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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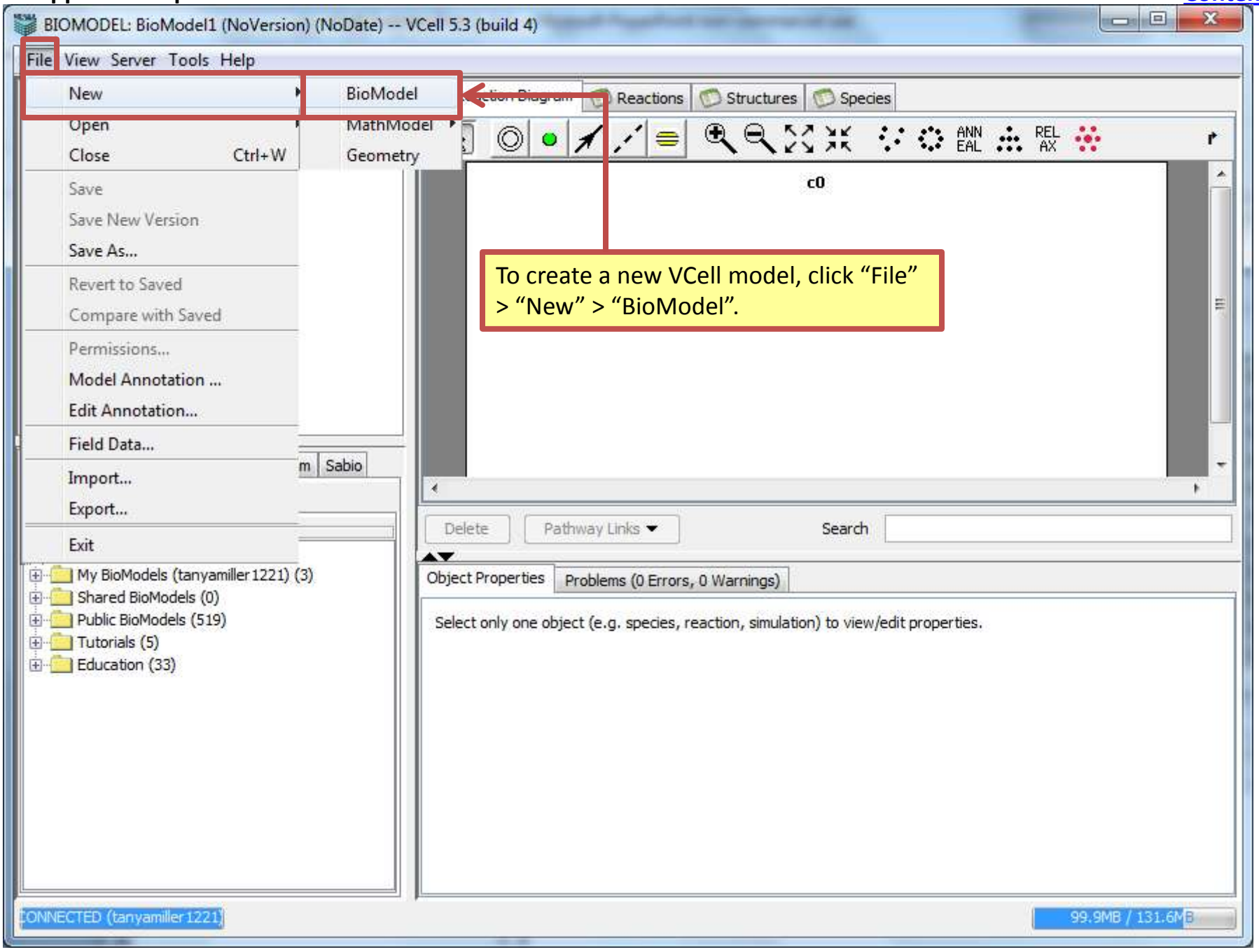
First time opening VCell

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.


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
File View Server Tools Help
New
Open
Close Ctrl+W
Save
Save New Version
Save As...
Revert to Saved
Compare with Saved
Permissions...
Model Annotation ...
Edit Annotation...
Field Data...
Import...
Export...
Exit
BioModel
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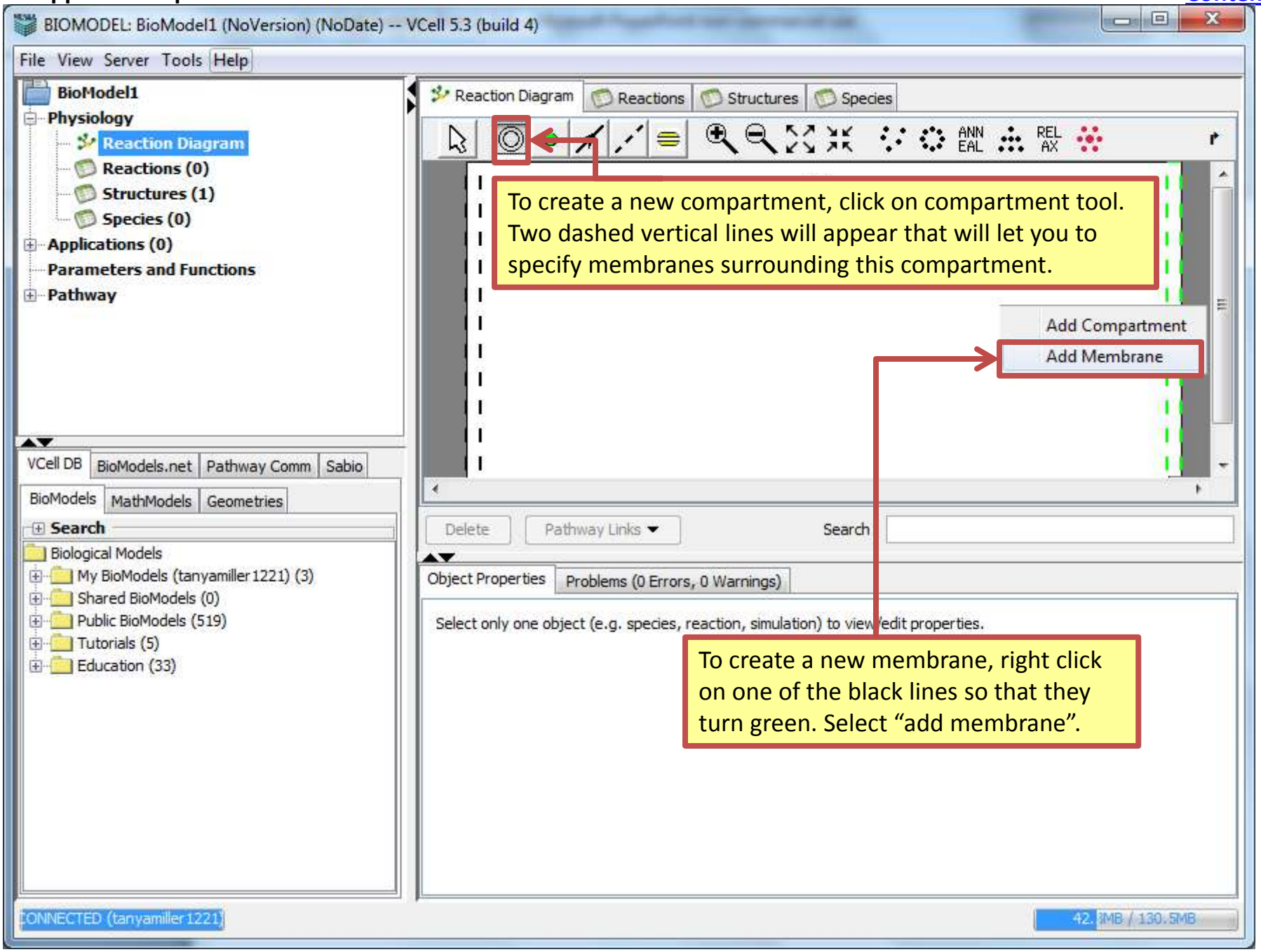
Structures
Species
c0
To create a new VCell model, click “File” > “New” > “BioModel”.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
My BioModels (tanyamiller1221) (3)
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
99.9MB / 131.6MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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To create a new compartment, click on compartment tool. Two dashed vertical lines will appear that will let you to specify membranes surrounding this compartment.
Add Compartment
Add Membrane
VCell DB
BioModels.net
Pathway Comm
Sabio
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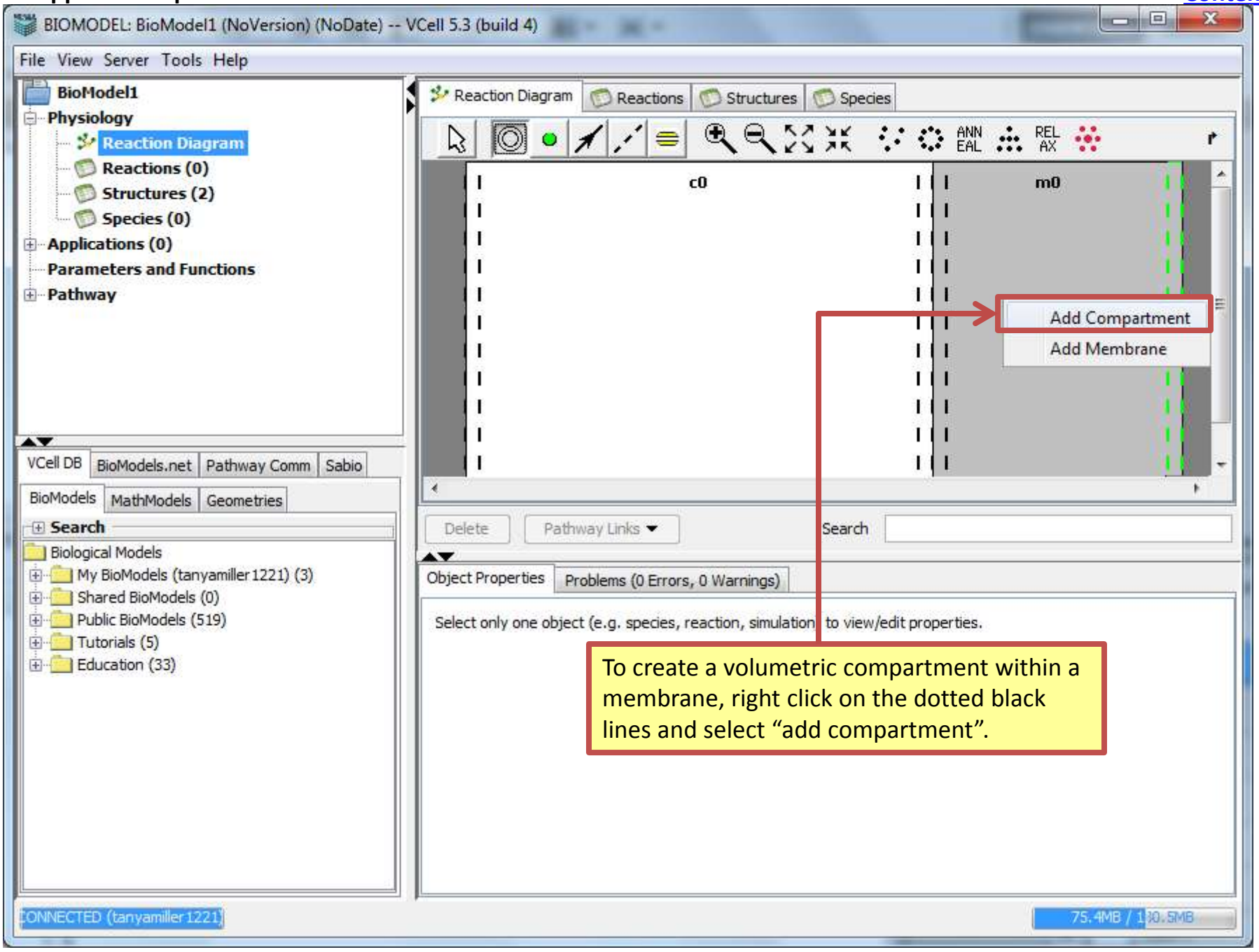
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
To create a new membrane, right click on one of the black lines so that they turn green. Select “add membrane”.
CONNECTED (tanyamiller1221)

Contents


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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m0
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Add Membrane
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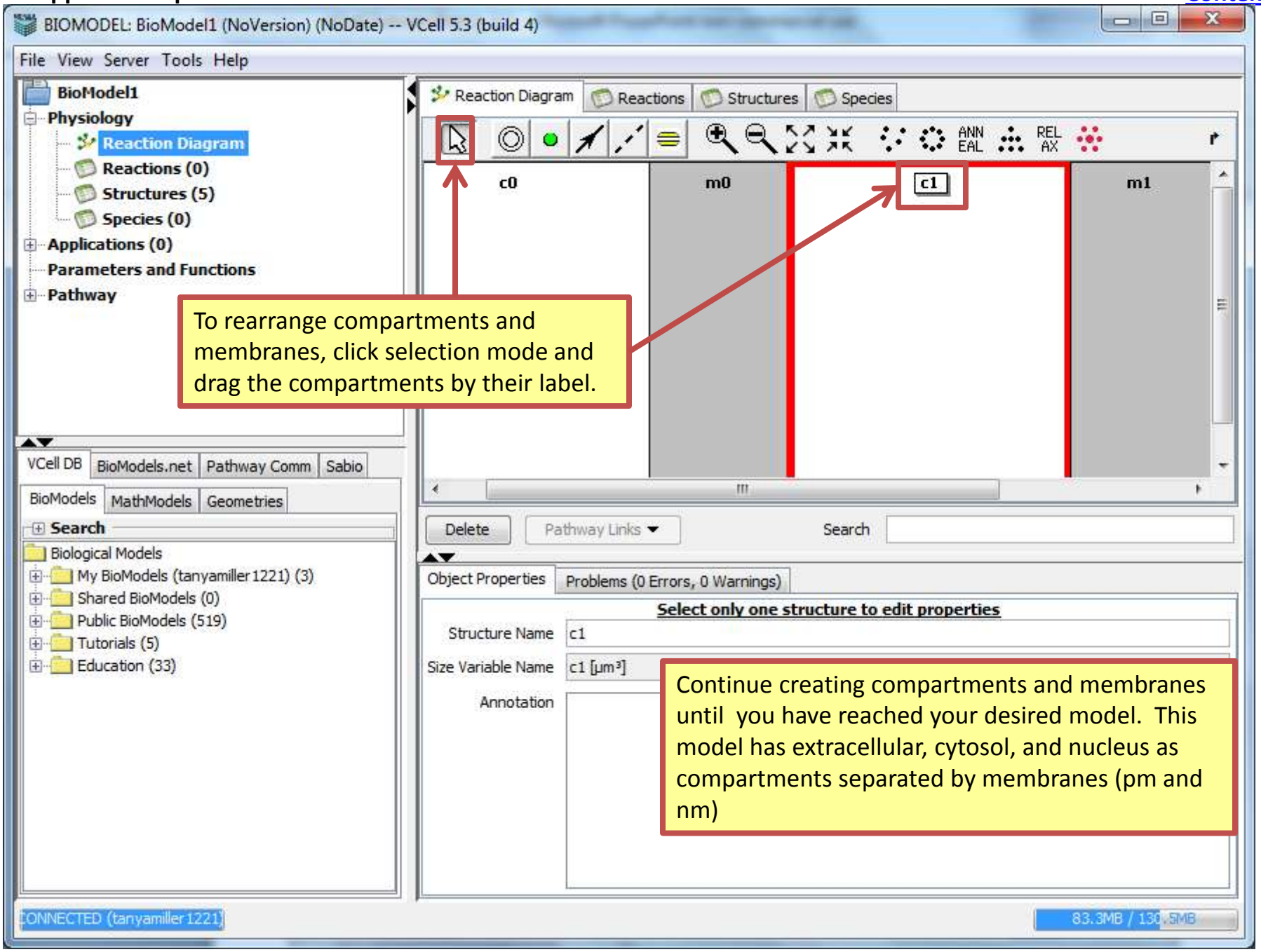
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation to view/edit properties.
To create a volumetric compartment within a membrane, right click on the dotted black lines and select “add compartment”.
CONNECTED (tanyamiller1221)

Contents


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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c0
m0
c1
m1
To rearrange compartments and membranes, click selection mode and drag the compartments by their label.
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Pathway Comm
Sabio
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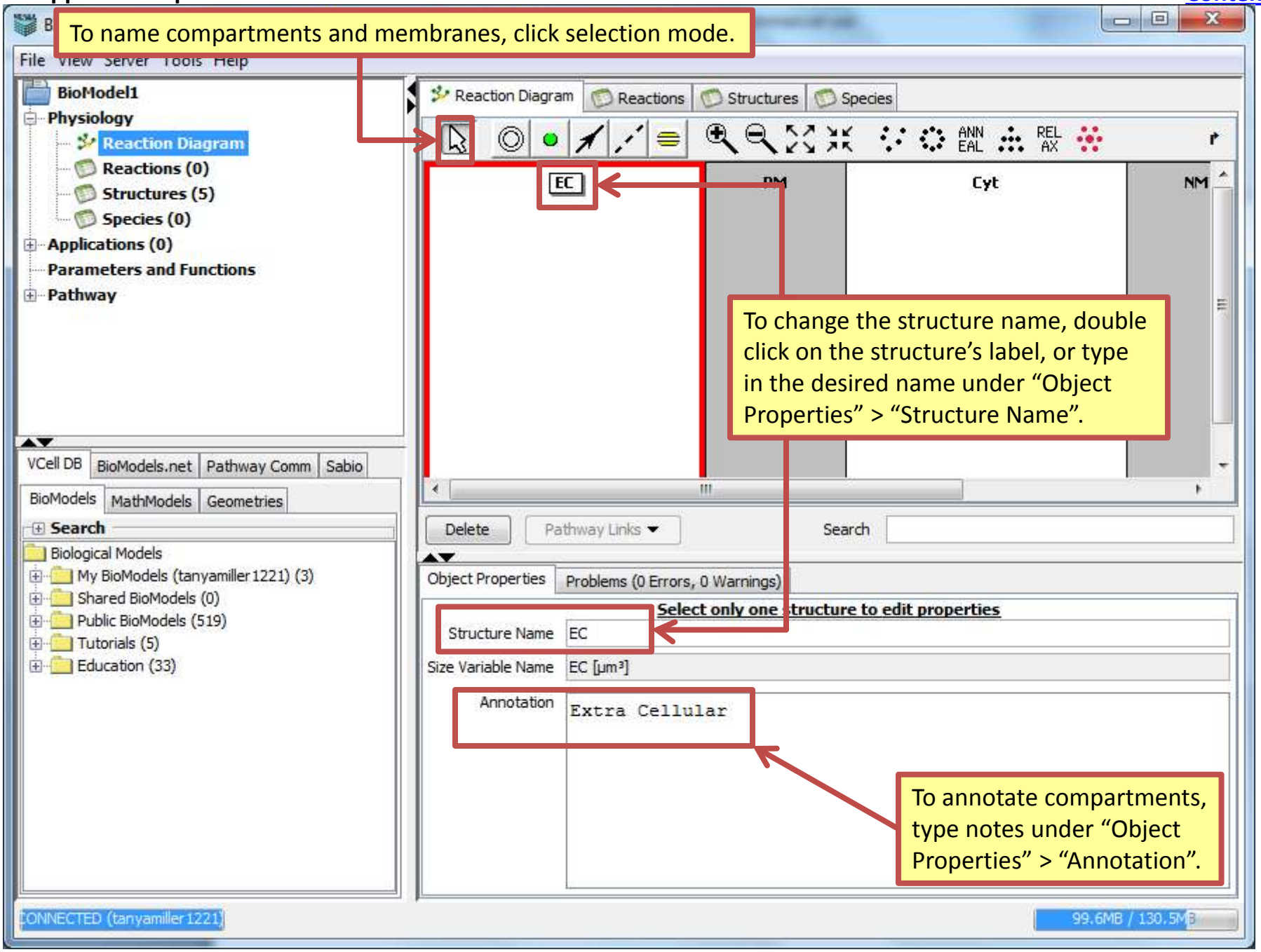
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name
c1
Size Variable Name
c1 [µm³]
Annotation
Continue creating compartments and membranes until you have reached your desired model. This model has extracellular, cytosol, and nucleus as compartments separated by membranes (pm and nm)
CONNECTED (tanyamiller1221)
83.3MB / 130.5MB


