VCell Tutorial

BioModel with Multiple Applications

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

Part 1: Spatial Deterministic Application using a 3D geometry derived from an image stack

The Multi-App Tutorial

- Part 1: Spatial Deterministic Application using a 3D geometry derived from an image stack

  Create the Physiology for a simple Biomodel of RAN nuclear transport, create a 3D geometry directly from a z-stack of microscopy images, and run a deterministic spatial simulation.

- Part 2: Additional Applications

  Compartmental stochastic application with data export; compartmental deterministic (ODE) application with parameter estimation parameters using external data; stochastic spatial application.

In Part 1 of this tutorial…

- Create a Biomodel Physiology with species, reactions and fluxes
- Create a spatial deterministic application of the Physiology
- Import a 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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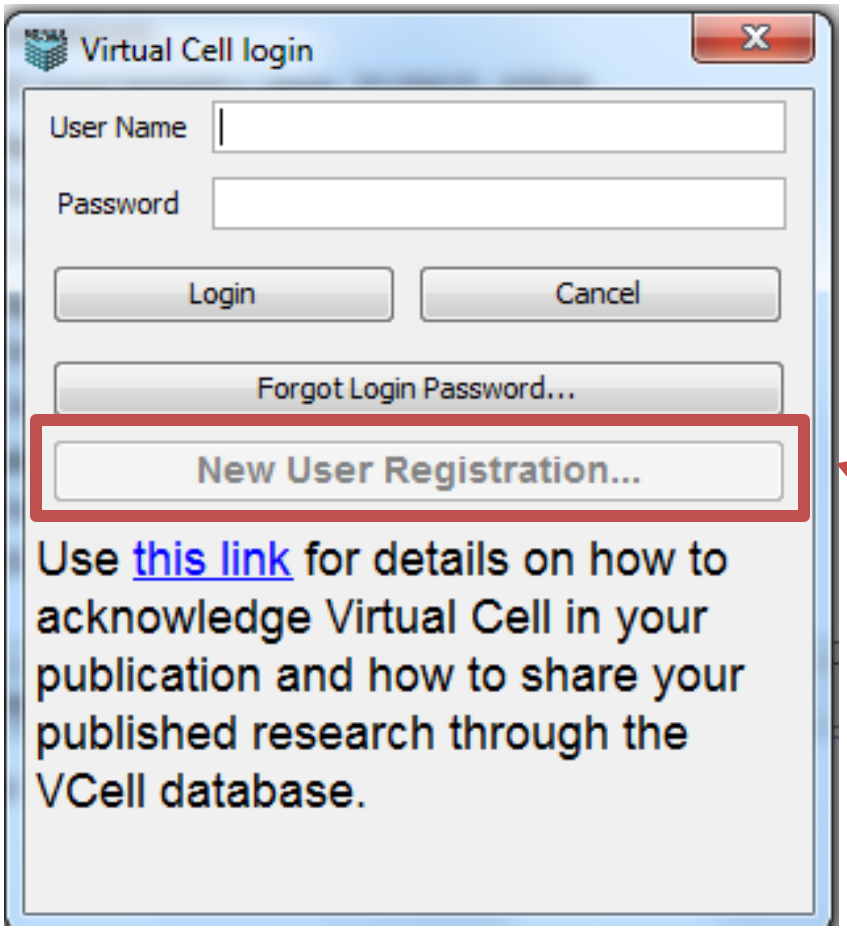
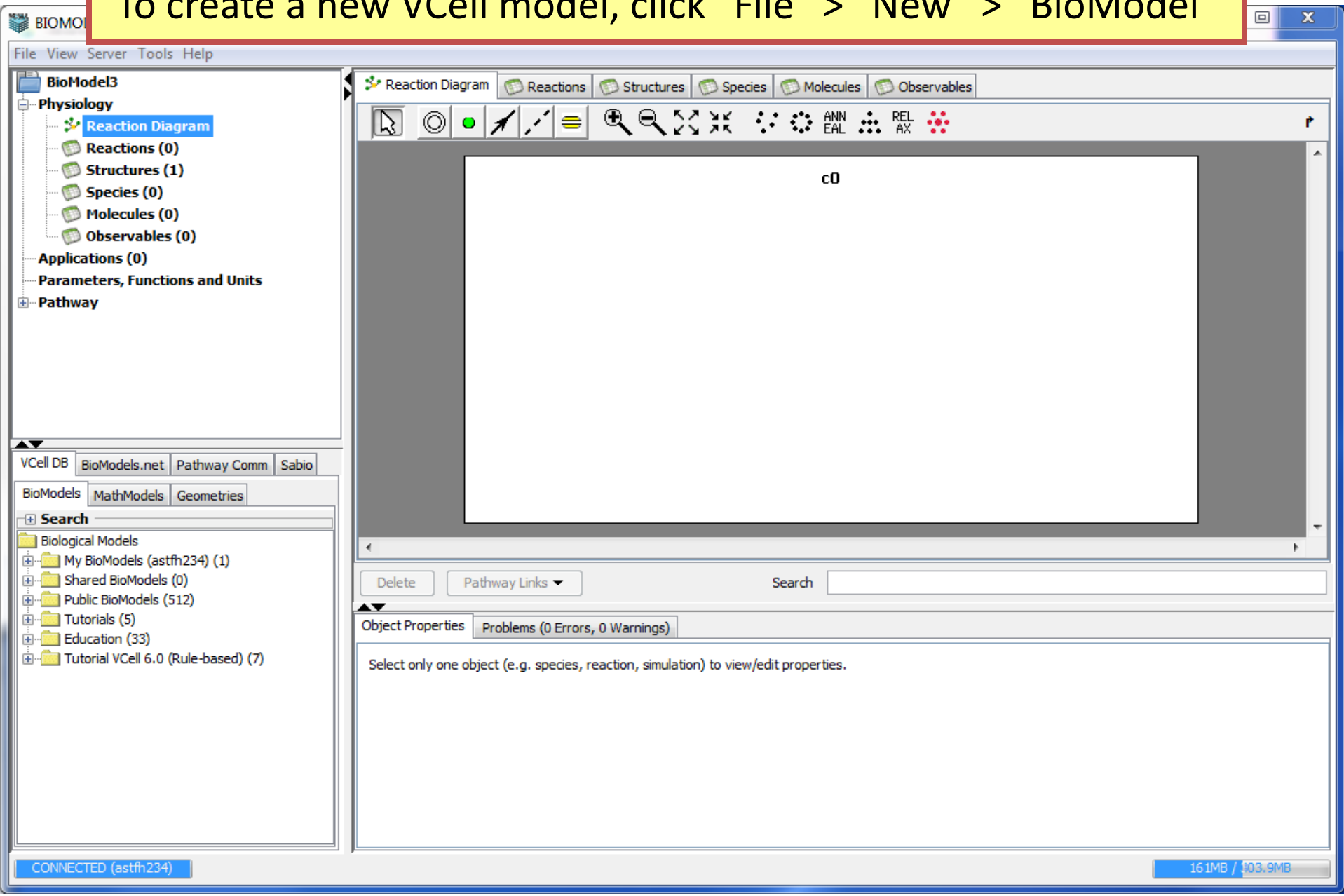
First time opening VCell

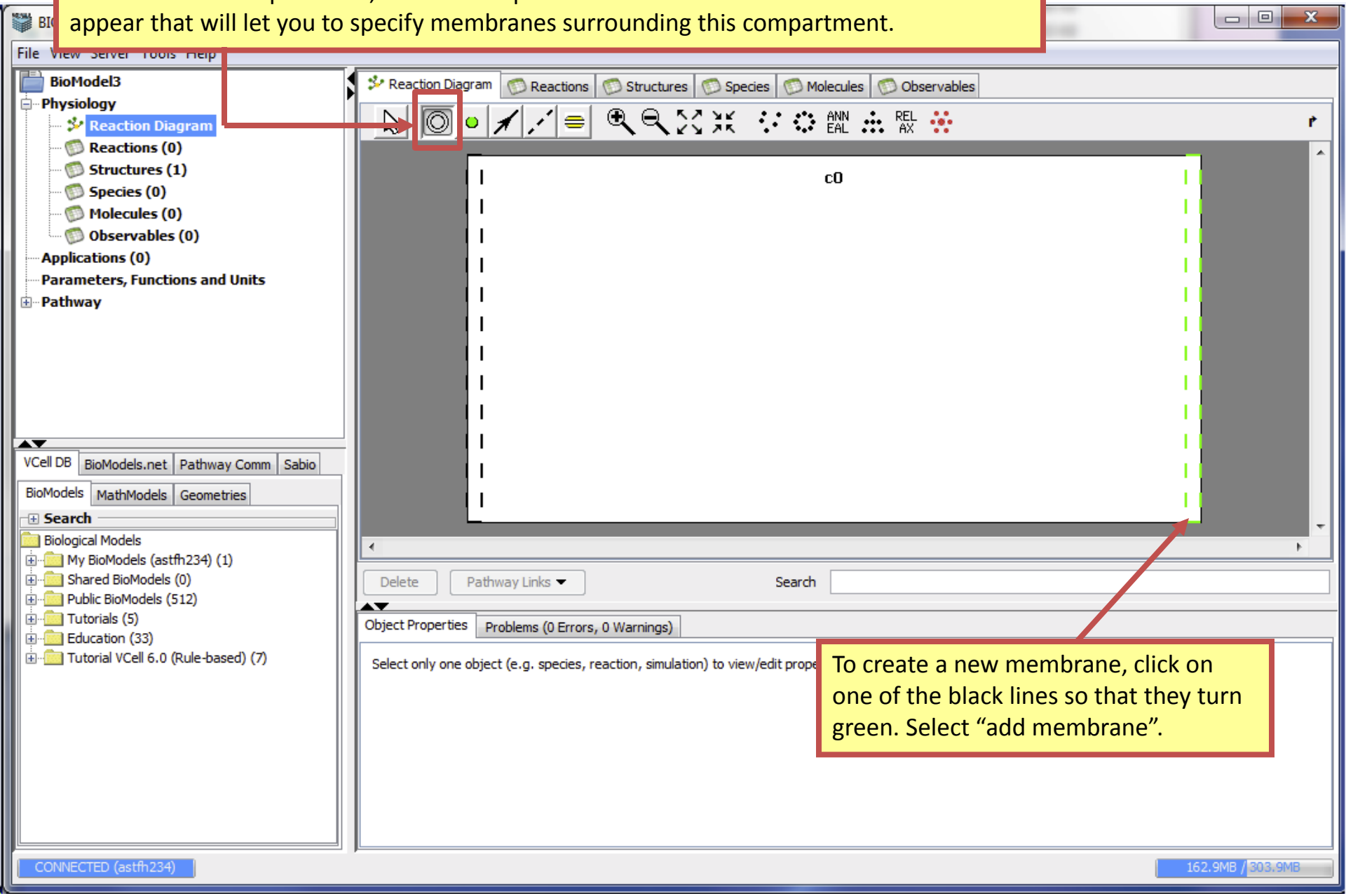


You need to register as a new user if you want to run simulations on VCell compute resources, or use the VCell database to store models that can be shared with collaborators.

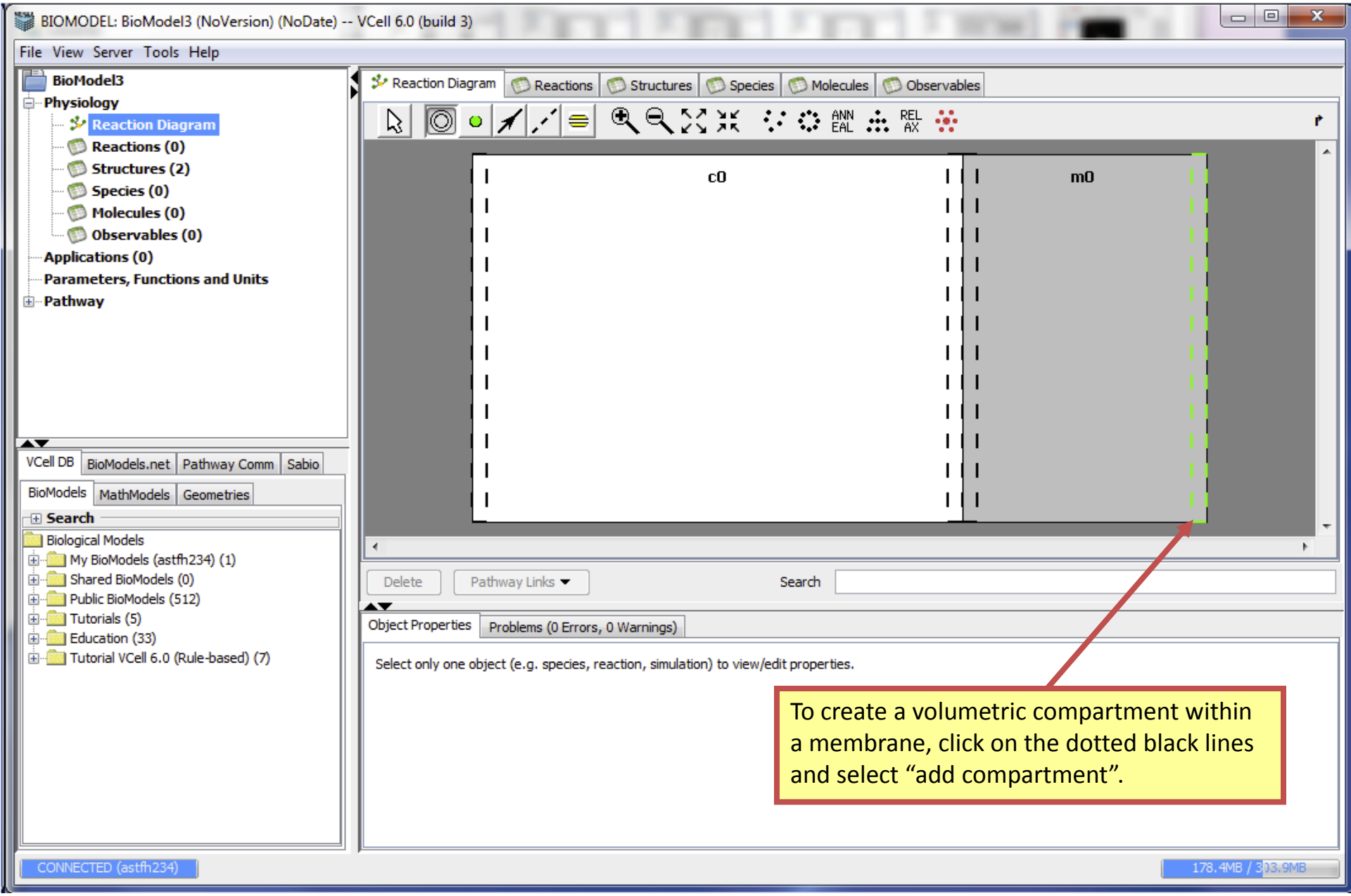
To create a new VCell model, click “File” > “New” > “BioModel”



To create new compartment, click on compartment tool. Two dashed vertical lines will appear that will let you to specify membranes surrounding this compartment.



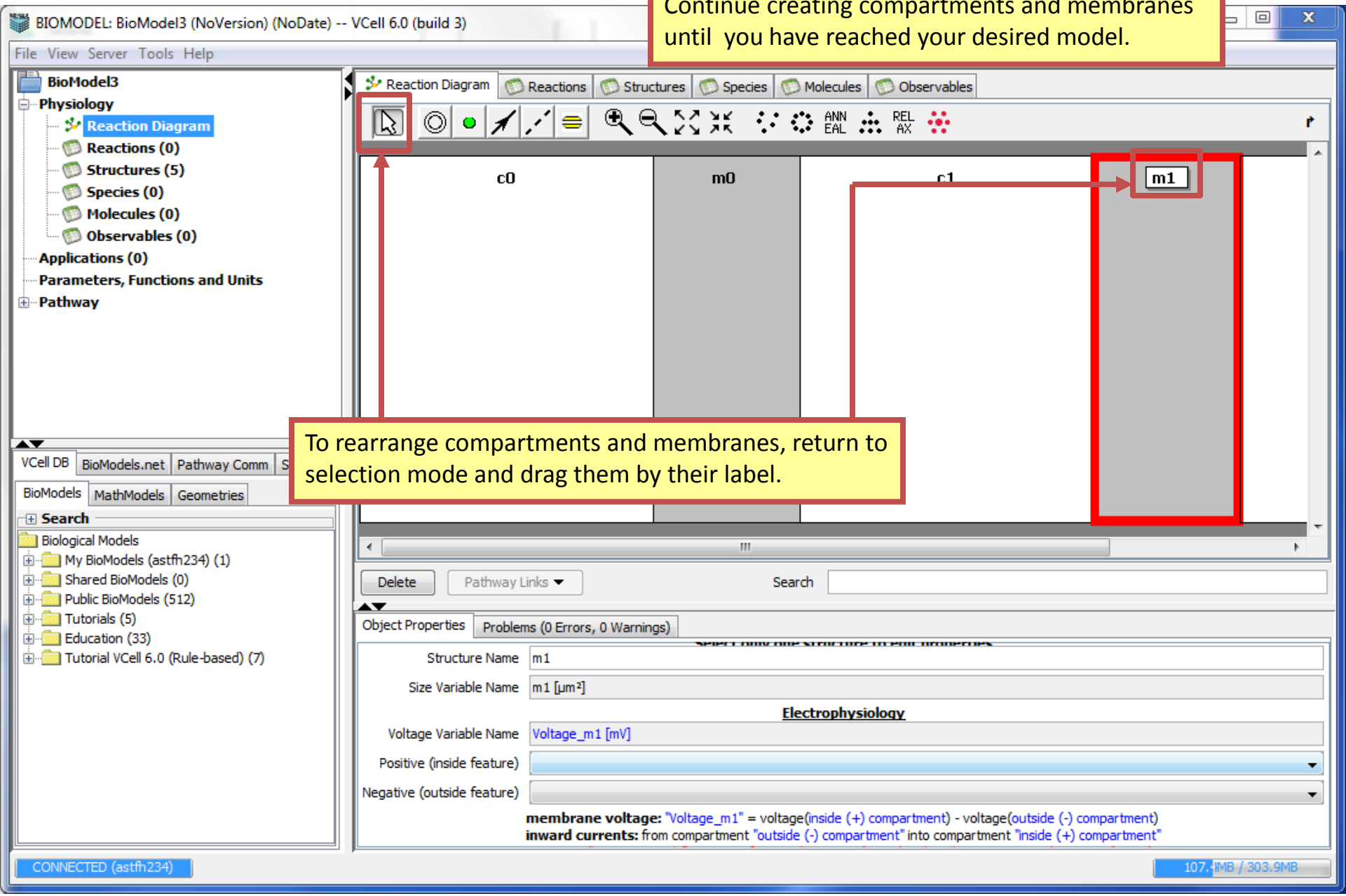
To create a new membrane, click on one of the black lines so that they turn green. Select “add membrane”.

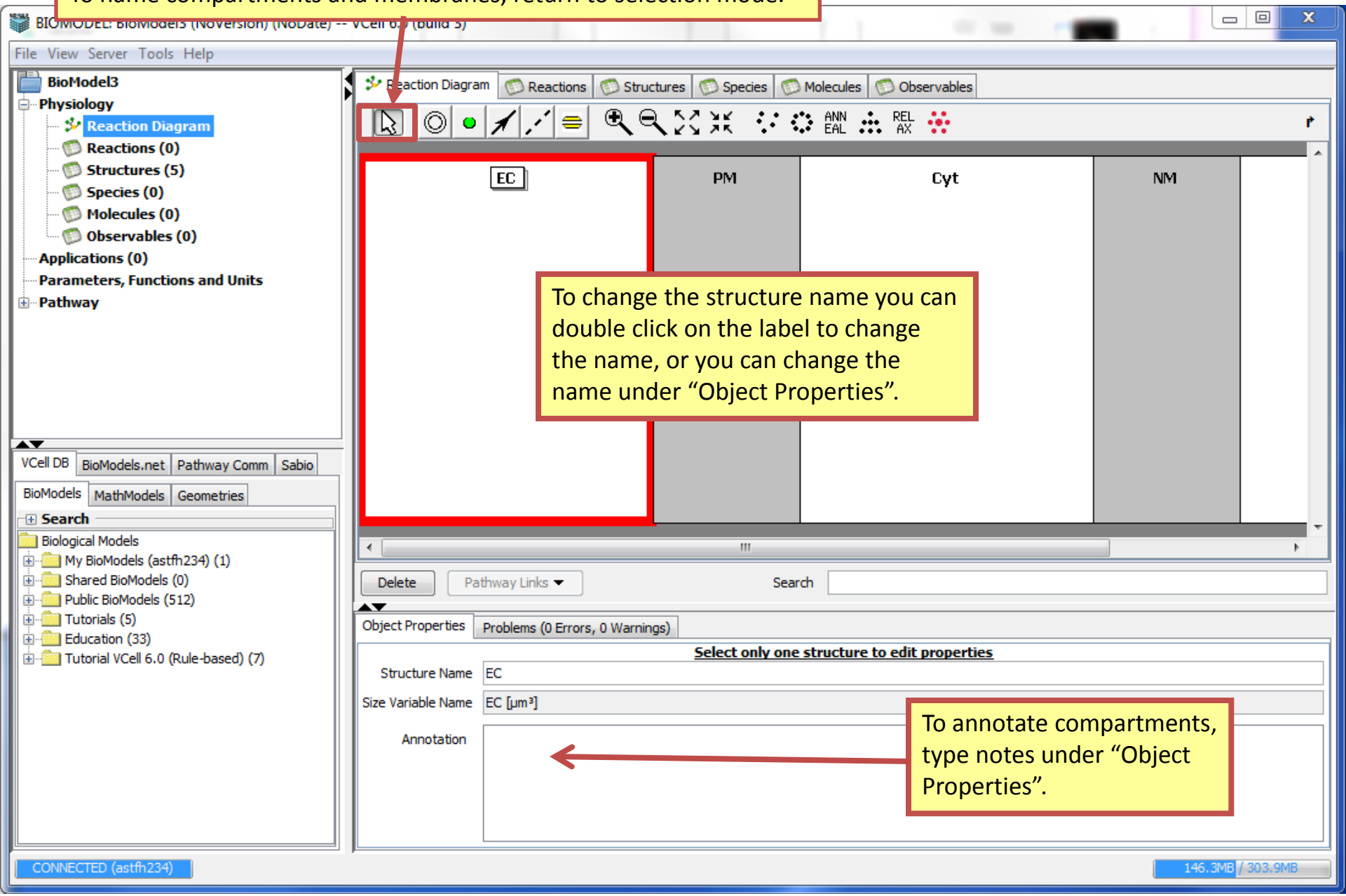


To create a volumetric compartment within a membrane, click on the dotted black lines and select “add compartment”.

Contents

Continue creating compartments and membranes until you have reached your desired model.




To name compartments and membranes, return to selection mode.
File View Server Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (0)
Structures (5)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
Cyt
NM
To change the structure name you can double click on the label to change the name, or you can change the name under “Object Properties”.
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
To annotate compartments, type notes under “Object Properties”.
VCell DB
BioModels.net
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My BioModels (astfh234) (1)
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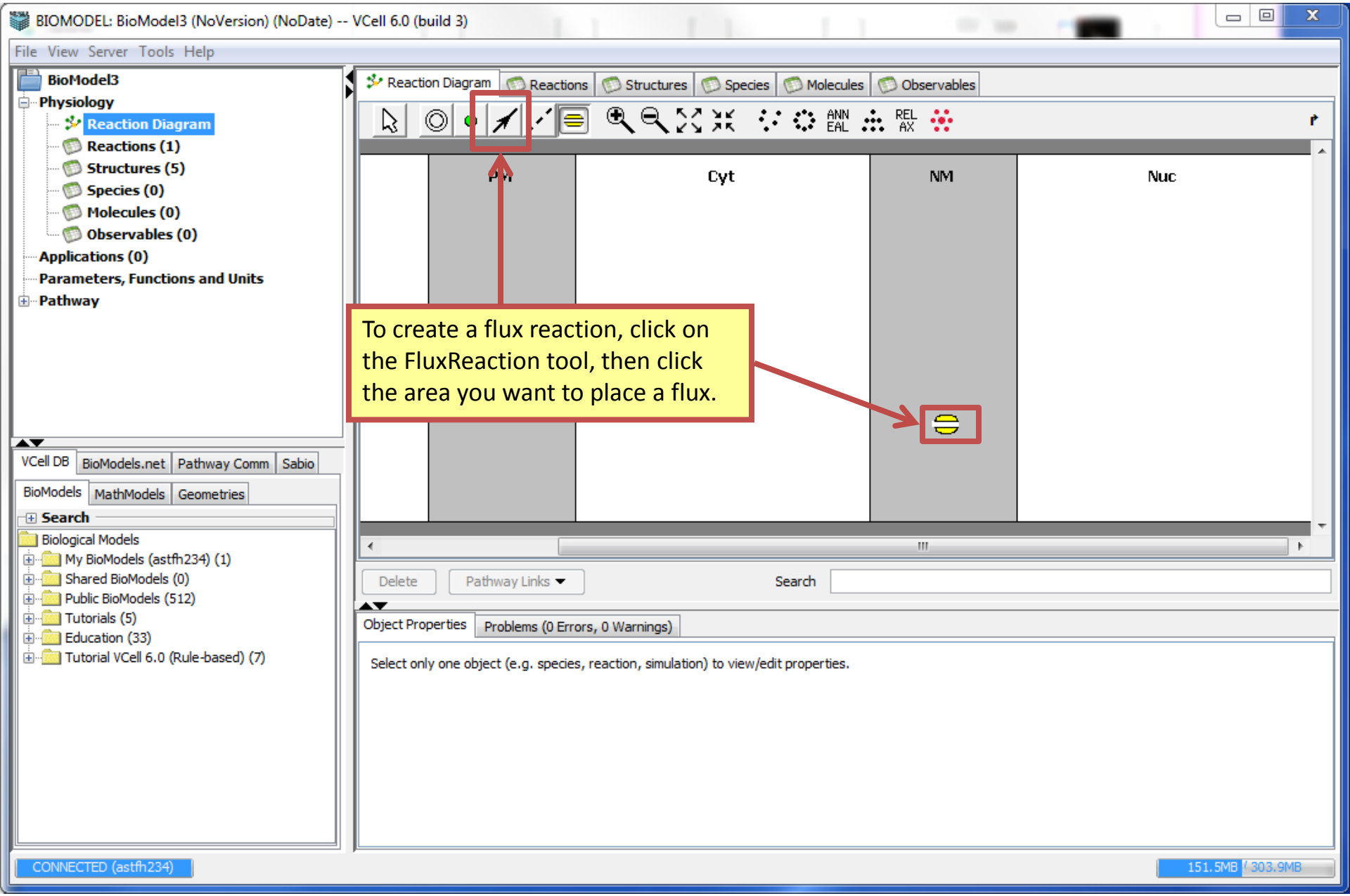
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
CONNECTED (astfh234)
146.3MB / 303.9MB


BIOMODEL: BioModel3 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
File View Server Tools Help
BioModel3
Physiology
Reaction Diagram
Reactions (1)
Structures (5)
Species (0)
Molecules (0)
Observables (0)
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Reaction Diagram
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Cyt
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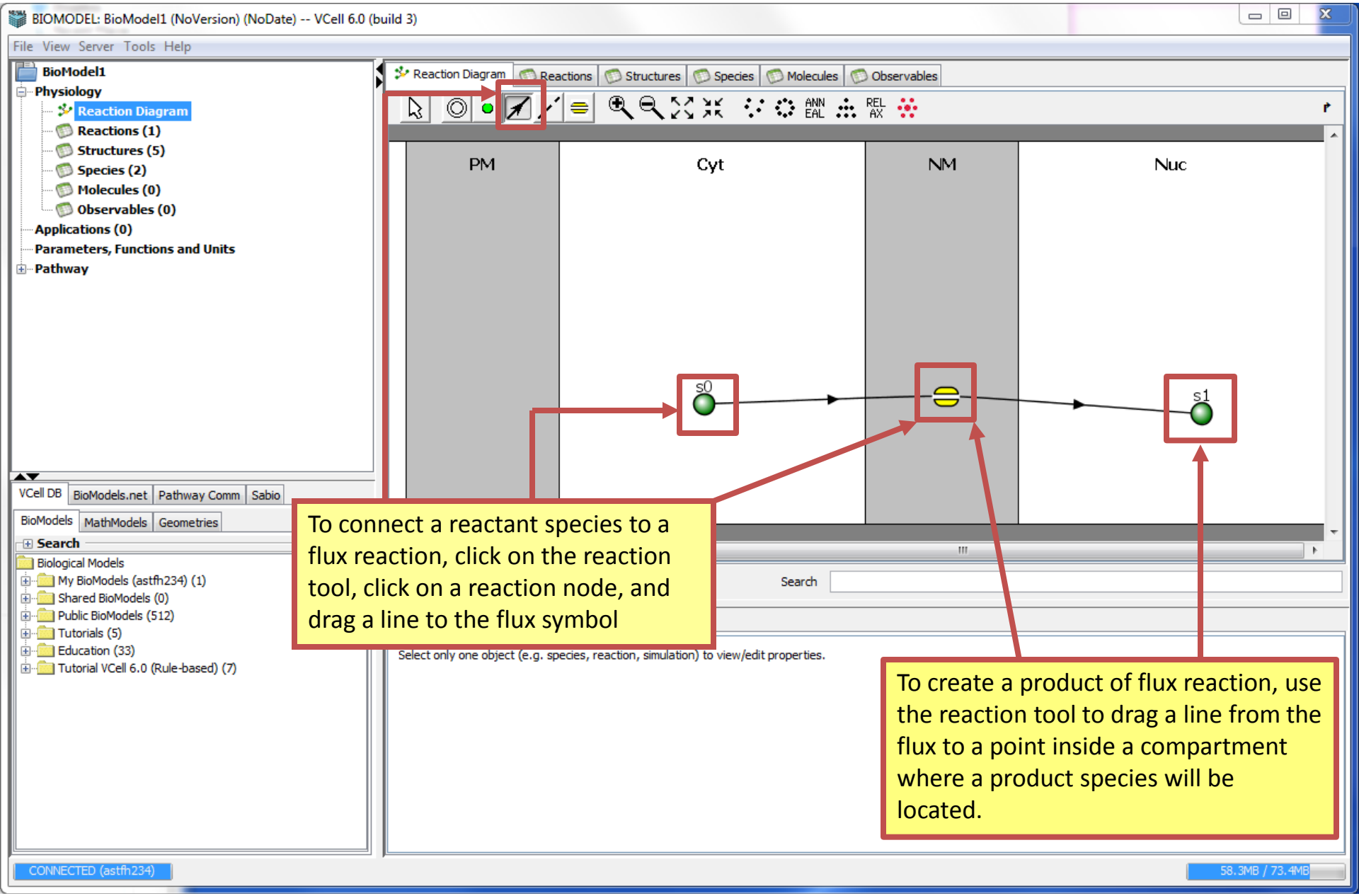
Nuc
To create a flux reaction, click on the FluxReaction tool, then click the area you want to place a flux.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
151.5MB
303.9MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Reactions (1)
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Observables (0)
Applications (0)
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Nuc
s0
s1
To connect a reactant species to a flux reaction, click on the reaction tool, click on a reaction node, and drag a line to the flux symbol
To create a product of flux reaction, use the reaction tool to drag a line from the flux to a point inside a compartment where a product species will be located.
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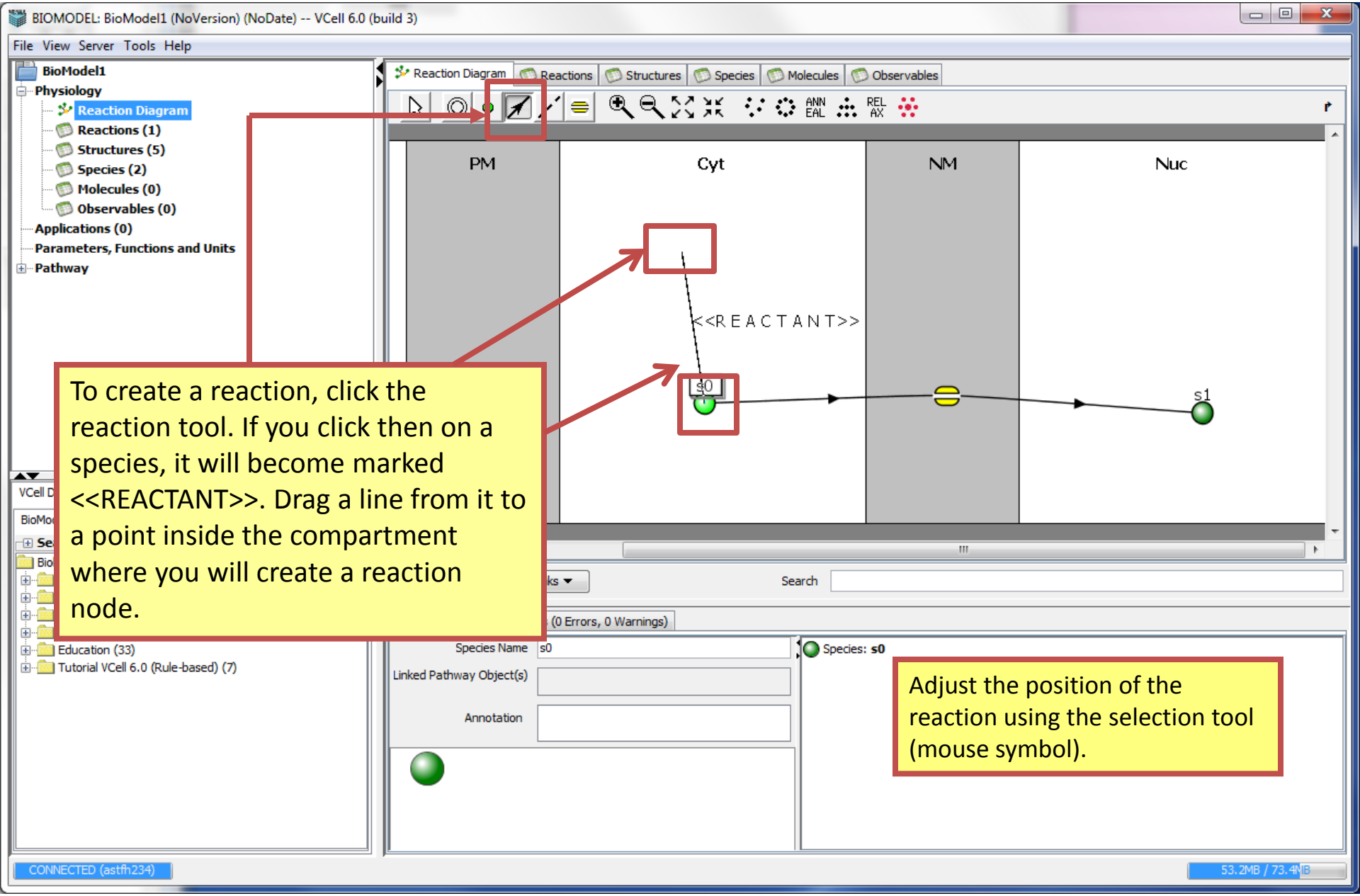
Search
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
58.3MB / 73.4MB

