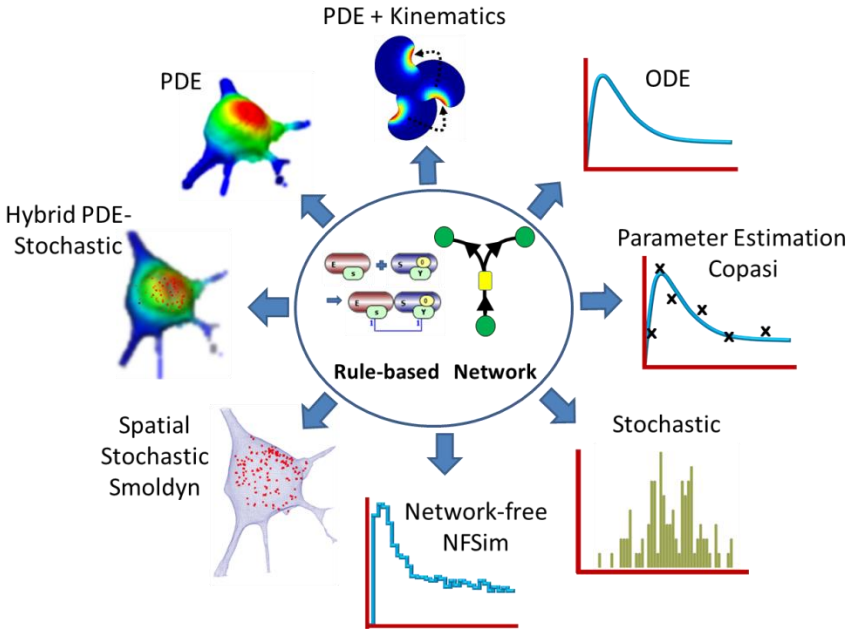
VCell

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 BioModel with Multiple Applications

Objective

Create a single Biomodel of RAN nuclear transport then use different modeling strategies to solve simulations.

Goals

- Create a Biomodel Physiology with species, reactions and fluxes
- Create a spatial deterministic application of the Physiology
- Import fluorescence images into VCell and segment a 3D image stack within VCell to create a geometry
- Create a simulation and specify solver, time, and computational mesh.
- Run the simulation, view results and create graphs

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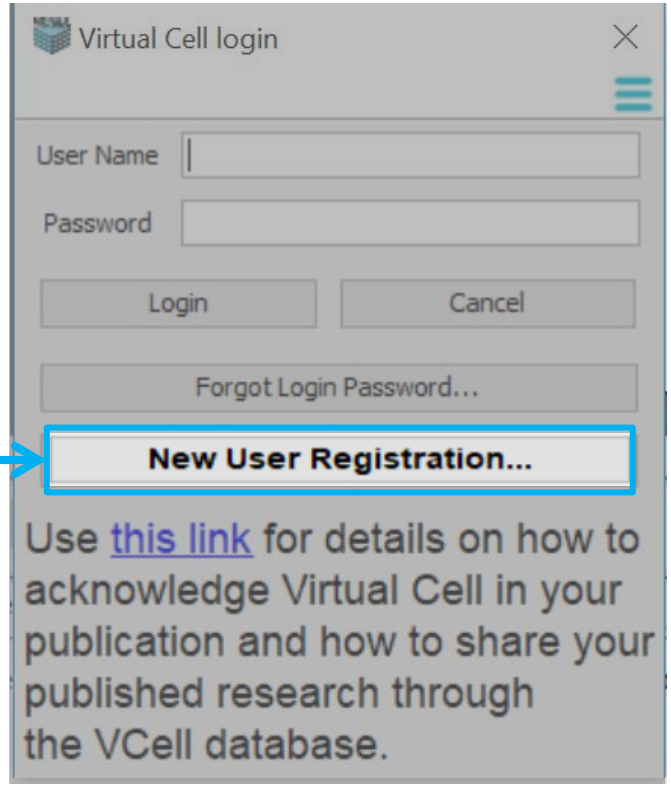
Your first time opening VCell

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.



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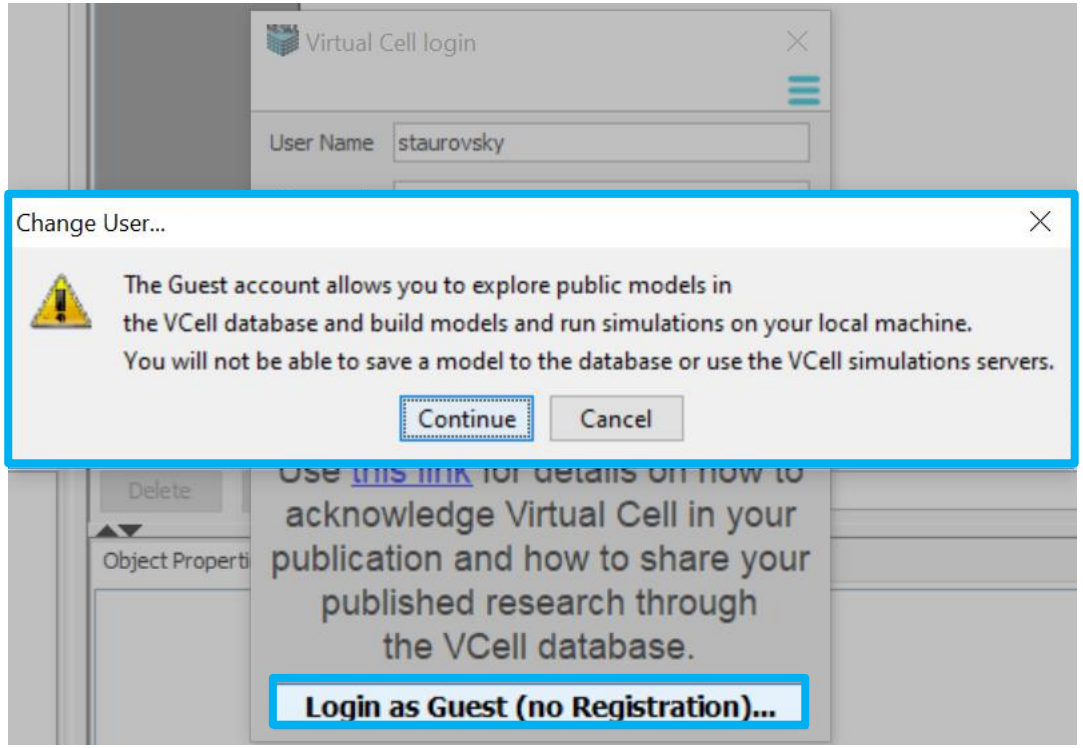
Guest Login Option



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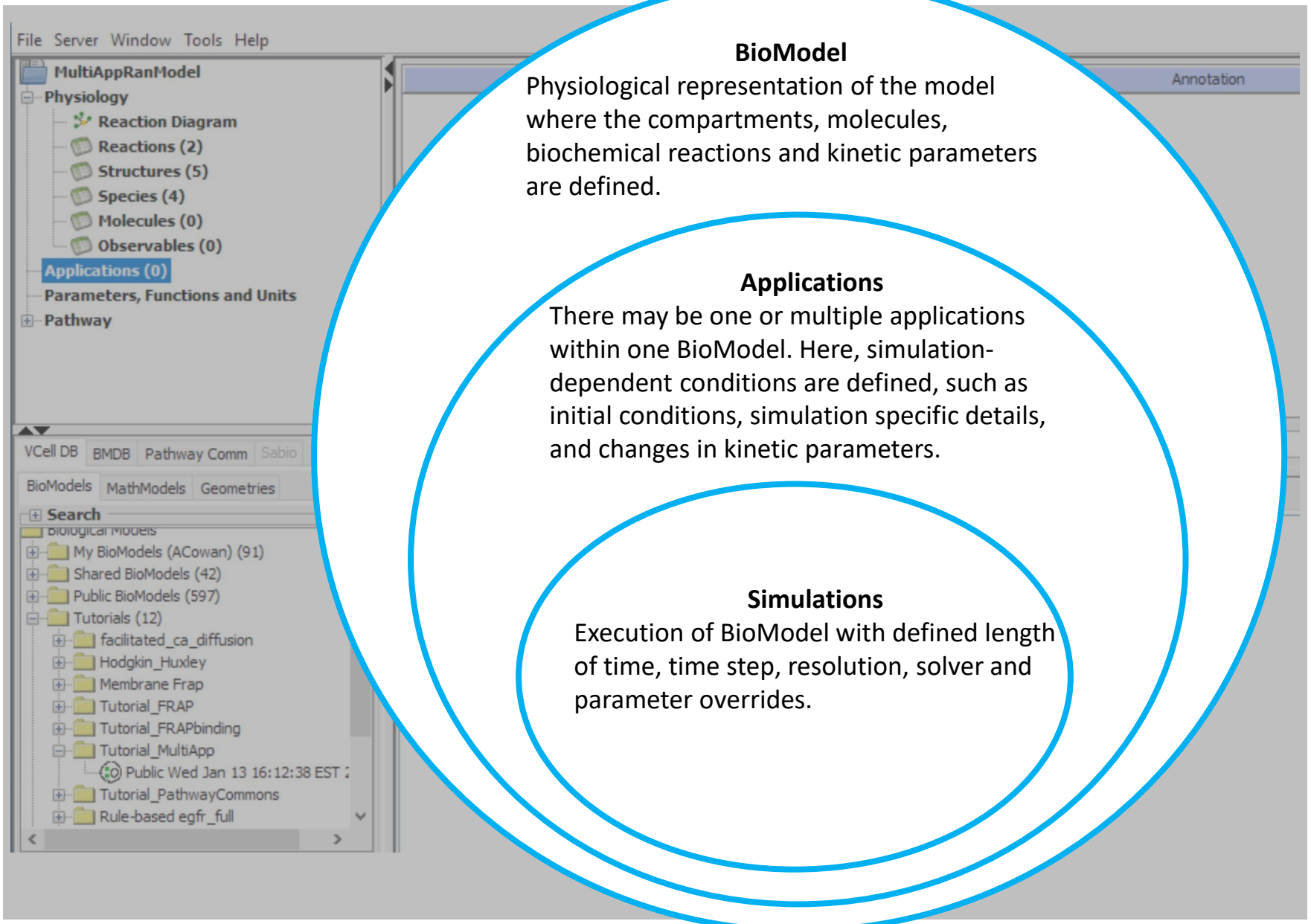
VCell BioModel Organization



BioModel

Physiological representation of the model where the compartments, molecules, biochemical reactions and kinetic parameters are defined.

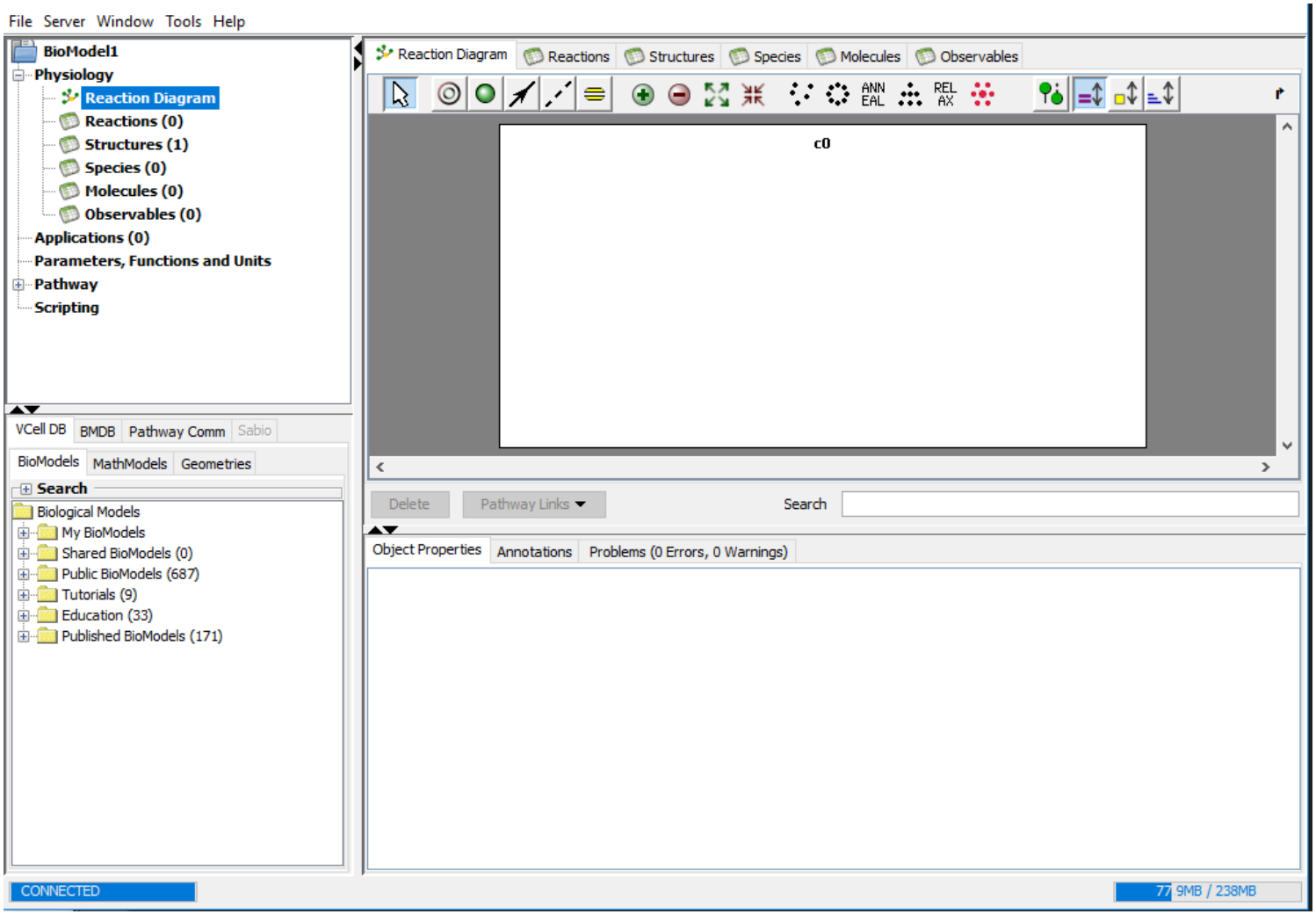
Applications

There may be one or multiple applications within one BioModel. Here, simulation-dependent conditions are defined, such as initial conditions, simulation specific details, and changes in kinetic parameters.

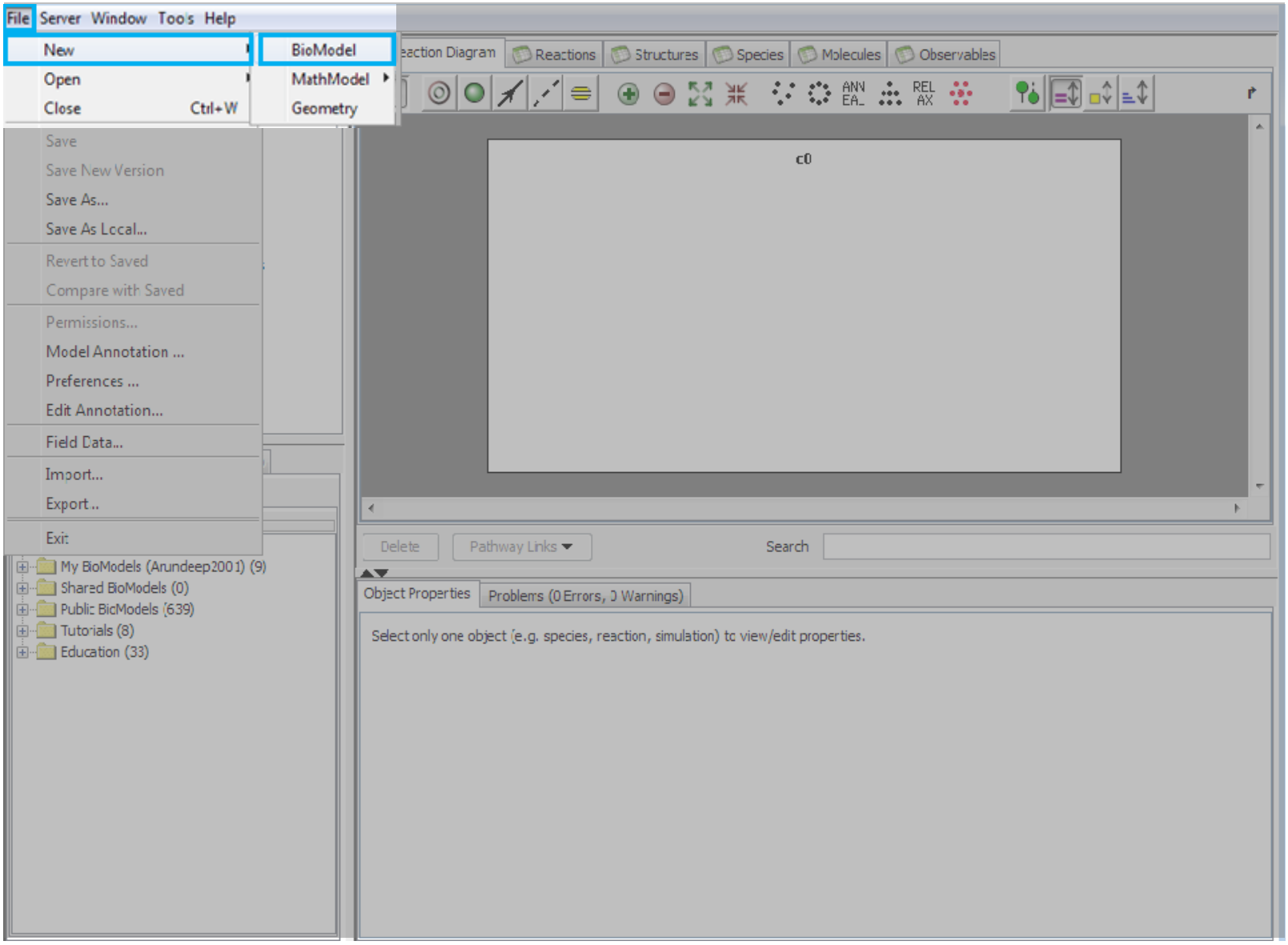
Simulations

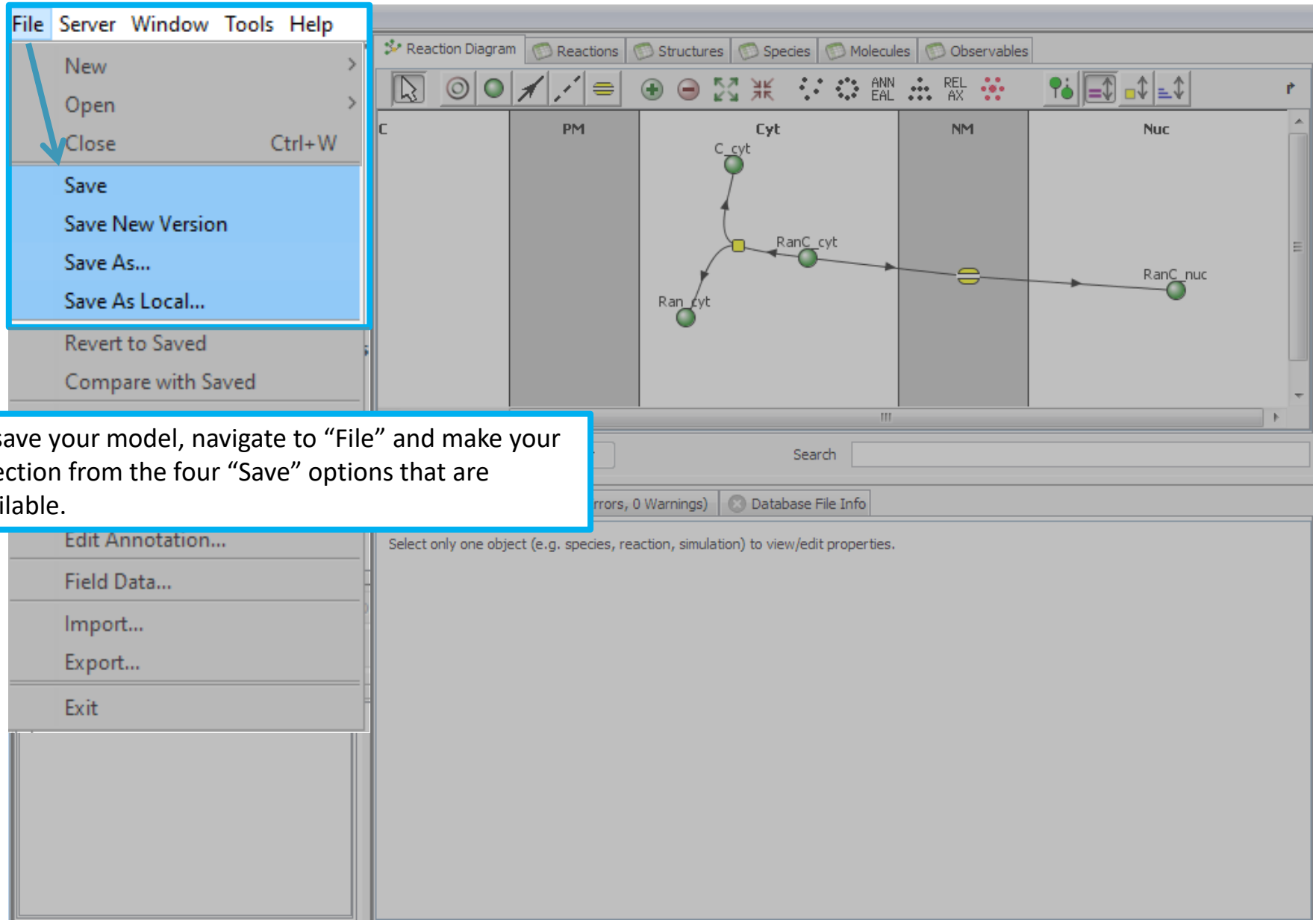
Execution of BioModel with defined length of time, time step, resolution, solver and parameter overrides.

The VCell Interface

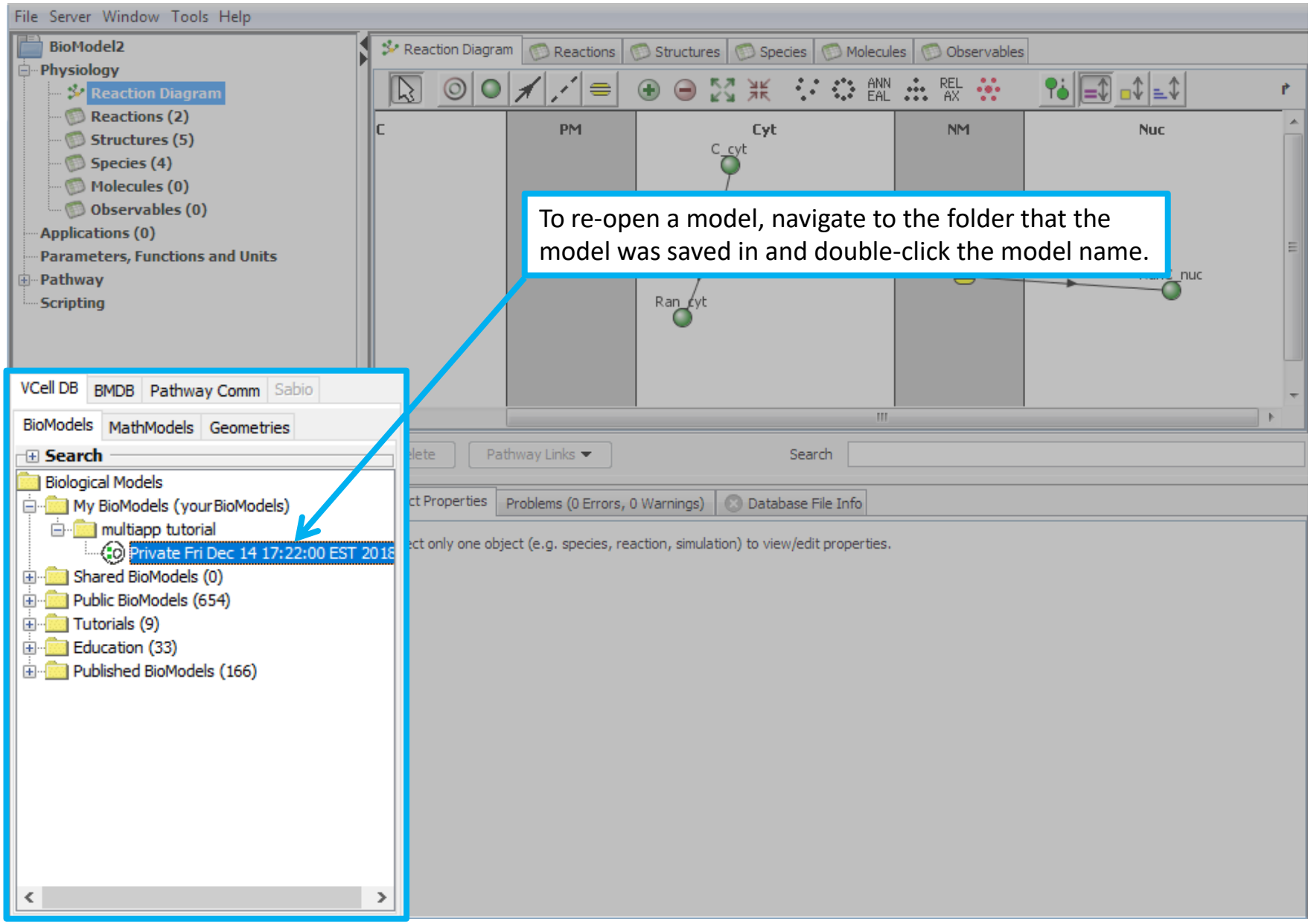


To create a new VCell model, click “File” > “New” > “BioModel”





To save your model, navigate to “File” and make your selection from the four “Save” options that are available.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multiapp tutorial
Private Fri Dec 14 17:22:00 EST 2018
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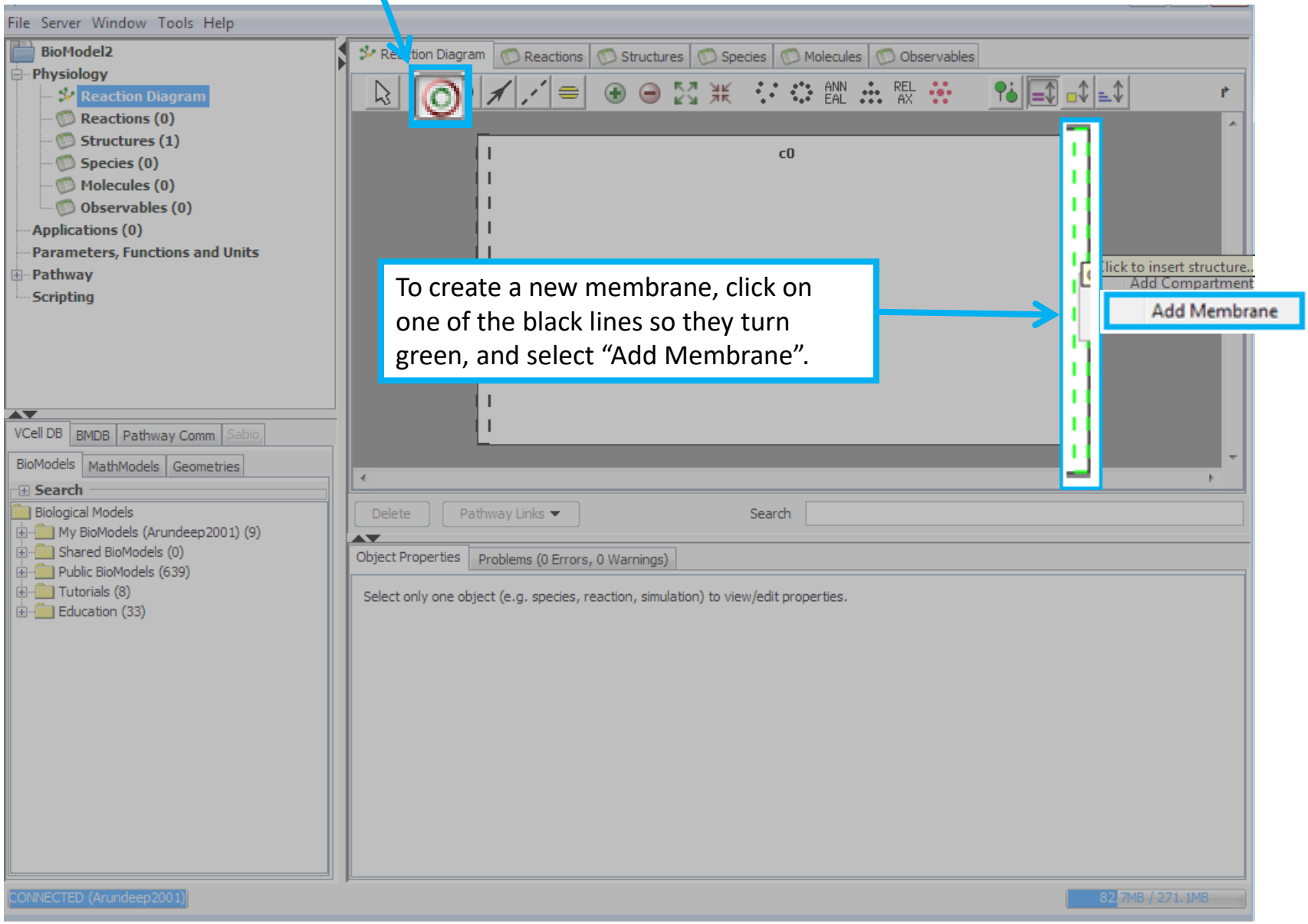
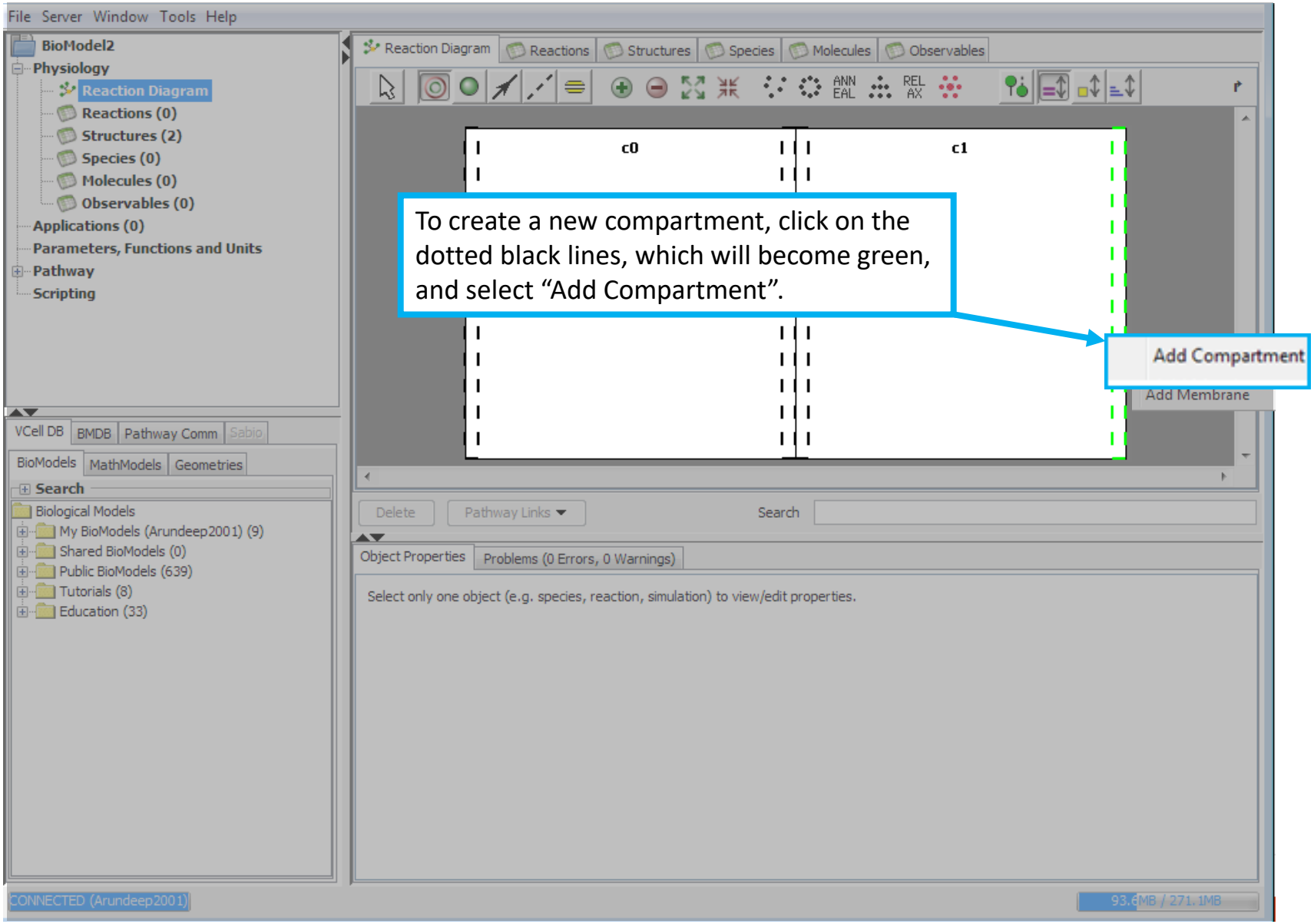
To re-open a model, navigate to the folder that the model was saved in and double-click the model name.

To create the components to your model, start with creating a volumetric compartment by selecting the Structure Tool. This will automatically create your first compartment.



To create a new membrane, click on one of the black lines so they turn green, and select “Add Membrane”.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To create a new compartment, click on the dotted black lines, which will become green, and select "Add Compartment".
Add Compartment
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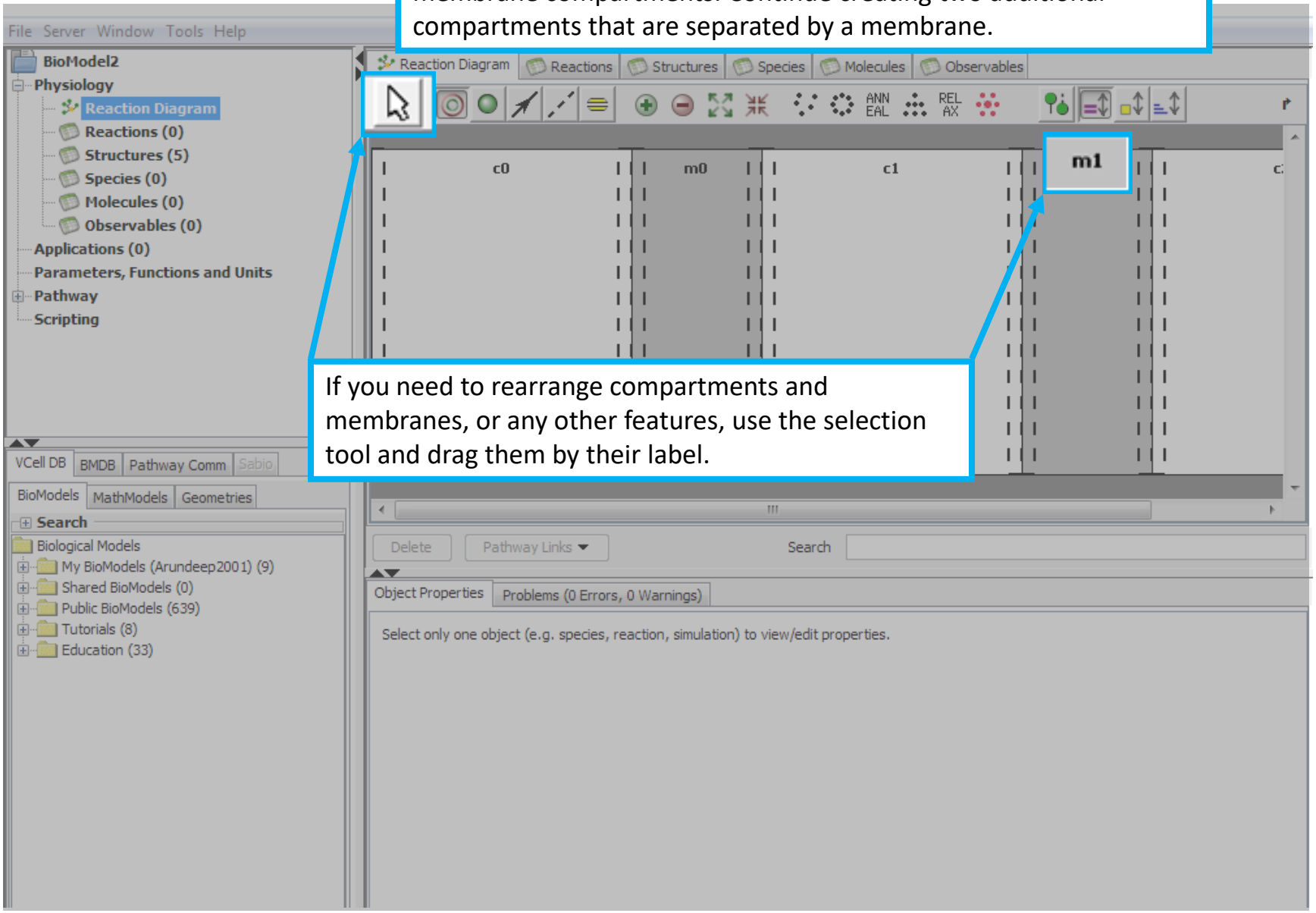
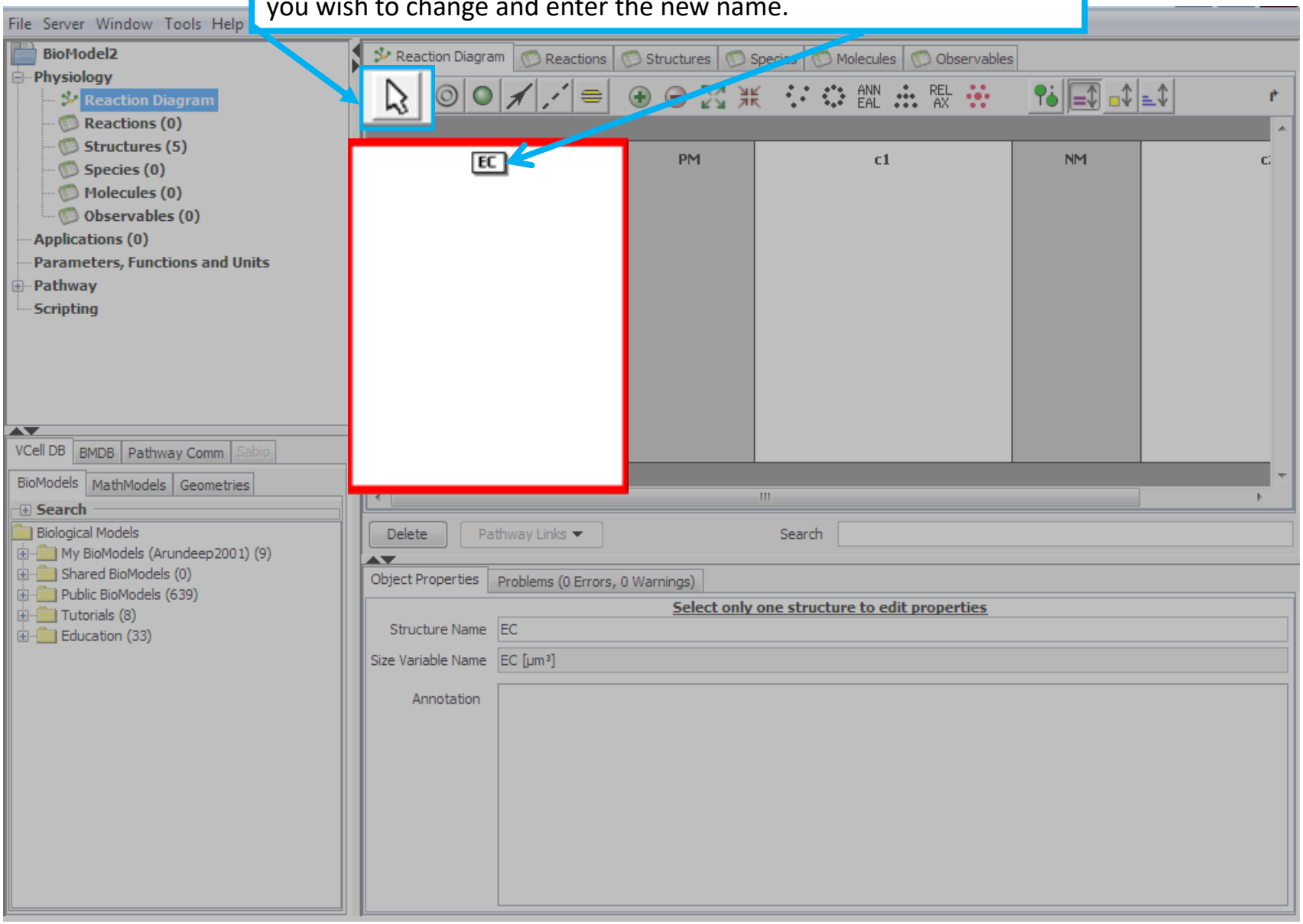
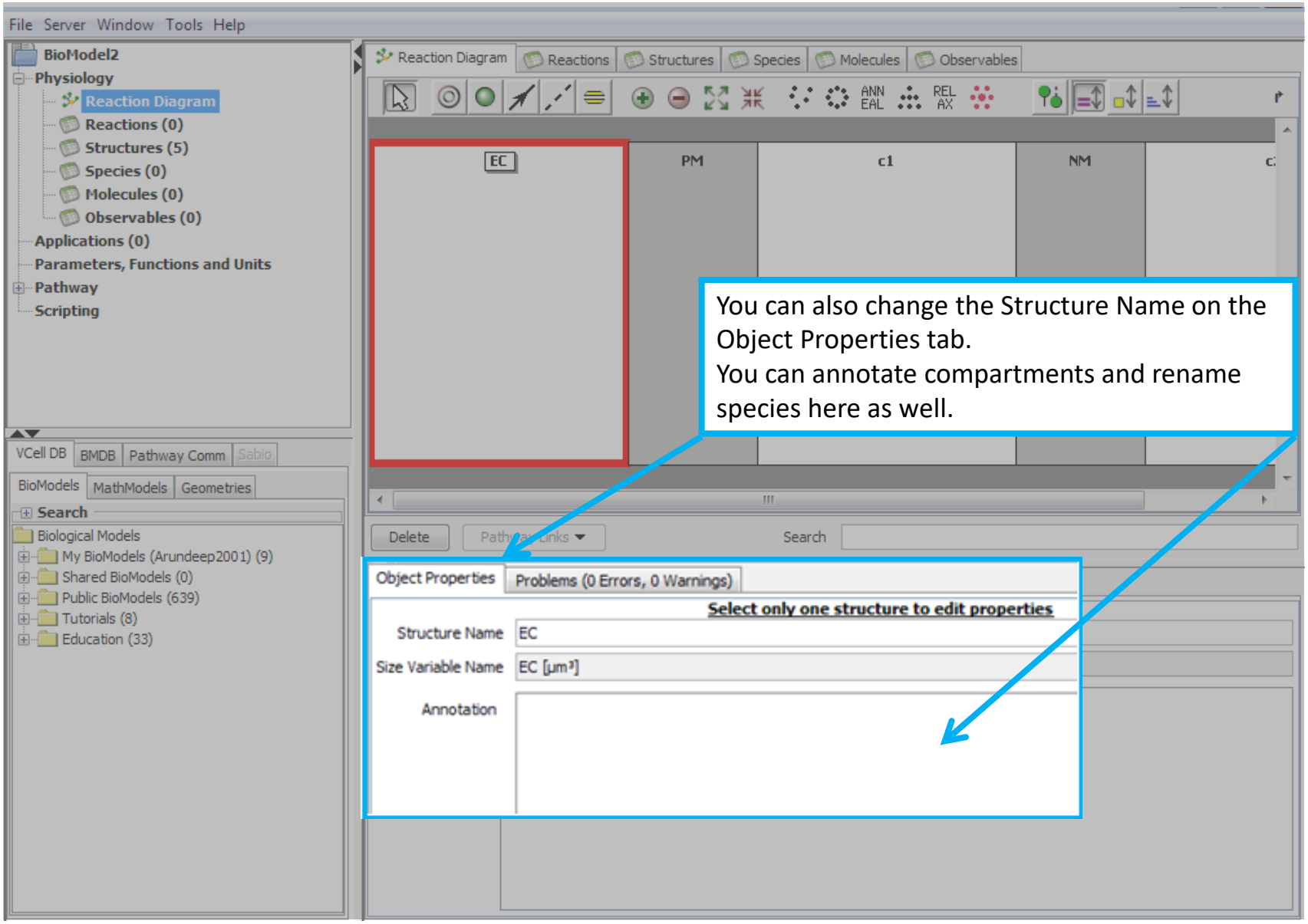
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (Arundeep2001)
93.6MB / 271.1MB

Your model requires 3 volumetric compartments separated by 2 membrane compartments. Continue creating two additional compartments that are separated by a membrane.



Use the selection tool to name compartments and membranes. The area will turn red upon selection. Double click the structure name you wish to change and enter the new name.

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You can also change the Structure Name on the Object Properties tab.
You can annotate compartments and rename species here as well.
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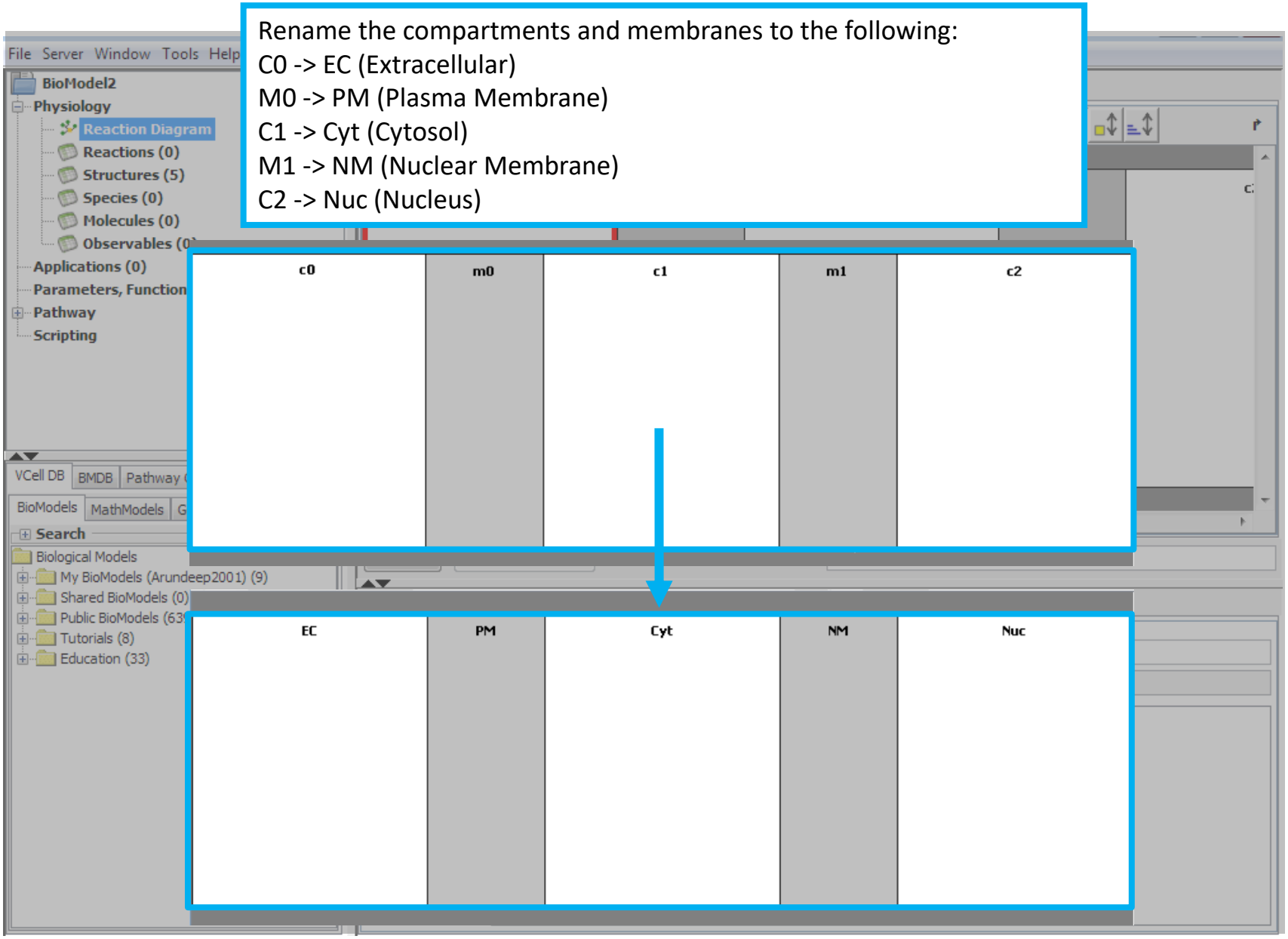
Select only one structure to edit properties
Structure Name
EC
Size Variable Name
EC [µm³]
Annotation