To name compartments and membranes, click selection mode.
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Species (0)
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Cyt
NM
To change the structure name, double click on the structure's label, or type in the desired name under "Object Properties" > "Structure Name".
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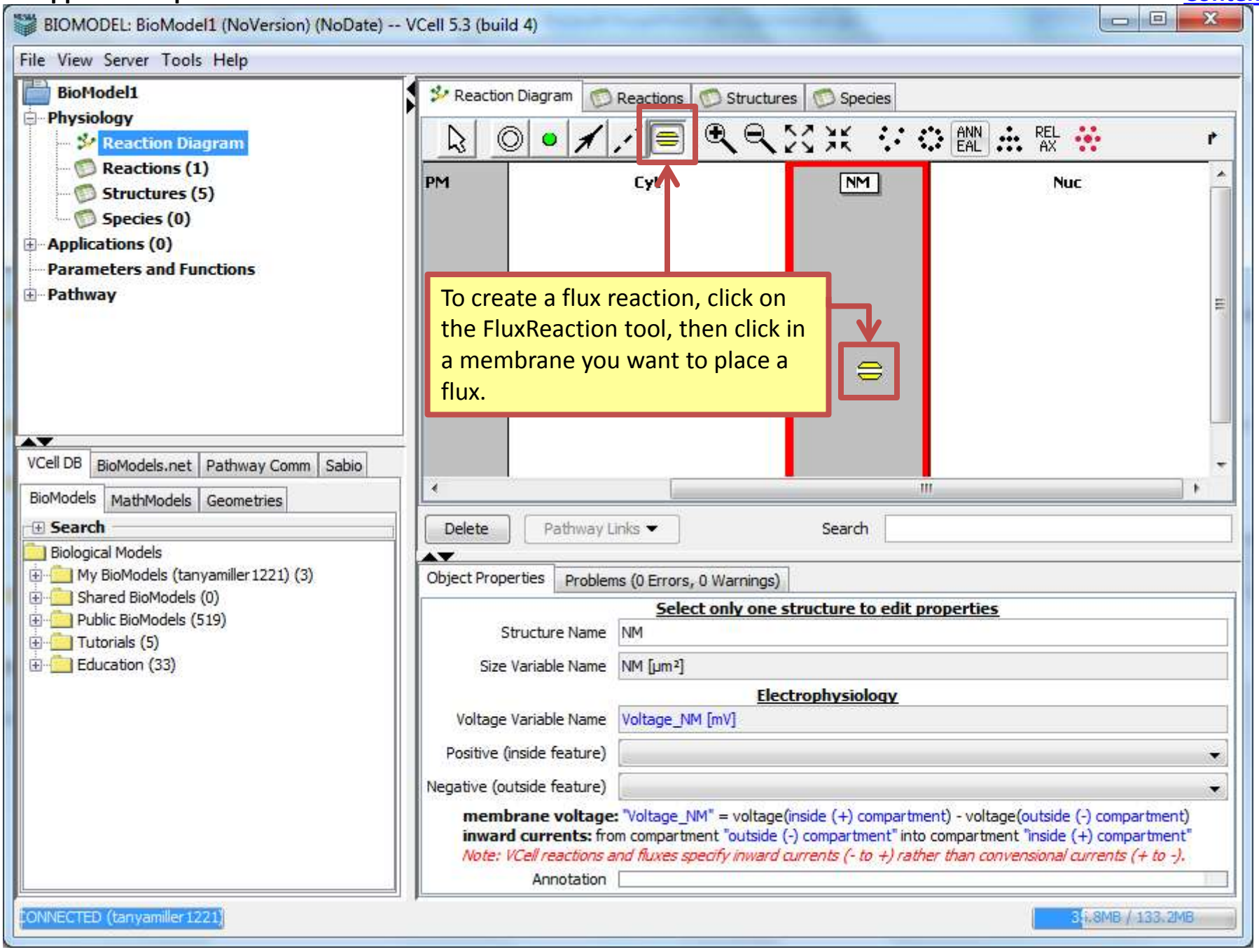
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name
EC
Size Variable Name
EC [µm³]
Annotation
Extra Cellular
To annotate compartments, type notes under "Object Properties" > "Annotation".
CONNECTED (tanyamiller1221)
99.6MB / 130.5MB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Cyt
NM
Nuc
To create a flux reaction, click on the FluxReaction tool, then click in a membrane you want to place a flux.
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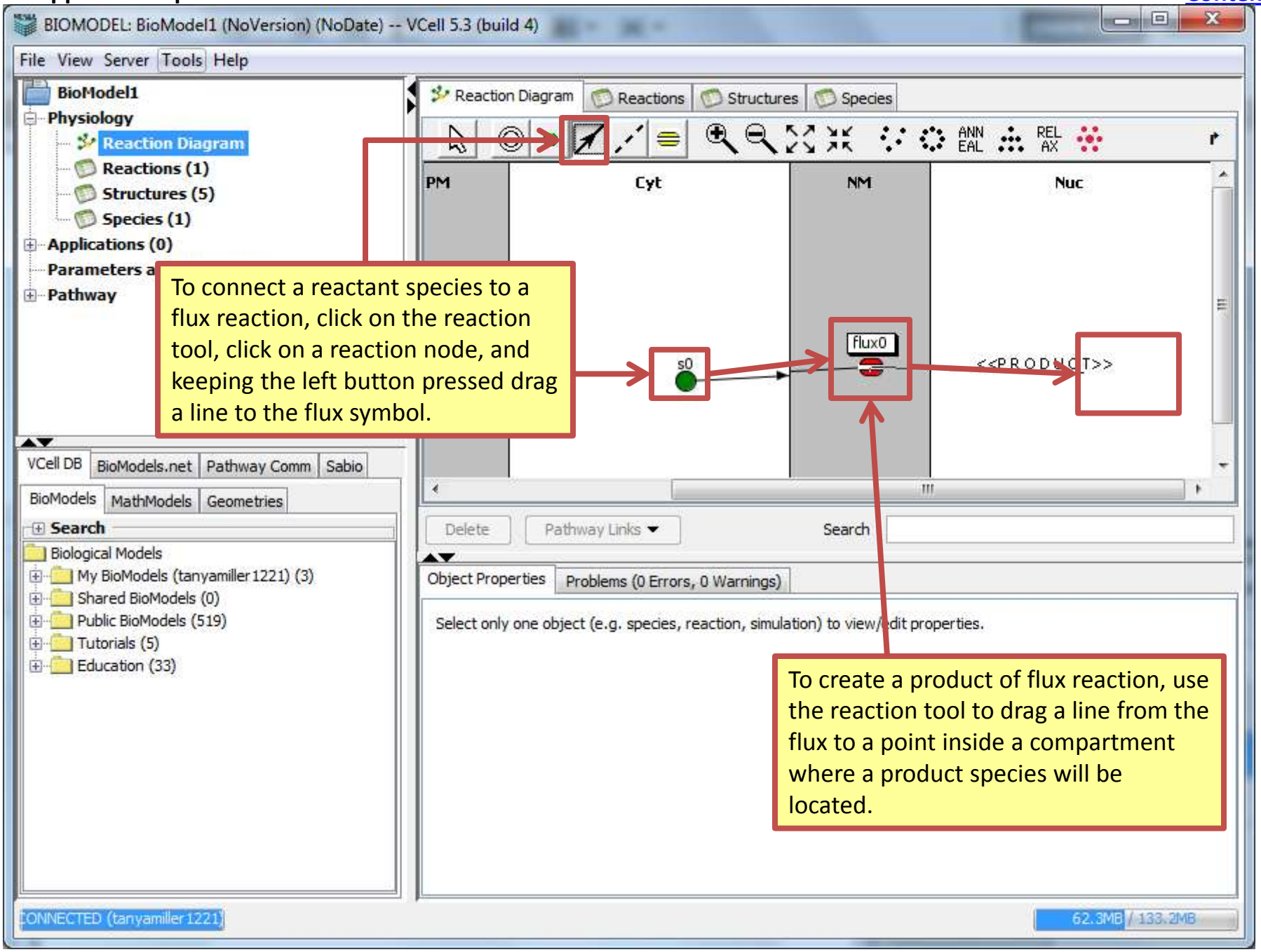
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name
NM
Size Variable Name
NM [µm²]
Electrophysiology
Voltage Variable Name
Voltage_NM [mV]
Positive (inside feature)
Negative (outside feature)
membrane voltage: "Voltage_NM" = 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 convensional currents (+ to -).
Annotation
ONNECTED (tanyamiller1221)

Contents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Nuc
s0
flux0
<<PRODUCT>>
To connect a reactant species to a flux reaction, click on the reaction tool, click on a reaction node, and keeping the left button pressed drag a line to the flux symbol.
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Public BioModels (519)
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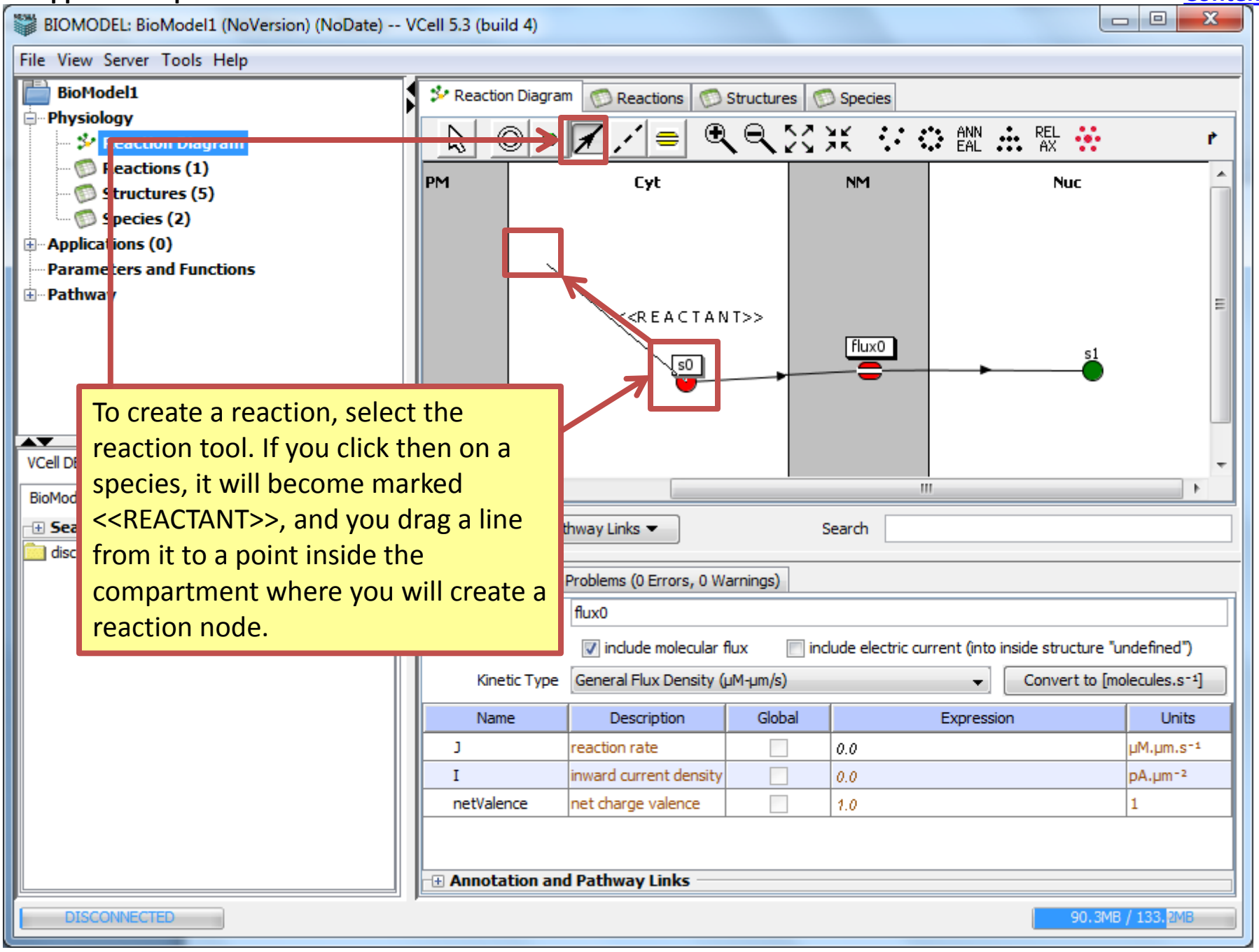
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
To create a product of flux reaction, use the reaction tool to drag a line from the flux to a point inside a compartment where a product species will be located.
CONNECTED (tanyamiller1221)
62.3MB / 133.2MB

Contents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Applications (0)
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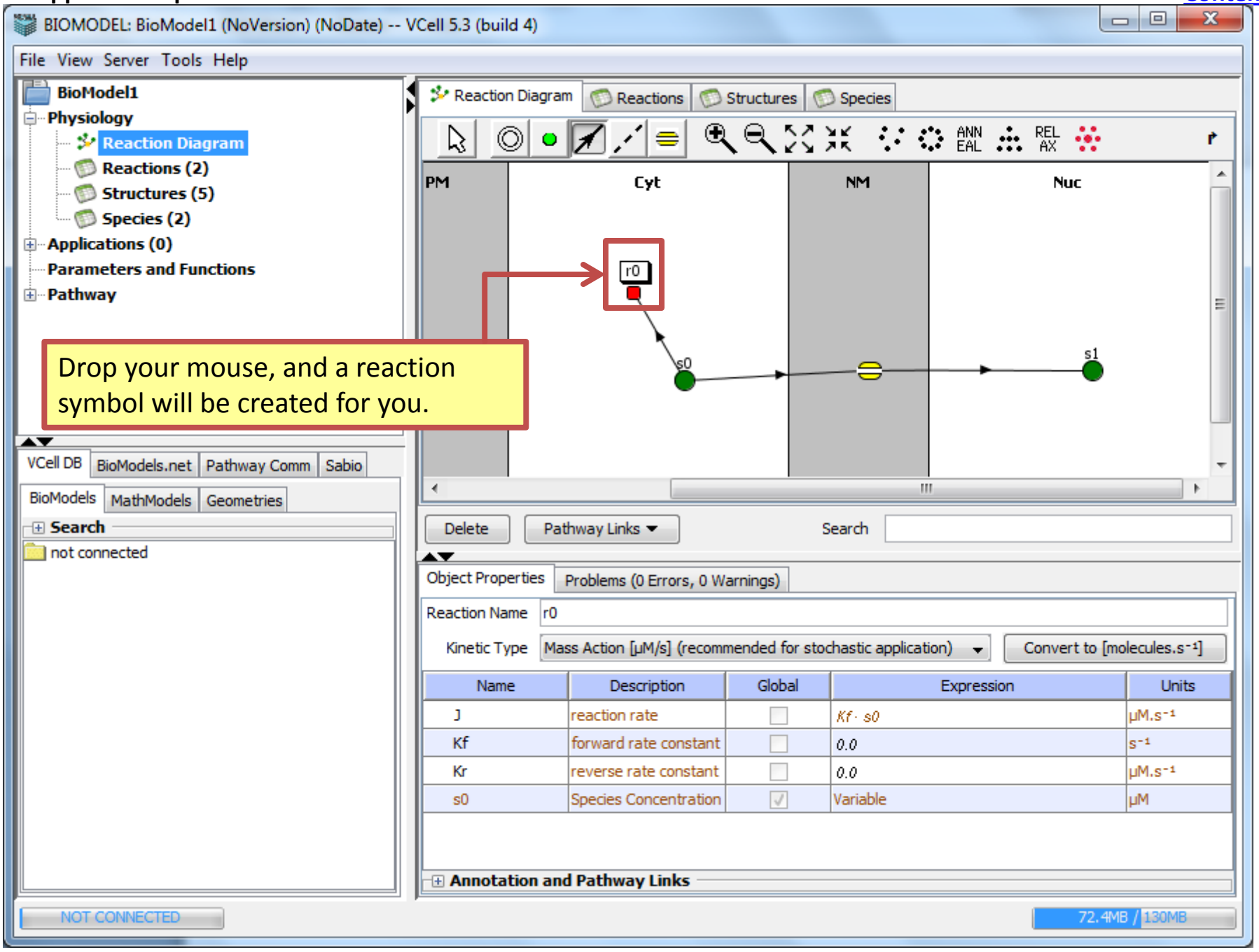
PM
Cyt
NM
Nuc
<<REACTANT>>
s0
flux0
s1
To create a reaction, select the reaction tool. If you click then on a species, it will become marked <<REACTANT>>, and you drag a line from it to a point inside the compartment where you will create a reaction node.
Search
Problems (0 Errors, 0 Warnings)
flux0
include molecular flux
include electric current (into inside structure "undefined")
Kinetic Type
General Flux Density (μM-μm/s)
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
0.0
μM.μm.s-1
I
inward current density
0.0
pA.μm-2
netValence
net charge valence
1.0
1
Annotation and Pathway Links
DISCONNECTED
90.3MB / 133.2MB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Applications (0)
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PM
Cyt
NM
Nuc
r0
s0
s1
Drop your mouse, and a reaction symbol will be created for you.
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Pathway Comm
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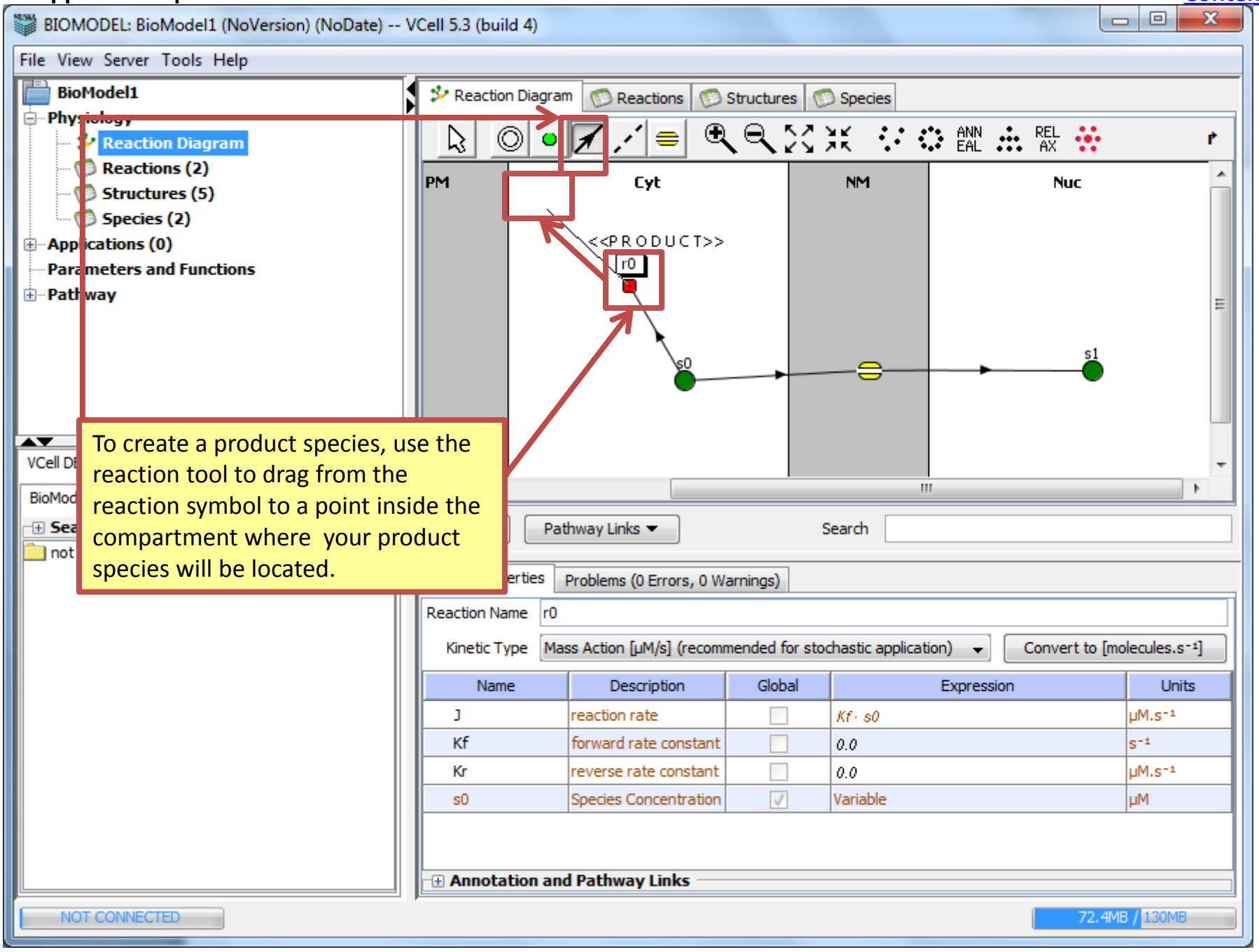
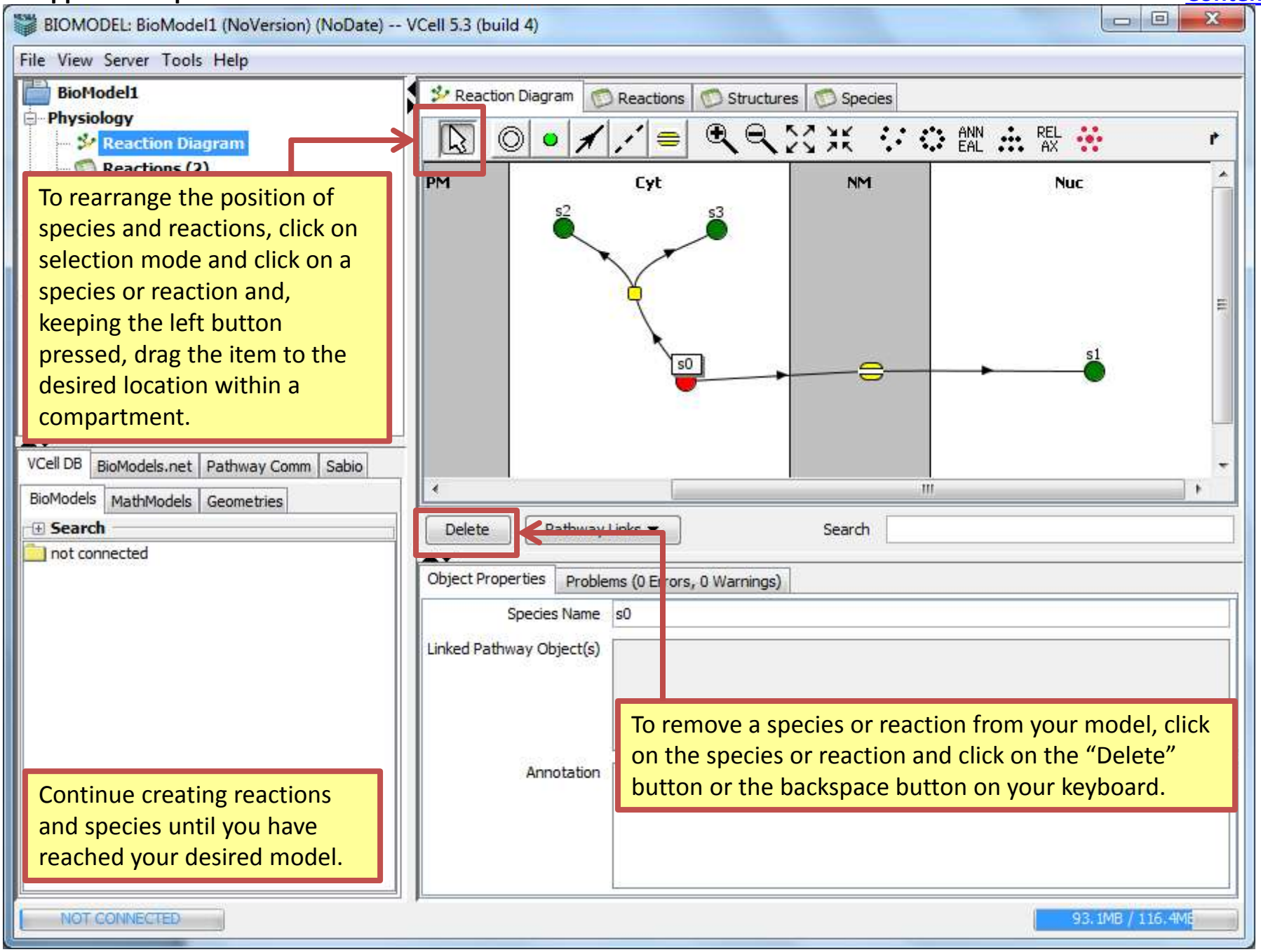
Search
not connected
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Reaction Name
r0
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
Kf· s0
μM.s-1
Kf
forward rate constant
0.0
s-1
Kr
reverse rate constant
0.0
μM.s-1
s0
Species Concentration
Variable
μM
Annotation and Pathway Links
NOT CONNECTED
72.4MB / 130MB