Contents


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Structures (5)
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Applications (0)
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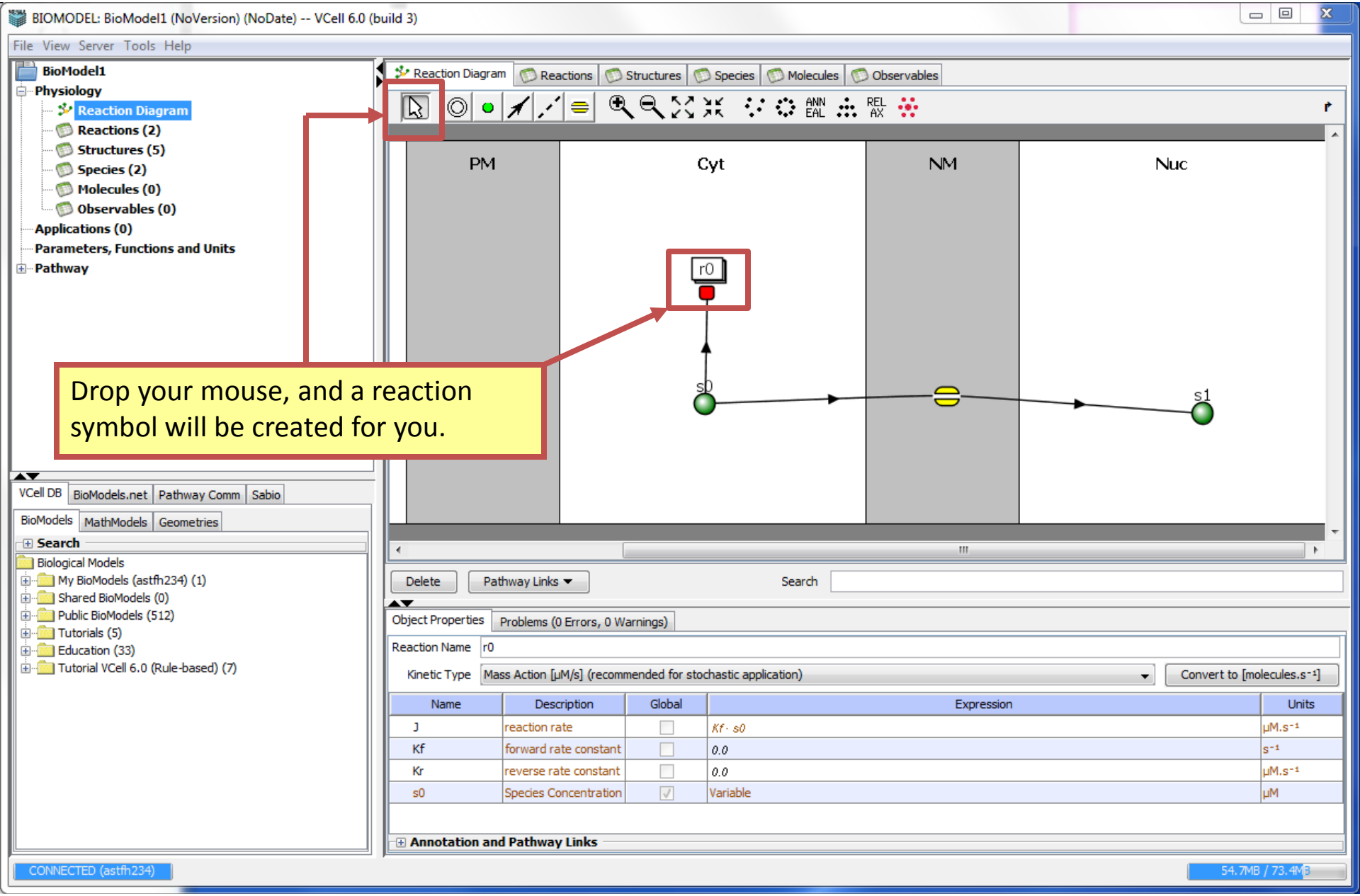
NM
Nuc
<<REACTANT>>
s0
s1
To create a reaction, click the reaction tool. If you click then on a species, it will become marked <<REACTANT>>. Drag a line from it to a point inside the compartment where you will create a reaction node.
Search
(0 Errors, 0 Warnings)
Species Name
s0
Linked Pathway Object(s)
Annotation
Species: s0
Adjust the position of the reaction using the selection tool (mouse symbol).
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
CONNECTED (astfh234)


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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s0
s1
Drop your mouse, and a reaction symbol will be created for you.
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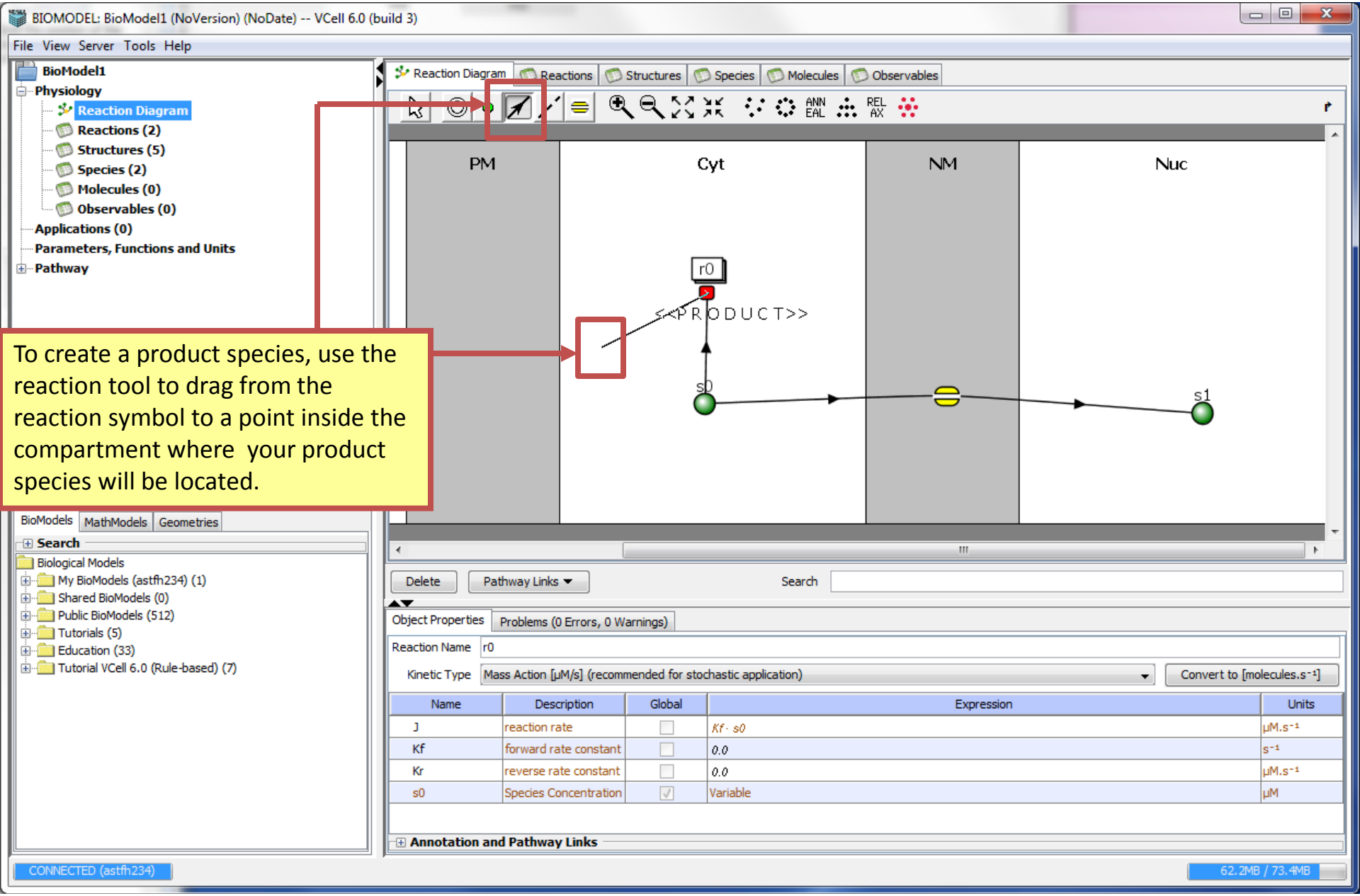
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Reaction Name
r0
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kf· s0
μM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹
Kr
reverse rate constant
0.0
μM.s⁻¹
s0
Species Concentration
Variable
μM
Annotation and Pathway Links
CONNECTED (astfh234)
54.7MB / 73.4MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Molecules (0)
Observables (0)
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Observables
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Cyt
NM
Nuc
r0
<<PRODUCT>>
s0
s1
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.
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Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Reaction Name
r0
Kinetic Type
Mass Action [µM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
Kf· s0
µM.s-1
Kf
forward rate constant
0.0
s-1
Kr
reverse rate constant
0.0
µM.s-1
s0
Species Concentration
Variable
µM
Annotation and Pathway Links
CONNECTED (astfh234)
62.2MB / 73.4MB

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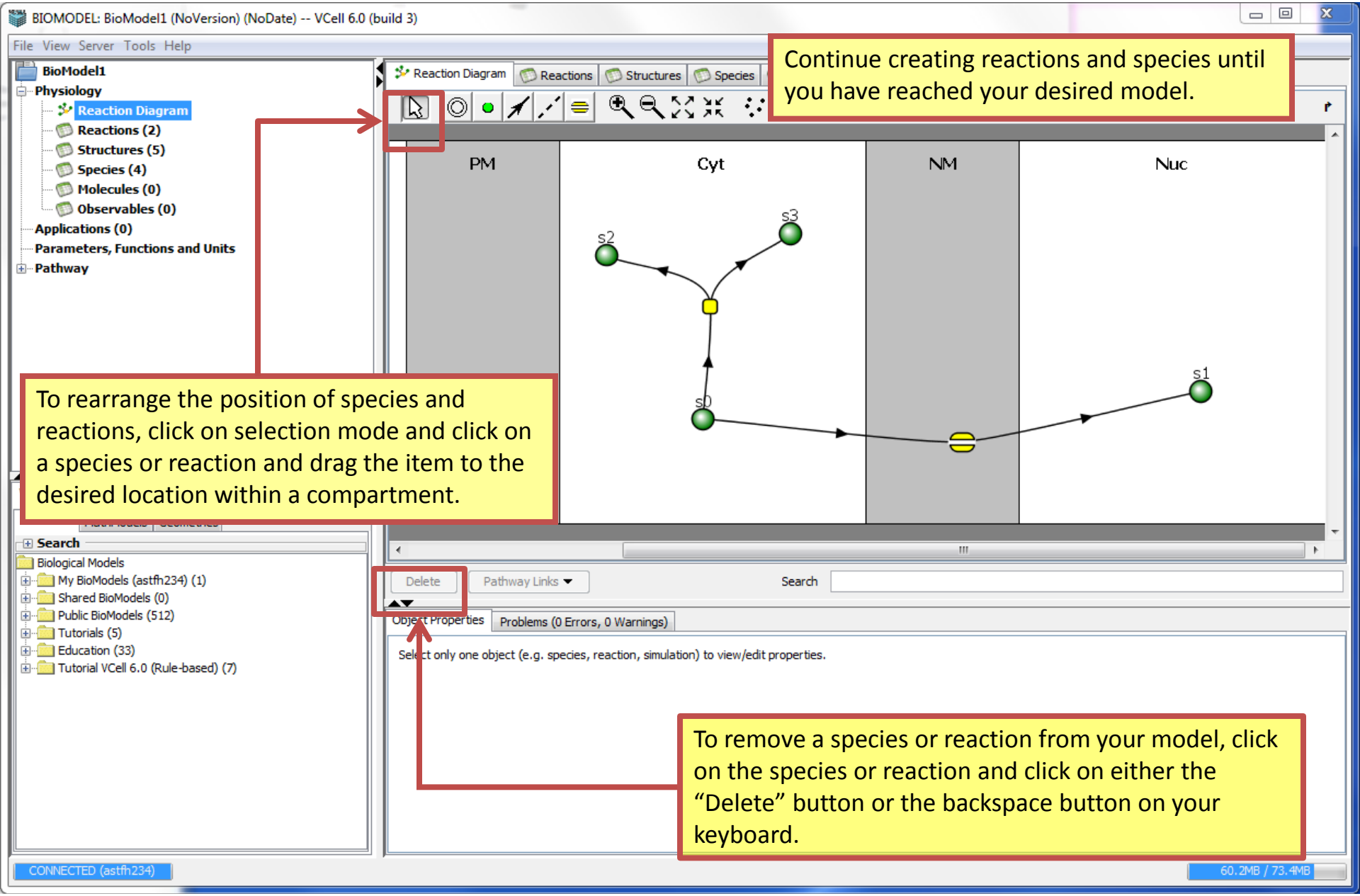
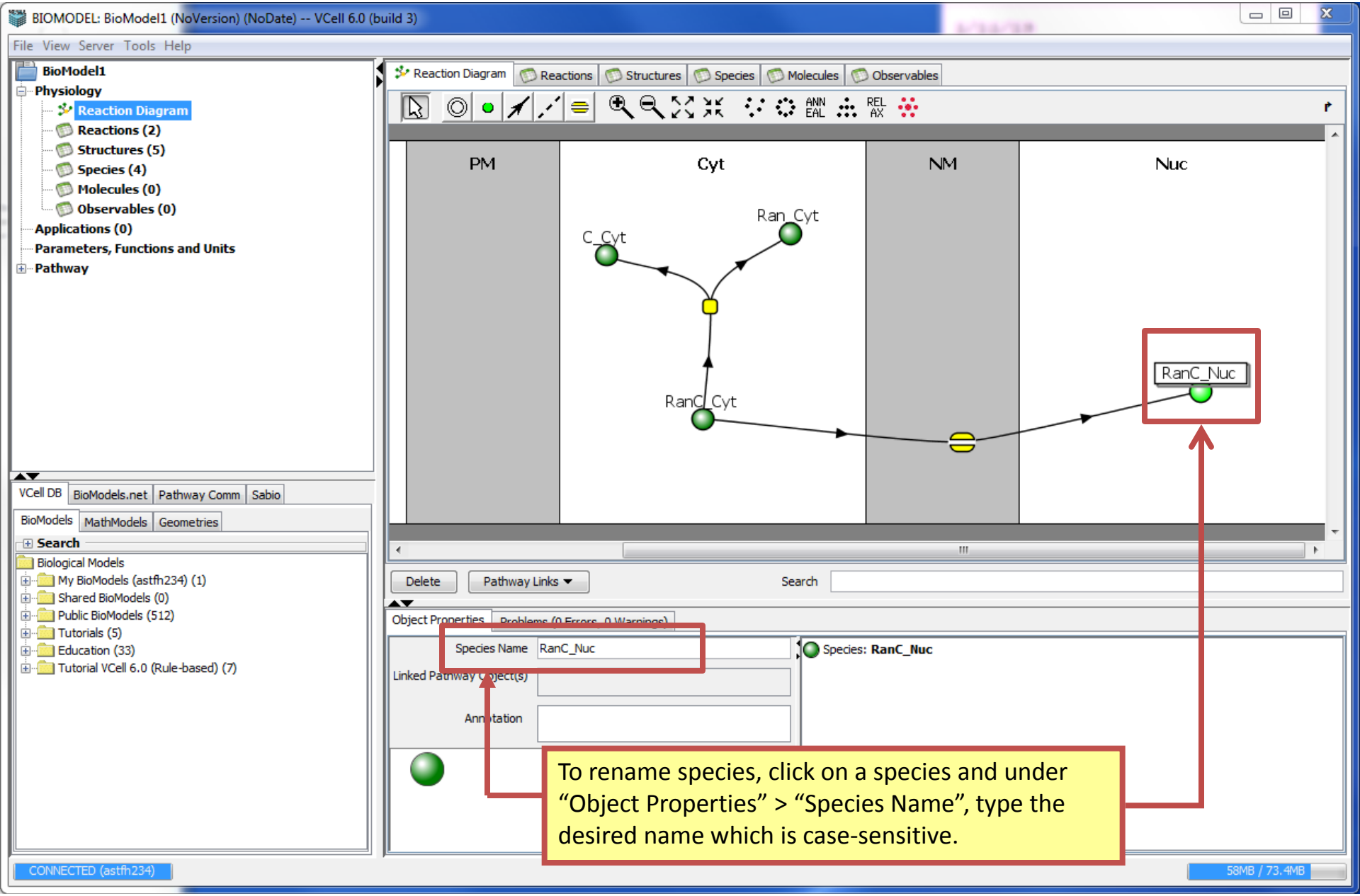


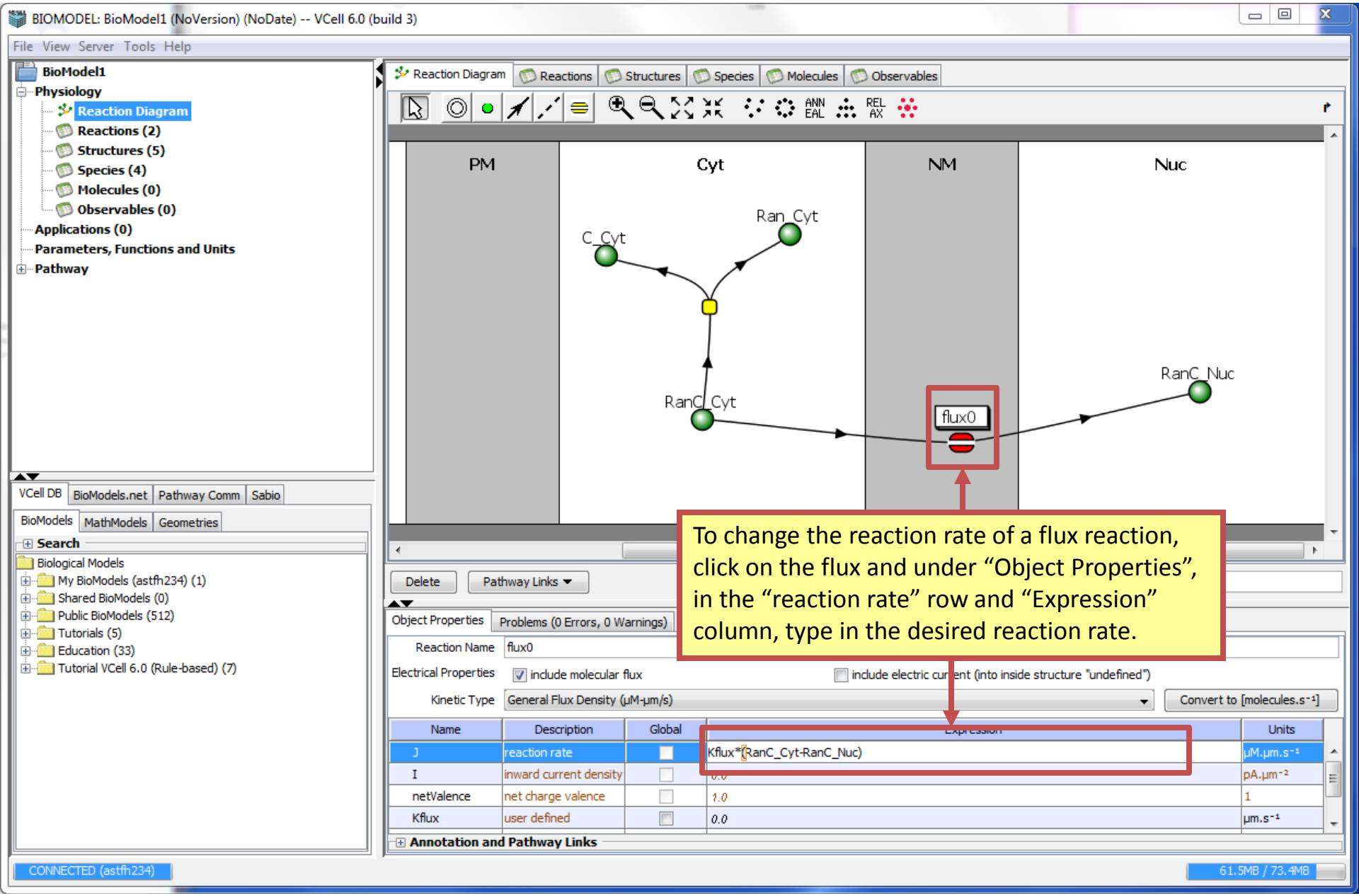
Continue creating reactions and species until you have reached your desired model.

To rearrange the position of species and reactions, click on selection mode and click on a species or reaction and drag the item to the desired location within a compartment.

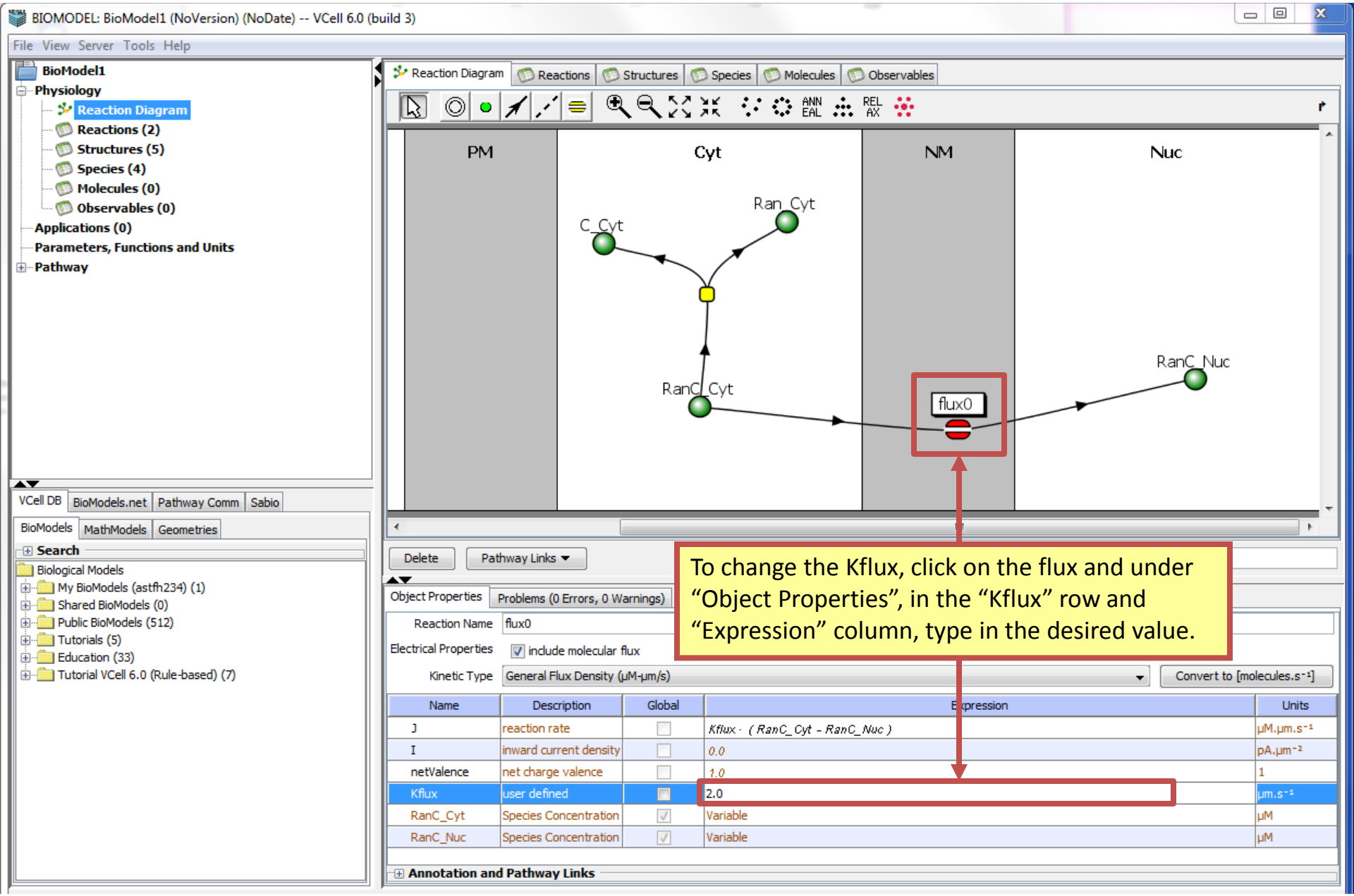
To remove a species or reaction from your model, click on the species or reaction and click on either the “Delete” button or the backspace button on your keyboard.



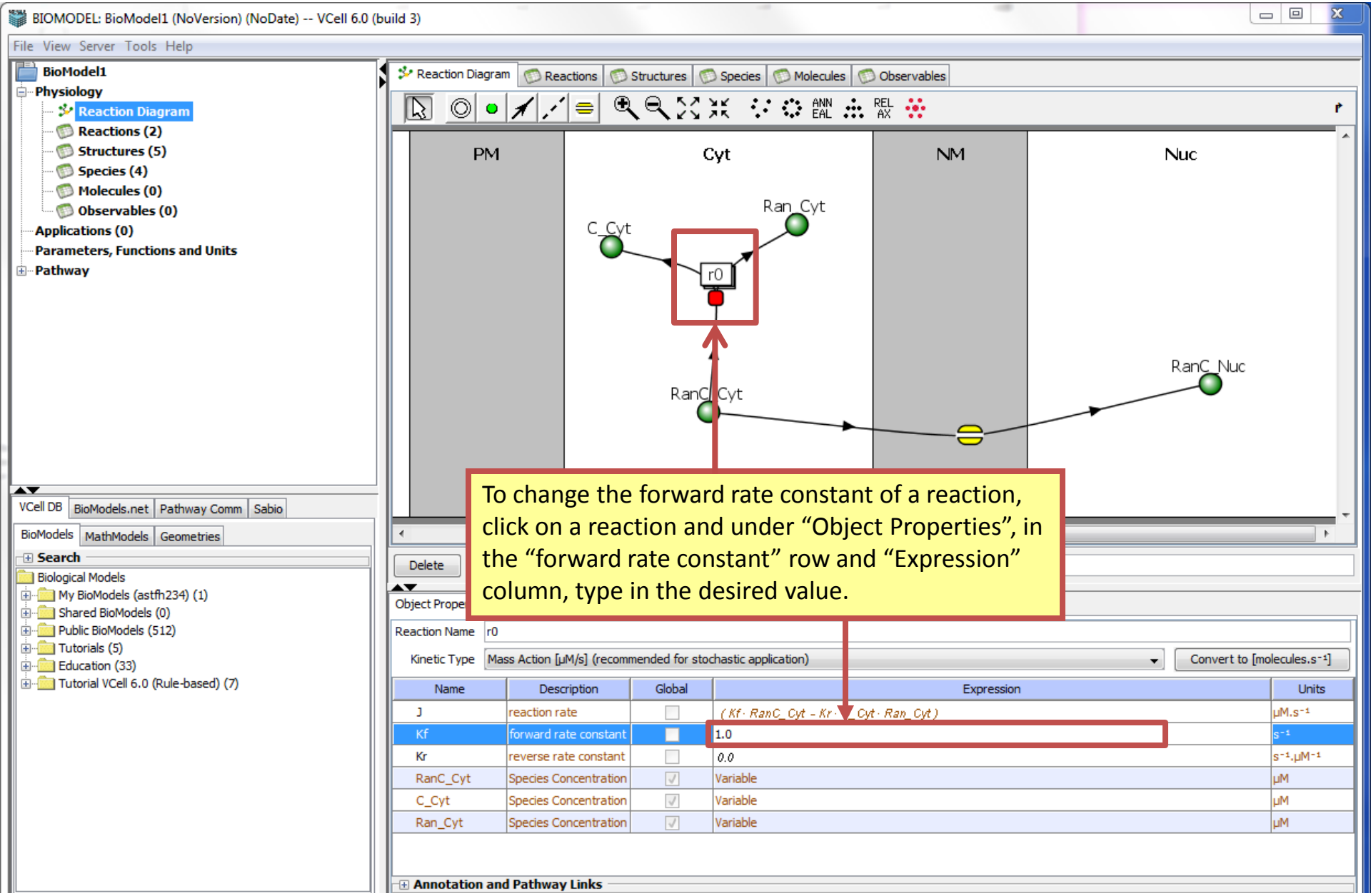
To rename species, click on a species and under “Object Properties” > “Species Name”, type the desired name which is case-sensitive.



To change the reaction rate of a flux reaction, click on the flux and under “Object Properties”, in the “reaction rate” row and “Expression” column, type in the desired reaction rate.



To change the Kflux, click on the flux and under "Object Properties", in the "Kflux" row and "Expression" column, type in the desired value.