Rename the compartments and membranes to the following:
C0 -> EC (Extracellular)
M0 -> PM (Plasma Membrane)
C1 -> Cyt (Cytosol)
M1 -> NM (Nuclear Membrane)
C2 -> Nuc (Nucleus)
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m0
c1
m1
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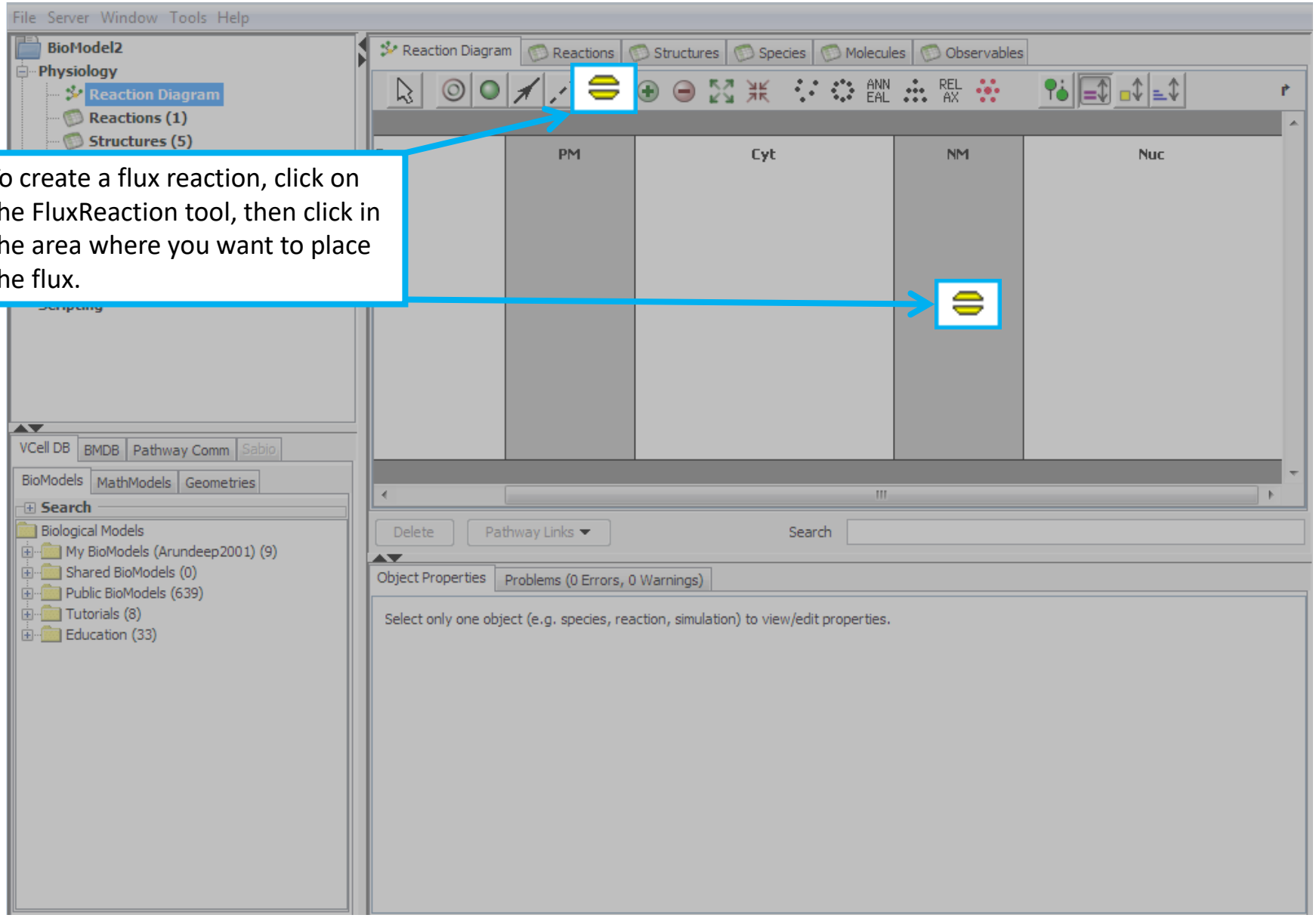
To create a flux reaction, click on the FluxReaction tool, then click in the area where you want to place the flux.
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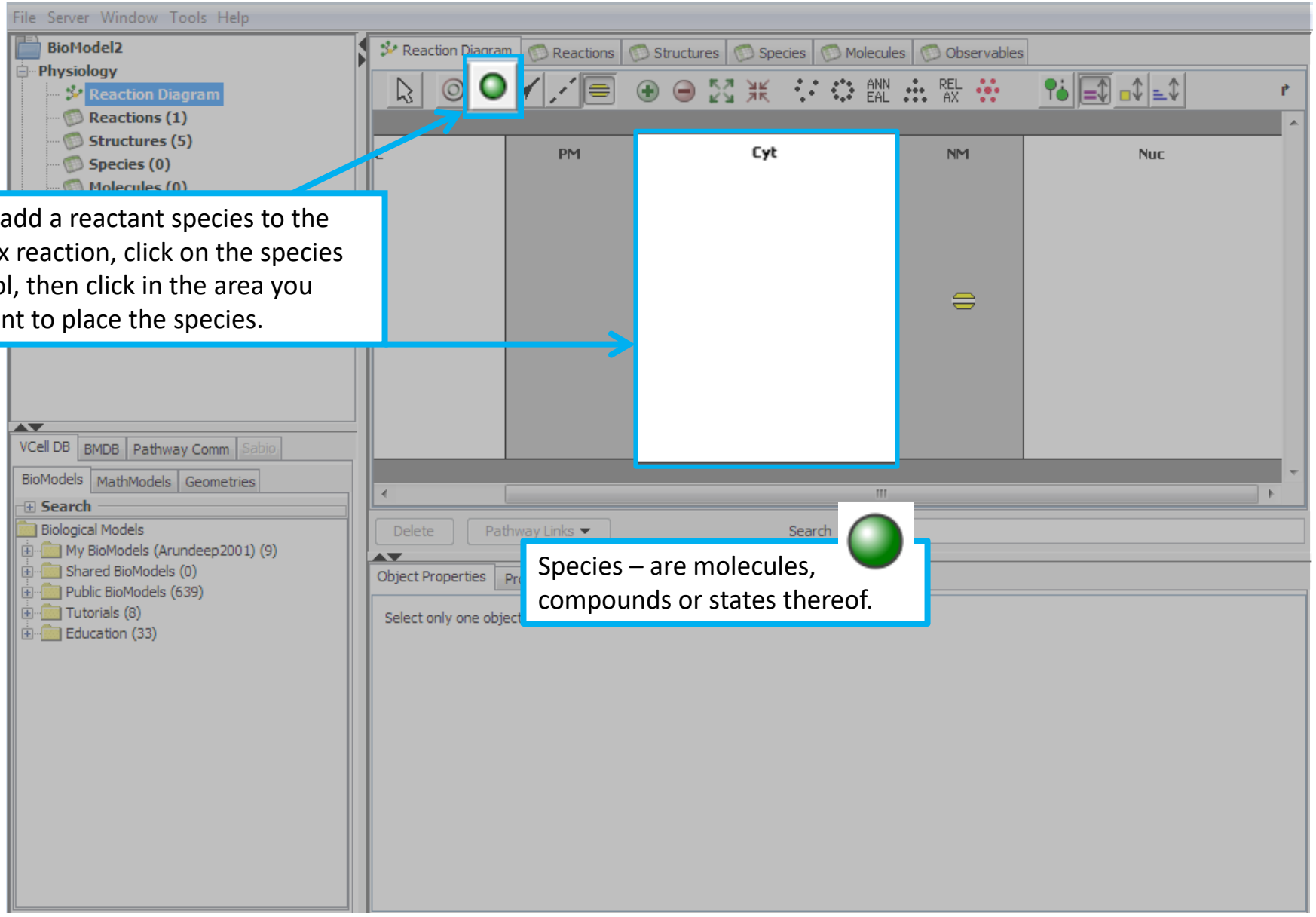
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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To add a reactant species to the flux reaction, click on the species tool, then click in the area you want to place the species.
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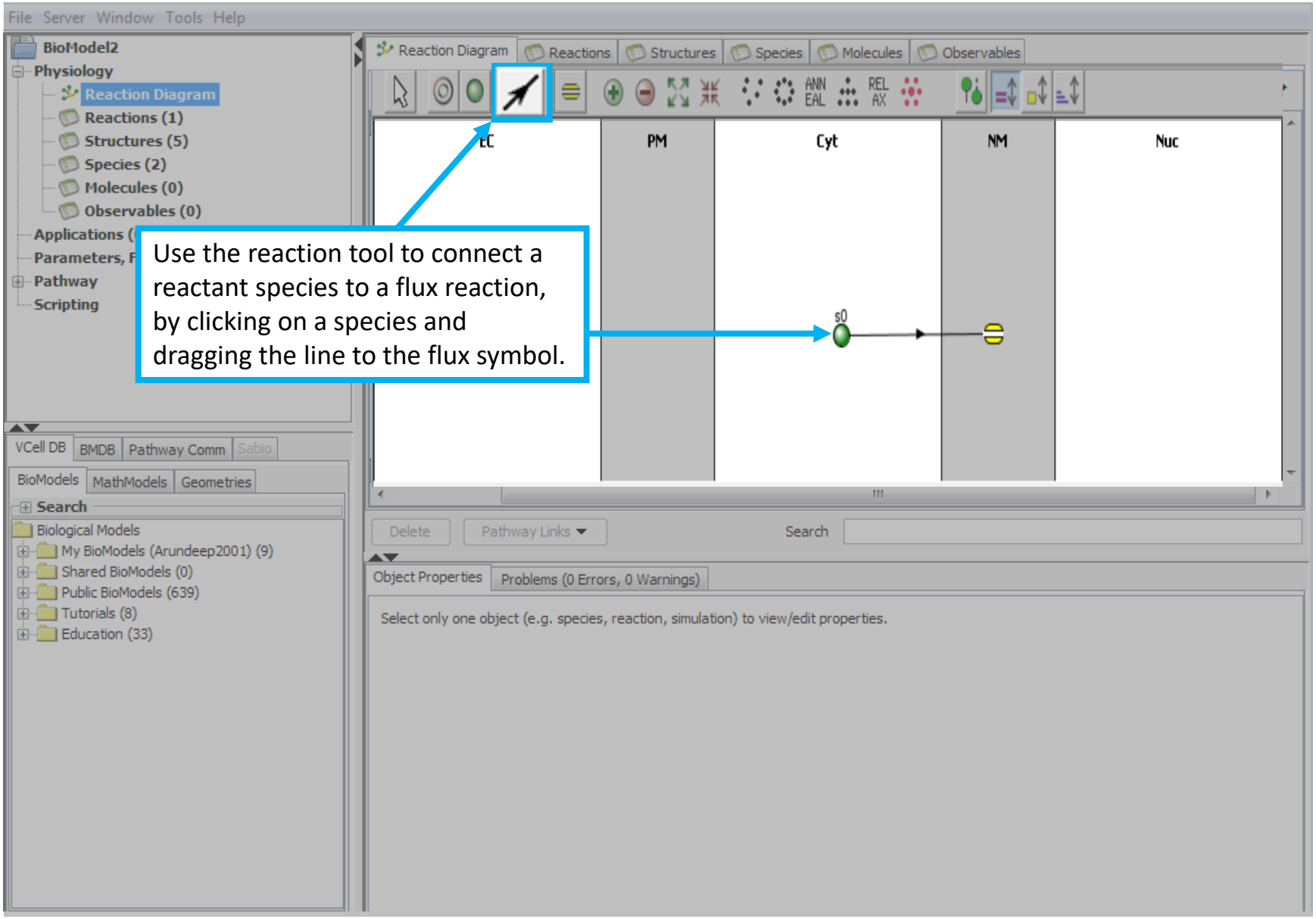
Species – are molecules, compounds or states thereof.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Use the reaction tool to connect a reactant species to a flux reaction, by clicking on a species and dragging the line to the flux symbol.
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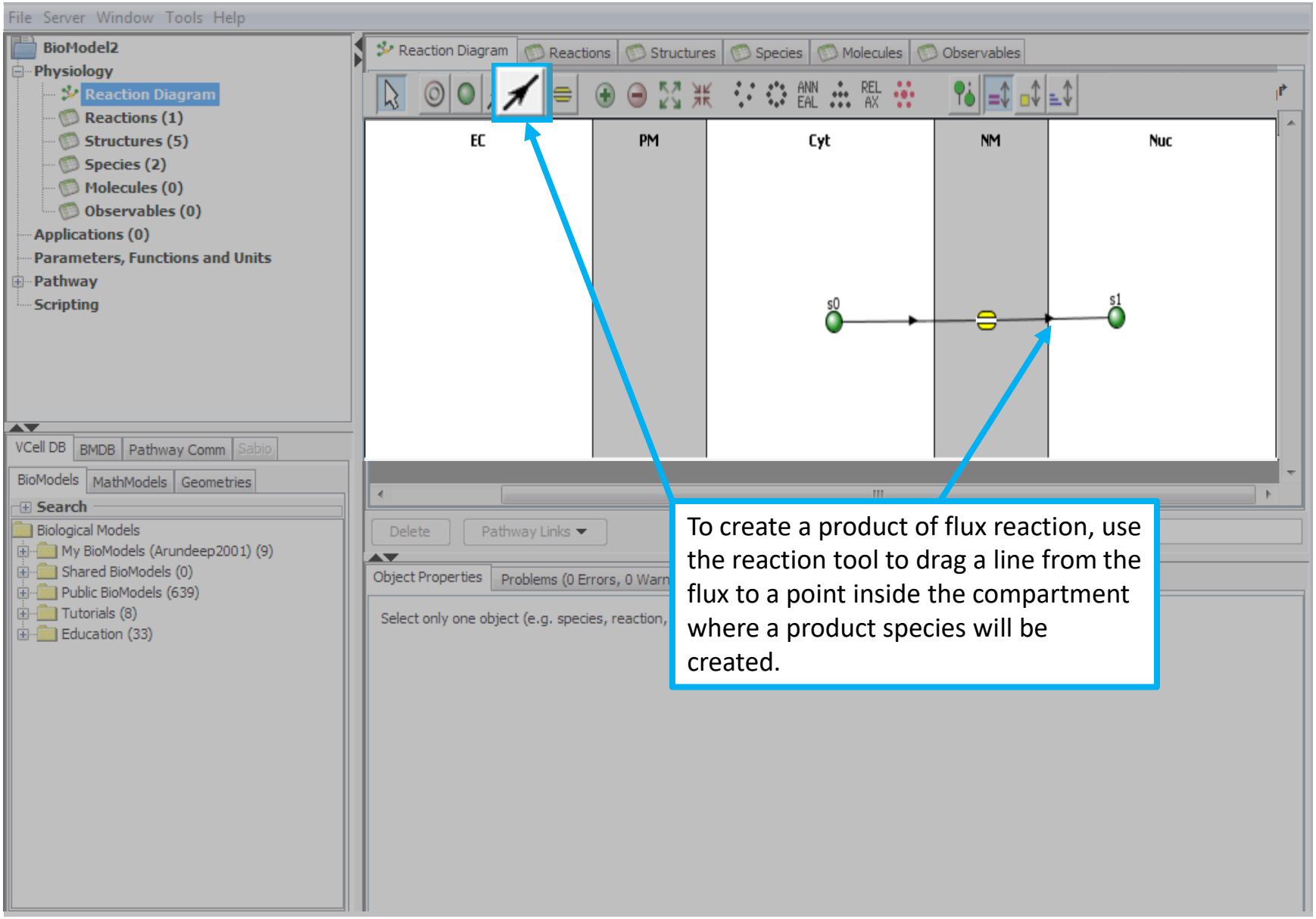
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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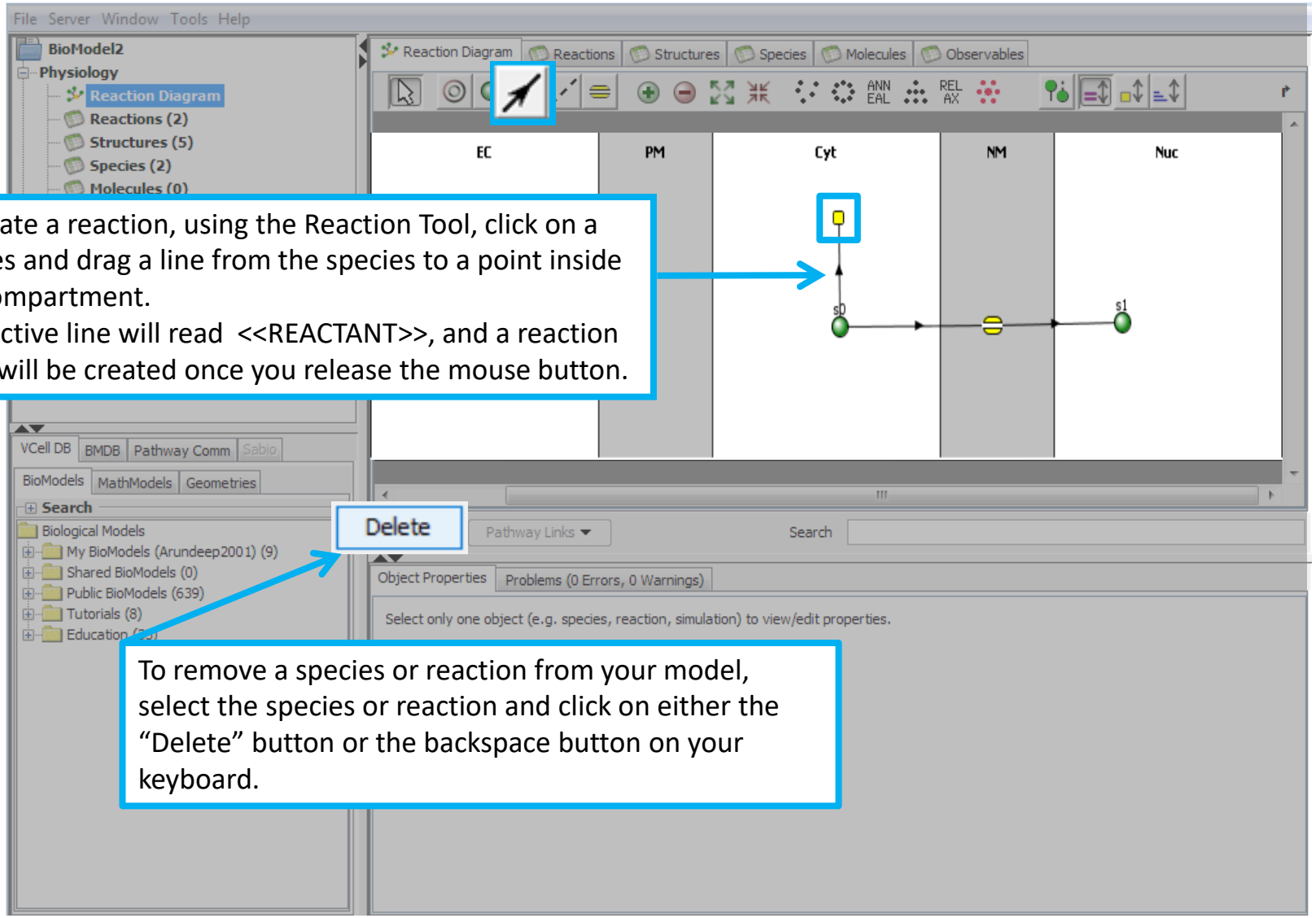
Select only one object (e.g. species, reaction,
To create a product of flux reaction, use the reaction tool to drag a line from the flux to a point inside the compartment where a product species will be created.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To create a reaction, using the Reaction Tool, click on a species and drag a line from the species to a point inside the compartment.
The active line will read <<REACTANT>>, and a reaction node will be created once you release the mouse button.
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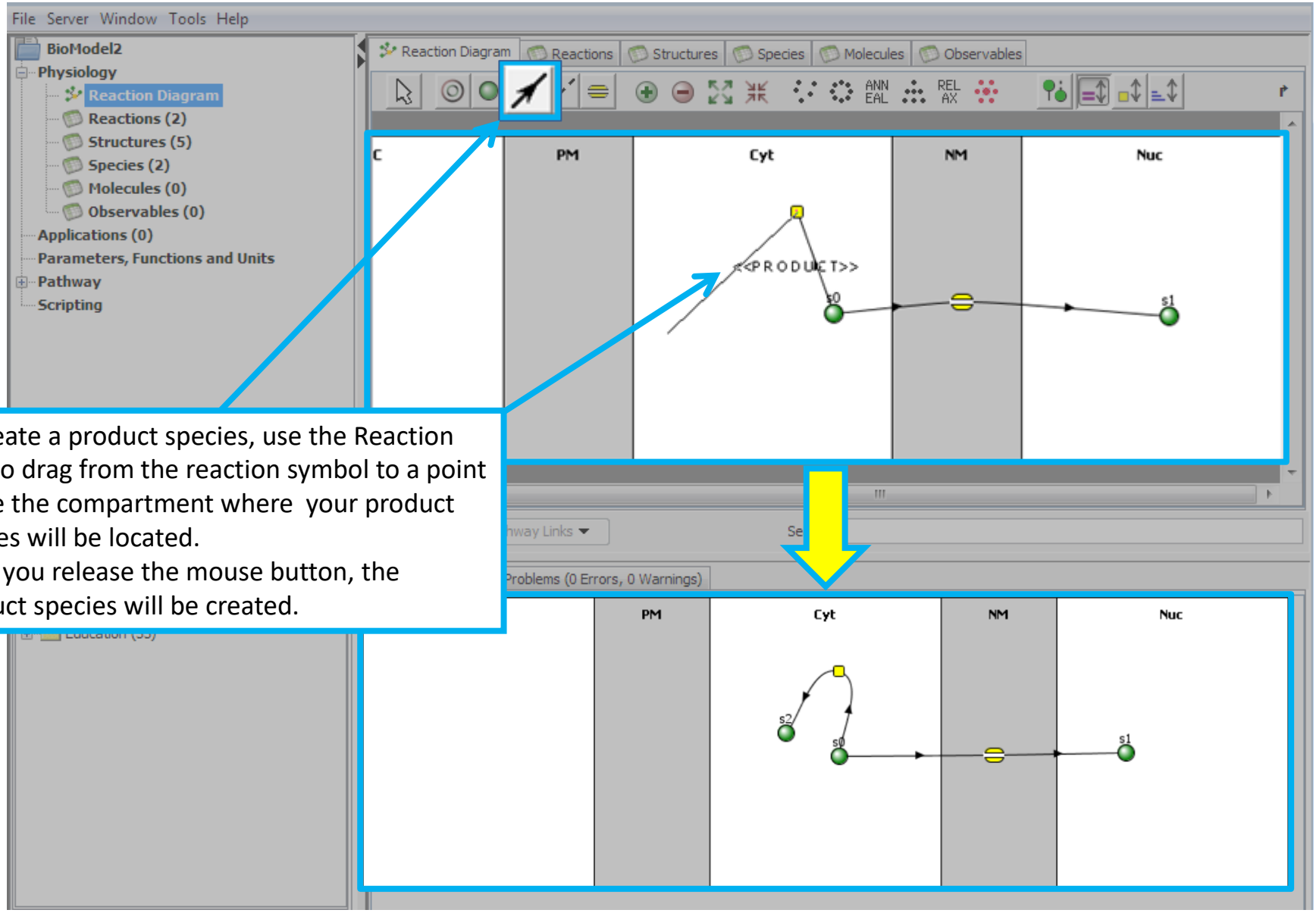
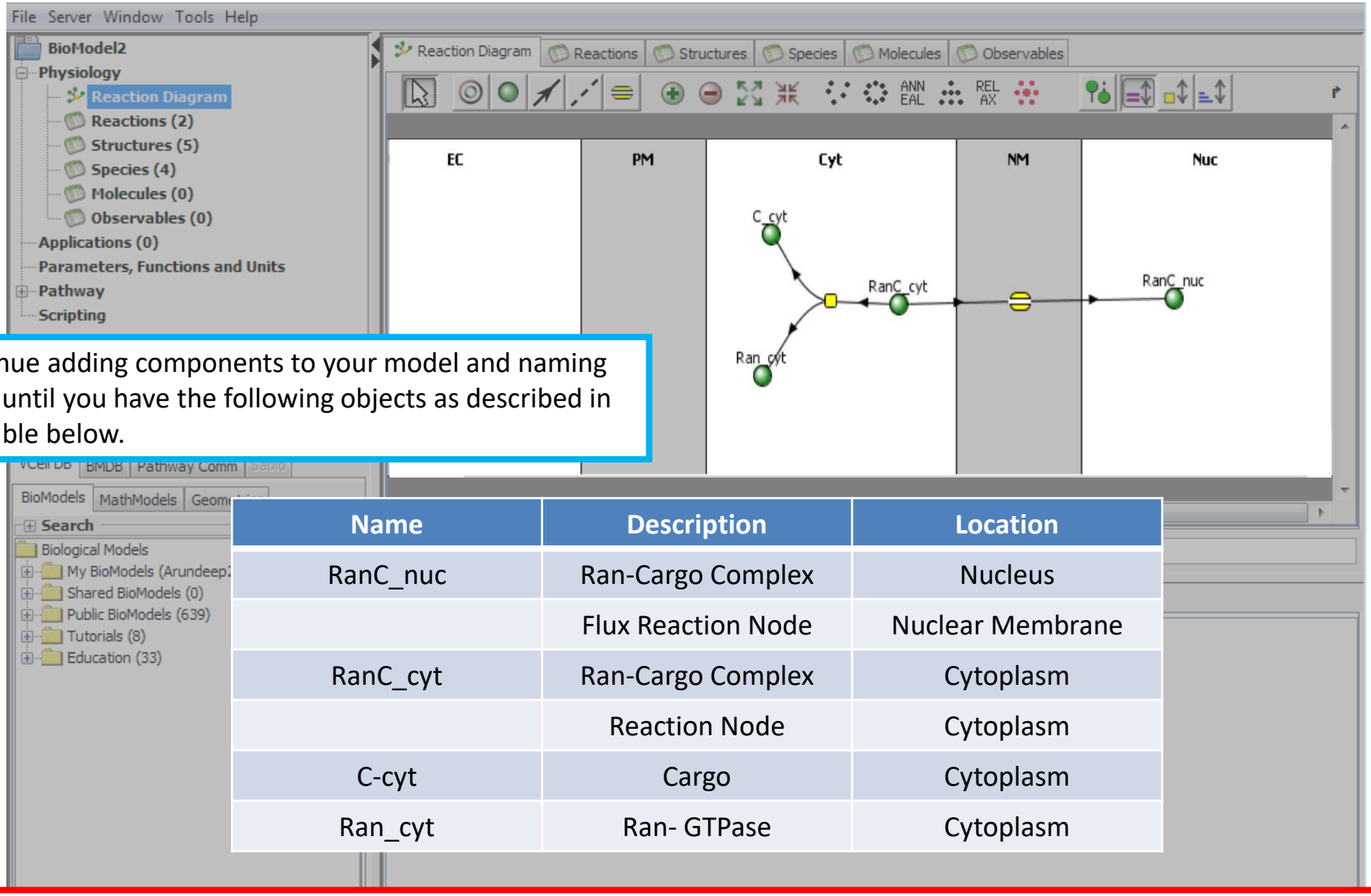
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
To remove a species or reaction from your model, select the species or reaction and click on either the "Delete" button or the backspace button on your keyboard.



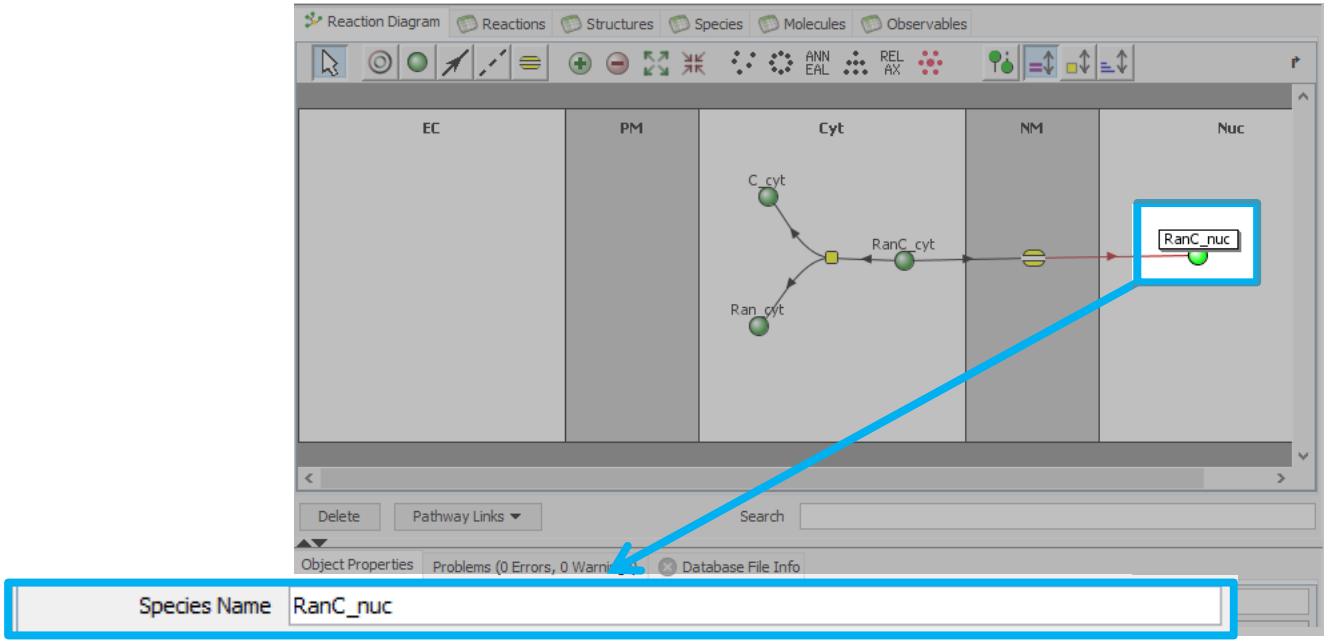
To create a product species, use the Reaction Tool to drag from the reaction symbol to a point inside the compartment where your product species will be located.
Once you release the mouse button, the product species will be created.



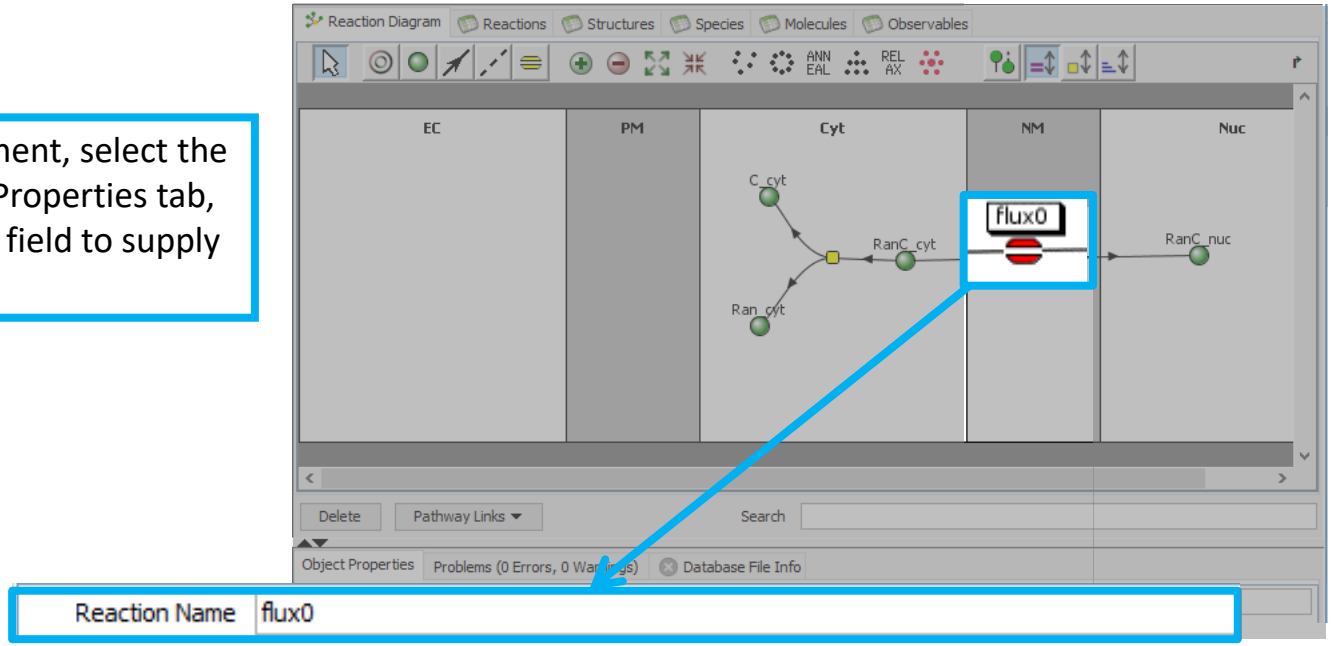
Continue adding components to your model and naming them until you have the following objects as described in the table below.

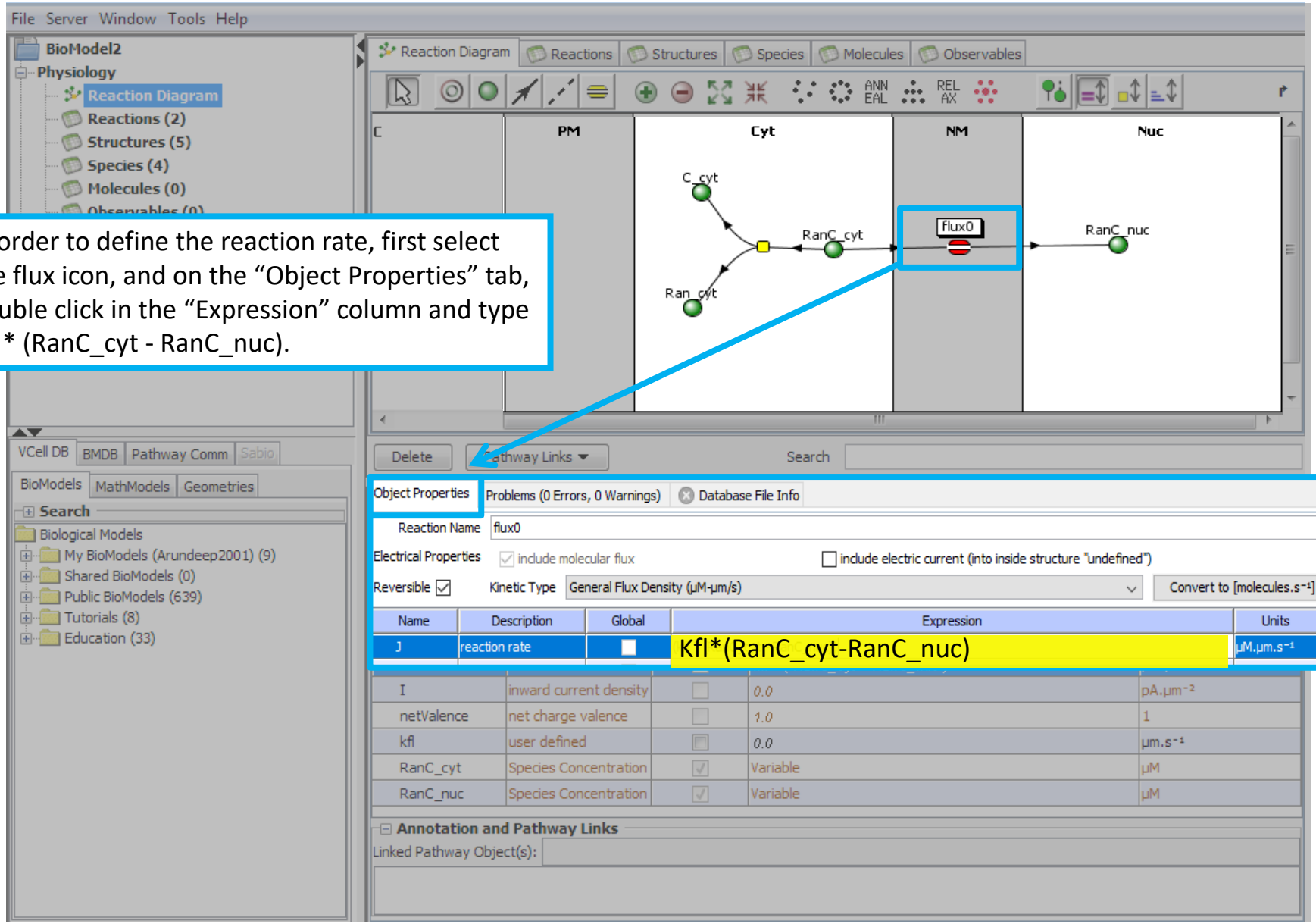
Name	Description	Location
RanC_nuc	Ran-Cargo Complex	Nucleus
	Flux Reaction Node	Nuclear Membrane
RanC_cyt	Ran-Cargo Complex	Cytoplasm
	Reaction Node	Cytoplasm
C-cyt	Cargo	Cytoplasm
Ran_cyt	Ran- GTPase	Cytoplasm

Note that you cannot move species, reactions, or fluxes from one compartment to another. You must delete a species, flux, or reaction from one compartment and then create it in another compartment.



If you need to rename a component, select the component, and on the Object Properties tab, use the component's name text field to supply the new name.




In order to define the reaction rate, first select the flux icon, and on the “Object Properties” tab, double click in the “Expression” column and type kfl * (RanC_cyt - RanC_nuc).
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Database File Info
Reaction Name
flux0
Electrical Properties
include molecular flux
include electric current (into inside structure "undefined")
Reversible
Kinetic Type
General Flux Density (μM-μm/s)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kfl*(RanC_cyt-RanC_nuc)
μM.μm.s⁻¹
I
inward current density
0.0
pA.μm⁻²
netValence
net charge valence
1.0
1
kfl
user defined
0.0
μm.s⁻¹
RanC_cyt
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μM
RanC_nuc
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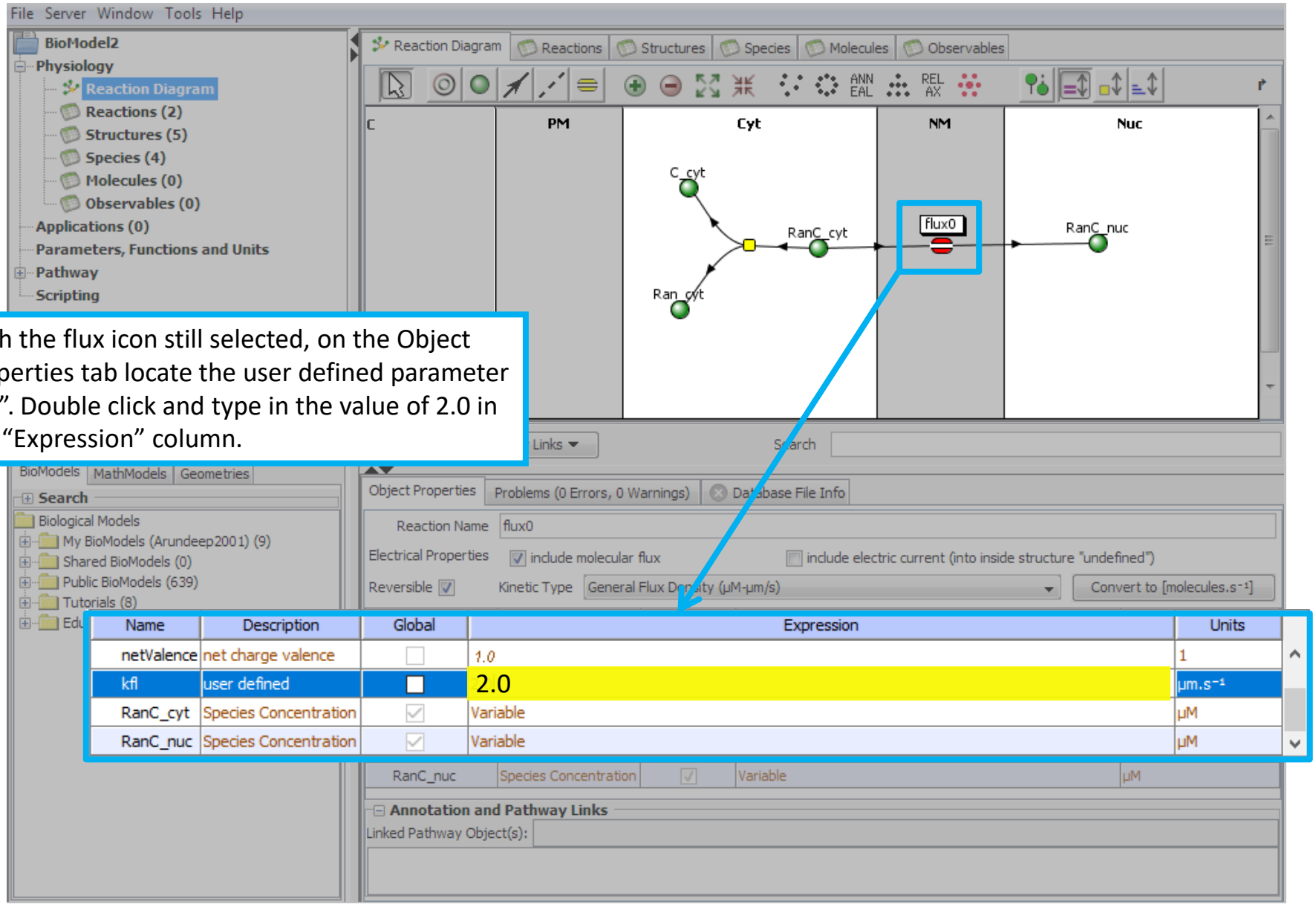
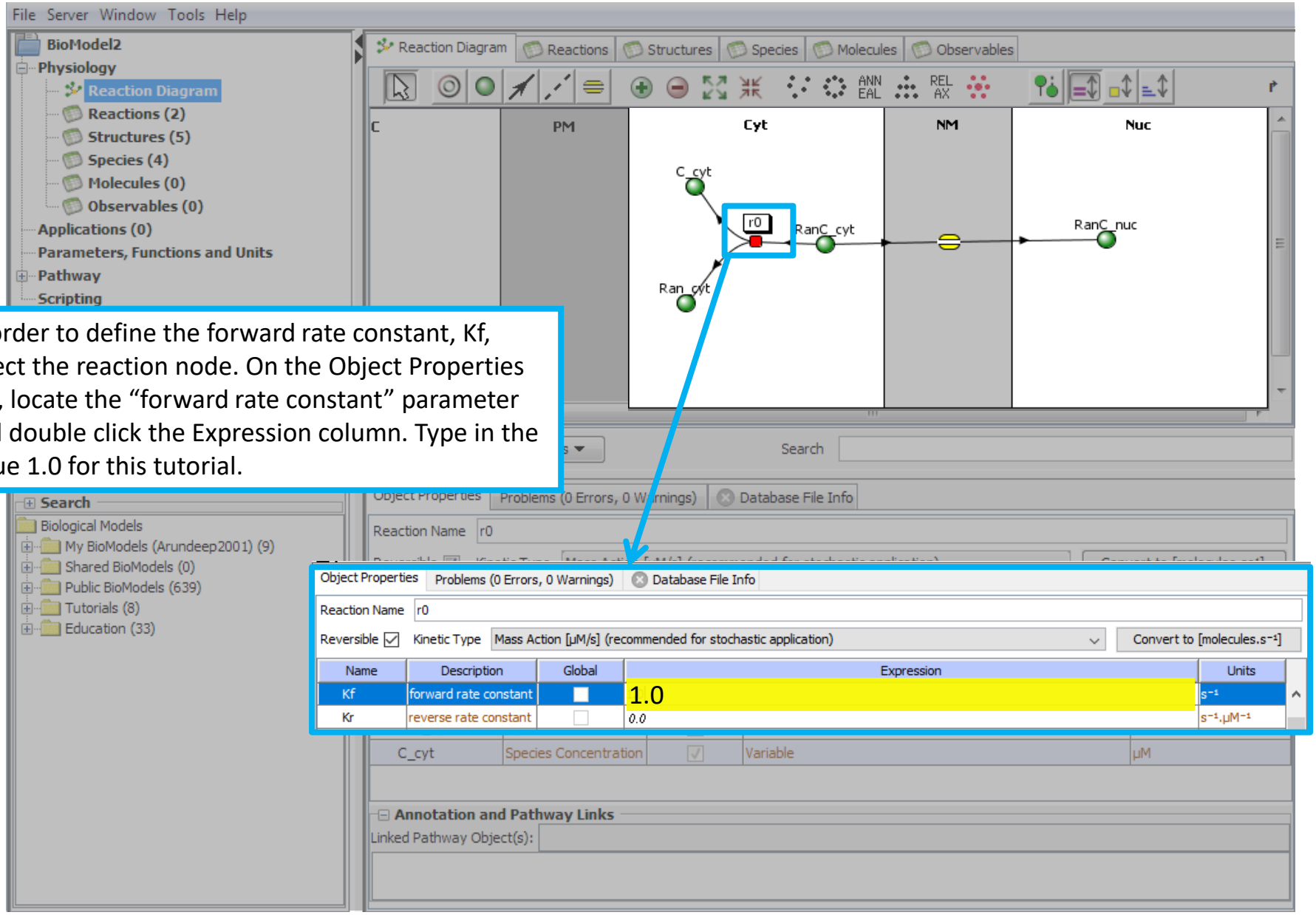
With the flux icon still selected, on the Object Properties tab locate the user defined parameter “Kfl”. Double click and type in the value of 2.0 in the “Expression” column.

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RanC_cyt
RanC_nuc
Ran_cyt
In order to define the forward rate constant, Kf, select the reaction node. On the Object Properties tab, locate the “forward rate constant” parameter and double click the Expression column. Type in the value 1.0 for this tutorial.
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Database File Info
Reaction Name
r0
Reversible
Kinetic Type
Mass Action [µM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
Kf
forward rate constant
1.0
s⁻¹
Kr
reverse rate constant
0.0
s⁻¹.µM⁻¹
C_cyt
Species Concentration
Variable
µM
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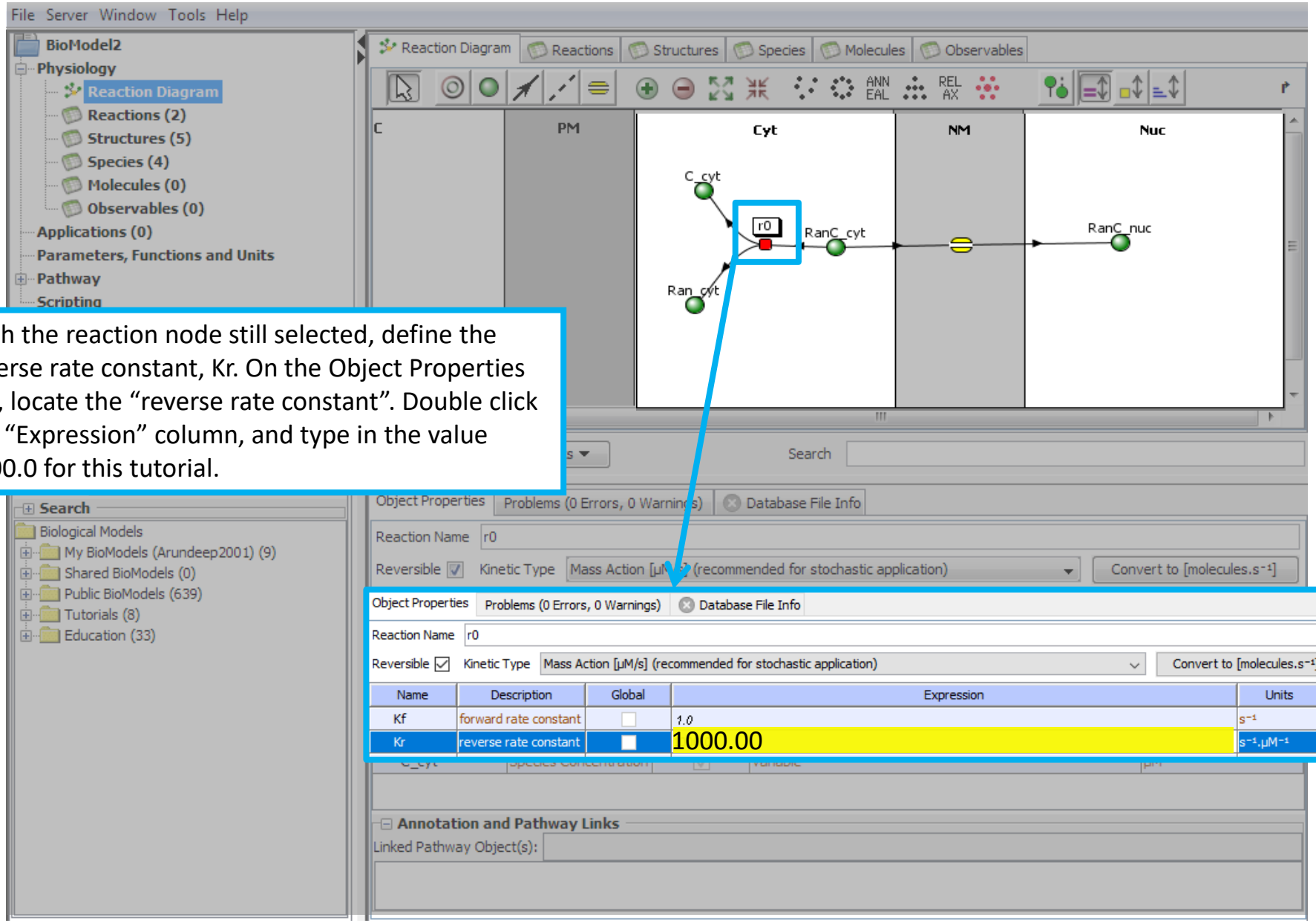
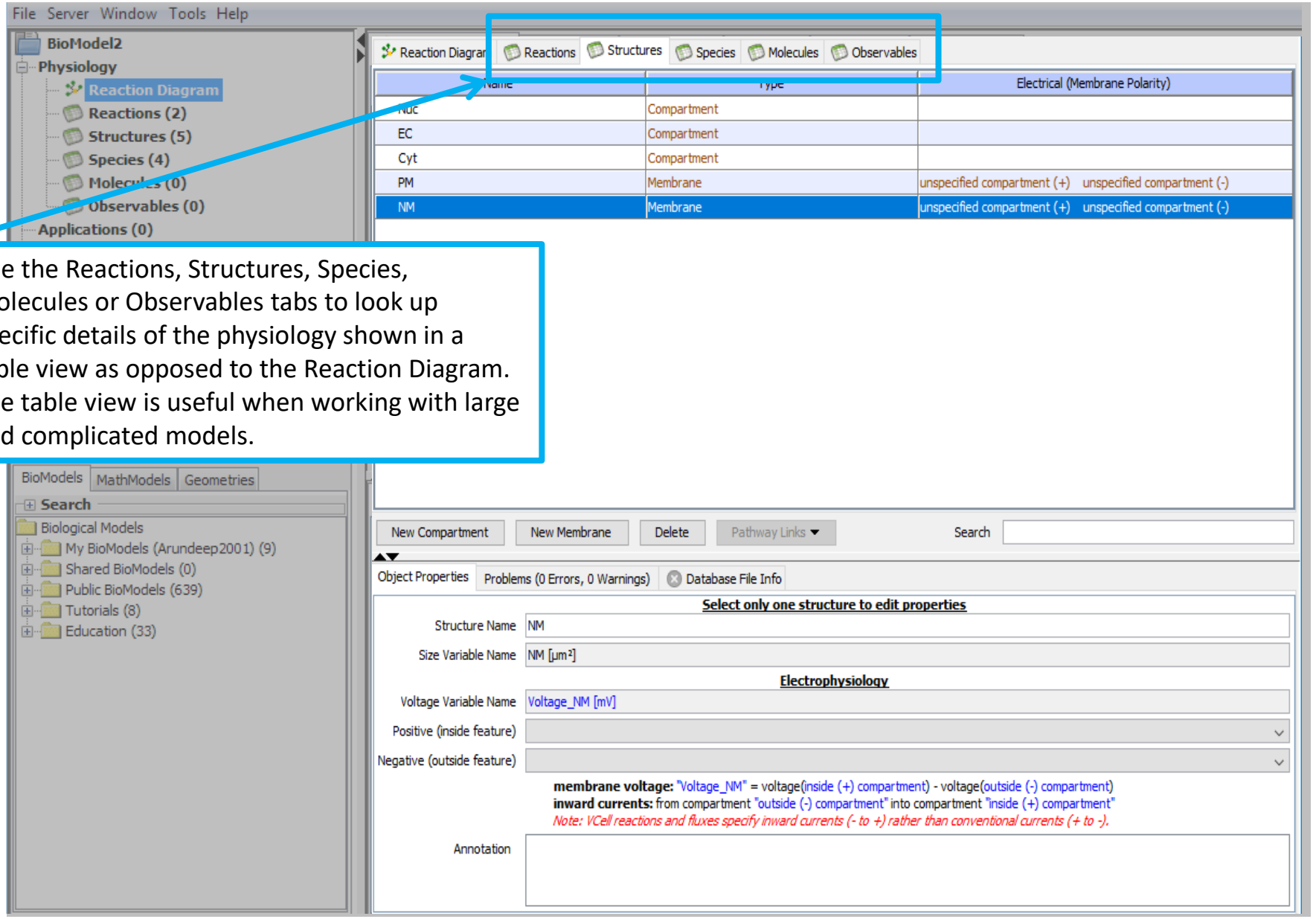
Linked Pathway Object(s):



With the reaction node still selected, define the reverse rate constant, Kr. On the Object Properties tab, locate the “reverse rate constant”. Double click the “Expression” column, and type in the value 1000.0 for this tutorial.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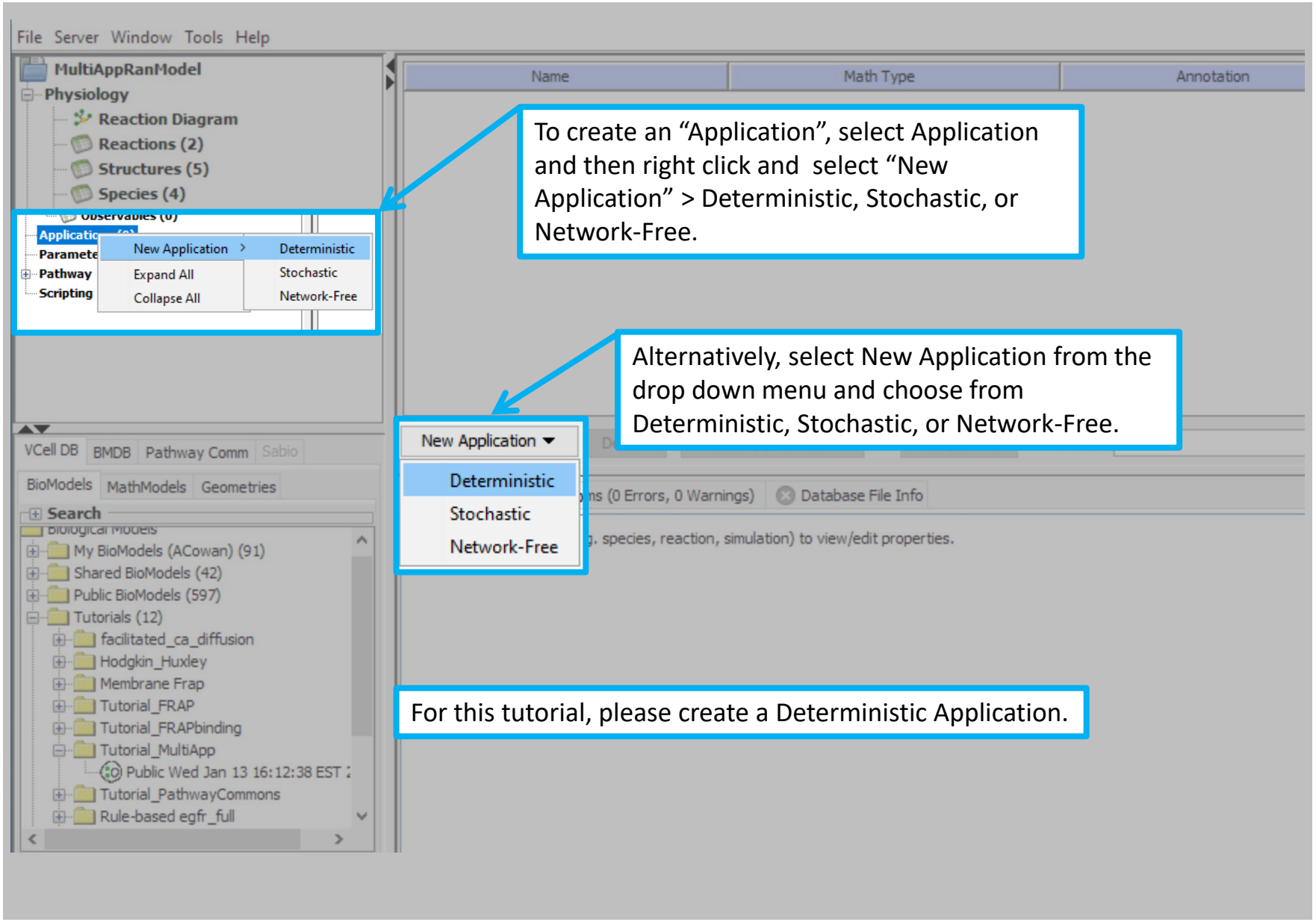
Name
Type
Electrical (Membrane Polarity)
Nuc
Compartment
EC
Compartment
Cyt
Compartment
PM
Membrane
unspecified compartment (+) unspecified compartment (-)
NM
Membrane
unspecified compartment (+) unspecified compartment (-)
Use the Reactions, Structures, Species, Molecules or Observables tabs to look up specific details of the physiology shown in a table view as opposed to the Reaction Diagram. The table view is useful when working with large and complicated models.
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (Arundeep2001) (9)
Shared BioModels (0)
Public BioModels (639)
Tutorials (8)
Education (33)
New Compartment
New Membrane
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one structure to edit properties
Structure Name
NM
Size Variable Name
NM [µm²]
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 -).
Annotation


File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
New Application
Deterministic
Stochastic
Network-Free
Expand All
Collapse All
Pathway
Scripting
Name
Math Type
Annotation
To create an “Application”, select Application and then right click and select “New Application” > Deterministic, Stochastic, or Network-Free.
Alternatively, select New Application from the drop down menu and choose from Deterministic, Stochastic, or Network-Free.
New Application
Deterministic
Stochastic
Network-Free
VCell DB
BMDB
Pathway Comm
BioModels
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Search
My BioModels (ACowan) (91)
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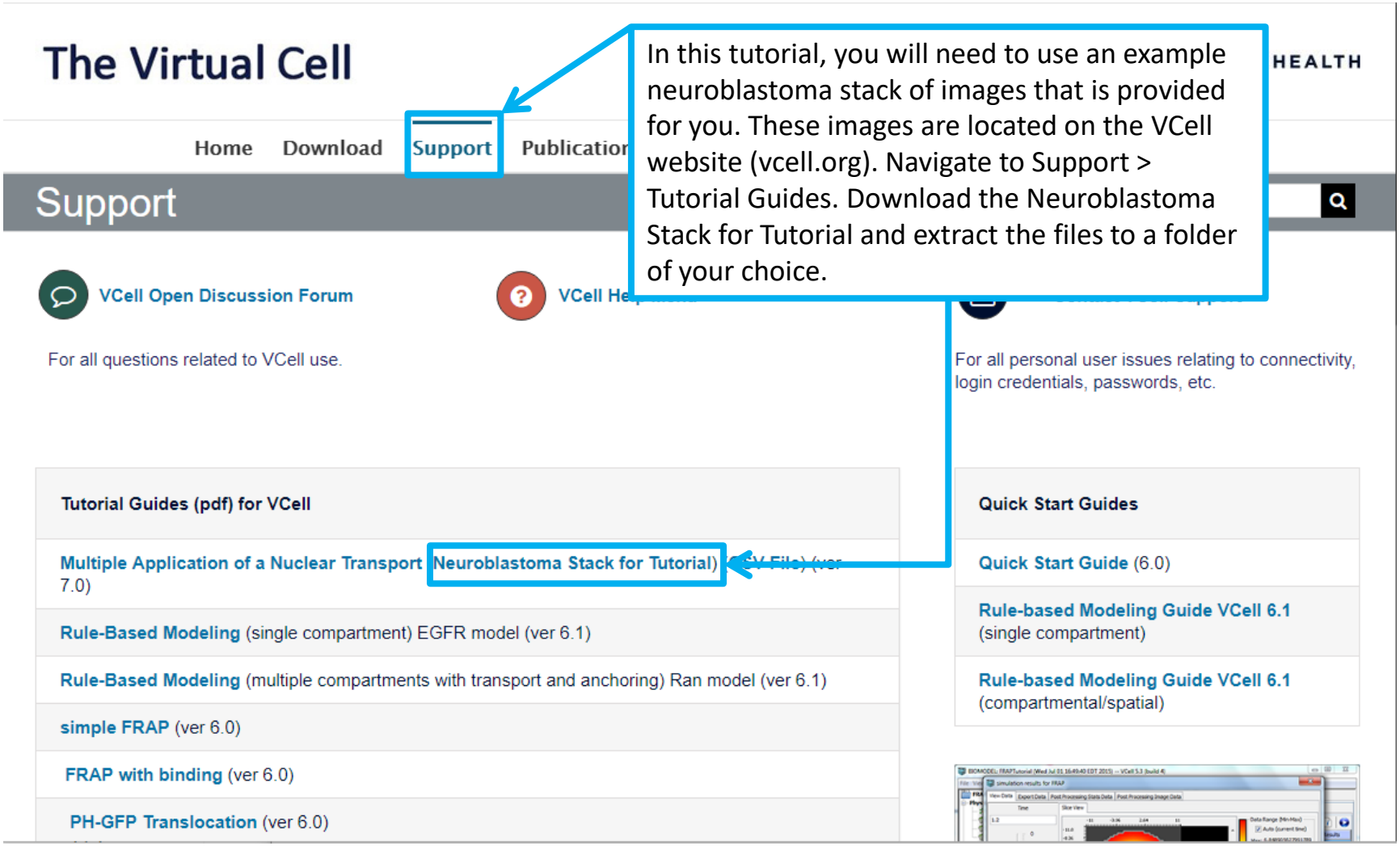
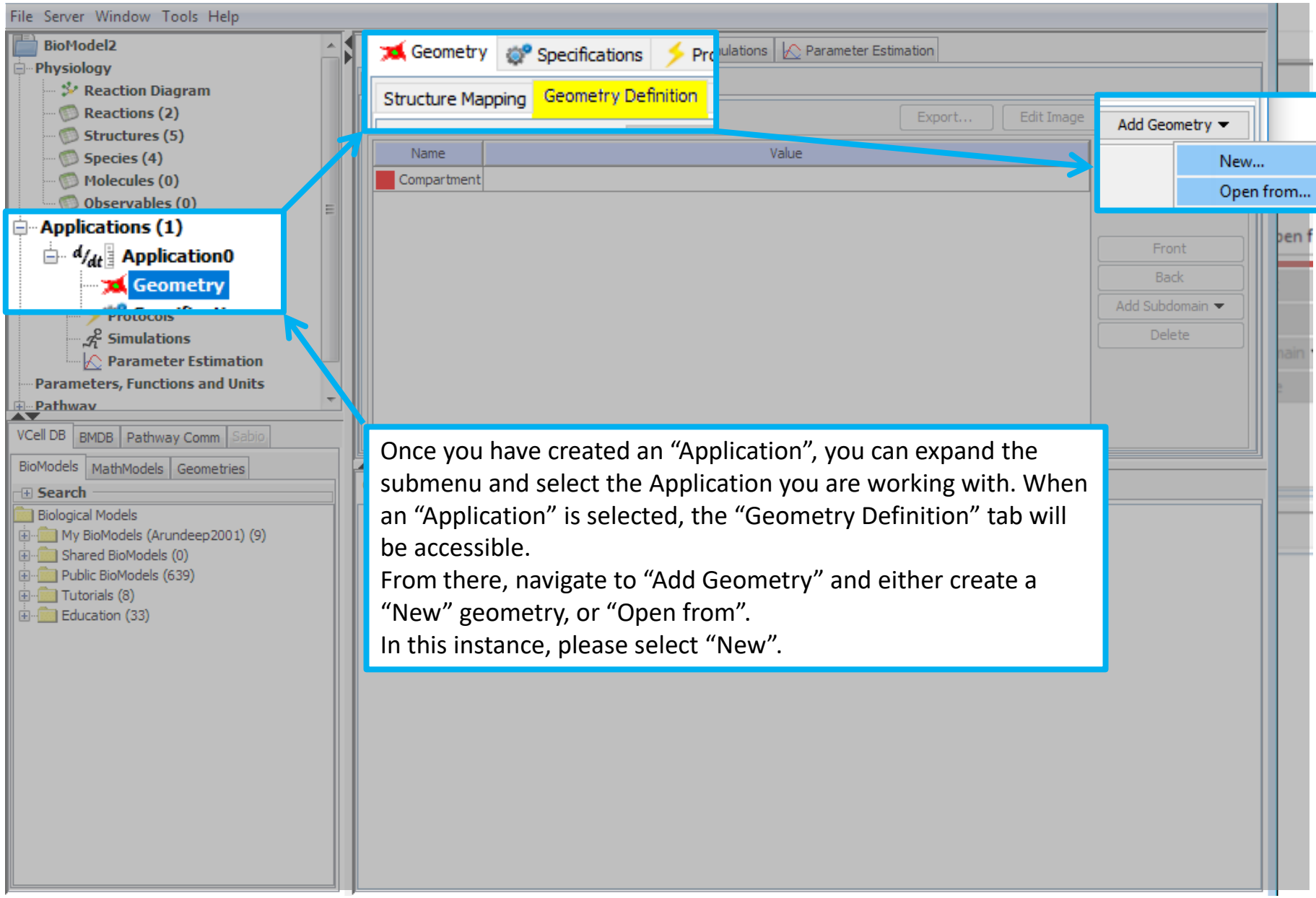
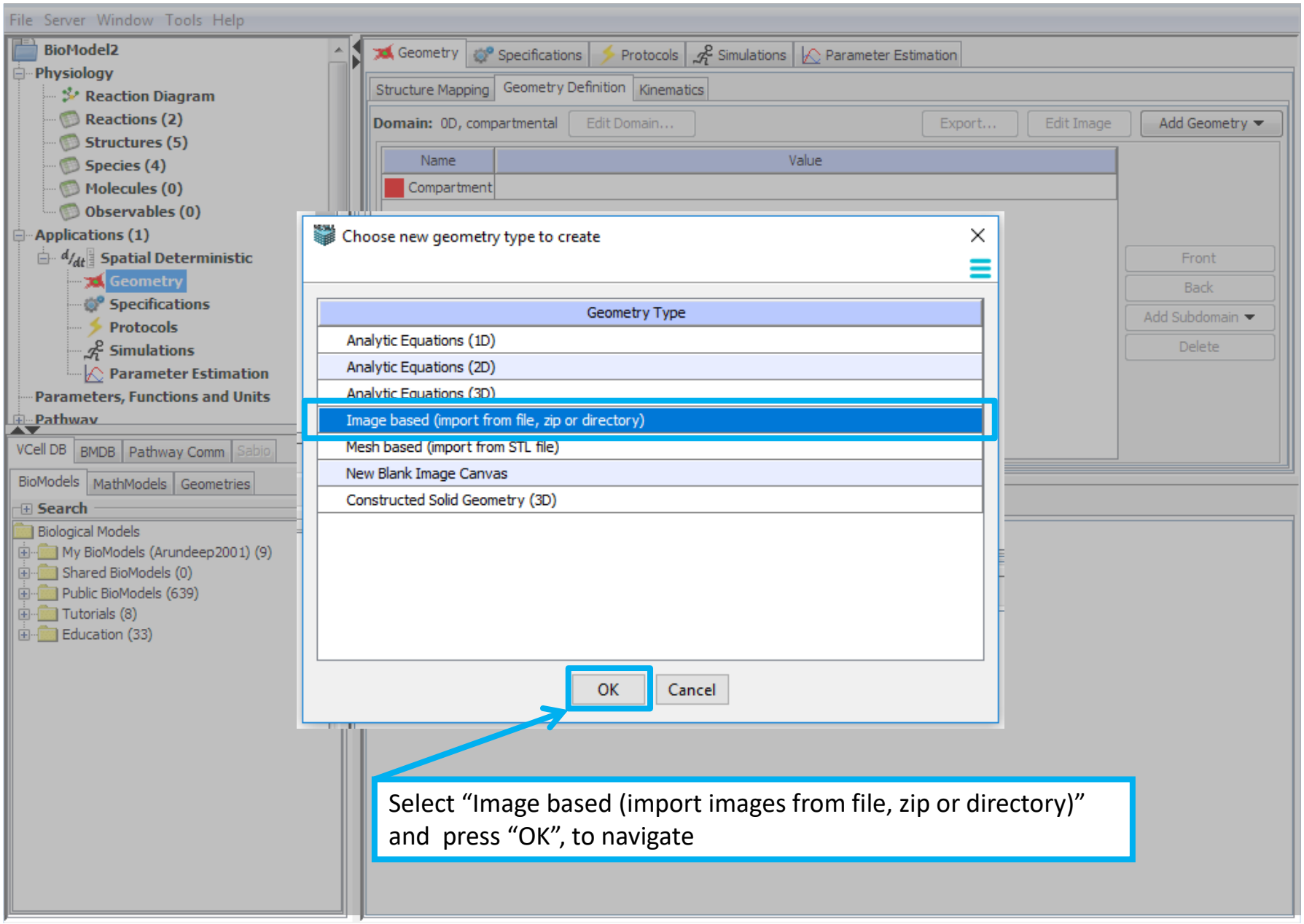
Tutorials (12)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Public Wed Jan 13 16:12:38 EST
Tutorial_PathwayCommons
Rule-based egfr_full
Database File Info
species, reaction, simulation) to view/edit properties.
For this tutorial, please create a Deterministic Application.