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.


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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Reactions (2)
Reaction Diagram
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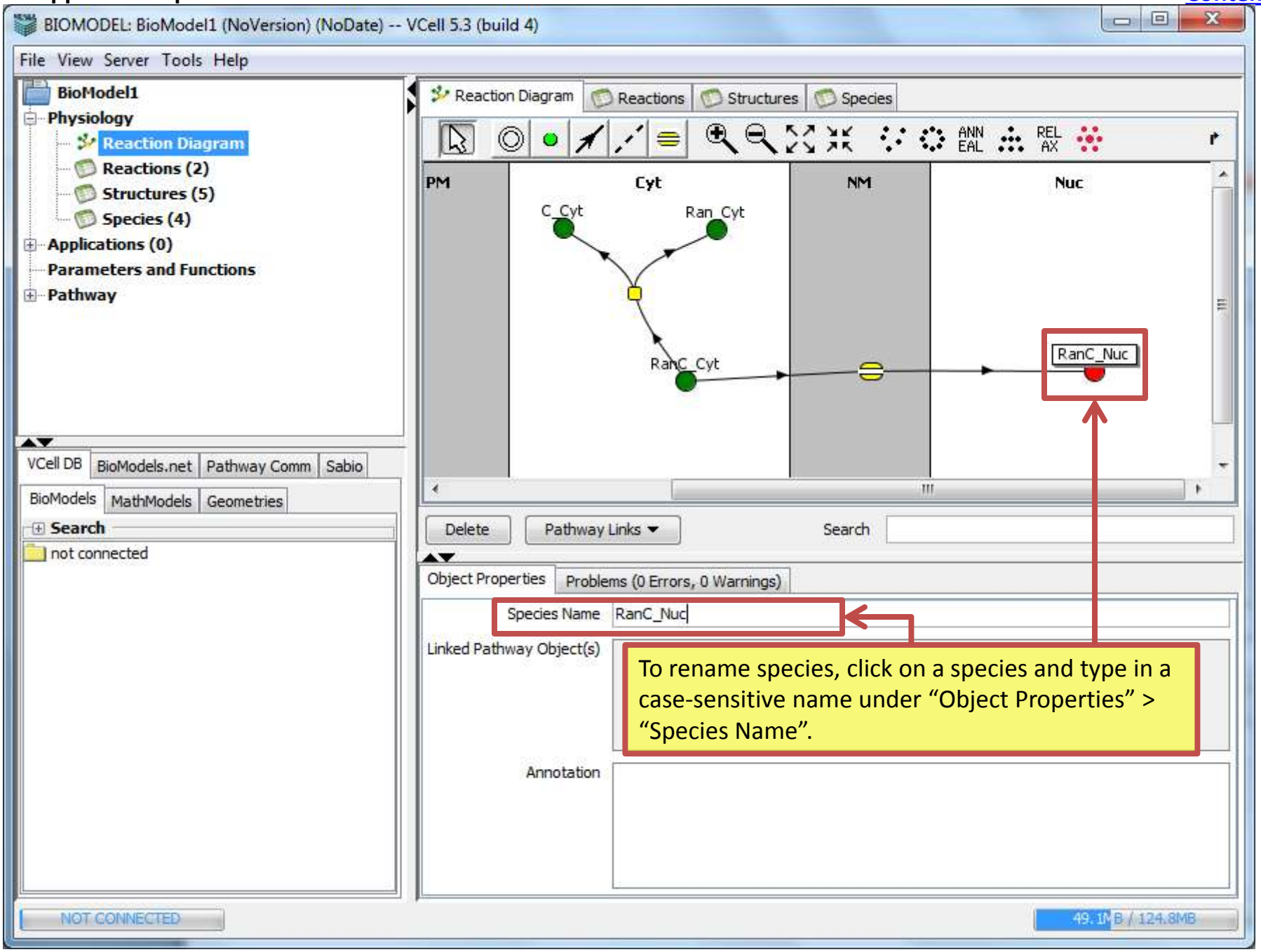
PM
Cyt
NM
Nuc
s2
s3
s0
s1
To rearrange the position of species and reactions, click on selection mode and click on a species or reaction and, keeping the left button pressed, drag the item to the desired location within a compartment.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
not connected
Delete
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Species Name
s0
Linked Pathway Object(s)
Annotation
To remove a species or reaction from your model, click on the species or reaction and click on the "Delete" button or the backspace button on your keyboard.
Continue creating reactions and species until you have reached your desired model.
NOT CONNECTED
93.1MB / 116.4MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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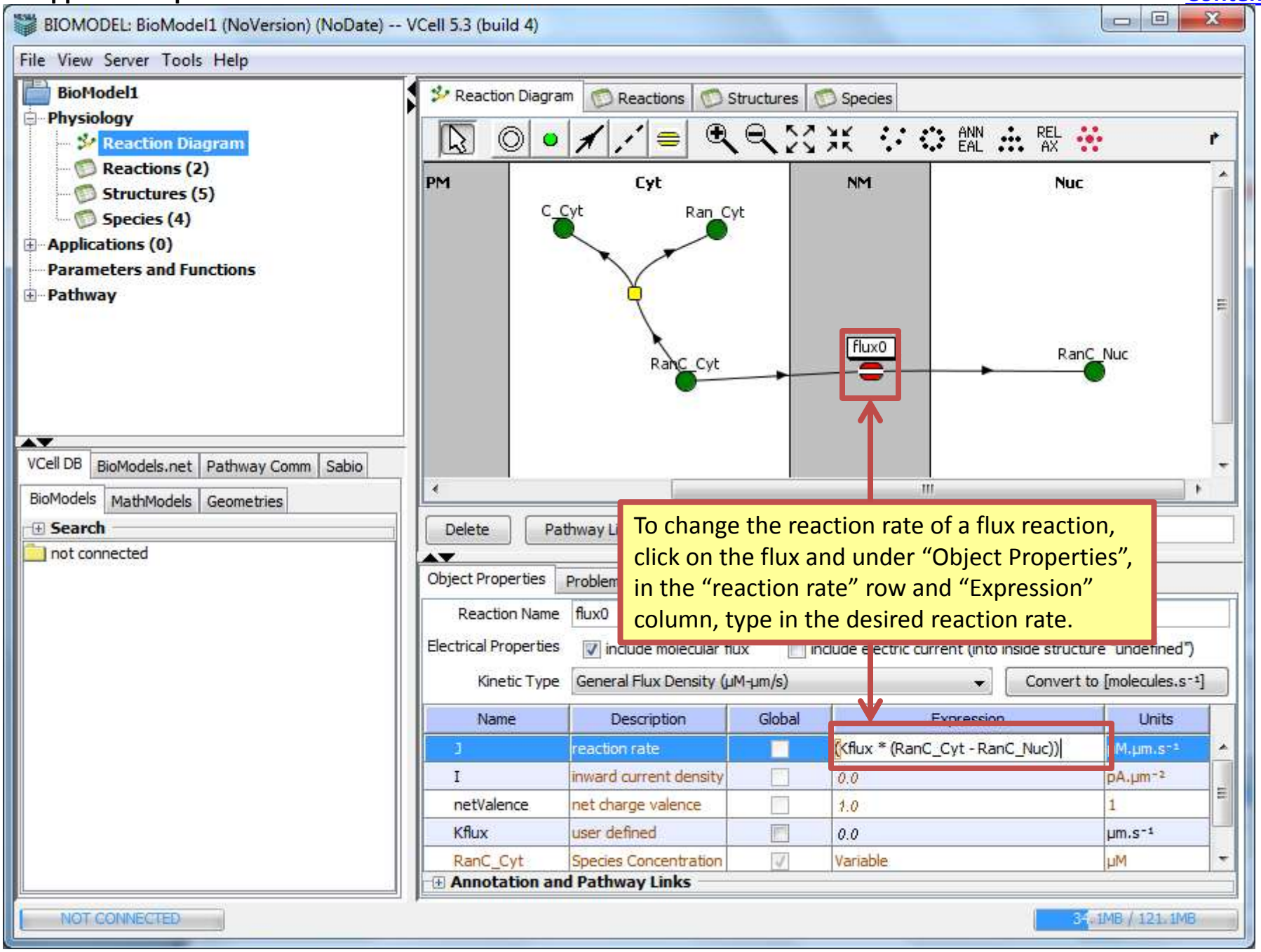
Cyt
NM
Nuc
C_Cyt
Ran_Cyt
RanC_Cyt
RanC_Nuc
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Species Name
RanC_Nuc
Linked Pathway Object(s)
Annotation
To rename species, click on a species and type in a case-sensitive name under “Object Properties” > “Species Name”.
NOT CONNECTED
49.1MB / 124.8MB

Contents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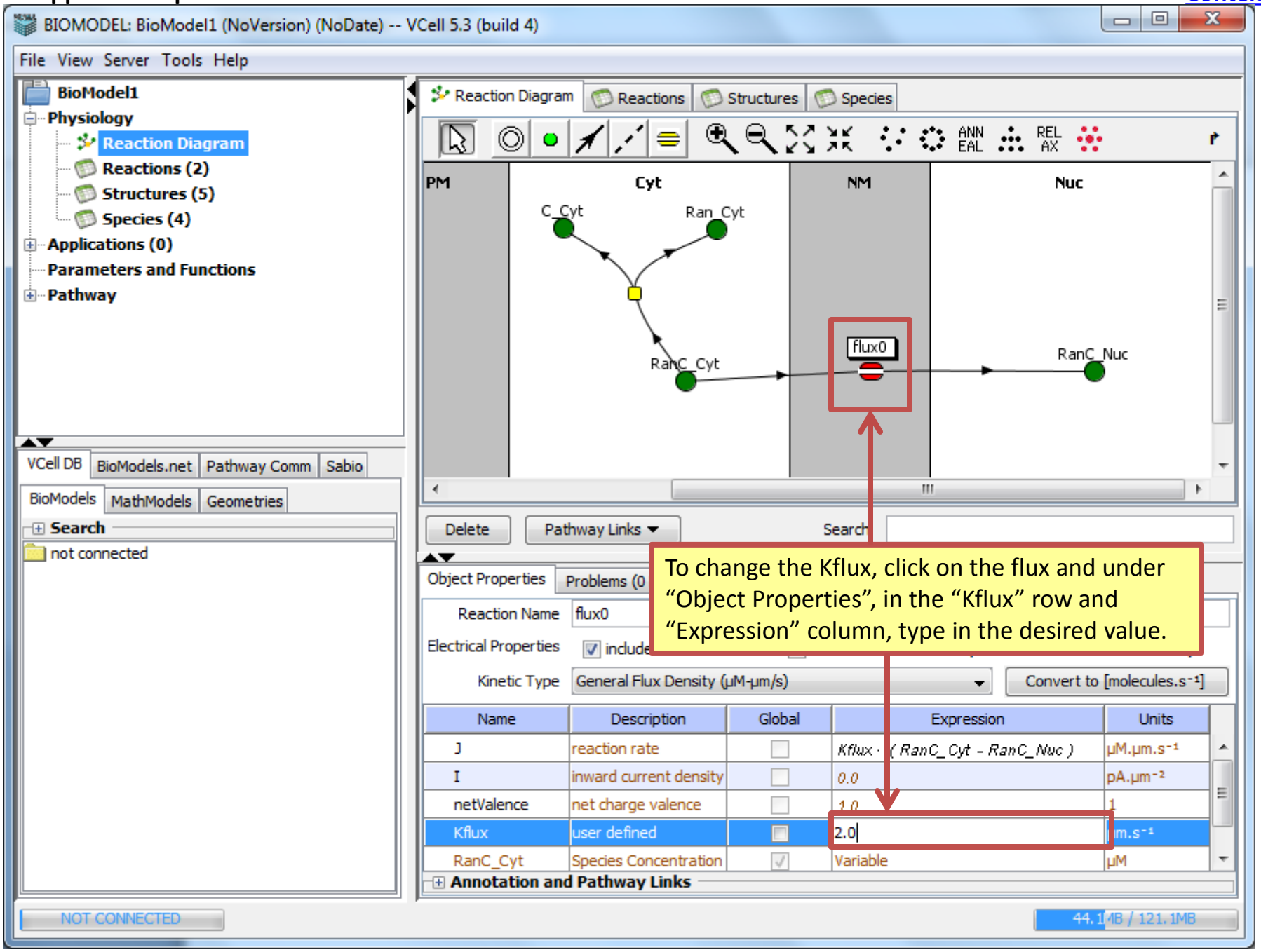
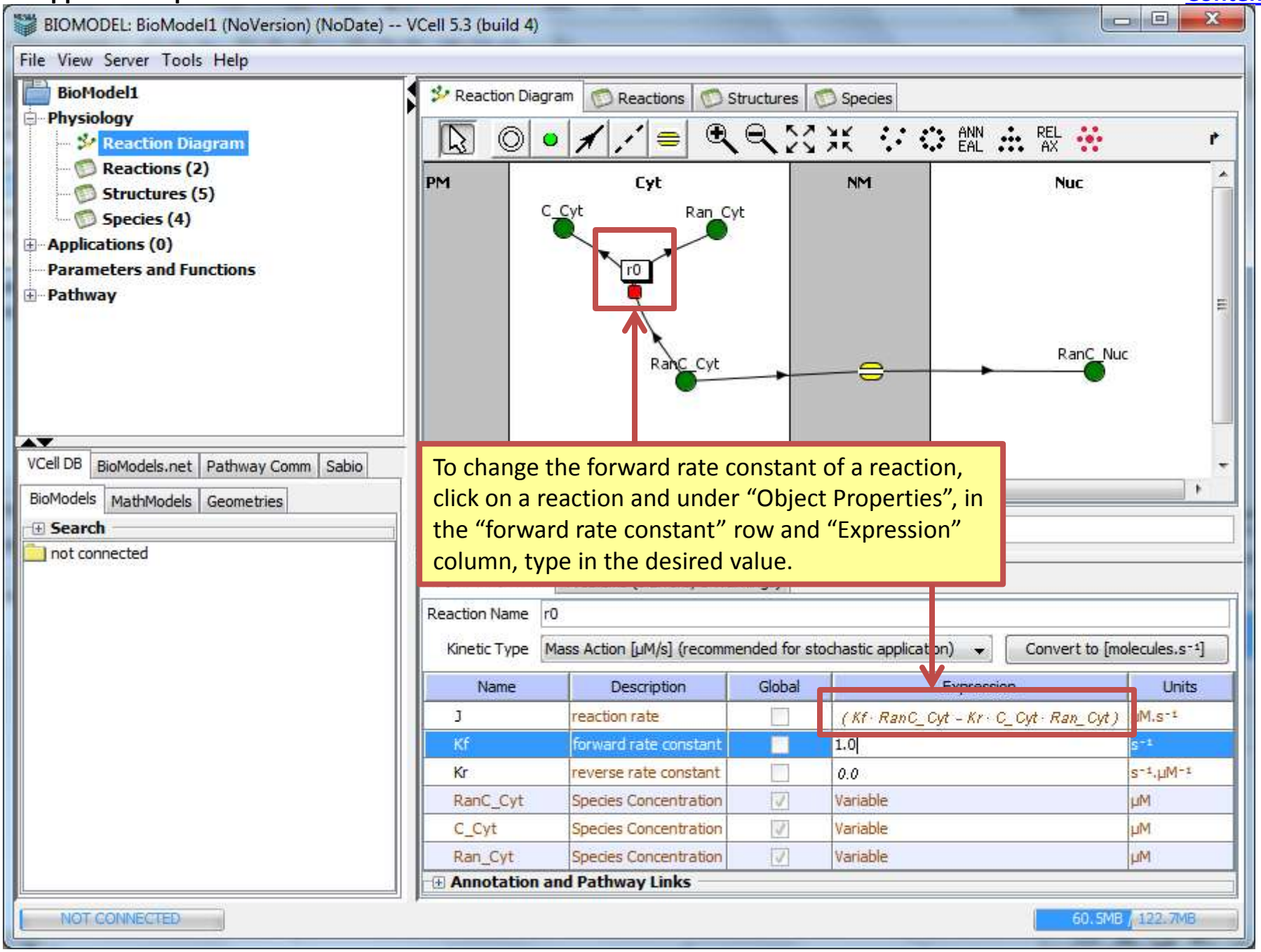
Ran_Cyt
RanC_Cyt
flux0
RanC_Nuc
Delete
Pathway Li
To change the reaction rate of a flux reaction, click on the flux and under "Object Properties", in the "reaction rate" row and "Expression" column, type in the desired reaction rate.
Object Properties
Problem
Reaction Name
flux0
Electrical Properties
include molecular flux
include electric current (into inside structure "undefined")
Kinetic Type
General Flux Density (μM-μm/s)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
(Kflux * (RanC_Cyt - RanC_Nuc))
M.μm.s⁻¹
I
inward current density
0.0
pA.μm⁻²
netValence
net charge valence
1.0
1
Kflux
user defined
0.0
μm.s⁻¹
RanC_Cyt
Species Concentration
Variable
μM
Annotation and Pathway Links
NOT CONNECTED
121.1MB



