan
CONNECTED (Zkhan)
60.2MB / 257.4MB
To change the time frame being viewed, type in a value under “Time” or hold down and drag the slider under “Time”.
The maximum and minimum values correspond to the colors shown


BIOMODEL: Tutorial_FRAP (Thu Jul 05 13:41:46 EDT 2018) -- VCell 7.0.0 (build 9)
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-1.76
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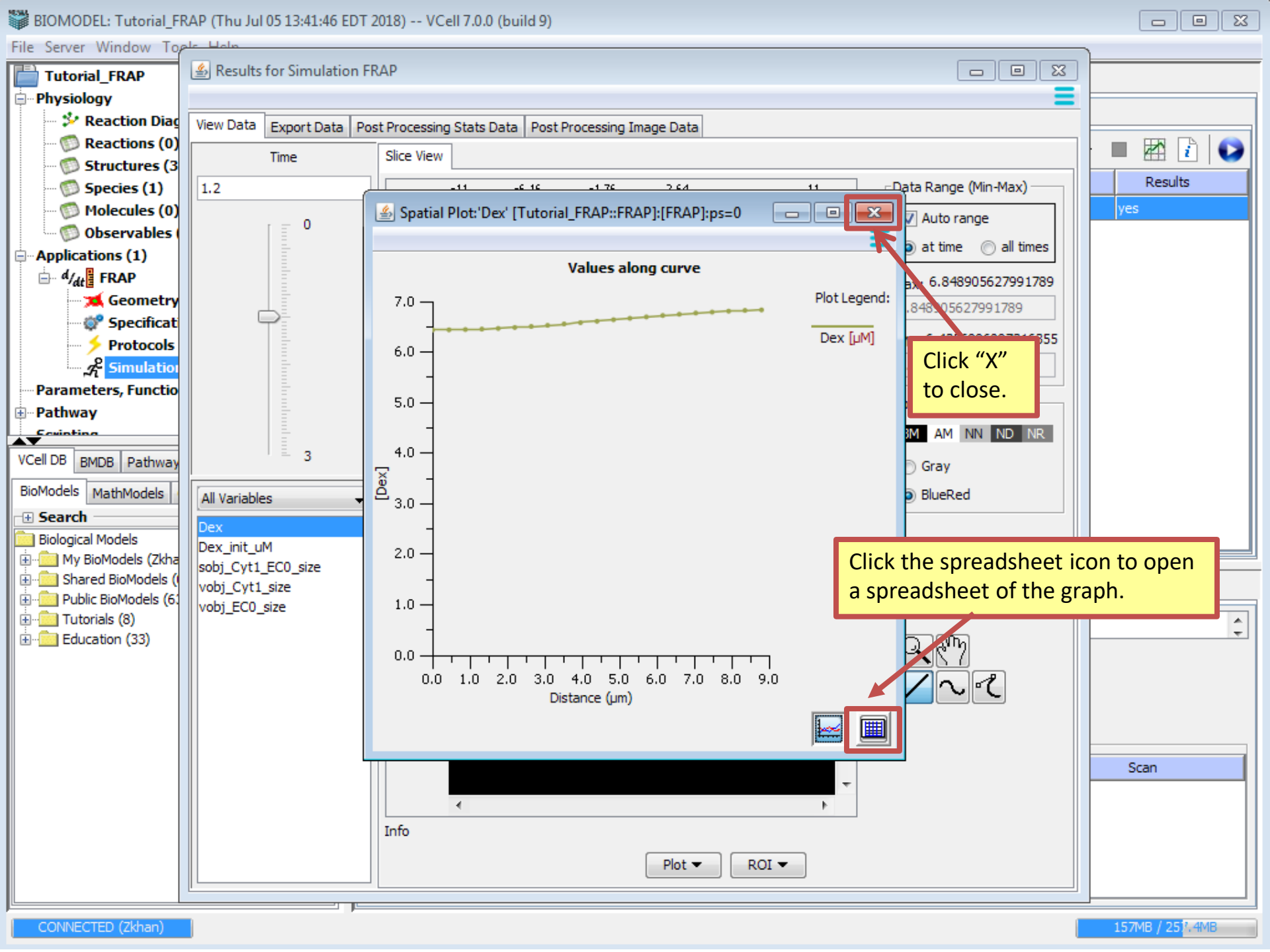
-7.48
-5.72
-3.96
-2.2
-0.44
1.32
3.08
4.84
6.6
8.36
Data Range (Min-Max)
Auto range
at time
all times
Max: 6.848905627991789
6.848905627991789
Min: 6.4356996097316355
6.4356996097316355
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
Dex
Dex_init_uM
Select the line tool, click on a point within the data and click on another point. A line will form and connect the two points.
Click “Plot” > “Spatial”.
Info
Plot
ROI
Results
yes
Scan
CONNECTED (Zkhan)
112.9MB / 257.4MB