The Virtual Cell
HEALTH
Home
Download
Support
Publicatior
Support
In this tutorial, you will need to use an example neuroblastoma stack of images that is provided for you. These images are located on the VCell website (vcell.org). Navigate to Support > Tutorial Guides. Download the Neuroblastoma Stack for Tutorial and extract the files to a folder of your choice.
VCell Open Discussion Forum
For all questions related to VCell use.
For all personal user issues relating to connectivity, login credentials, passwords, etc.
Tutorial Guides (pdf) for VCell
Multiple Application of a Nuclear Transport
Neuroblastoma Stack for Tutorial)
7.0)
Rule-Based Modeling (single compartment) EGFR model (ver 6.1)
Rule-Based Modeling (multiple compartments with transport and anchoring) Ran model (ver 6.1)
simple FRAP (ver 6.0)
FRAP with binding (ver 6.0)
PH-GFP Translocation (ver 6.0)
Quick Start Guides
Quick Start Guide (6.0)
Rule-based Modeling Guide VCell 6.1 (single compartment)
Rule-based Modeling Guide VCell 6.1 (compartmental/spatial)



Once you have created an “Application”, you can expand the submenu and select the Application you are working with. When an “Application” is selected, the “Geometry Definition” tab will be accessible.
From there, navigate to “Add Geometry” and either create a “New” geometry, or “Open from”.
In this instance, please select “New”.


File Server Window Tools Help
BioModel2
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Spatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions and Units
Pathway
VCell DB
BMDB
Pathway Comm
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My BioModels (Arundeep2001) (9)
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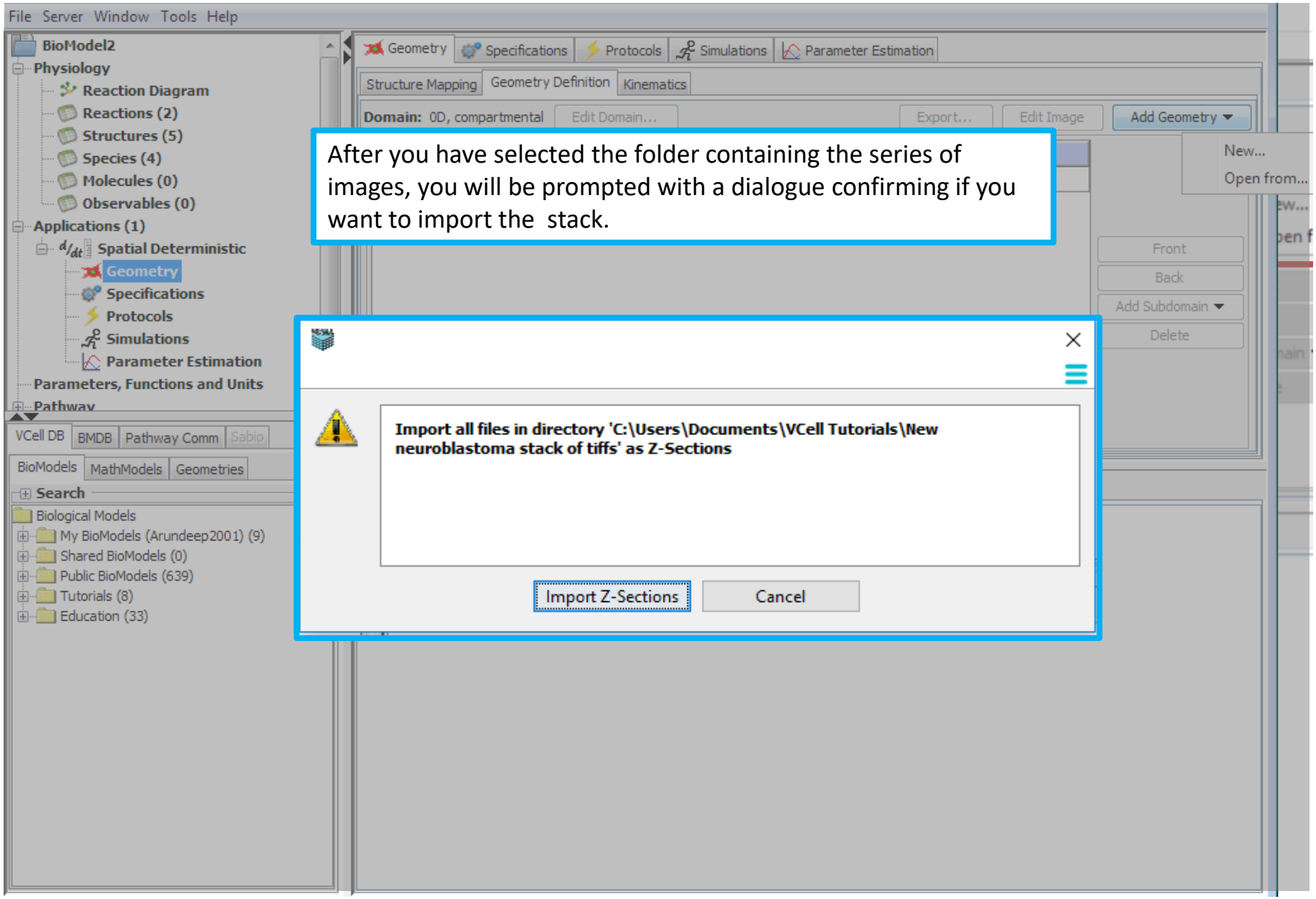
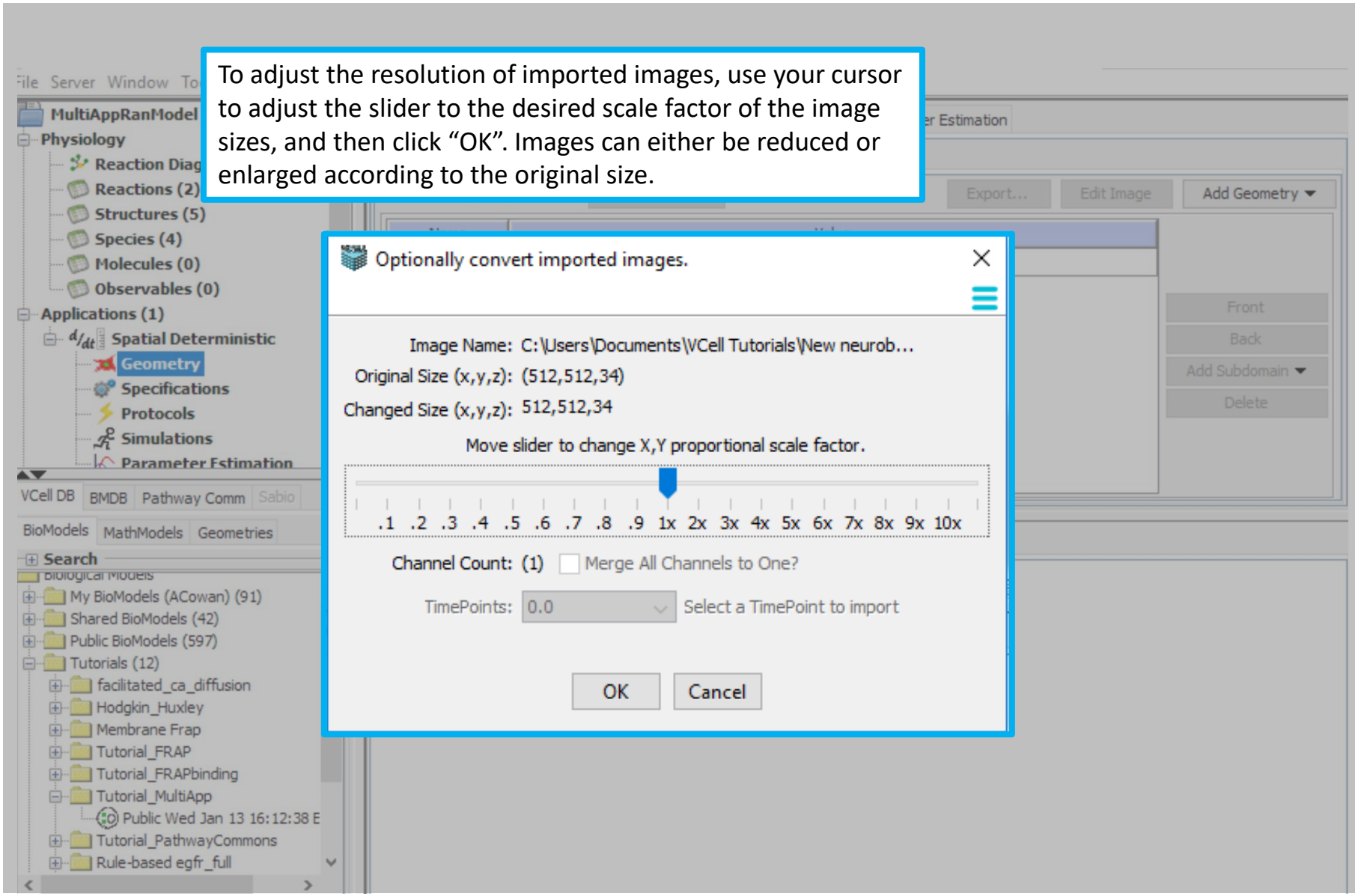
Structure Mapping
Geometry Definition
Kinematics
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
Choose new geometry type to create
Geometry Type
Analytic Equations (1D)
Analytic Equations (2D)
Analytic Equations (3D)
Image based (import from file, zip or directory)
Mesh based (import from STL file)
New Blank Image Canvas
Constructed Solid Geometry (3D)
OK
Cancel
Select “Image based (import images from file, zip or directory)” and press “OK”, to navigate



After you have selected the folder containing the series of images, you will be prompted with a dialogue confirming if you want to import the stack.


To adjust the resolution of imported images, use your cursor to adjust the slider to the desired scale factor of the image sizes, and then click “OK”. Images can either be reduced or enlarged according to the original size.
Optionally convert imported images.
Image Name: C:\Users\Documents\VCell Tutorials\New neurob...
Original Size (x,y,z): (512,512,34)
Changed Size (x,y,z): 512,512,34
Move slider to change X,Y proportional scale factor.
.1 .2 .3 .4 .5 .6 .7 .8 .9 1x 2x 3x 4x 5x 6x 7x 8x 9x 10x
Channel Count: (1)
Merge All Channels to One?
TimePoints: 0.0
Select a TimePoint to import
OK
Cancel
MultiAppRanModel
Physiology
Reaction Diag
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Spatial Deterministic
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My BioModels (ACowan) (91)
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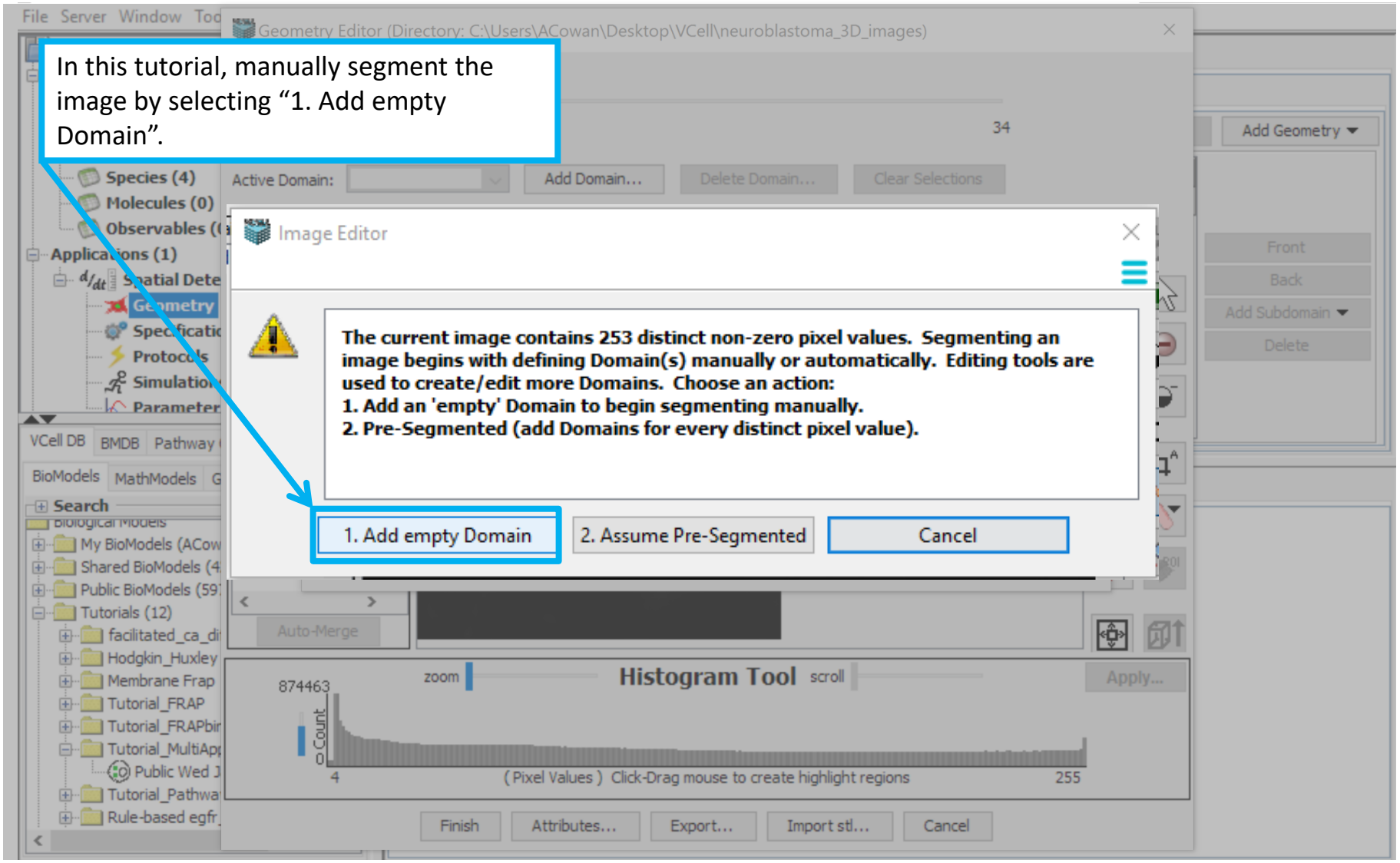
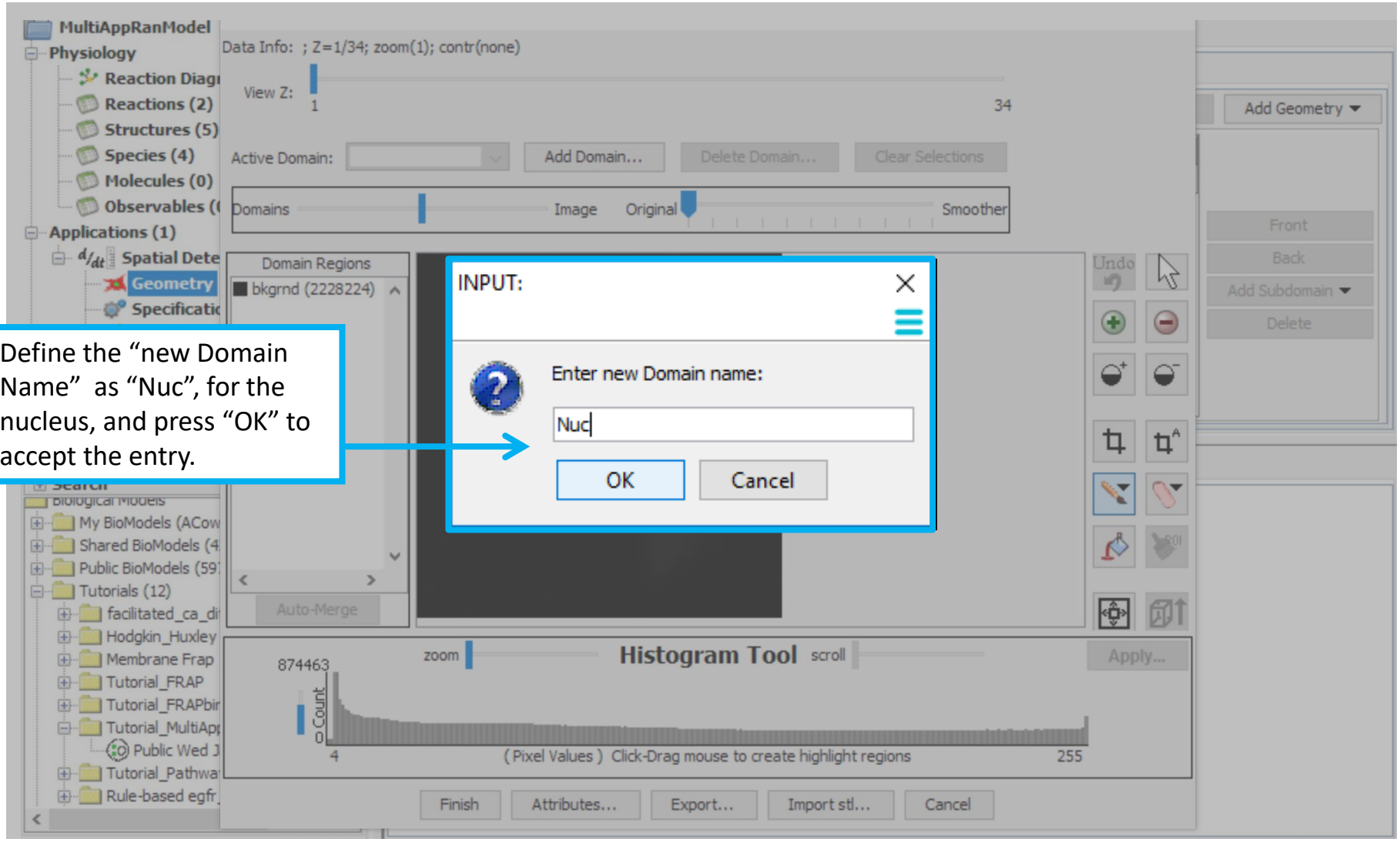
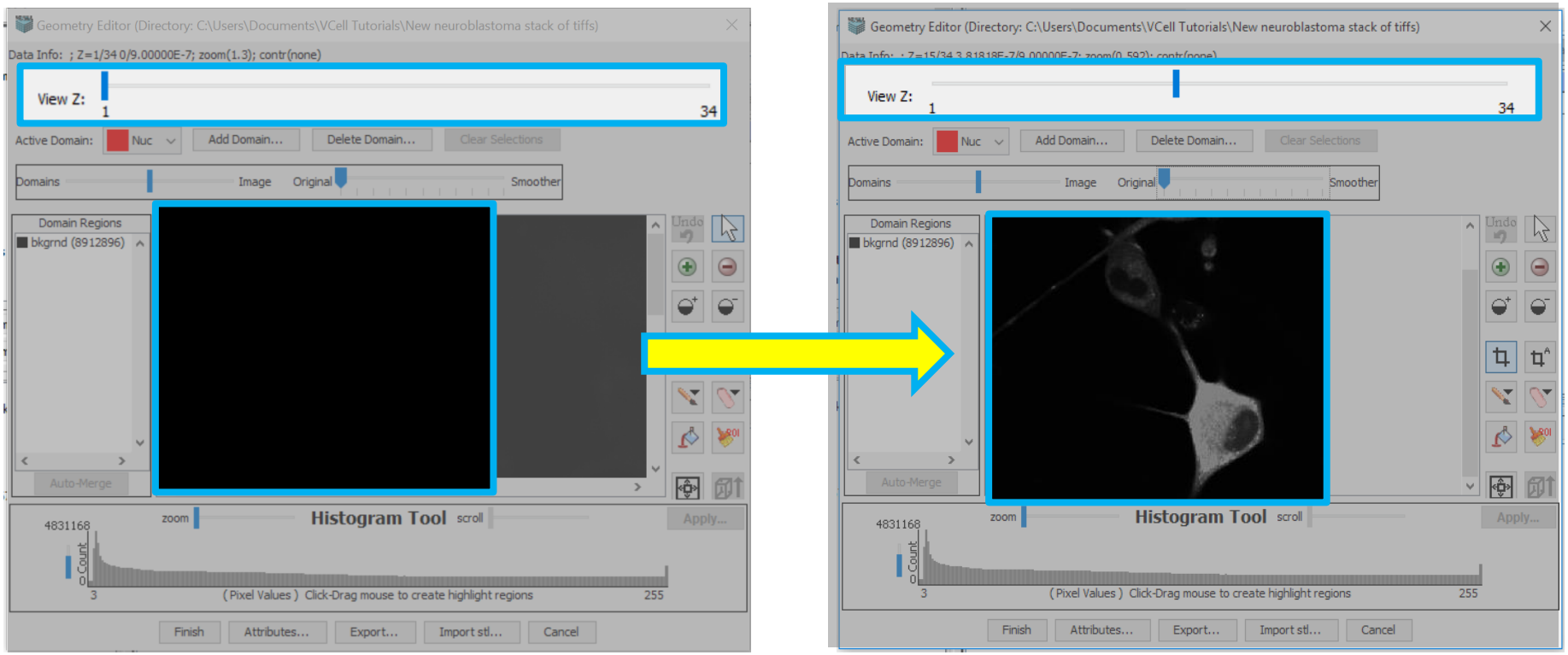
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based egfr_full
Export...
Edit Image
Add Geometry
Front
Back
Add Subdomain
Delete

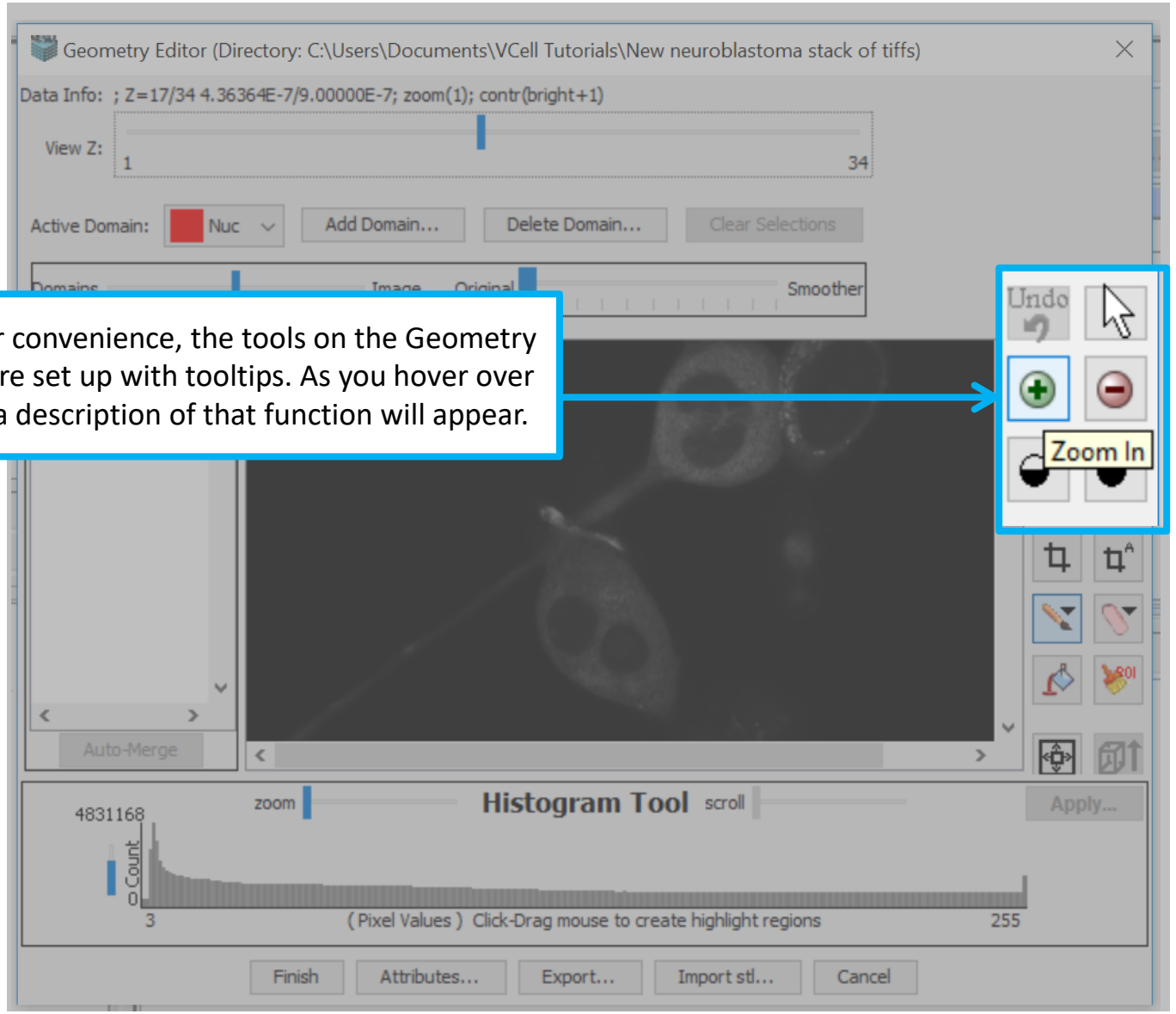

In this tutorial, manually segment the image by selecting “1. Add empty Domain”.
Geometry Editor (Directory: C:\Users\ACowan\Desktop\VCell\neuroblastoma_3D_images)
Image Editor
The current image contains 253 distinct non-zero pixel values. Segmenting an image begins with defining Domain(s) manually or automatically. Editing tools are used to create/edit more Domains. Choose an action:
1. Add an 'empty' Domain to begin segmenting manually.
2. Pre-Segmented (add Domains for every distinct pixel value).
1. Add empty Domain
2. Assume Pre-Segmented
Cancel
Histogram Tool
zoom
scroll
Apply...
874463
0 Count
4
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel
Add Geometry
Active Domain:
Add Domain...
Delete Domain...
Clear Selections
Species (4)
Molecules (0)
Applications (1)
Geometry
Protocols
Front
Back
Add Subdomain
Delete
Auto-Merge



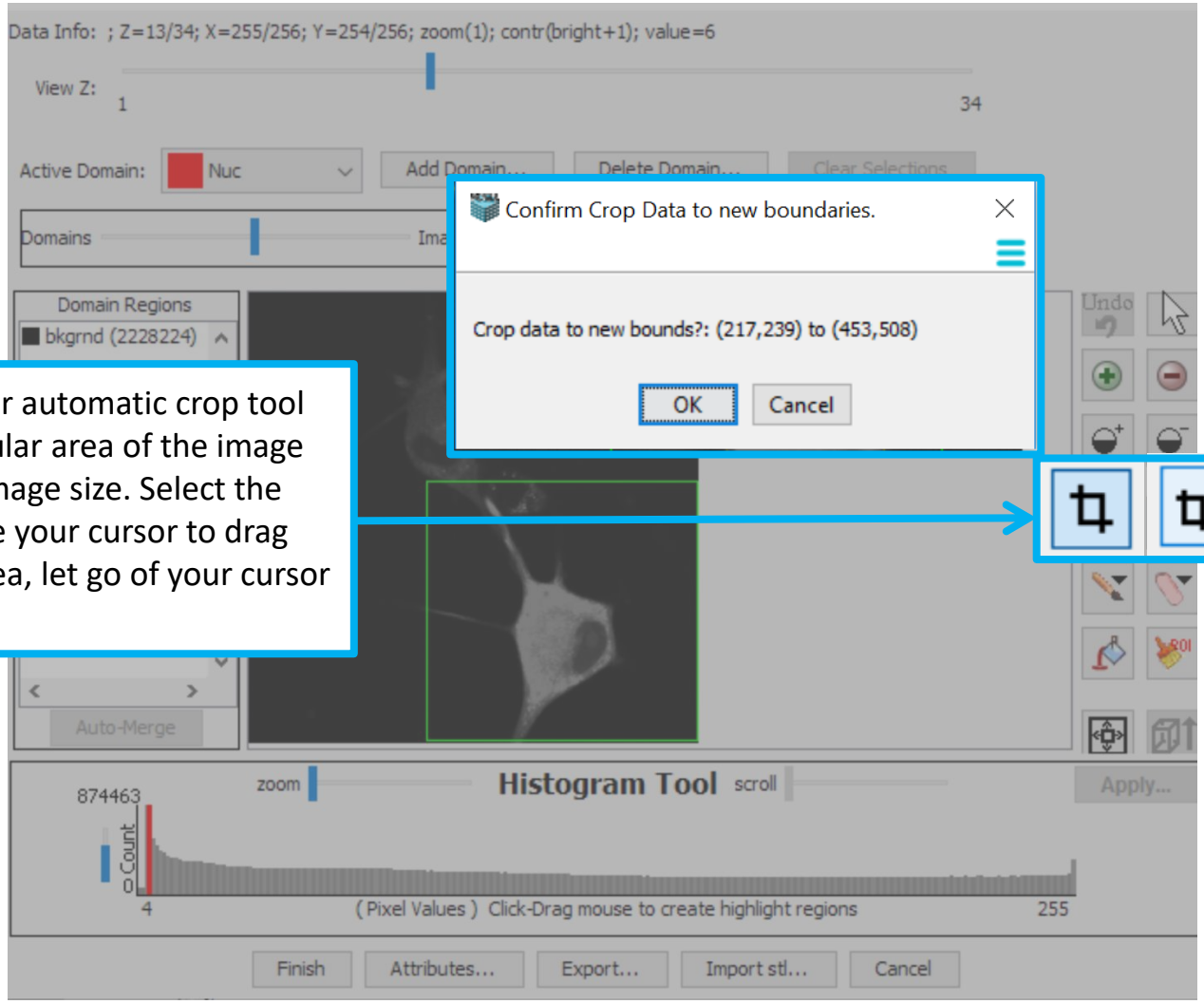
Define the “new Domain Name” as “Nuc”, for the nucleus, and press “OK” to accept the entry.

After importing the images, be sure to adjust the z plane so you can see your cells. The stack defaults to the first z level therefore you may not be able to see your cells until you focus up through the stack.

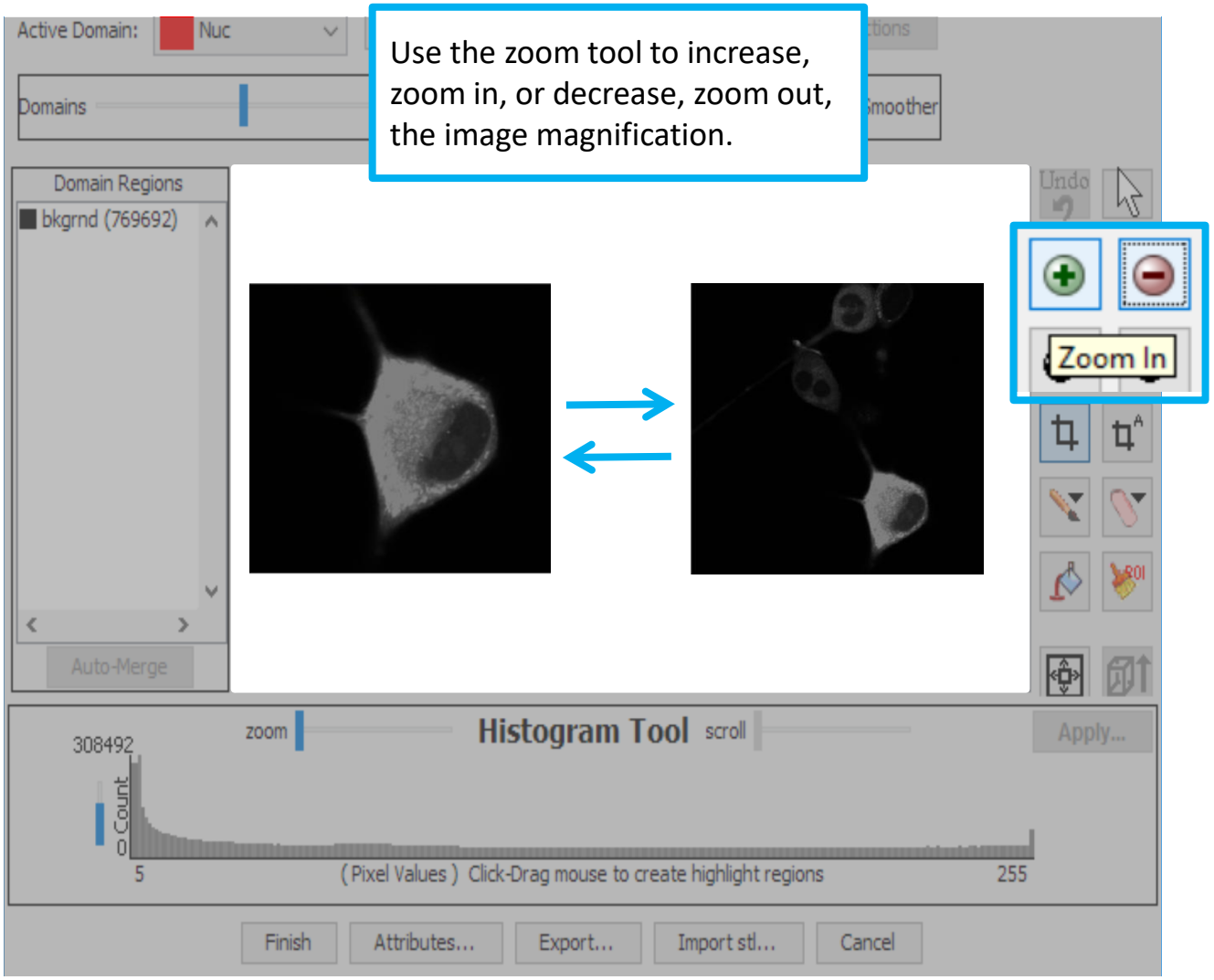




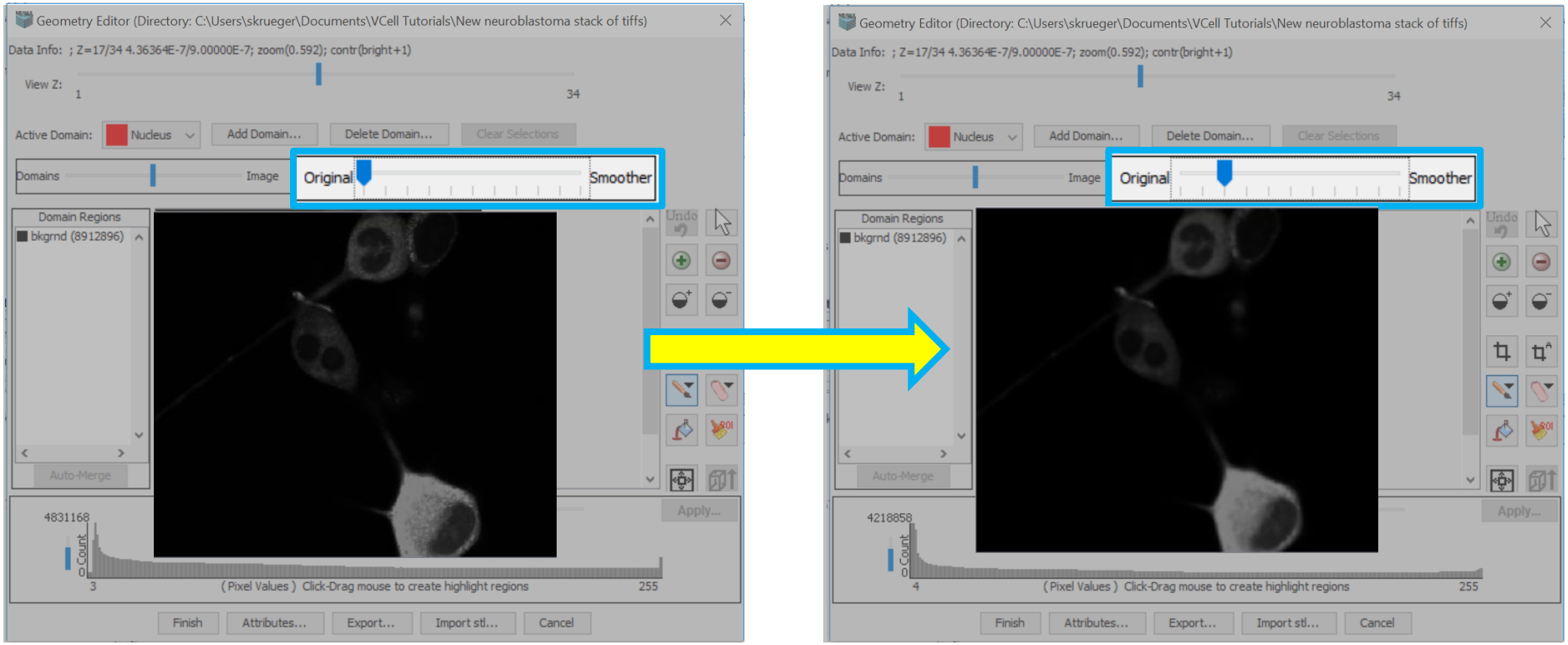
For your convenience, the tools on the Geometry Editor are set up with tooltips. As you hover over a tool, a description of that function will appear.



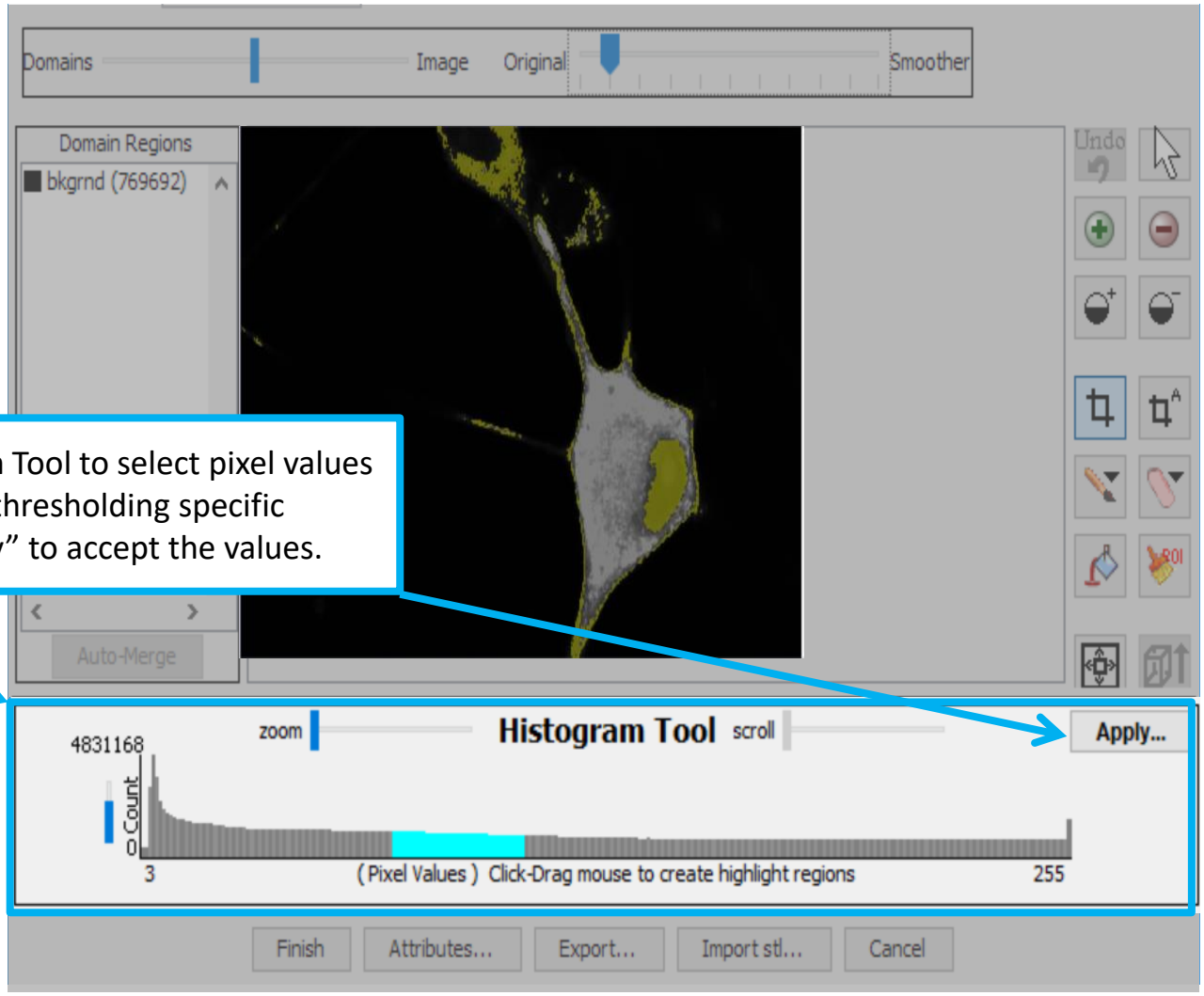
Use the manual or automatic crop tool to select a particular area of the image and reduce the image size. Select the crop tool, and use your cursor to drag over a specific area, let go of your cursor and click “OK”.


Use the zoom tool to increase, zoom in, or decrease, zoom out, the image magnification.
Active Domain:
Nuc
Domains
Domain Regions
bkgrnd (769692)
Auto-Merge
Undo
Zoom In
zoom
Histogram Tool
scroll
Apply...
308492
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel

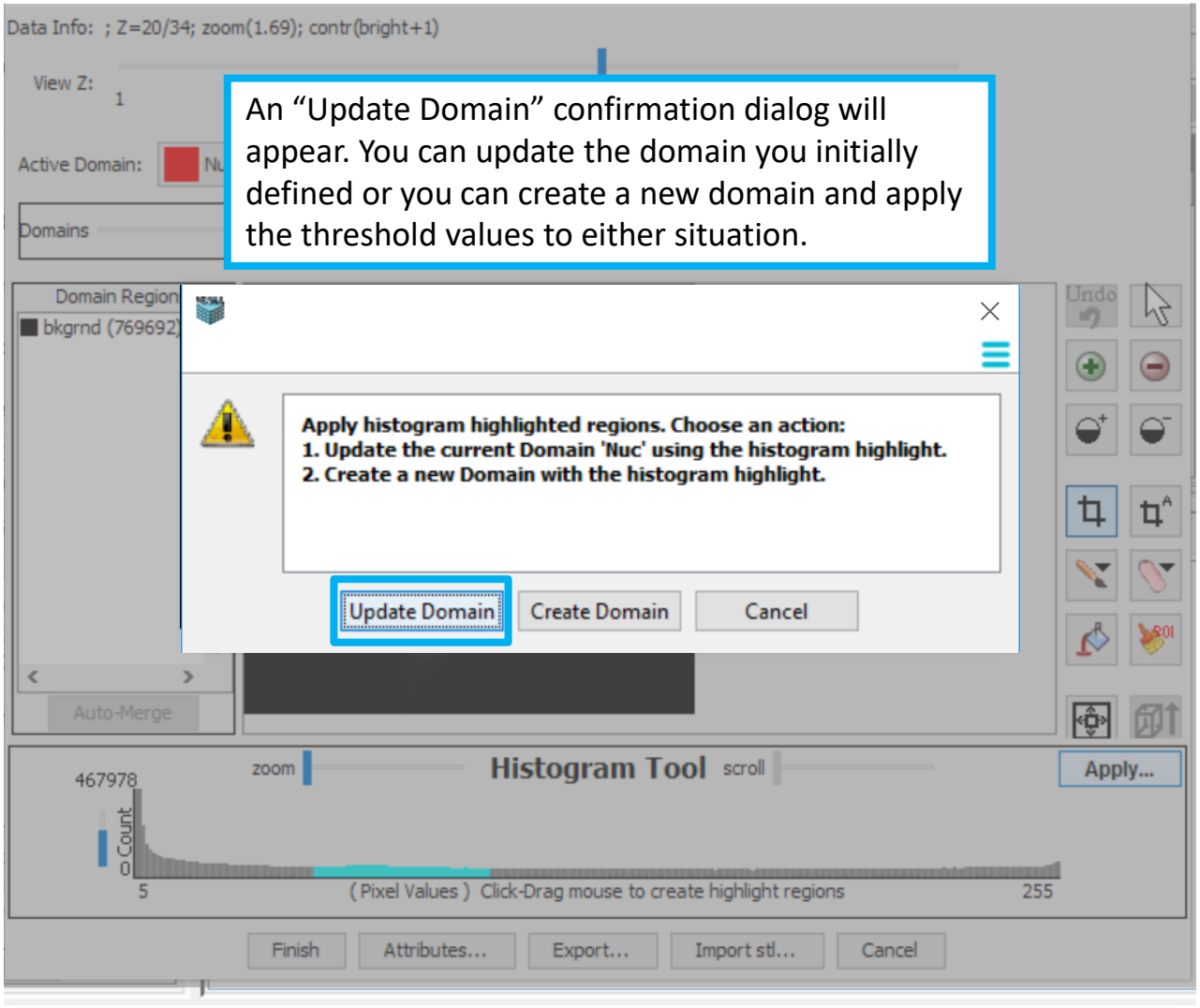
In order to reduce noise in the images, you can apply an averaging filter to the stack.



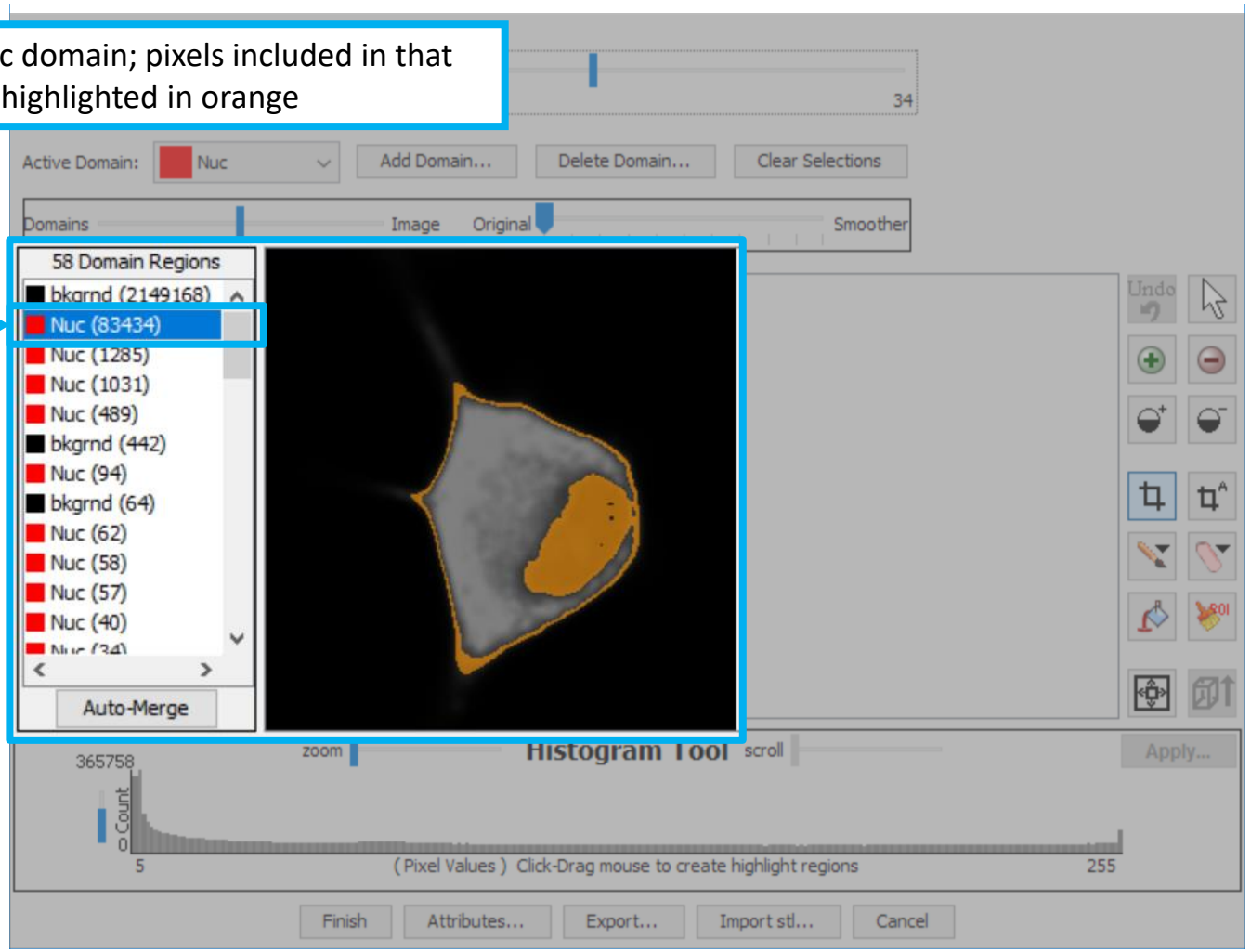
With the Averaging Filter, each pixel and it's immediate neighbor's intensity values are added together and the sum is divided by the number of neighbors. For example, in a 2-D image, each pixel has 8 surrounding neighbors. The 9 values are added together and divided by 9 and that value replaces the original pixel value.



Use the Histogram Tool to select pixel values in your image for thresholding specific regions. Hit “Apply” to accept the values.