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
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Molecules
Observables
PM
Cyt
NM
Nuc
C_Cyt
Ran_Cyt
r0
RanC_Cyt
RanC_Nuc
To change the forward rate constant of a reaction, click on a reaction and under “Object Properties”, in the “forward rate constant” row and “Expression” column, type in the desired value.
Delete
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BioModels.net
Pathway Comm
Sabio
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Public BioModels (512)
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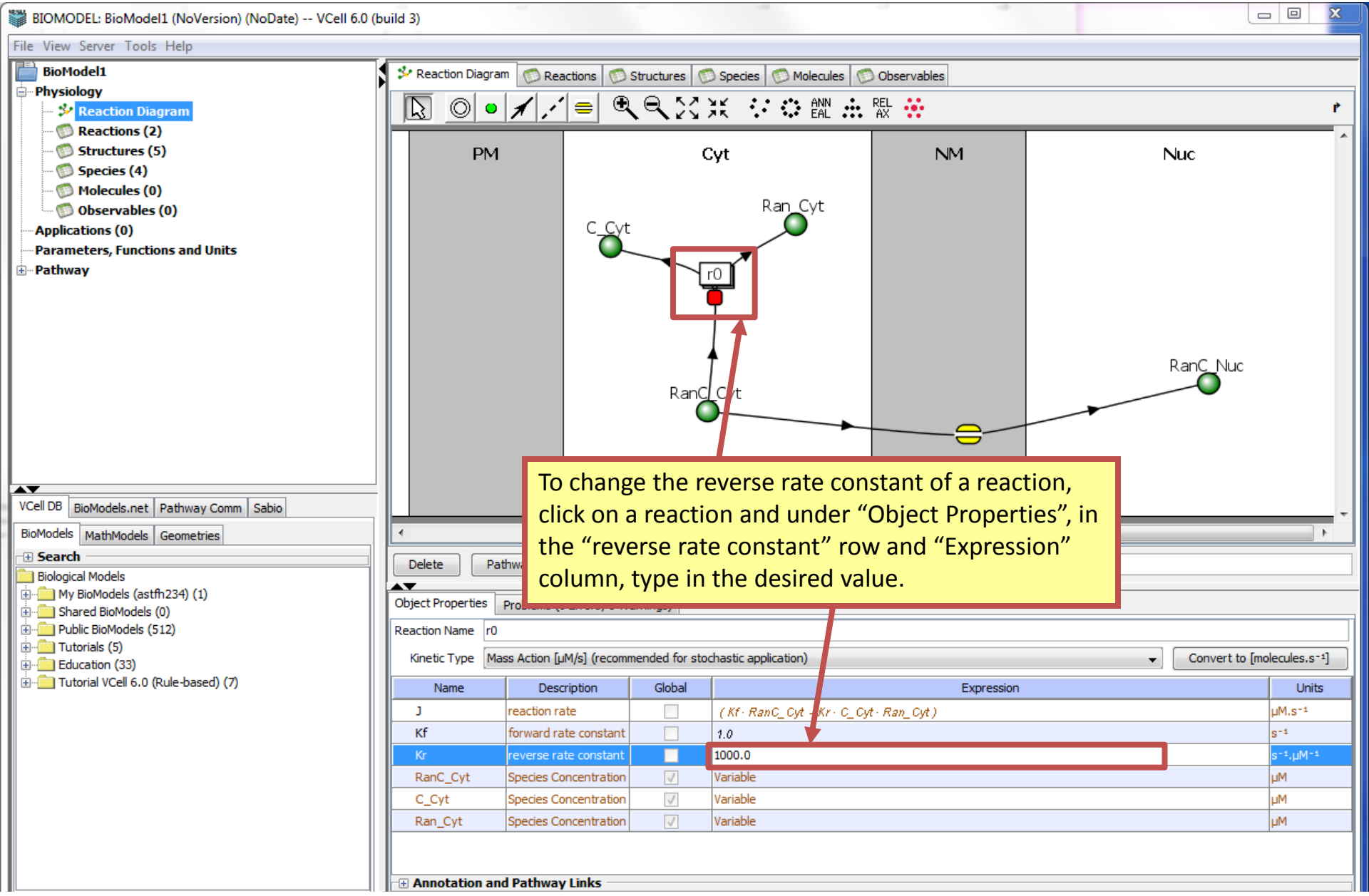
Reaction Name
r0
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
(Kf · RanC_Cyt - Kr · C_Cyt · Ran_Cyt)
μM.s-1
Kf
forward rate constant
1.0
s-1
Kr
reverse rate constant
0.0
s-1.μM-1
RanC_Cyt
Species Concentration
Variable
μM
C_Cyt
Species Concentration
Variable
μM
Ran_Cyt
Species Concentration
Variable
μM
Annotation and Pathway Links


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Species (4)
Molecules (0)
Observables (0)
Applications (0)
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Species
Molecules
Observables
PM
Cyt
NM
Nuc
Ran_Cyt
C_Cyt
r0
RanC_Cyt
RanC_Nuc
To change the reverse rate constant of a reaction, click on a reaction and under “Object Properties”, in the “reverse rate constant” row and “Expression” column, type in the desired value.
VCell DB
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My BioModels (astfh234) (1)
Shared BioModels (0)
Public BioModels (512)
Tutorials (5)
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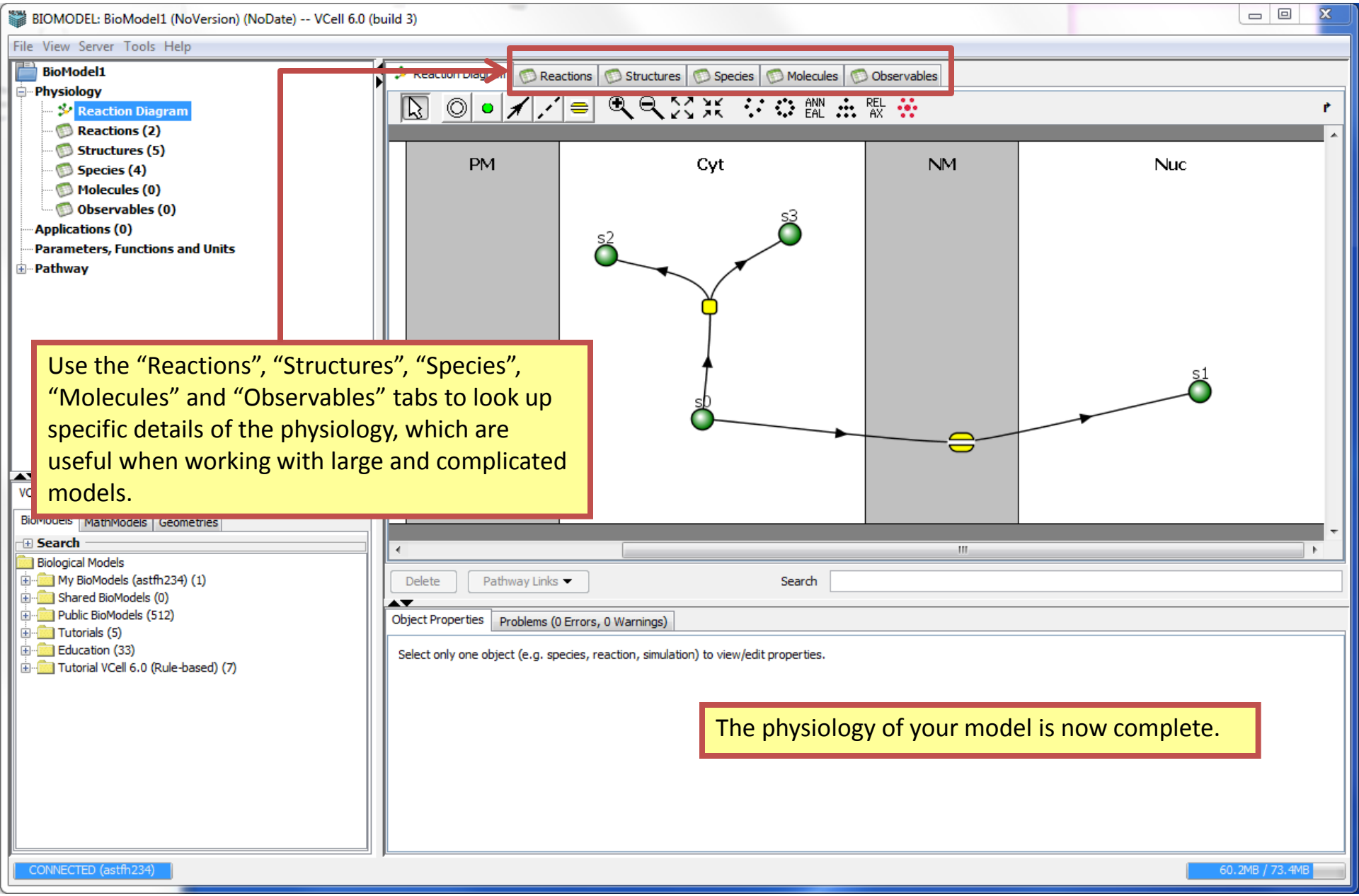
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Object Properties
Reaction Name r0
Kinetic Type Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name Description Global Expression Units
J reaction rate (Kf · RanC_Cyt - Kr · C_Cyt · Ran_Cyt) μM.s-1
Kf forward rate constant 1.0 s-1
Kr reverse rate constant 1000.0 s-1.μM-1
RanC_Cyt Species Concentration Variable μM
C_Cyt Species Concentration Variable μM
Ran_Cyt Species Concentration Variable μM
Annotation and Pathway Links


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Cyt
NM
Nuc
s0
s1
s2
s3
Use the “Reactions”, “Structures”, “Species”, “Molecules” and “Observables” tabs to look up specific details of the physiology, which are useful when working with large and complicated models.
BioModels
MathModels
Geometries
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My BioModels (astfh234) (1)
Shared BioModels (0)
Public BioModels (512)
Tutorials (5)
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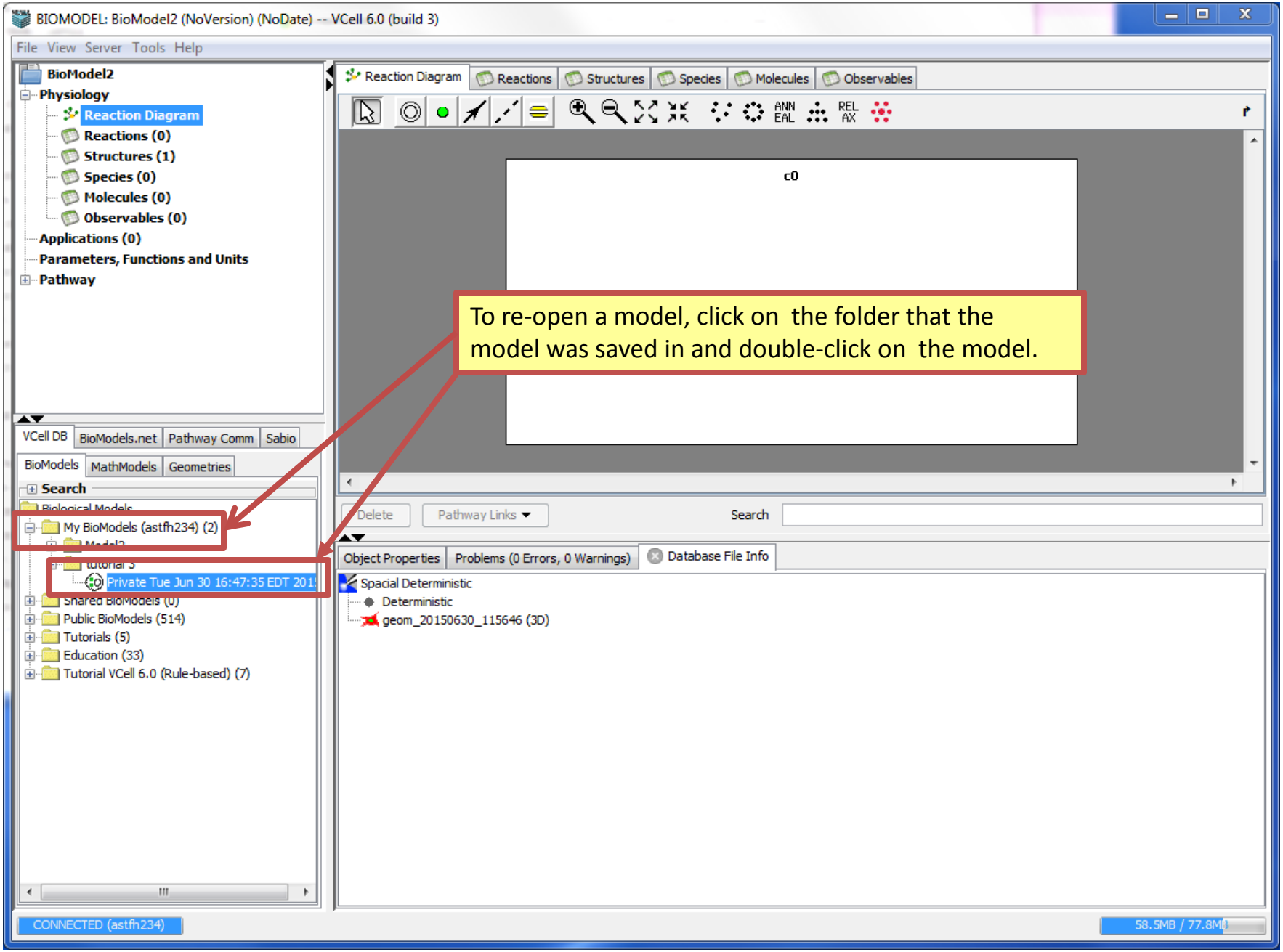
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
The physiology of your model is now complete.
CONNECTED (astfh234)
60.2MB / 73.4MB


BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
File View Server 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
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Sabio
BioModels
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Geometries
Search
My BioModels (astfh234) (2)
Private Tue Jun 30 16:47:35 EDT 201
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
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Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Spacial Deterministic
Deterministic
geom_20150630_115646 (3D)
CONNECTED (astfh234)
58.5MB / 77.8MB

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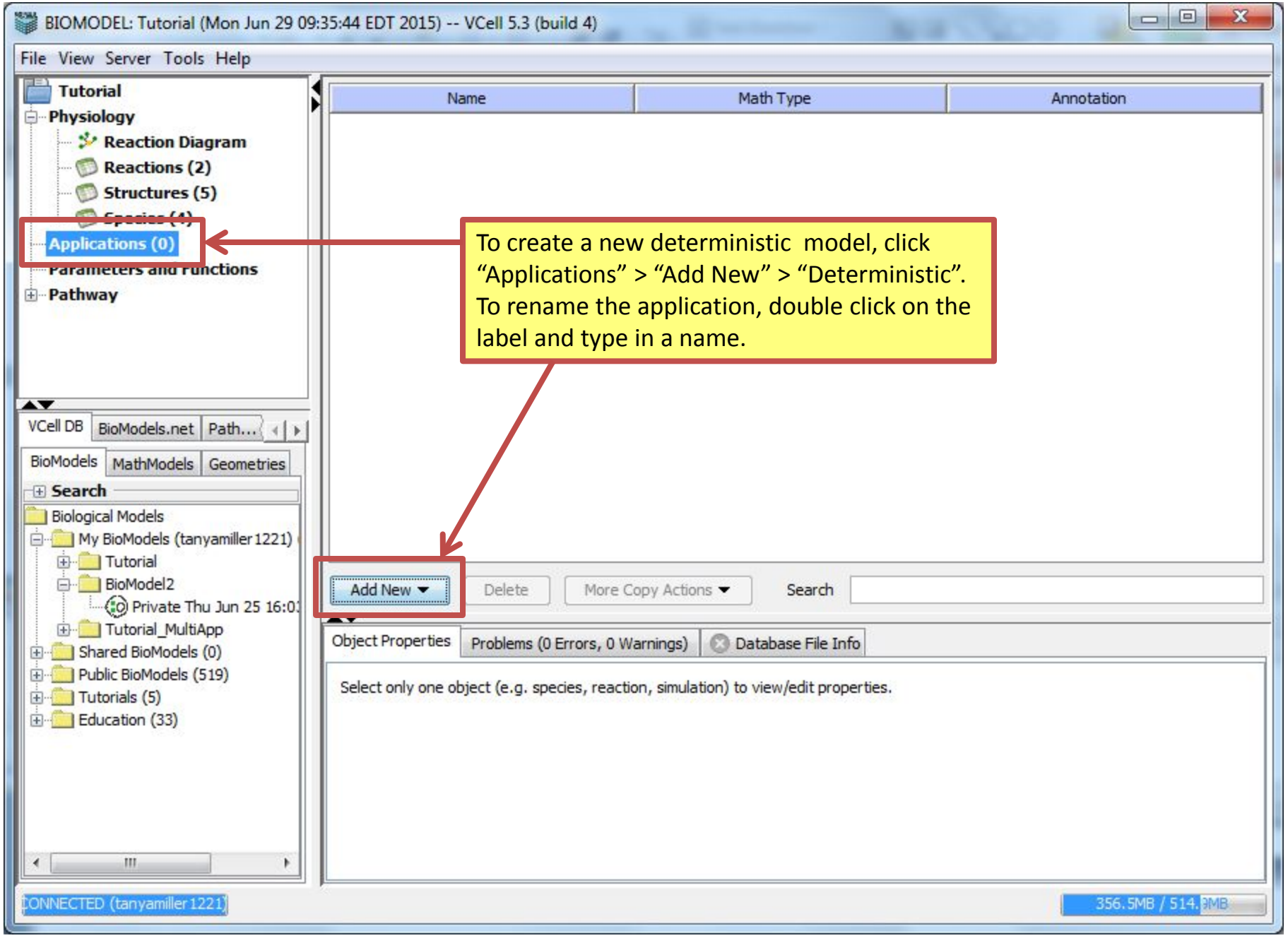
BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
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Reactions (2)
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Applications (0)
Pathway
Name
Math Type
Annotation
To create a new deterministic model, click "Applications" > "Add New" > "Deterministic". To rename the application, double click on the label and type in a name.
VCell DB
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Add New
Delete
More Copy Actions
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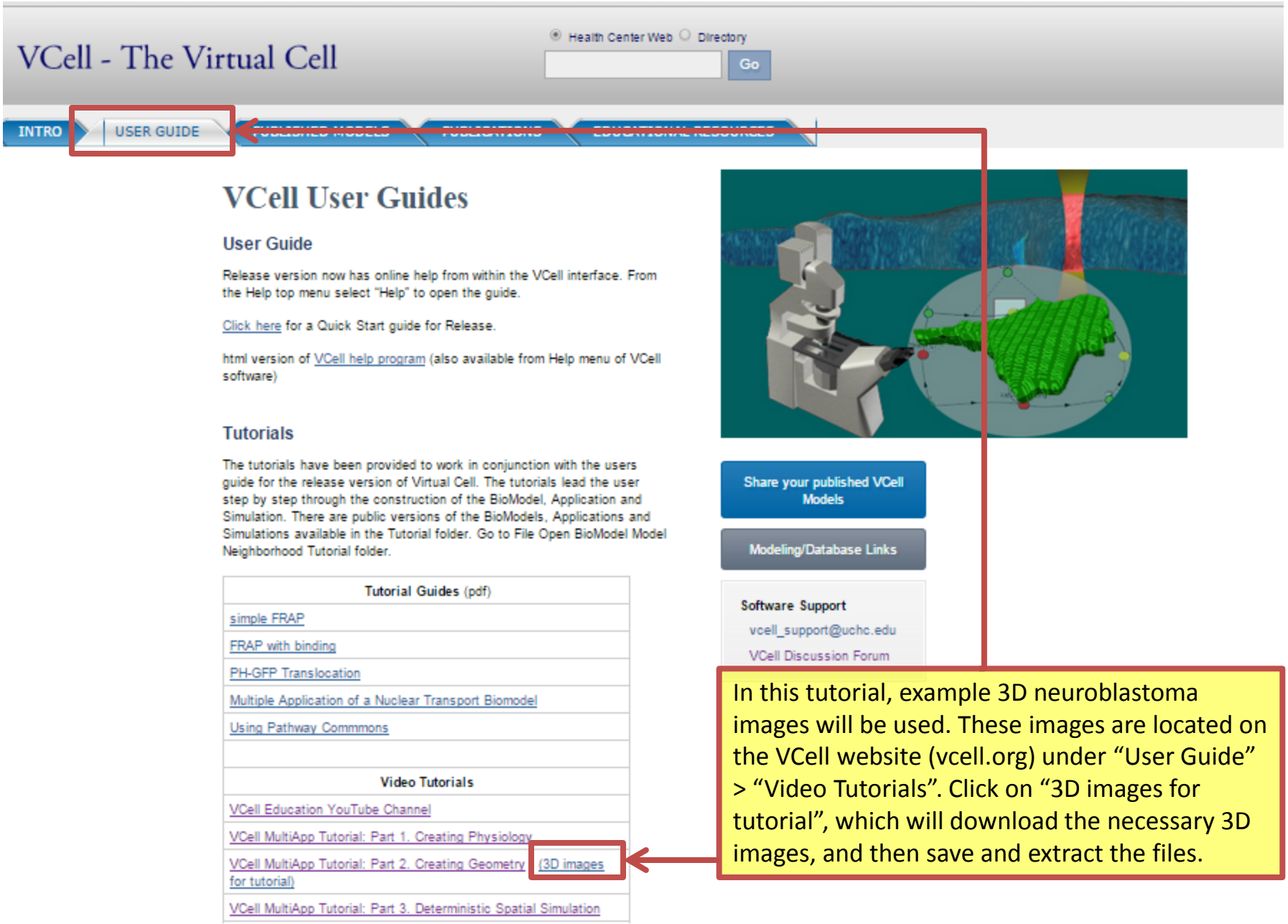
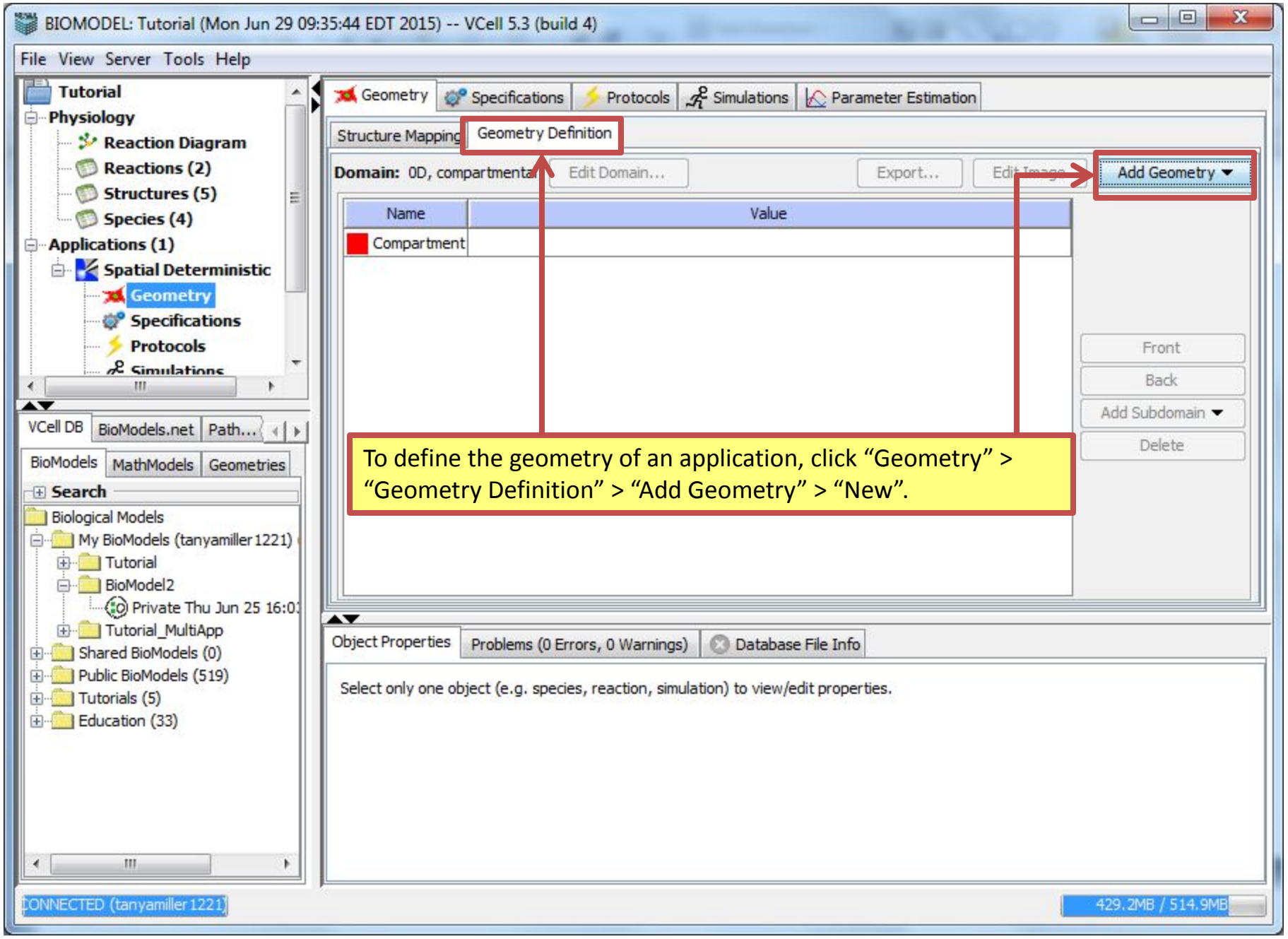
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
356.5MB / 514.3MB



In this tutorial, example 3D neuroblastoma images will be used. These images are located on the VCell website (vcell.org) under "User Guide" > "Video Tutorials". Click on "3D images for tutorial", which will download the necessary 3D images, and then save and extract the files.


BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Applications (1)
Spatial Deterministic
Geometry
Specifications
Protocols
Simulations
VCell DB
BioModels.net
Path...
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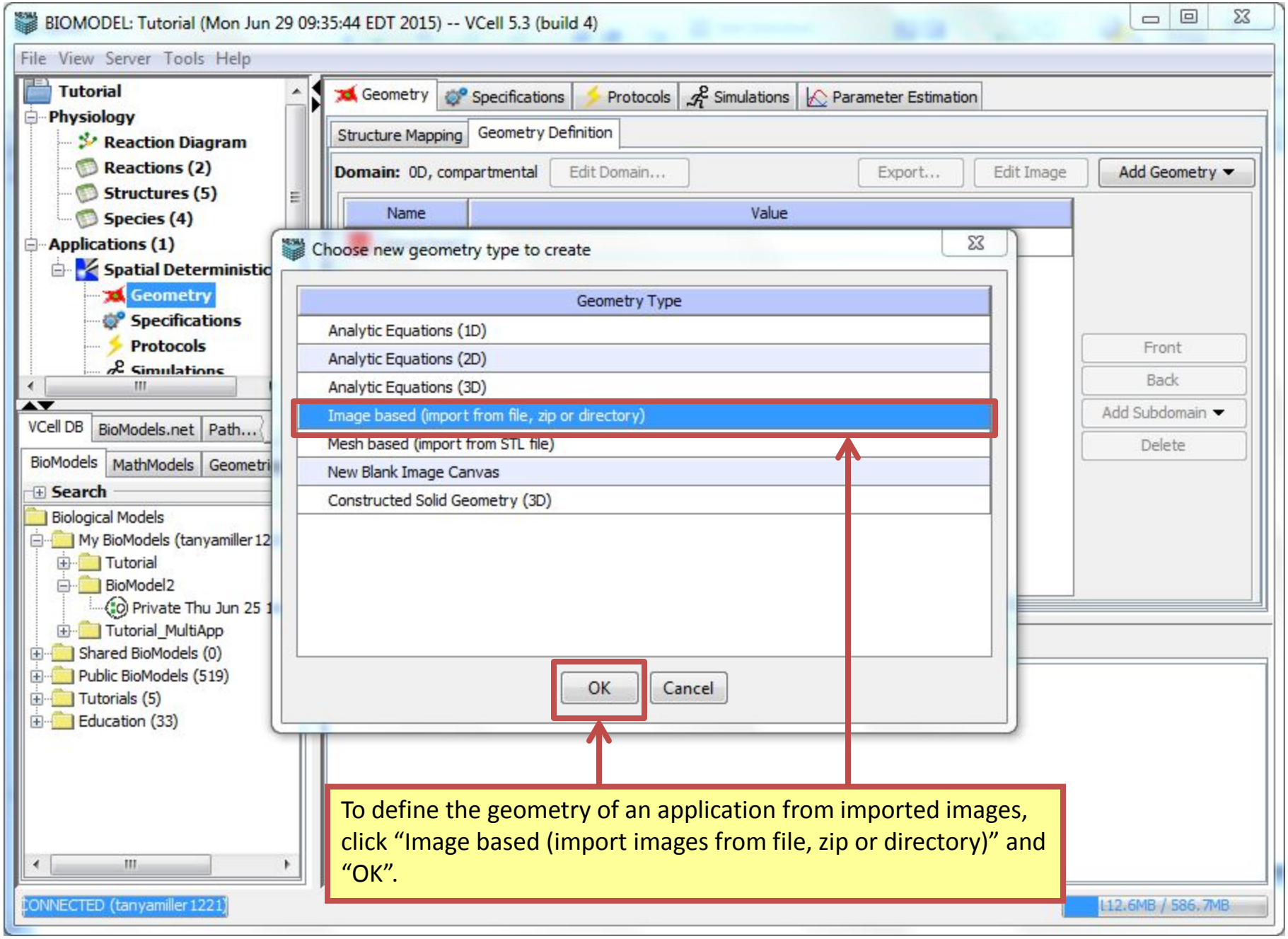
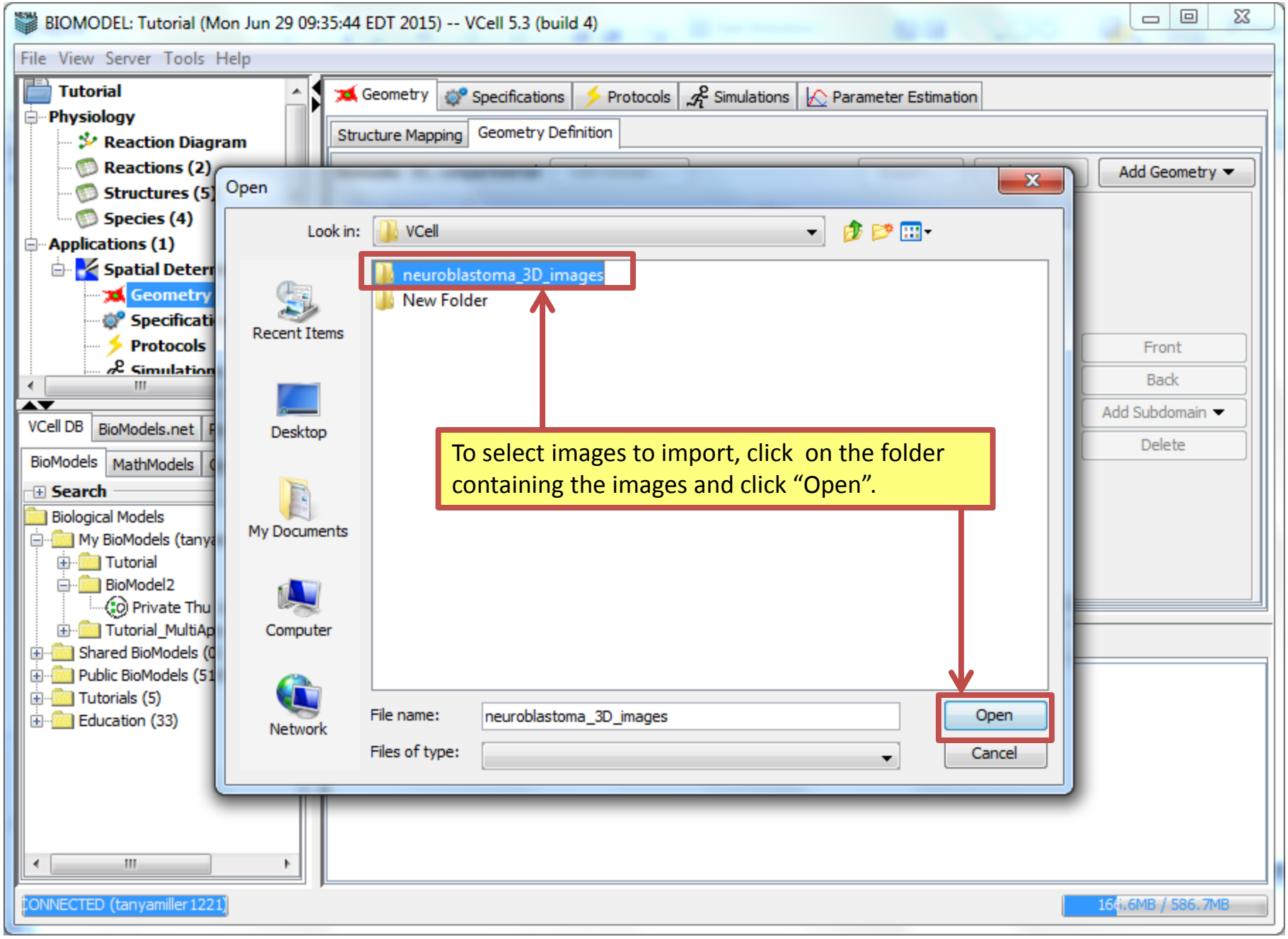
Search
Biological Models
My BioModels (tanyamiller1221)
Tutorial
BioModel2
Private Thu Jun 25 16:0
Tutorial_MultiApp
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image...
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
To define the geometry of an application, click “Geometry” > “Geometry Definition” > “Add Geometry” > “New”.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
429.2MB / 514.9MB

Contents



To define the geometry of an application from imported images, click “Image based (import images from file, zip or directory)” and “OK”.