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

Contents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NM
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Ran_Cyt
r0
RanC_Cyt
RanC_Nuc
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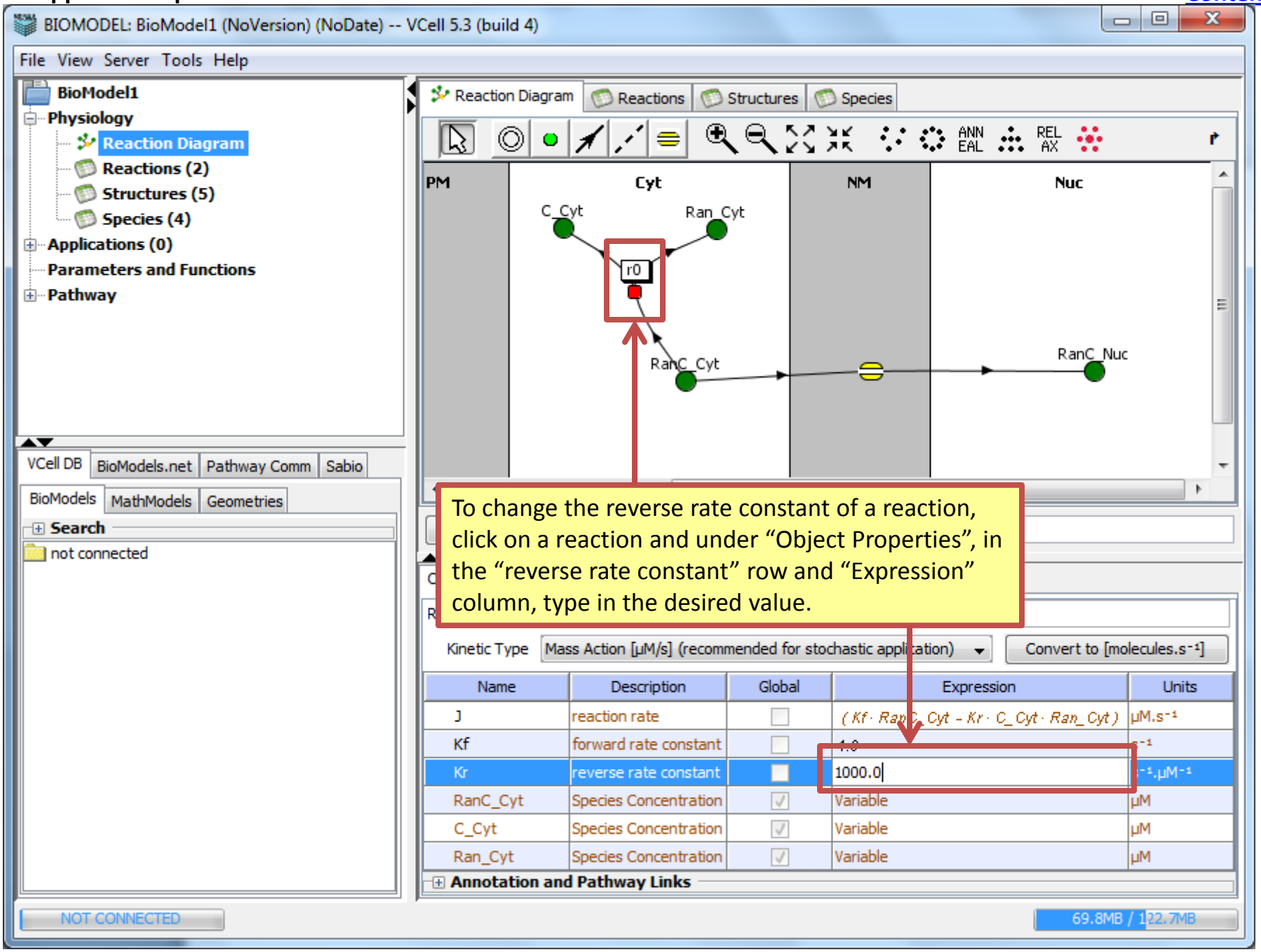
Geometries
Search
not connected
To change the forward rate constant of a reaction, click on a reaction and under "Object Properties", in the "forward rate constant" row and "Expression" column, type in the desired value.
Reaction Name
r0
Kinetic Type
Mass Action [µM/s] (recommended for stochastic application)
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
NOT CONNECTED
60.5MB
122.7MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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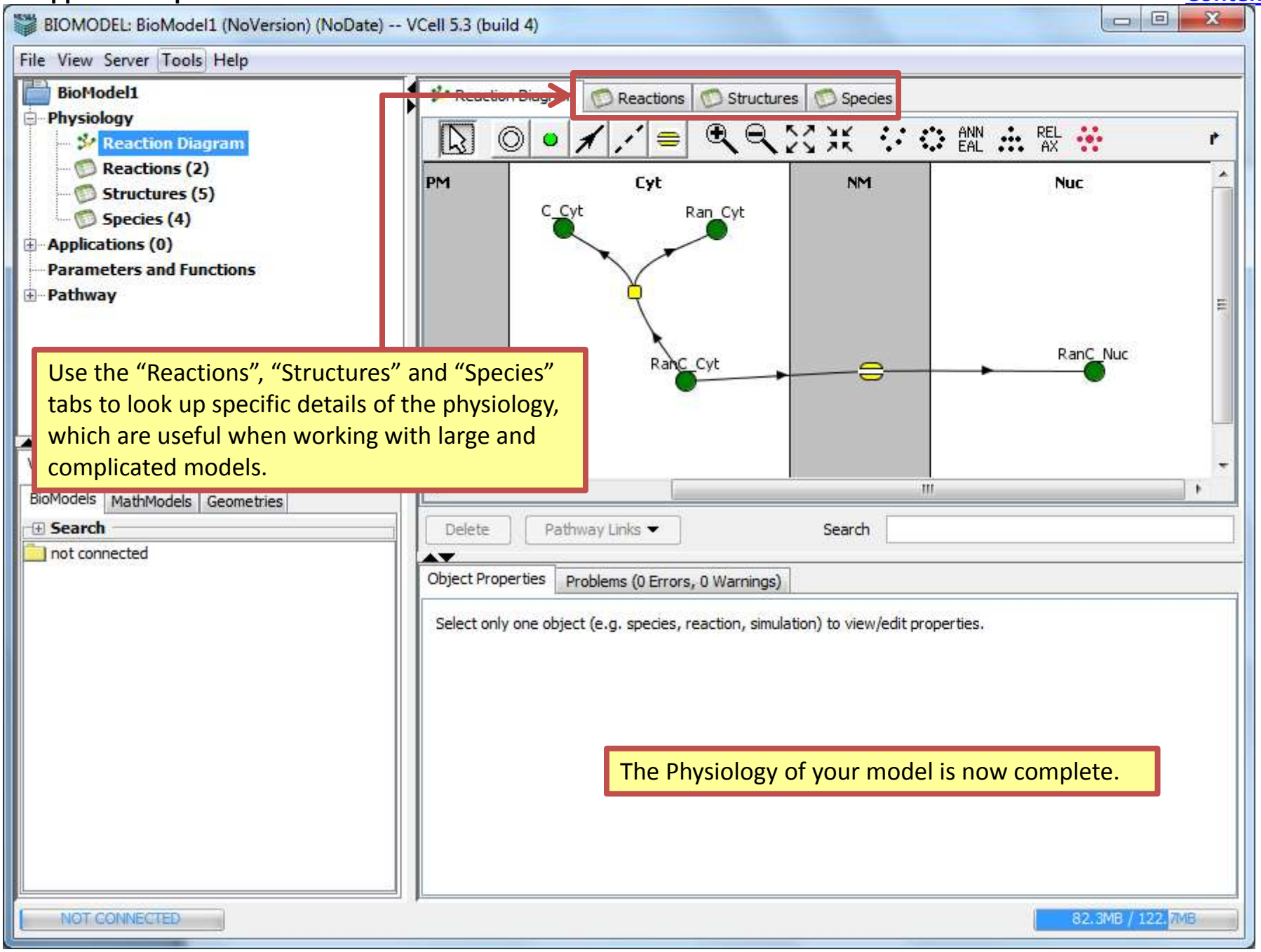
PM
Cyt
NM
Nuc
C_Cyt
Ran_Cyt
r0
RanC_Cyt
RanC_Nuc
To change the reverse rate constant of a reaction, click on a reaction and under "Object Properties", in the "reverse rate constant" row and "Expression" column, type in the desired value.
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
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
NOT CONNECTED
69.8MB / 122.7MB