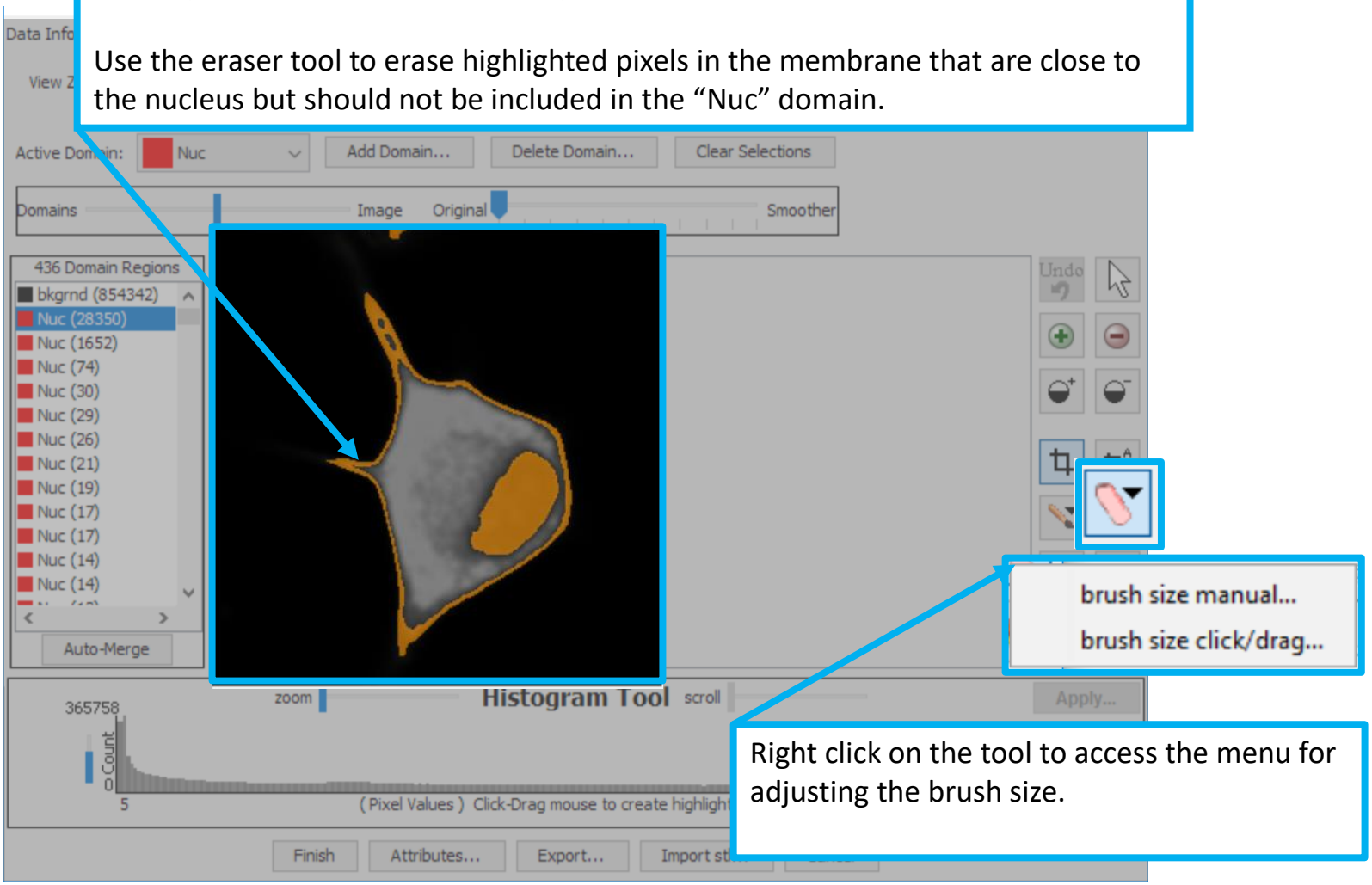

Data Info: ; Z=20/34; zoom(1.69); contr(bright+1)
View Z:
1
Active Domain:
Domains
An “Update Domain” confirmation dialog will appear. You can update the domain you initially defined or you can create a new domain and apply the threshold values to either situation.
Domain Region
bkgrnd (769692)
Apply histogram highlighted regions. Choose an action:
1. Update the current Domain 'Nuc' using the histogram highlight.
2. Create a new Domain with the histogram highlight.
Update Domain
Create Domain
Cancel
Undo
Auto-Merge
zoom
Histogram Tool
scroll
Apply...
467978
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel

Click on the Nuc domain; pixels included in that domain will be highlighted in orange



The largest "Nuc" domain includes pixels that are outside of the actual nucleus.

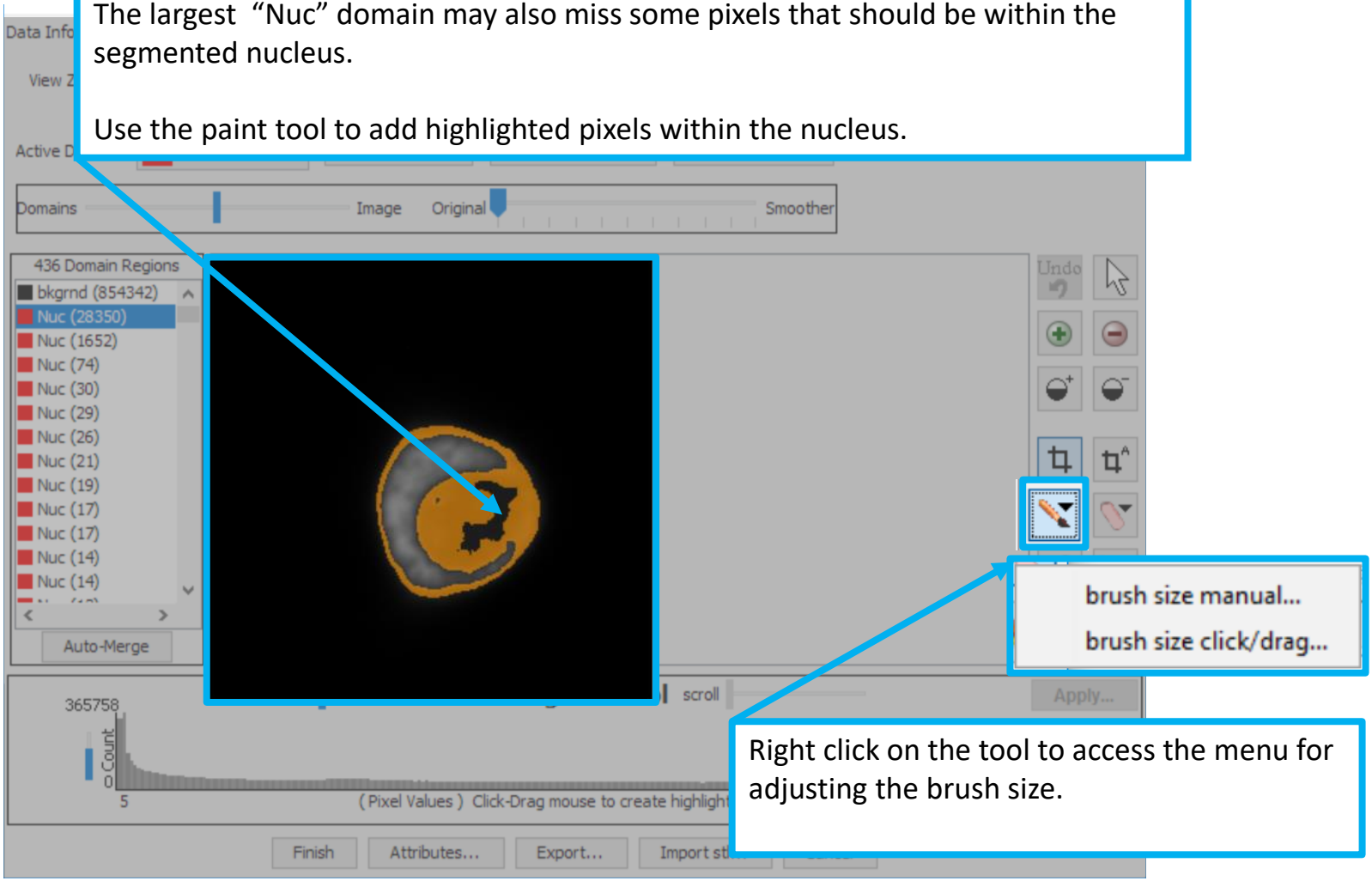
Use the eraser tool to erase highlighted pixels in the membrane that are close to the nucleus but should not be included in the "Nuc" domain.



Right click on the tool to access the menu for adjusting the brush size.

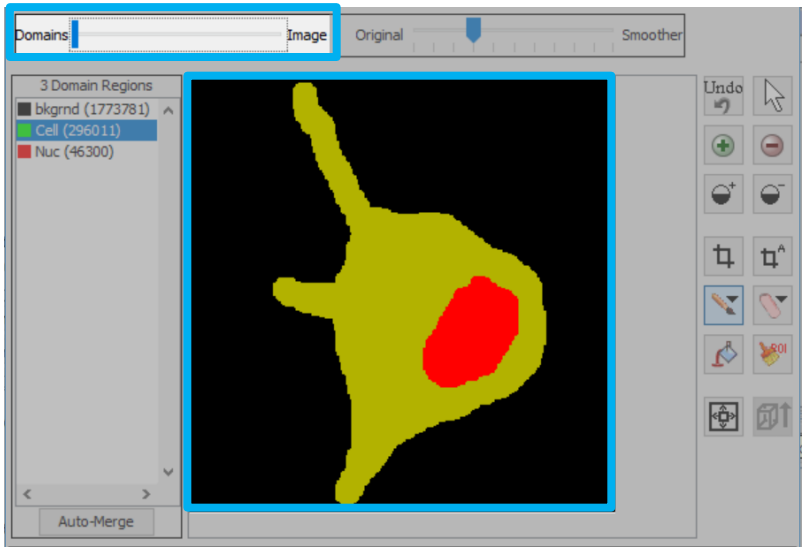
The largest "Nuc" domain may also miss some pixels that should be within the segmented nucleus.

Use the paint tool to add highlighted pixels within the nucleus.



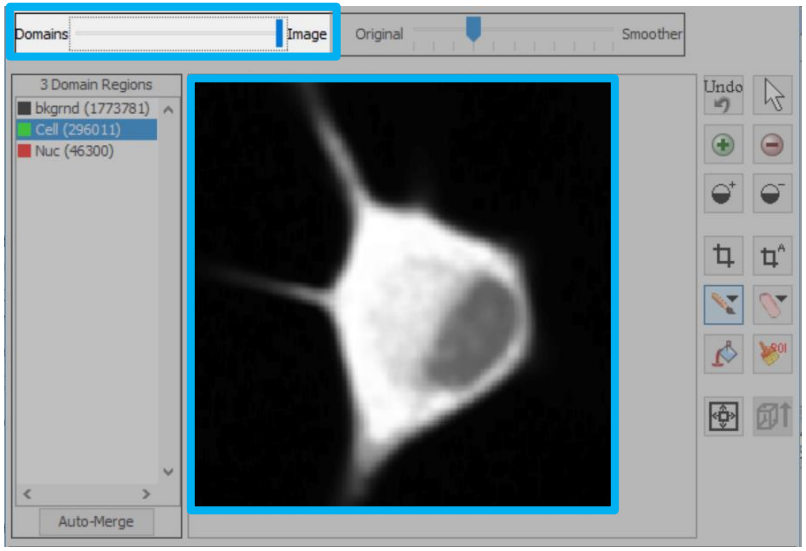
Right click on the tool to access the menu for adjusting the brush size.

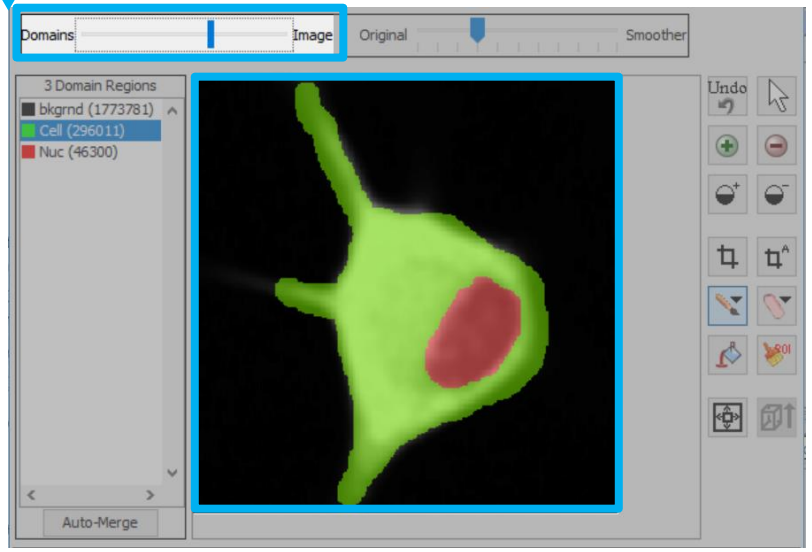
Contents



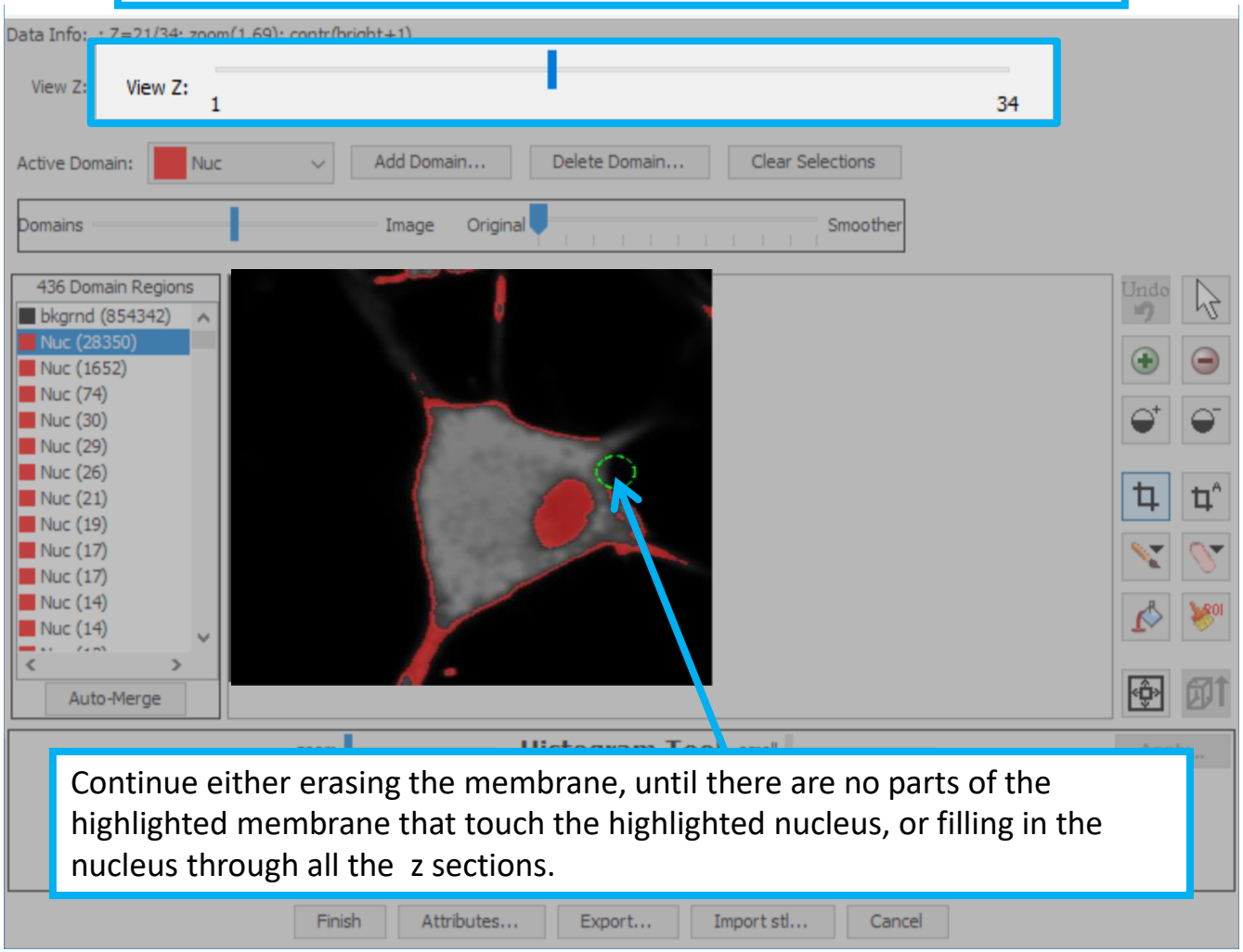
Use the Domains to Image display slider to adjust the way your image is displayed. This can show the image as segmented domains, the image only, or a overlay of the two.

This tool is helpful for visualizing your cell while defining the domains.

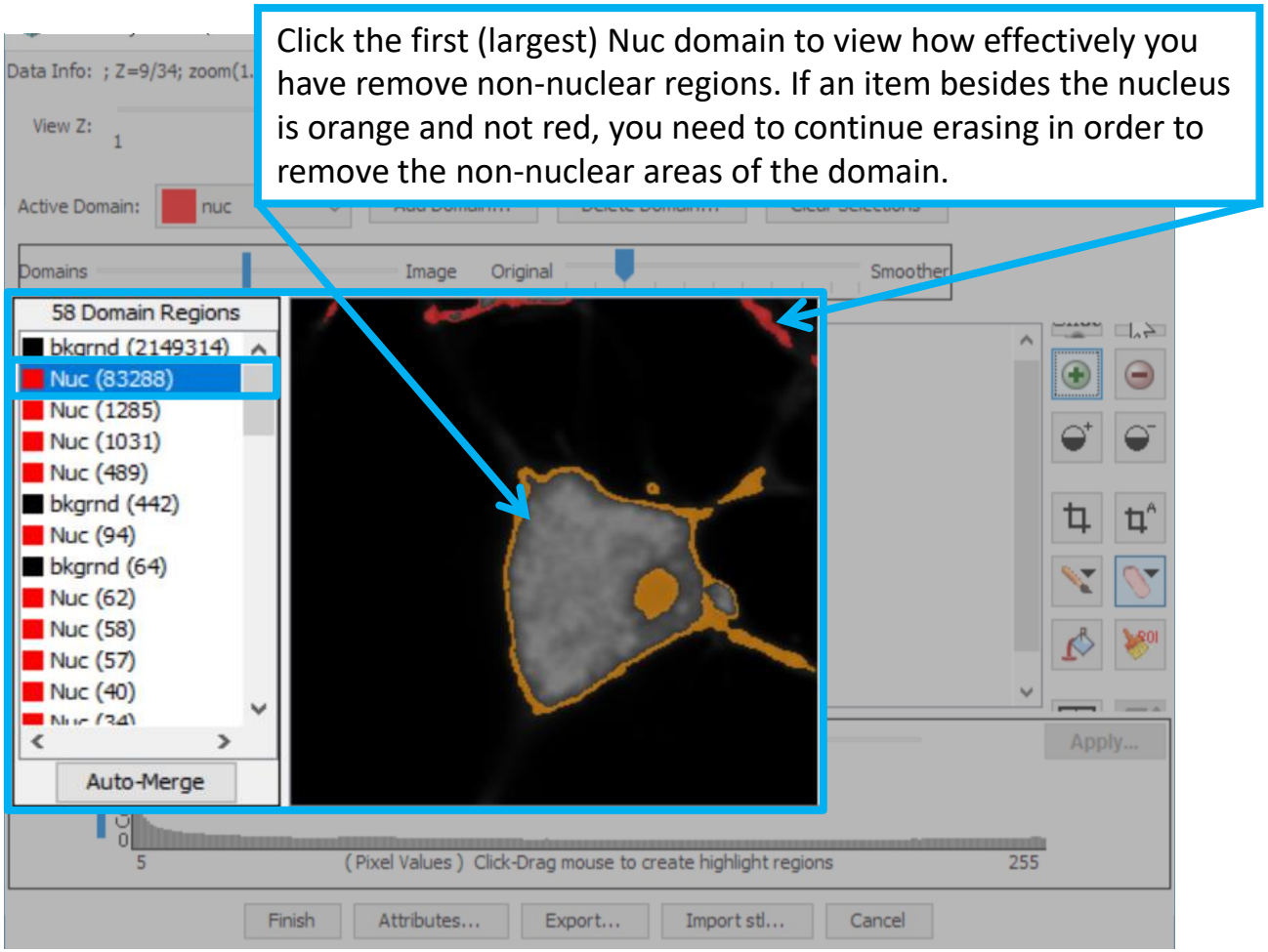


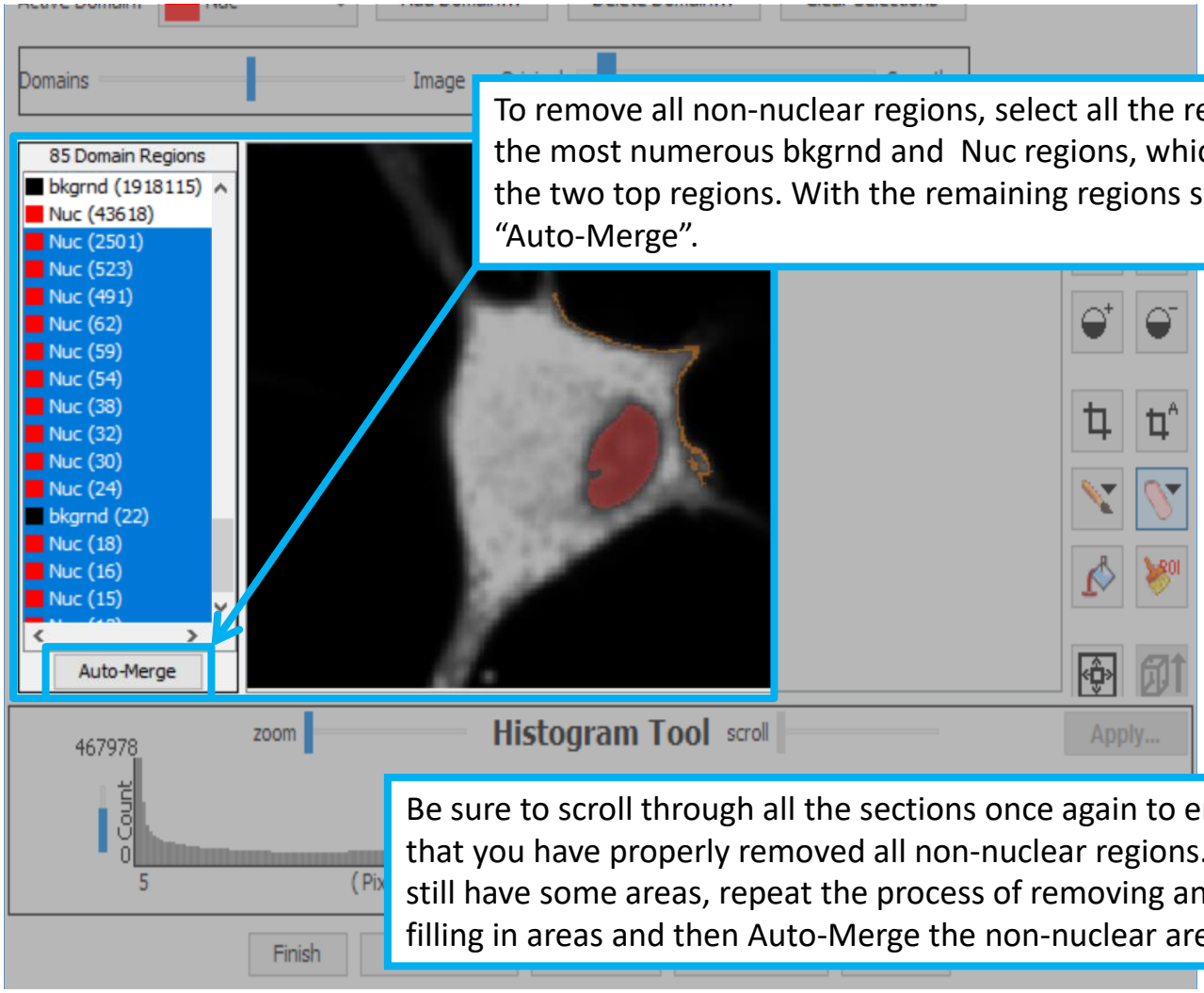


Scroll through the Z slider to view more slices in which the nucleus and membrane are in close proximity or where you need to fill in regions within the nucleus.



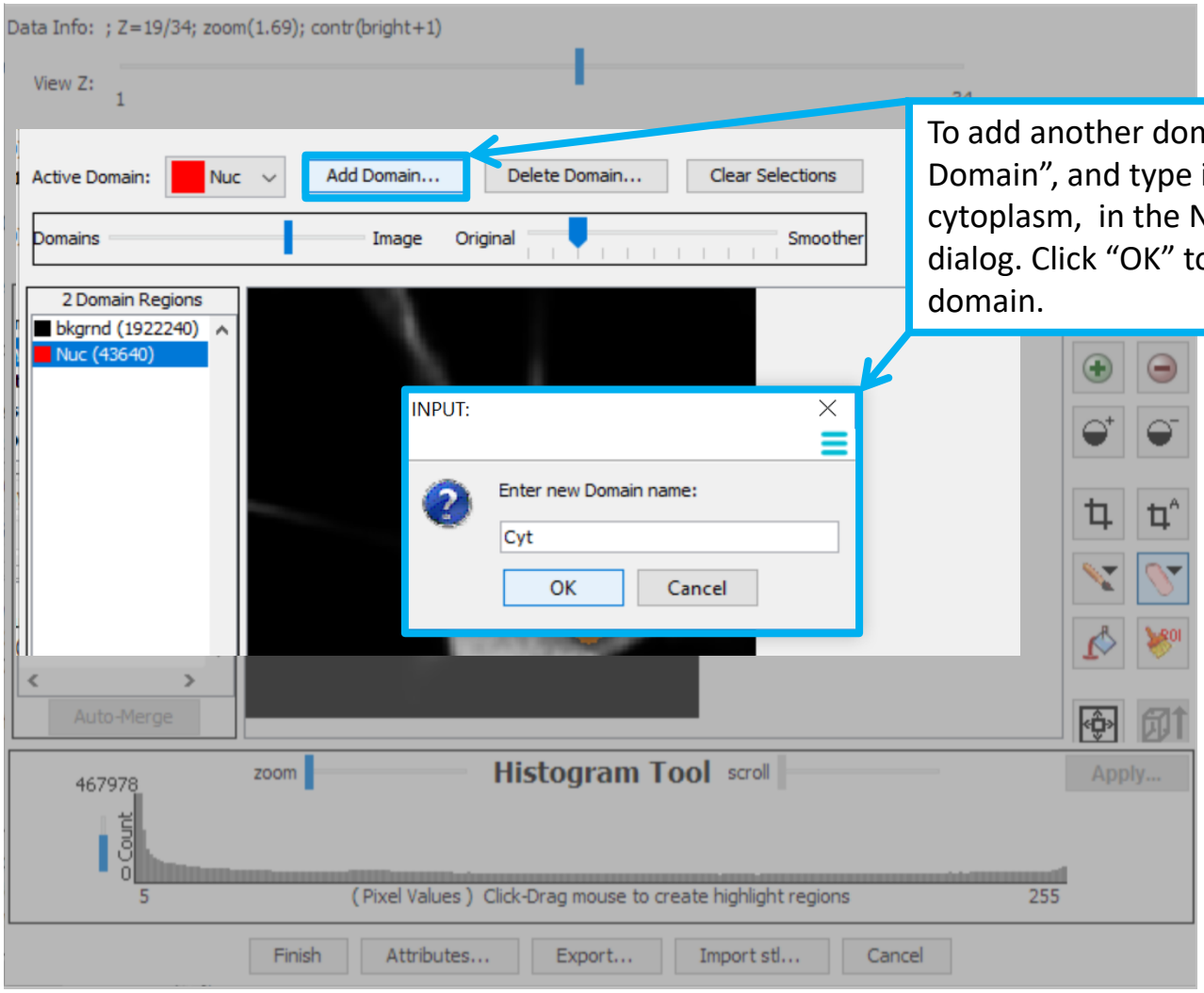
Continue either erasing the membrane, until there are no parts of the highlighted membrane that touch the highlighted nucleus, or filling in the nucleus through all the z sections.


Click the first (largest) Nuc domain to view how effectively you have remove non-nuclear regions. If an item besides the nucleus is orange and not red, you need to continue erasing in order to remove the non-nuclear areas of the domain.
Data Info: ; Z=9/34; zoom(1.
View Z:
1
Active Domain:
nuc
Domains
Image
Original
Smoother
58 Domain Regions
bkgrnd (2149314)
Nuc (83288)
Nuc (1285)
Nuc (1031)
Nuc (489)
bkgrnd (442)
Nuc (94)
bkgrnd (64)
Nuc (62)
Nuc (58)
Nuc (57)
Nuc (40)
Auto-Merge
Apply...
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel

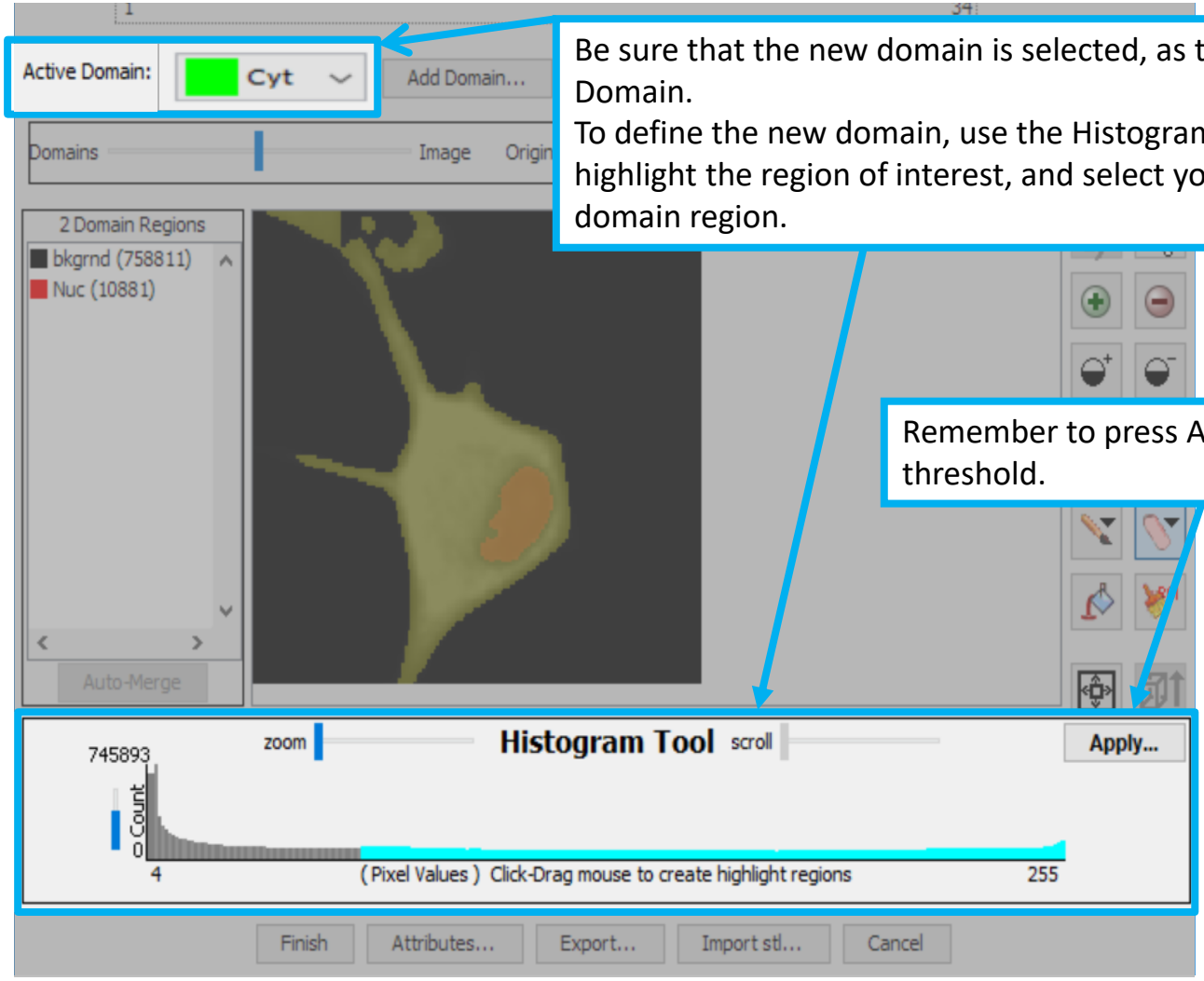


To remove all non-nuclear regions, select all the regions except the most numerous bkgrnd and Nuc regions, which are usually the two top regions. With the remaining regions selected, click "Auto-Merge".

Be sure to scroll through all the sections once again to ensure that you have properly removed all non-nuclear regions. If you still have some areas, repeat the process of removing and/or filling in areas and then Auto-Merge the non-nuclear areas.



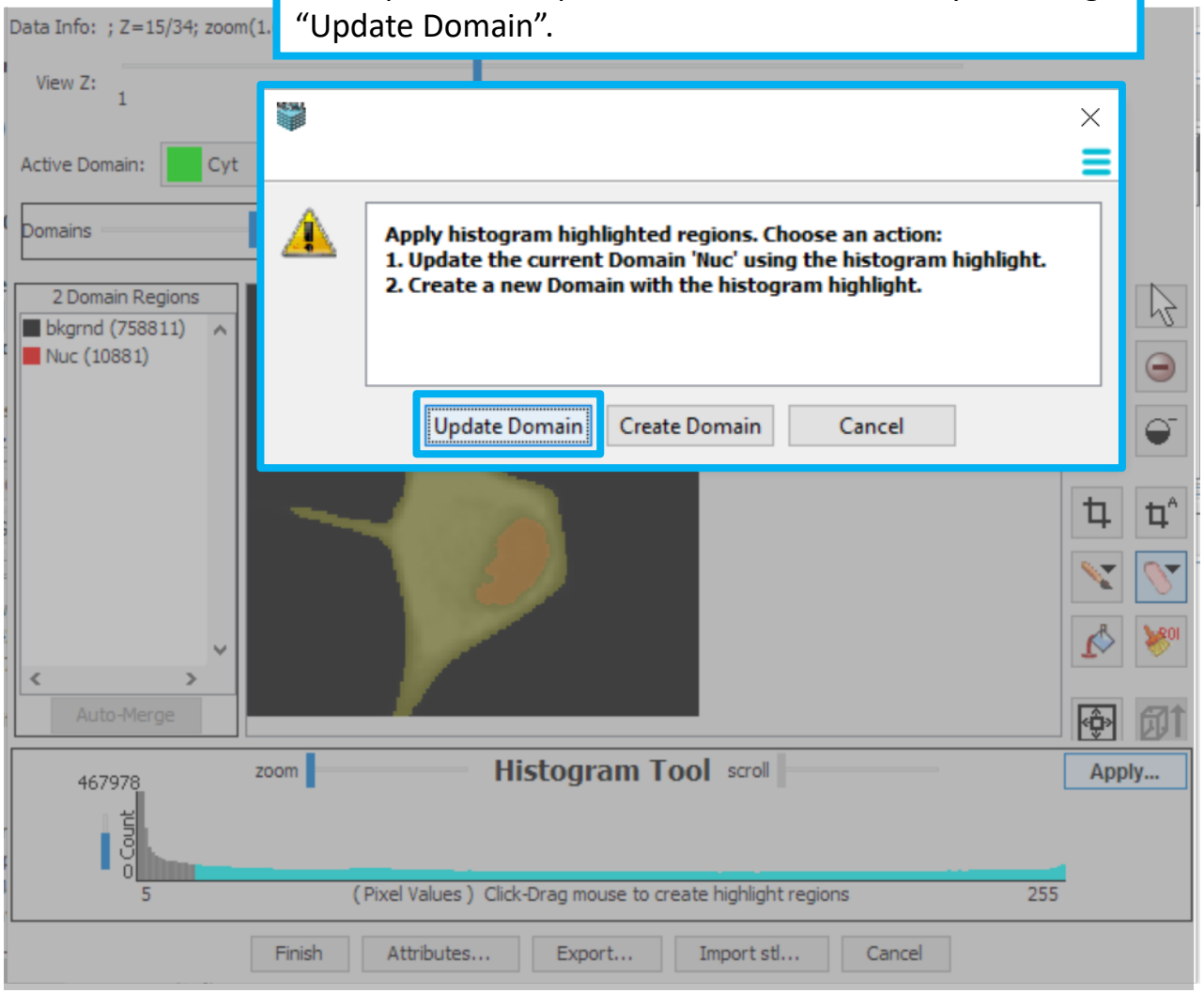
To add another domain, click “Add Domain”, and type in Cyt for cytoplasm, in the New Domain dialog. Click “OK” to accept the new domain.



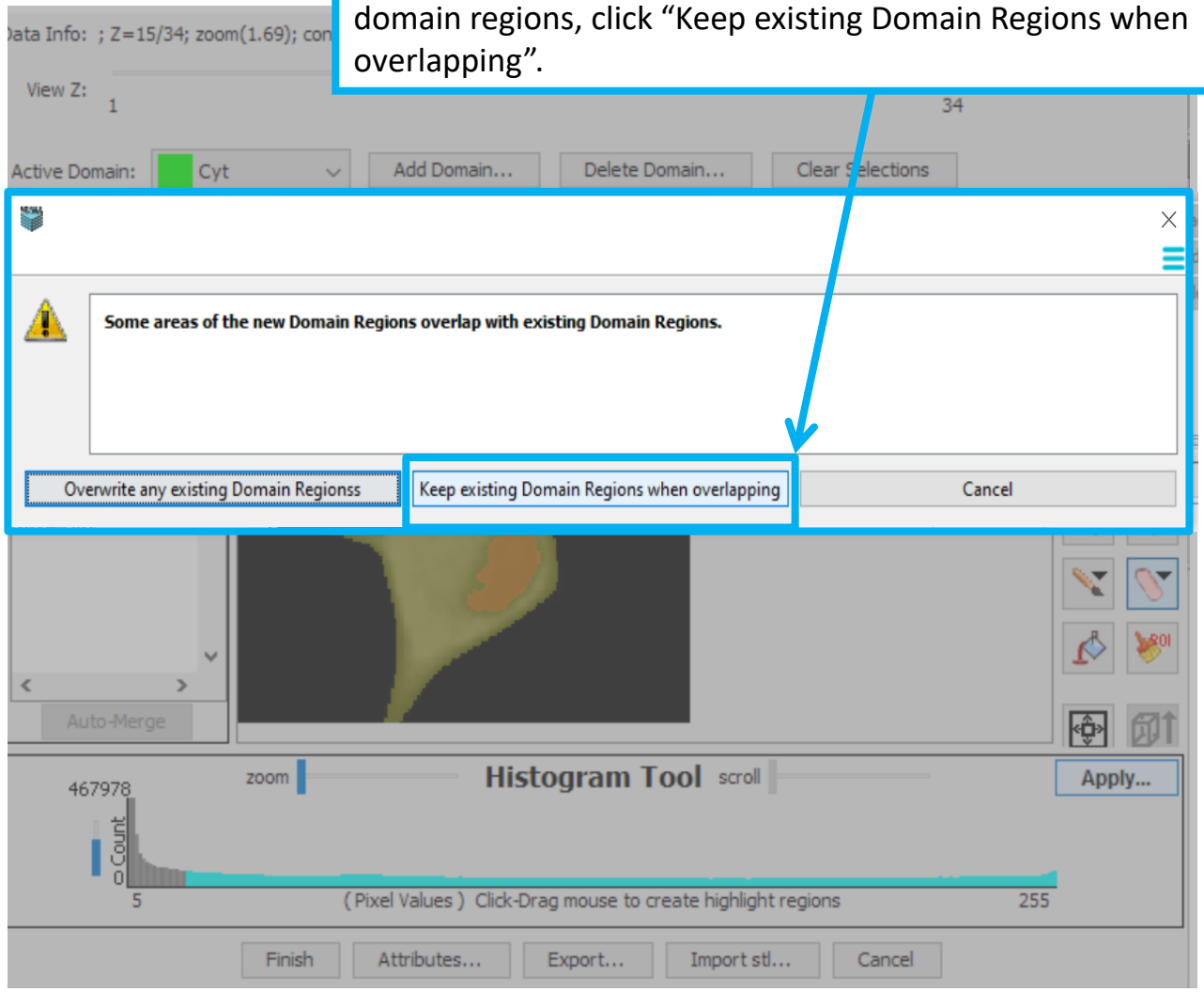
Be sure that the new domain is selected, as the Active Domain.
To define the new domain, use the Histogram Tool to highlight the region of interest, and select your desired domain region.

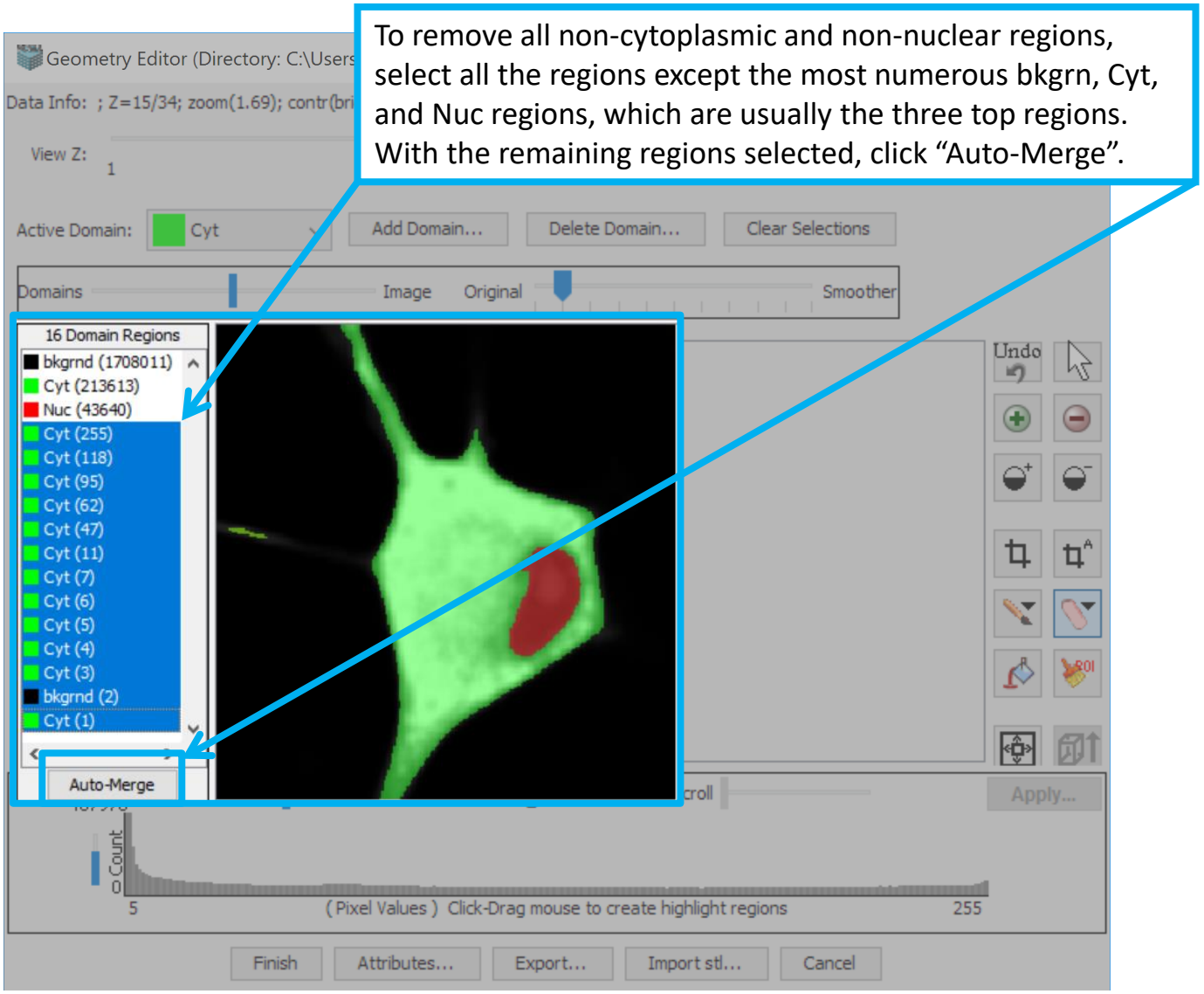
Remember to press Apply to accept the threshold.

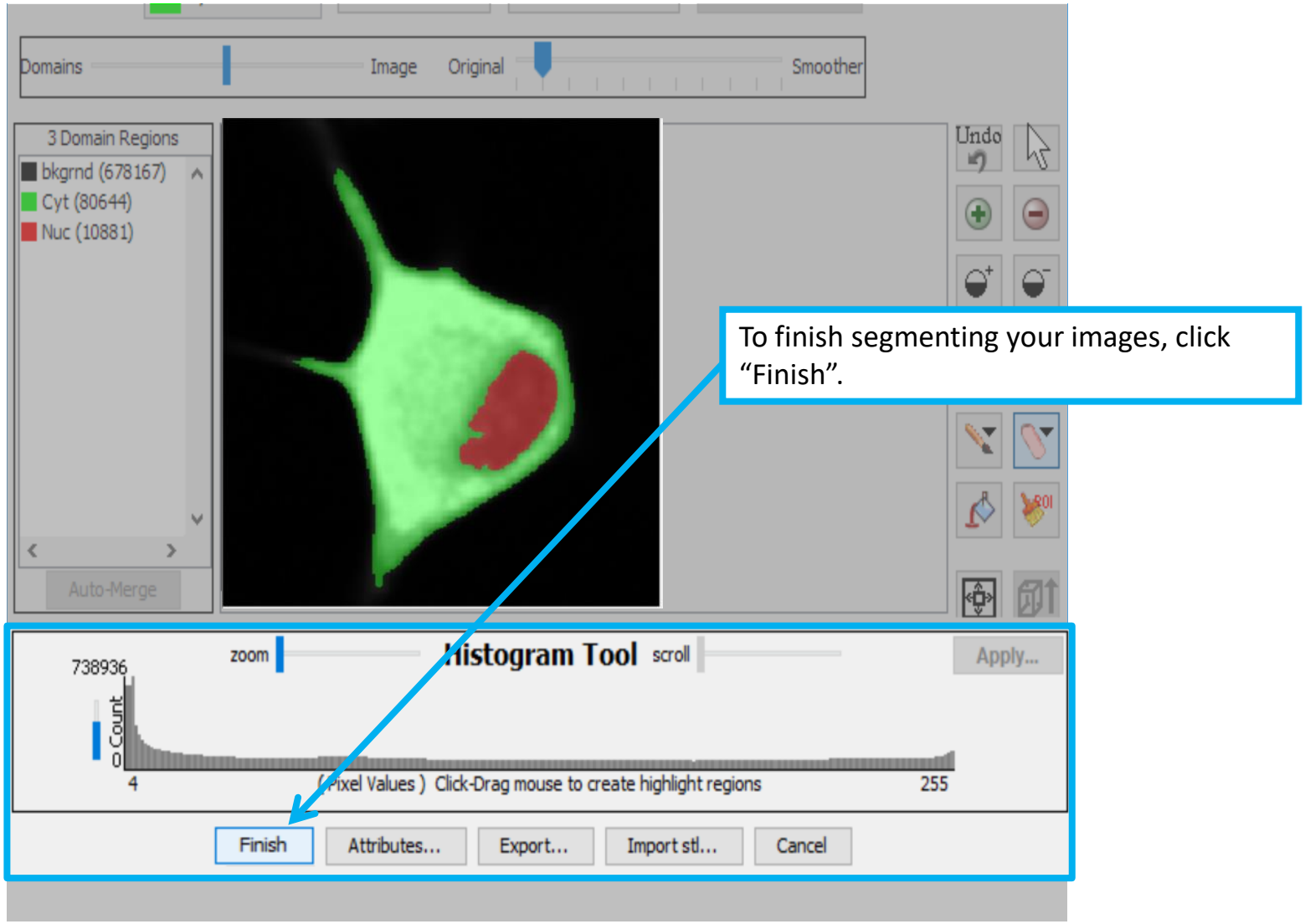
Since you have already created the cytoplasmic domain, in the previous steps, confirm the threshold by selecting "Update Domain".

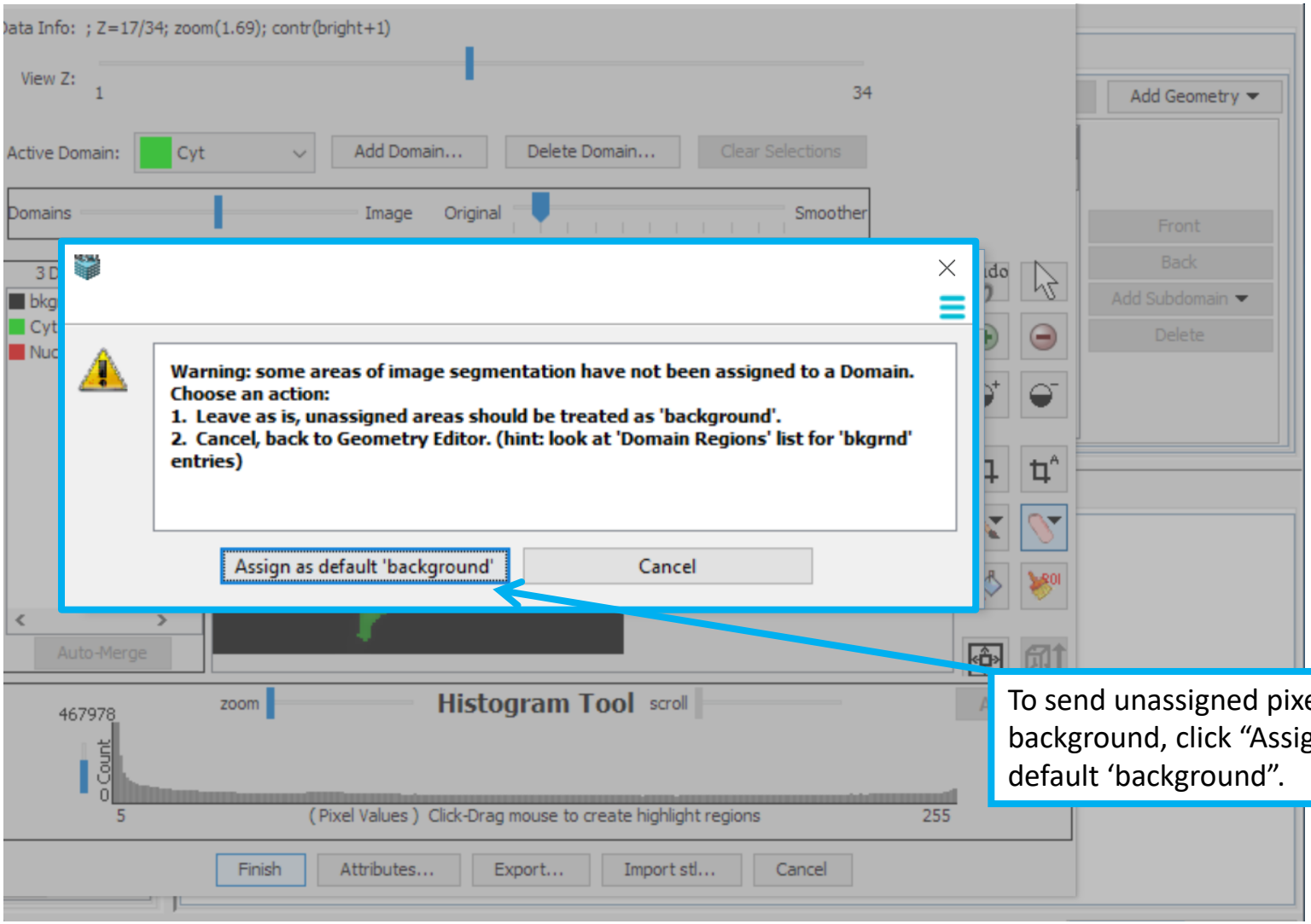


To prevent the new domain selection from over-writing existing domain regions, click “Keep existing Domain Regions when overlapping”.

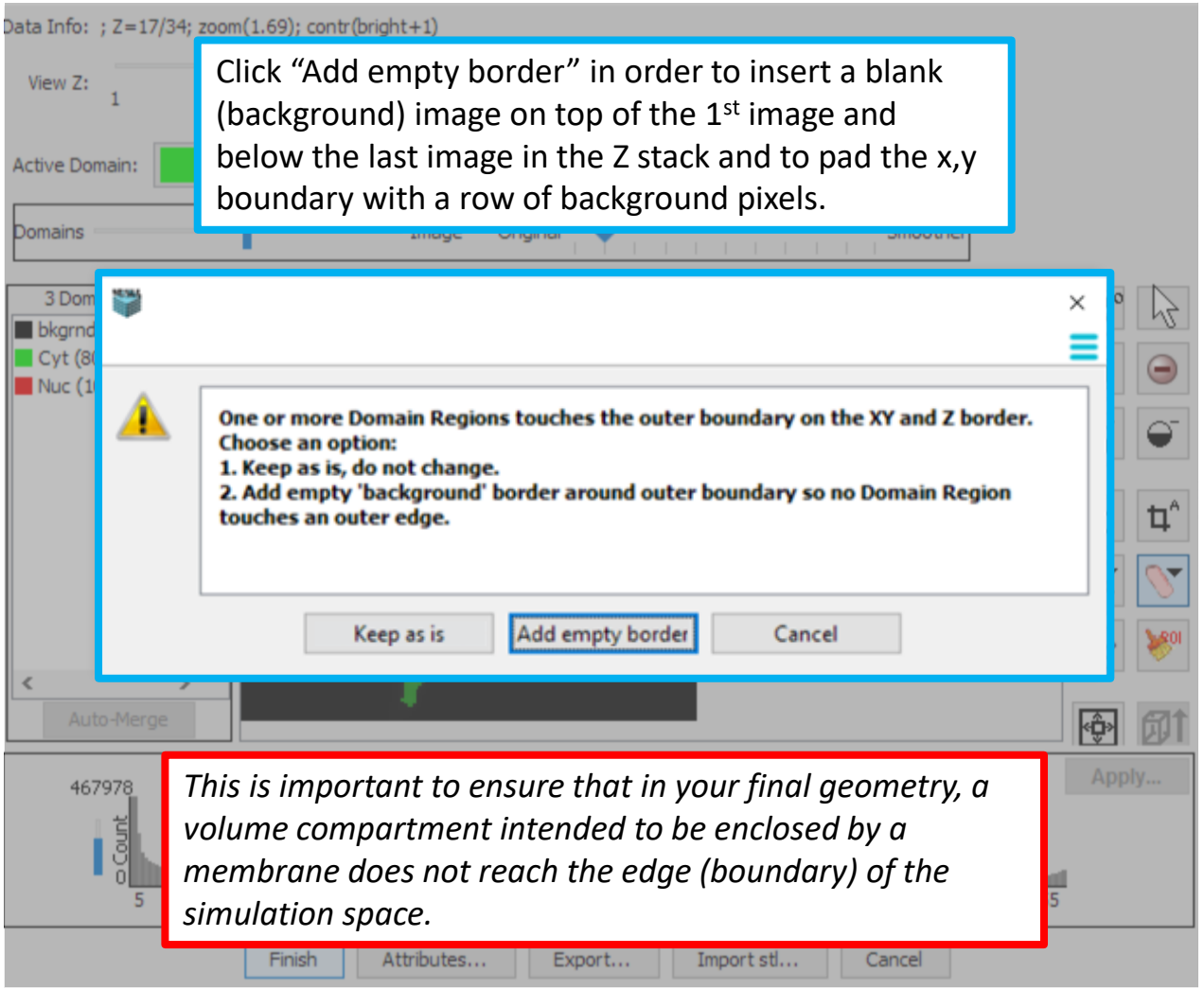



To remove all non-cytoplasmic and non-nuclear regions, select all the regions except the most numerous bkgrn, Cyt, and Nuc regions, which are usually the three top regions. With the remaining regions selected, click “Auto-Merge”.
Geometry Editor (Directory: C:\Users
Data Info: ; Z=15/34; zoom(1.69); contr(bri
View Z:
1
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
16 Domain Regions
bkgrnd (1708011)
Cyt (213613)
Nuc (43640)
Cyt (255)
Cyt (118)
Cyt (95)
Cyt (62)
Cyt (47)
Cyt (11)
Cyt (7)
Cyt (6)
Cyt (5)
Cyt (4)
Cyt (3)
bkgrnd (2)
Cyt (1)
Auto-Merge
Undo
Apply...
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel


Domains
Image
Original
Smoother
3 Domain Regions
bkgrnd (678167)
Cyt (80644)
Nuc (10881)
Auto-Merge
Undo
To finish segmenting your images, click "Finish".
zoom
Histogram Tool
scroll
Apply...
738936
Count
0
4
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Import stl...
Cancel



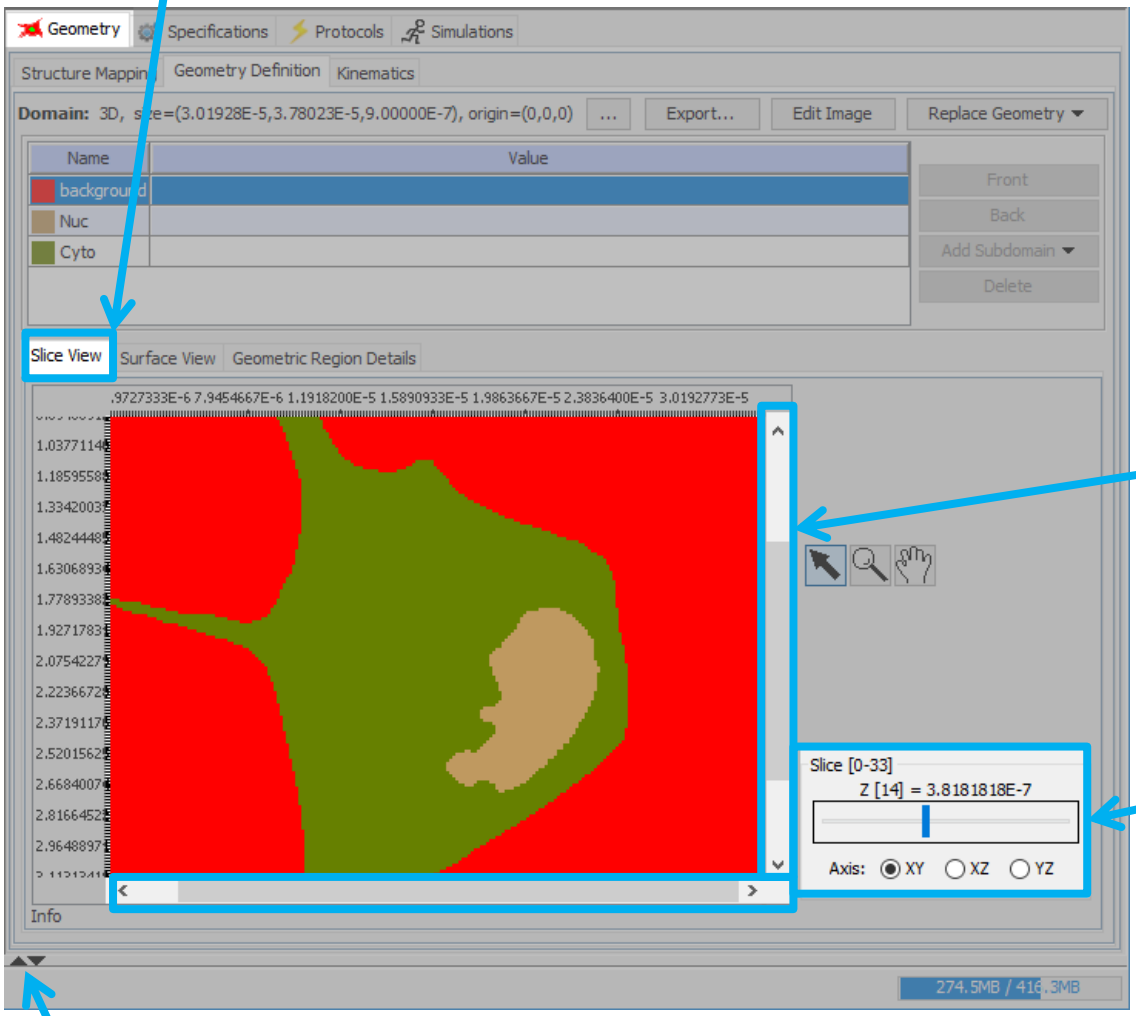
To send unassigned pixels to the background, click “Assign as default ‘background”.