BIOMODEL: Tutorial_FRAP (Thu Jul 05 13:41:46 EDT 2018) -- VCell 7.0.0 (build 9)
File Server Window Tools Help
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All Variables
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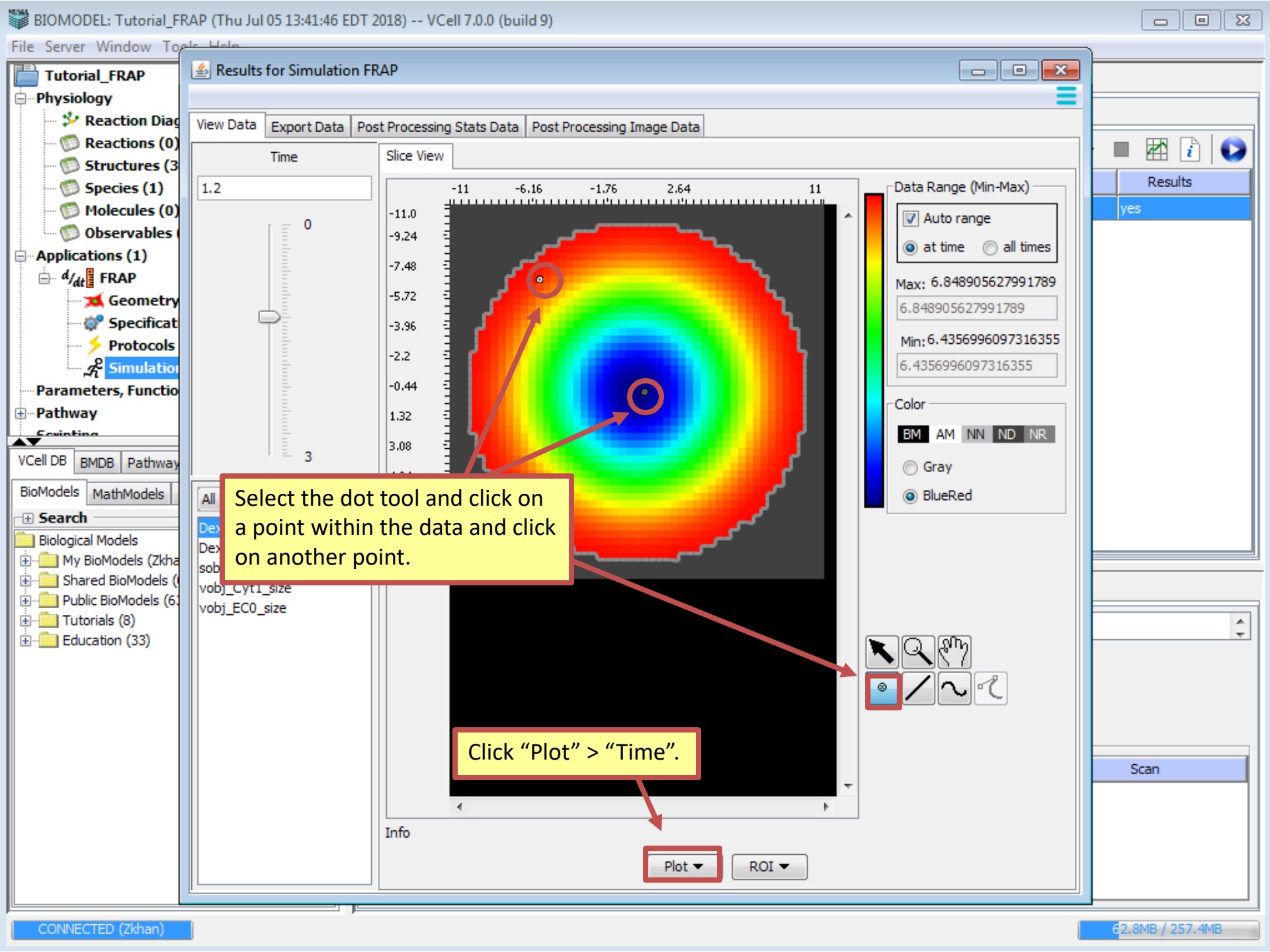
Dex_init_uM
sobj_Cyt1_EC0_size
vobj_Cyt1_size
vobj_EC0_size
Data Range (Min-Max)
Auto range
at time
all times
6.848905627991789
AM
NN
ND
NR
Gray
BlueRed
Info
Plot
ROI
Results
yes
Scan
Spatial Plot:'Dex' [Tutorial_FRAP::FRAP]:[FRAP]:ps=0
Values along curve
Plot Legend:
Dex [μM]
[Dex]
Distance (μm)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
Click "X" to close.
Click the spreadsheet icon to open a spreadsheet of the graph.
CONNECTED (Zkhan)
157MB / 25