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)
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Applications (0)
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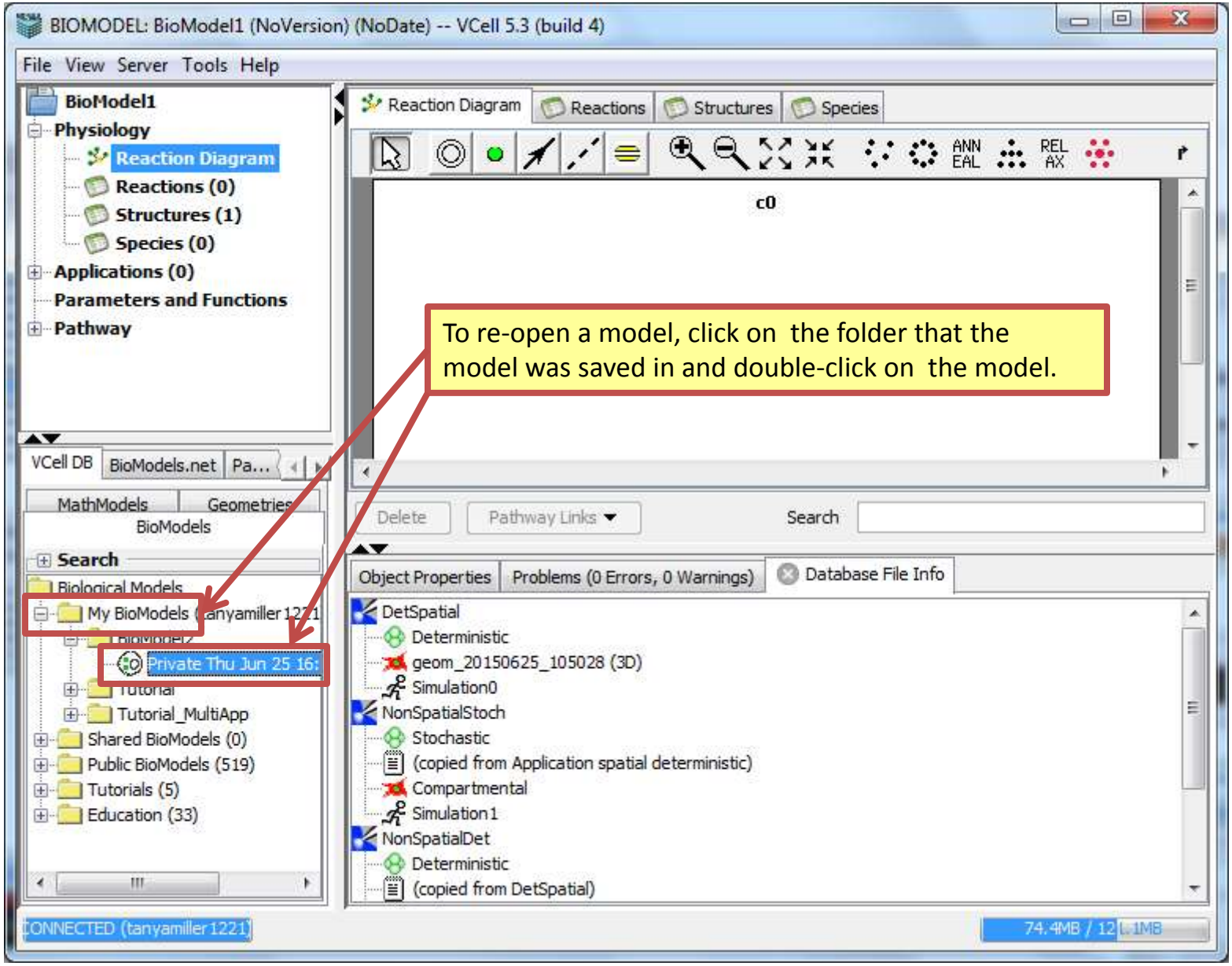
Pathway
Reactions
Structures
Species
PM
Cyt
NM
Nuc
C_Cyt
Ran_Cyt
RanC_Cyt
RanC_Nuc
Use the "Reactions", "Structures" and "Species" tabs to look up specific details of the physiology, which are useful when working with large and complicated models.
BioModels
MathModels
Geometries
Search
not connected
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.
NOT CONNECTED
82.3MB / 122.7MB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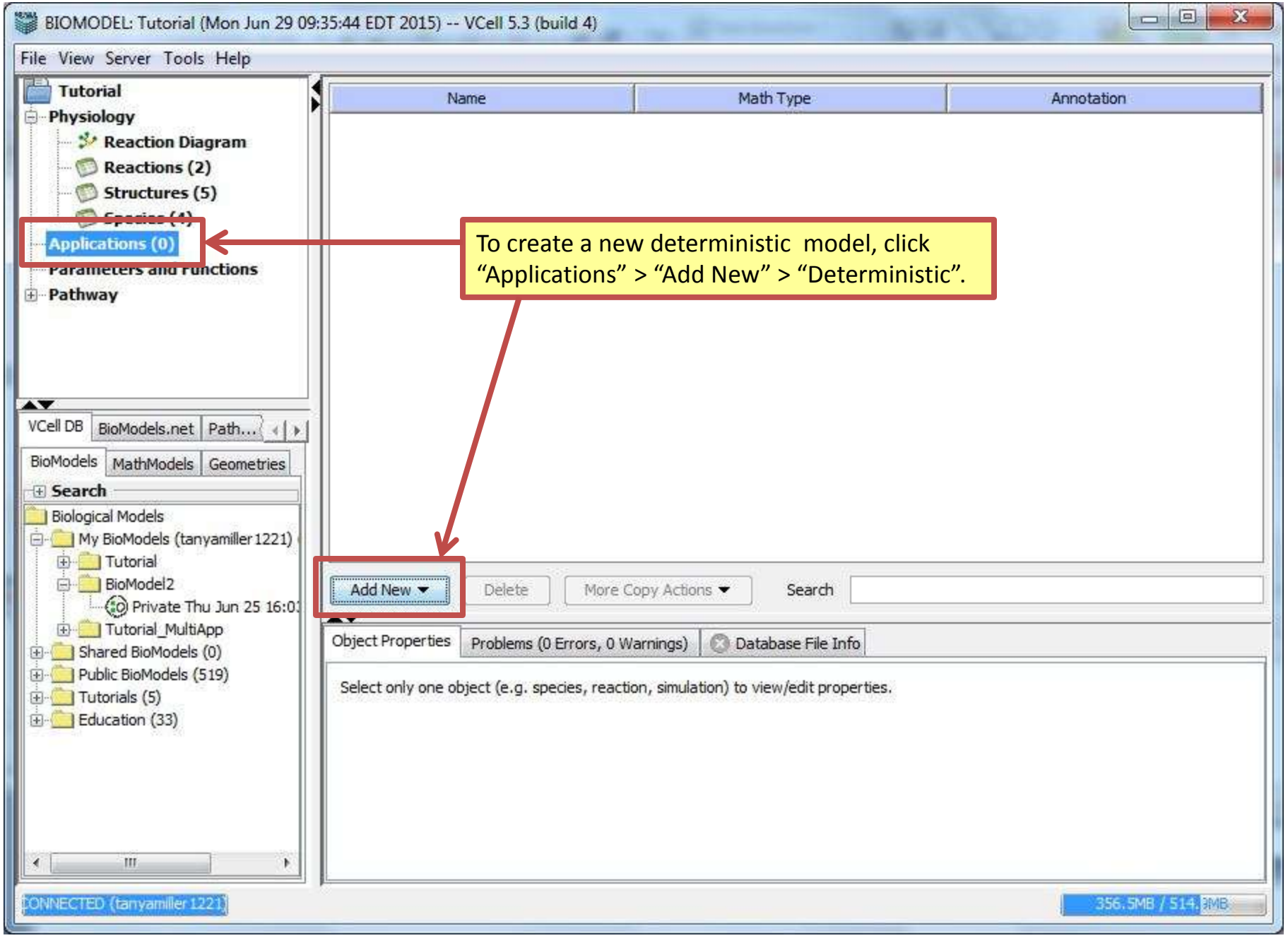
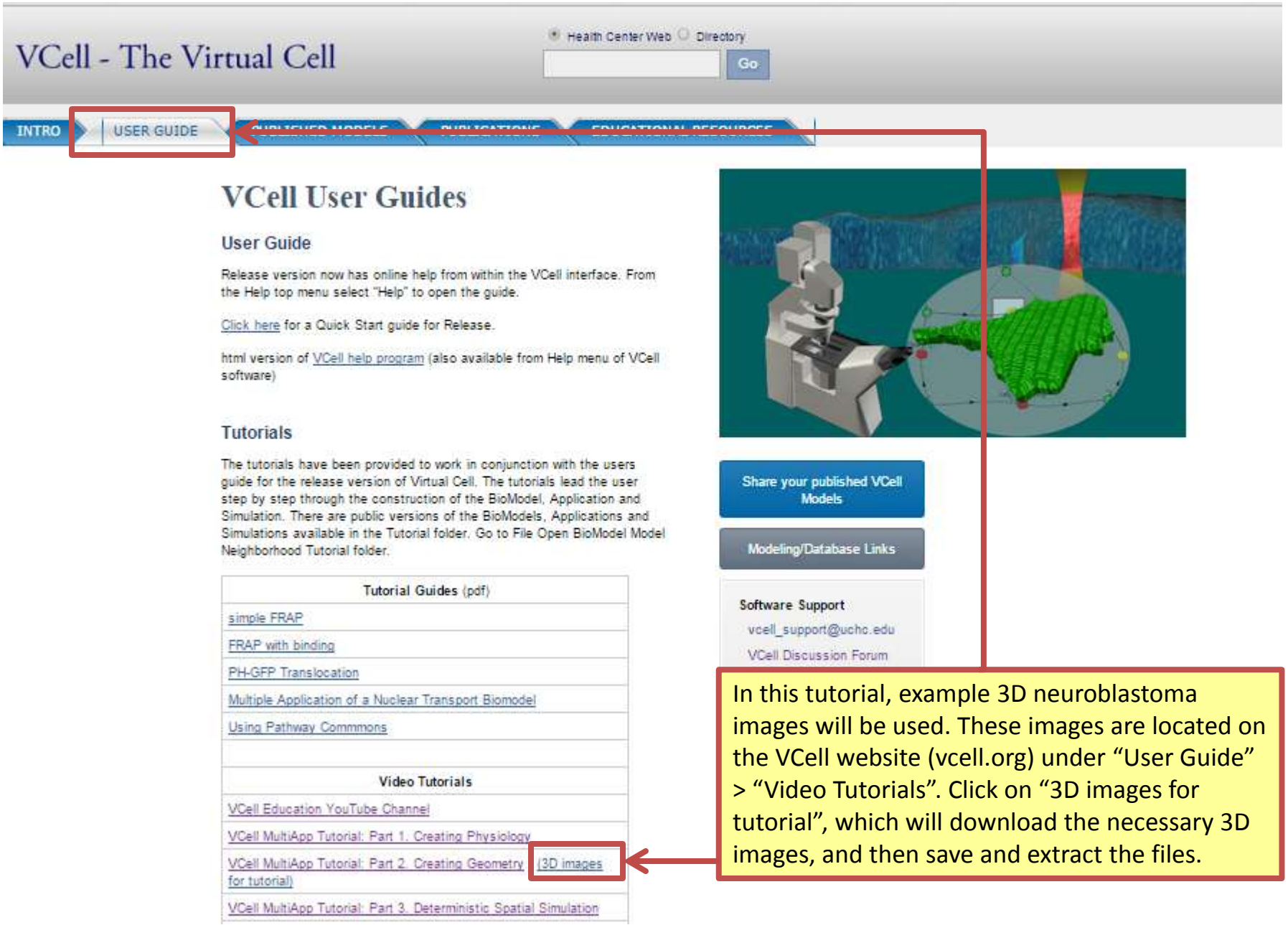
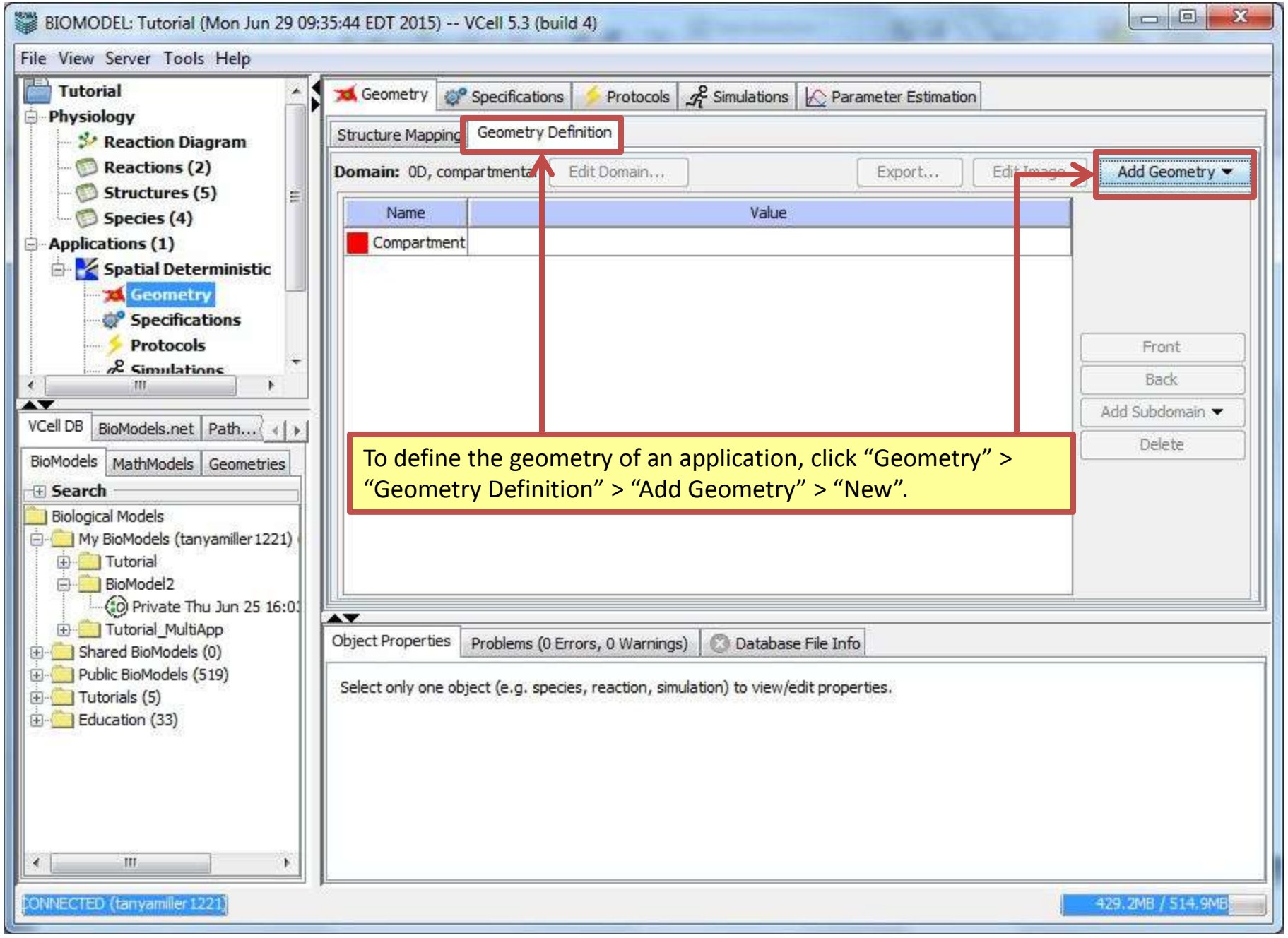
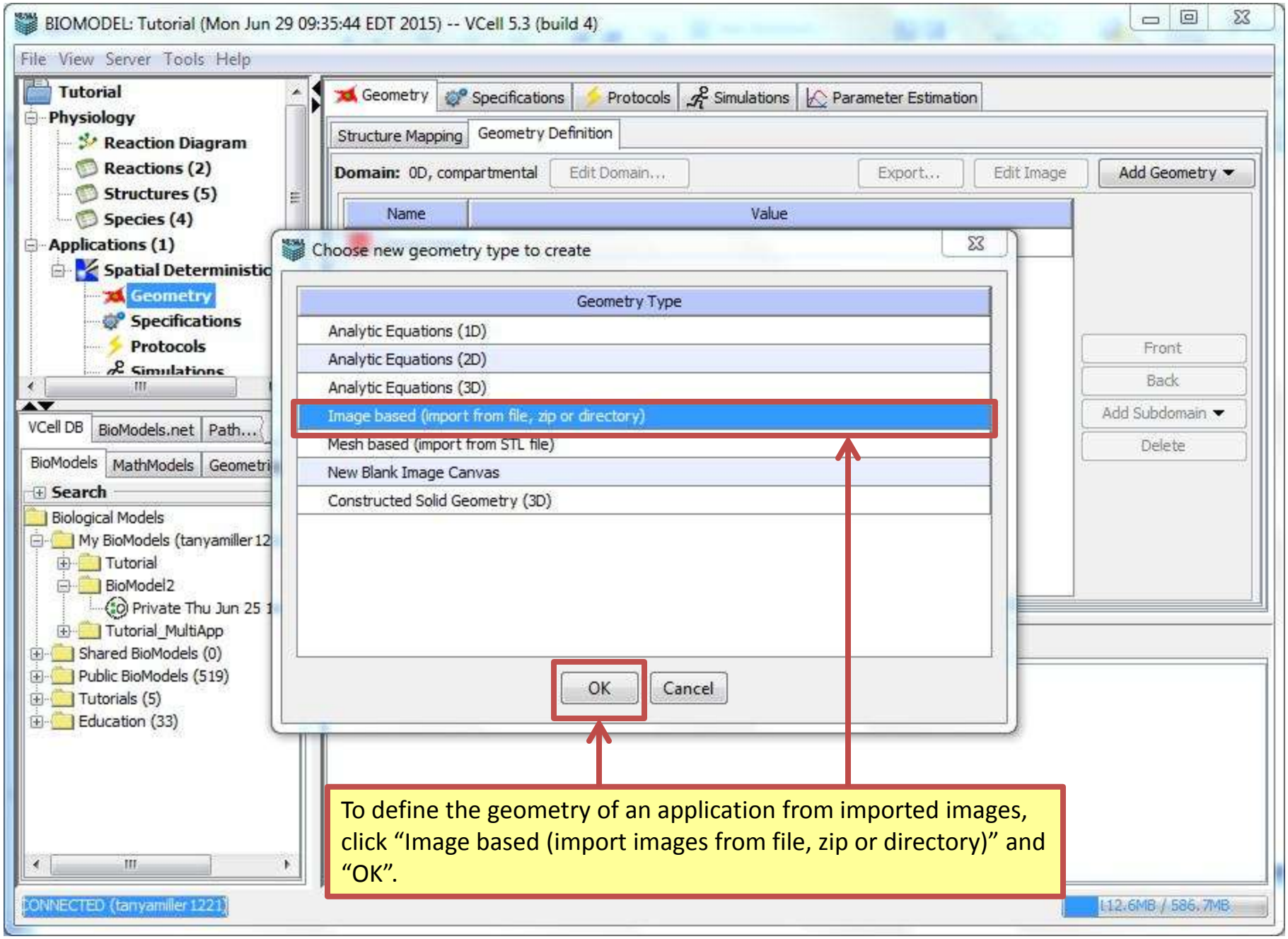
Species
c0
To re-open a model, click on the folder that the model was saved in and double-click on the model.
VCell DB
BioModels.net
MathModels
Geometries
BioModels
Search
Biological Models
My BioModels (tanyamiller1221)
Private Thu Jun 25 16:
Tutorial_MultiApp
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
DetSpatial
Deterministic
geom_20150625_105028 (3D)
Simulation0
NonSpatialStoch
Stochastic
(copied from Application spatial deterministic)
Compartmental
Simulation1
NonSpatialDet
Deterministic
(copied from DetSpatial)
CONNECTED (tanyamiller1221)
74.4MB / 12

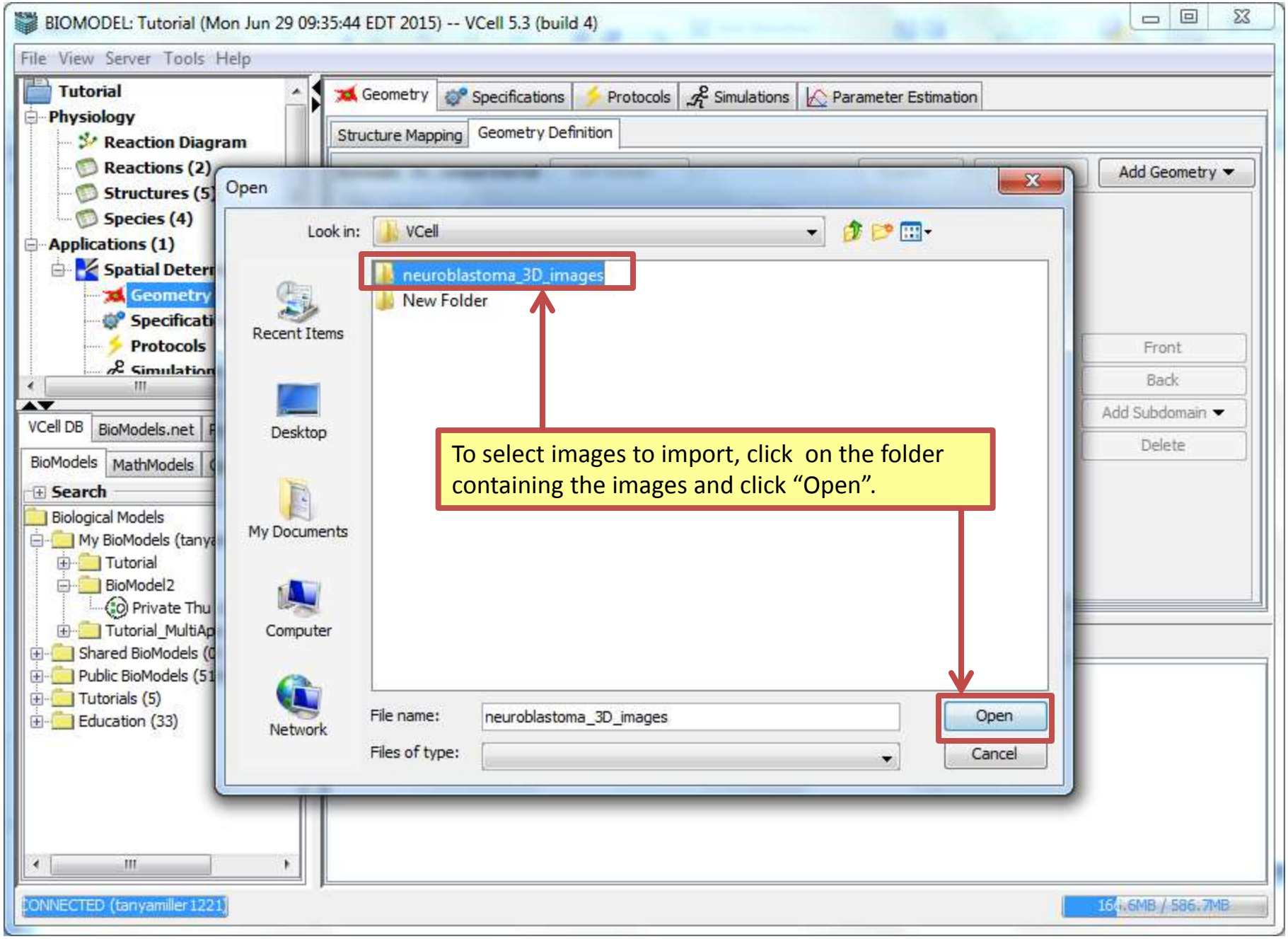

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Applications (0)
Pathway
Name
Math Type
Annotation
To create a new deterministic model, click "Applications" > "Add New" > "Deterministic".
VCell DB
BioModels.net
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221)
Tutorial
BioModel2
Tutorial_MultiApp
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
Add New
Delete
More Copy Actions
Search
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