Click “Add empty border” in order to insert a blank (background) image on top of the 1st image and below the last image in the Z stack and to pad the x,y boundary with a row of background pixels.

This is important to ensure that in your final geometry, a volume compartment intended to be enclosed by a membrane does not reach the edge (boundary) of the simulation space.

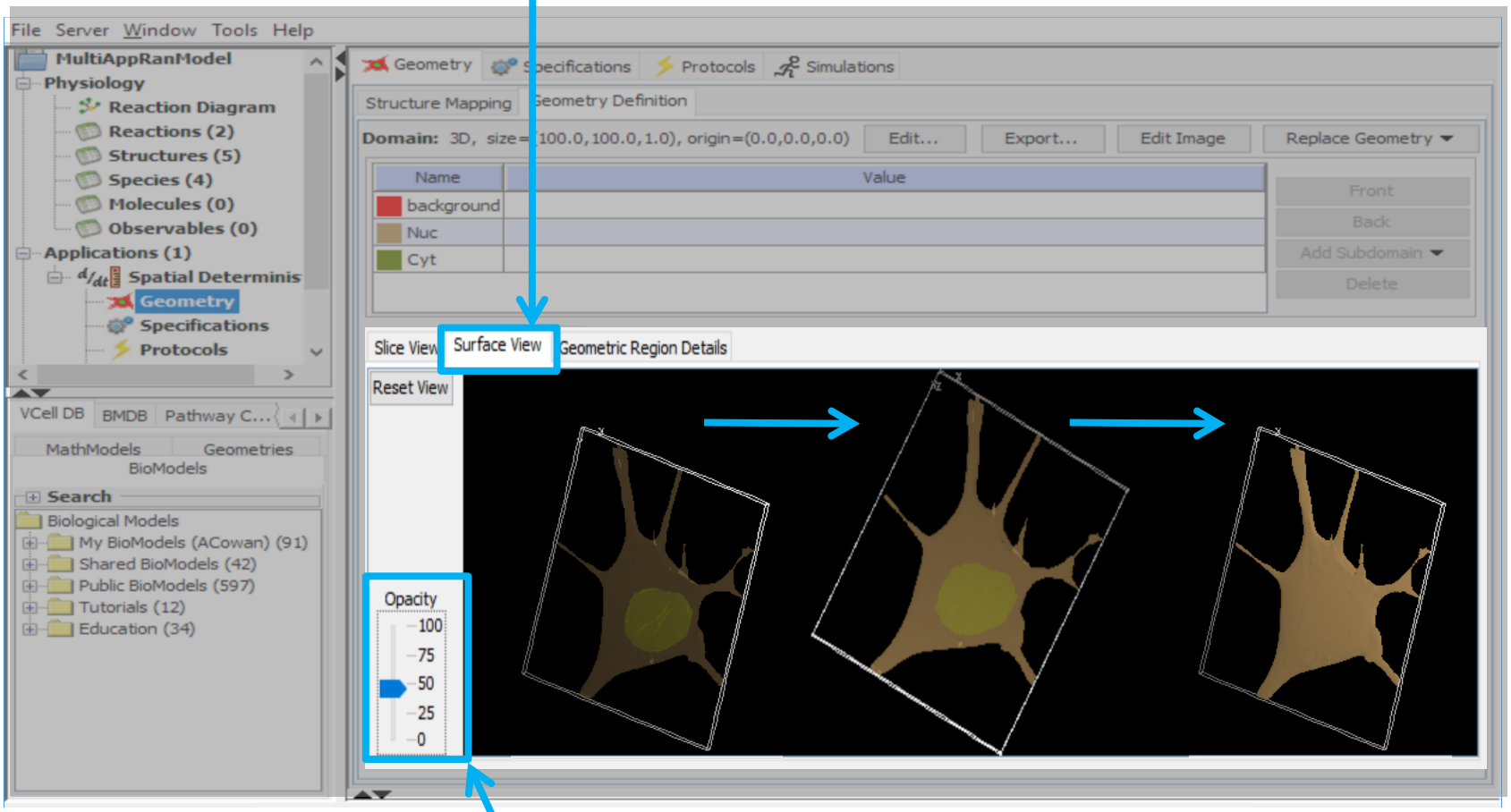
Click “Slice View” in order to view the segmented compartments by individual slices.



Be sure to adjust the scroll bars and Slice indicator to ensure you are able to see the displayed image.

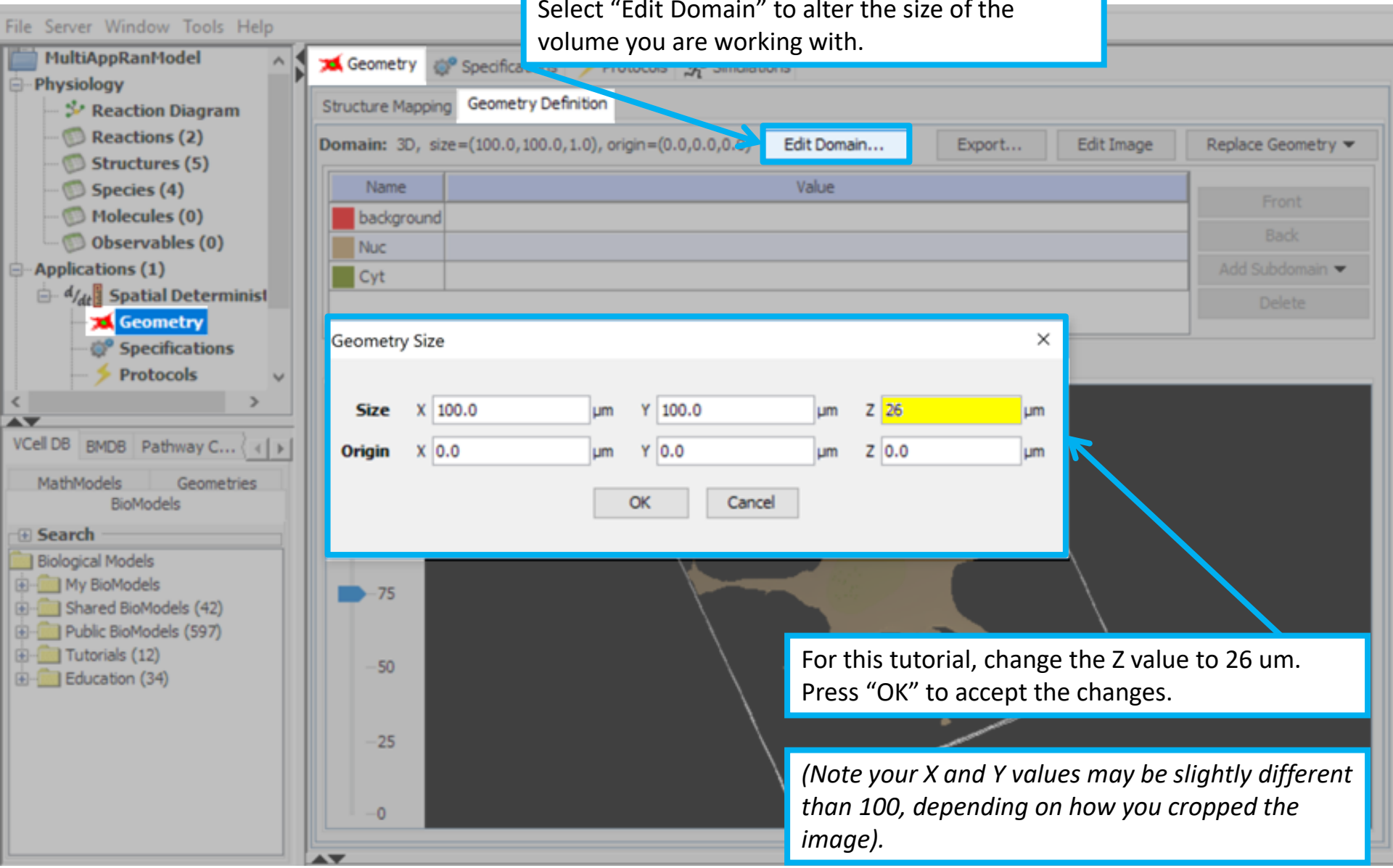
Press the up or down arrow to increase or decrease the window size in order to view more or less of the displayed image.

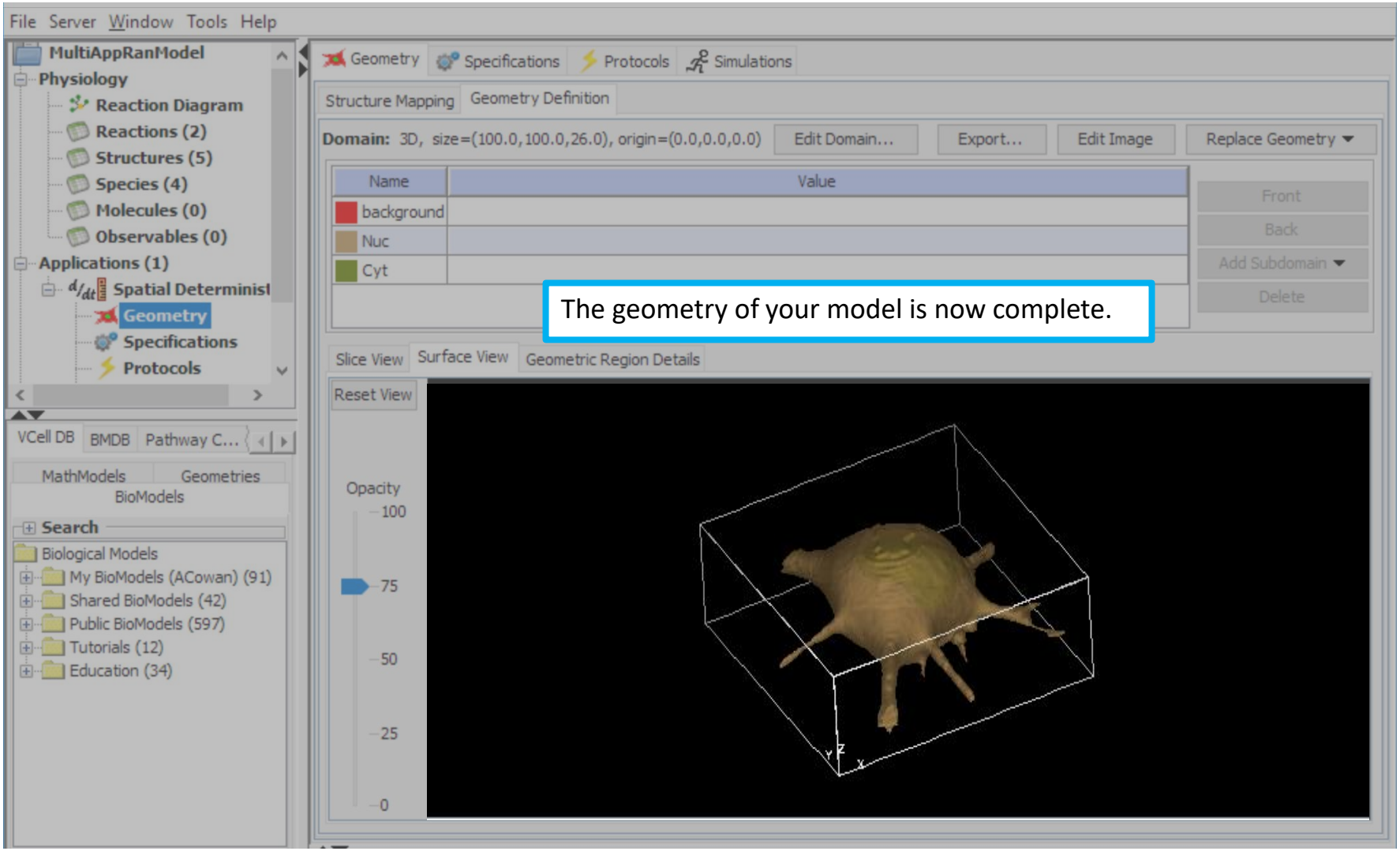
Click “Surface View” in order to view the volume in 3-D.



Adjust the opacity, from 0 – 100%, to allow for the ease of visualizing the different domains within the volume.

The cell here looks flat because there was no Z step information in the images to use to define the domain size. This will be corrected in the next slide by adjusting the domain size for Z.


Select “Edit Domain” to alter the size of the volume you are working with.
File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Spatial Determinist
Geometry
Specifications
Protocols
Geometry
Structure Mapping
Geometry Definition
Domain: 3D, size=(100.0,100.0,1.0), origin=(0.0,0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
Geometry Size
Size X 100.0 µm Y 100.0 µm Z 26 µm
Origin X 0.0 µm Y 0.0 µm Z 0.0 µm
OK
Cancel
VCell DB
BMDB
Pathway C...
MathModels
Geometries
BioModels
Search
Biological Models
My BioModels
Shared BioModels (42)
Public BioModels (597)
Tutorials (12)
Education (34)
75
50
25
0
For this tutorial, change the Z value to 26 um. Press “OK” to accept the changes.
(Note your X and Y values may be slightly different than 100, depending on how you cropped the image).


File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Spatial Determinist
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Specifications
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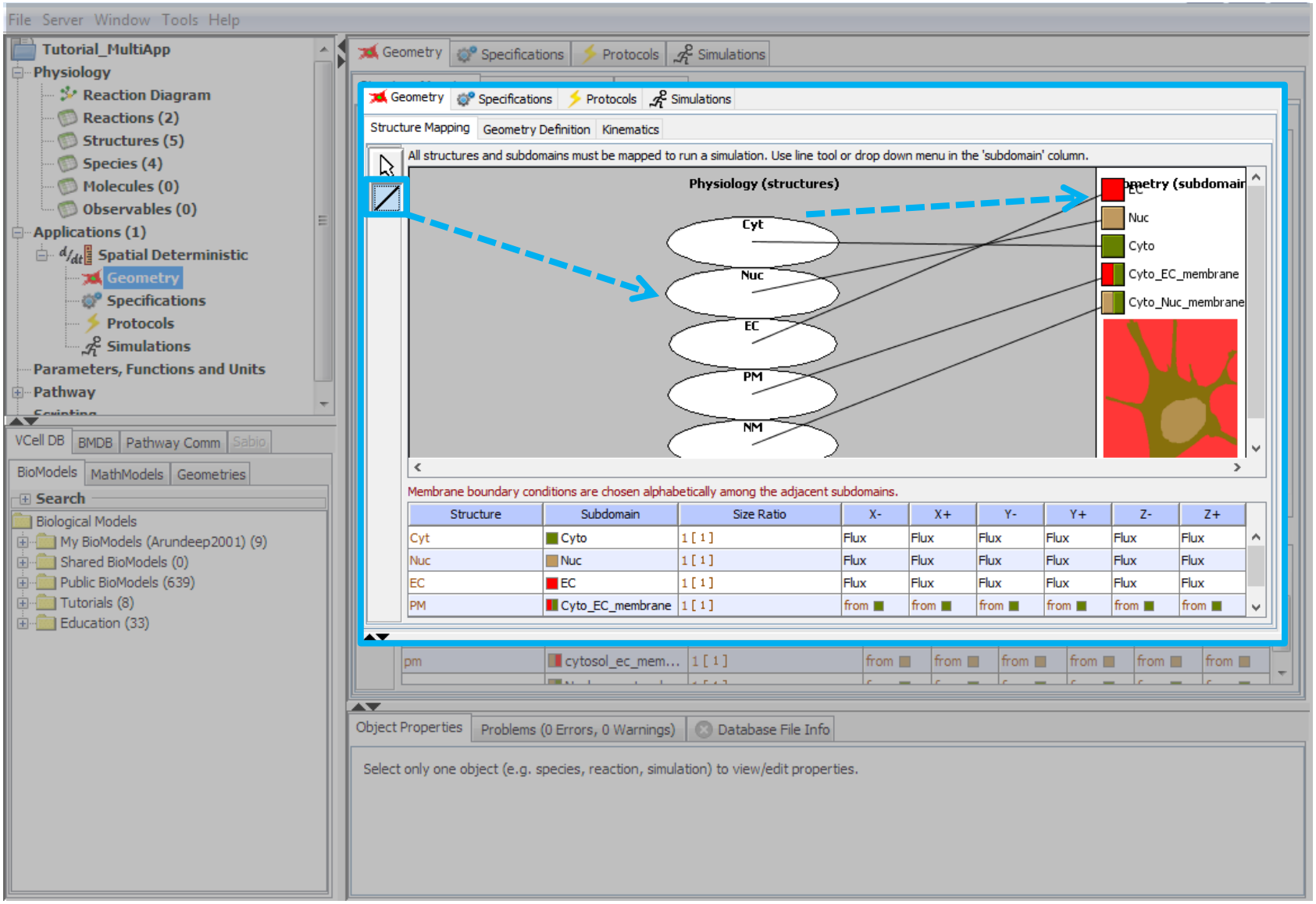
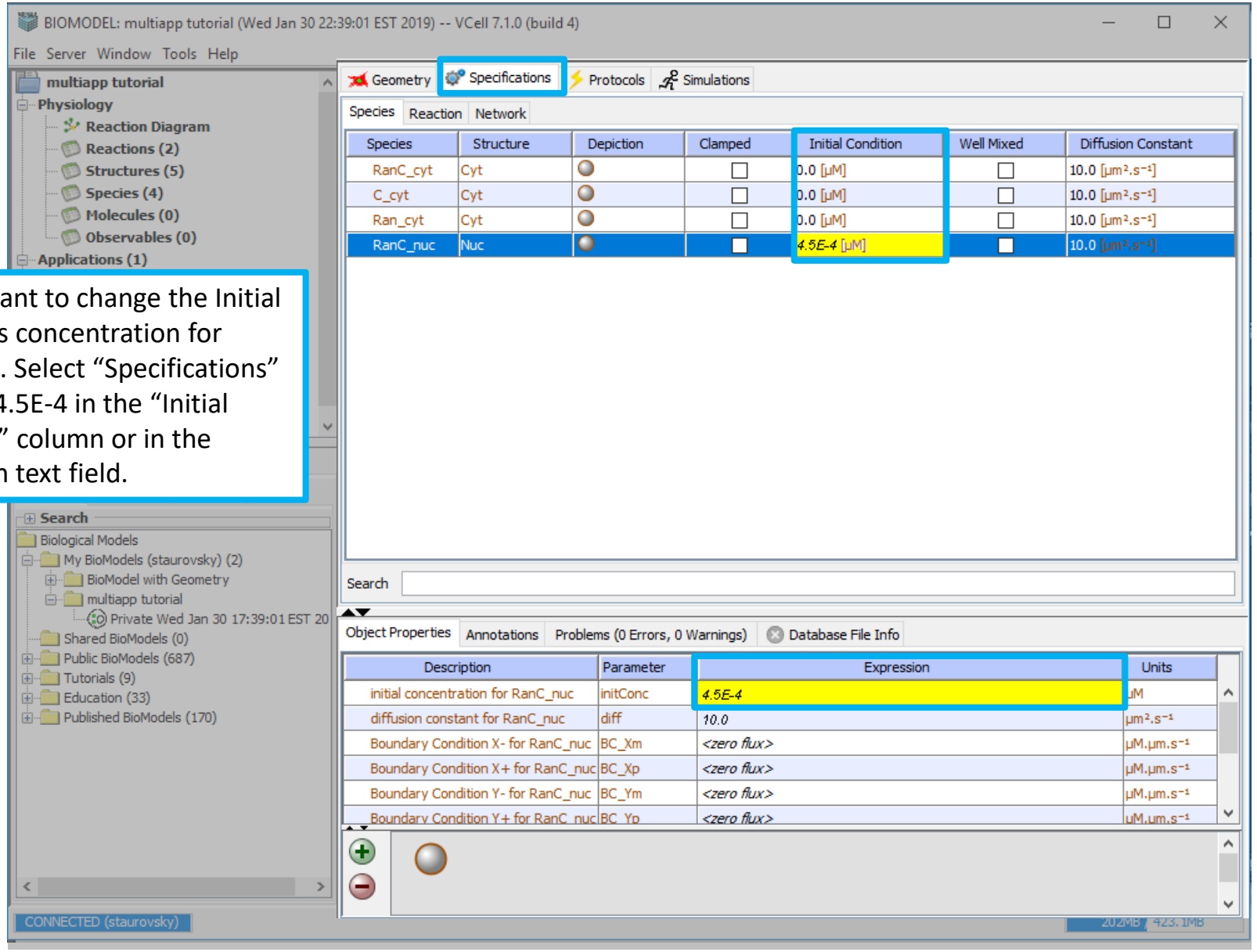
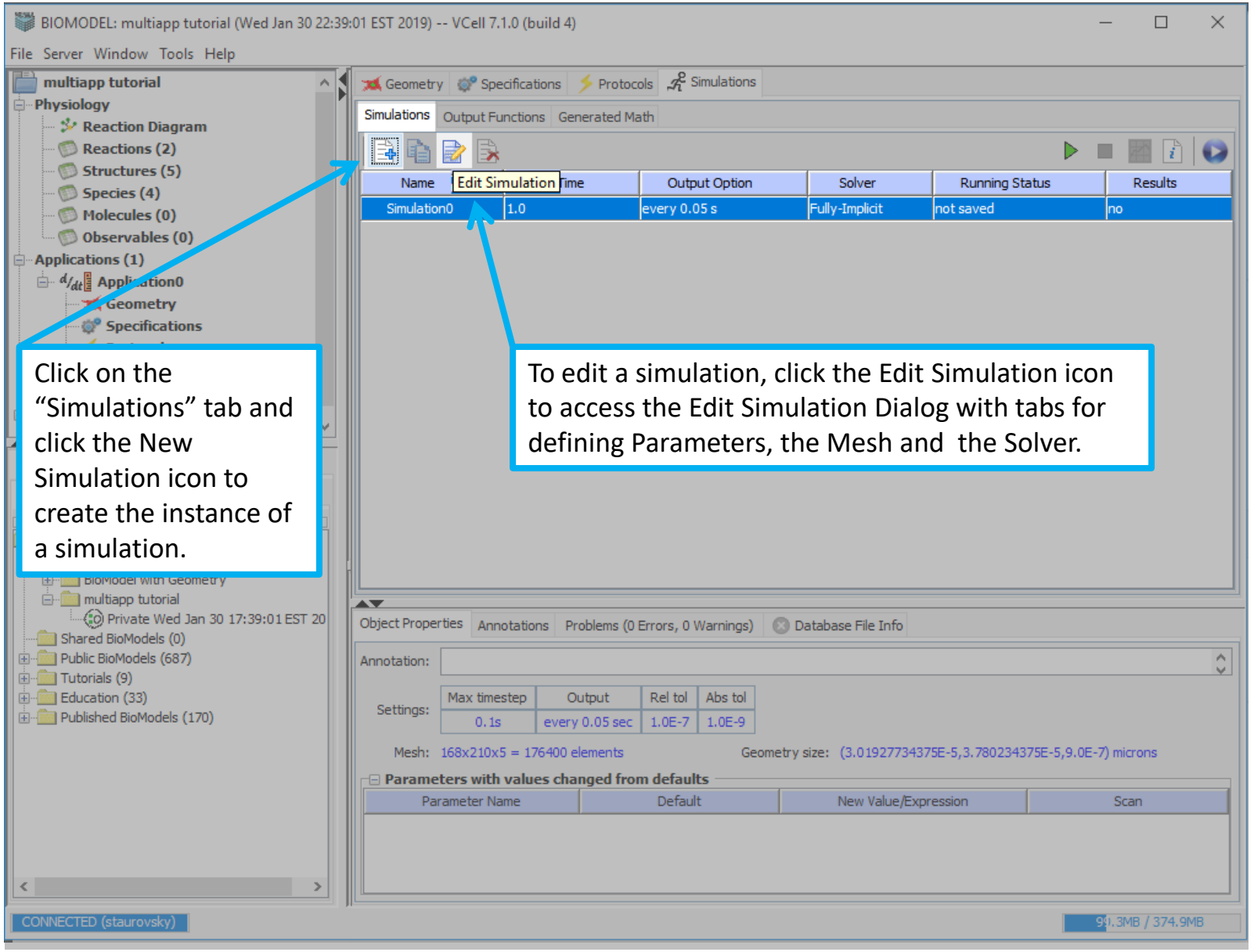
VCell DB
BMDB
Pathway C...
MathModels
Geometries
BioModels
Search
Biological Models
My BioModels (ACowan) (91)
Shared BioModels (42)
Public BioModels (597)
Tutorials (12)
Education (34)
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(100.0,100.0,26.0), origin=(0.0,0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
The geometry of your model is now complete.
Slice View
Surface View
Geometric Region Details
Reset View
Opacity
100
75
50
25
0

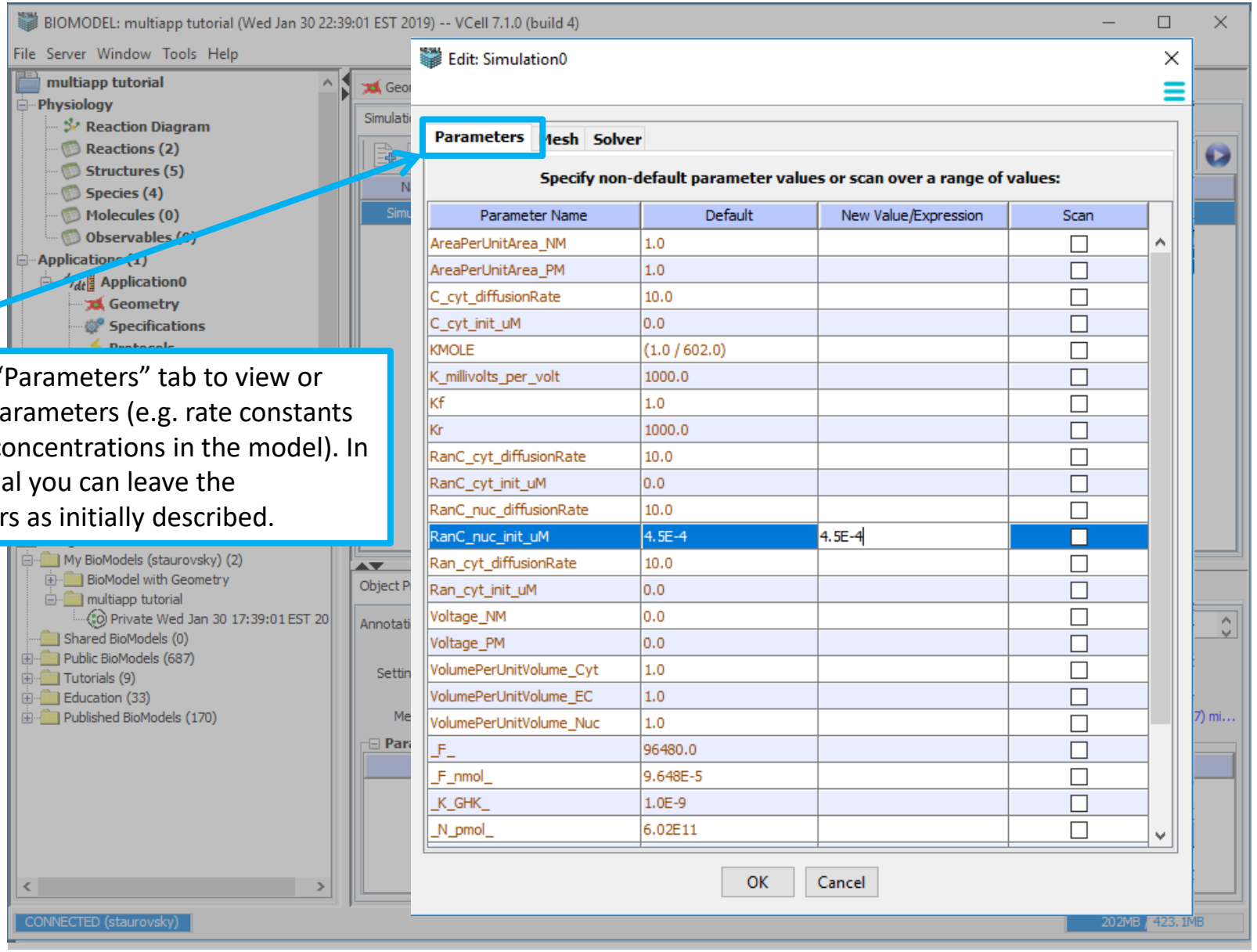
On the Geometry tab > Structure Mapping tab, use the line tool to link the physiology to the geometry. You must select the line tool each time and drag your cursor from a structure to its corresponding subdomain.





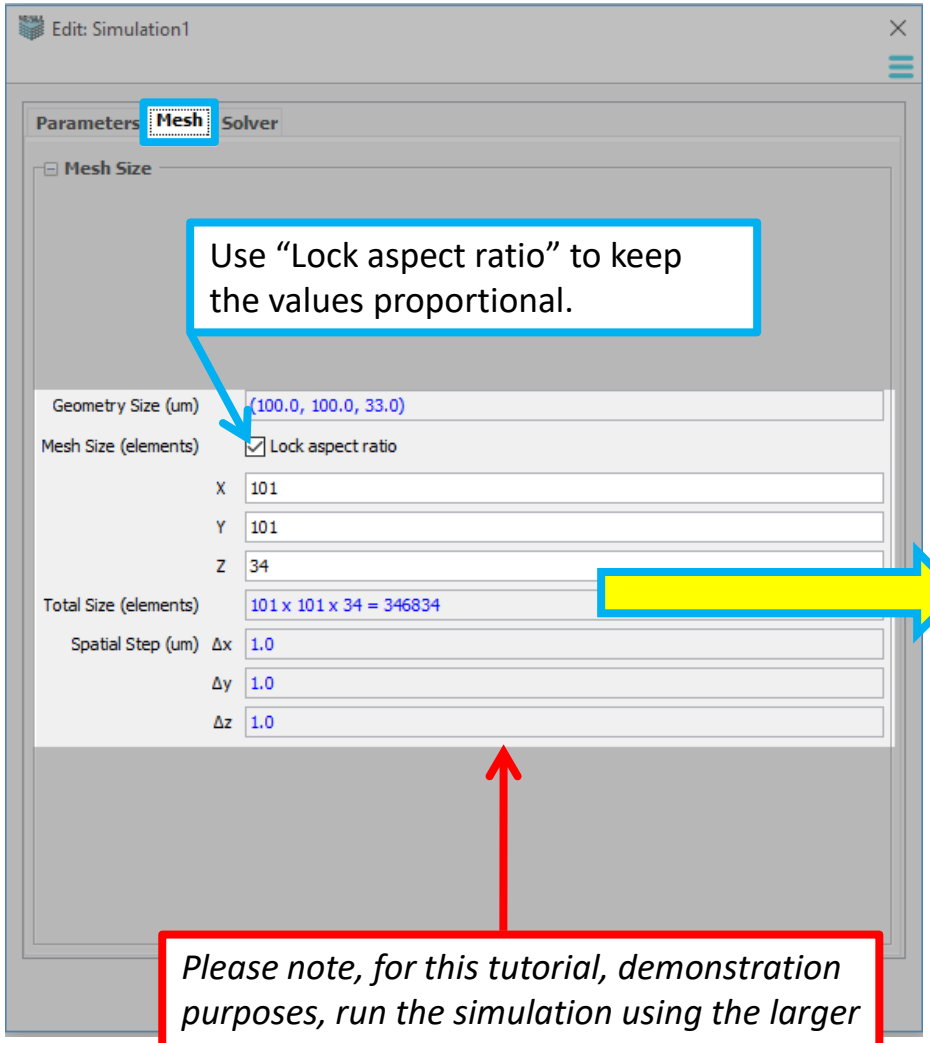
You will want to change the Initial Conditions concentration for RanC_nuc. Select “Specifications” and type 4.5E-4 in the “Initial Condition” column or in the Expression text field.

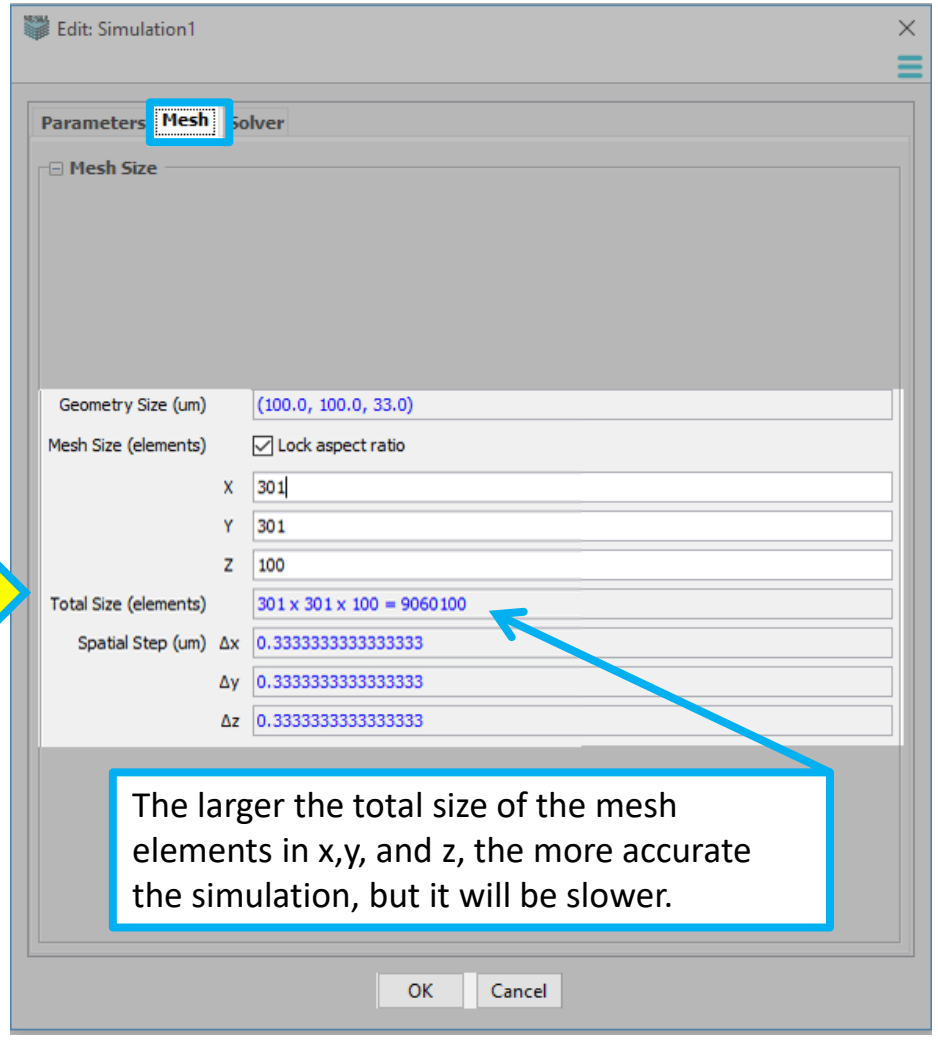

BIOMODEL: multiapp tutorial (Wed Jan 30 22:39:01 EST 2019) -- VCell 7.1.0 (build 4)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Application0
Geometry
Specifications
Geometry Specifications Protocols Simulations
Simulations Output Functions Generated Math
Name Edit Simulation ime Output Option Solver Running Status Results
Simulation0 1.0 every 0.05 s Fully-Implicit not saved no
Click on the "Simulations" tab and click the New Simulation icon to create the instance of a simulation.
To edit a simulation, click the Edit Simulation icon to access the Edit Simulation Dialog with tabs for defining Parameters, the Mesh and the Solver.
multiapp tutorial
Private Wed Jan 30 17:39:01 EST 20
Shared BioModels (0)
Public BioModels (687)
Tutorials (9)
Education (33)
Published BioModels (170)
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: 168x210x5 = 176400 elements
Geometry size: (3.01927734375E-5,3.780234375E-5,9.0E-7) microns
Parameters with values changed from defaults
Parameter Name Default New Value/Expression Scan
CONNECTED (staurovsky)



Click the “Parameters” tab to view or edit the parameters (e.g. rate constants or initial concentrations in the model). In this tutorial you can leave the parameters as initially described.

Select the “Mesh” tab to edit the mesh resolution for the simulation in the X, Y, and Z planes. Select “OK” to accept your changes.

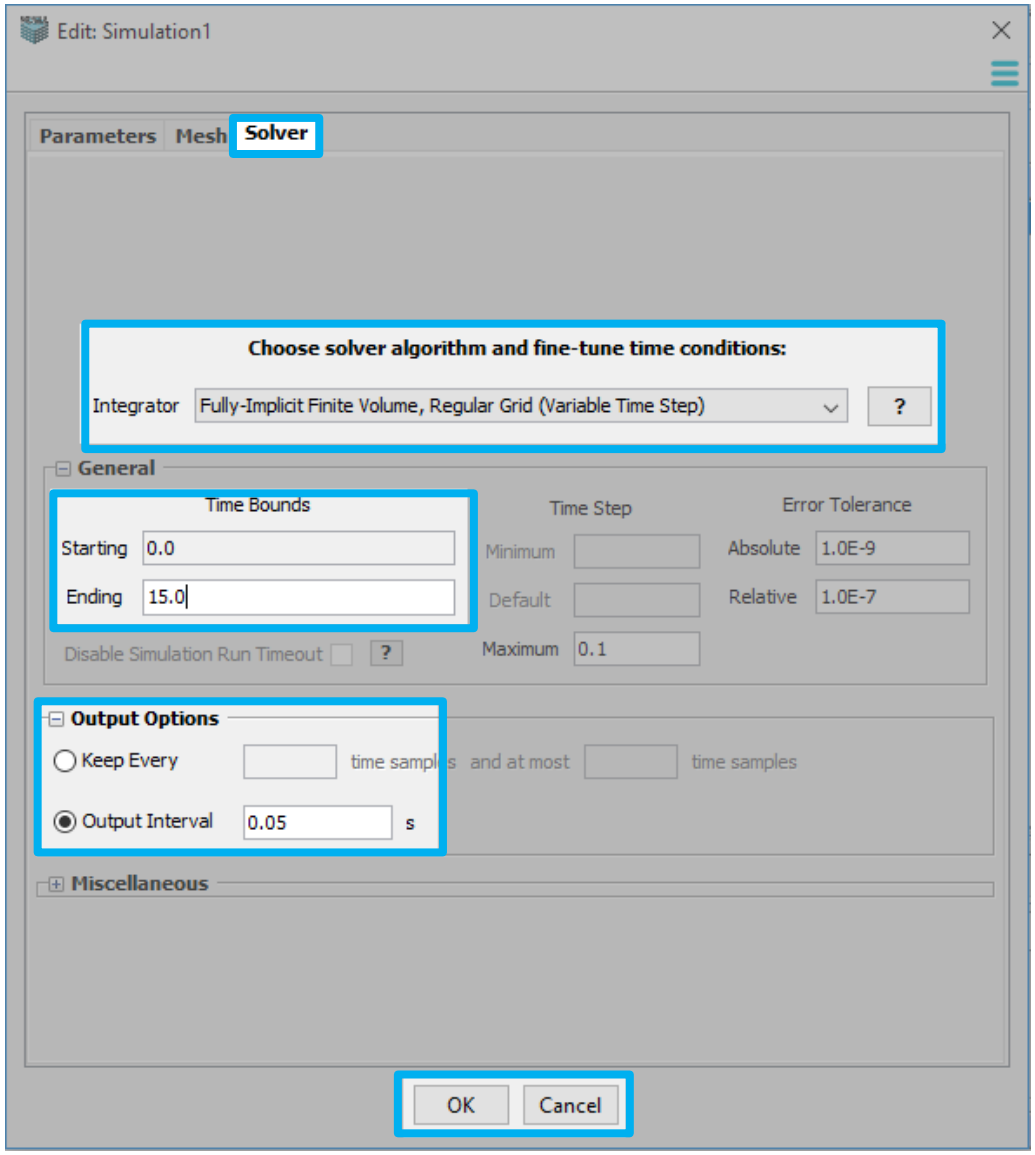


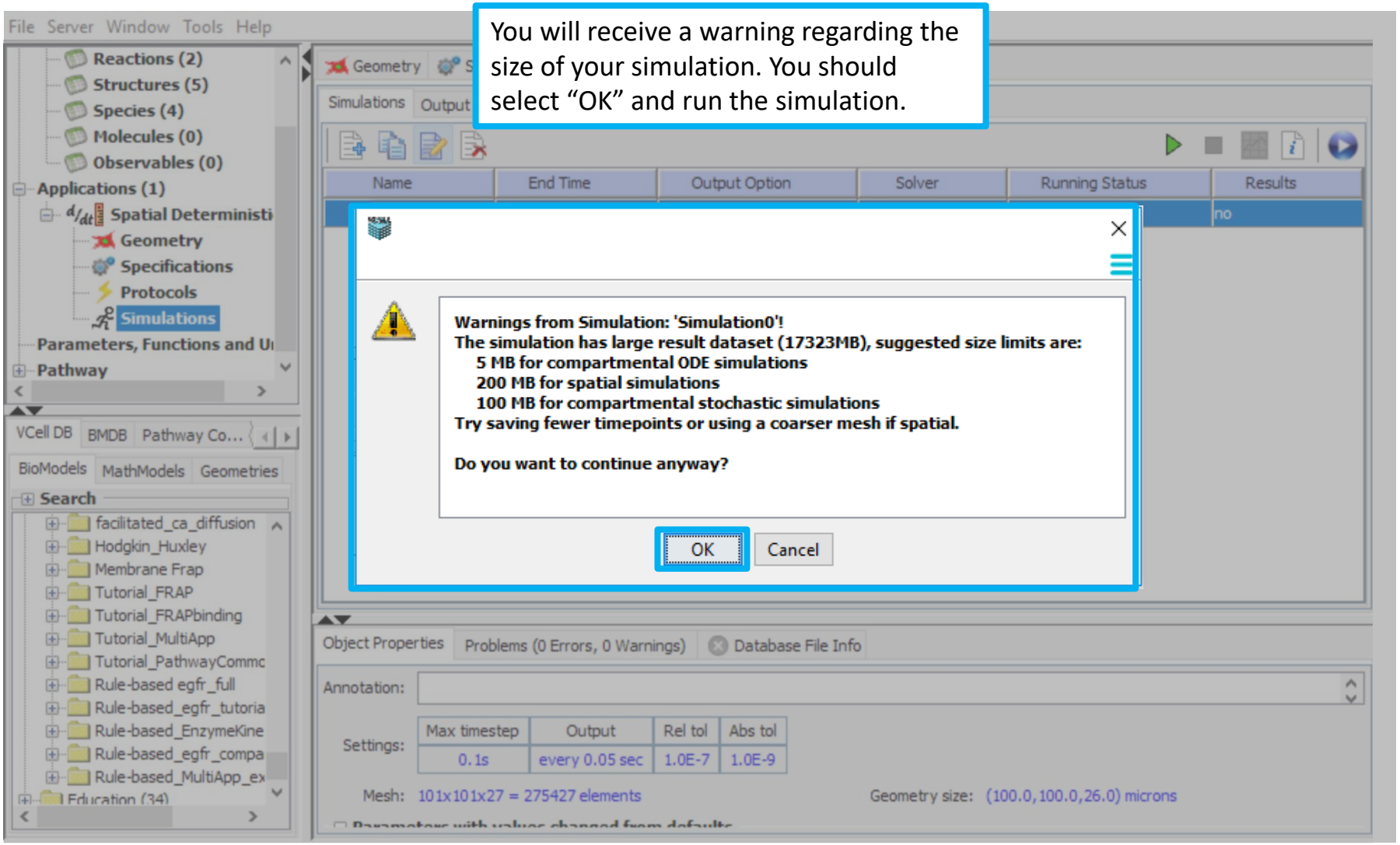


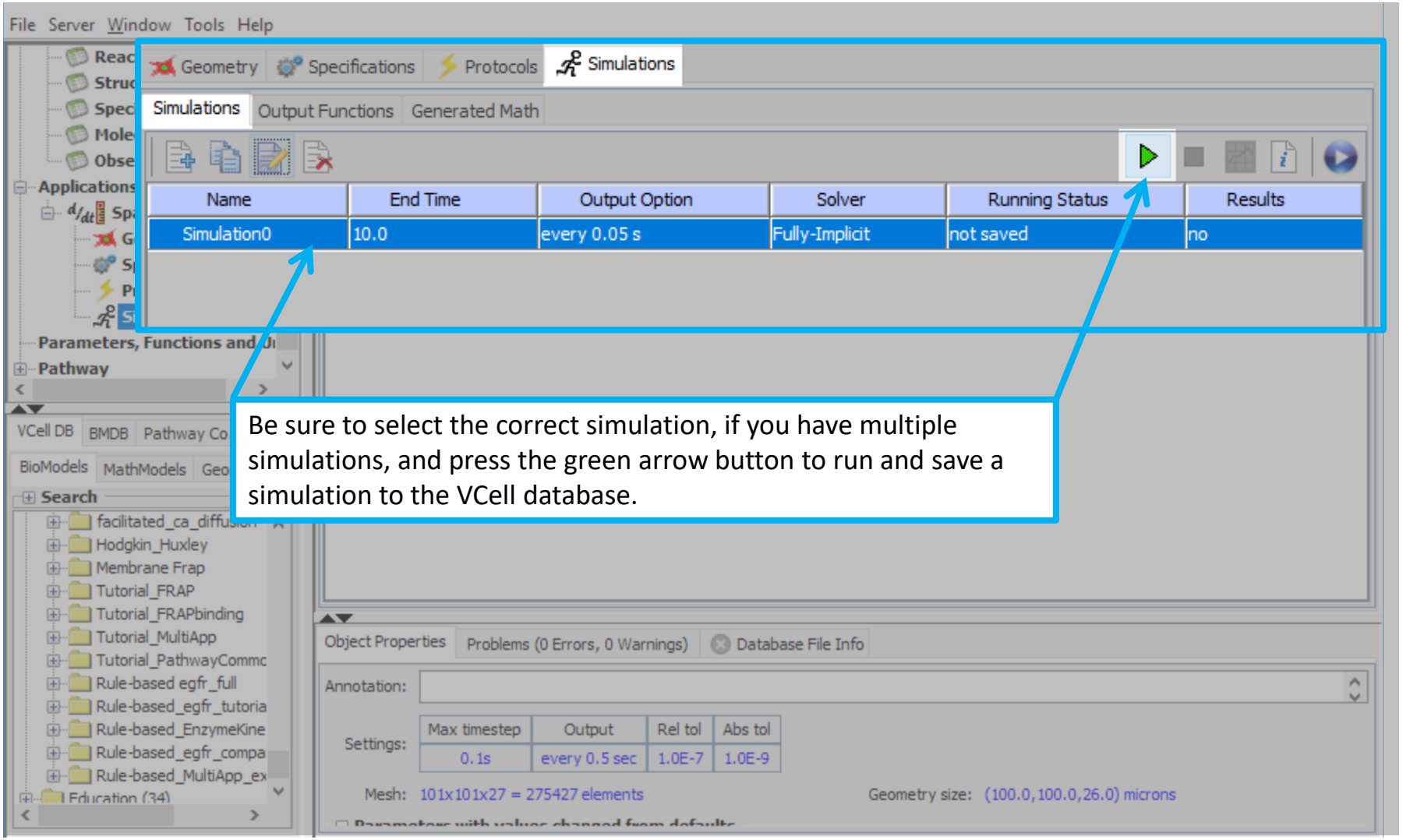
The larger the total size of the mesh elements in x,y, and z, the more accurate the simulation, but it will be slower.

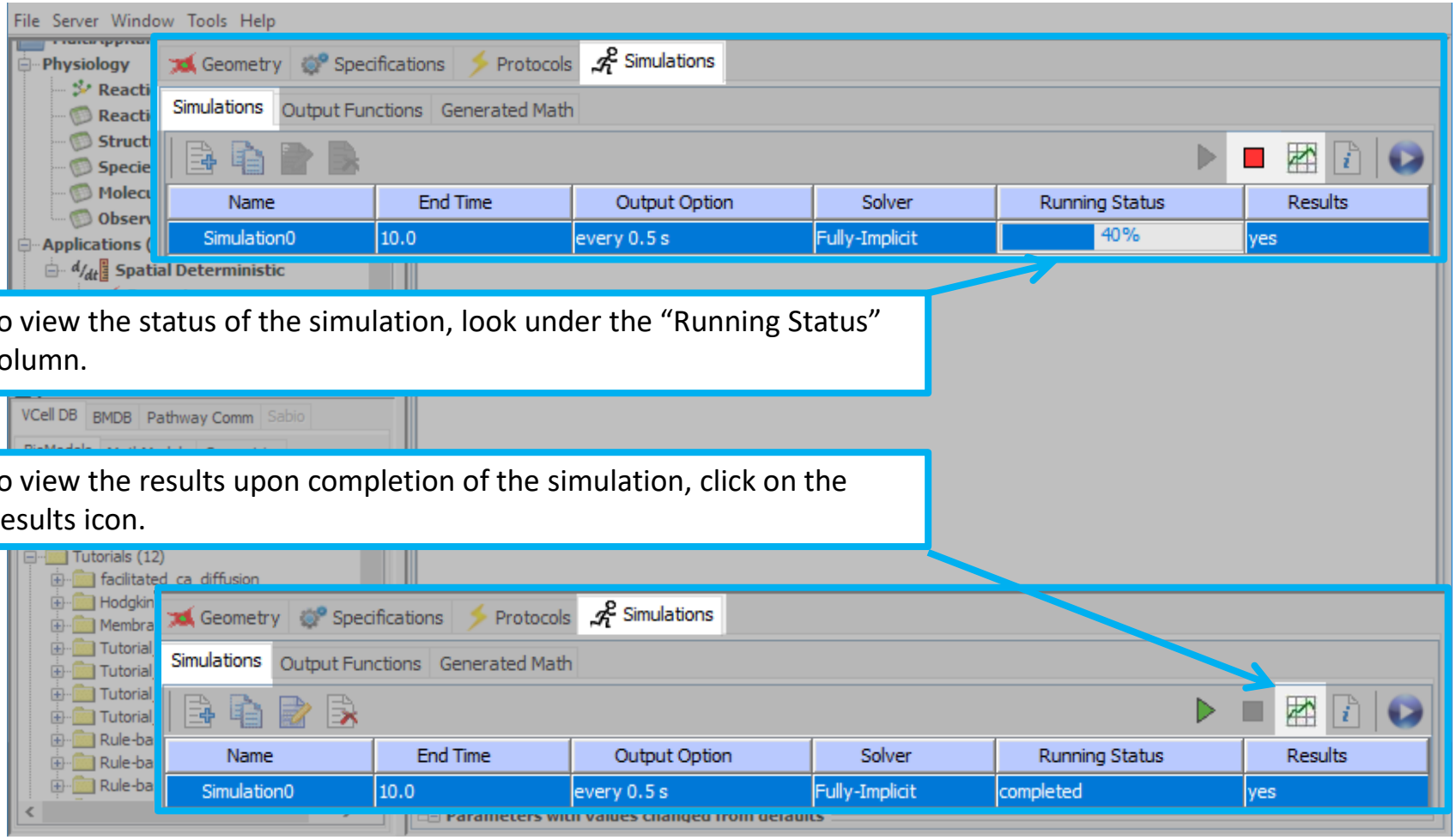
Please note, for this tutorial, demonstration purposes, run the simulation using the larger mesh elements to save on your simulation time.

Select the “Solver” tab to edit the solver run configuration as shown. Be sure to press “OK” to accept your changes.