Contents


BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
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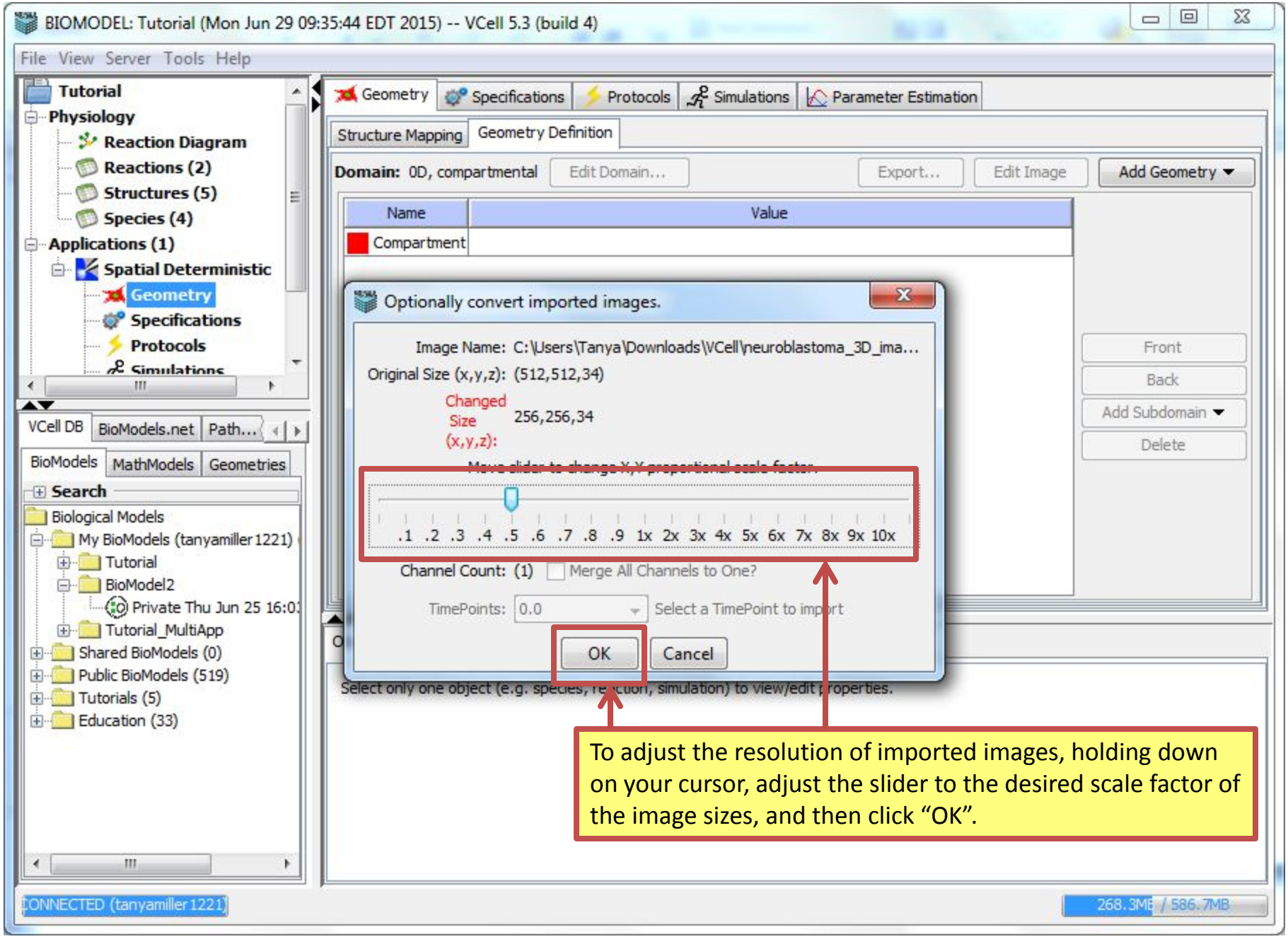
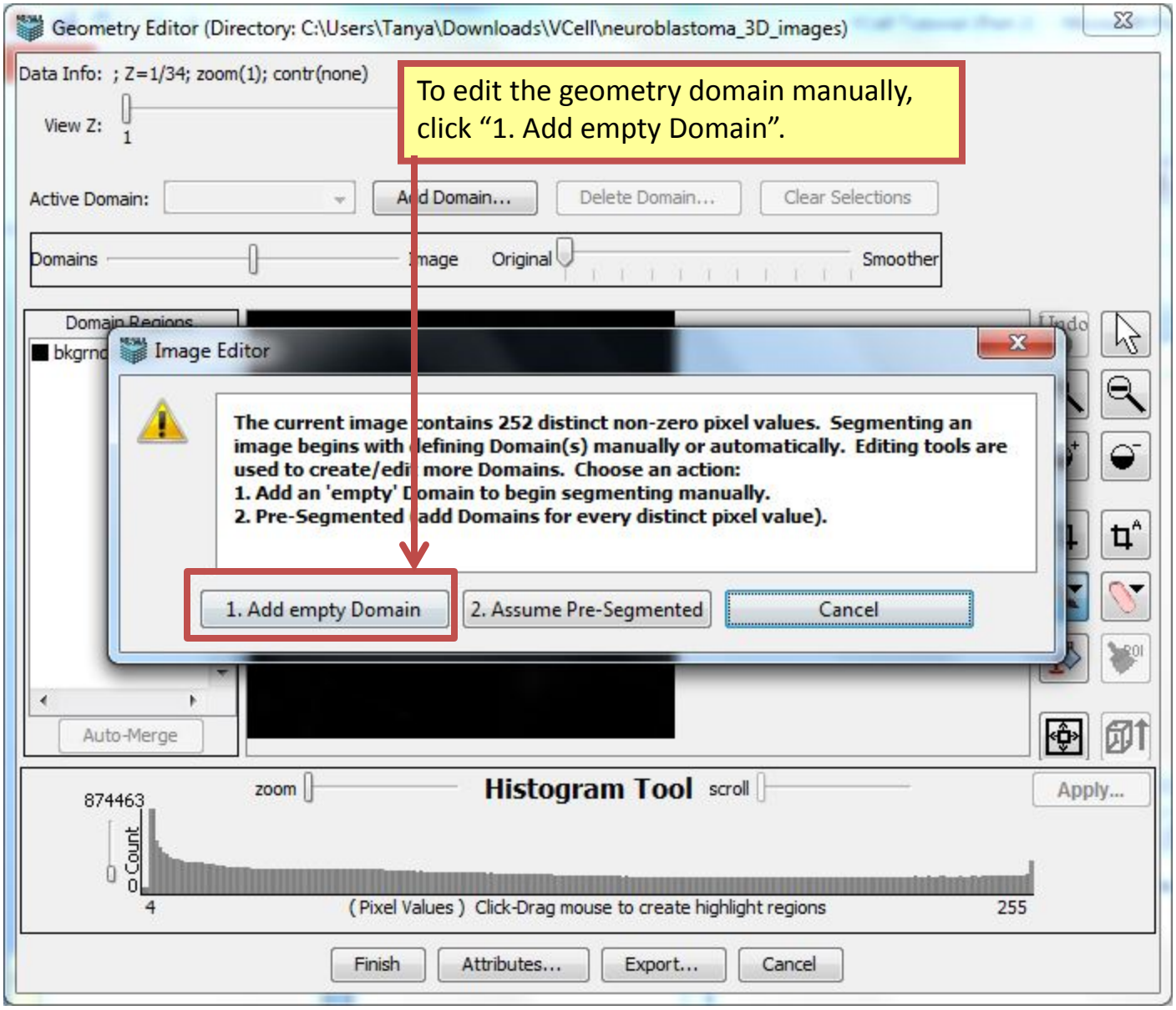
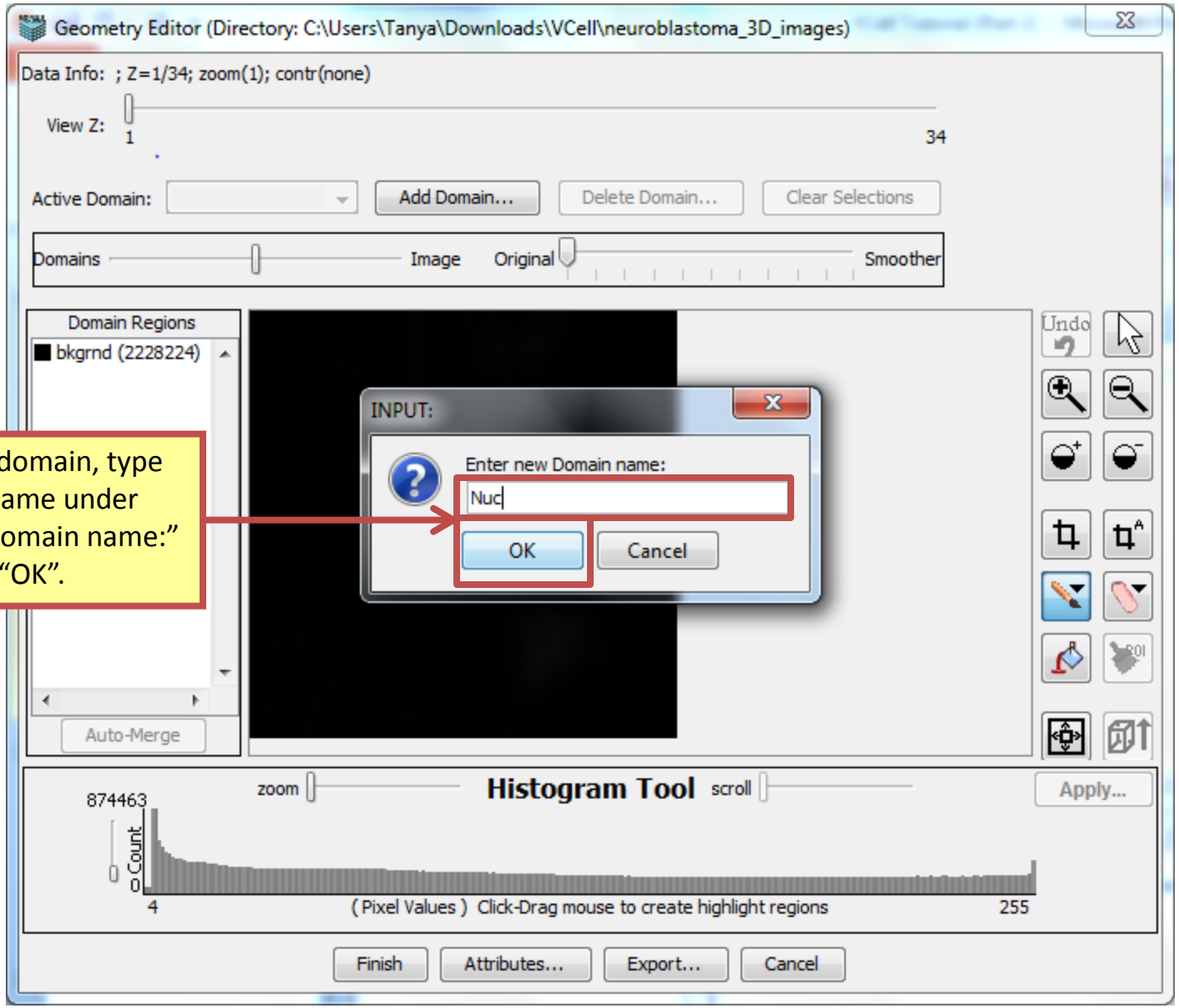
Geometry Definition
Add Geometry
Front
Back
Add Subdomain
Delete
Open
Look in:
VCell
neuroblastoma_3D_images
New Folder
Recent Items
Desktop
My Documents
Computer
Network
To select images to import, click on the folder containing the images and click “Open”.
File name:
neuroblastoma_3D_images
Files of type:
Open
Cancel
CONNECTED (tanyamiller1221)
164.6MB / 586.7MB

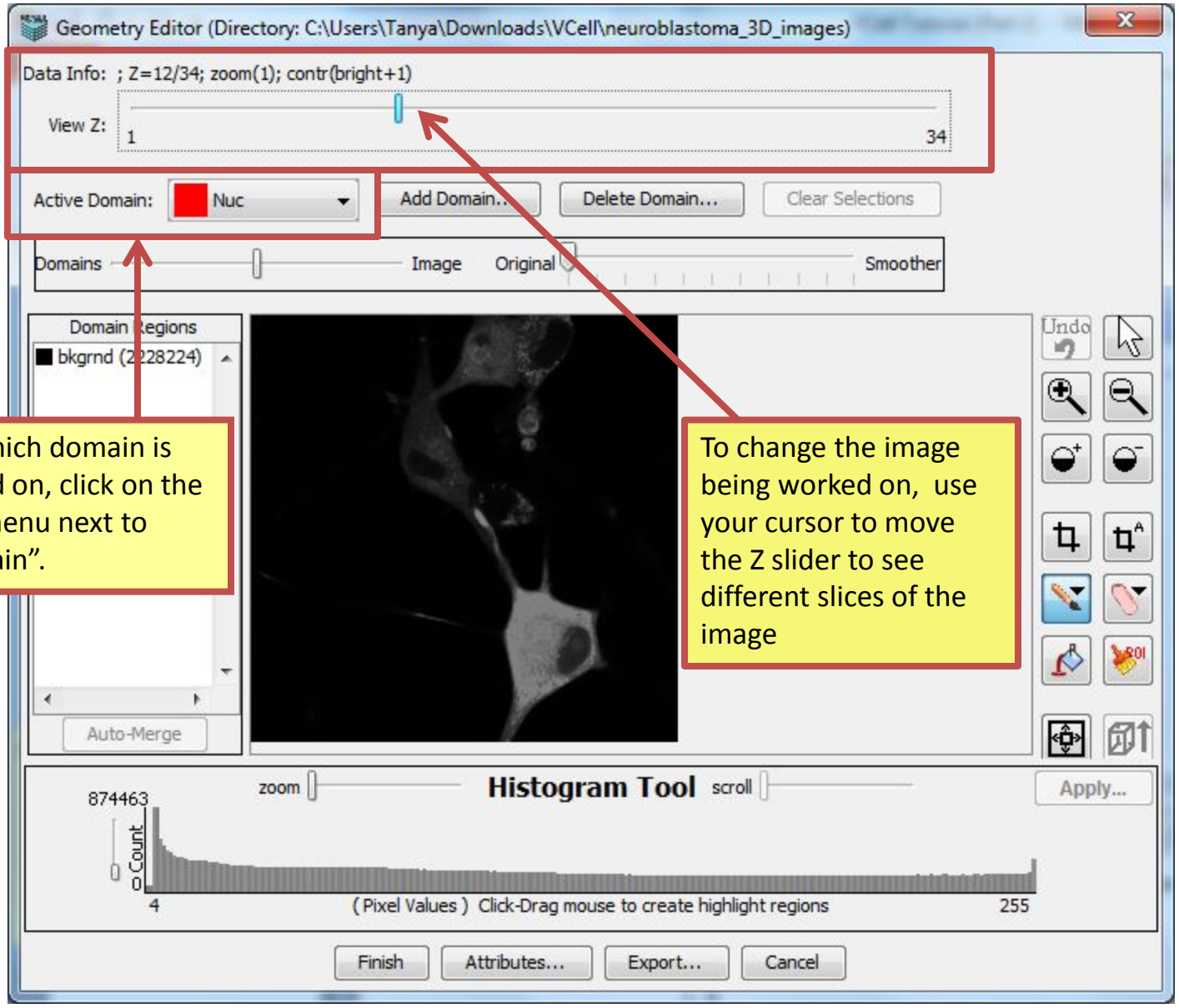


To adjust the resolution of imported images, holding down on your cursor, adjust the slider to the desired scale factor of the image sizes, and then click “OK”.


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=1/34; zoom(1); contr(none)
View Z:
1
To edit the geometry domain manually, click “1. Add empty Domain”.
Active Domain:
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd
Image Editor
The current image contains 252 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
Undo
Auto-Merge
zoom
Histogram Tool
scroll
Apply...
874463
Count
0
4
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

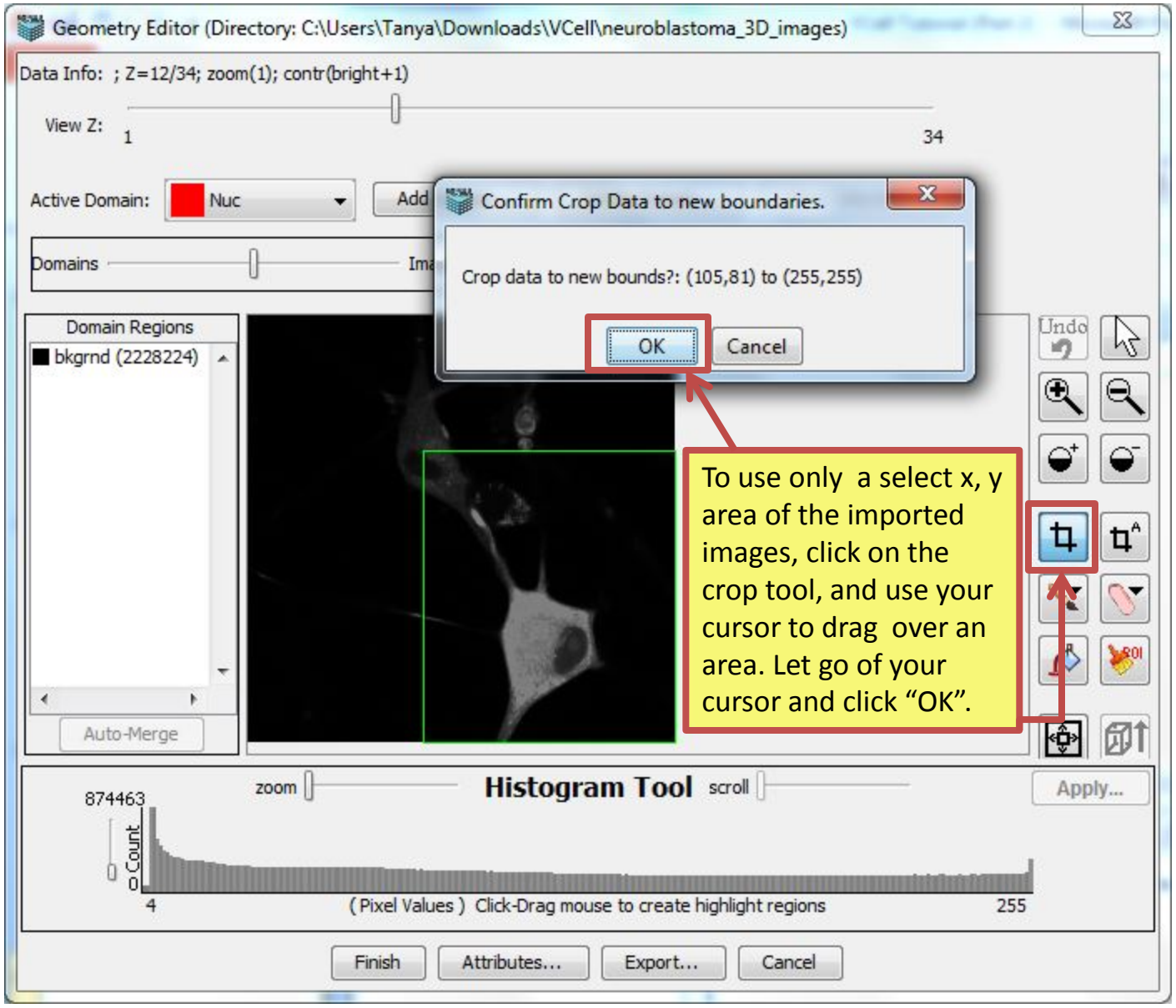


To name the domain, type the domain name under "Enter new Domain name:" and the click "OK".

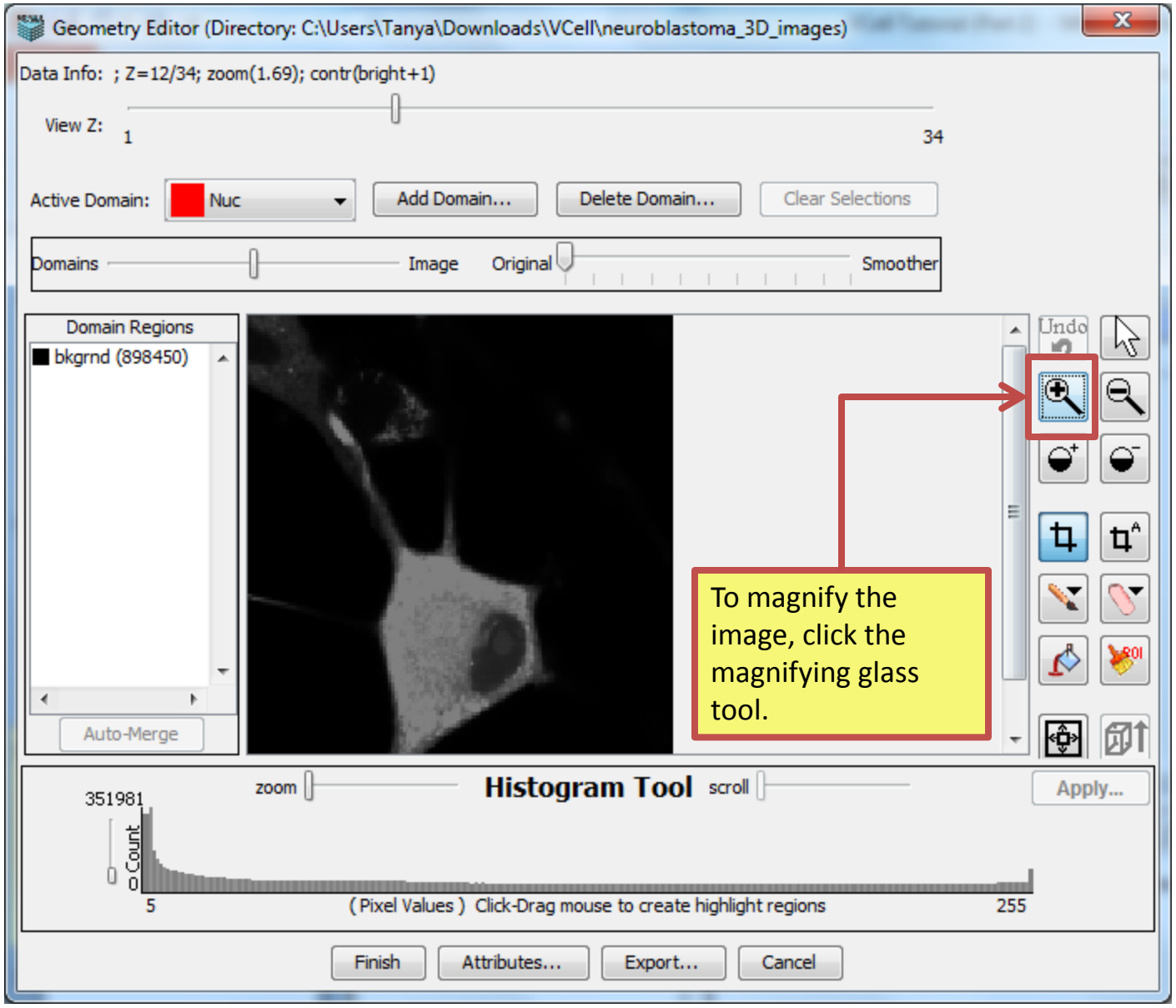


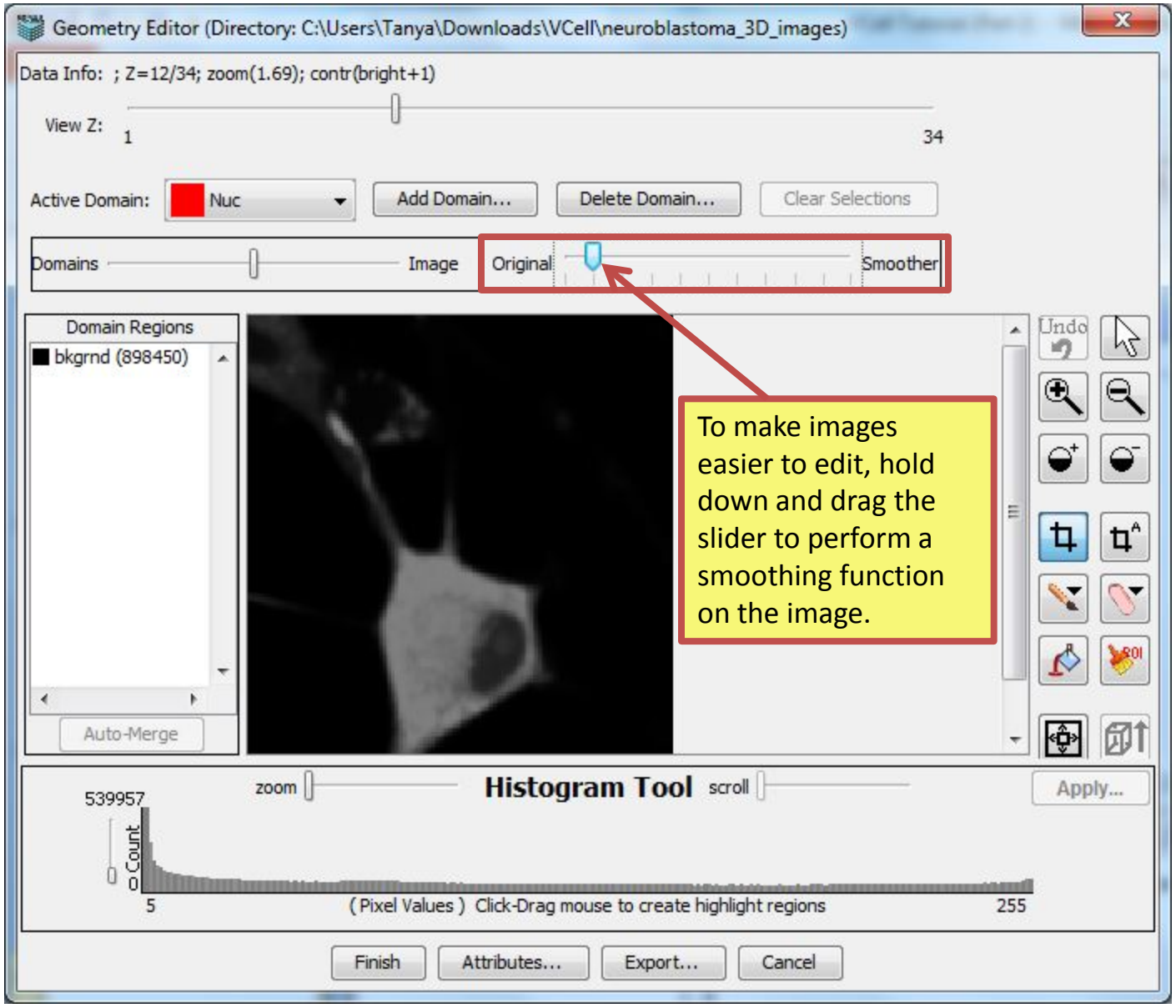
To change which domain is being worked on, click on the drop down menu next to "Active Domain".

To change the image being worked on, use your cursor to move the Z slider to see different slices of the image

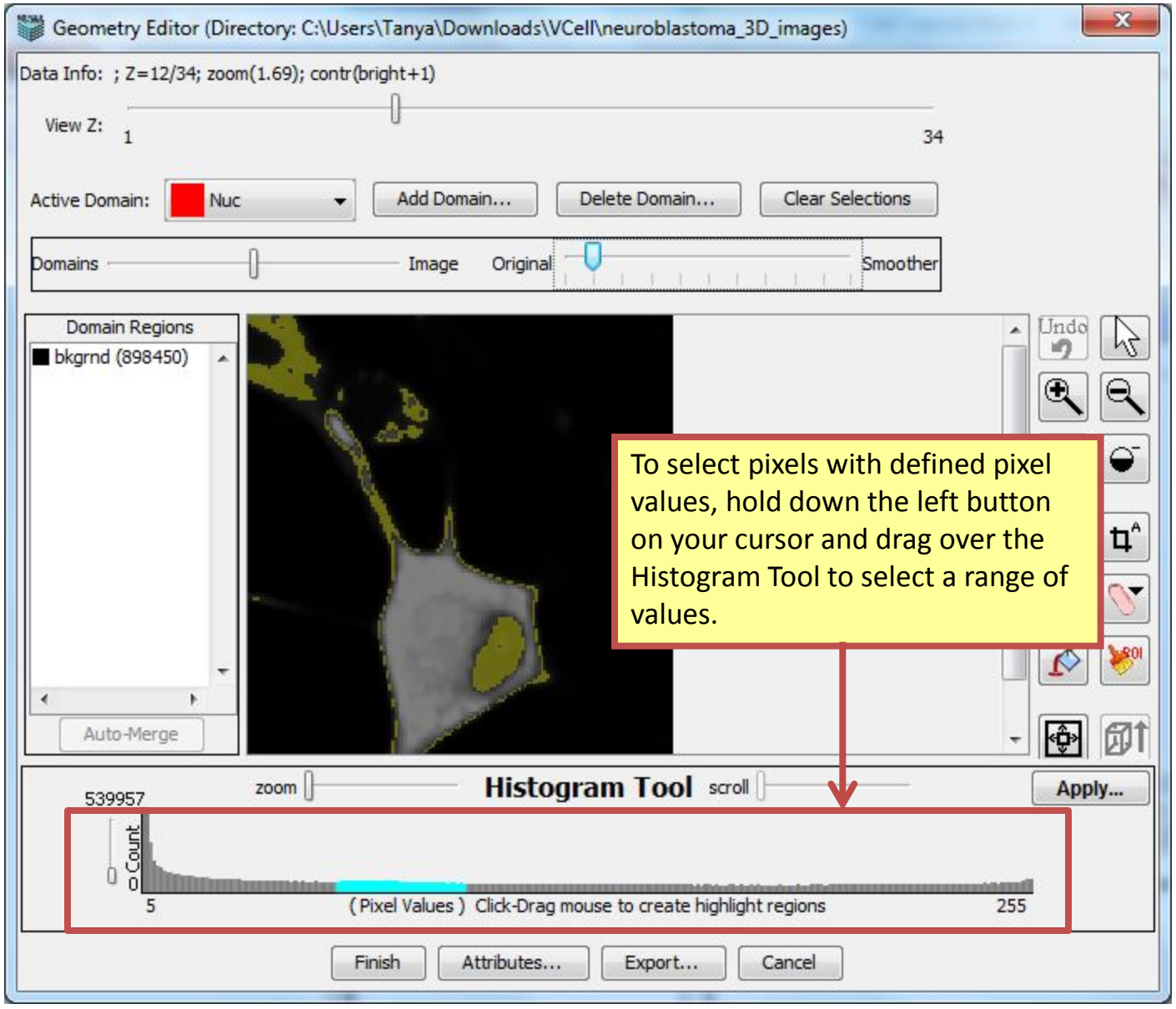

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add
Domains
Confirm Crop Data to new boundaries.
Crop data to new bounds?: (105,81) to (255,255)
OK
Cancel
Domain Regions
bkgrnd (2228224)
Auto-Merge
Undo
To use only a select x, y area of the imported images, click on the crop tool, and use your cursor to drag over an area. Let go of your cursor and click "OK".
zoom
Histogram Tool
scroll
Apply...
874463
Count
0
4
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

Contents

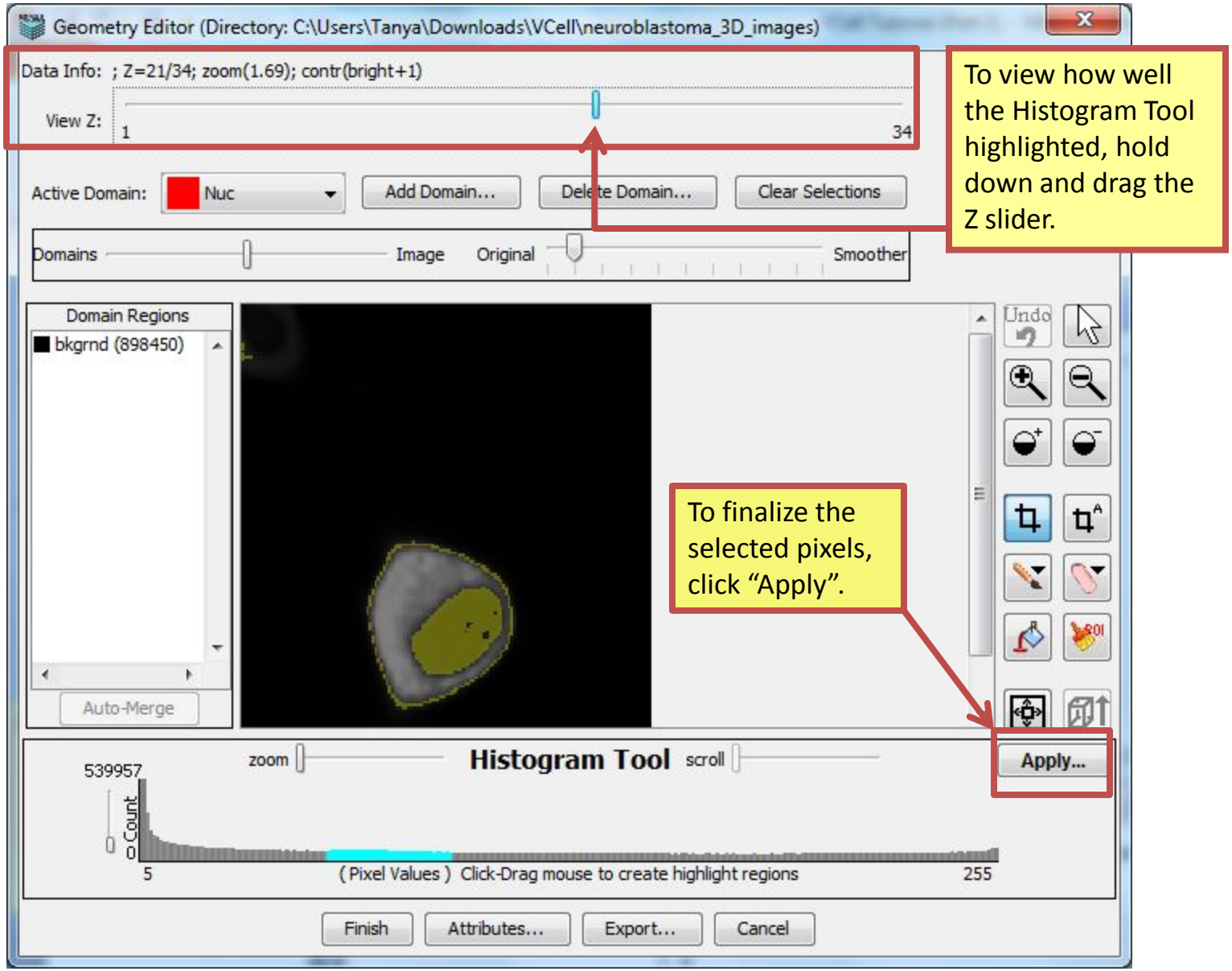

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To magnify the image, click the magnifying glass tool.
zoom
Histogram Tool
scroll
Apply...
351981
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

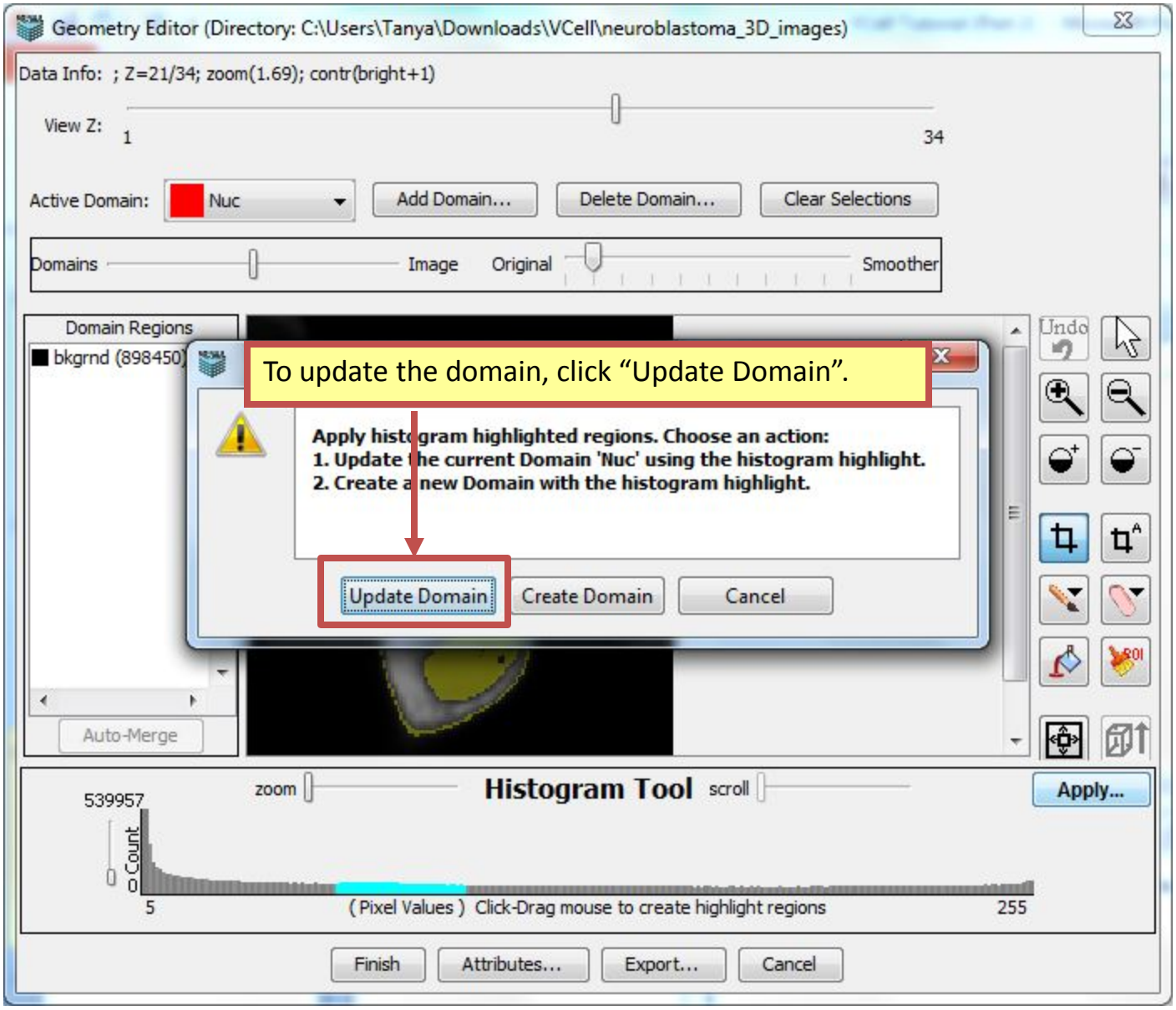

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To make images easier to edit, hold down and drag the slider to perform a smoothing function on the image.
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