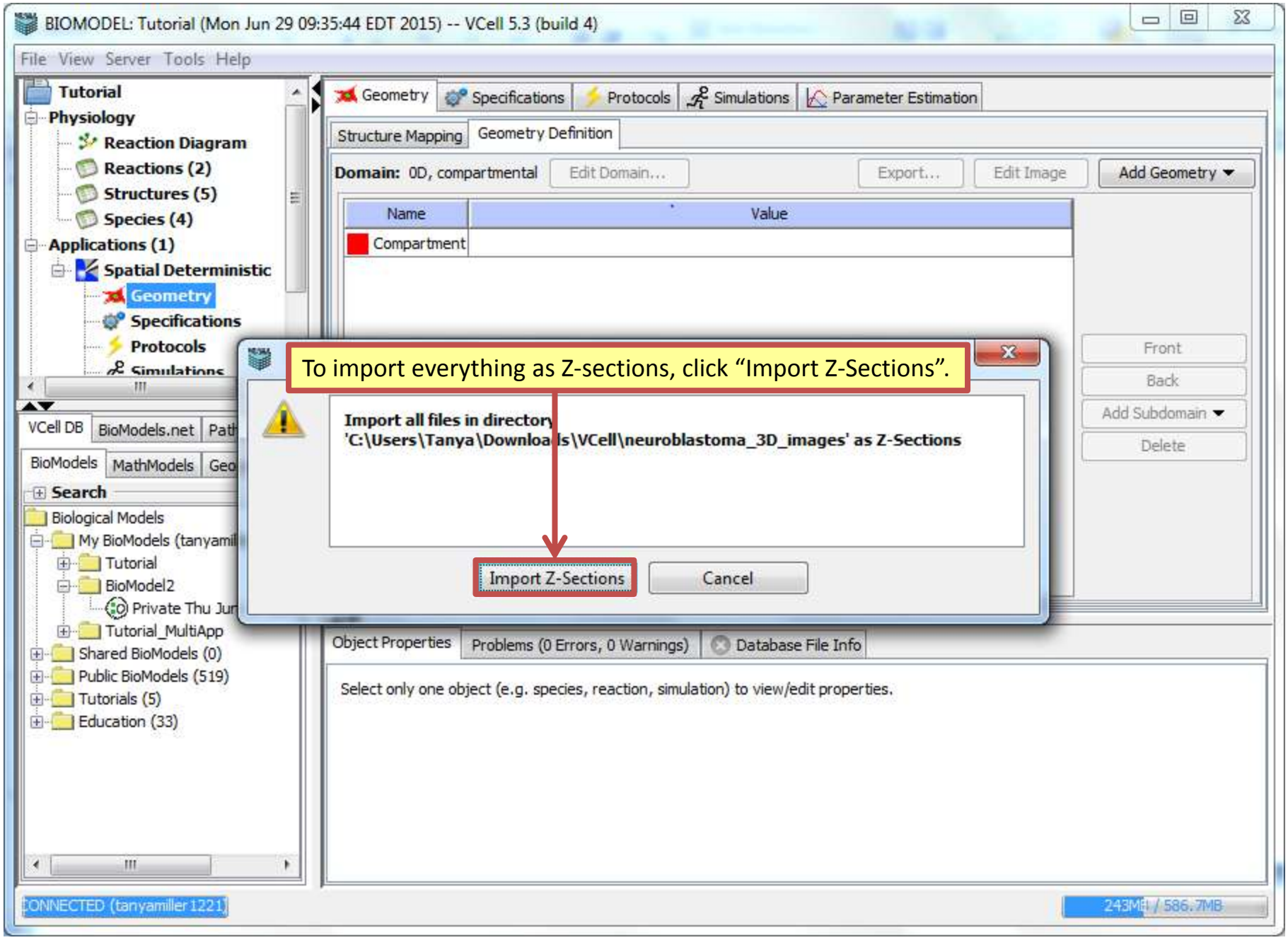


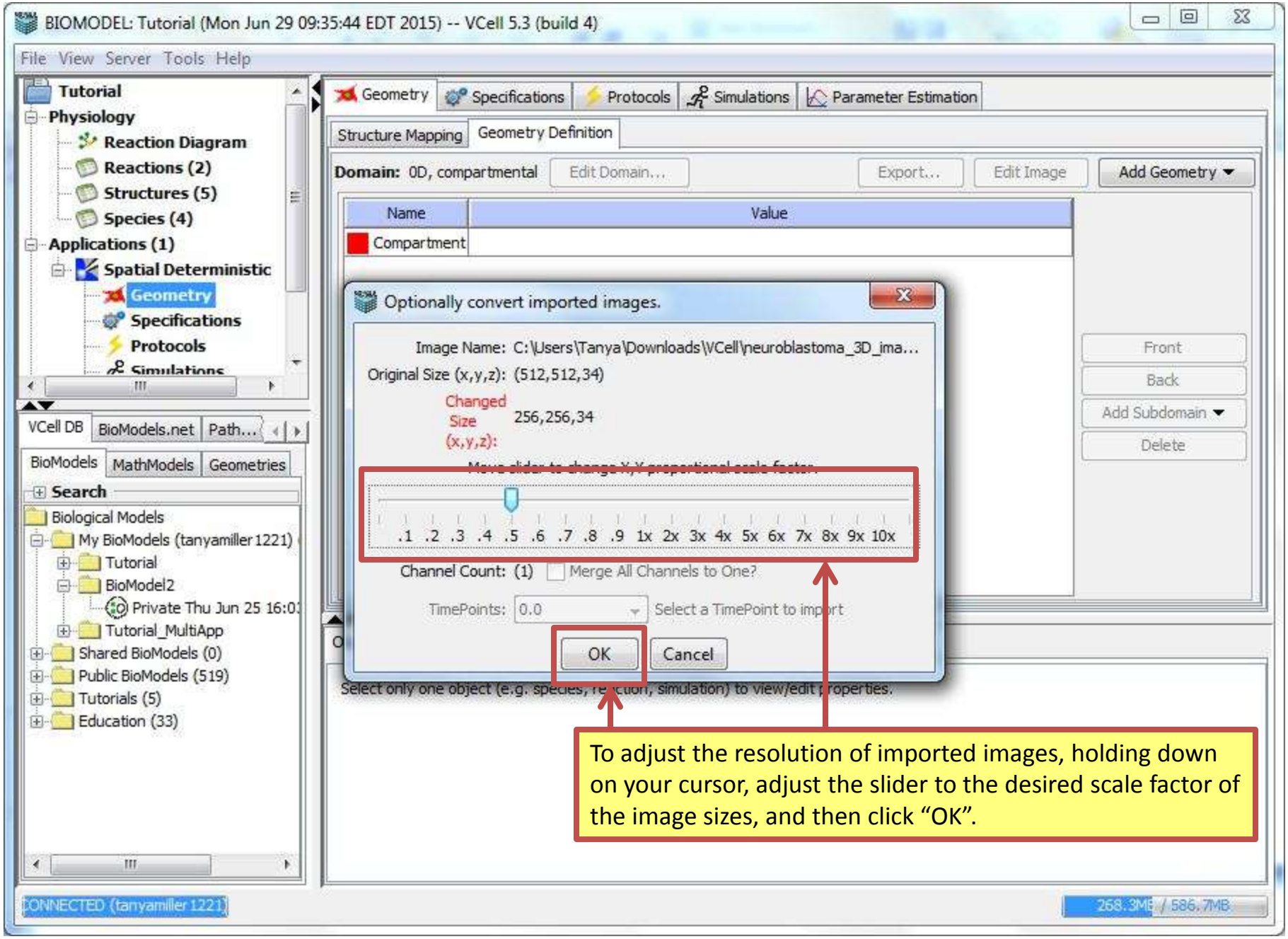
In this tutorial, example 3D neuroblastoma images will be used. These images are located on the VCell website (vcell.org) under "User Guide" > "Video Tutorials". Click on "3D images for tutorial", which will download the necessary 3D images, and then save and extract the files.


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...
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221)
Tutorial
BioModel2
Private Thu Jun 25 16:01
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

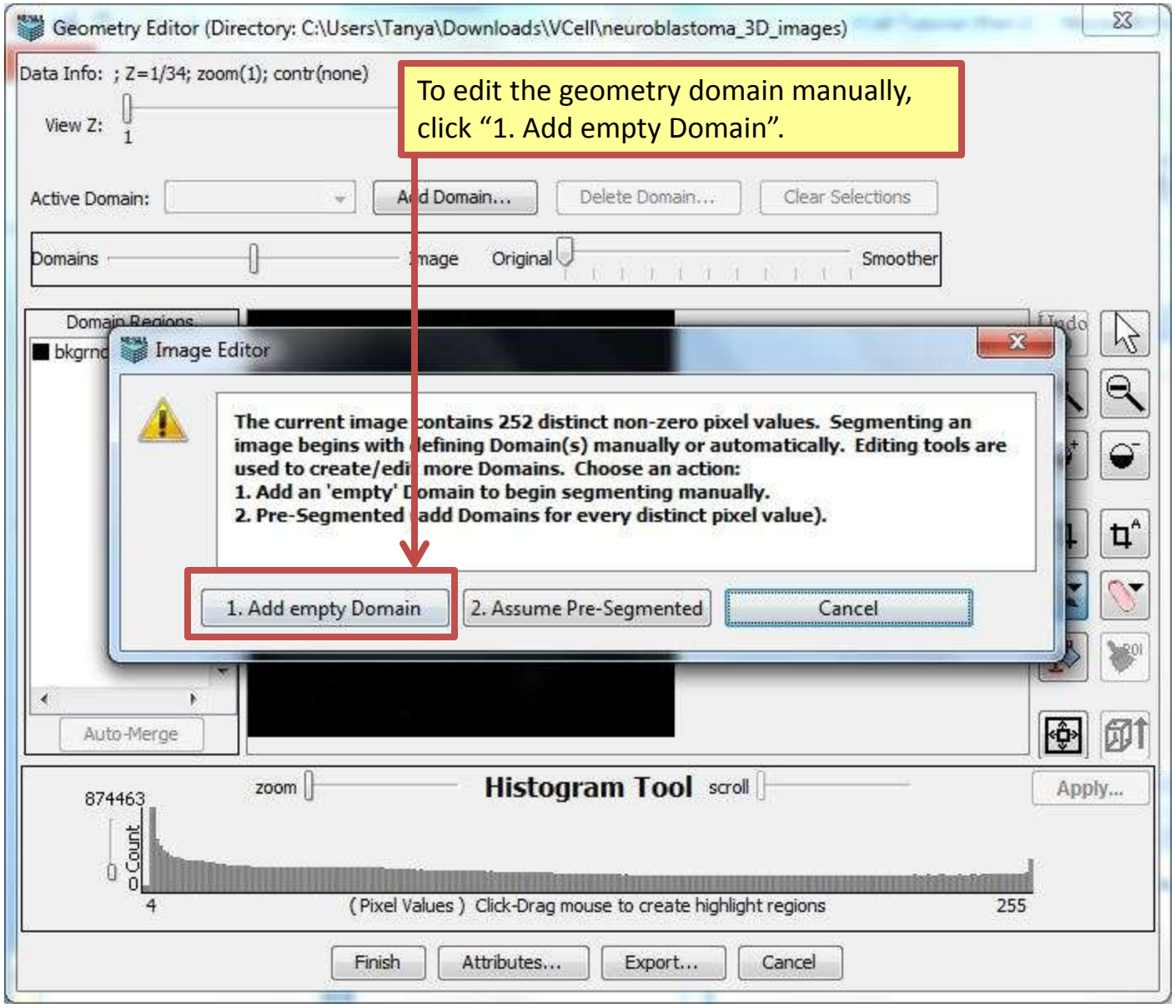

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Applications (1)
Spatial Deterministic
Geometry
Specifications
Protocols
Simulations
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
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
VCell DB
BioModels.net
Path...
BioModels
MathModels
Search
Biological Models
My BioModels (tanyamiller12
Tutorial
BioModel2
Private Thu Jun 25
Tutorial_MultiApp
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
112.6MB / 586.7MB
To define the geometry of an application from imported images, click “Image based (import images from file, zip or directory)” and “OK”.

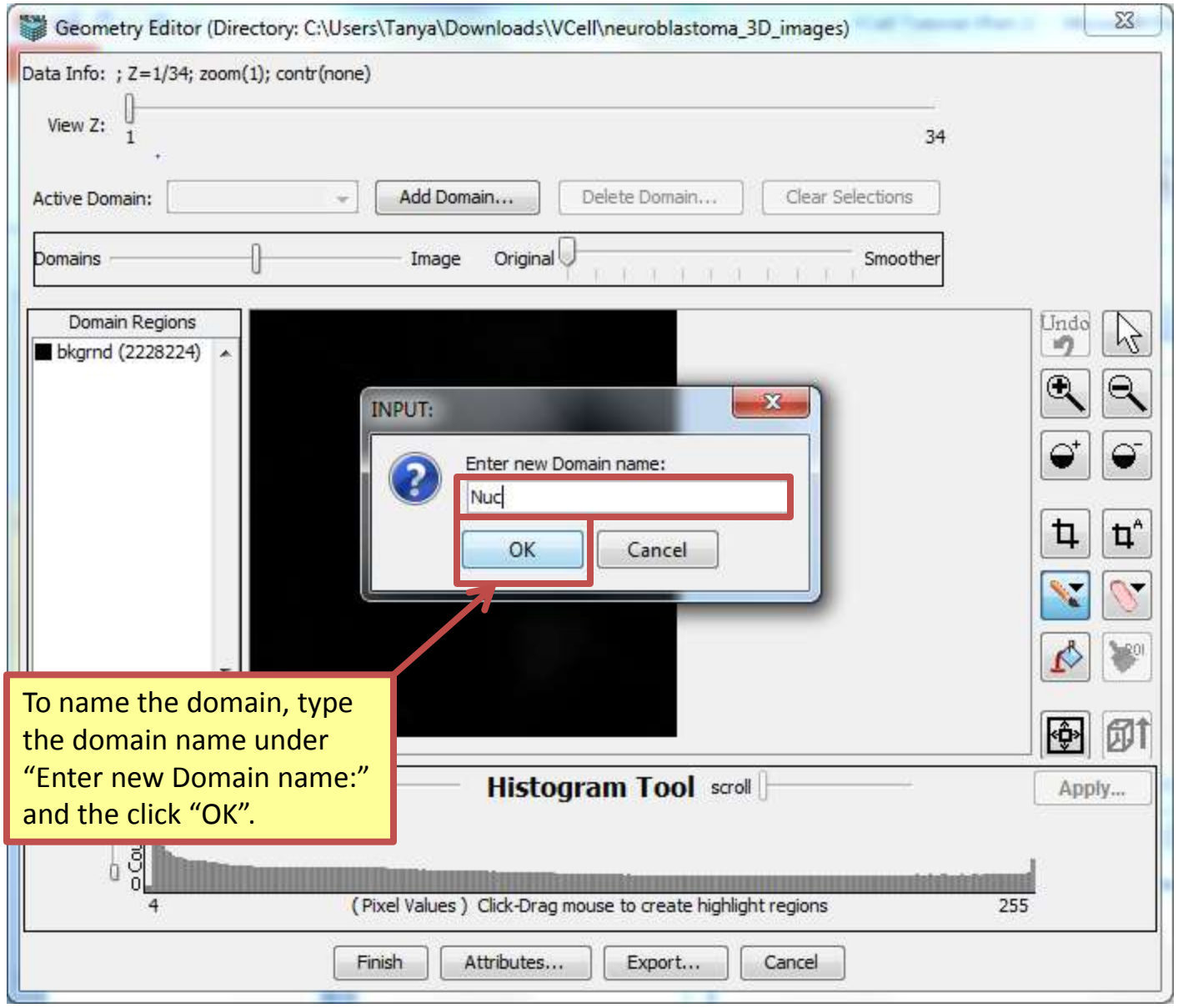

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Applications (1)
Spatial Deterr
Geometry
Specificati
Protocols
Simulation
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Add Geometry
Front
Back
Add Subdomain
Delete
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (tanya
Tutorial
BioModel2
Private Thu
Tutorial_MultiAp
Shared BioModels (0
Public BioModels (51
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
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

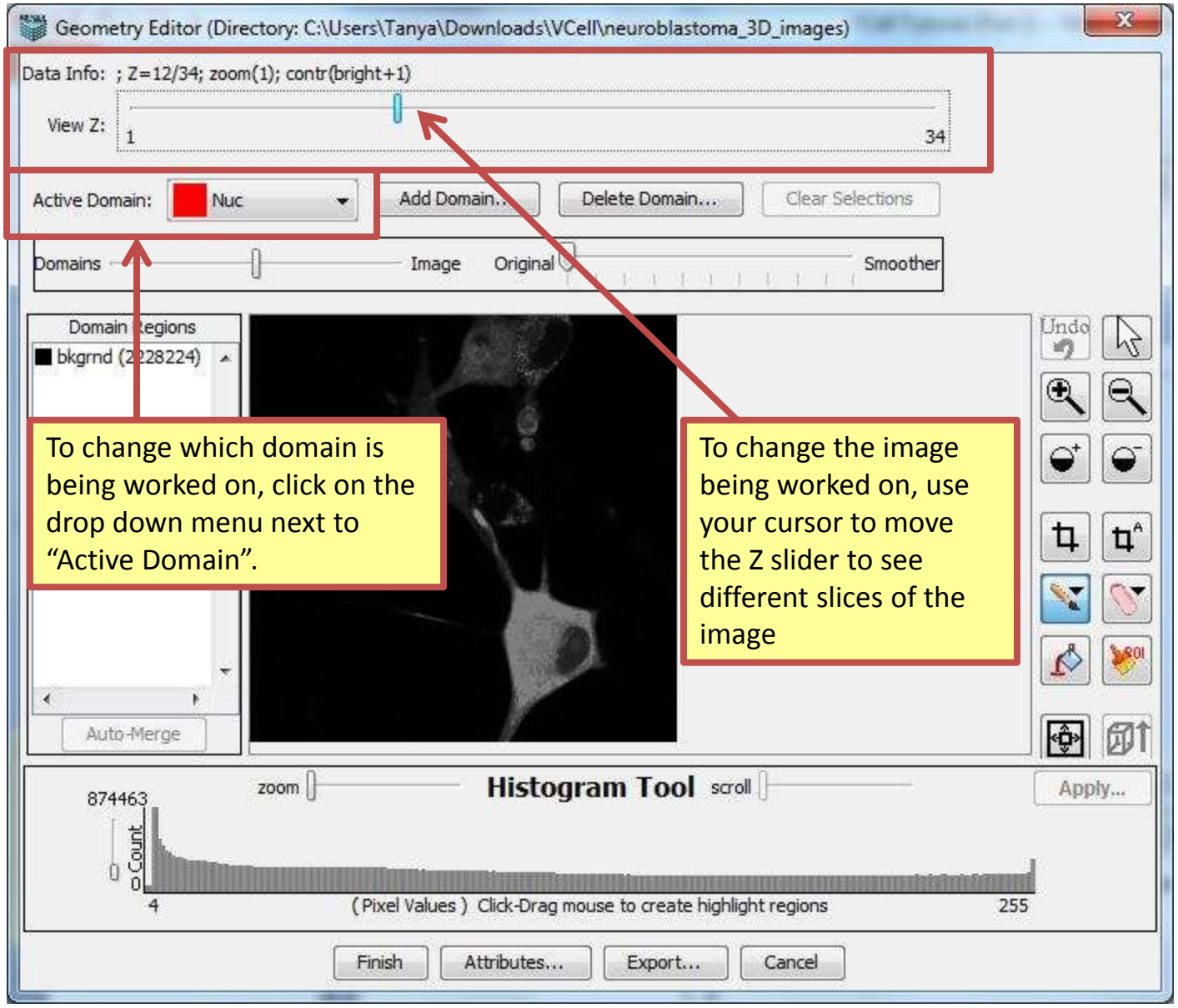

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Applications (1)
Spatial Deterministic
Geometry
Specifications
Protocols
Simulations
Geometry
Specifications
Protocols
Simulations
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 import everything as Z-sections, click “Import Z-Sections”.
Import all files in directory
'C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images' as Z-Sections
Import Z-Sections
Cancel
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (tanyamil
Tutorial
BioModel2
Tutorial_MultiApp
Shared BioModels (0)
Public BioModels (519)
Tutorials (5)
Education (33)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
243ME / 586.7MB