You will receive a warning regarding the size of your simulation. You should select “OK” and run the simulation.
Warnings from Simulation: 'Simulation0'!
The simulation has large result dataset (17323MB), suggested size limits are:
5 MB for compartmental ODE simulations
200 MB for spatial simulations
100 MB for compartmental stochastic simulations
Try saving fewer timepoints or using a coarser mesh if spatial.
Do you want to continue anyway?
OK
Cancel


File Server Window Tools Help
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
10.0
every 0.05 s
Fully-Implicit
not saved
no
Be sure to select the correct simulation, if you have multiple simulations, and press the green arrow button to run and save a simulation to the VCell database.
Applications
Parameters, Functions and
Pathway
VCell DB
BMDB
BioModels
MathModels
Search
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Rule-based egfr_full
Rule-based_EnzymeKine
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
Max timestep
Output
Rel tol
Abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 101x101x27 = 275427 elements
Geometry size: (100.0,100.0,26.0) microns



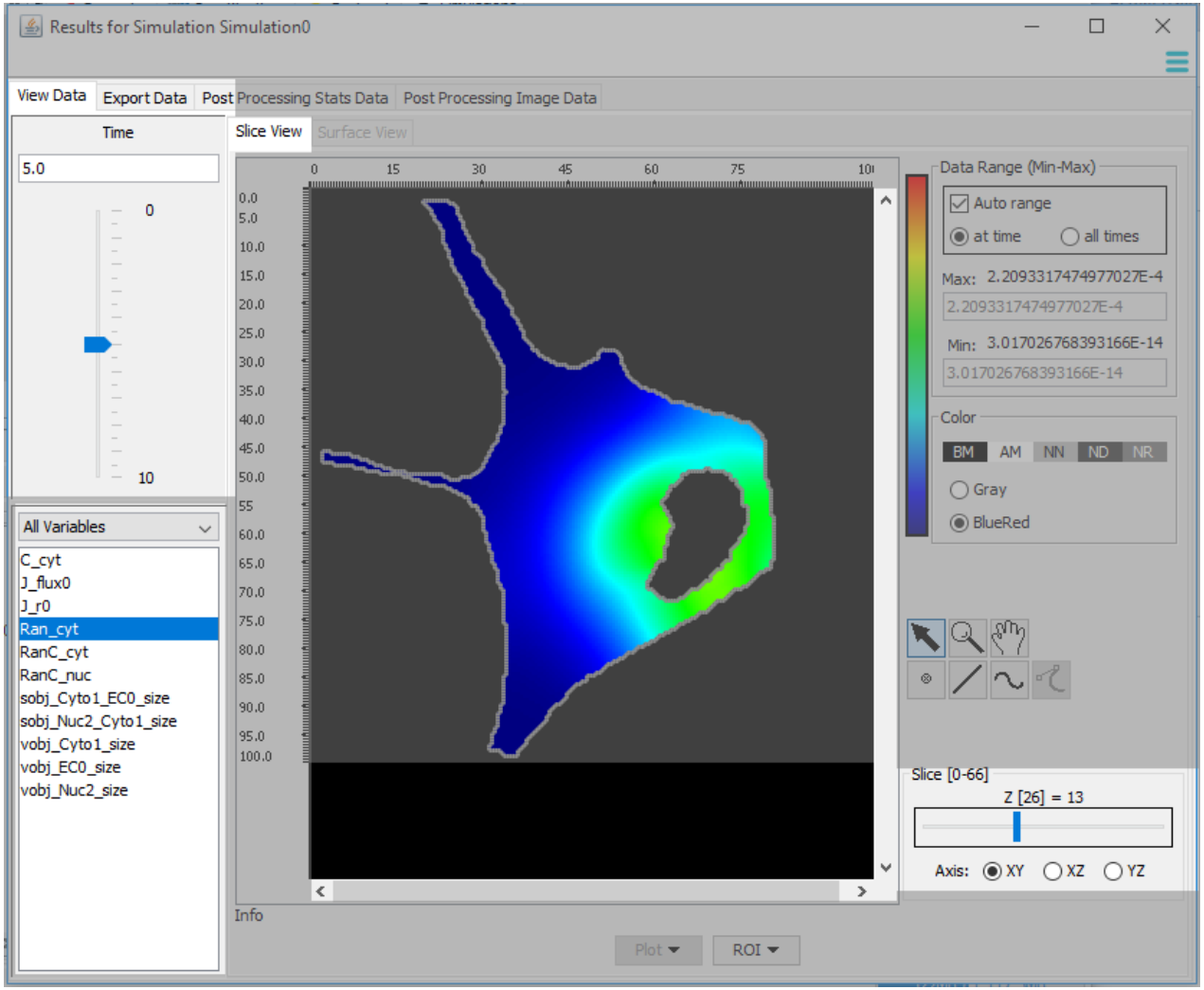
To view the status of the simulation, look under the “Running Status” column.

To view the results upon completion of the simulation, click on the Results icon.

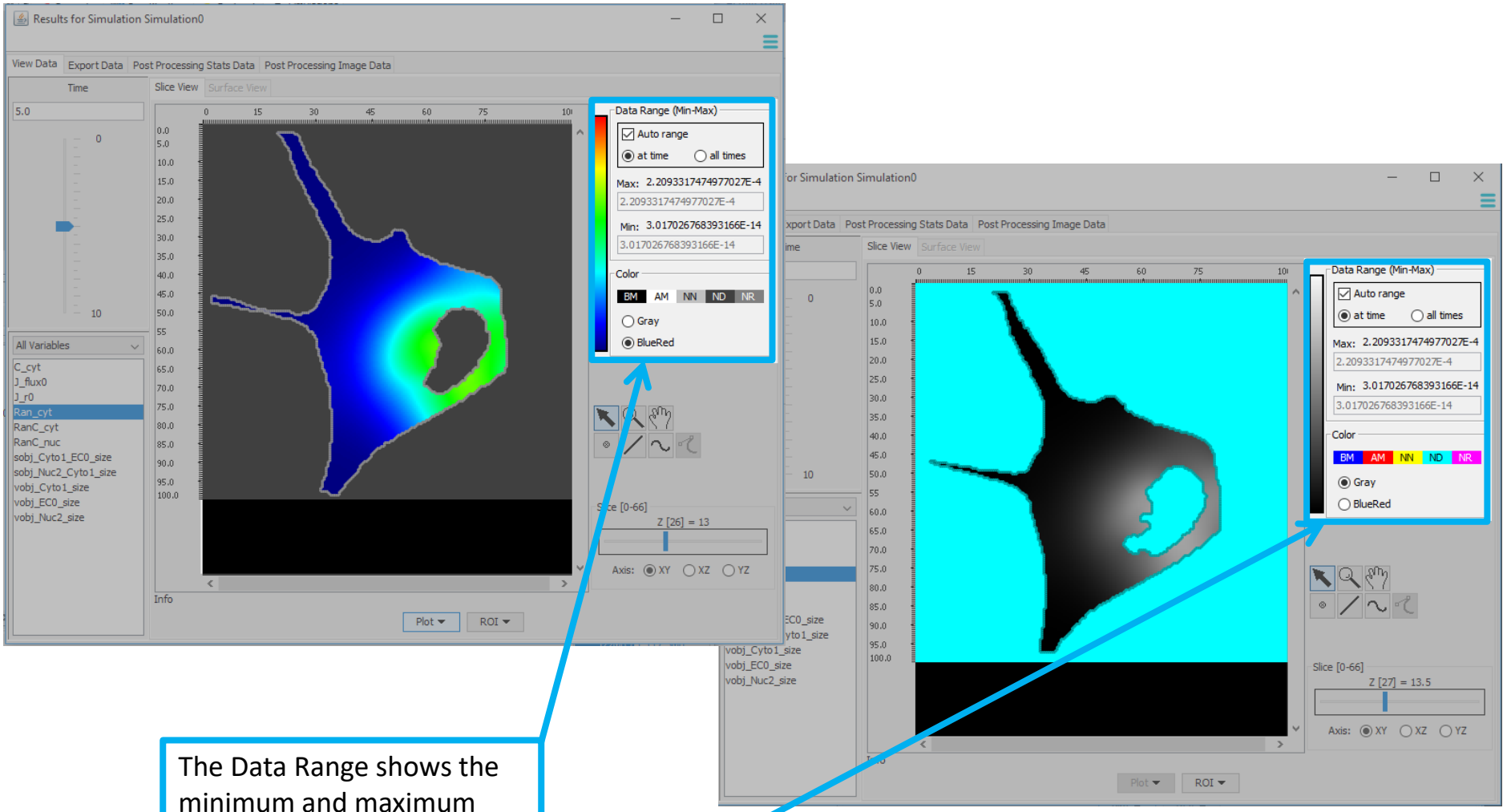
In order to view your results, be sure to adjust the following three parameters:

1. Time Point

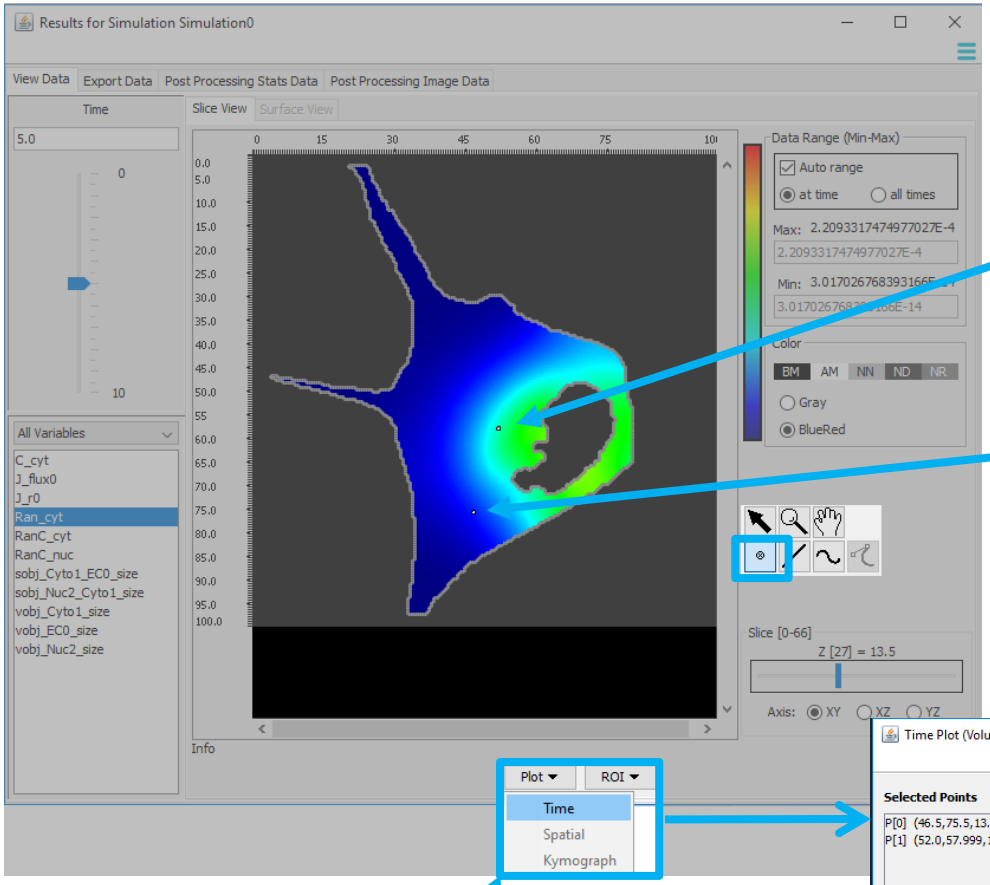
2. Variable



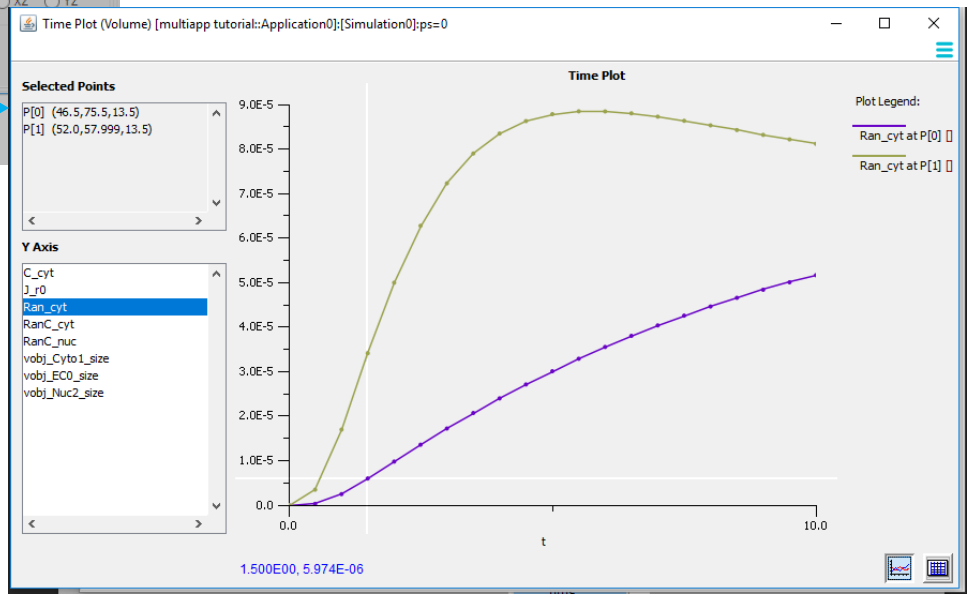
3. Z-Slice



The Data Range shows the minimum and maximum concentrations displayed in the blue-red or greyscale/ black-white, color map.

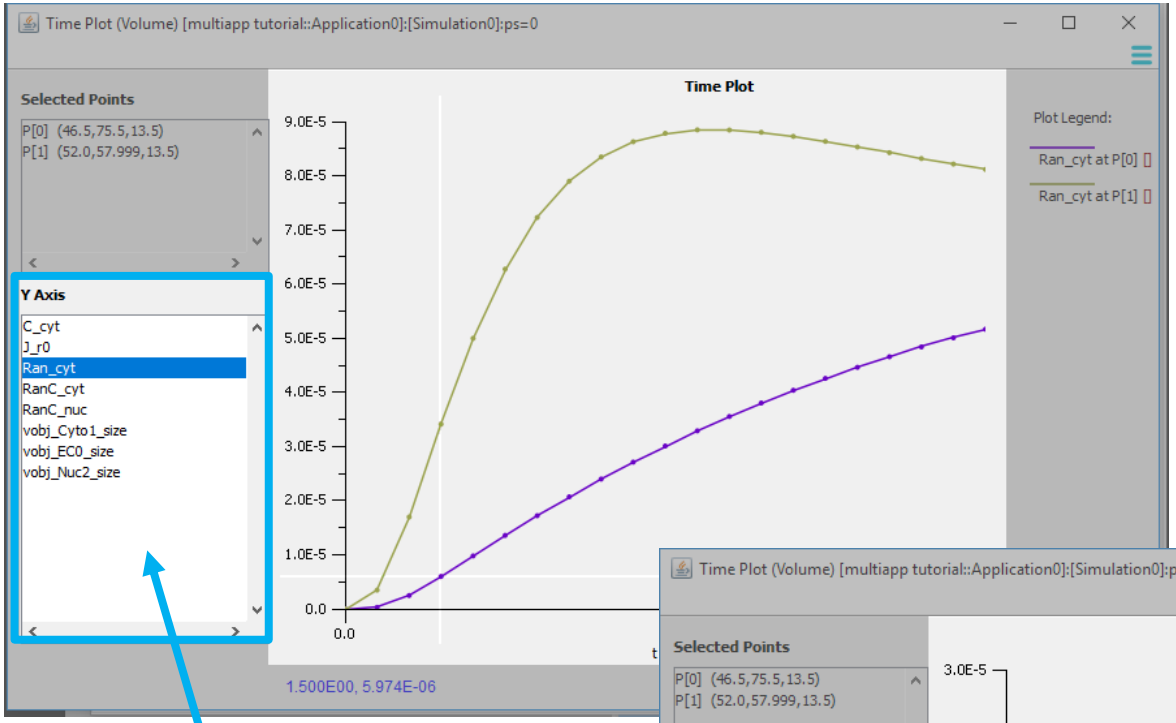


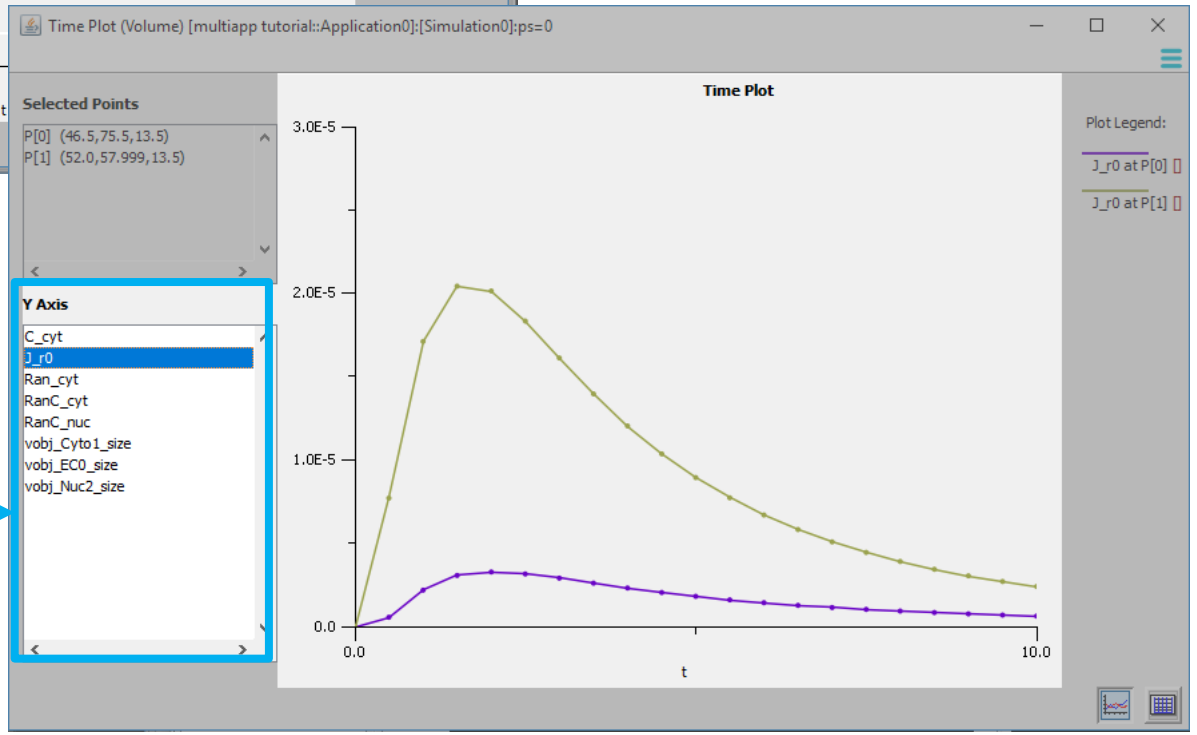
To create a time plot, select the time point tool and click within the geometry to create the desired point. You can define multiple time points within the geometry.



To view the time plot, click “Plot” > “Time”.

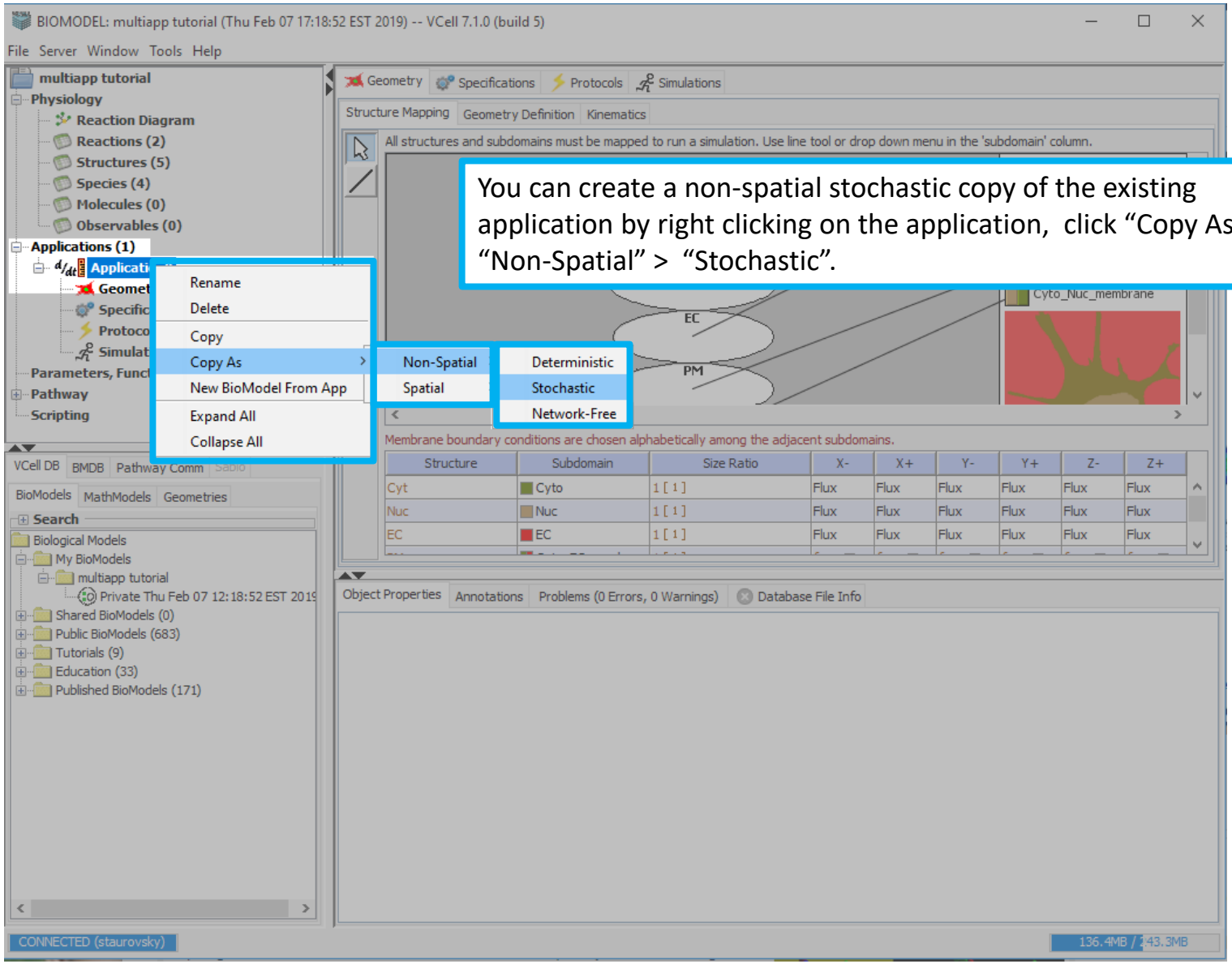
Contents



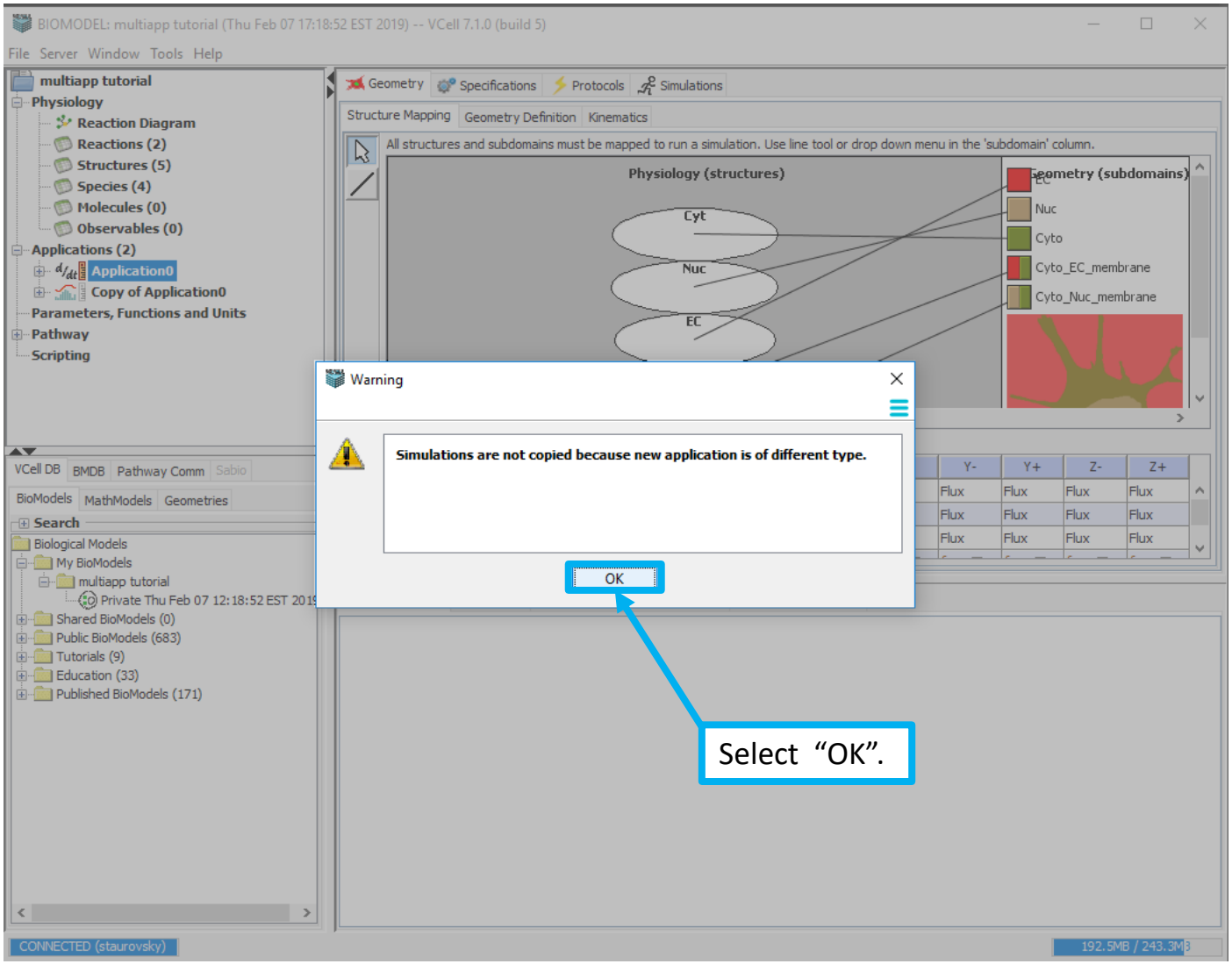


To change what species concentrations are being viewed, click on different species under “Y Axis”.

Creating a New Application from an Existing Application



You can create a non-spatial stochastic copy of the existing application by right clicking on the application, click “Copy As” > “Non-Spatial” > “Stochastic”.


BIOMODEL: multiapp tutorial (Thu Feb 07 17:18:52 EST 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
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Species (4)
Molecules (0)
Observables (0)
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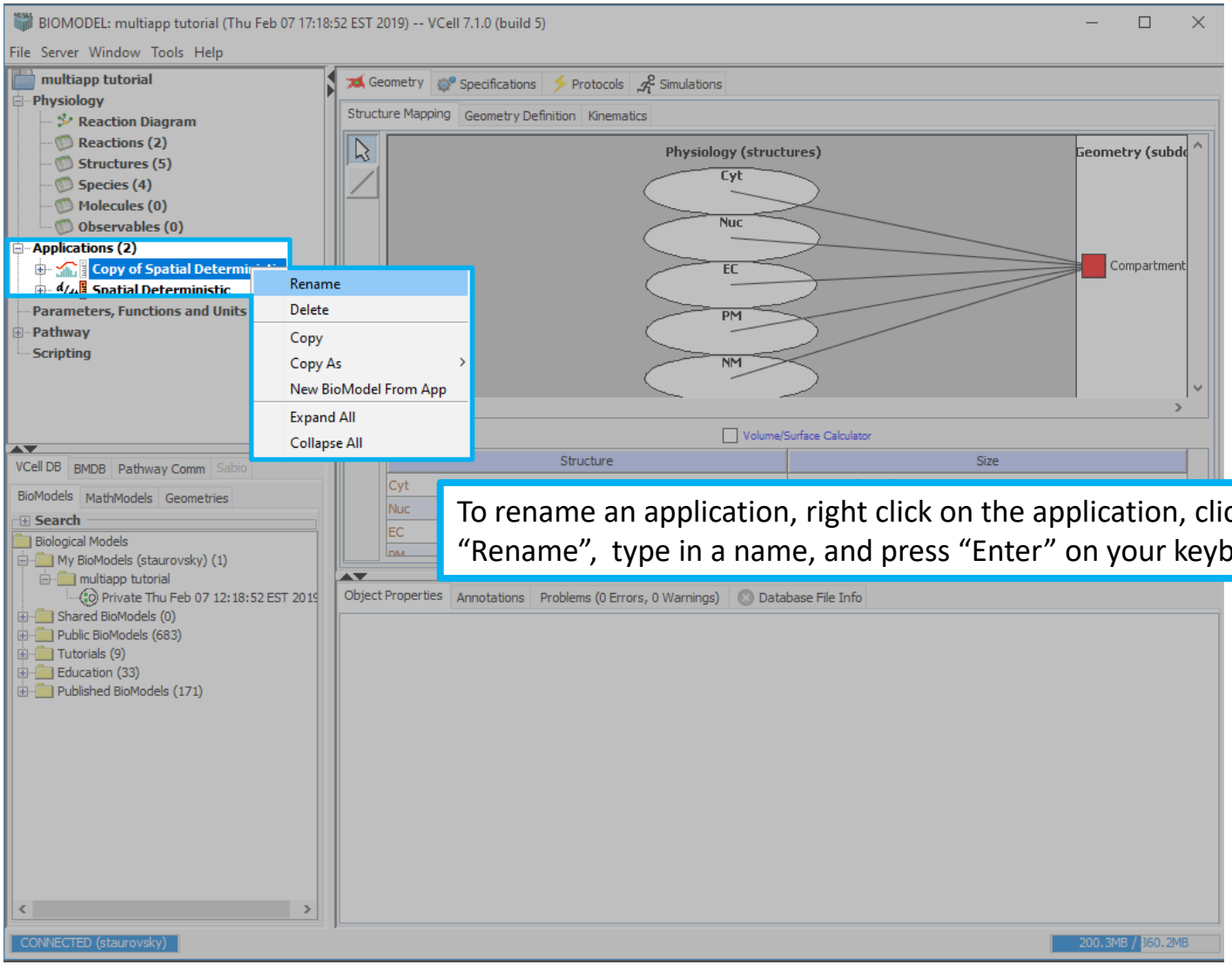
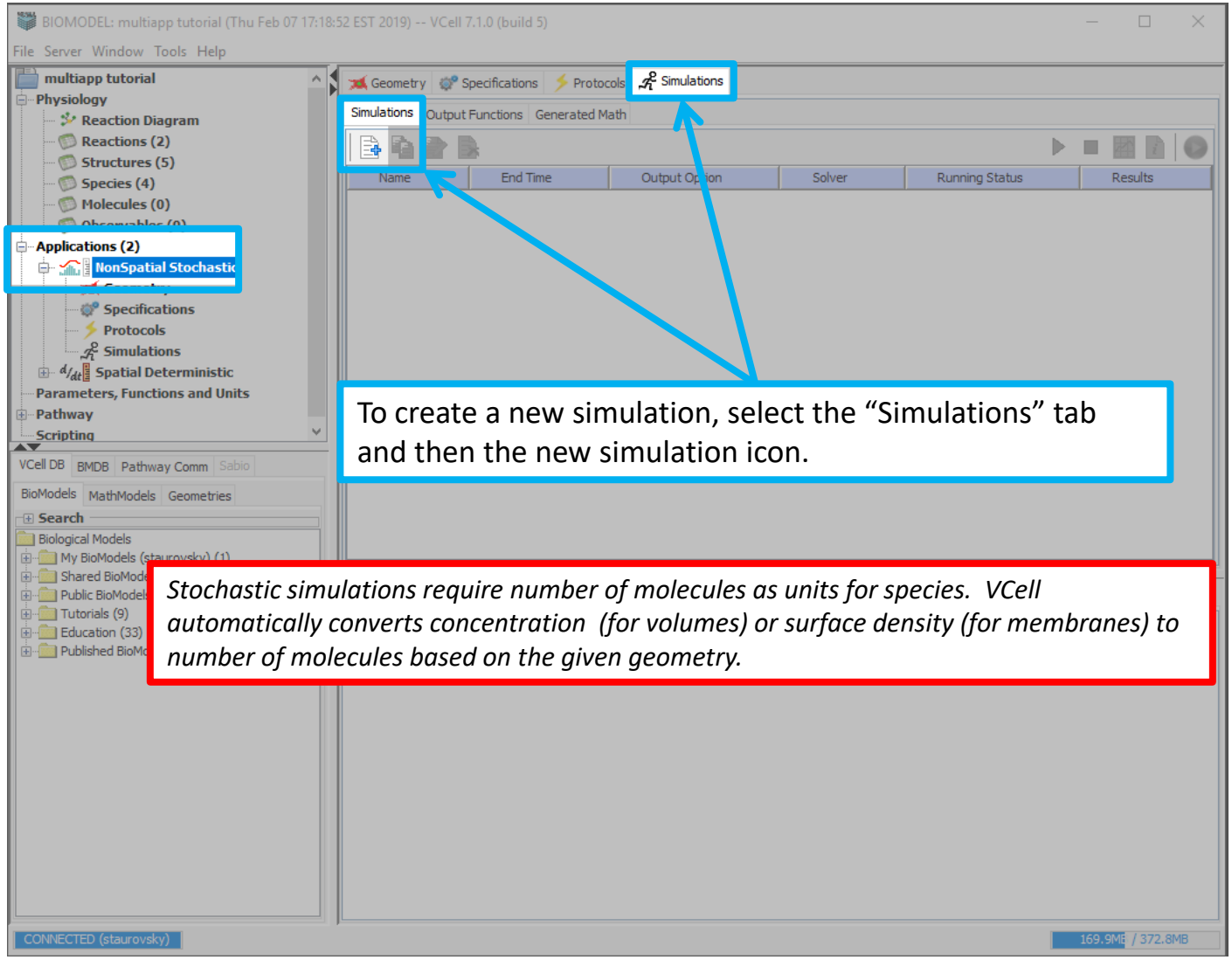
Application0
Copy of Application0
Parameters, Functions and Units
Pathway
Scripting
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Kinematics
All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.
Physiology (structures)
Cyt
Nuc
EC
Geometry (subdomains)
EC
Nuc
Cyto
Cyto_EC_membrane
Cyto_Nuc_membrane
Warning
Simulations are not copied because new application is of different type.
OK
Select "OK".
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
multiapp tutorial
Private Thu Feb 07 12:18:52 EST 2019
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
Y-
Y+
Z-
Z+
Flux
CONNECTED (staurovsky)
192.5MB / 243.3MB



To rename an application, right click on the application, click “Rename”, type in a name, and press “Enter” on your keyboard.


BIOMODEL: multiapp tutorial (Thu Feb 07 17:18:52 EST 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
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Reactions (2)
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NonSpatial Stochastic
Specifications
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Spatial Deterministic
Parameters, Functions and Units
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VCell DB
BMDB
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Sabio
BioModels
MathModels
Geometries
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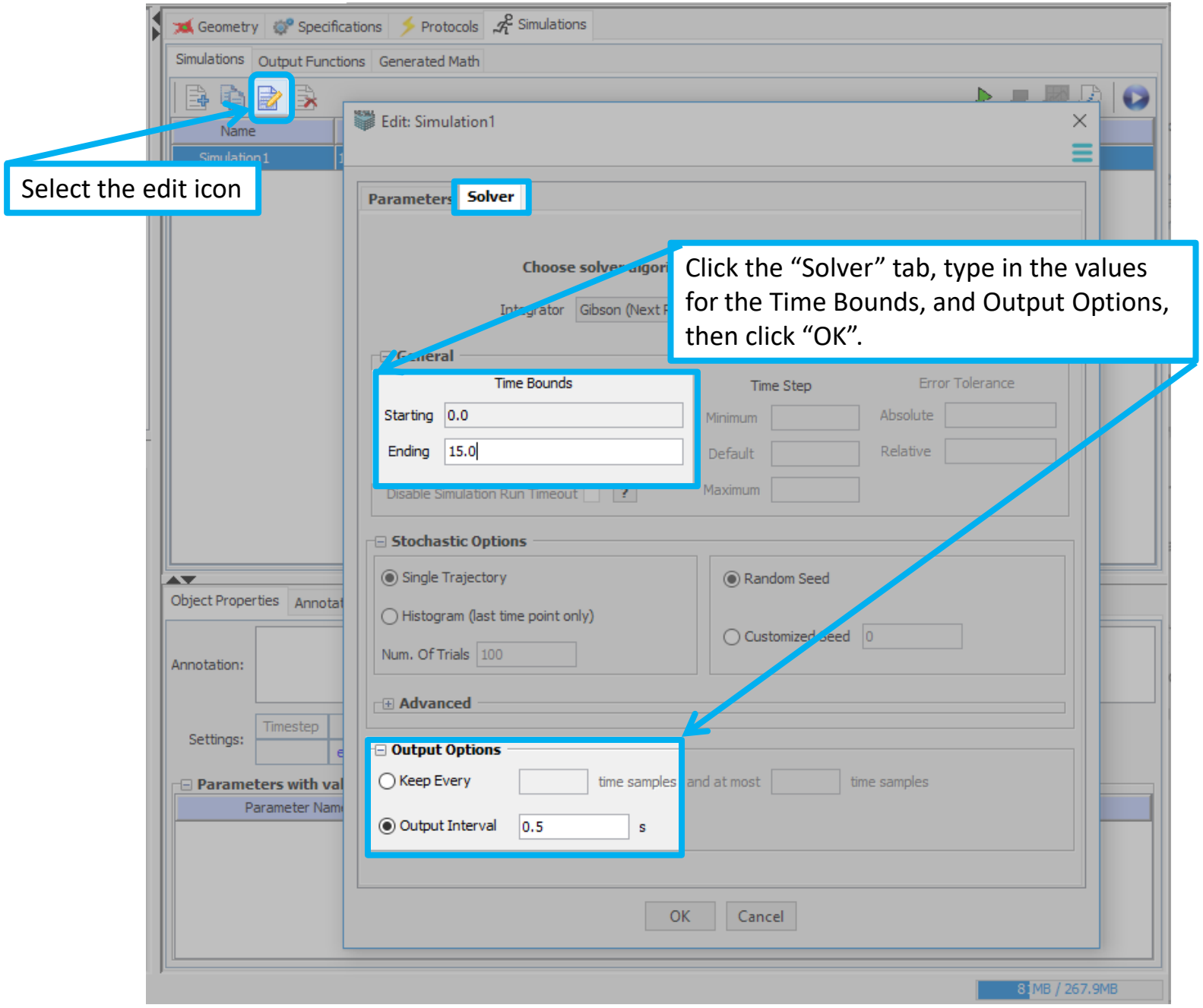
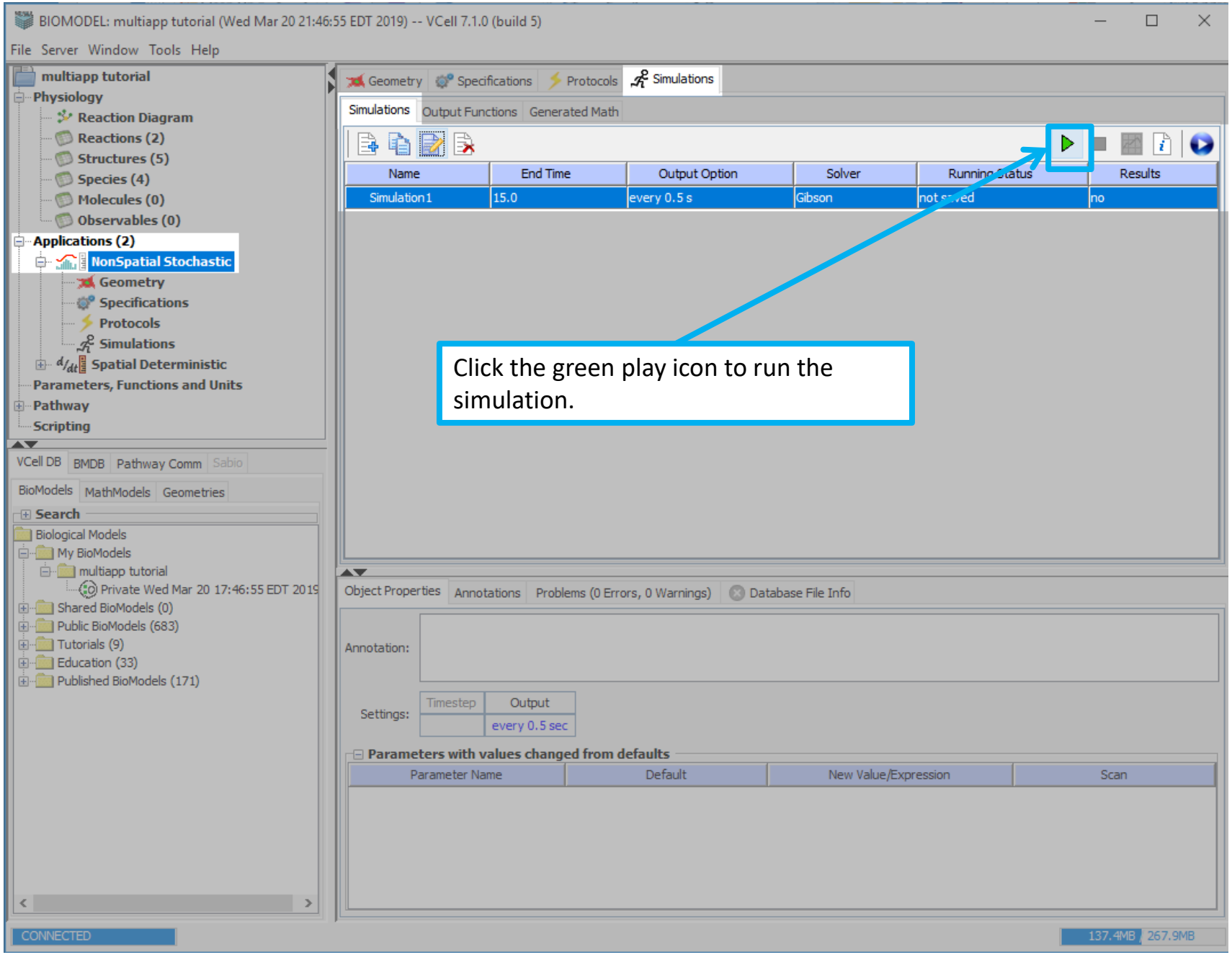
Tutorials (9)
Education (33)
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To create a new simulation, select the “Simulations” tab and then the new simulation icon.
Stochastic simulations require number of molecules as units for species. VCell automatically converts concentration (for volumes) or surface density (for membranes) to number of molecules based on the given geometry.
CONNECTED (staurovsky)
169.9MB / 372.8MB


Select the edit icon
Click the “Solver” tab, type in the values for the Time Bounds, and Output Options, then click “OK”.
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
Simulation1
Edit: Simulation1
Parameters
Solver
Integrator
Gibson (Next
General
Time Bounds
Starting
0.0
Ending
15.0
Time Step
Minimum
Default
Maximum
Error Tolerance
Absolute
Relative
Disable Simulation Run Timeout
Stochastic Options
Single Trajectory
Histogram (last time point only)
Num. Of Trials
100
Random Seed
Customized Seed
0
Advanced
Output Options
Keep Every
time samples
and at most
time samples
Output Interval
0.5
s
OK
Cancel
Object Properties
Annotation:
Settings:
Timestep
Parameters with val
Parameter Nam
MB / 267.9MB


BIOMODEL: multiapp tutorial (Wed Mar 20 21:46:55 EDT 2019) -- VCell 7.1.0 (build 5)
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Physiology
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Species (4)
Molecules (0)
Observables (0)
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Private Wed Mar 20 17:46:55 EDT 2019
Shared BioModels (0)
Public BioModels (683)
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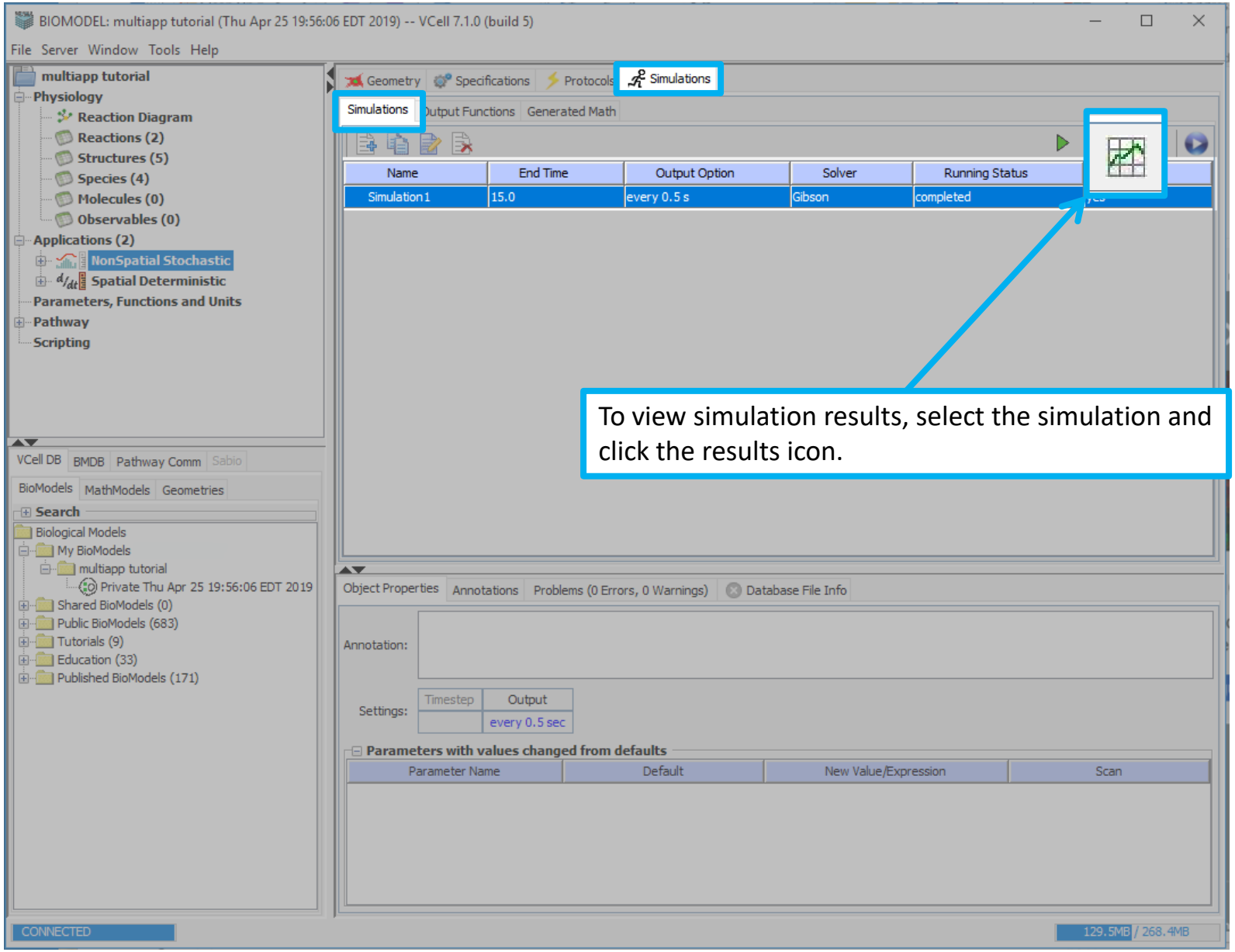
Published BioModels (171)
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
15.0
every 0.5 s
Gibson
not solved
no
Click the green play icon to run the simulation.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
Timestep
Output
every 0.5 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED
137.4MB
267.9MB


BIOMODEL: multiapp tutorial (Thu Apr 25 19:56:06 EDT 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
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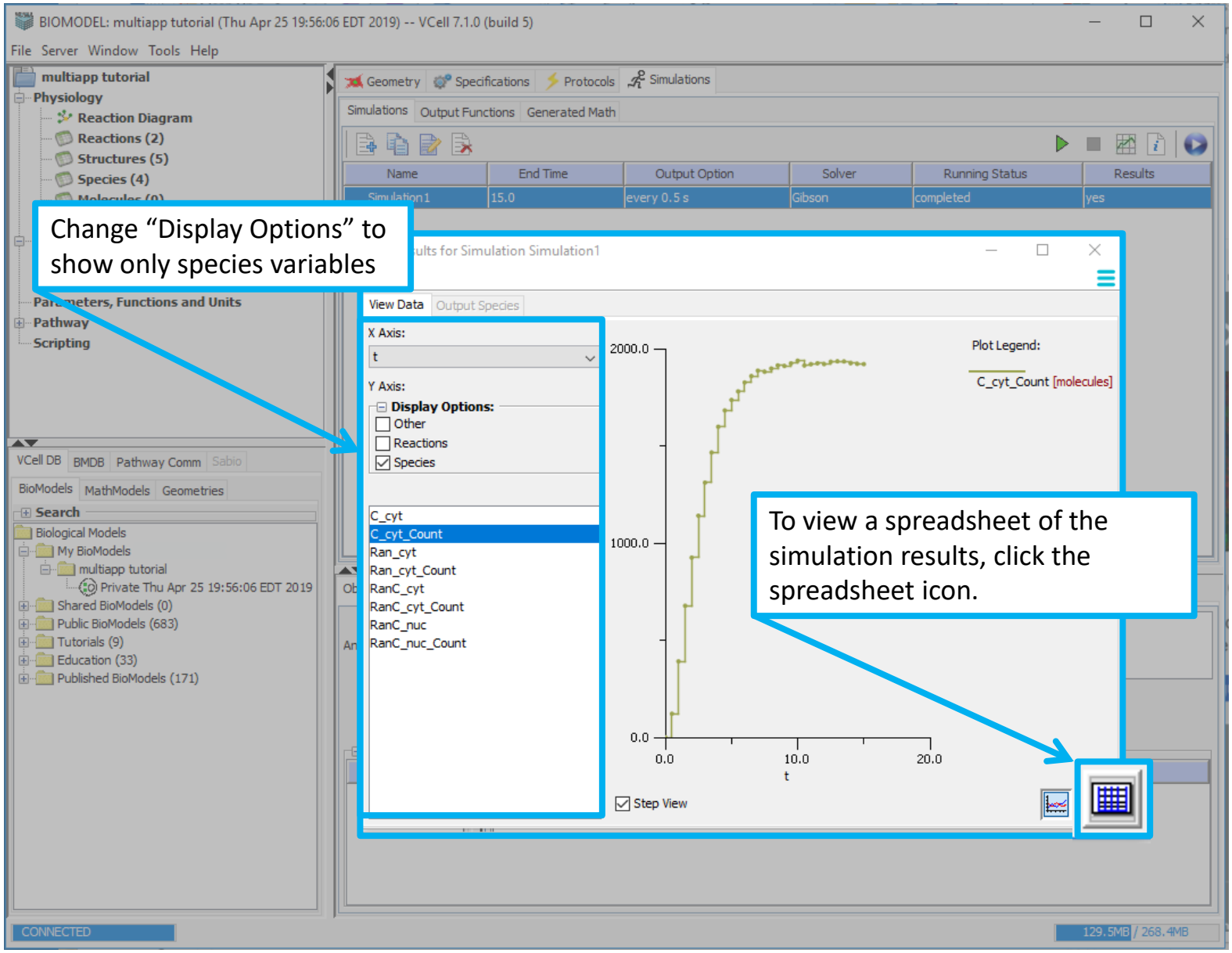
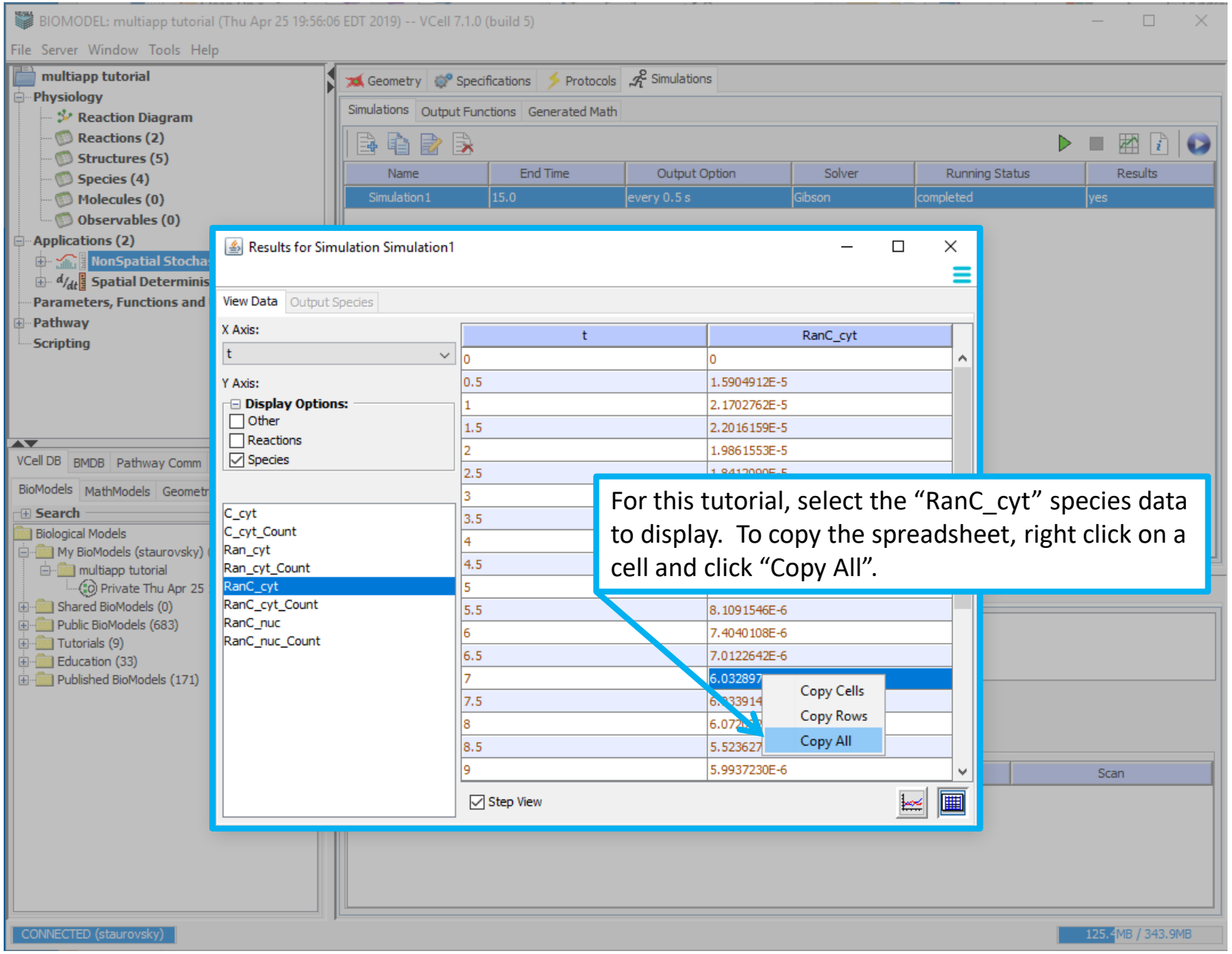
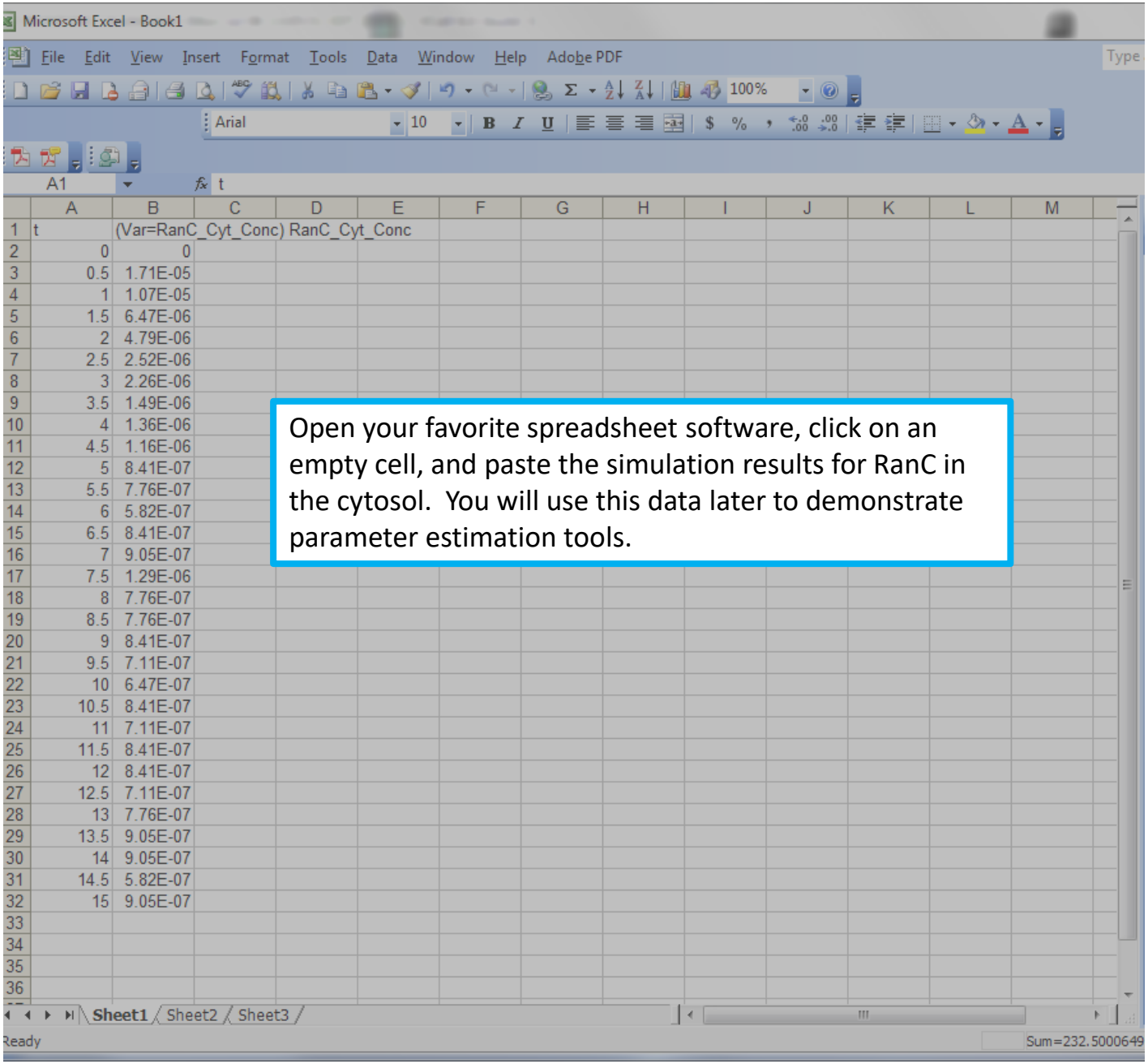
NonSpatial Stochastic
Spatial Deterministic
Parameters, Functions and Units
Pathway
Scripting
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Simulation 1
15.0
every 0.5 s
Gibson
completed
To view simulation results, select the simulation and click the results icon.
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
multiapp tutorial
Private Thu Apr 25 19:56:06 EDT 2019
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
Timestep
Output
every 0.5 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED
129.5MB / 268.4MB