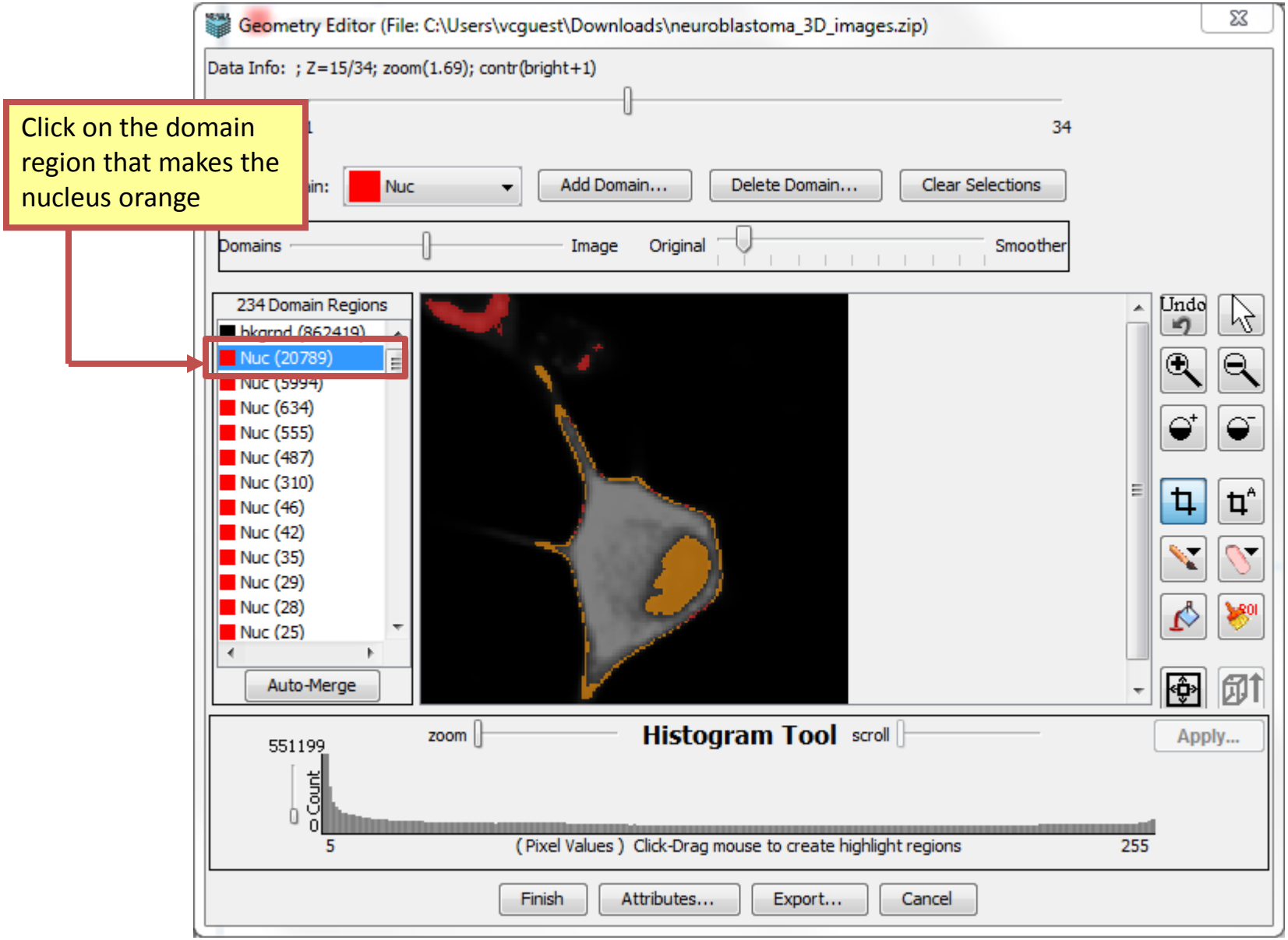
Contents

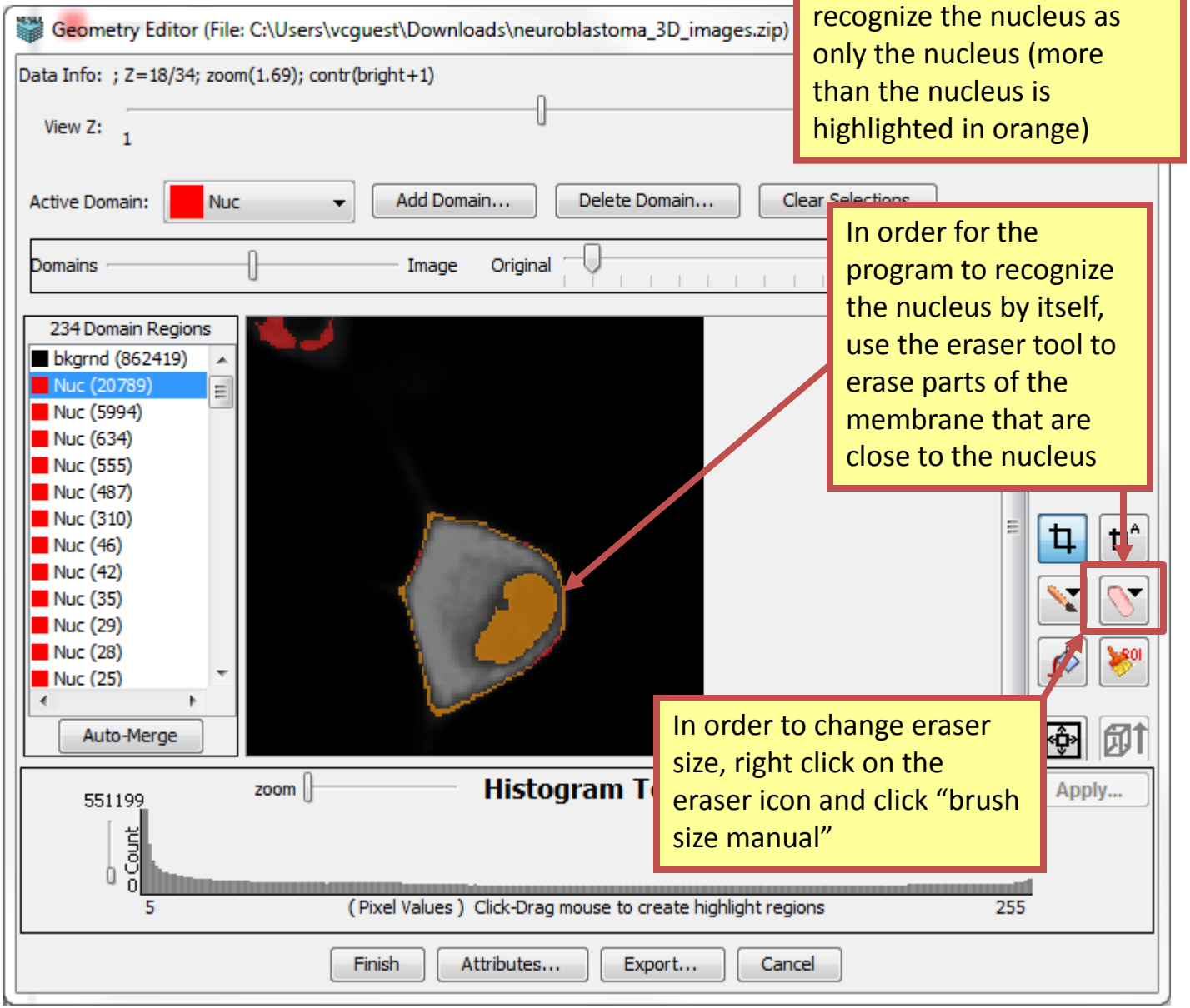

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To select pixels with defined pixel values, hold down the left button on your cursor and drag over the Histogram Tool to select a range of values.
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

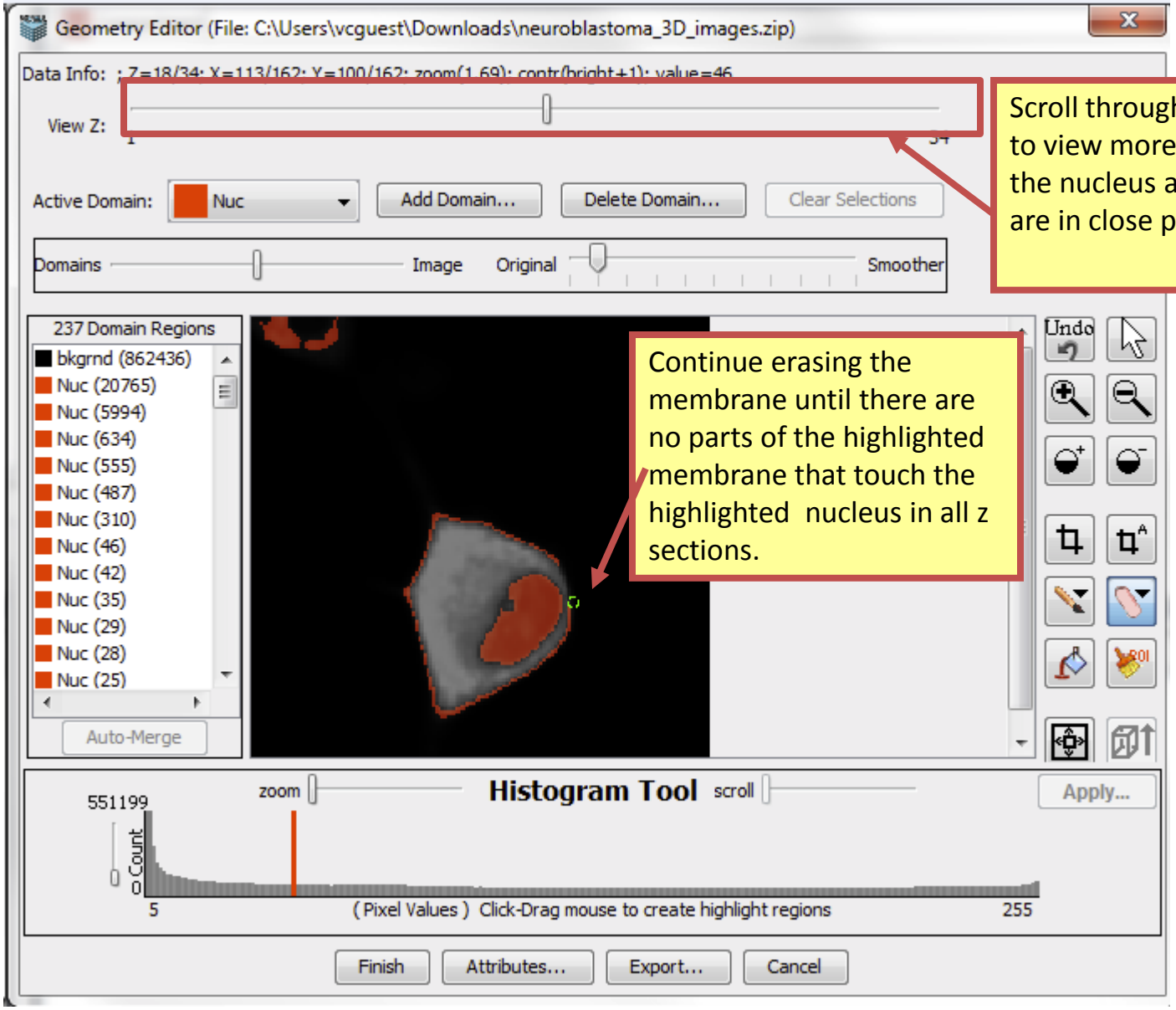
Contents


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=21/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To view how well the Histogram Tool highlighted, hold down and drag the Z slider.
To finalize the selected pixels, click “Apply”.
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=21/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
To update the domain, click "Update Domain".
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
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

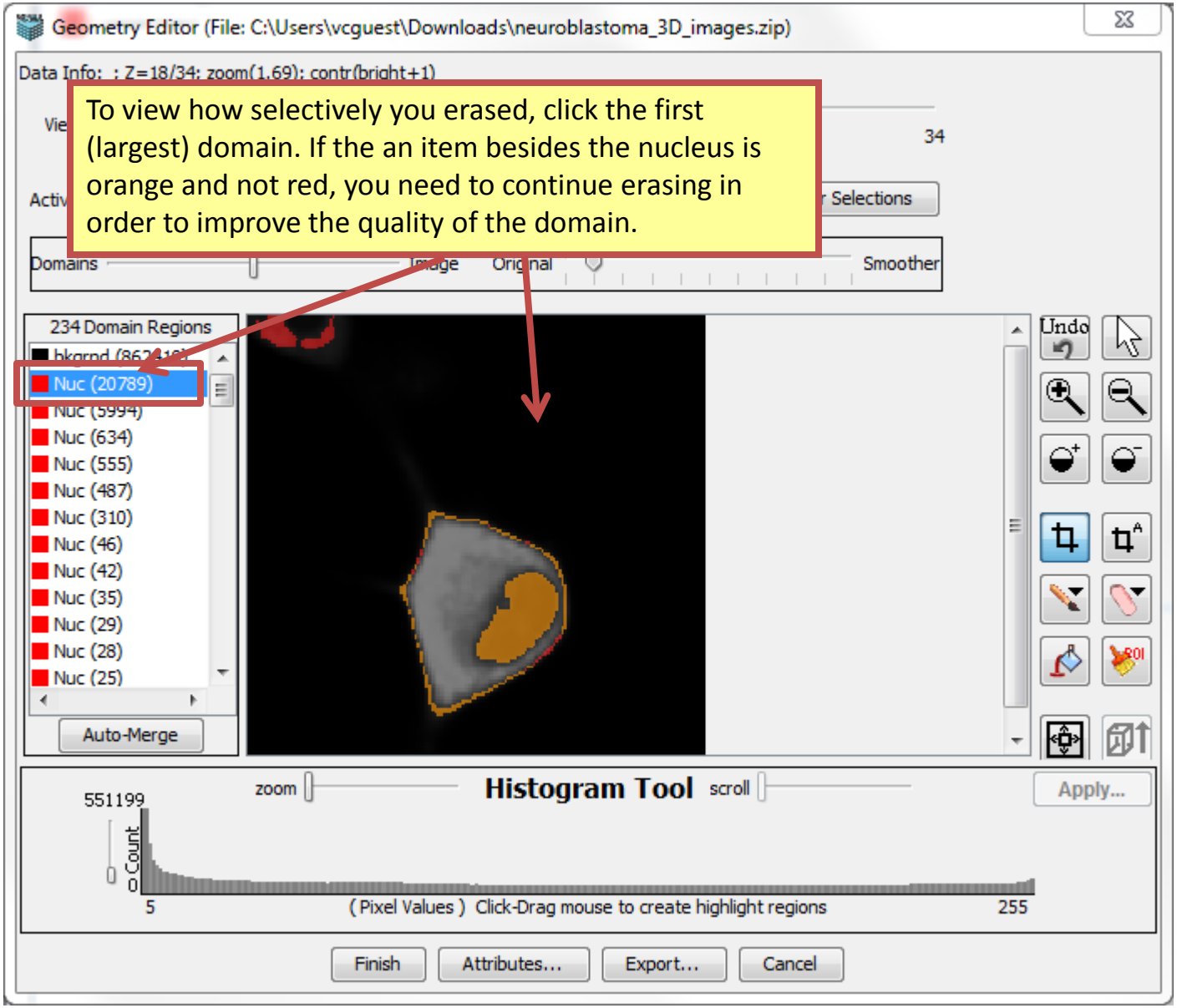

Click on the domain region that makes the nucleus orange
Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=15/34; zoom(1.69); contr(bright+1)
34
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
234 Domain Regions
Nuc (20789)
Nuc (5994)
Nuc (634)
Nuc (555)
Nuc (487)
Nuc (310)
Nuc (46)
Nuc (42)
Nuc (35)
Nuc (29)
Nuc (28)
Nuc (25)
Auto-Merge
Undo
zoom
Histogram Tool
scroll
Apply...
551199
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

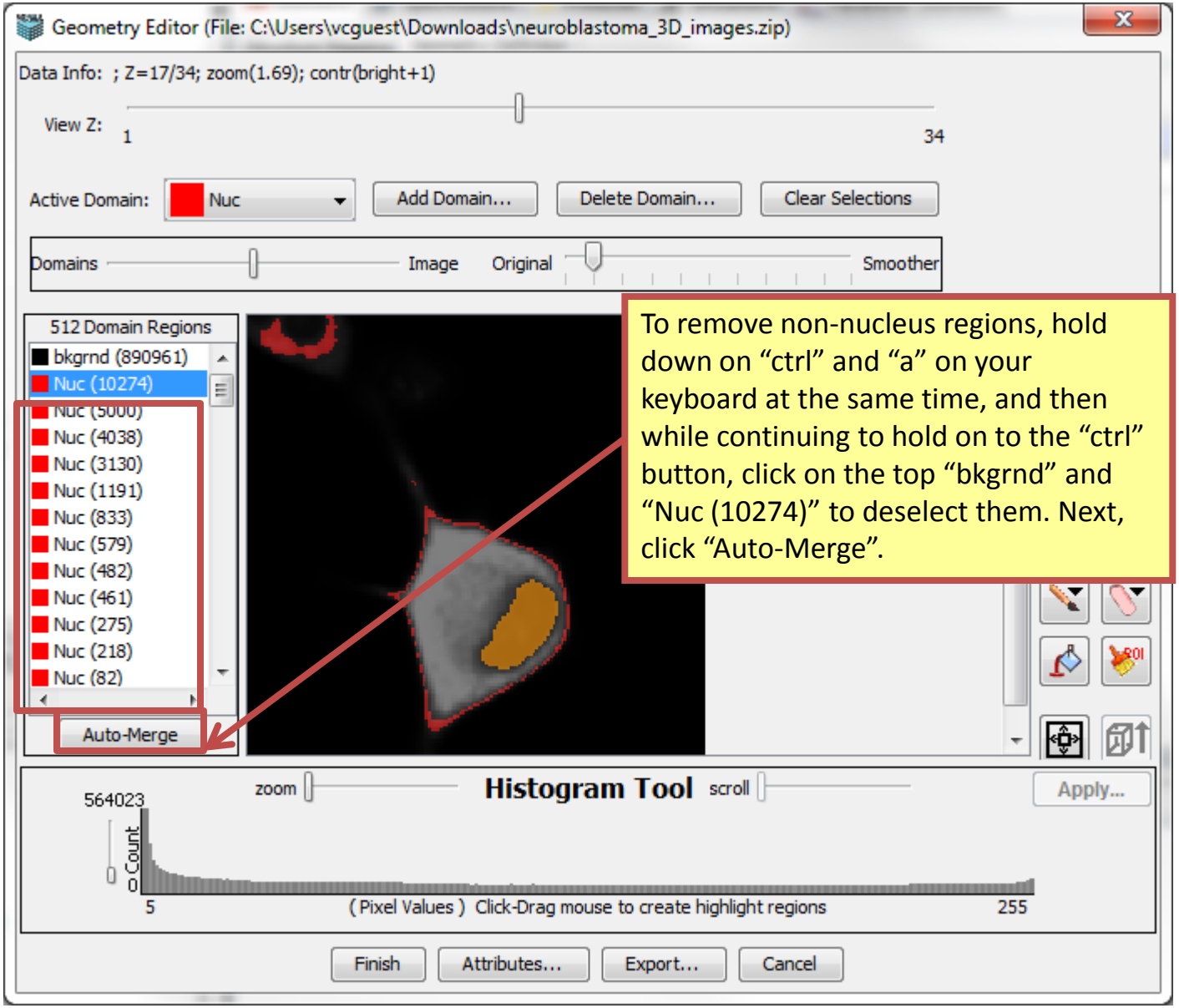

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=18/34; zoom(1.69); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
234 Domain Regions
bkgrnd (862419)
Nuc (20789)
Nuc (5994)
Nuc (634)
Nuc (555)
Nuc (487)
Nuc (310)
Nuc (46)
Nuc (42)
Nuc (35)
Nuc (29)
Nuc (28)
Nuc (25)
Auto-Merge
zoom
Histogram T
Apply...
551199
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel
The program does not recognize the nucleus as only the nucleus (more than the nucleus is highlighted in orange)
In order for the program to recognize the nucleus by itself, use the eraser tool to erase parts of the membrane that are close to the nucleus
In order to change eraser size, right click on the eraser icon and click “brush size manual”

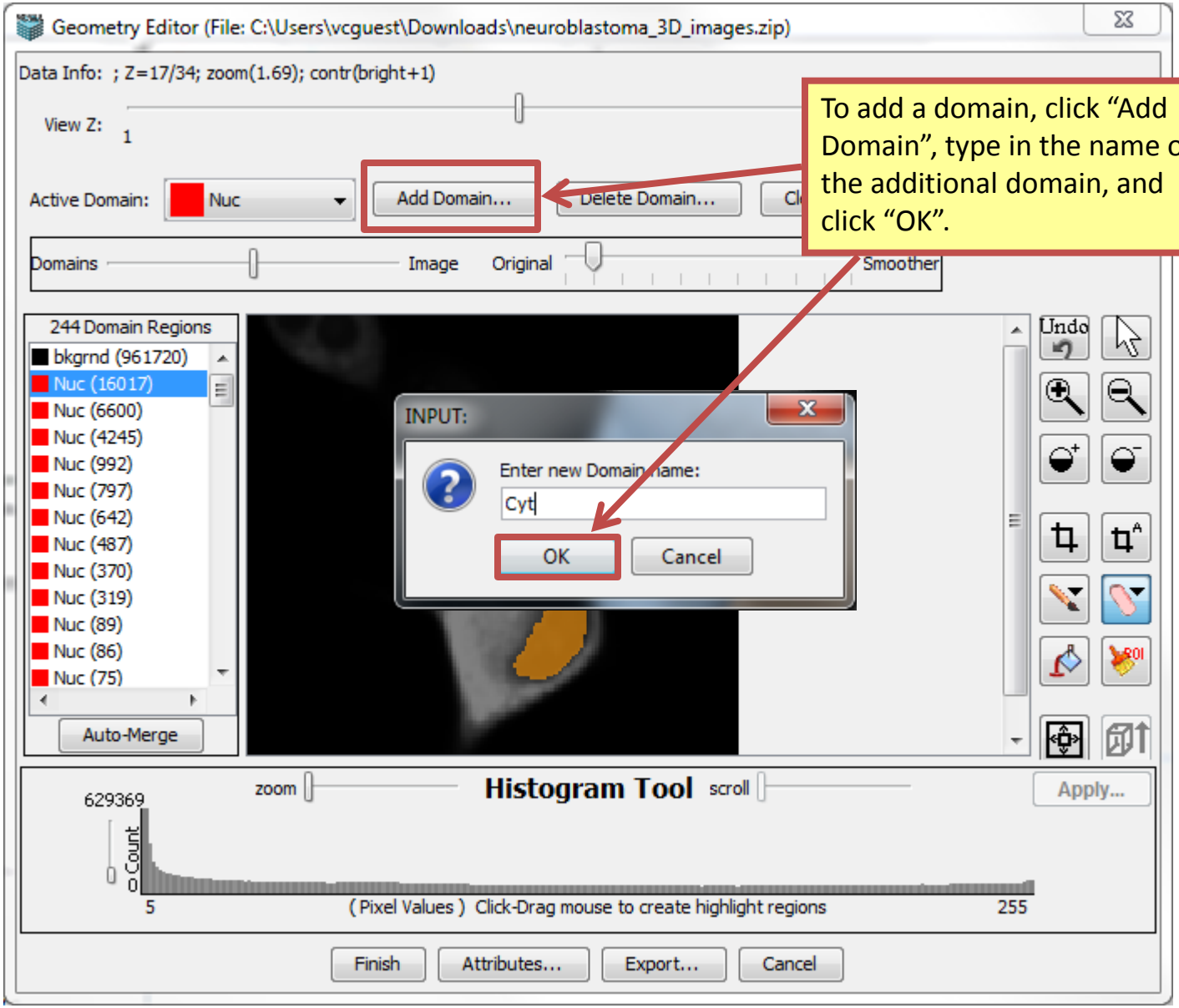


Scroll through the Z slider to view more slices in which the nucleus and membrane are in close proximity

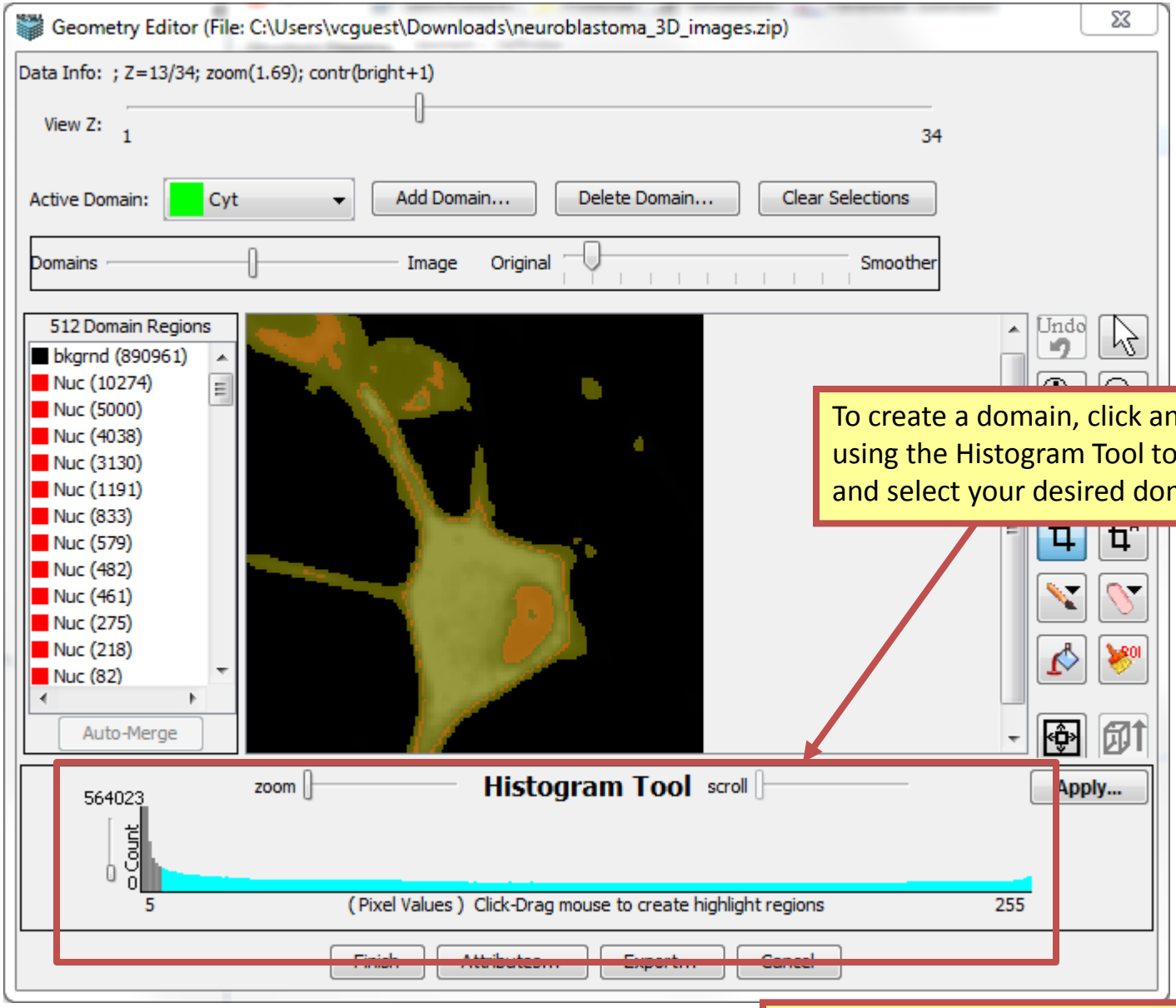
Continue erasing the membrane until there are no parts of the highlighted membrane that touch the highlighted nucleus in all z sections.

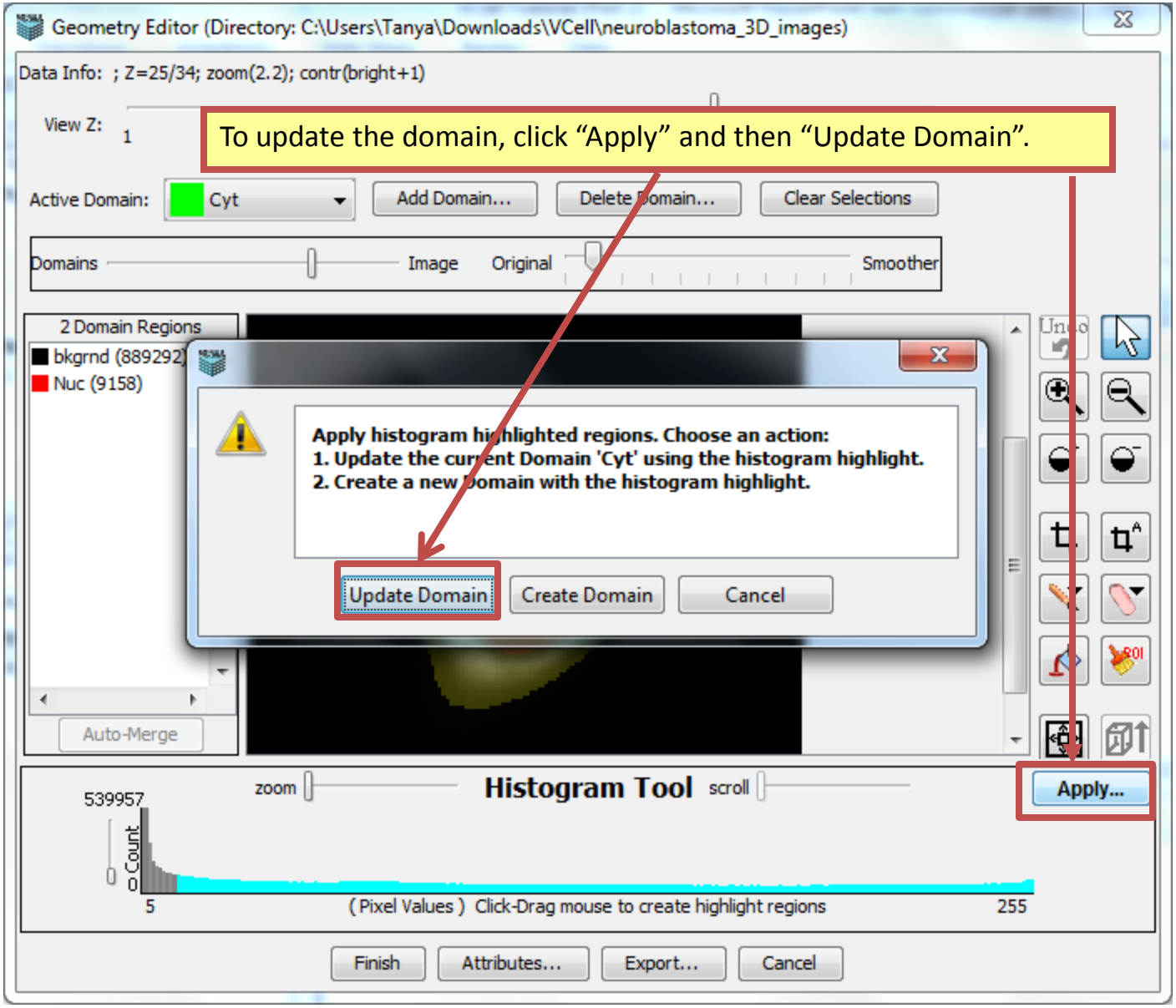

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=18/34; zoom(1.69); contr(bright+1)
34
Selections
Domains
Smoother
To view how selectively you erased, click the first (largest) domain. If the an item besides the nucleus is orange and not red, you need to continue erasing in order to improve the quality of the domain.
234 Domain Regions
Nuc (20789)
Nuc (5994)
Nuc (634)
Nuc (555)
Nuc (487)
Nuc (310)
Nuc (46)
Nuc (42)
Nuc (35)
Nuc (29)
Nuc (28)
Nuc (25)
Auto-Merge
Undo
zoom
Histogram Tool
scroll
Apply...
551199
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

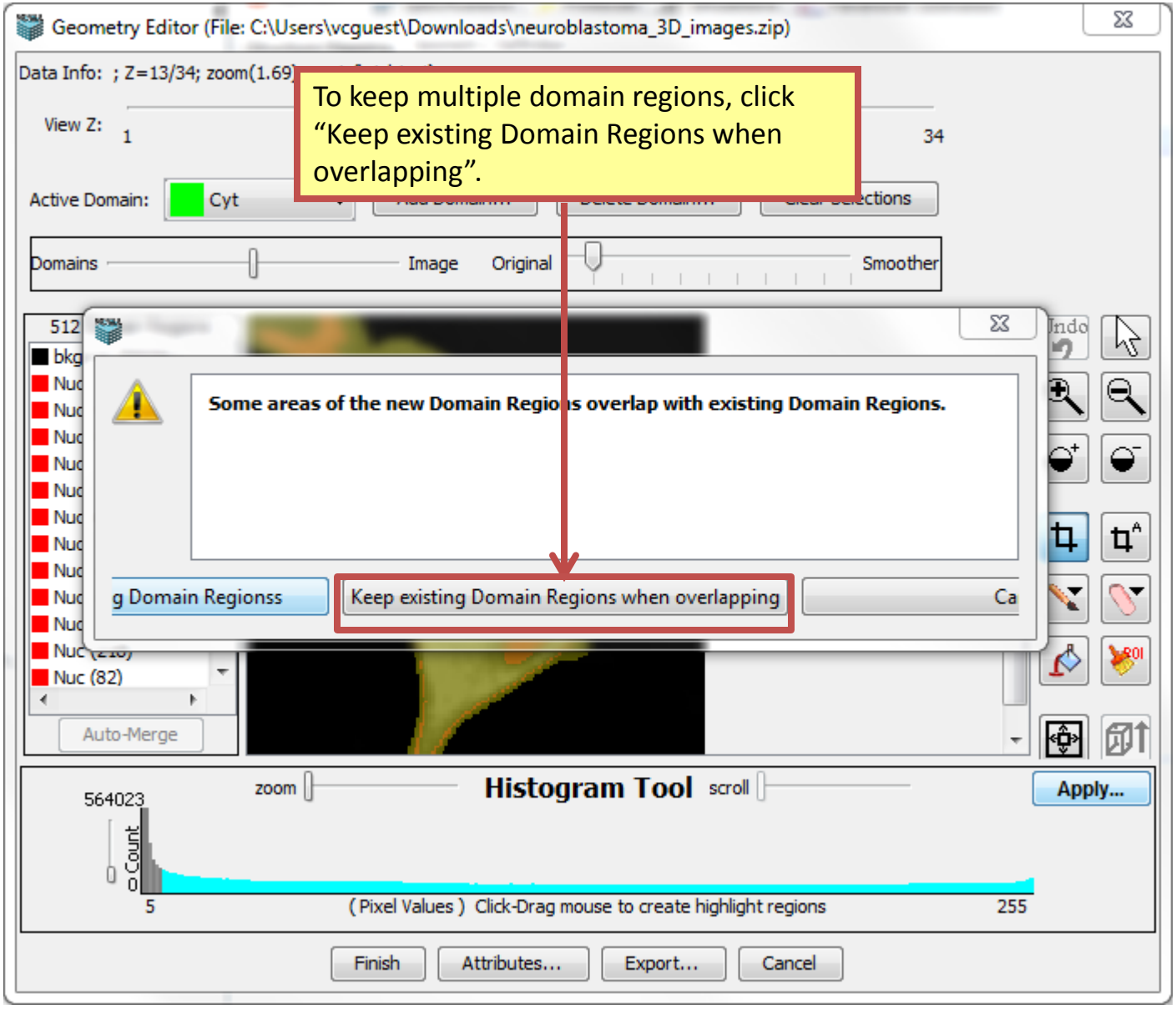

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=17/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
512 Domain Regions
bkgrnd (890961)
Nuc (10274)
Nuc (5000)
Nuc (4038)
Nuc (3130)
Nuc (1191)
Nuc (833)
Nuc (579)
Nuc (482)
Nuc (461)
Nuc (275)
Nuc (218)
Nuc (82)
Auto-Merge
To remove non-nucleus regions, hold down on “ctrl” and “a” on your keyboard at the same time, and then while continuing to hold on to the “ctrl” button, click on the top “bkgrnd” and “Nuc (10274)” to deselect them. Next, click “Auto-Merge”.
zoom
Histogram Tool
scroll
Apply...
564023
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