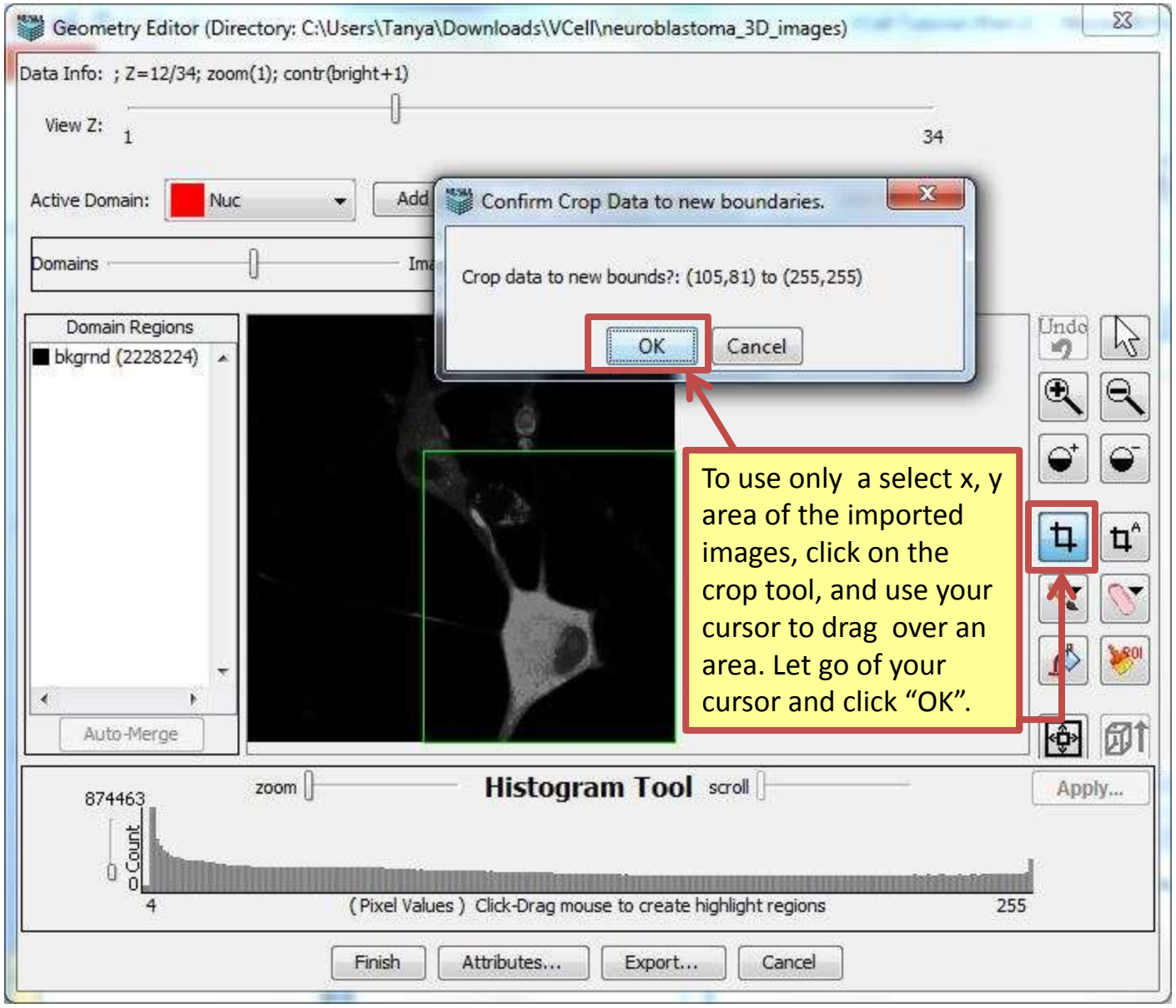


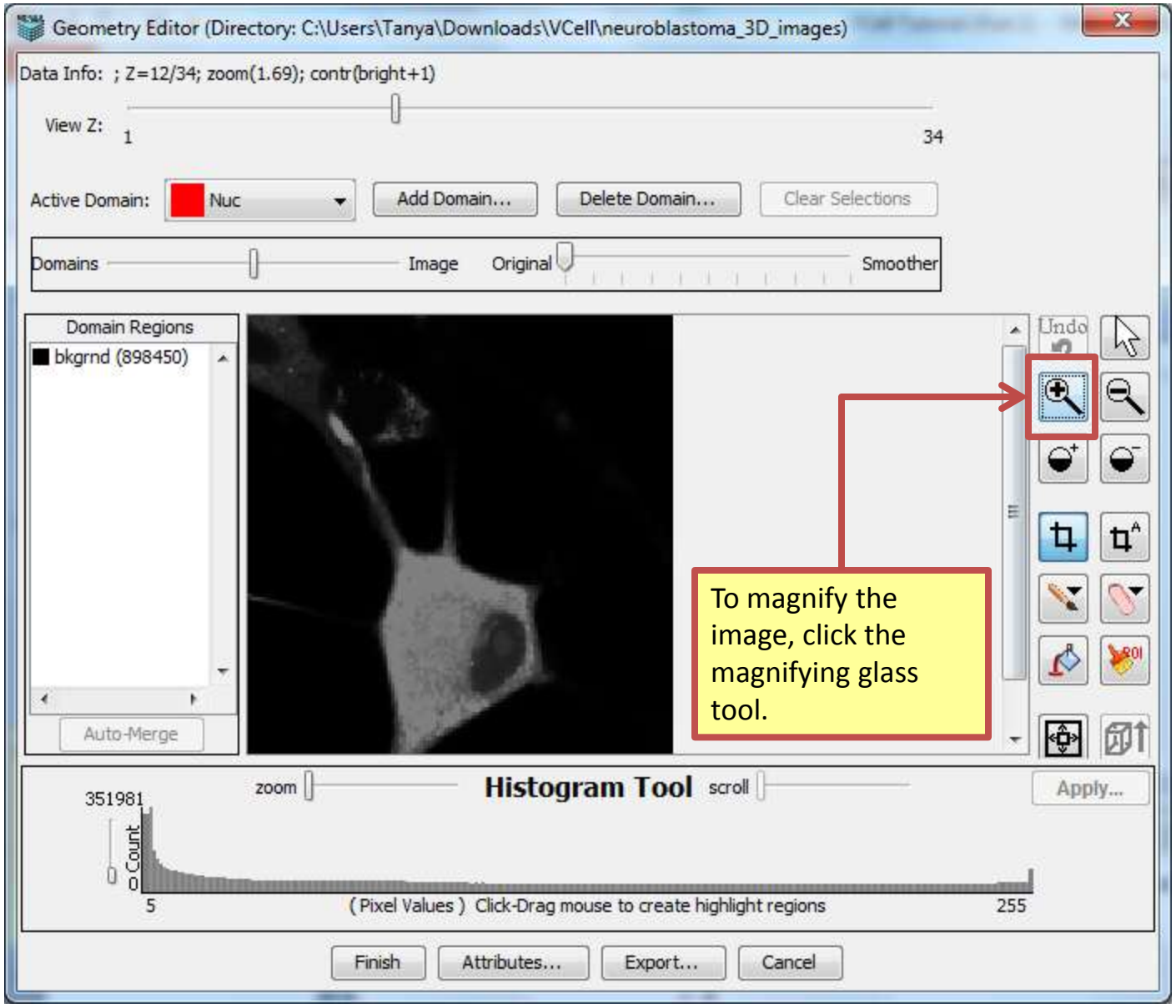
To adjust the resolution of imported images, holding down on your cursor, adjust the slider to the desired scale factor of the image sizes, and then click “OK”.

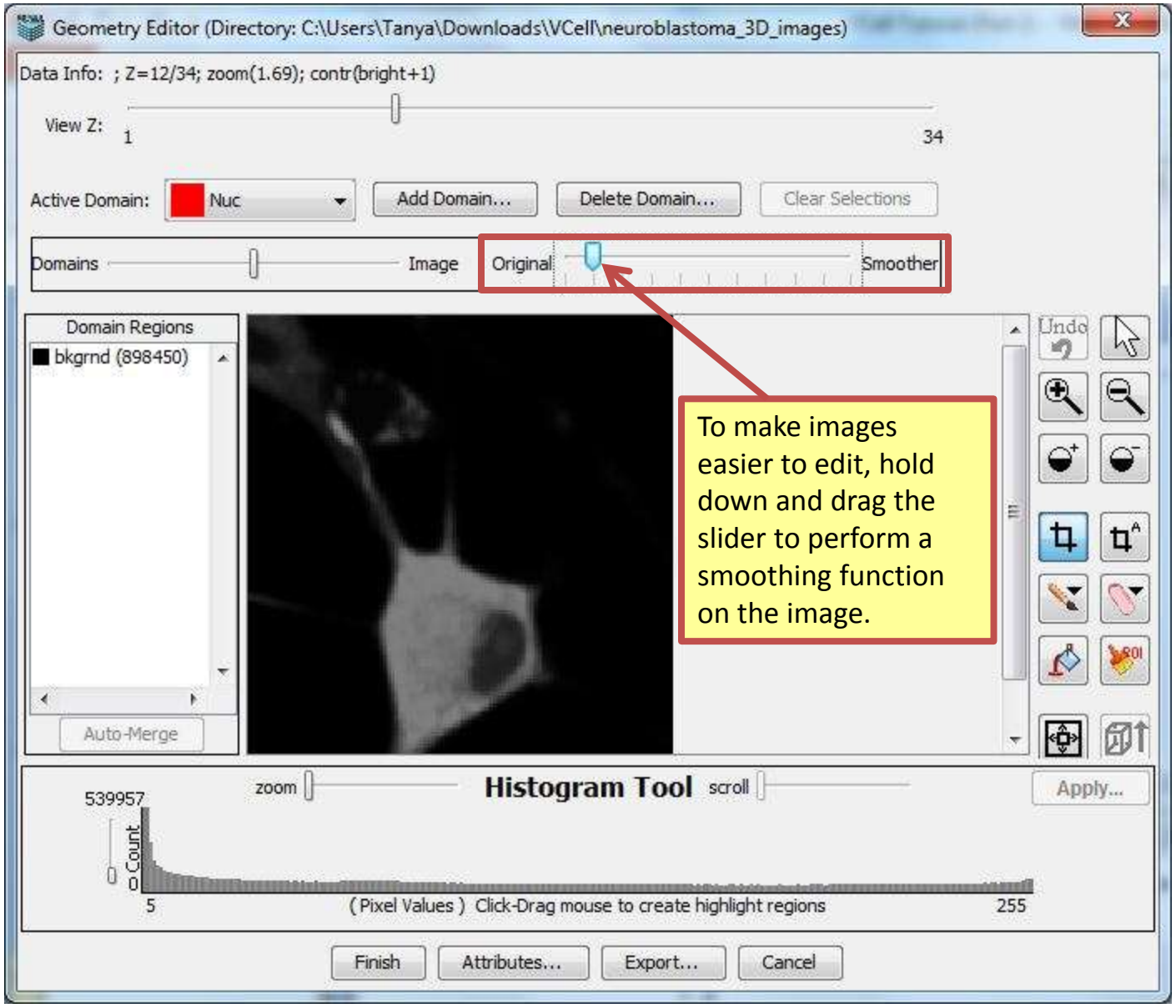

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=1/34; zoom(1); contr(none)
View Z:
1
To edit the geometry domain manually, click "1. Add empty Domain".
Active Domain:
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain 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
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

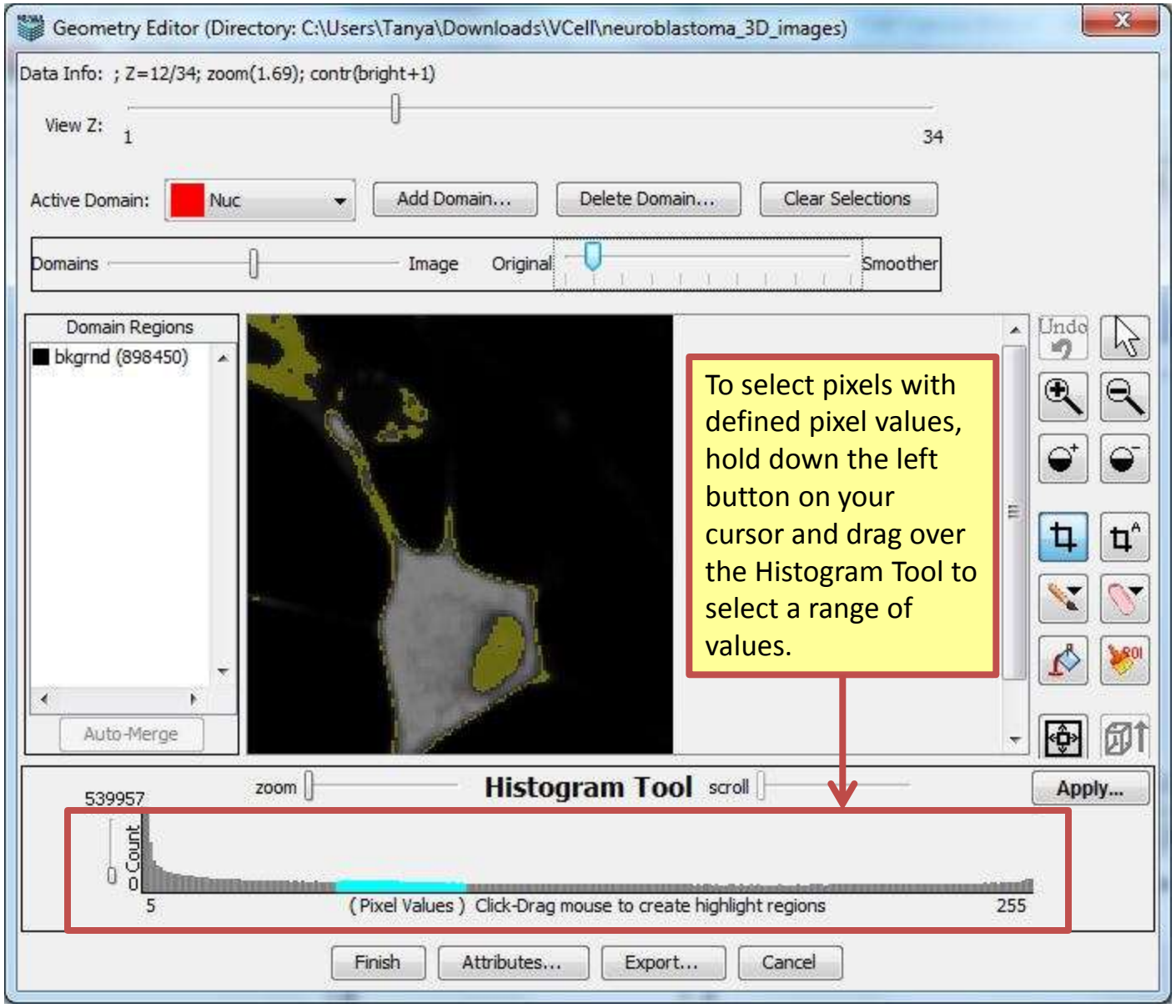

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=1/34; zoom(1); contr(none)
View Z:
1
34
Active Domain:
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (2228224)
INPUT:
Enter new Domain name:
Nuc
OK
Cancel
Undo
Histogram Tool
scroll
Apply...
Col
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".

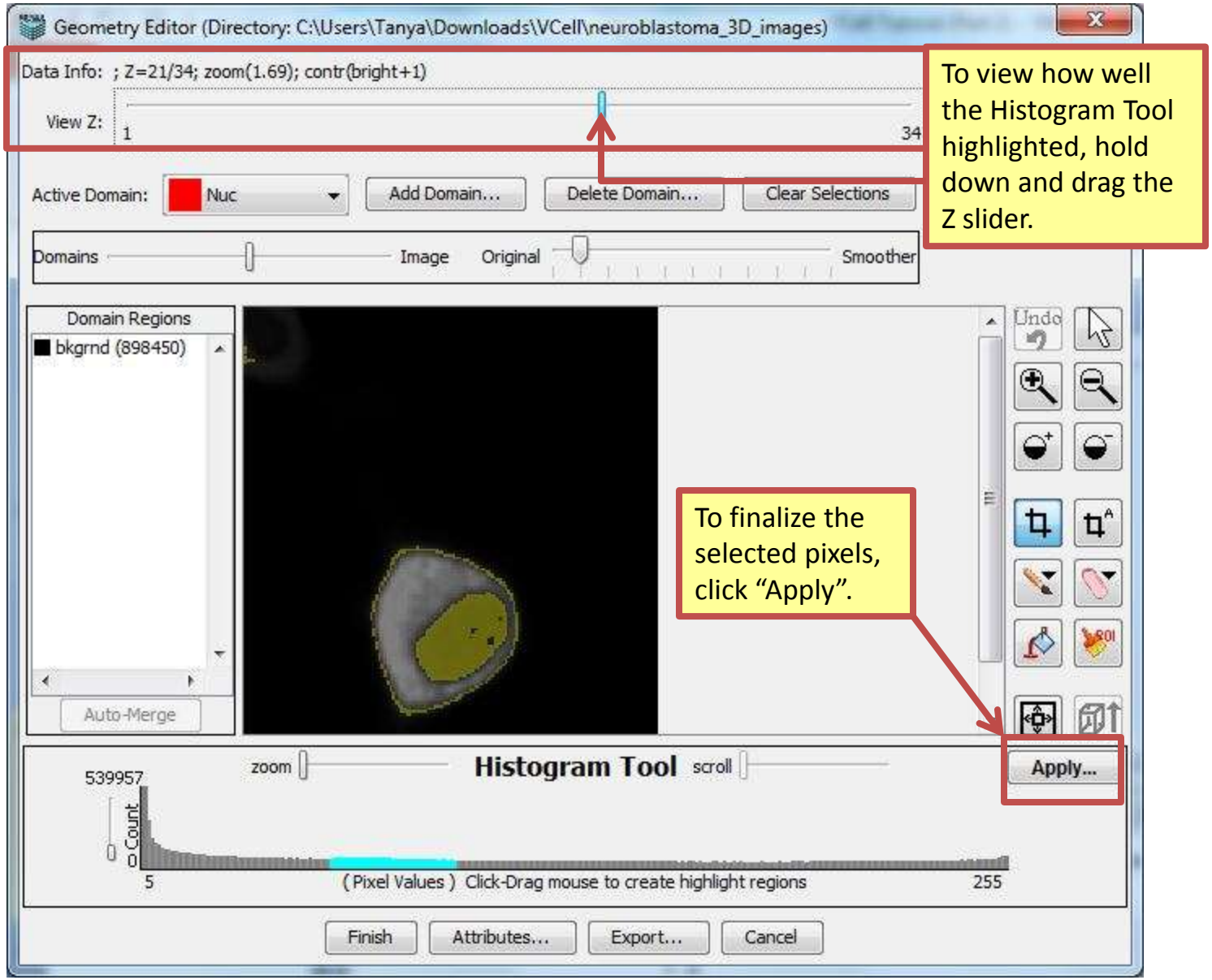

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (2228224)
Auto-Merge
Undo
To change 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
zoom
Histogram Tool
scroll
Apply...
874463
Count
0
4
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

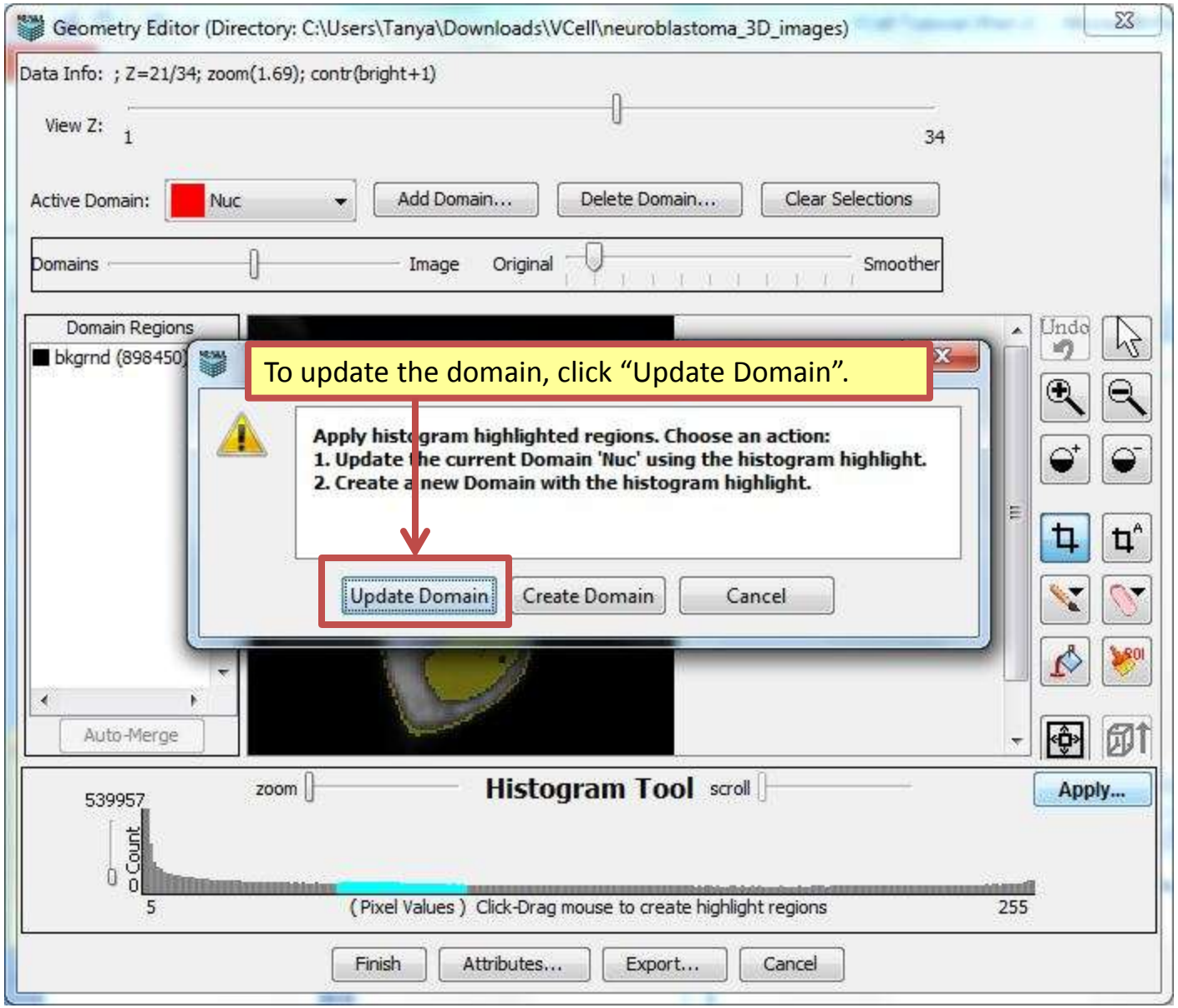

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add
Domains
Confirm Crop Data to new boundaries.
Crop data to new bounds?: (105,81) to (255,255)
OK
Cancel
Domain Regions
bkgrnd (2228224)
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