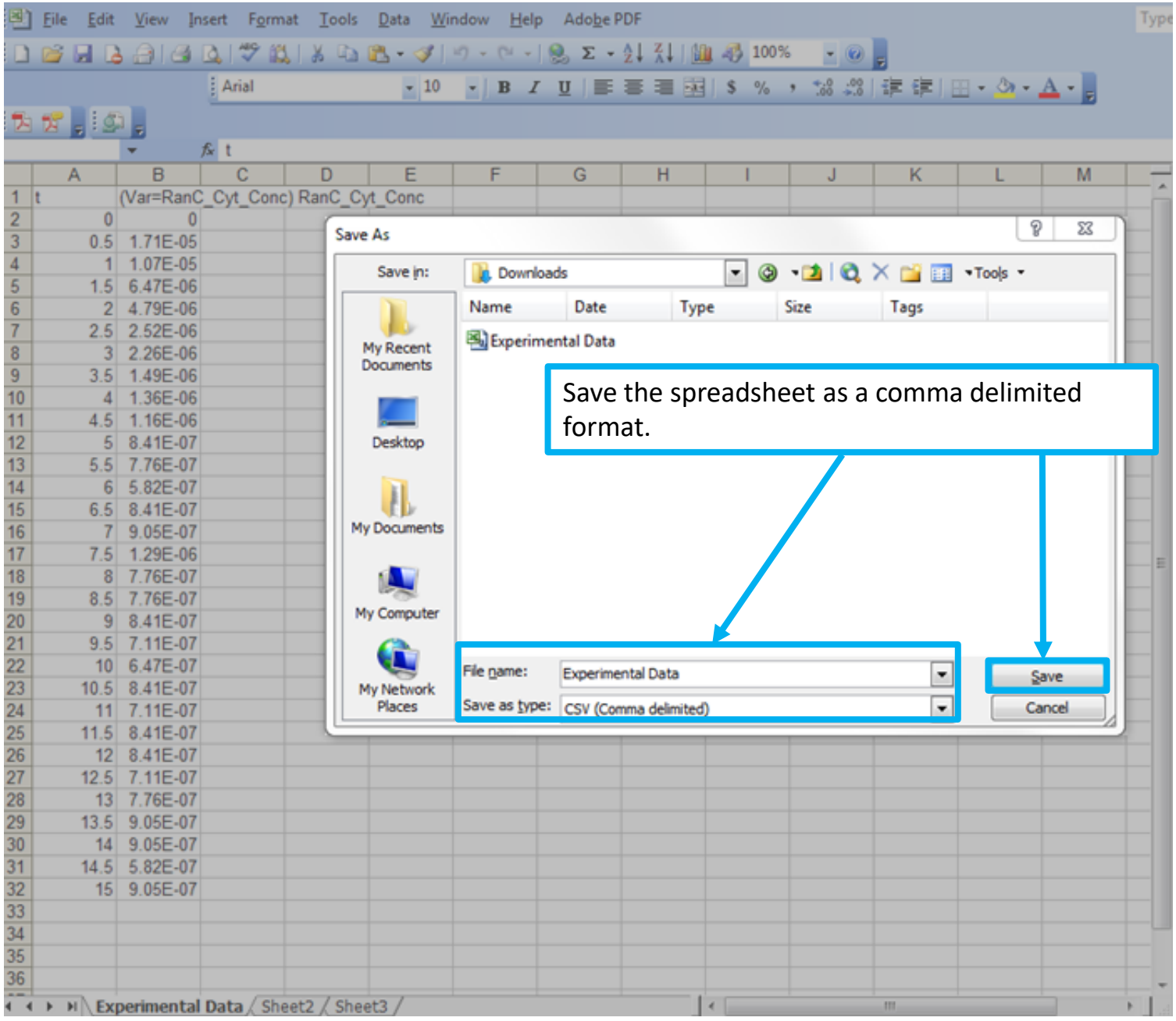

BIOMODEL: multiapp tutorial (Thu Apr 25 19:56:06 EDT 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Parameters, Functions and Units
Pathway
Scripting
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
15.0
every 0.5 s
Gibson
completed
yes
Change “Display Options” to show only species variables
ults for Simulation Simulation1
View Data
Output Species
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
C_cyt
C_cyt_Count
Ran_cyt
Ran_cyt_Count
RanC_cyt
RanC_cyt_Count
RanC_nuc
RanC_nuc_Count
2000.0
1000.0
0.0
0.0
10.0
20.0
t
Plot Legend:
C_cyt_Count [molecules]
Step View
To view a spreadsheet of the simulation results, click the spreadsheet icon.
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
multiapp tutorial
Private Thu Apr 25 19:56:06 EDT 2019
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
CONNECTED
129.5MB / 268.4MB

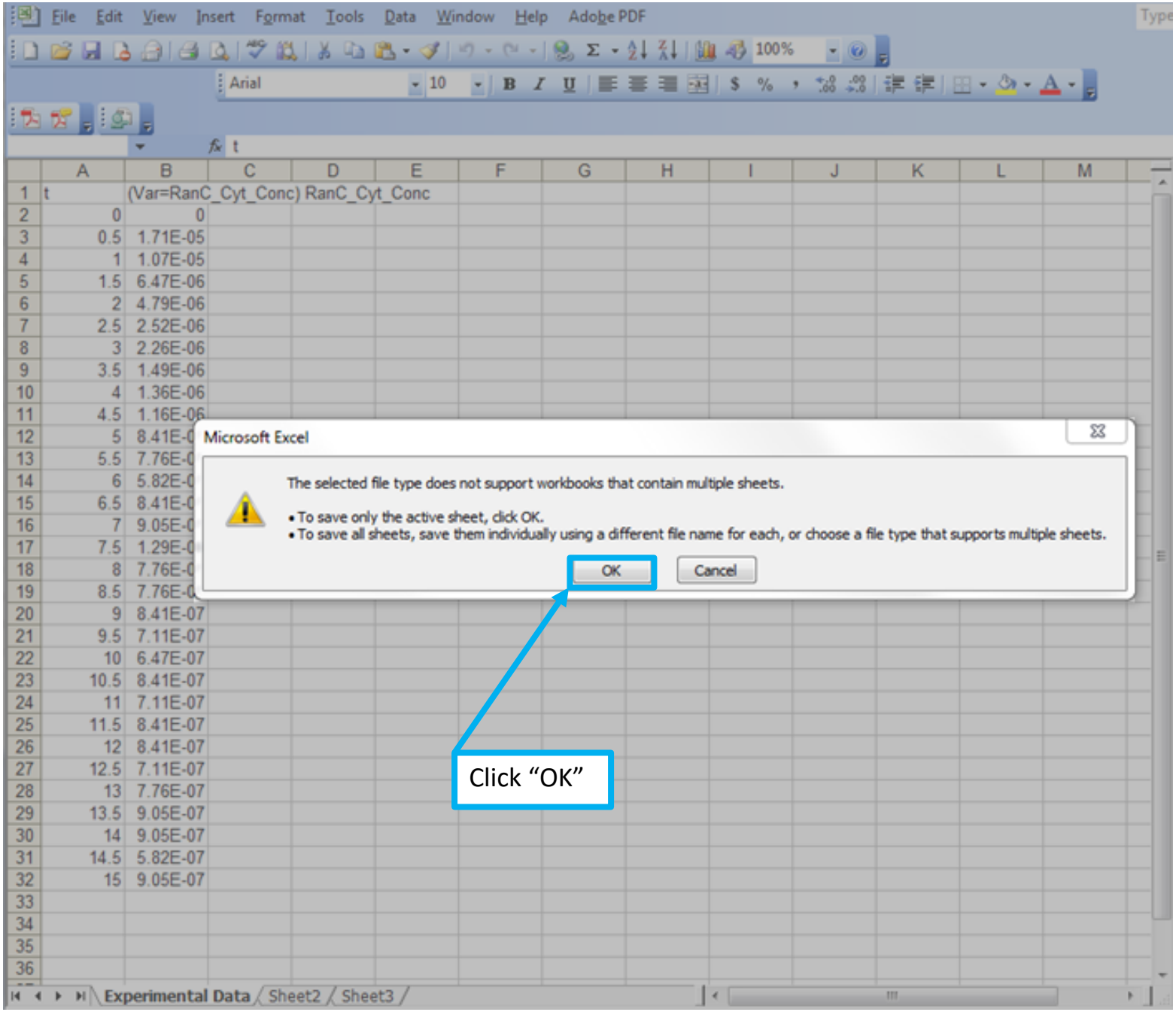

BIOMODEL: multiapp tutorial (Thu Apr 25 19:56:06 EDT 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stocha
Spatial Determinis
Parameters, Functions and
Pathway
Scripting
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
15.0
every 0.5 s
Gibson
completed
yes
Results for Simulation Simulation1
View Data
Output Species
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
C_cyt
C_cyt_Count
Ran_cyt
Ran_cyt_Count
RanC_cyt
RanC_cyt_Count
RanC_nuc
RanC_nuc_Count
t
RanC_cyt
0
0
0.5
1.5904912E-5
1
2.1702762E-5
1.5
2.2016159E-5
2
1.9861553E-5
5.5
8.1091546E-6
6
7.4040108E-6
6.5
7.0122642E-6
7
6.032897
7.5
8
6.072
8.5
5.523627
9
5.9937230E-6
Copy Cells
Copy Rows
Copy All
Step View
For this tutorial, select the “RanC_cyt” species data to display. To copy the spreadsheet, right click on a cell and click “Copy All”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Search
Biological Models
My BioModels (staurovsky)
multiapp tutorial
Private Thu Apr 25
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
Scan
CONNECTED (staurovsky)
125.4MB / 343.9MB



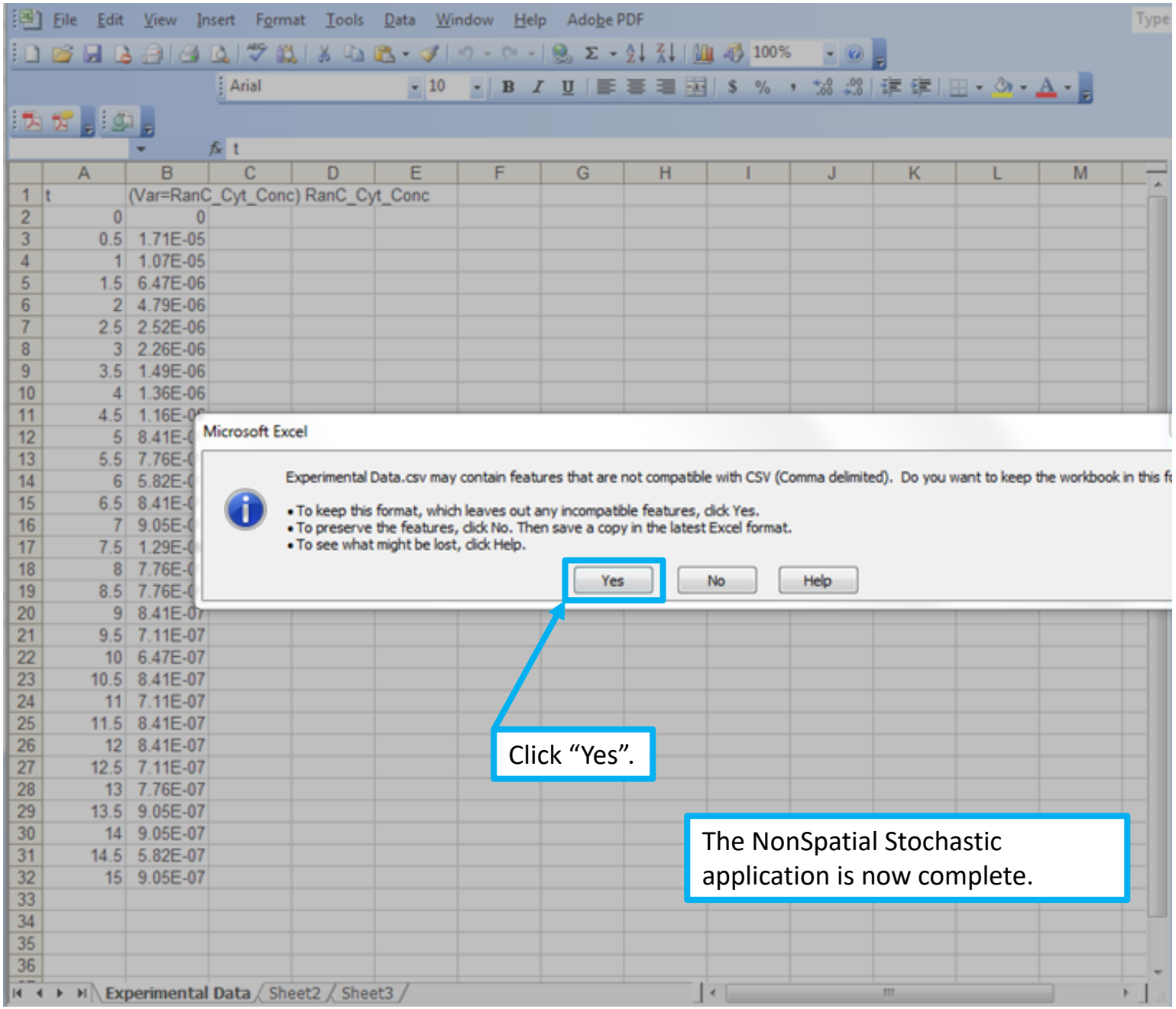
	A	B
1	t	(Var=RanC_Cyt_Conc) RanC_Cyt_Conc
2	0	0
3	0.5	1.71E-05
4	1	1.07E-05
5	1.5	6.47E-06
6	2	4.79E-06
7	2.5	2.52E-06
8	3	2.26E-06
9	3.5	1.49E-06
10	4	1.36E-06
11	4.5	1.16E-06
12	5	8.41E-07
13	5.5	7.76E-07
14	6	5.82E-07
15	6.5	8.41E-07
16	7	9.05E-07
17	7.5	1.29E-06
18	8	7.76E-07
19	8.5	7.76E-07
20	9	8.41E-07
21	9.5	7.11E-07
22	10	6.47E-07
23	10.5	8.41E-07
24	11	7.11E-07
25	11.5	8.41E-07
26	12	8.41E-07
27	12.5	7.11E-07
28	13	7.76E-07
29	13.5	9.05E-07
30	14	9.05E-07
31	14.5	5.82E-07
32	15	9.05E-07

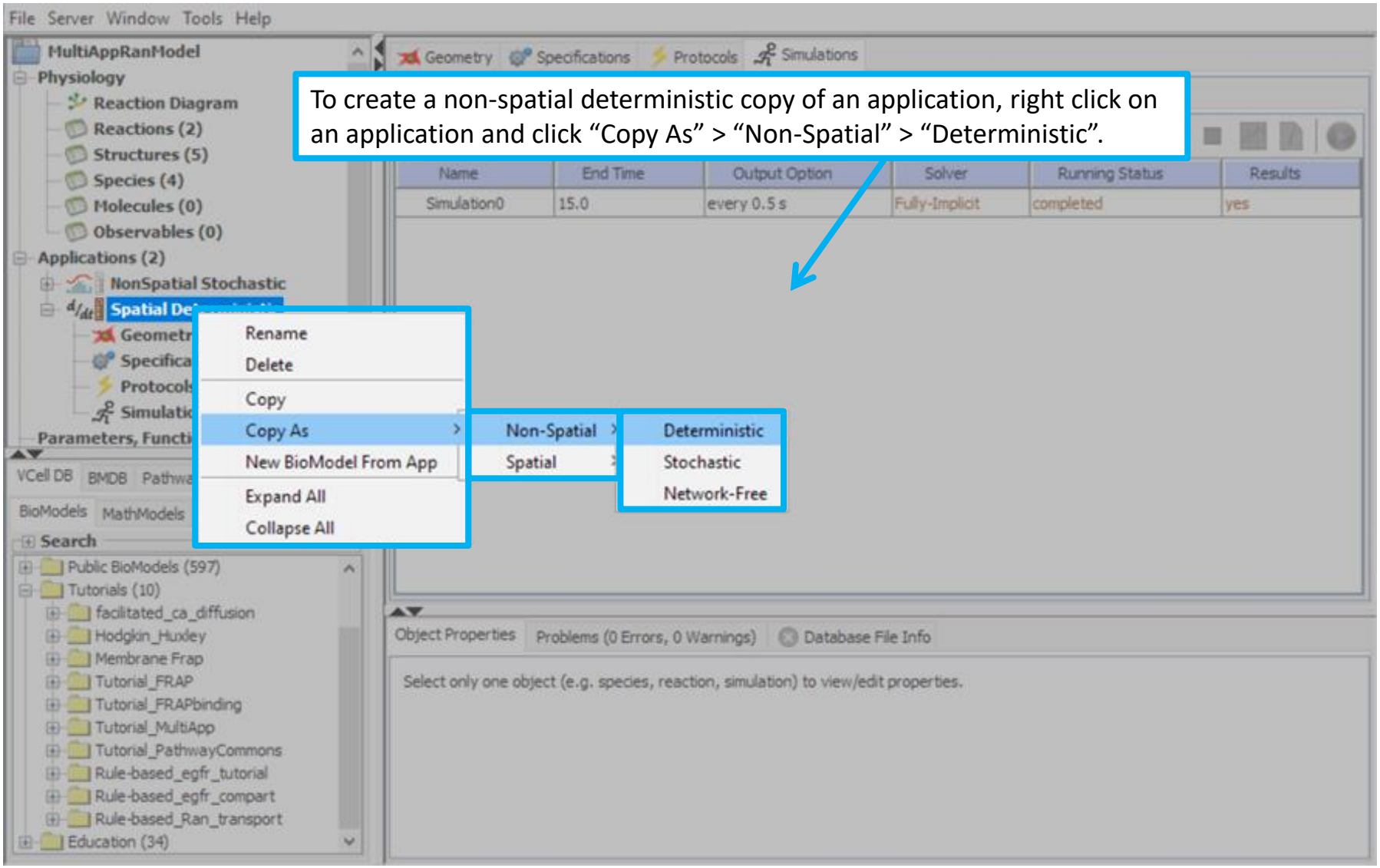
Open your favorite spreadsheet software, click on an empty cell, and paste the simulation results for RanC in the cytosol. You will use this data later to demonstrate parameter estimation tools.

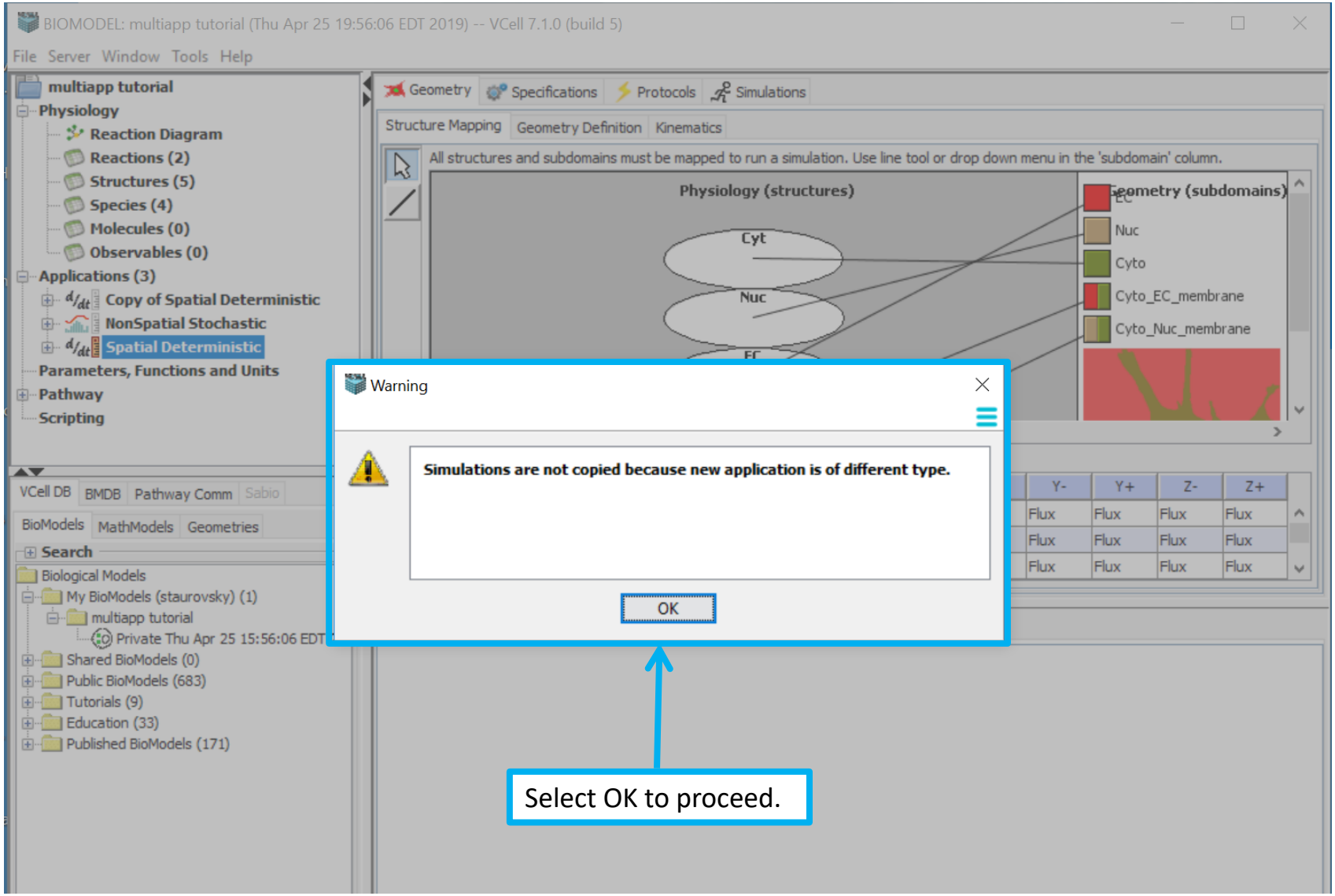

Save As
Save in:
Downloads
Tools
Name
Date
Type
Size
Tags
Experimental Data
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
Save the spreadsheet as a comma delimited format.
File name:
Experimental Data
Save as type:
CSV (Comma delimited)
Save
Cancel
Experimental Data
Sheet2
Sheet3

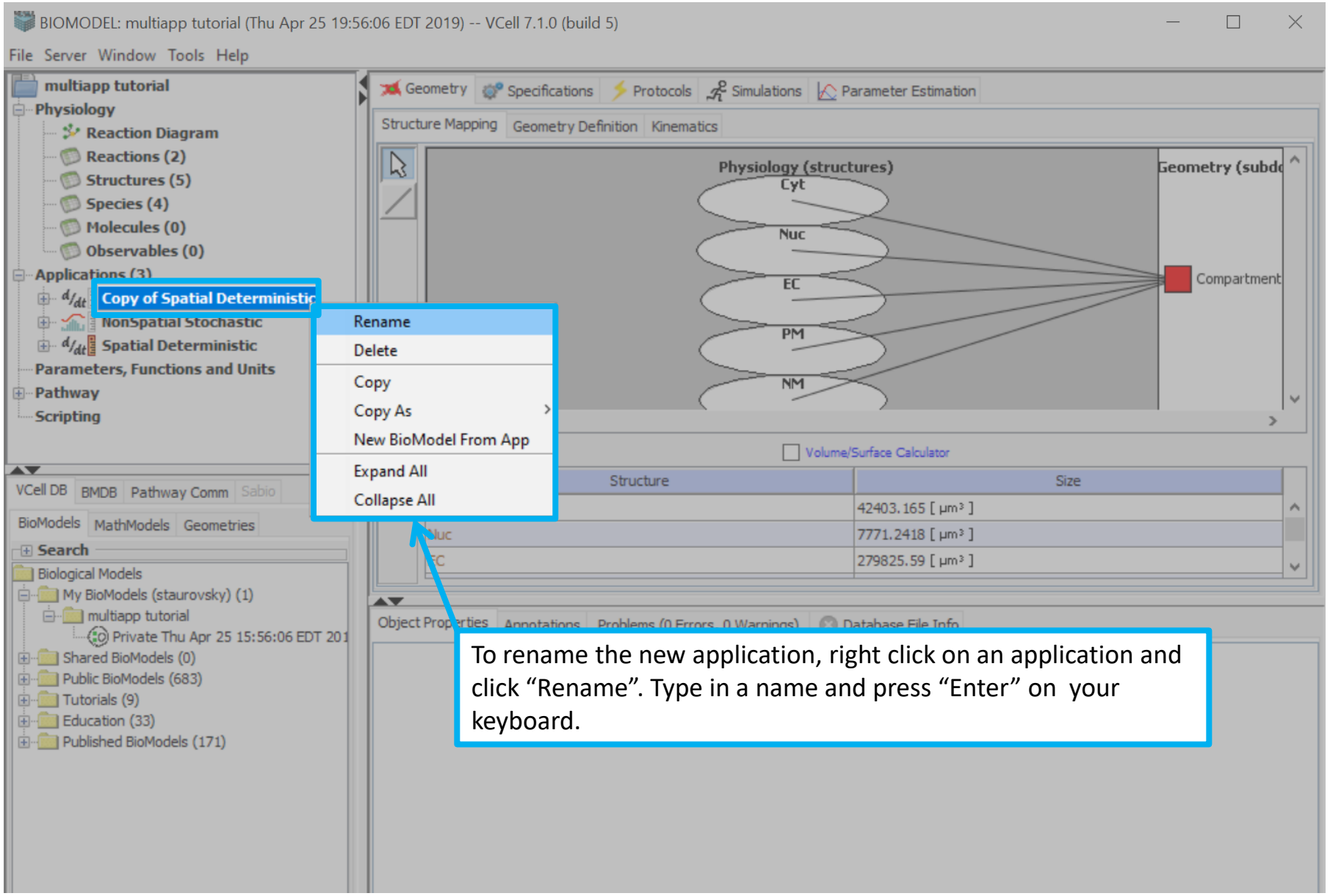


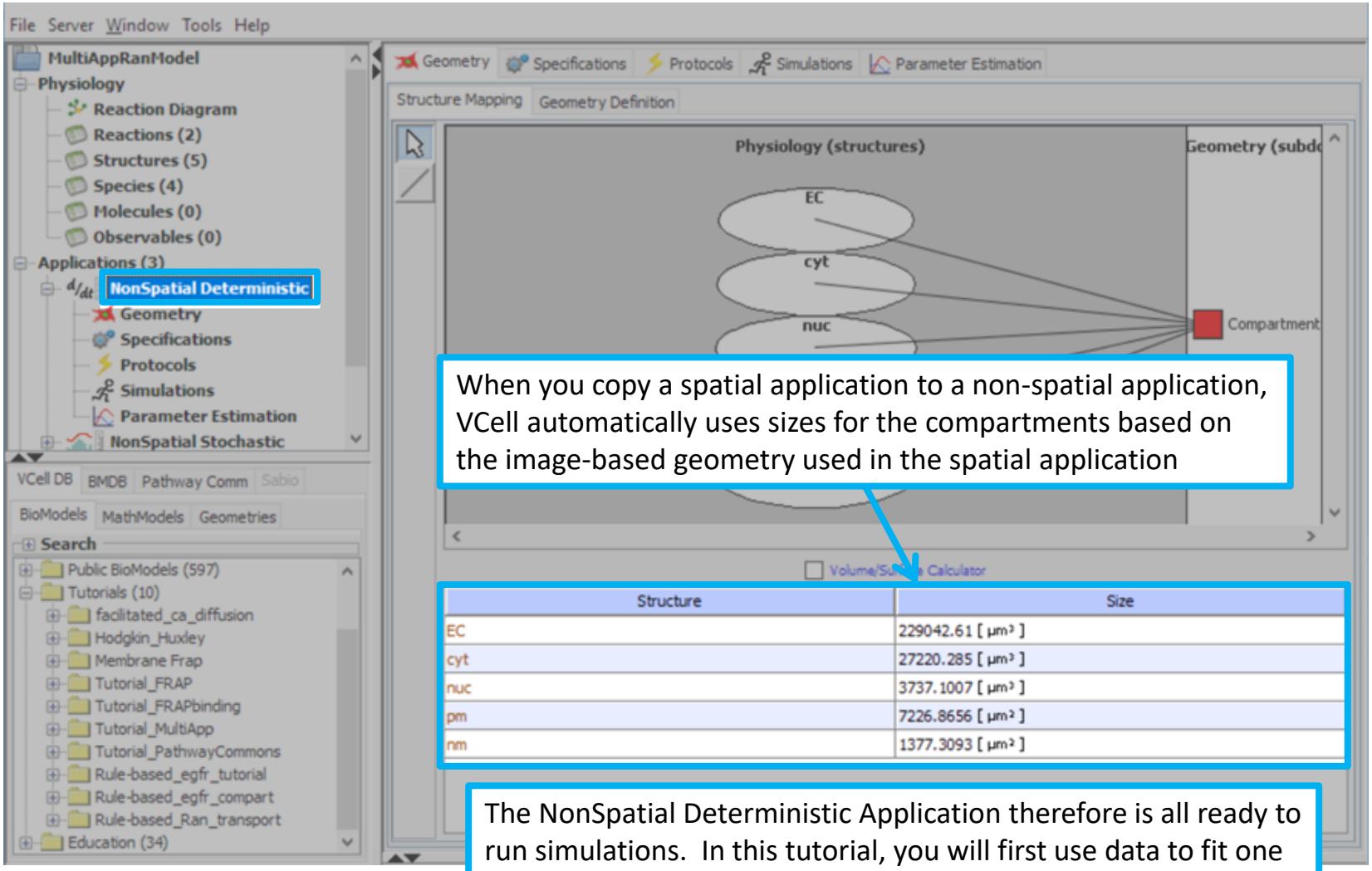
	A	B
1	t	(Var=RanC_Cyt_Conc) RanC_Cyt_Conc
2	0	0
3	0.5	1.71E-05
4	1	1.07E-05
5	1.5	6.47E-06
6	2	4.79E-06
7	2.5	2.52E-06
8	3	2.26E-06
9	3.5	1.49E-06
10	4	1.36E-06
11	4.5	1.16E-06
12	5	8.41E-0
13	5.5	7.76E-0
14	6	5.82E-0
15	6.5	8.41E-0
16	7	9.05E-0
17	7.5	1.29E-0
18	8	7.76E-0
19	8.5	7.76E-0
20	9	8.41E-07
21	9.5	7.11E-07
22	10	6.47E-07
23	10.5	8.41E-07
24	11	7.11E-07
25	11.5	8.41E-07
26	12	8.41E-07
27	12.5	7.11E-07
28	13	7.76E-07
29	13.5	9.05E-07
30	14	9.05E-07
31	14.5	5.82E-07
32	15	9.05E-07
33		
34		
35		
36		

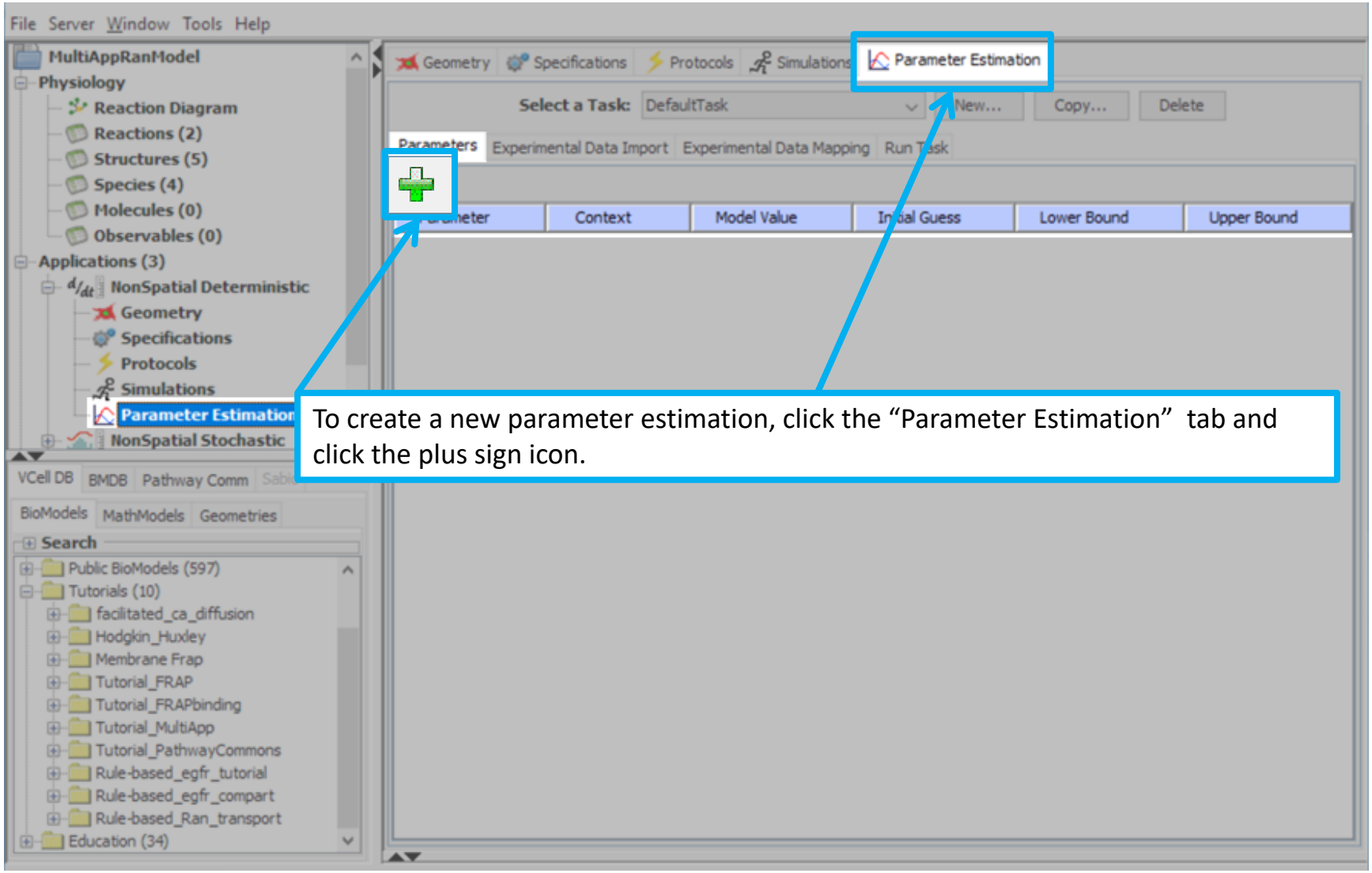

Microsoft Excel
Experimental Data.csv may contain features that are not compatible with CSV (Comma delimited). Do you want to keep the workbook in this f
• To keep this format, which leaves out any incompatible features, click Yes.
• To preserve the features, click No. Then save a copy in the latest Excel format.
• To see what might be lost, click Help.
Yes
No
Help
Click “Yes”.
The NonSpatial Stochastic application is now complete.
Experimental Data
Sheet2
Sheet3

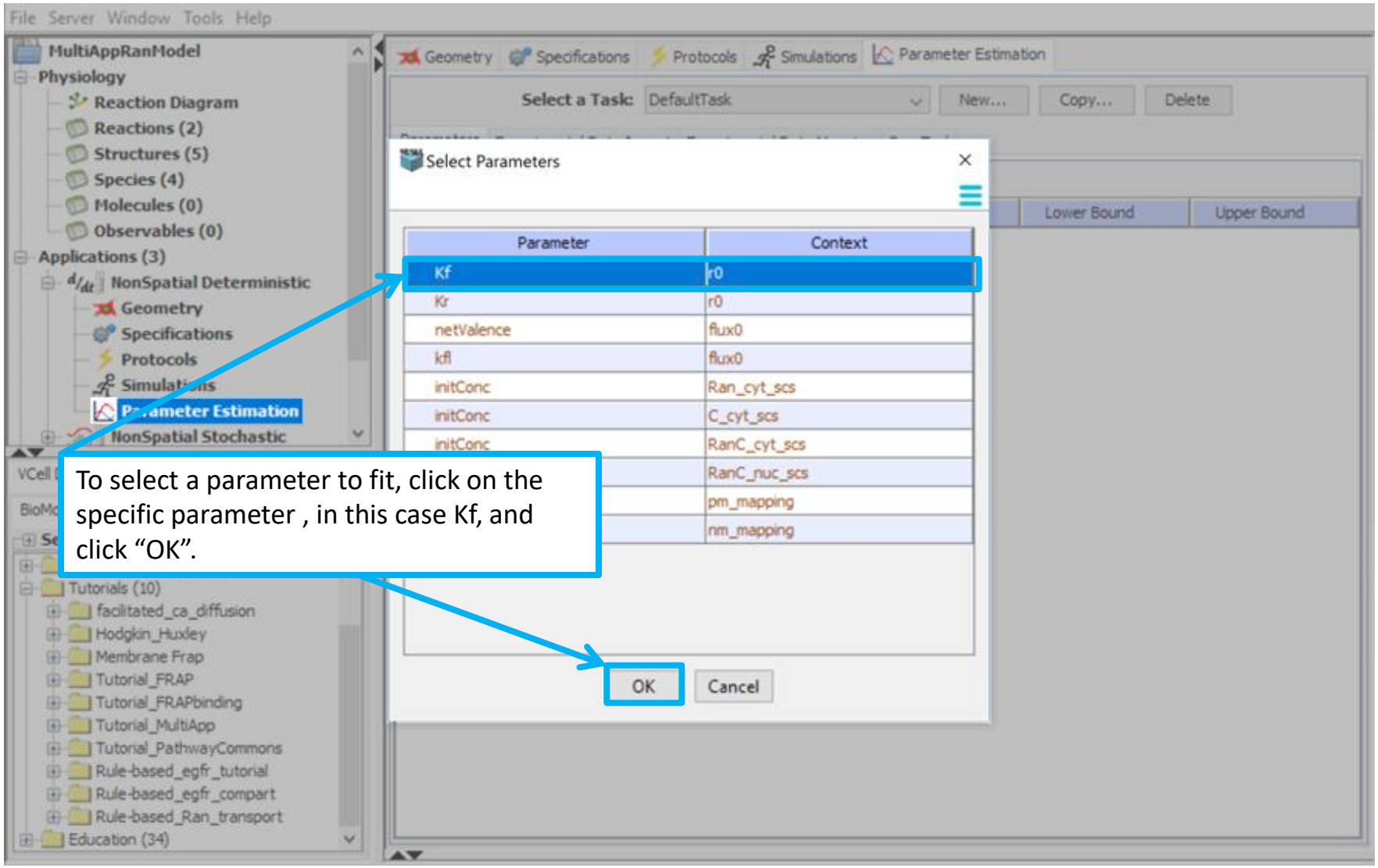

To create a non-spatial deterministic copy of an application, right click on an application and click “Copy As” > “Non-Spatial” > “Deterministic”.
File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Non-Spatial
Spatial
Deterministic
Stochastic
Network-Free
Geometry
Specifications
Protocols
Simulations
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 s
Fully-Implicit
completed
yes
VCell DB
BMDB
BioModels
MathModels
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

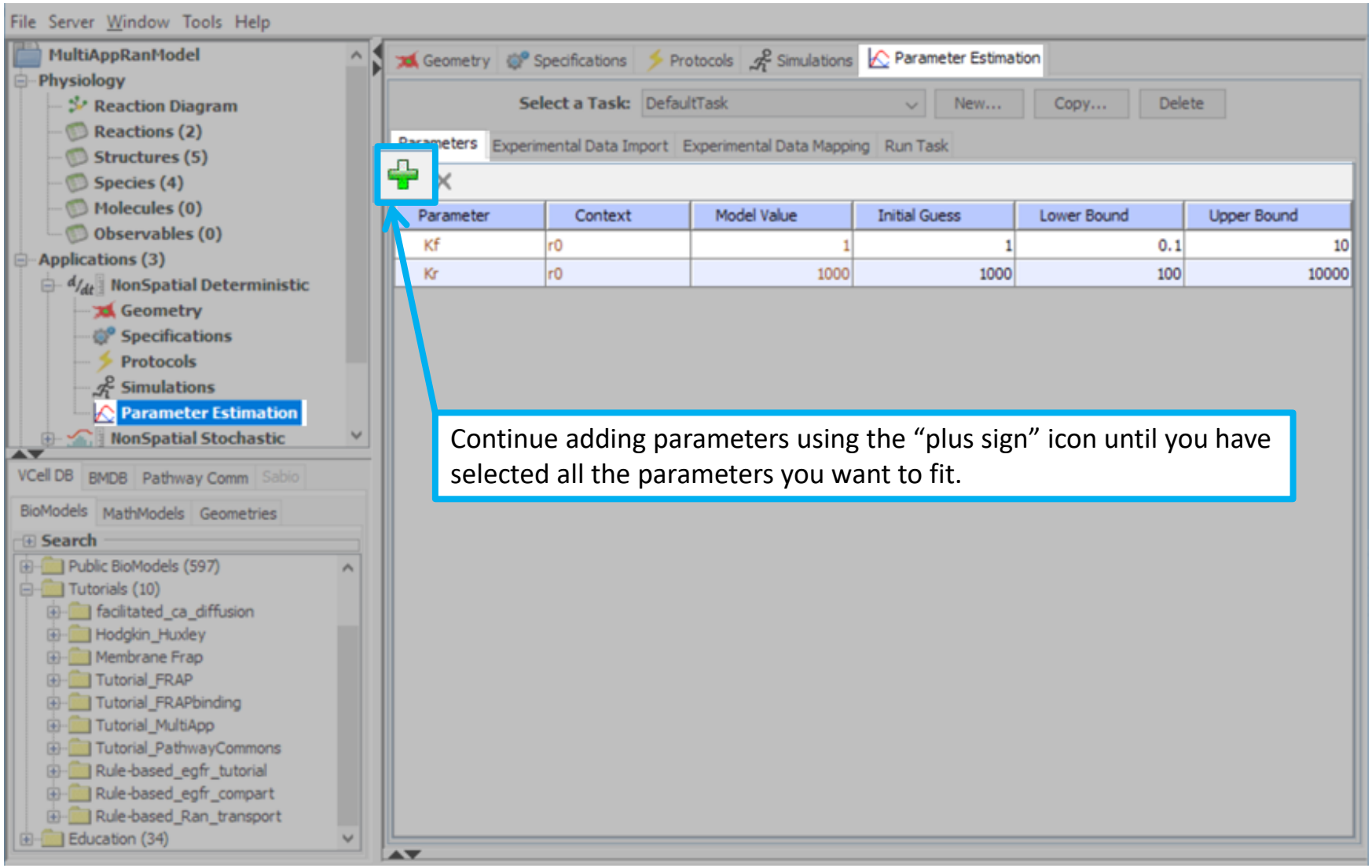

BIOMODEL: multiapp tutorial (Thu Apr 25 19:56:06 EDT 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
Copy of Spatial Deterministic
NonSpatial Stochastic
Spatial Deterministic
Parameters, Functions and Units
Pathway
Scripting
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.
Physiology (structures)
Cyt
Nuc
Geometry (subdomains)
Nuc
Cyto
Cyto_EC_membrane
Cyto_Nuc_membrane
Warning
Simulations are not copied because new application is of different type.
OK
Y-
Y+
Z-
Z+
Flux
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (staurovsky) (1)
multiapp tutorial
Private Thu Apr 25 15:56:06 EDT
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
Select OK to proceed.

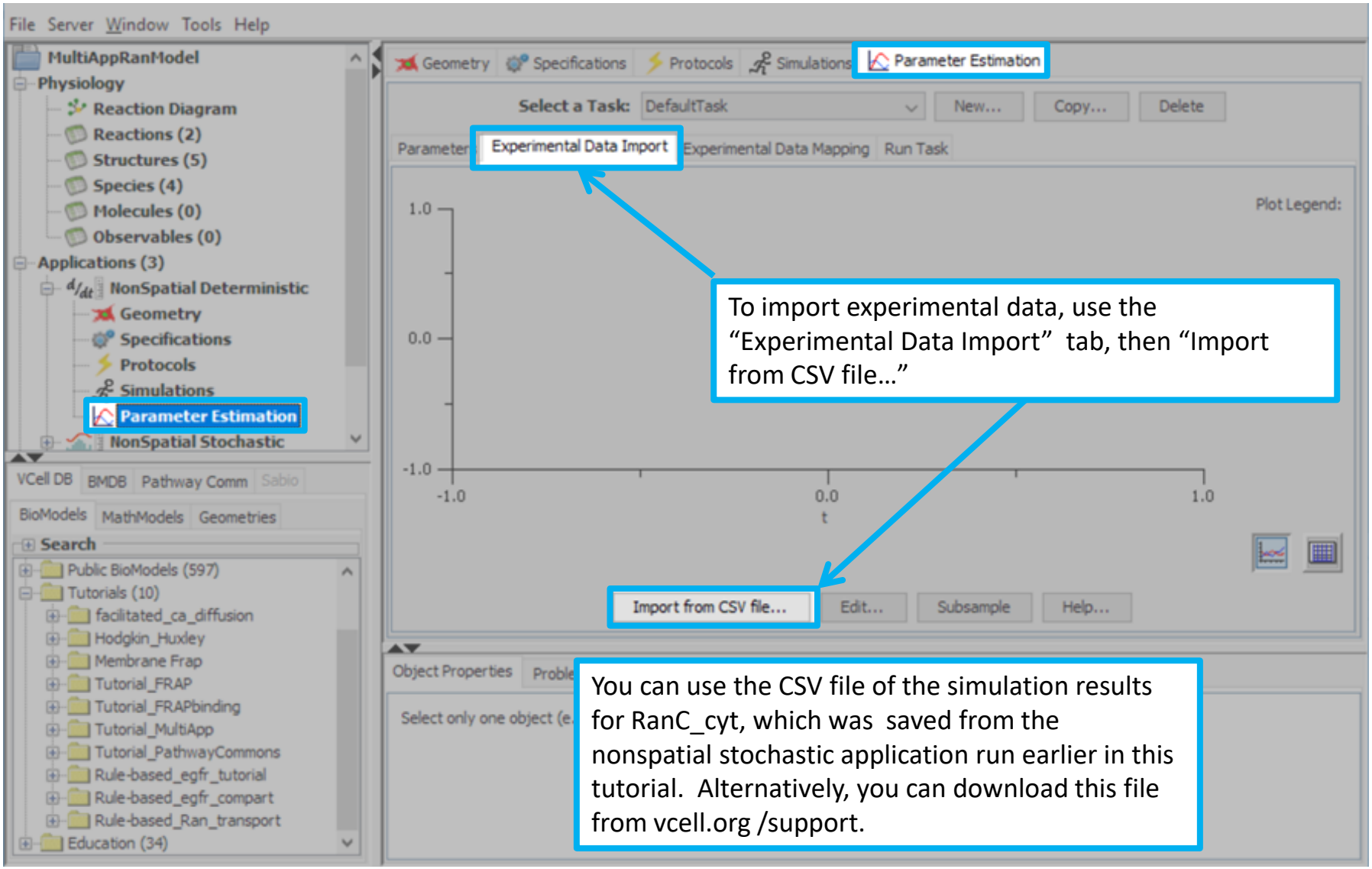

BIOMODEL: multiapp tutorial (Thu Apr 25 19:56:06 EDT 2019) -- VCell 7.1.0 (build 5)
File Server Window Tools Help
multiapp tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
Copy of Spatial Deterministic
NonSpatial Stochastic
Spatial Deterministic
Parameters, Functions and Units
Pathway
Scripting
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Kinematics
Physiology (structures)
Cyt
Nuc
EC
PM
NM
Compartment
Volume/Surface Calculator
Structure
Size
42403.165 [µm³]
7771.2418 [µm³]
279825.59 [µm³]
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (staurovsky) (1)
multiapp tutorial
Shared BioModels (0)
Public BioModels (683)
Tutorials (9)
Education (33)
Published BioModels (171)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
To rename the new application, right click on an application and click “Rename”. Type in a name and press “Enter” on your keyboard.

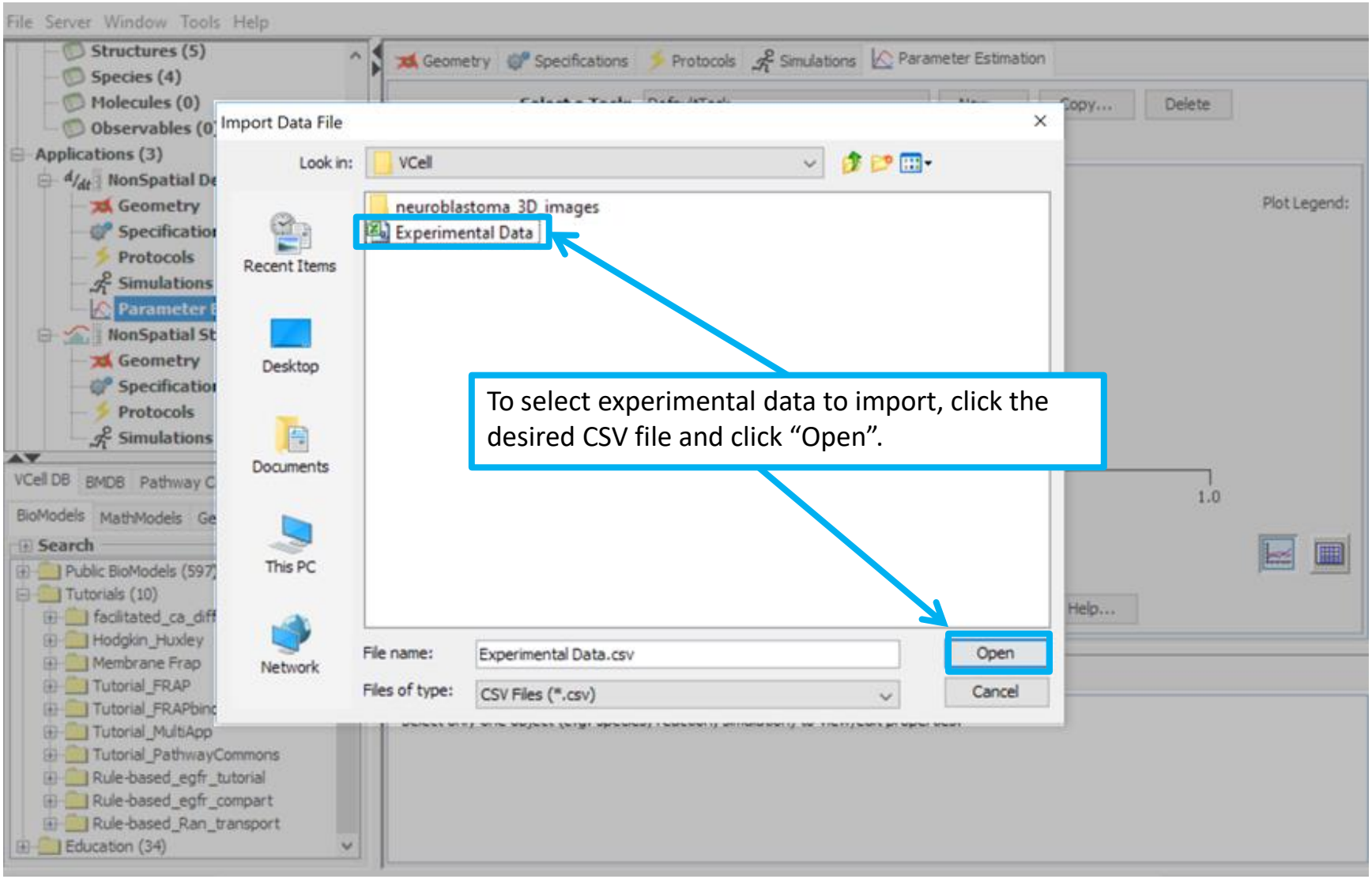

File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Physiology (structures)
EC
cyt
nuc
Compartment
When you copy a spatial application to a non-spatial application, VCell automatically uses sizes for the compartments based on the image-based geometry used in the spatial application
Structure
Size
EC
229042.61 [µm³]
cyt
27220.285 [µm³]
nuc
3737.1007 [µm³]
pm
7226.8656 [µm²]
nm
1377.3093 [µm²]
The NonSpatial Deterministic Application therefore is all ready to run simulations. In this tutorial, you will first use data to fit one of the parameters for the model

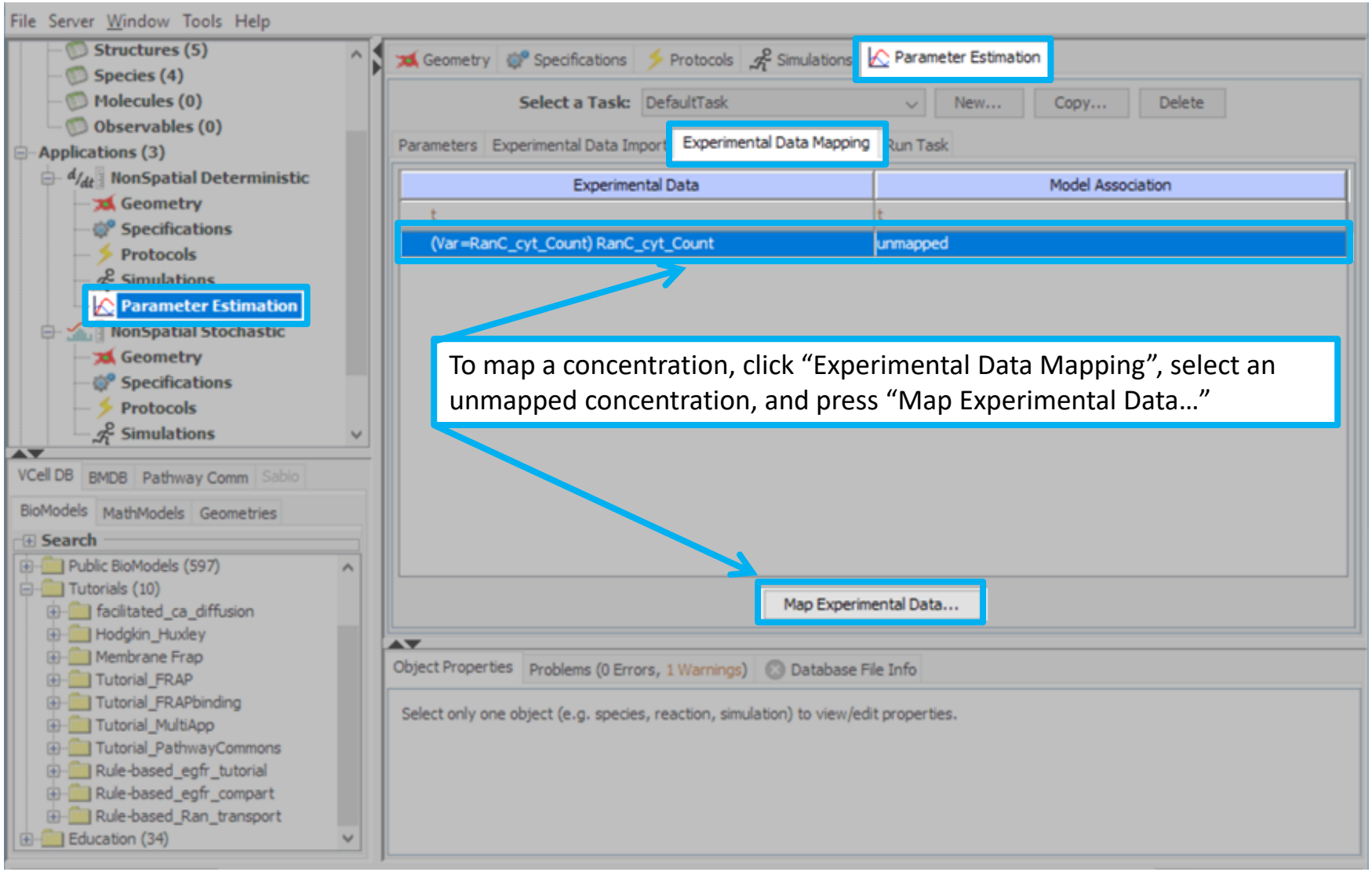

File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Context
Model Value
Lower Bound
Upper Bound
To create a new parameter estimation, click the “Parameter Estimation” tab and click the plus sign icon.