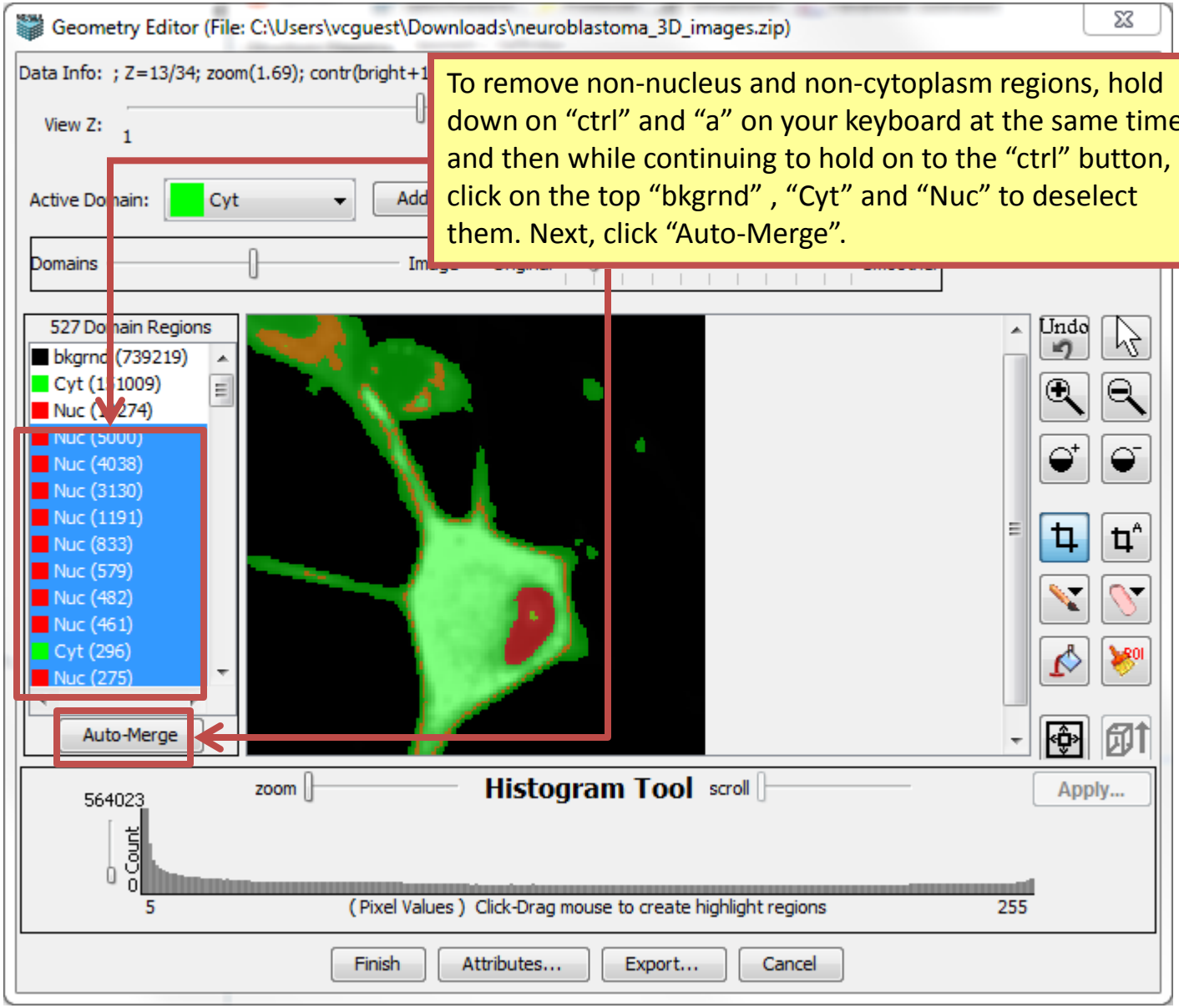

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=17/34; zoom(1.69); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Delete Domain...
Domains
Image
Original
Smoother
244 Domain Regions
bkgrnd (961720)
Nuc (16017)
Nuc (6600)
Nuc (4245)
Nuc (992)
Nuc (797)
Nuc (642)
Nuc (487)
Nuc (370)
Nuc (319)
Nuc (89)
Nuc (86)
Nuc (75)
Auto-Merge
INPUT:
Enter new Domain name:
Cyt
OK
Cancel
Undo
zoom
Histogram Tool
scroll
Apply...
629369
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel
To add a domain, click “Add Domain”, type in the name of the additional domain, and click “OK”.

Contents

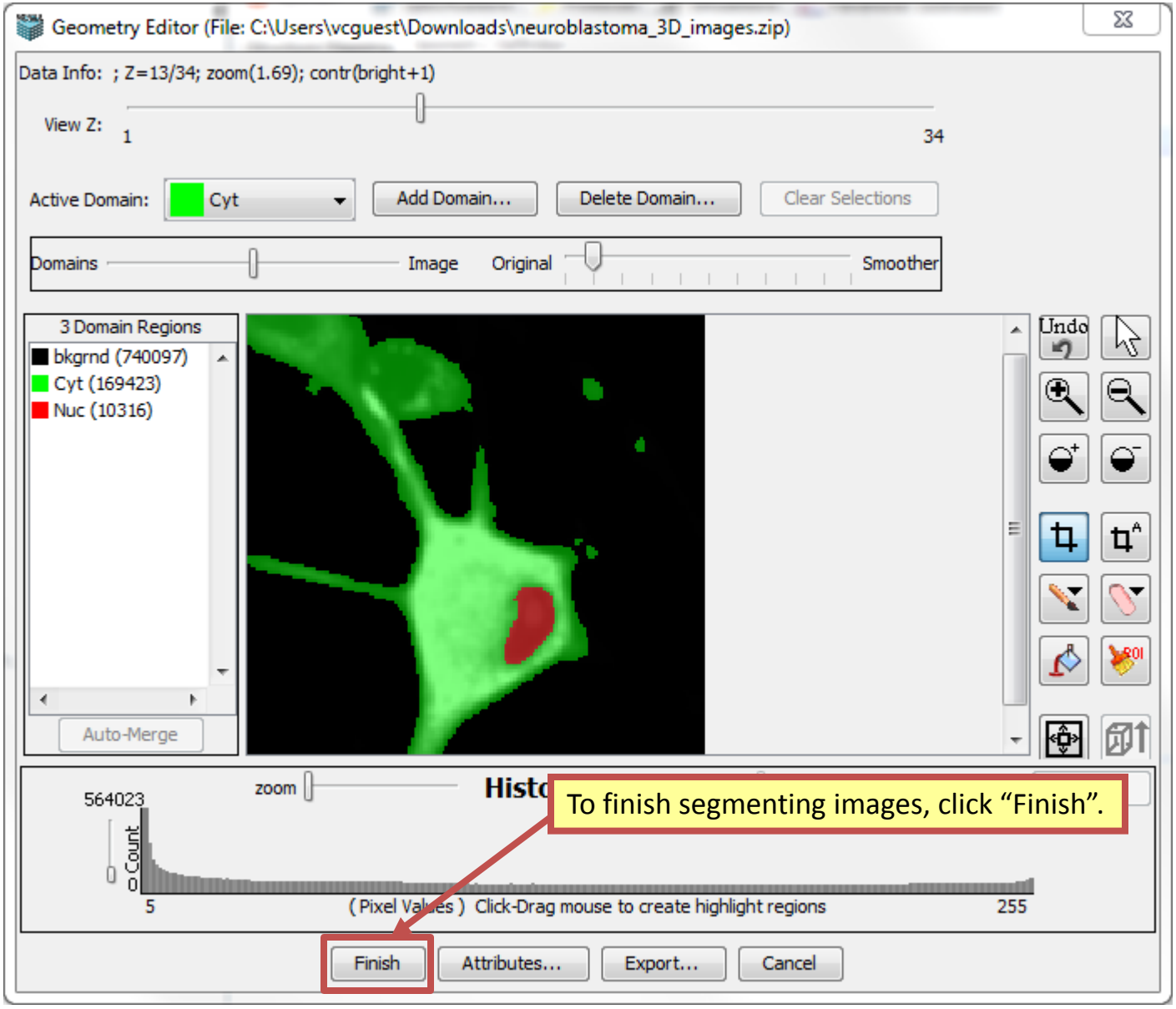

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=13/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
512 Domain Regions
bkgrnd (890961)
Nuc (10274)
Nuc (5000)
Nuc (4038)
Nuc (3130)
Nuc (1191)
Nuc (833)
Nuc (579)
Nuc (482)
Nuc (461)
Nuc (275)
Nuc (218)
Nuc (82)
Auto-Merge
Undo
zoom
Histogram Tool
scroll
Apply...
564023
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel
To create a domain, click and drag using the Histogram Tool to highlight and select your desired domain region.
Use the Z slider to make sure all parts of the cytoplasm are highlighted

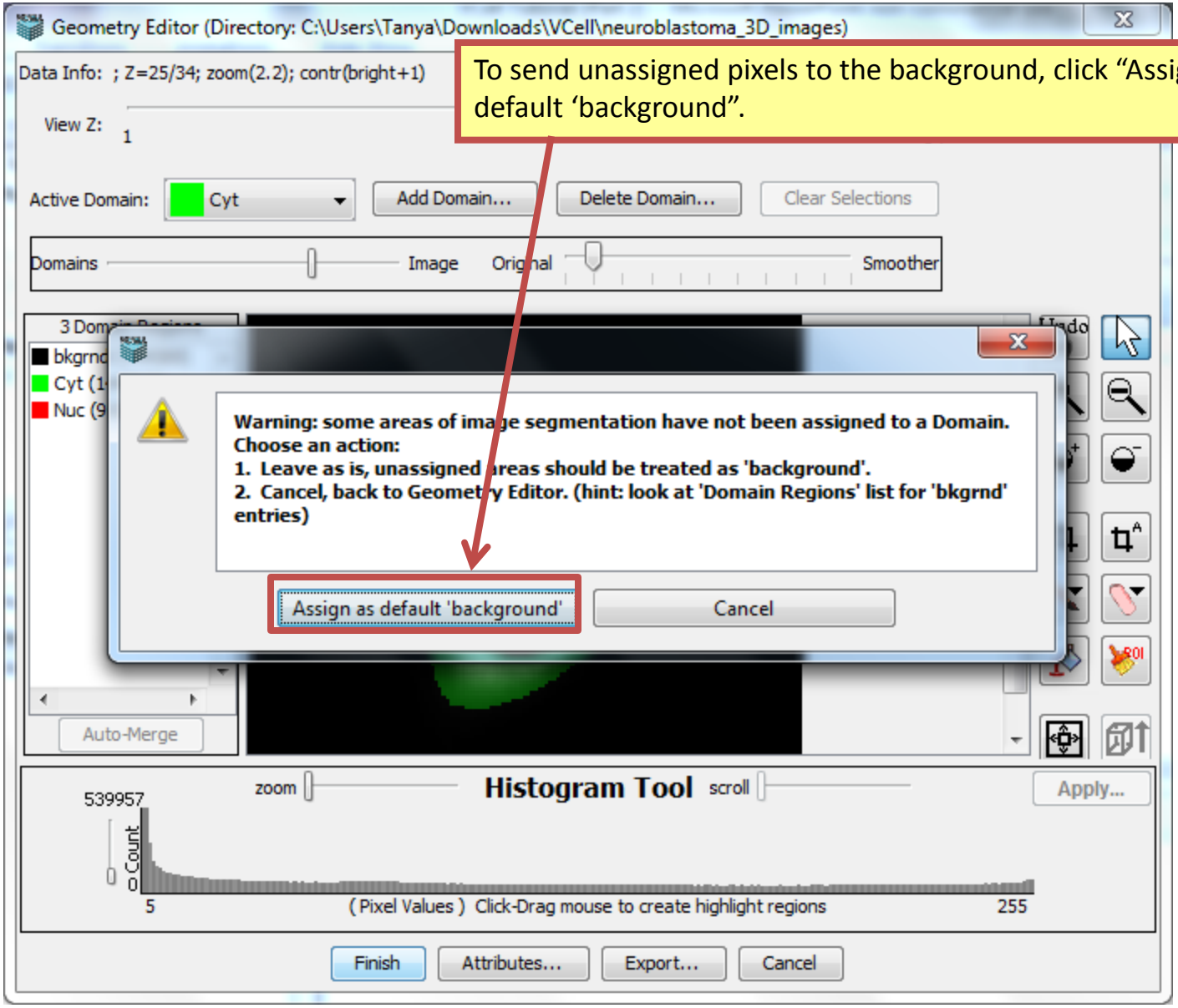

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=25/34; zoom(2.2); contr(bright+1)
View Z:
1
To update the domain, click “Apply” and then “Update Domain”.
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
2 Domain Regions
bkgrnd (889292)
Nuc (9158)
Auto-Merge
Apply histogram highlighted regions. Choose an action:
1. Update the current Domain 'Cyt' using the histogram highlight.
2. Create a new Domain with the histogram highlight.
Update Domain
Create Domain
Cancel
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel


Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=13/34; zoom(1.69)
View Z:
1
34
Active Domain:
Cyt
Domains
Image
Original
Smoother
To keep multiple domain regions, click "Keep existing Domain Regions when overlapping".
Some areas of the new Domain Regions overlap with existing Domain Regions.
g Domain Regionss
Keep existing Domain Regions when overlapping
Ca
Nuc (82)
Auto-Merge
zoom
Histogram Tool
scroll
Apply...
564023
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

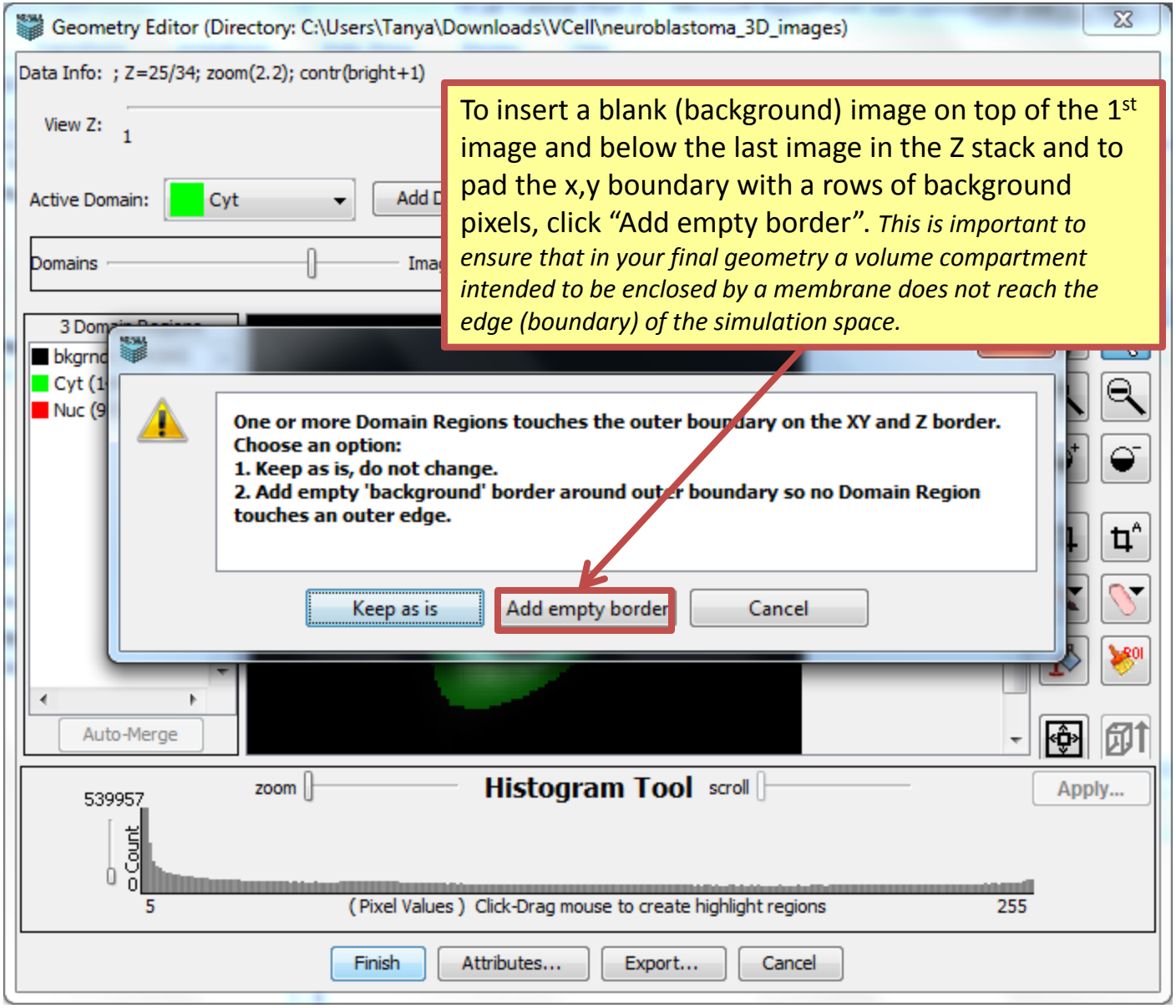


To remove non-nucleus and non-cytoplasm regions, hold down on “ctrl” and “a” on your keyboard at the same time, and then while continuing to hold on to the “ctrl” button, click on the top “bkgrnd” , “Cyt” and “Nuc” to deselect them. Next, click “Auto-Merge”.

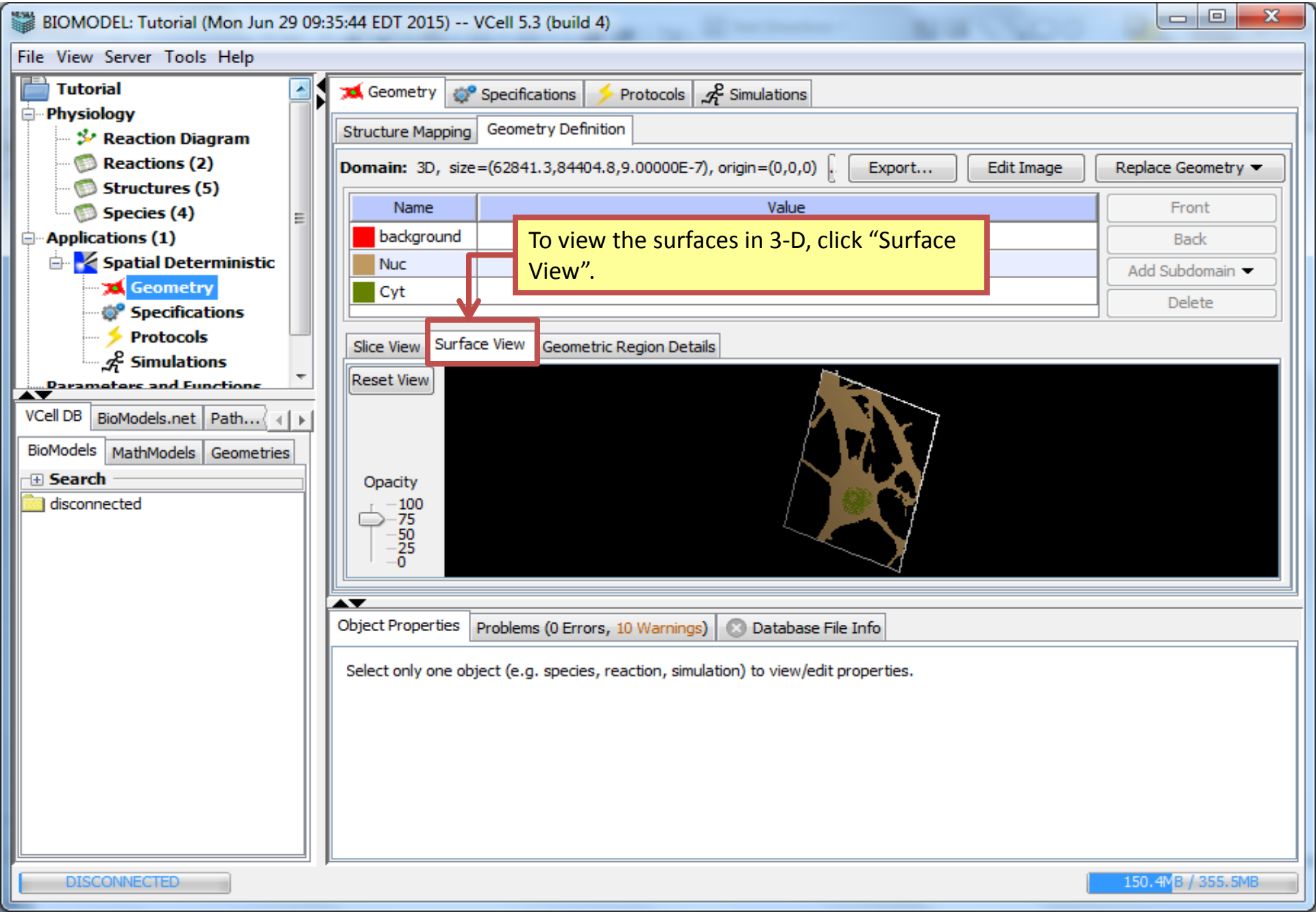

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=13/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
3 Domain Regions
bkgrnd (740097)
Cyt (169423)
Nuc (10316)
Auto-Merge
Undo
zoom
564023
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
To finish segmenting images, click “Finish”.
Finish
Attributes...
Export...
Cancel



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



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 rows of background pixels, click "Add empty border". *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.*


BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
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disconnected
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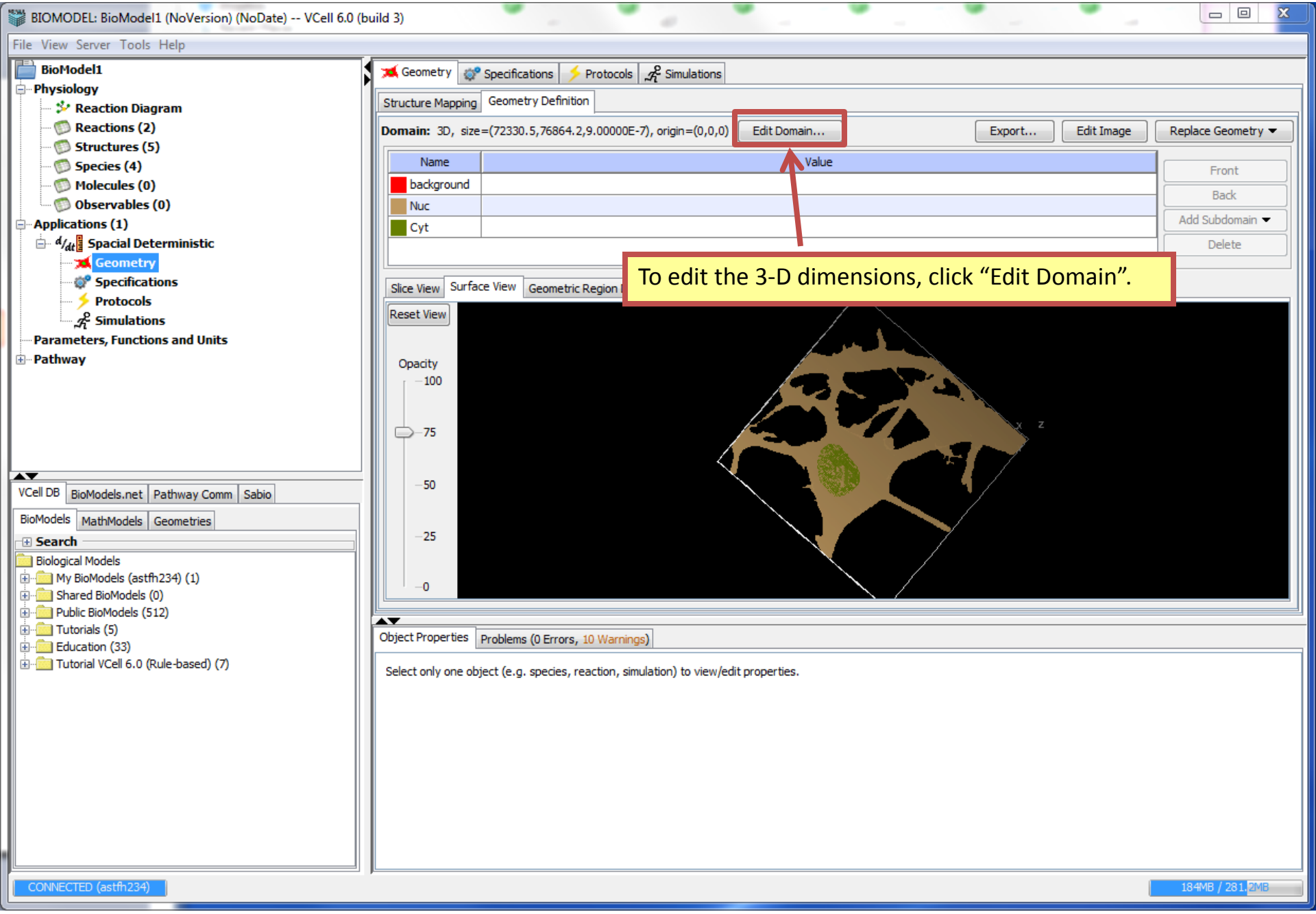
Structure Mapping
Geometry Definition
Domain: 3D, size=(62841.3,84404.8,9.00000E-7), origin=(0,0,0)
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To view the surfaces in 3-D, click “Surface View”.
Slice View
Surface View
Geometric Region Details
Reset View
Opacity
100
75
50
25
0
Object Properties
Problems (0 Errors, 10 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
DISCONNECTED
150.4MB / 355.5MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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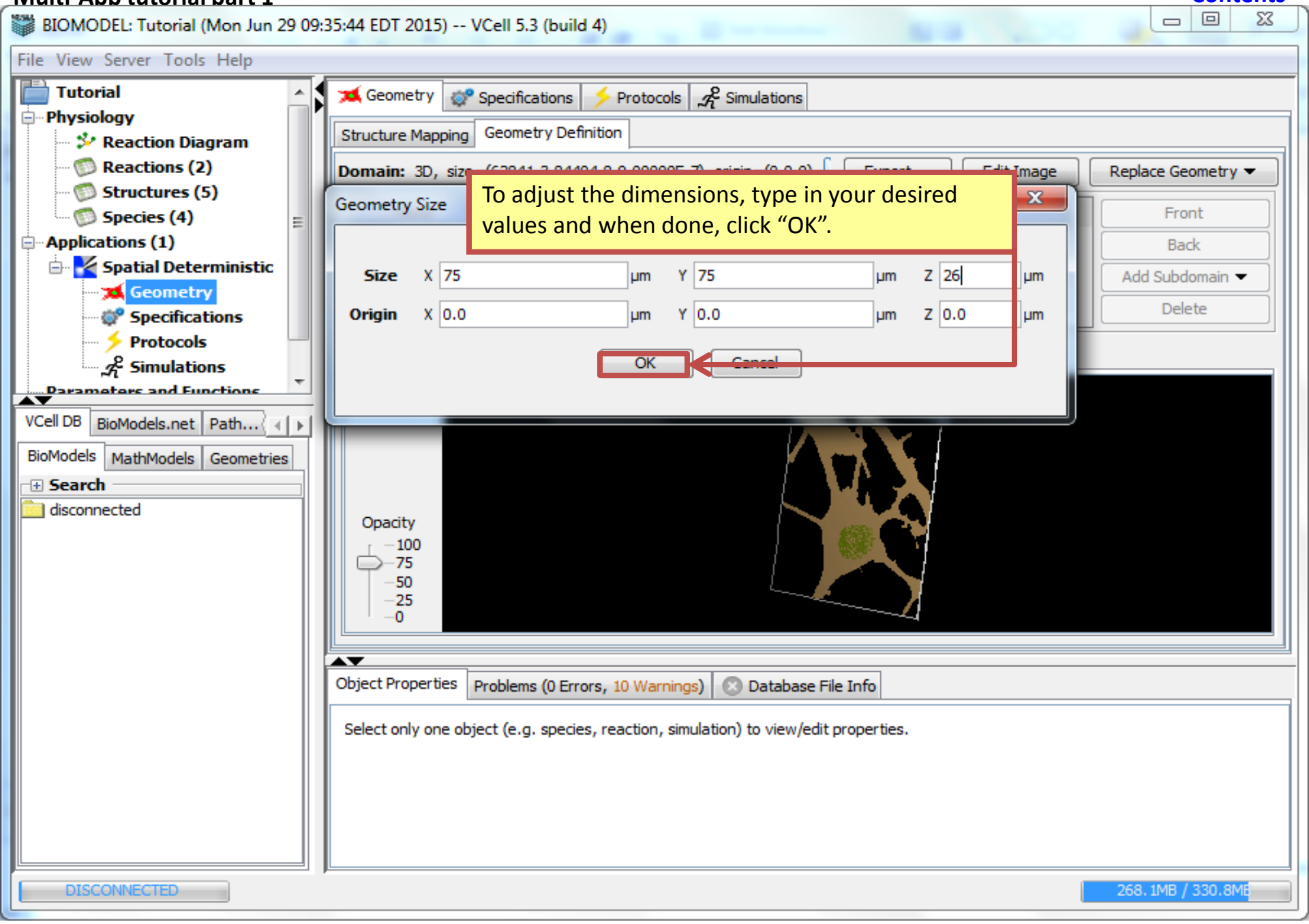
Geometry Definition
Domain: 3D, size=(72330.5,76864.2,9.00000E-7), origin=(0,0,0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To edit the 3-D dimensions, click “Edit Domain”.
Slice View
Surface View
Geometric Region
Reset View
Opacity
100
75
50
25
0
Object Properties
Problems (0 Errors, 10 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
184MB / 281.2MB


BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
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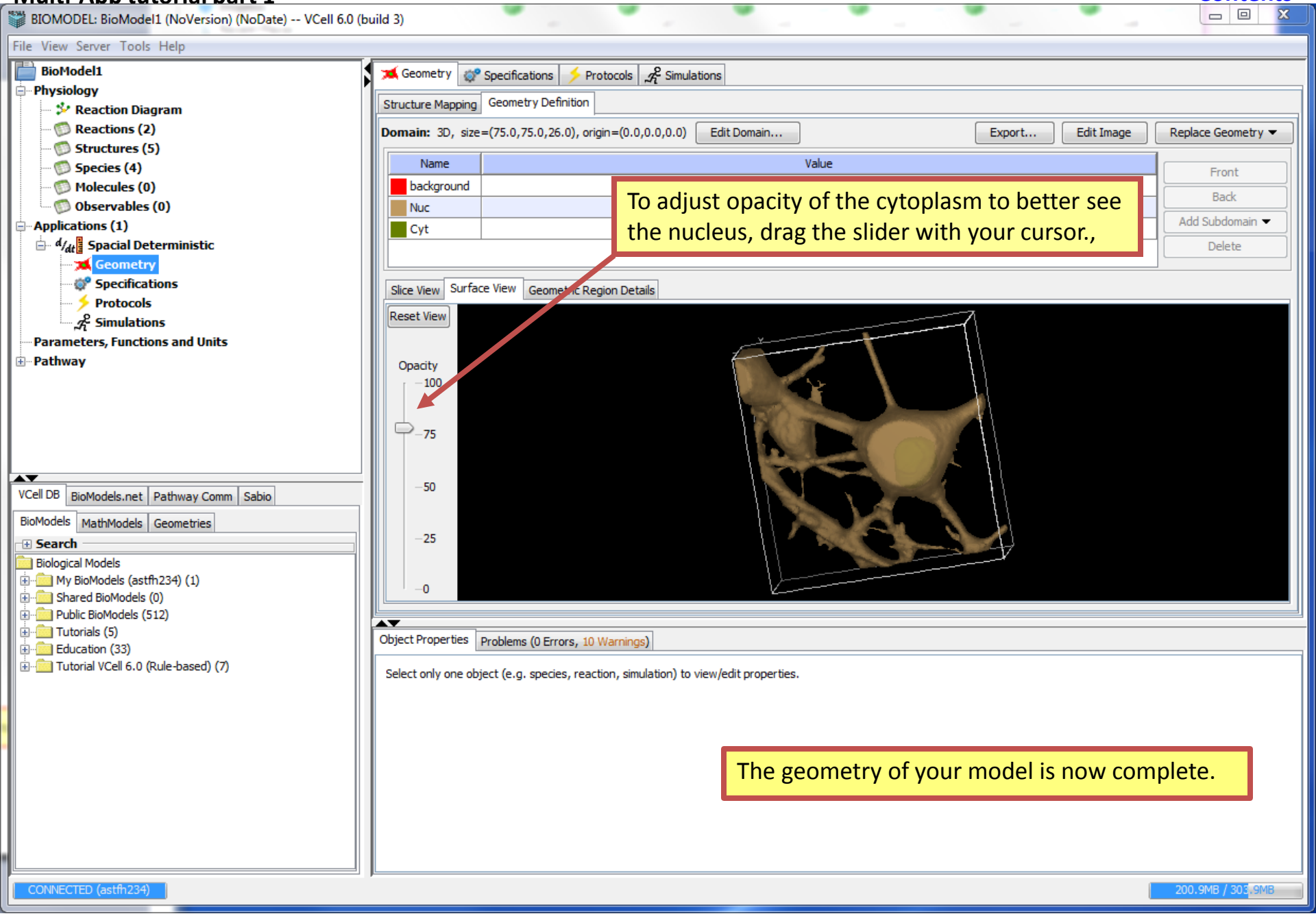
BioModels.net
Path...
BioModels
MathModels
Geometries
Search
disconnected
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D,
Export...
Edit Image
Replace Geometry
Front
Back
Add Subdomain
Delete
Geometry Size
To adjust the dimensions, type in your desired values and when done, click "OK".
Size X 75 µm Y 75 µm Z 26 µm
Origin X 0.0 µm Y 0.0 µm Z 0.0 µm
OK
Cancel
Opacity
100
75
50
25
0
Object Properties
Problems (0 Errors, 10 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
DISCONNECTED
268.1MB / 330.8MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(75.0,75.0,26.0), origin=(0.0,0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To adjust opacity of the cytoplasm to better see the nucleus, drag the slider with your cursor.,
Slice View
Surface View
Geometric Region Details
Reset View
Opacity
100
75
50
25
0
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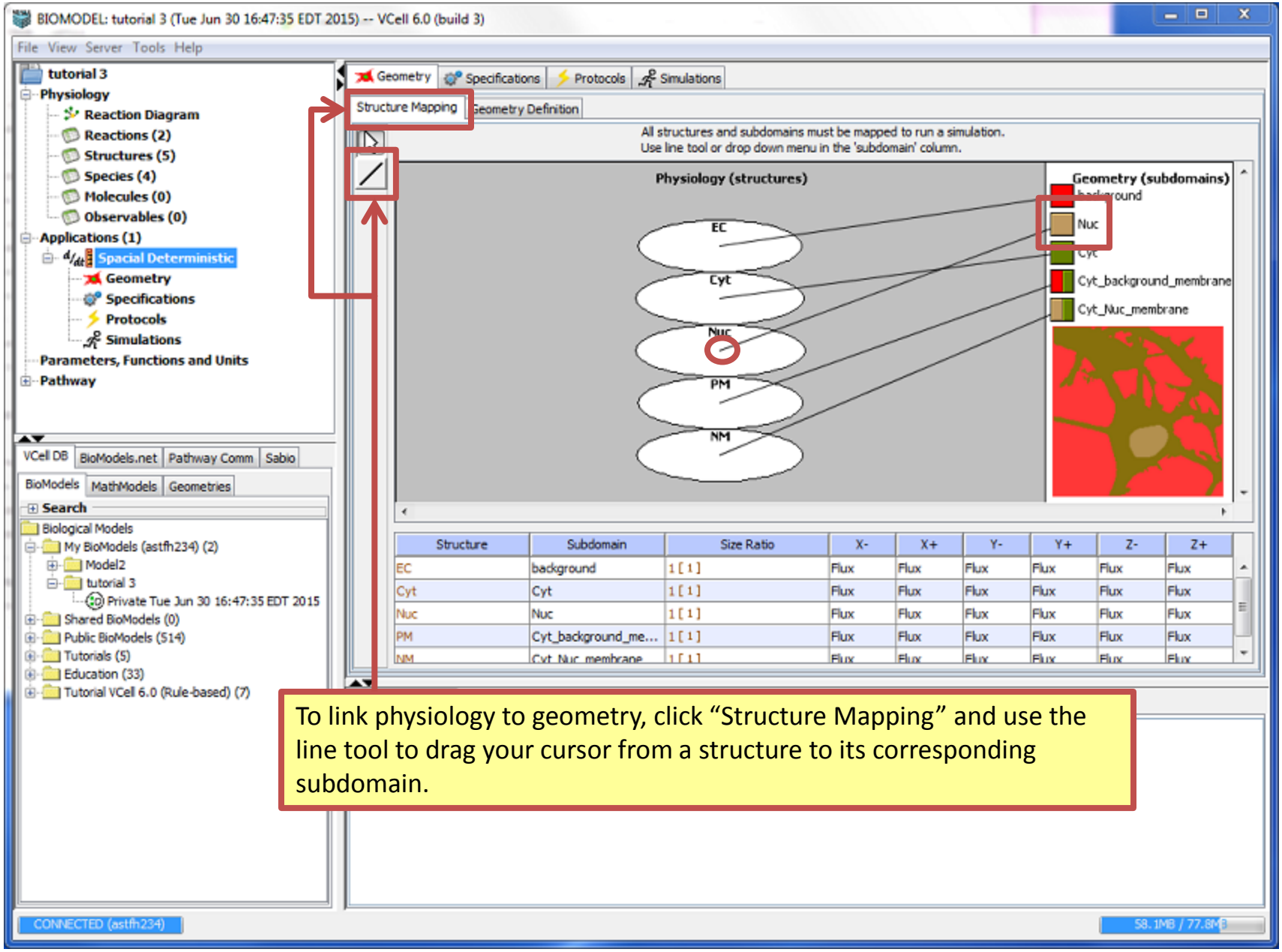
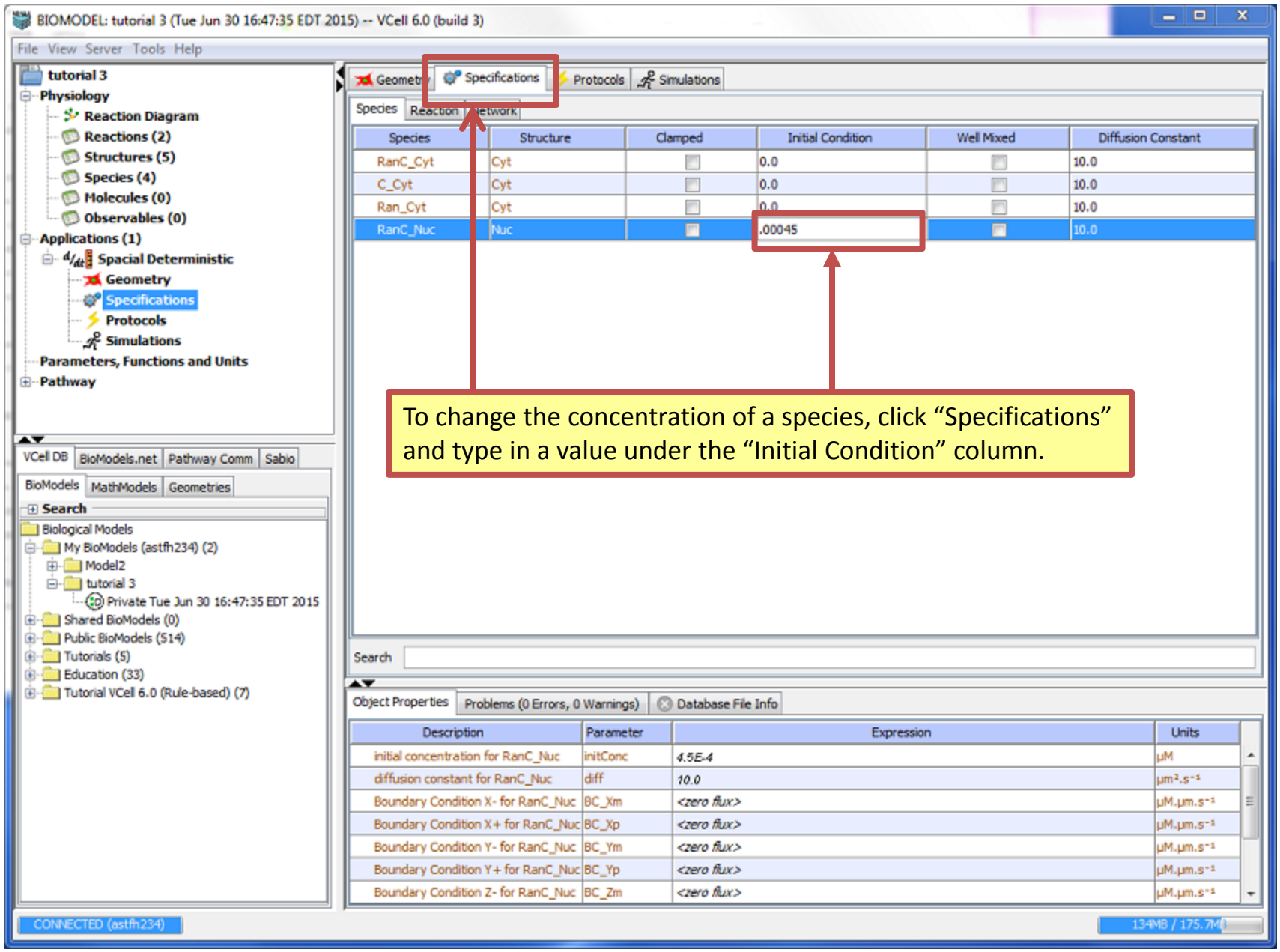
Object Properties
Problems (0 Errors, 10 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
The geometry of your model is now complete.
CONNECTED (astfh234)
200.9MB / 303.9MB

Contents



To link physiology to geometry, click “Structure Mapping” and use the line tool to drag your cursor from a structure to its corresponding subdomain.

Contents


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
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Reaction
Network
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
RanC_Cyt
Cyt
0.0
10.0
C_Cyt
Cyt
0.0
10.0
Ran_Cyt
Cyt
0.0
10.0
RanC_Nuc
Nuc
.00045
10.0
To change the concentration of a species, click “Specifications” and type in a value under the “Initial Condition” column.
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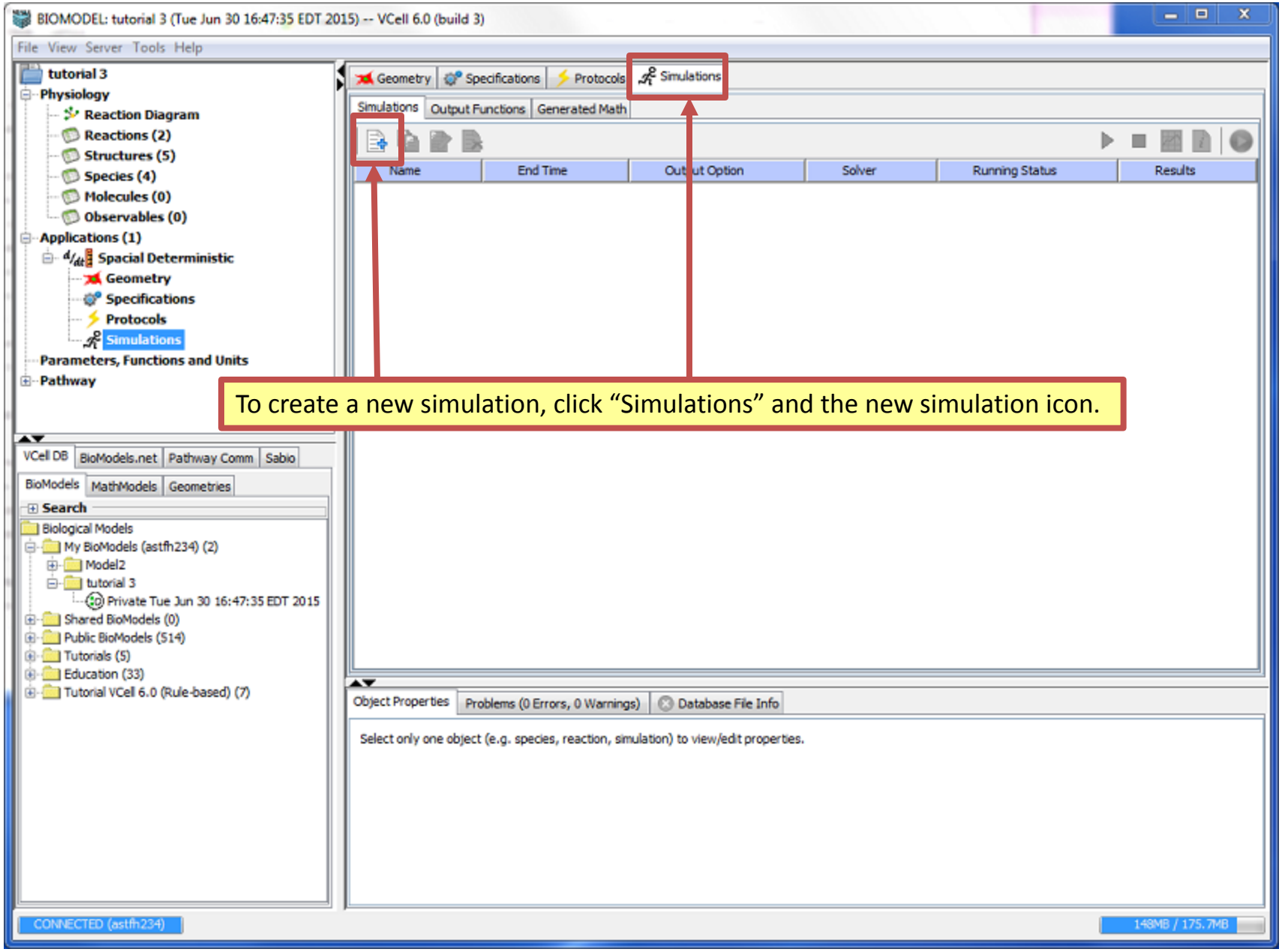
Tutorial VCell 6.0 (Rule-based) (7)
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for RanC_Nuc
initConc
4.5E-4
μM
diffusion constant for RanC_Nuc
diff
10.0
μm².s⁻¹
Boundary Condition X- for RanC_Nuc
BC_Xm
<zero flux>
μM.μm.s⁻¹
Boundary Condition X+ for RanC_Nuc
BC_Xp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y- for RanC_Nuc
BC_Ym
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y+ for RanC_Nuc
BC_Yp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Z- for RanC_Nuc
BC_Zm
<zero flux>
μM.μm.s⁻¹
CONNECTED (astfh234)
134MB / 175.7MB

Contents


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
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Geometry
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Protocols
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Simulations
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Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To create a new simulation, click “Simulations” and the new simulation icon.
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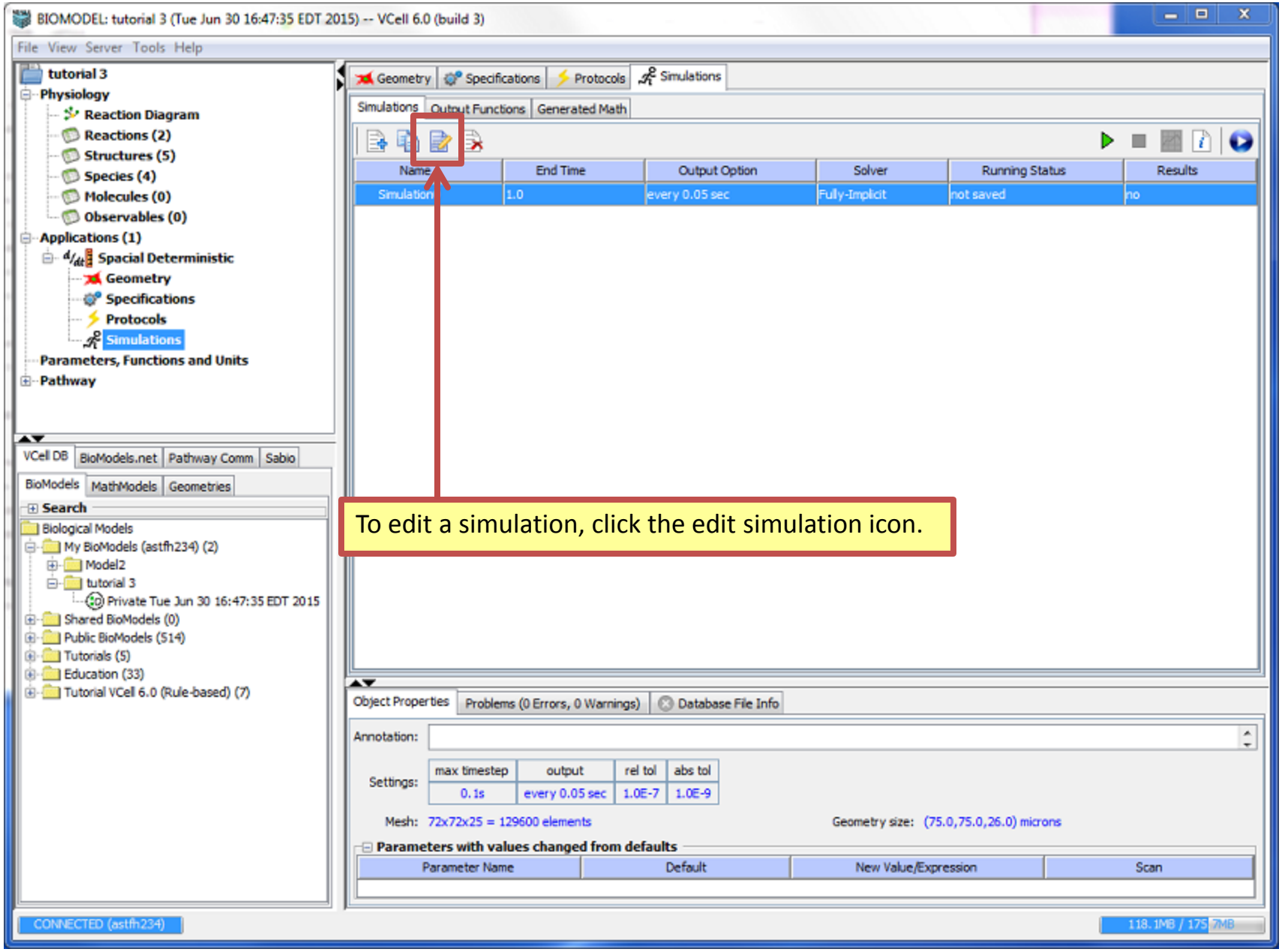
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
148MB / 175.7MB

Contents


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
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Simulations
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Generated Math
Name
End Time
Output Option
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Running Status
Results
Simulation
1.0
every 0.05 sec
Fully-Implicit
not saved
no
To edit a simulation, click the edit simulation icon.
VCell DB
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Pathway Comm
Sabio
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Geometries
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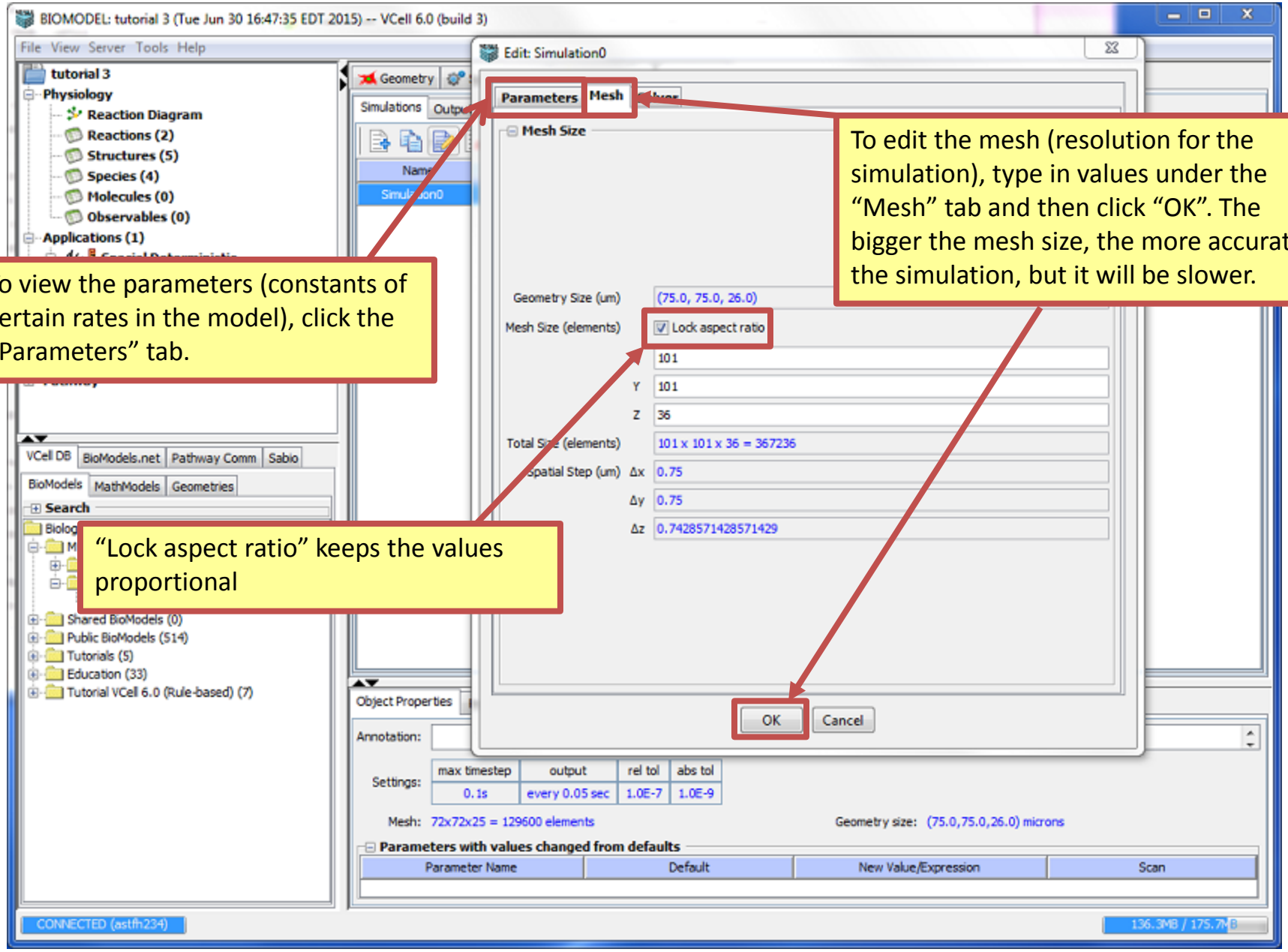
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
118.1MB / 175.7MB

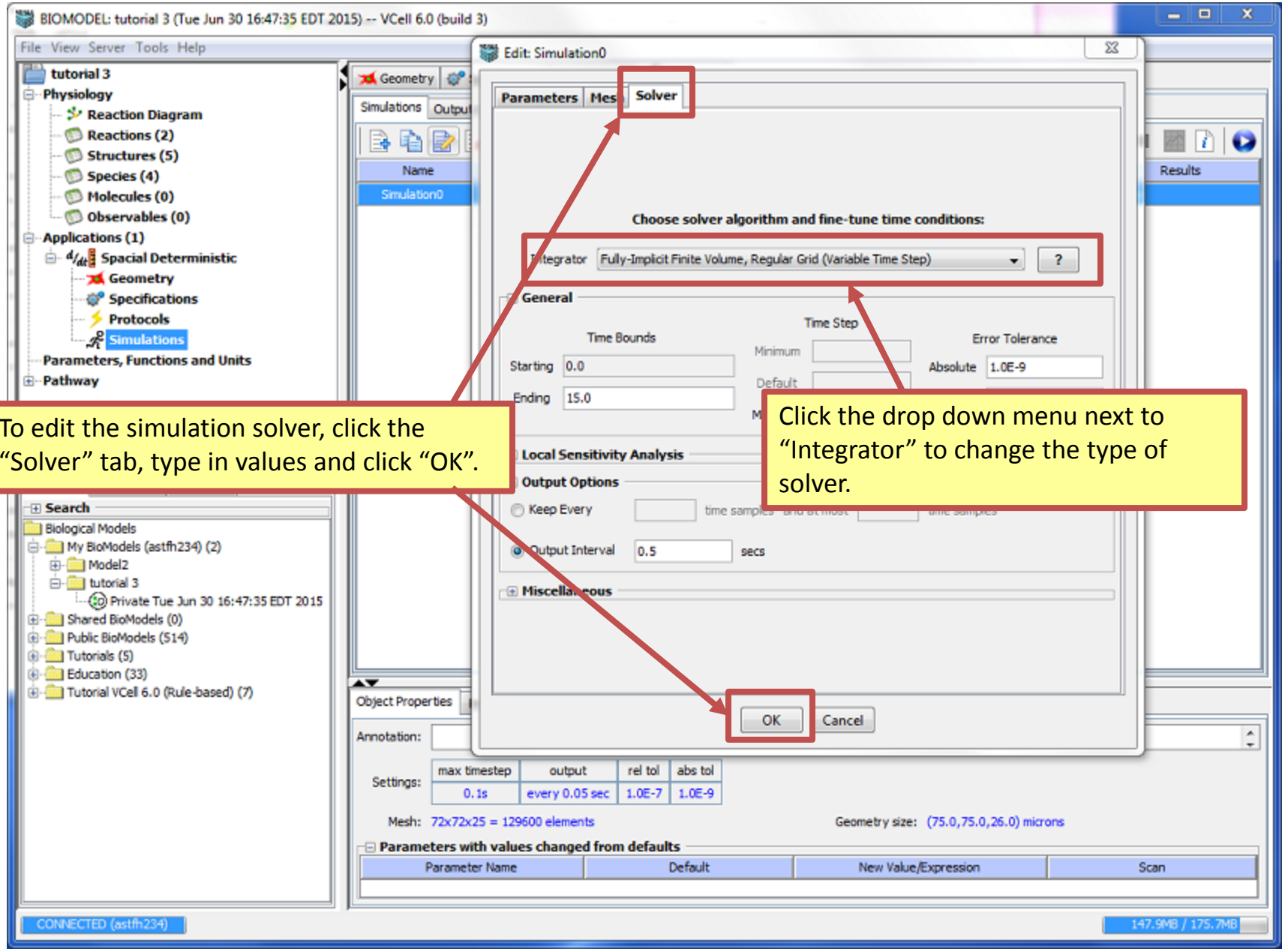


To view the parameters (constants of certain rates in the model), click the "Parameters" tab.

To edit the mesh (resolution for the simulation), type in values under the "Mesh" tab and then click "OK". The bigger the mesh size, the more accurate the simulation, but it will be slower.

"Lock aspect ratio" keeps the values proportional

Contents


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
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Geometry
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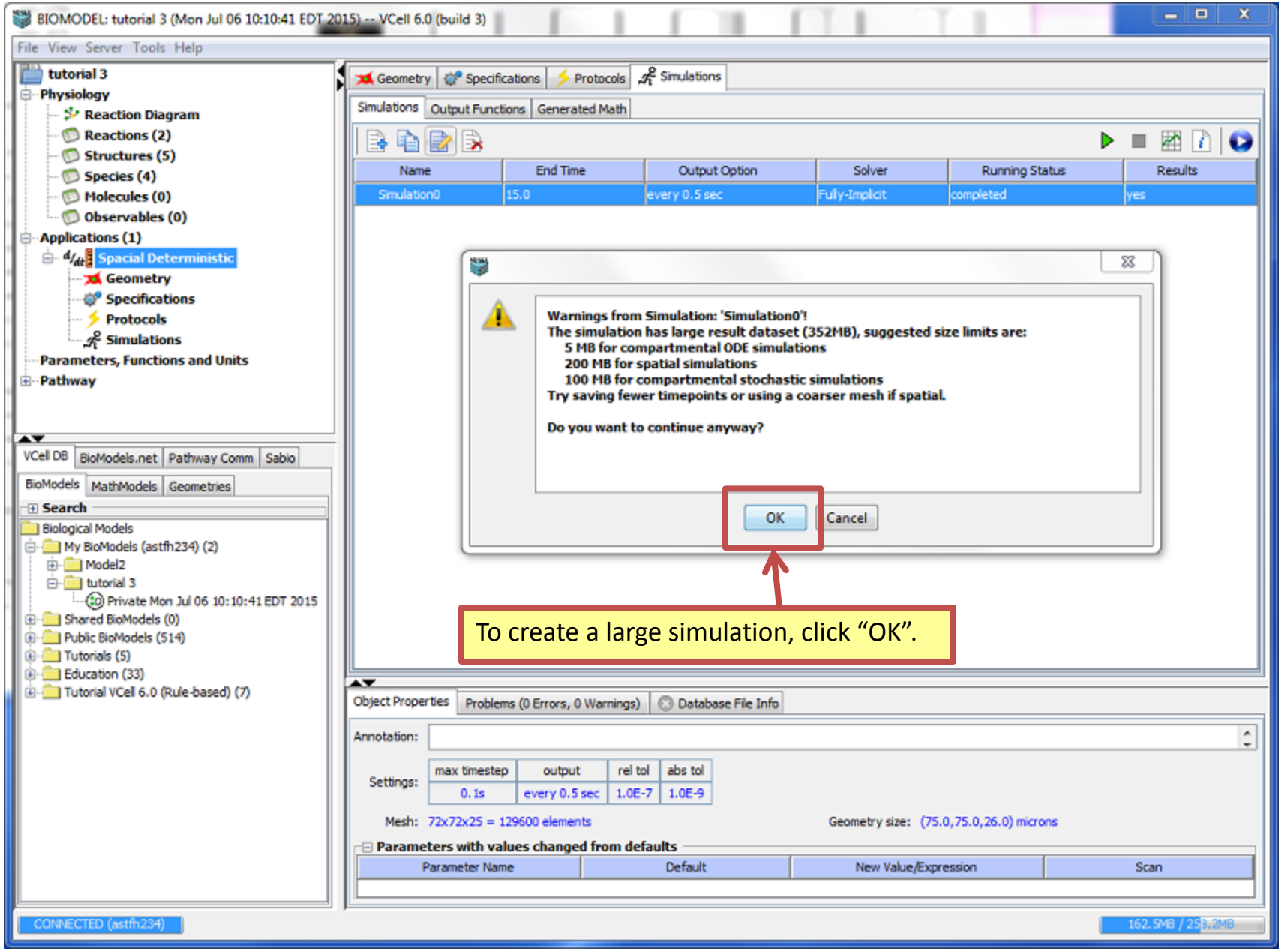
Output
Name
Simulation0
Results
Edit: Simulation0
Parameters
Mes
Solver
Choose solver algorithm and fine-tune time conditions:
Integrator
Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)
?
General
Time Bounds
Starting
0.0
Ending
15.0
Time Step
Minimum
Default
Error Tolerance
Absolute
1.0E-9
Local Sensitivity Analysis
Output Options
Keep Every
time samples
Output Interval
0.5
secs
Miscellaneous
OK
Cancel
To edit the simulation solver, click the "Solver" tab, type in values and click "OK".
Click the drop down menu next to "Integrator" to change the type of solver.
Object Properties
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05 sec
1.0E-7
1.0E-9
Mesh:
72x72x25 = 129600 elements
Geometry size:
(75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
147.9MB / 175.7MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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Simulations
Output Functions
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Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 sec
Fully-Implicit
completed
yes
Warnings from Simulation: 'Simulation0'!
The simulation has large result dataset (352MB), 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
To create a large simulation, click “OK”.
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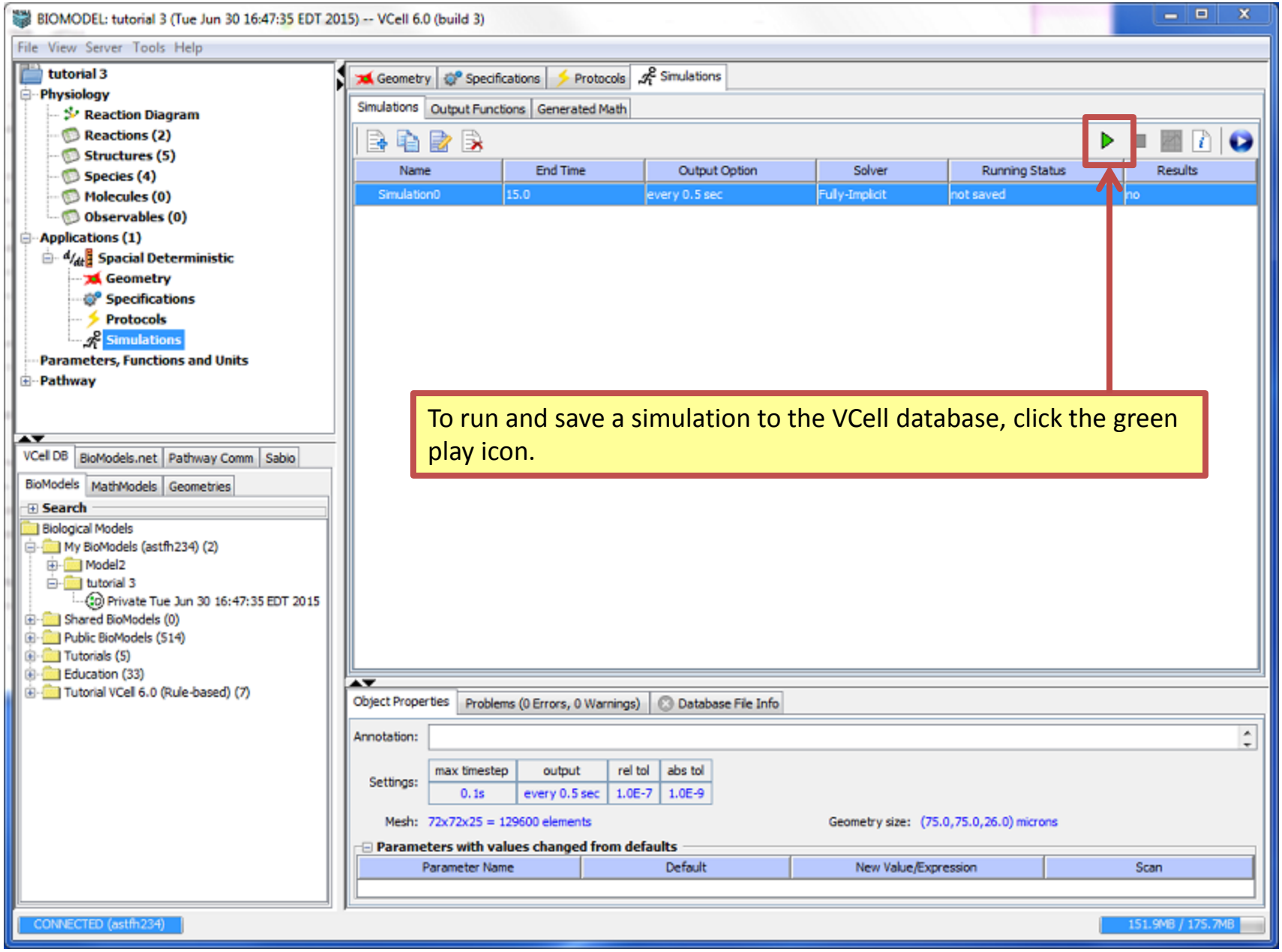
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
162.5MB / 253.2MB