BIOMODEL: Tutorial_FRAP (Thu Jul 05 13:41:46 EDT 2018) -- VCell 7.0.0 (build 9)
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Slice View
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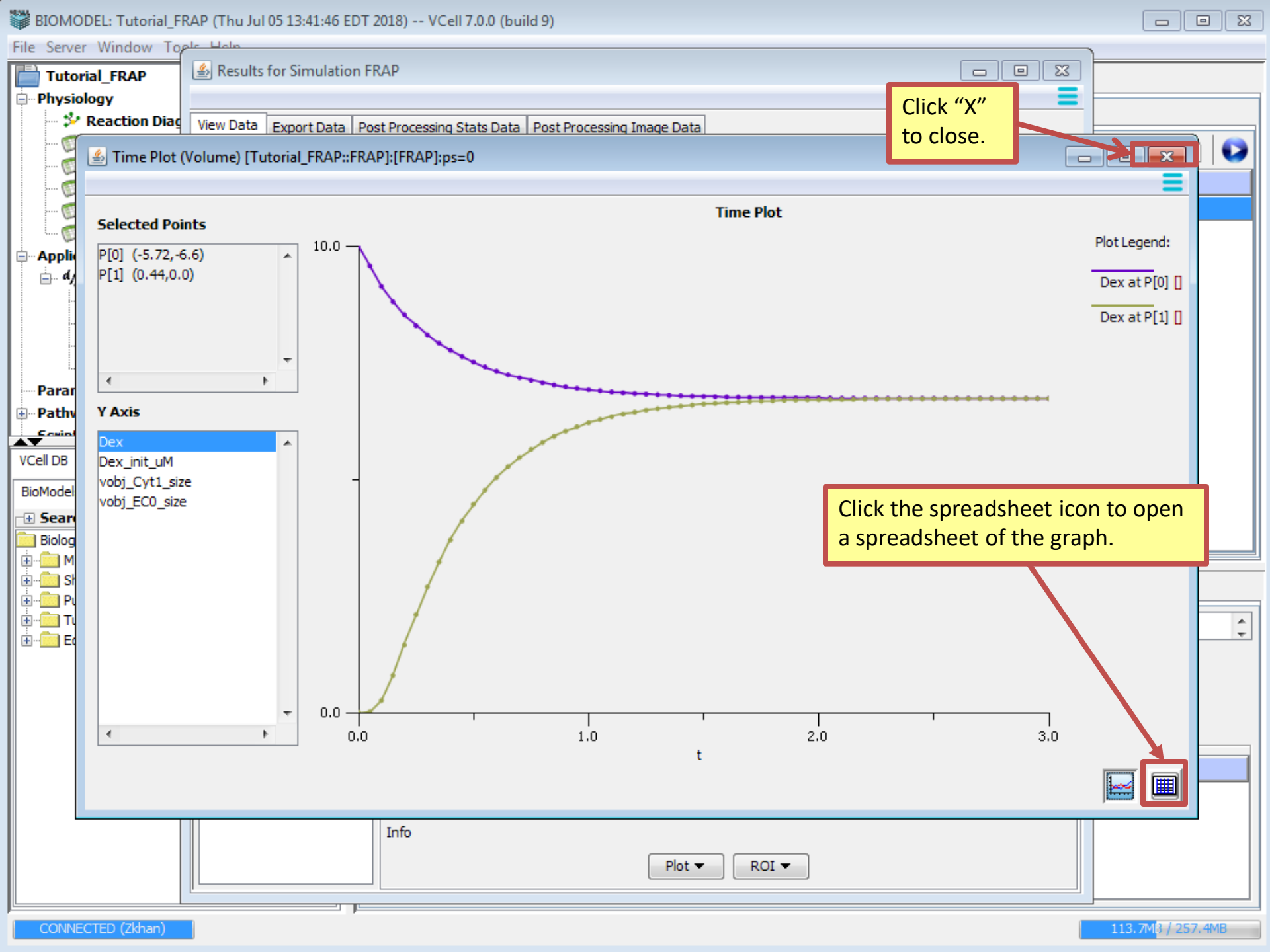
-6.16
-1.76
2.64
11
-11.0
-9.24
-7.48
-5.72
-3.96
-2.2
-0.44
1.32
3.08
All
vobj_Cyt1_size
vobj_EC0_size
Data Range (Min-Max)
Auto range
at time
all times
Max: 6.848905627991789
6.848905627991789
Min: 6.4356996097316355
6.4356996097316355
Color
BM
AM
NN
ND
NR
Gray
BlueRed
Select the dot tool and click on a point within the data and click on another point.
Click “Plot” > “Time”.
Info
Plot
ROI
Results
yes
Scan
CONNECTED (Zkhan)
62.8MB / 257.4MB


BIOMODEL: Tutorial_FRAP (Thu Jul 05 13:41:46 EDT 2018) -- VCell 7.0.0 (build 9)
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Results for Simulation FRAP
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time Plot (Volume) [Tutorial_FRAP::FRAP]:[FRAP]:ps=0
Selected Points
P[0] (-5.72,-6.6)
P[1] (0.44,0.0)
Y Axis
Dex
Dex_init_uM
vobj_Cyt1_size
vobj_EC0_size
Time Plot
Plot Legend:
Dex at P[0]
Dex at P[1]
10.0
0.0
0.0
1.0
2.0
3.0
t
Click "X" to close.
Click the spreadsheet icon to open a spreadsheet of the graph.
Info
Plot
ROI
CONNECTED (Zkhan)
113.7MB / 257.4MB

Acknowledgements

The following students worked on this tutorial:

Arundeep Singh (2018) – Sport and Medical Sciences Academy
Zaiba Khan (2018) – East Windsor High School

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