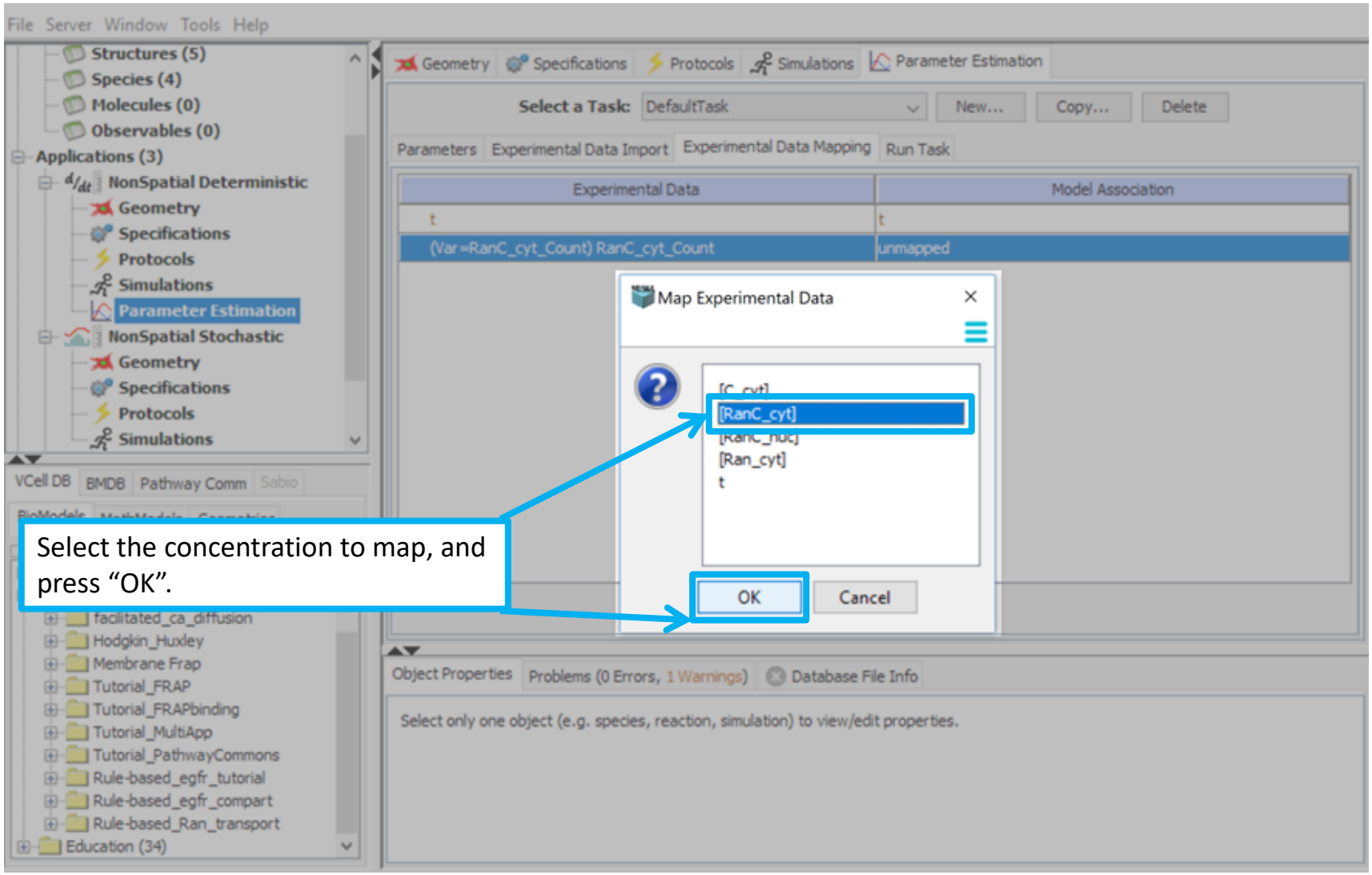

File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Lower Bound
Upper Bound
Select Parameters
Parameter
Context
Kf
r0
Kr
r0
netValence
flux0
kfl
flux0
initConc
Ran_cyt_scs
initConc
C_cyt_scs
initConc
RanC_cyt_scs
RanC_nuc_scs
pm_mapping
nm_mapping
OK
Cancel
To select a parameter to fit, click on the specific parameter , in this case Kf, and click “OK”.


File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Experimental Data Import
Experimental Data Mapping
Run Task
Parameter
Context
Model Value
Initial Guess
Lower Bound
Upper Bound
Kf
r0
1
1
0.1
10
Kr
r0
1000
1000
100
10000
Continue adding parameters using the “plus sign” icon until you have selected all the parameters you want to fit.

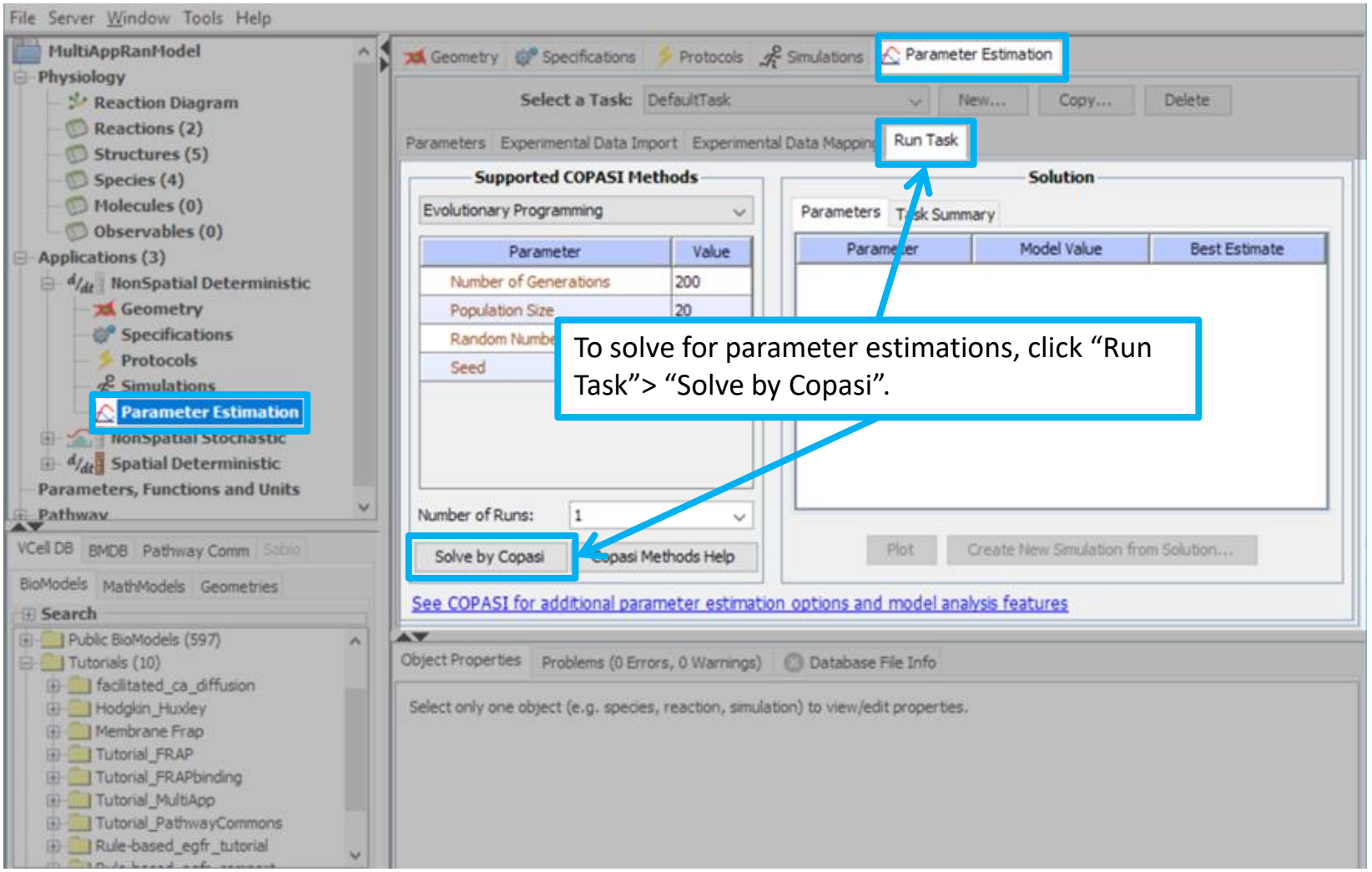

File Server Window Tools Help
MultiAppRanModel
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameter
Experimental Data Import
Experimental Data Mapping
Run Task
Plot Legend:
1.0
0.0
-1.0
-1.0
0.0
1.0
t
Import from CSV file...
Edit...
Subsample
Help...
Object Properties
Select only one object (e
To import experimental data, use the "Experimental Data Import" tab, then "Import from CSV file…"
You can use the CSV file of the simulation results for RanC_cyt, which was saved from the nonspatial stochastic application run earlier in this tutorial. Alternatively, you can download this file from vcell.org /support.


Import Data File
Look in:
VCell
neuroblastoma_3D_images
Experimental Data
Recent Items
Desktop
Documents
This PC
Network
File name:
Experimental Data.csv
Files of type:
CSV Files (*.csv)
Open
Cancel
To select experimental data to import, click the desired CSV file and click “Open”.
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Plot Legend:
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
Tutorials (10)


File Server Window Tools Help
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
NonSpatial Stochastic
Geometry
Specifications
Protocols
Simulations
VCell DB
BMDB
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Public BioModels (597)
Tutorials (10)
facilitated_ca_diffusion
Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
Rule-based_egfr_compart
Rule-based_Ran_transport
Education (34)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Experimental Data
Model Association
(Var=RanC_cyt_Count) RanC_cyt_Count
unmapped
To map a concentration, click “Experimental Data Mapping”, select an unmapped concentration, and press “Map Experimental Data…”
Map Experimental Data...
Object Properties
Problems (0 Errors, 1 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.



Select the concentration to map, and press “OK”.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Hodgkin_Huxley
Membrane Frap
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_PathwayCommons
Rule-based_egfr_tutorial
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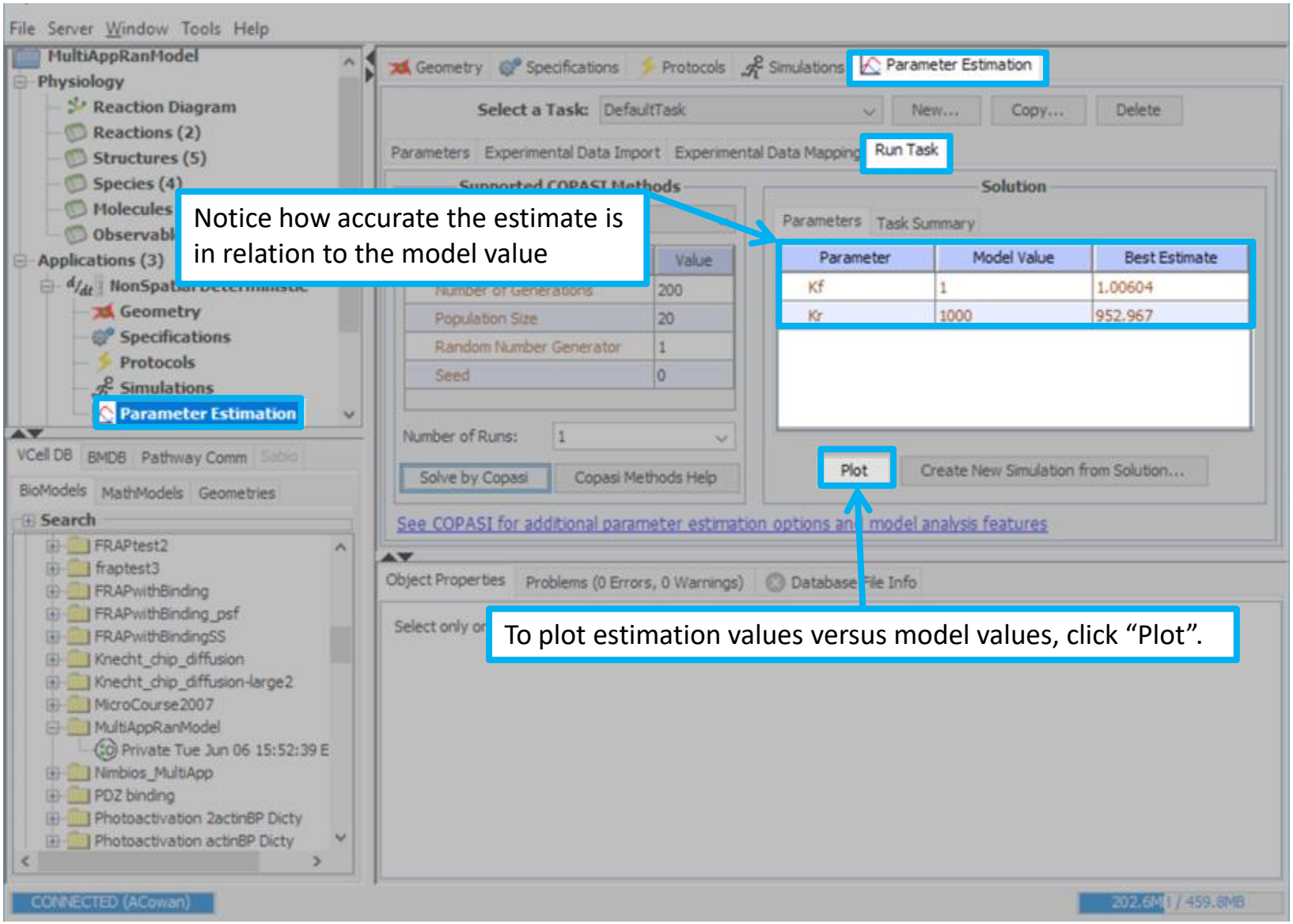
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Supported COPASI Methods
Evolutionary Programming
Parameter
Value
Number of Generations
200
Population Size
20
Random Numbe
Seed
Number of Runs:
1
Solve by Copasi
Copasi Methods Help
Solution
Parameters
Task Summary
Parameter
Model Value
Best Estimate
Plot
Create New Simulation from Solution...
See COPASI for additional parameter estimation options and model analysis features
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
To solve for parameter estimations, click “Run Task”> “Solve by Copasi”.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Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Solution
Parameters
Task Summary
Parameter
Model Value
Best Estimate
Kf
1
1.00604
Kr
1000
952.967
Value
200
20
1
0
Number of Runs:
1
Solve by Copasi
Copasi Methods Help
Plot
Create New Simulation from Solution...
See COPASI for additional parameter estimation options and model analysis features
Object Properties
Problems (0 Errors, 0 Warnings)
Database
File Info
Notice how accurate the estimate is in relation to the model value
To plot estimation values versus model values, click “Plot”.
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Knecht_chip_diffusion-large2
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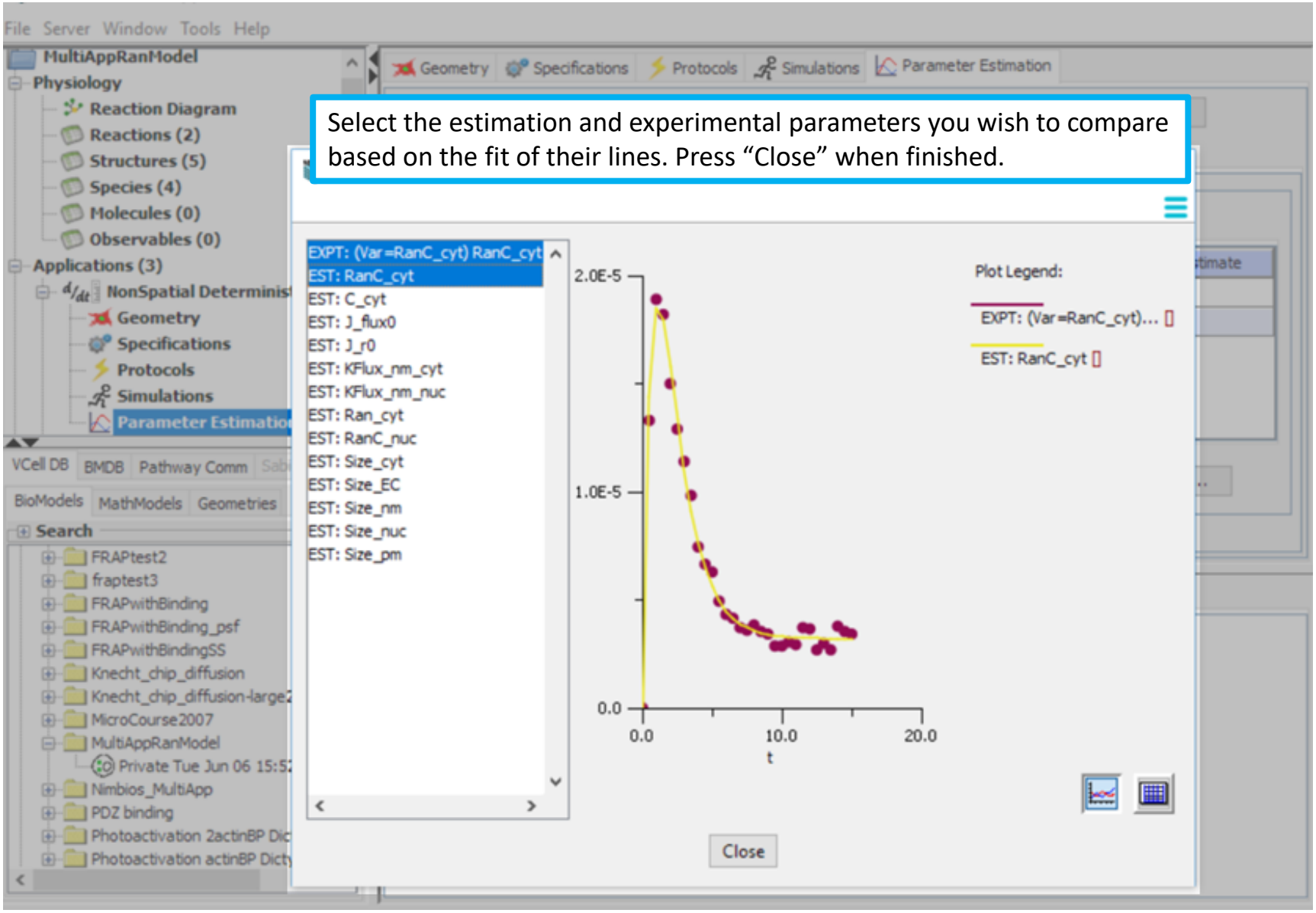
MultiAppRanModel
Private Tue Jun 06 15:52:39 E
Nimbios_MultiApp
PDZ binding
Photoactivation 2actinBP Dicty
Photoactivation actinBP Dicty
CONNECTED (ACowan)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Geometry
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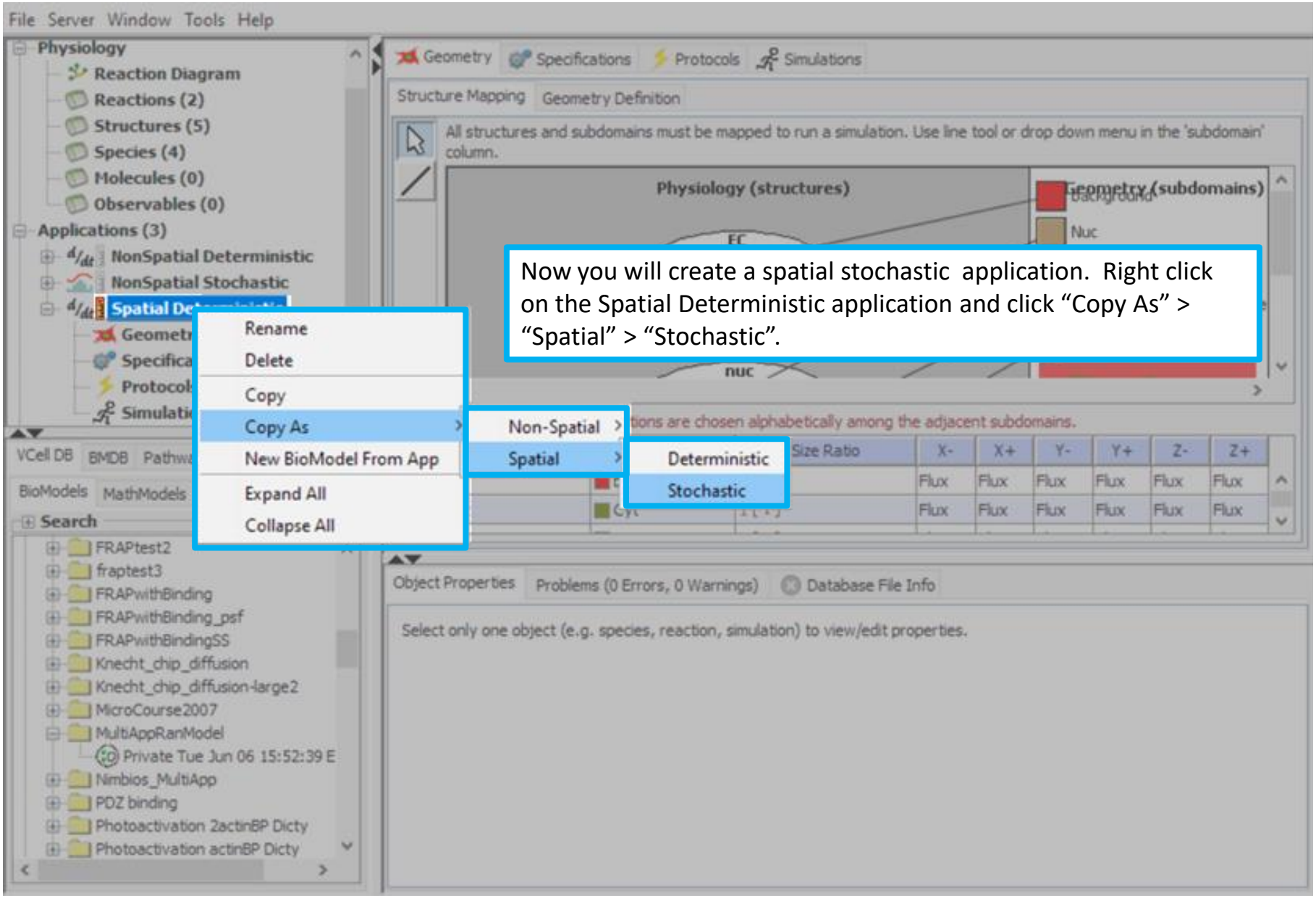
Parameter Estimation
Select the estimation and experimental parameters you wish to compare based on the fit of their lines. Press “Close” when finished.
EXPT: (Var=RanC_cyt) RanC_cyt
EST: RanC_cyt
EST: C_cyt
EST: J_flux0
EST: J_r0
EST: KFlux_nm_cyt
EST: KFlux_nm_nuc
EST: Ran_cyt
EST: RanC_nuc
EST: Size_cyt
EST: Size_EC
EST: Size_nm
EST: Size_nuc
EST: Size_pm
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
Plot Legend:
EXPT: (Var=RanC_cyt)...
EST: RanC_cyt
Close


File Server Window Tools Help
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NonSpatial Deterministic
NonSpatial Stochastic
Spatial Deterministic
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.
Physiology (structures)
Geometry (subdomains)
Background
Nuc
EC
nuc
Now you will create a spatial stochastic application. Right click on the Spatial Deterministic application and click "Copy As" > "Spatial" > "Stochastic".
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Non-Spatial
Spatial
Deterministic
Stochastic
tions are chosen alphabetically among the adjacent subdomains.
Size Ratio
X-
X+
Y-
Y+
Z-
Z+
Flux
VCell DB
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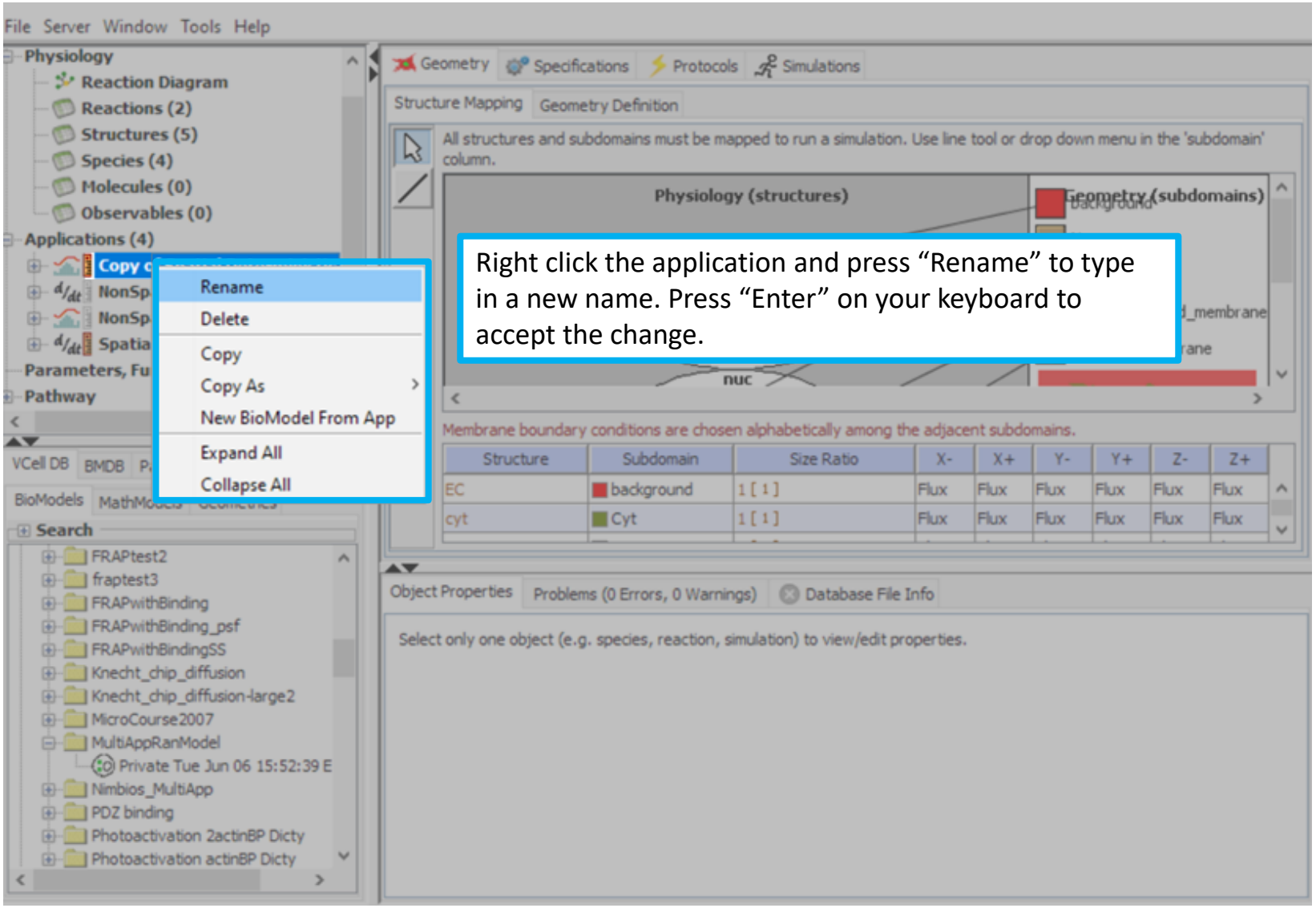
Nimbios_MultiApp
PDZ binding
Photoactivation 2actinBP Dicty
Photoactivation actinBP Dicty
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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Observables (0)
Applications (4)
Parameters, Fu
Pathway
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Right click the application and press “Rename” to type in a new name. Press “Enter” on your keyboard to accept the change.
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.
Physiology (structures)
Geometry (subdomains)
nuc
Membrane boundary conditions are chosen alphabetically among the adjacent subdomains.
Structure
Subdomain
Size Ratio
X-
X+
Y-
Y+
Z-
Z+
EC
background
1 [1]
Flux
cyt
Cyt
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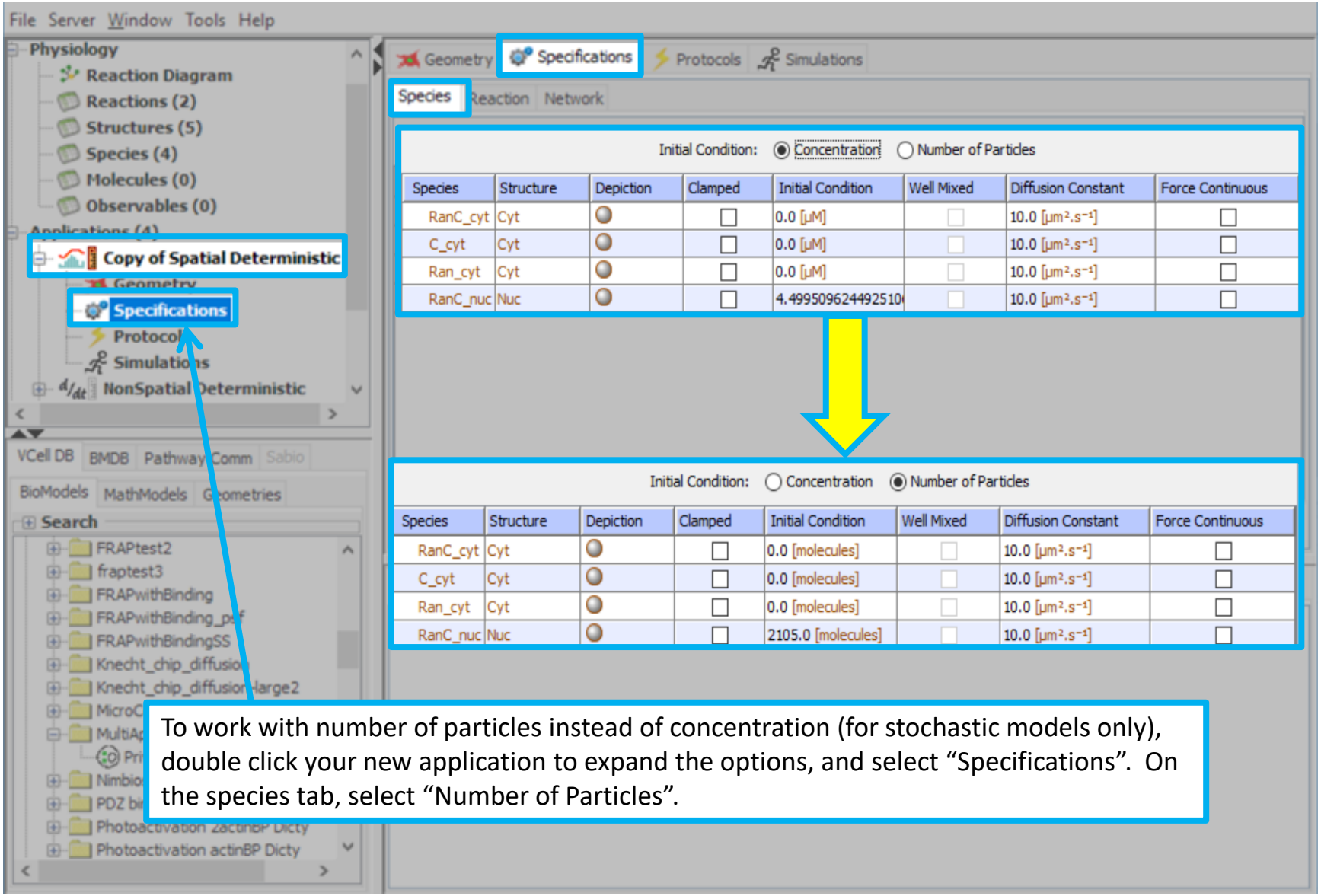
Photoactivation actinBP Dicty
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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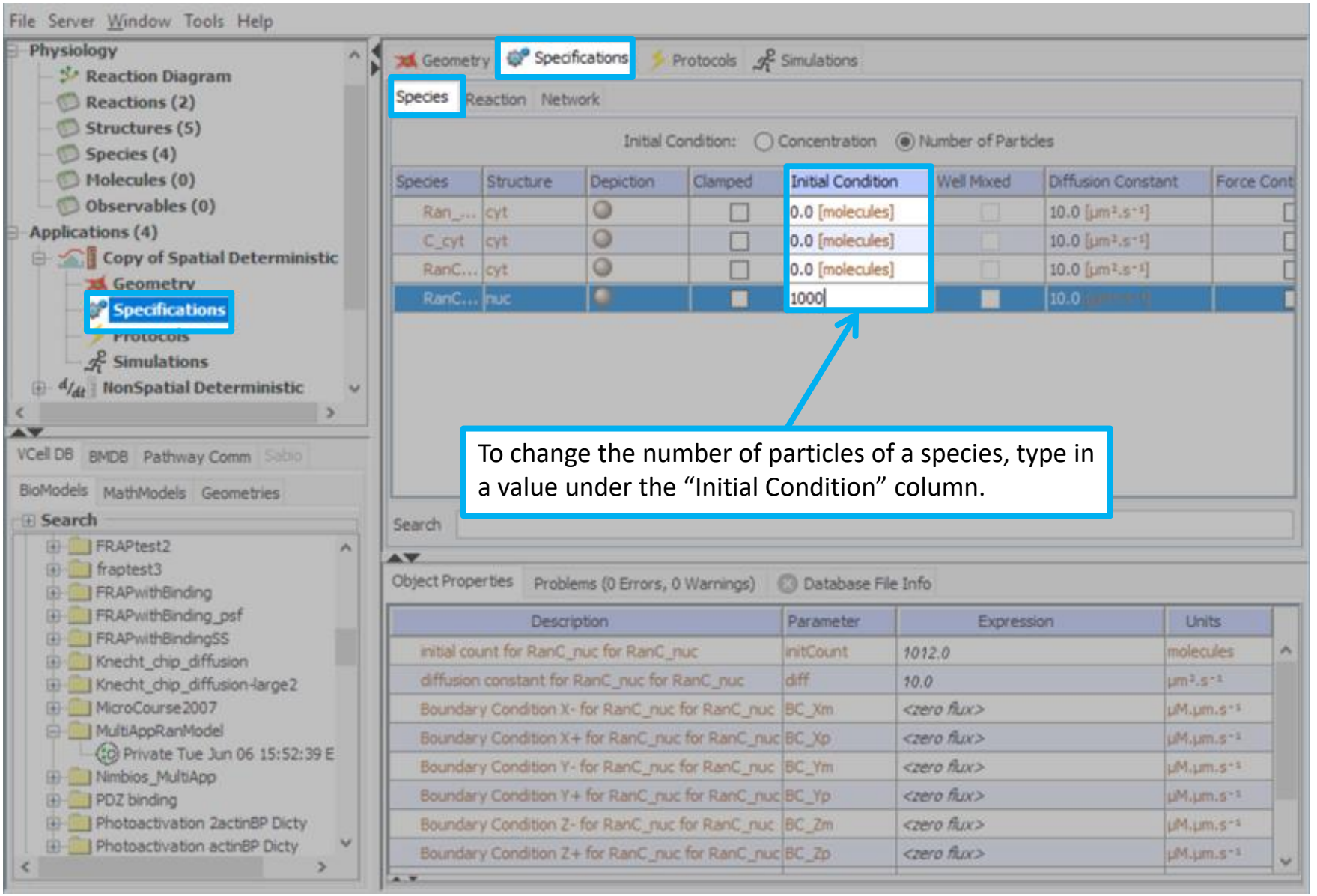
Initial Condition: Concentration Number of Particles
Species Structure Depiction Clamped Initial Condition Well Mixed Diffusion Constant Force Continuous
RanC_cyt Cyt 0.0 [µM] 10.0 [µm².s⁻¹]
C_cyt Cyt 0.0 [µM] 10.0 [µm².s⁻¹]
Ran_cyt Cyt 0.0 [µM] 10.0 [µm².s⁻¹]
RanC_nuc Nuc 10.0 [µm².s⁻¹]
Initial Condition: Concentration Number of Particles
Species Structure Depiction Clamped Initial Condition Well Mixed Diffusion Constant Force Continuous
RanC_cyt Cyt 0.0 [molecules] 10.0 [µm².s⁻¹]
C_cyt Cyt 0.0 [molecules] 10.0 [µm².s⁻¹]
Ran_cyt Cyt 0.0 [molecules] 10.0 [µm².s⁻¹]
RanC_nuc Nuc 2105.0 [molecules] 10.0 [µm².s⁻¹]
To work with number of particles instead of concentration (for stochastic models only), double click your new application to expand the options, and select “Specifications”. On the species tab, select “Number of Particles”.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Network
Initial Condition: Concentration Number of Particles
Species
Structure
Depiction
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Force Cont
Ran_...
cyt
0.0 [molecules]
10.0 [μm².s⁻¹]
C_cyt
cyt
0.0 [molecules]
10.0 [μm².s⁻¹]
RanC...
cyt
0.0 [molecules]
10.0 [μm².s⁻¹]
RanC...
nuc
1000
10.0
To change the number of particles of a species, type in a value under the “Initial Condition” column.
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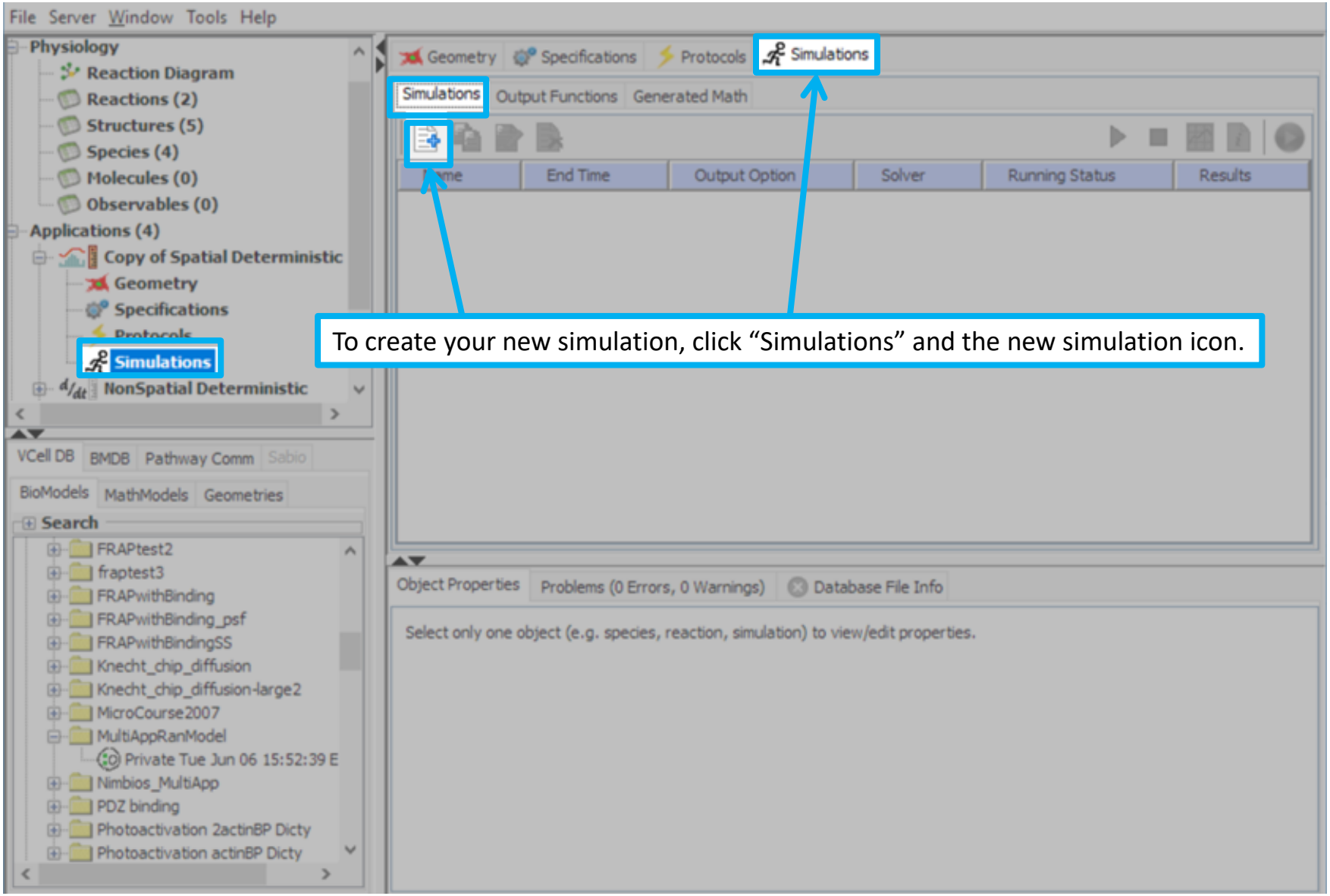
Photoactivation actinBP Dicty
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial count for RanC_nuc for RanC_nuc
initCount
1012.0
molecules
diffusion constant for RanC_nuc for RanC_nuc
diff
10.0
μm².s⁻¹
Boundary Condition X- for RanC_nuc for RanC_nuc
BC_Xm
<zero flux>
μM.μm.s⁻¹
Boundary Condition X+ for RanC_nuc for RanC_nuc
BC_Xp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y- for RanC_nuc for RanC_nuc
BC_Ym
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y+ for RanC_nuc for RanC_nuc
BC_Yp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Z- for RanC_nuc for RanC_nuc
BC_Zm
<zero flux>
μM.μm.s⁻¹
Boundary Condition Z+ for RanC_nuc for RanC_nuc
BC_Zp
<zero flux>
μM.μm.s⁻¹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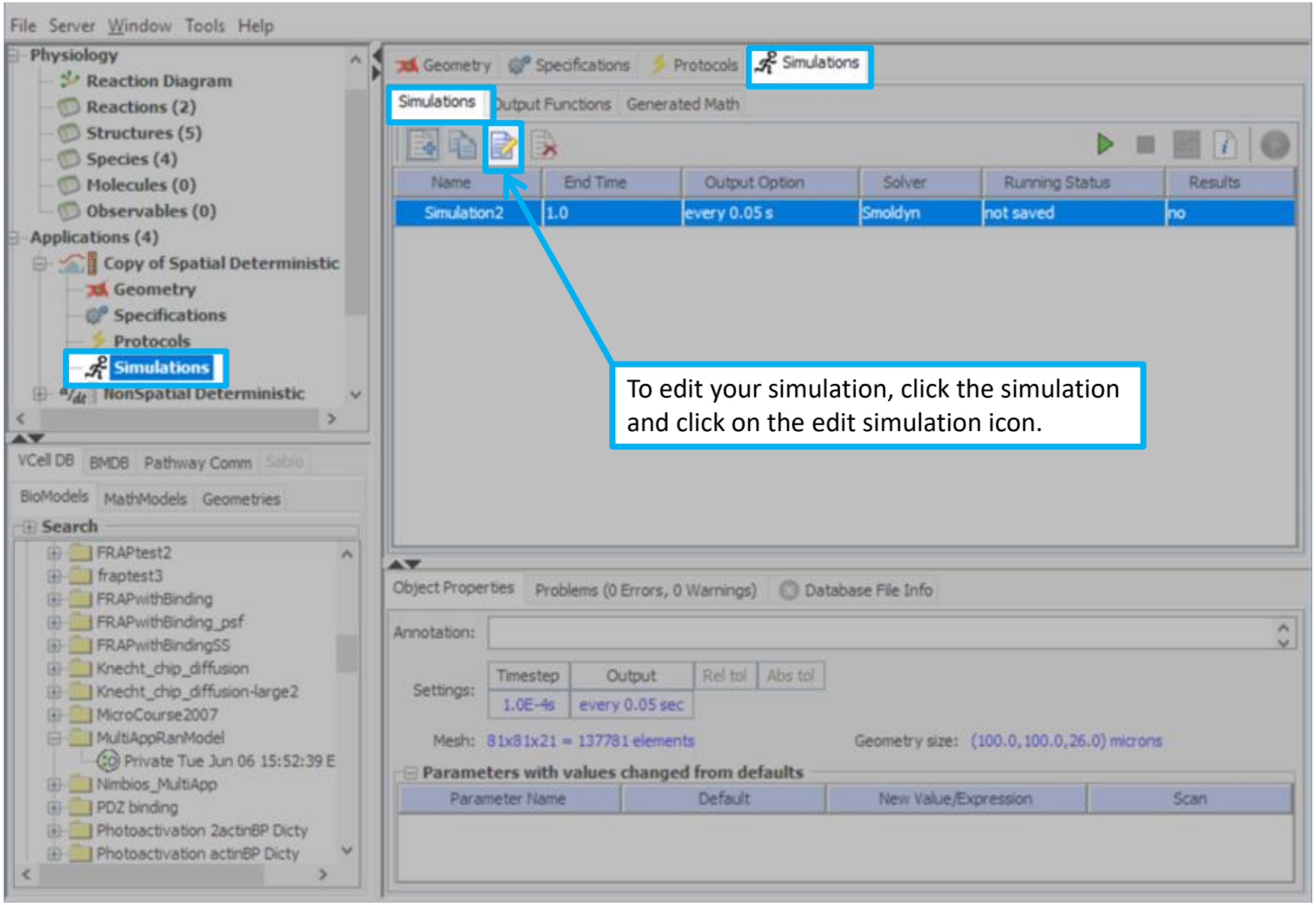
Output Functions
Generated Math
End Time
Output Option
Solver
Running Status
Results
To create your new simulation, click “Simulations” and the new simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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Simulations
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End Time
Output Option
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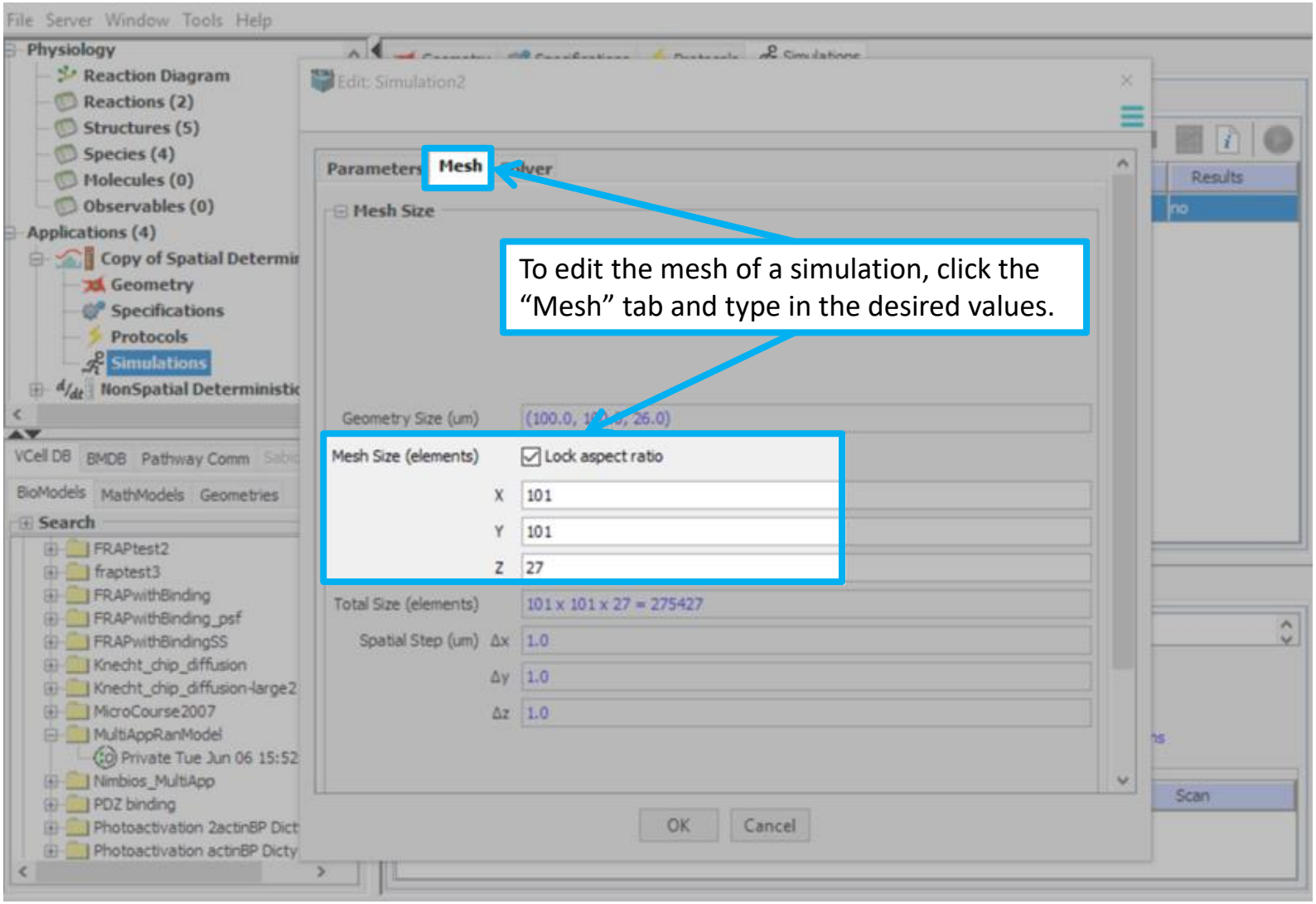
Results
Simulation2
1.0
every 0.05 s
Smoldyn
not saved
no
To edit your simulation, click the simulation and click on the edit simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
Timestep
Output
Rel tol
Abs tol
1.0E-4s
every 0.05 sec
Mesh: 81x81x21 = 137781 elements
Geometry size: (100.0,100.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan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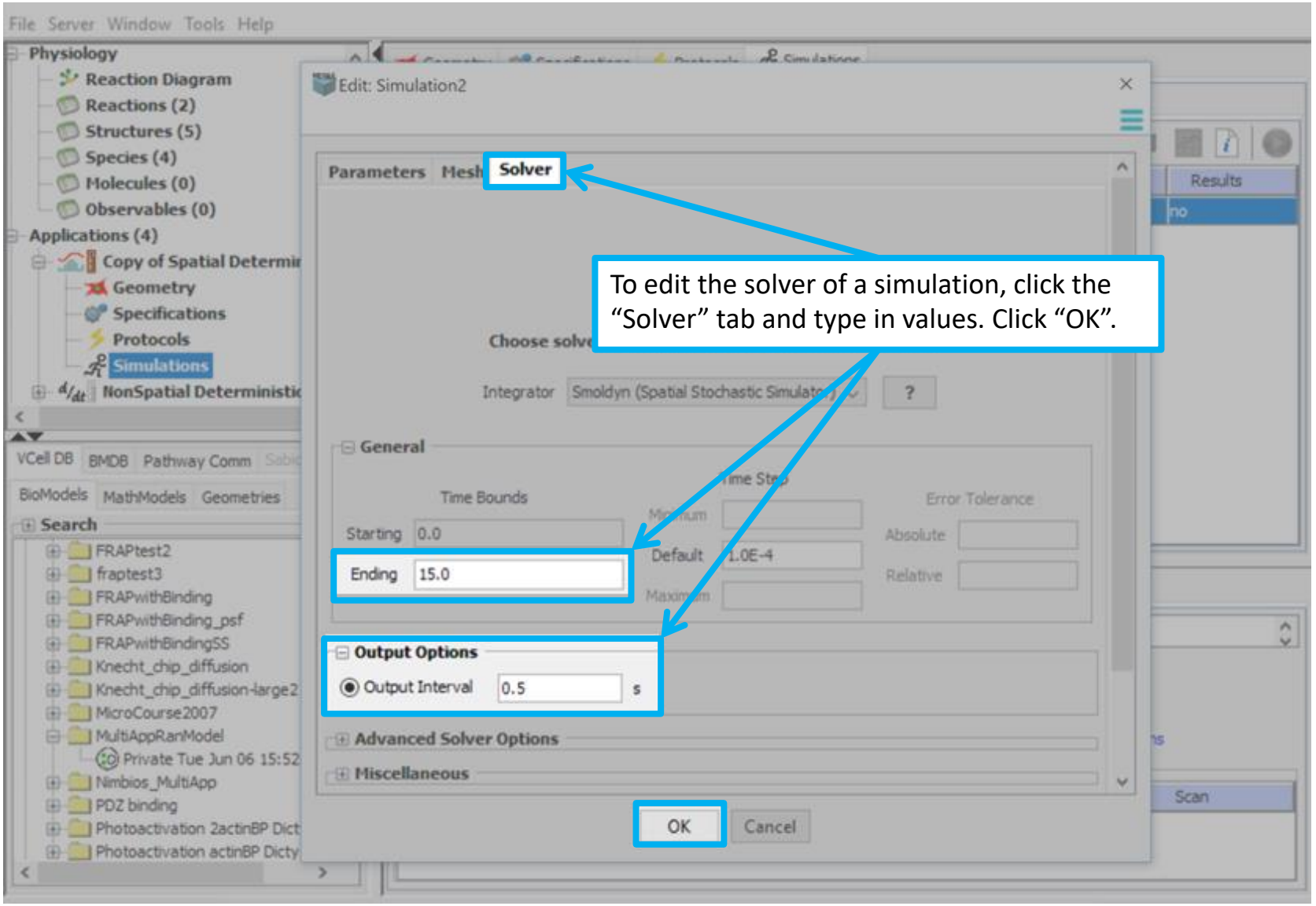
Photoactivation actinBP Dicty
Edit: Simulation2
Parameters
Mesh
Mesh Size
To edit the mesh of a simulation, click the "Mesh" tab and type in the desired values.
Geometry Size (um)
Mesh Size (elements)
Lock aspect ratio
X
101
Y
101
Z
27
Total Size (elements)
101 x 101 x 27 = 275427
Spatial Step (um)
Δx
1.0
Δy
1.0
Δz
1.0
OK
Cancel
Results
Scan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PDZ binding
Photoactivation 2actinBP Dict
Photoactivation actinBP Dicty
Edit: Simulation2
Parameters
Mesh
Solver
Choose solve
Integrator
Smoldyn (Spatial Stochastic Simulate
?
General
Time Bounds
Starting 0.0
Ending 15.0
Time Step
Minimum
Default 1.0E-4
Maximum
Error Tolerance
Absolute
Relative
Output Options
Output Interval 0.5 s
Advanced Solver Options
Miscellaneous
OK
Cancel
Results
no
Scan
To edit the solver of a simulation, click the "Solver" tab and type in values. Click "OK".

You can now run your simulation, and view your results as previously described in this tutorial.