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
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Observables (0)
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Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 sec
Fully-Implicit
not saved
no
To run and save a simulation to the VCell database, click the green play icon.
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BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
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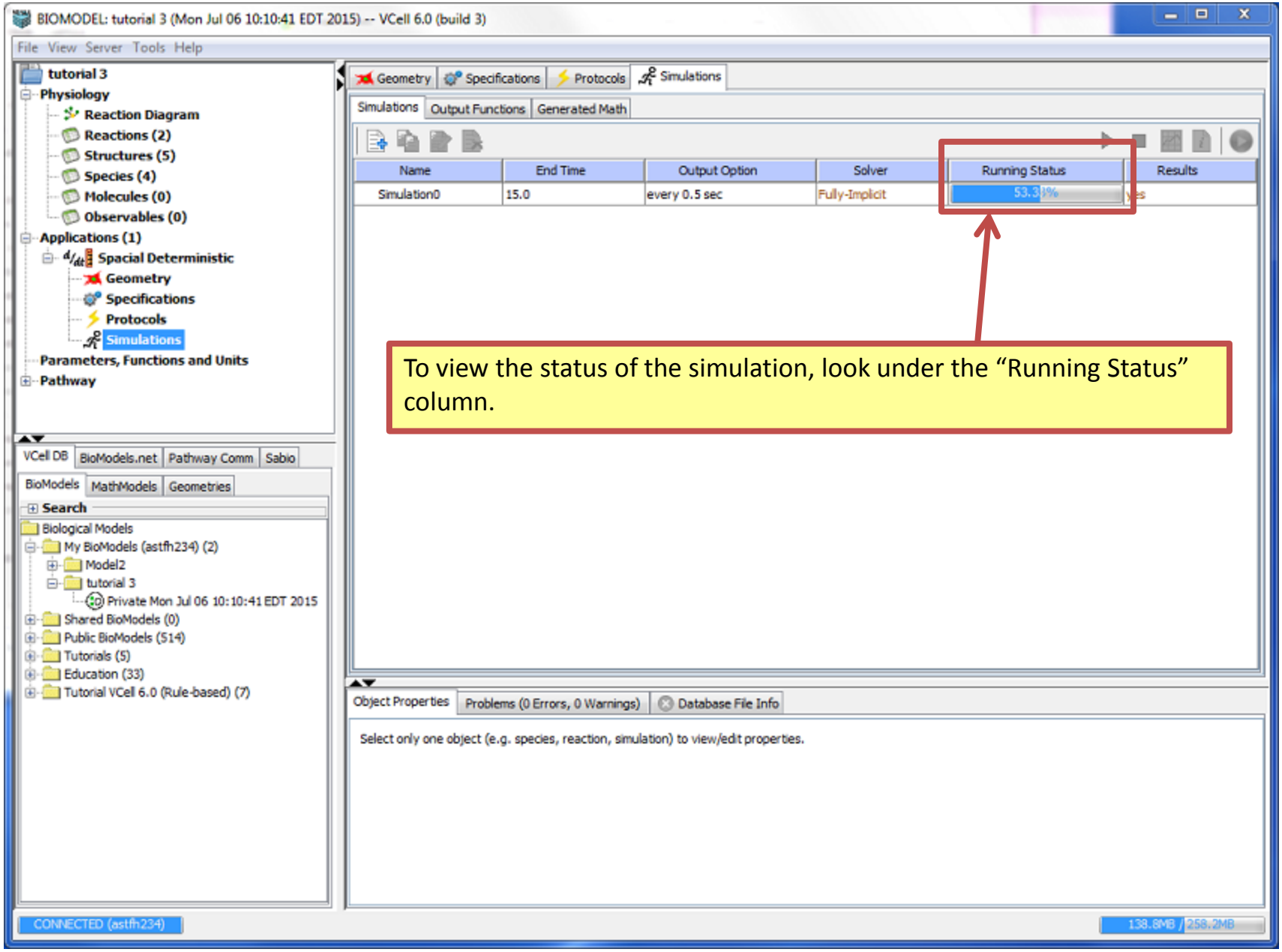
Private Tue Jun 30 16:47:35 EDT 2015
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
151.9MB / 175.7MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 sec
Fully-Implicit
53.3%
To view the status of the simulation, look under the “Running Status” column.
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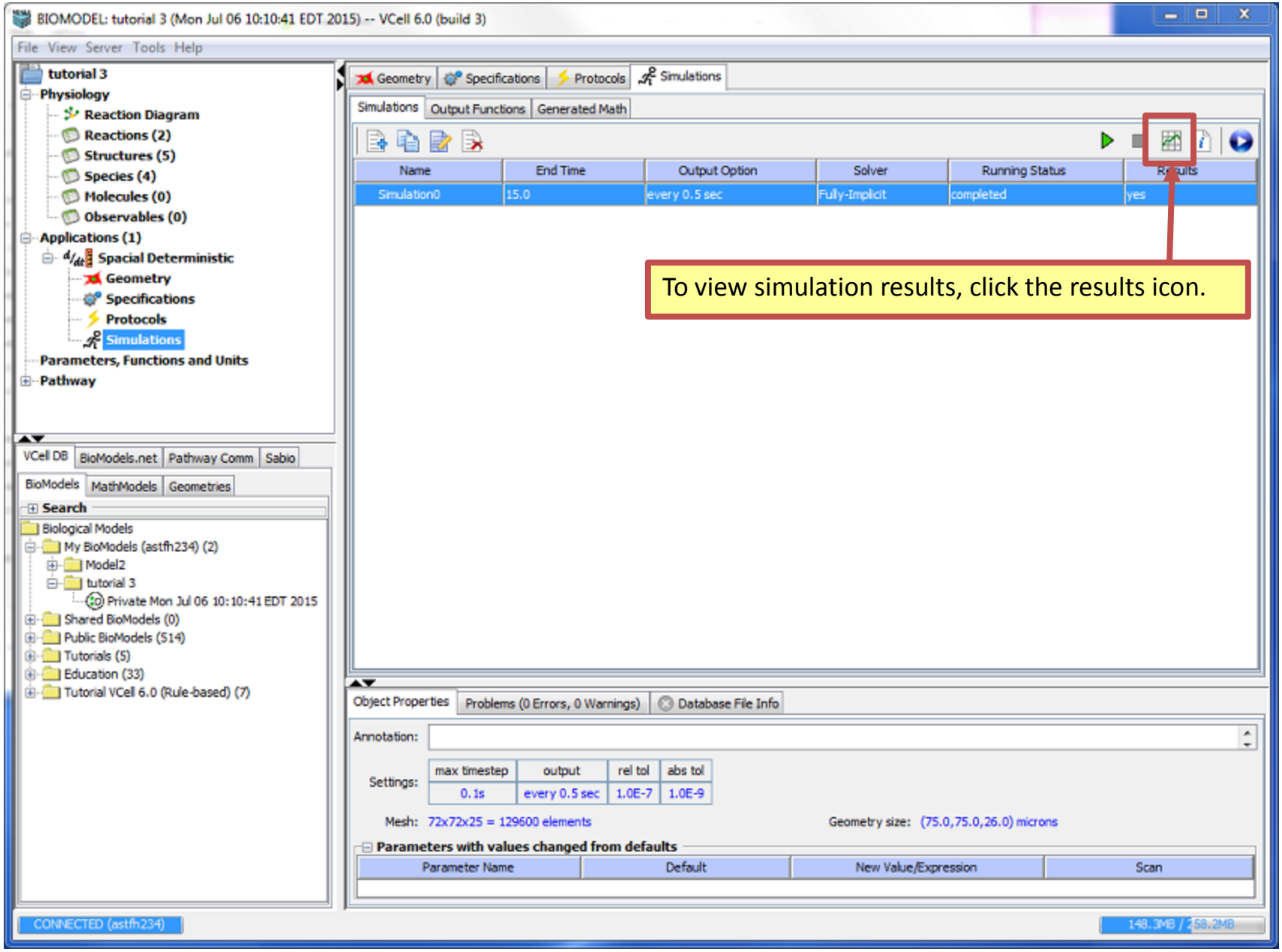
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
138.8MB / 258.2MB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Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 sec
Fully-Implicit
completed
yes
To view simulation results, click the results icon.
VCell DB
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Pathway Comm
Sabio
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MathModels
Geometries
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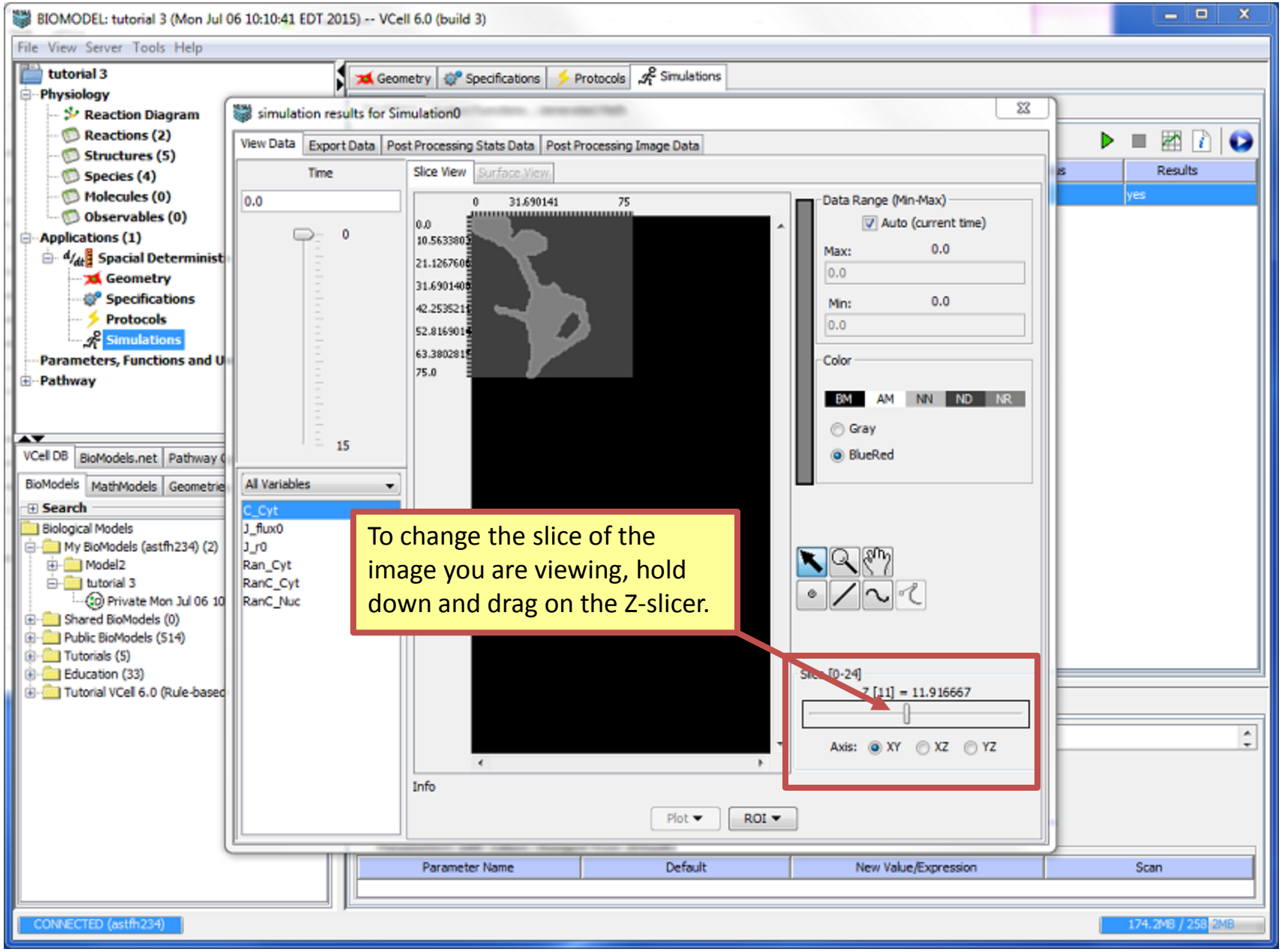
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
148.3MB / 258.2MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
0.0
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max:
0.0
Min:
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
To change the slice of the image you are viewing, hold down and drag on the Z-slicer.
Axis:
XY
XZ
YZ
Info
Plot
ROI
Parameter Name
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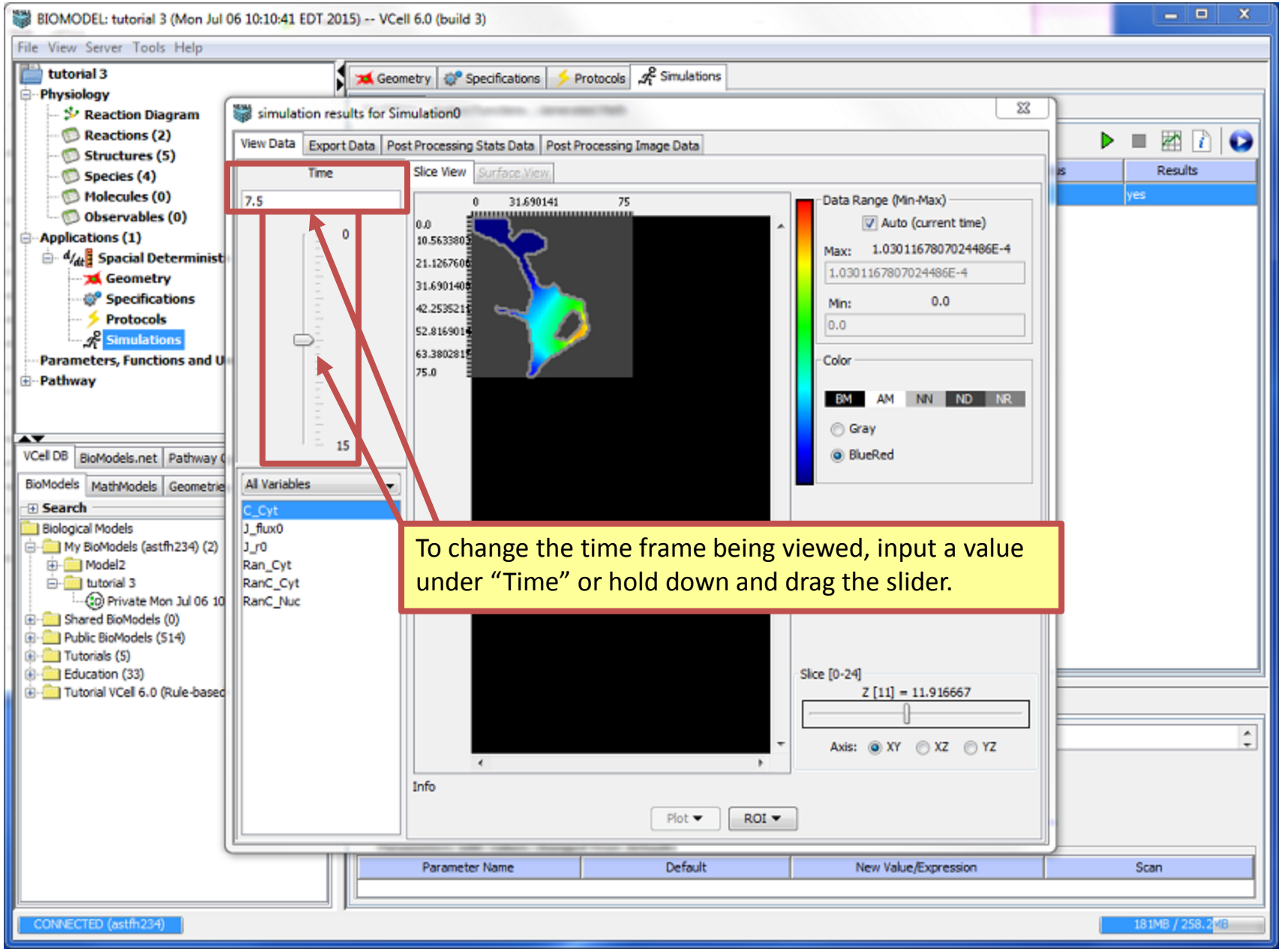
Results
yes

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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View Data
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Time
7.5
0
15
Slice View
Surface View
0
31.690141
75
0.0
10.563380
21.126760
31.690140
42.253521
52.816901
63.380281
75.0
Data Range (Min-Max)
Auto (current time)
Max:
1.0301167807024486E-4
1.0301167807024486E-4
Min:
0.0
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Slice [0-24]
Z [11] = 11.916667
Axis:
XY
XZ
YZ
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Results
yes
Parameter Name
Default
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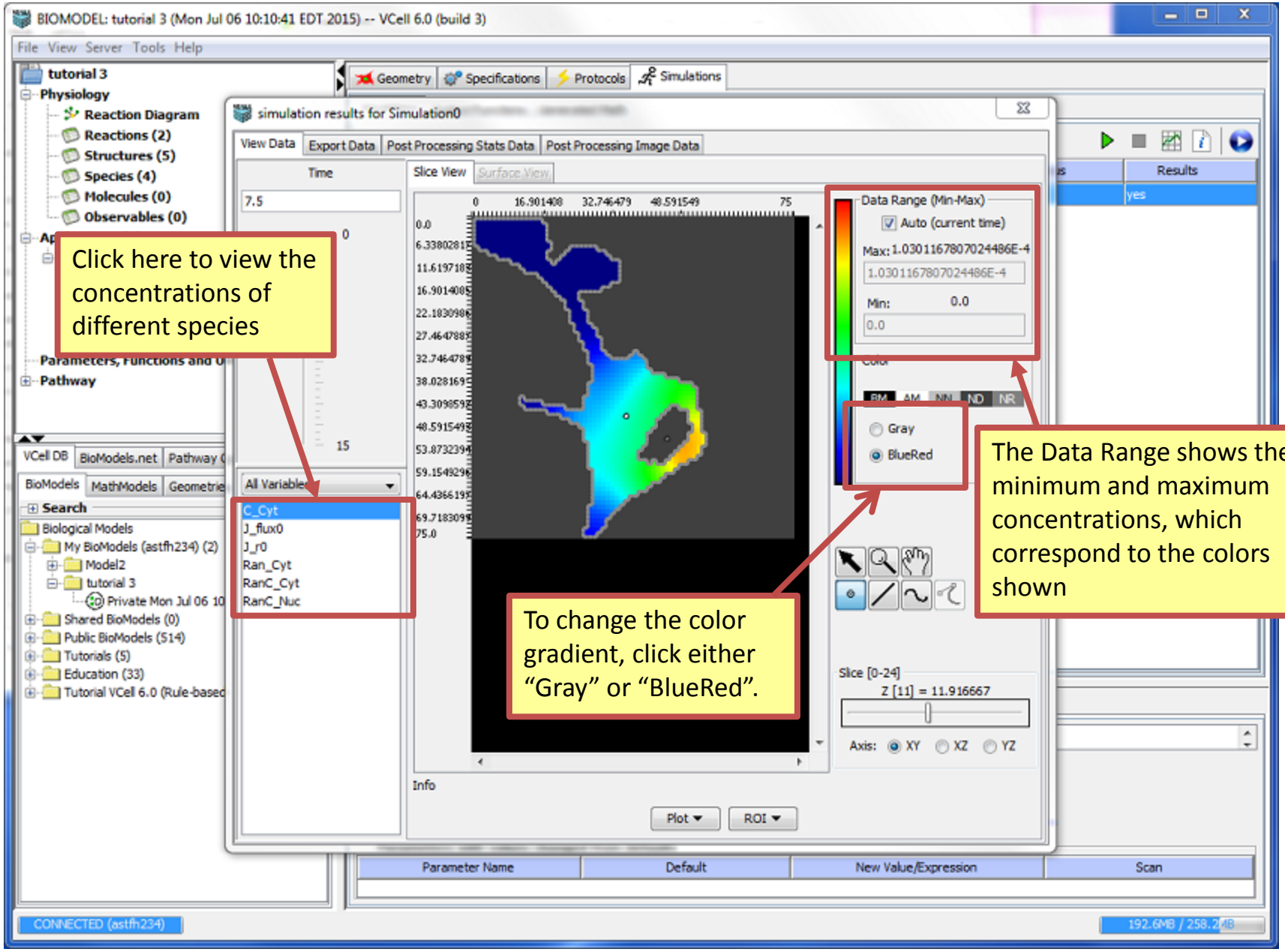
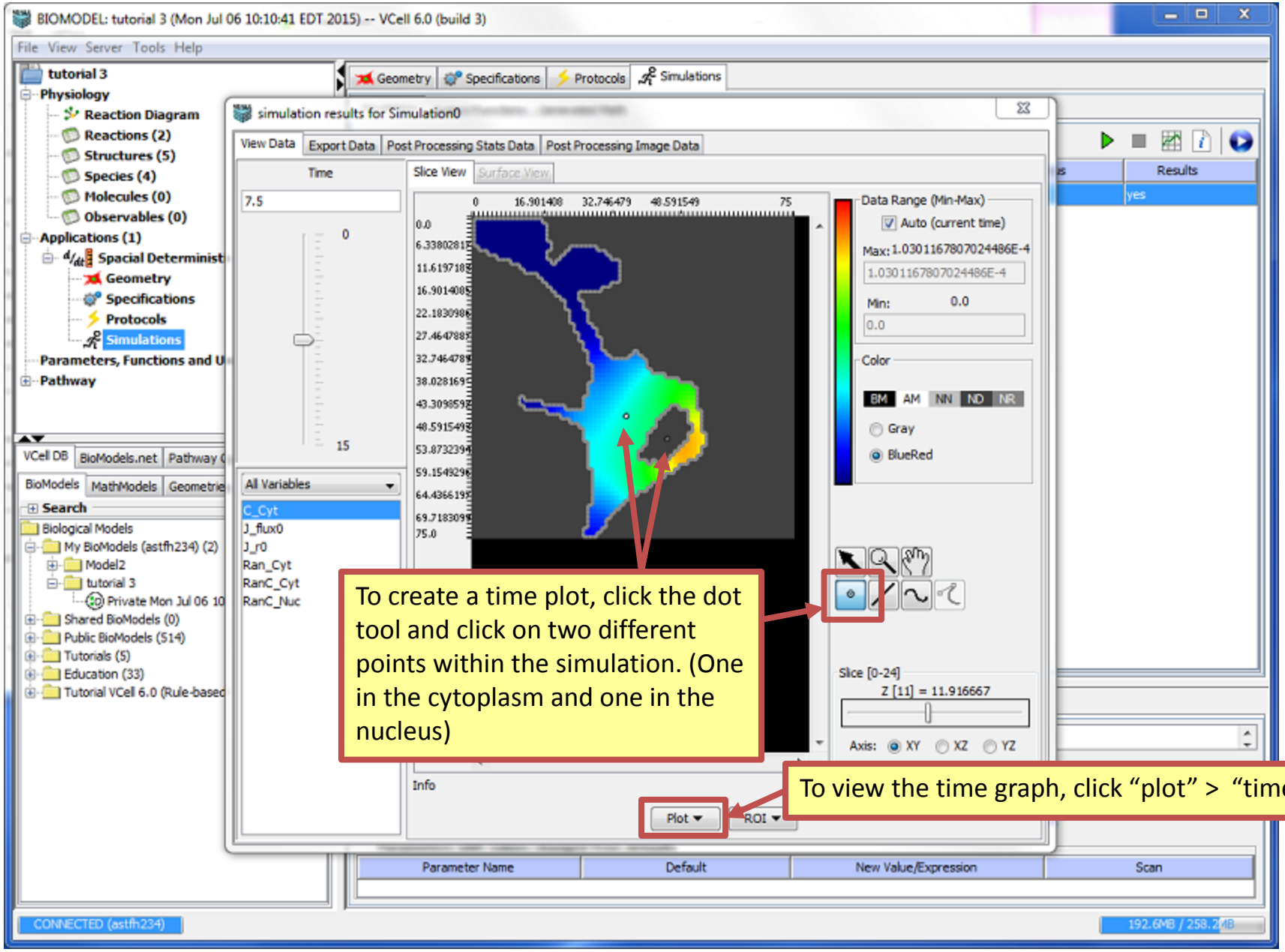
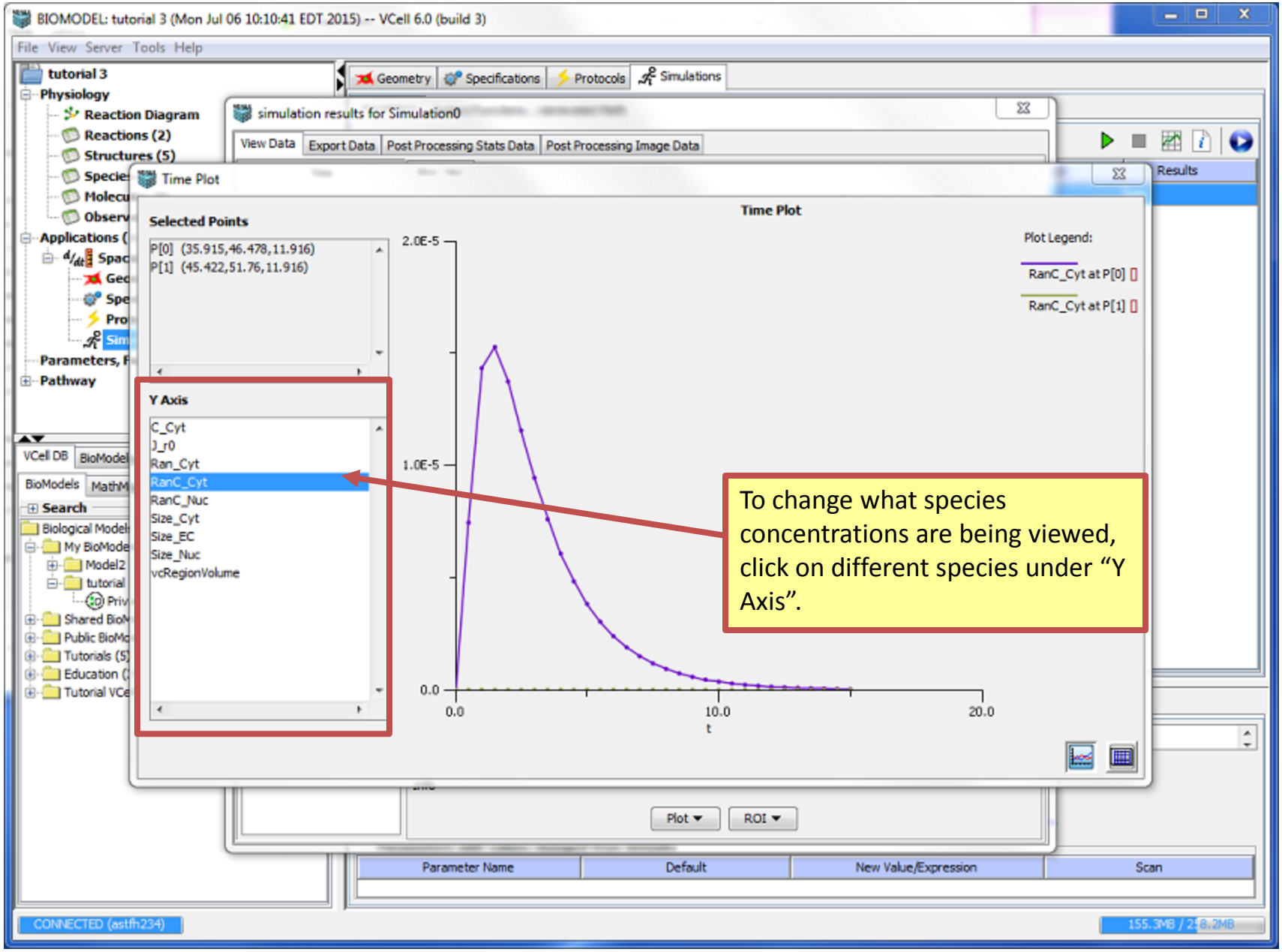
181MB / 258.2MB
To change the time frame being viewed, input a value under “Time” or hold down and drag the slider.

Contents


Click here to view the concentrations of different species
To change the color gradient, click either “Gray” or “BlueRed”.
The Data Range shows the minimum and maximum concentrations, which correspond to the colors shown


To create a time plot, click the dot tool and click on two different points within the simulation. (One in the cytoplasm and one in the nucleus)
To view the time graph, click “plot” > “time”.

Contents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Time Plot
Selected Points
P[0] (35.915,46.478,11.916)
P[1] (45.422,51.76,11.916)
Time Plot
Plot Legend:
RanC_Cyt at P[0]
RanC_Cyt at P[1]
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
Y Axis
C_Cyt
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Size_Cyt
Size_EC
Size_Nuc
vcRegionVolume
To change what species concentrations are being viewed, click on different species under “Y Axis”.
Plot
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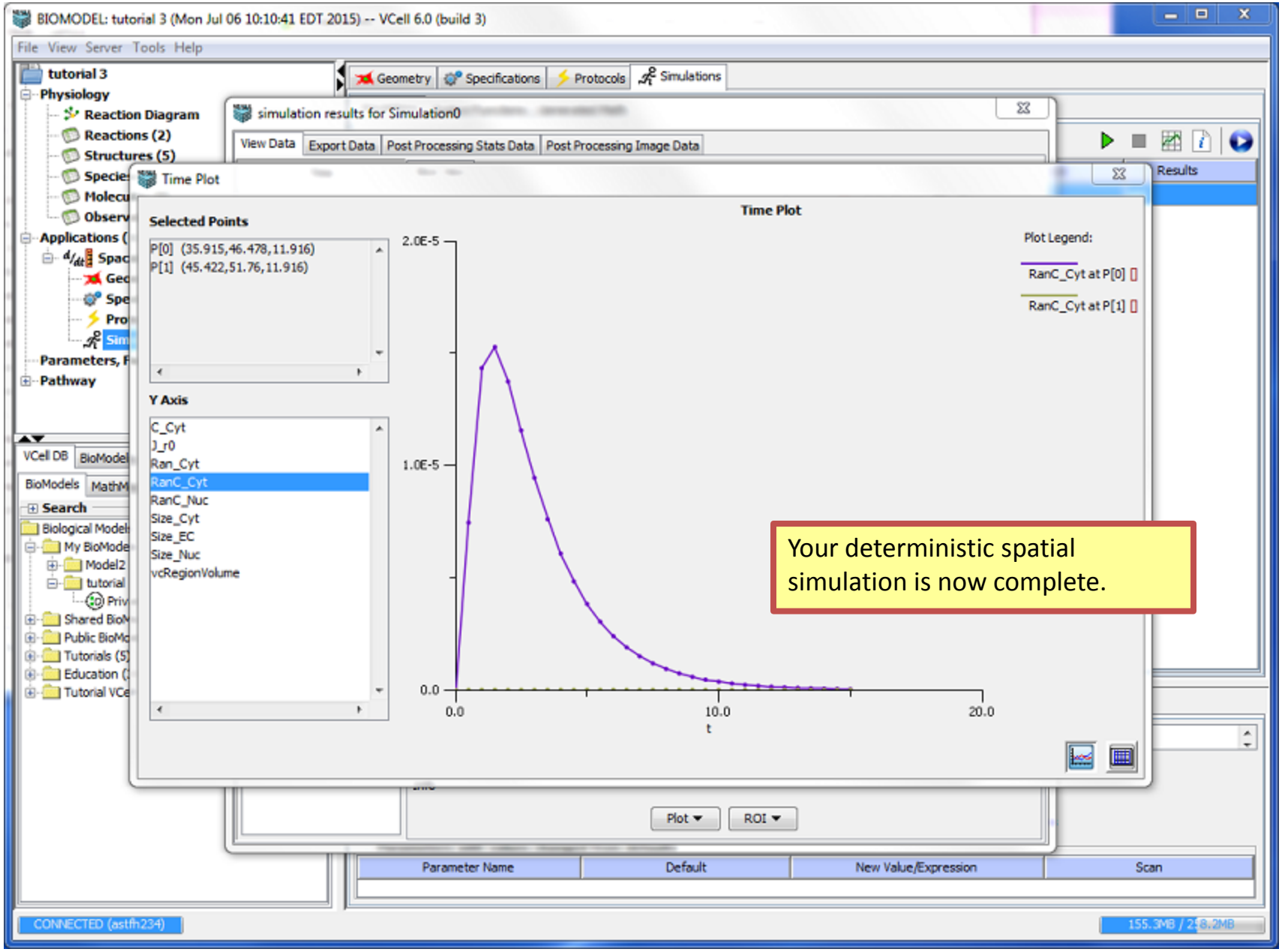
BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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P[1] (45.422,51.76,11.916)
Y Axis
C_Cyt
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Size_Cyt
Size_EC
Size_Nuc
vcRegionVolume
Time Plot
Plot Legend:
RanC_Cyt at P[0]
RanC_Cyt at P[1]
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
Your deterministic spatial simulation is now complete.
Plot
ROI
Parameter Name
Default
New Value/Expression
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VCell DB
BioModels
Search
CONNECTED (astfh234)

Next: VCell Tutorial
BioModel with Multiple Applications

Part 2 Compartmental Applications and Parameter Estimation