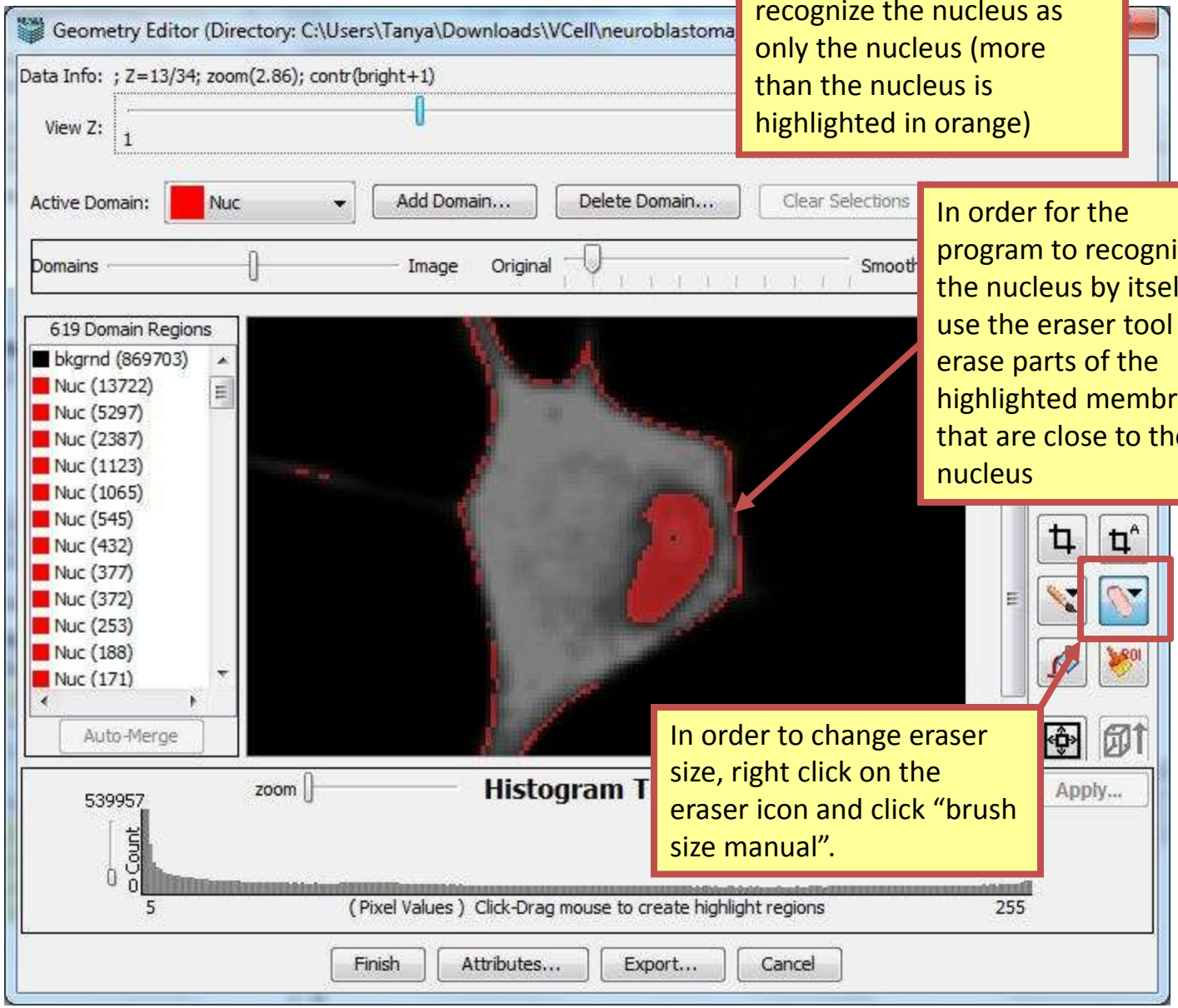

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To magnify 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
To make images easier to edit, hold down and drag the slider to perform a smoothing function on the image.
Undo
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=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


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
To view how well the Histogram Tool highlighted, hold down and drag the Z slider.
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
To finalize the selected pixels, click “Apply”.
Undo
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

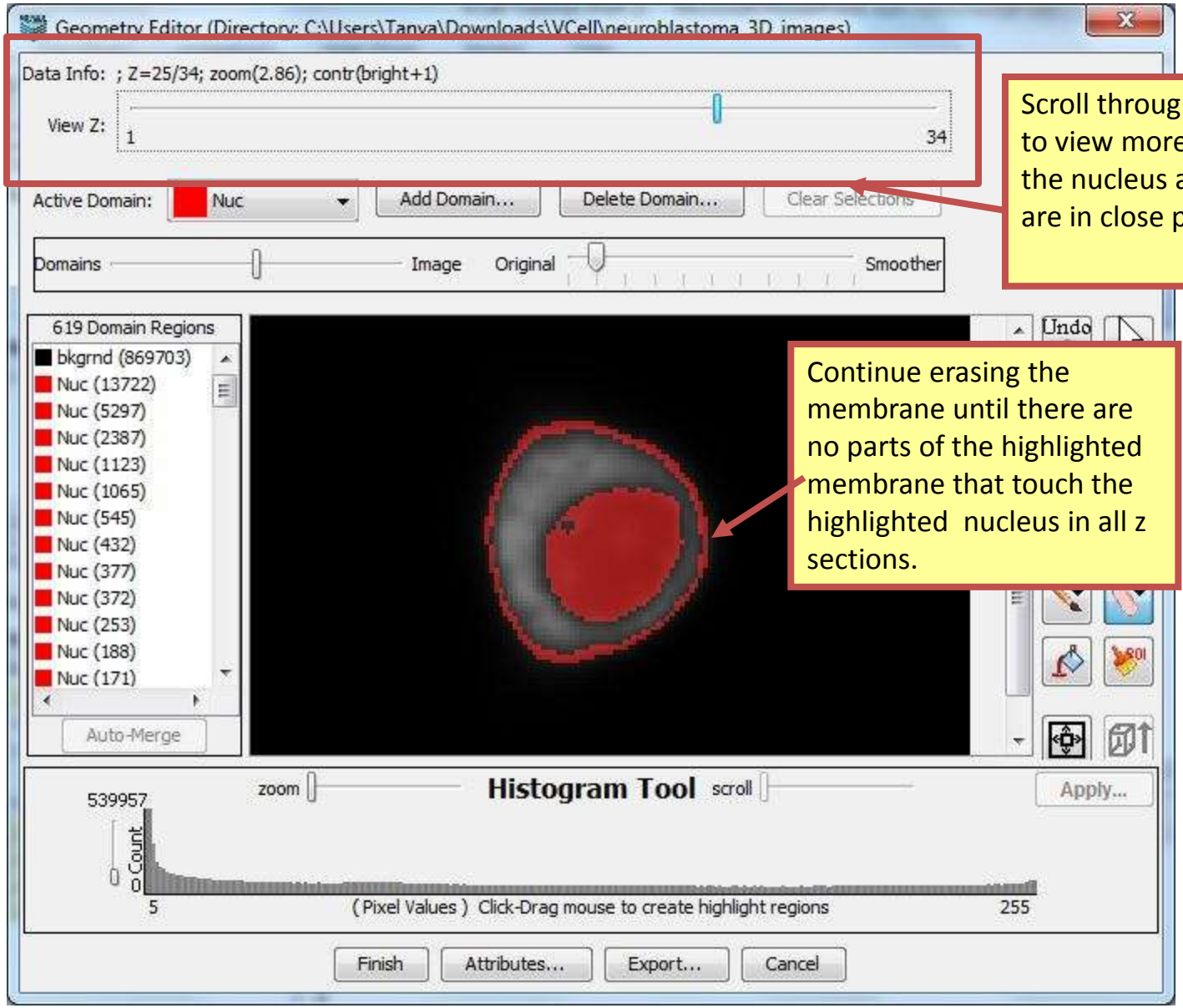

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=21/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
To update the 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



The program does not recognize the nucleus as only the nucleus (more than the nucleus is highlighted in orange)

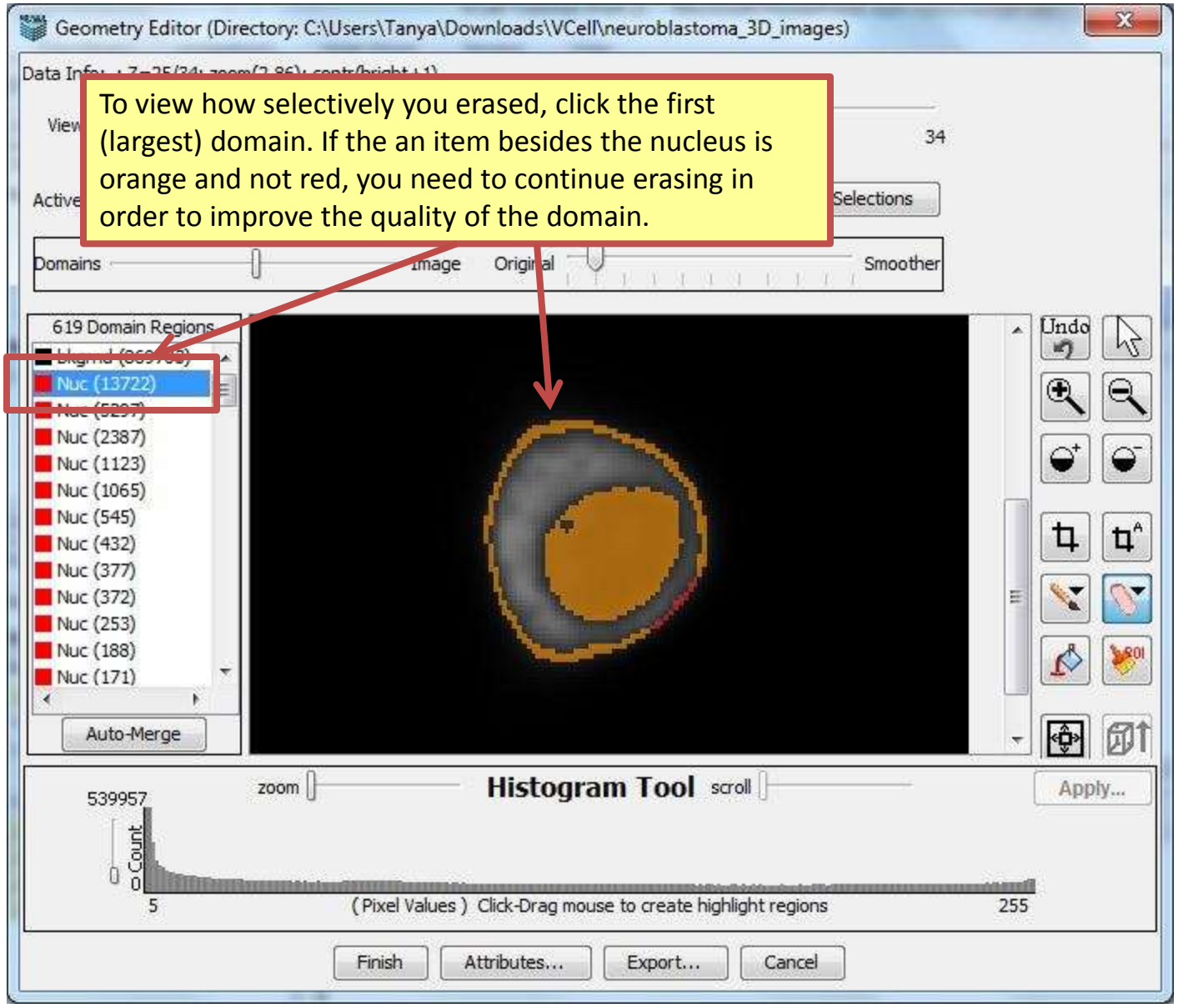
In order for the program to recognize the nucleus by itself, use the eraser tool to erase parts of the highlighted membrane that are close to the nucleus

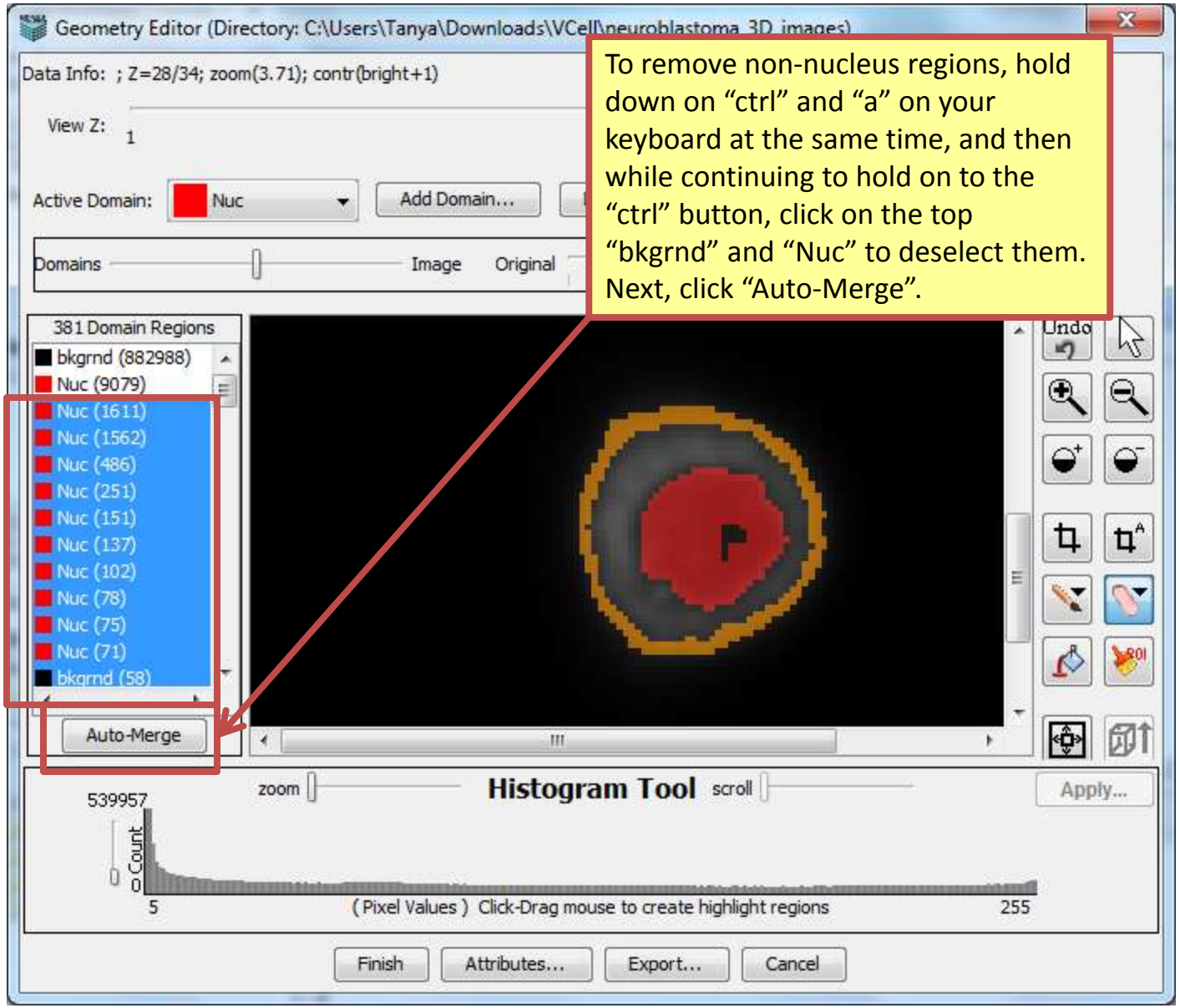
In order to change eraser size, right click on the eraser icon and click “brush size manual”.

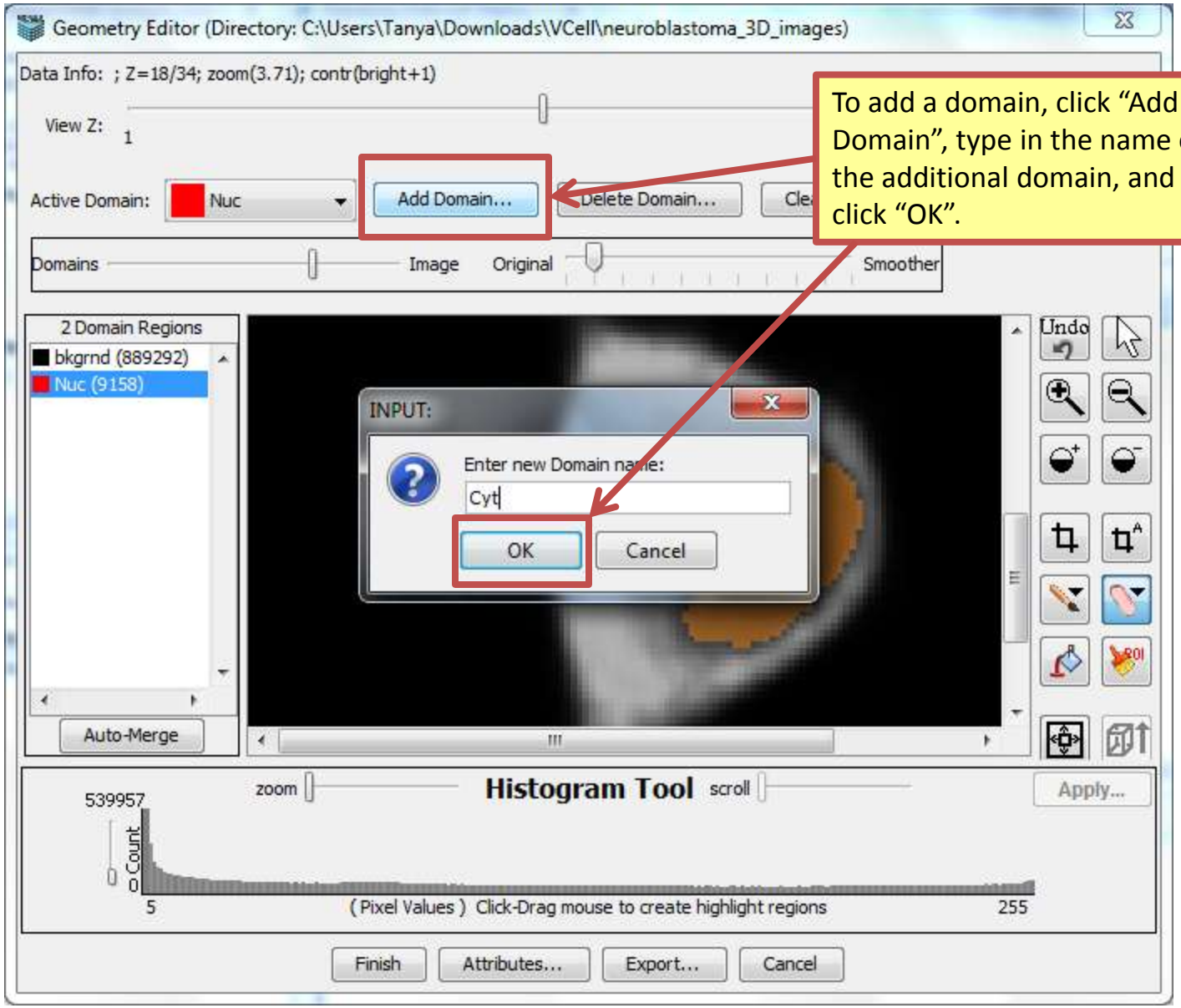


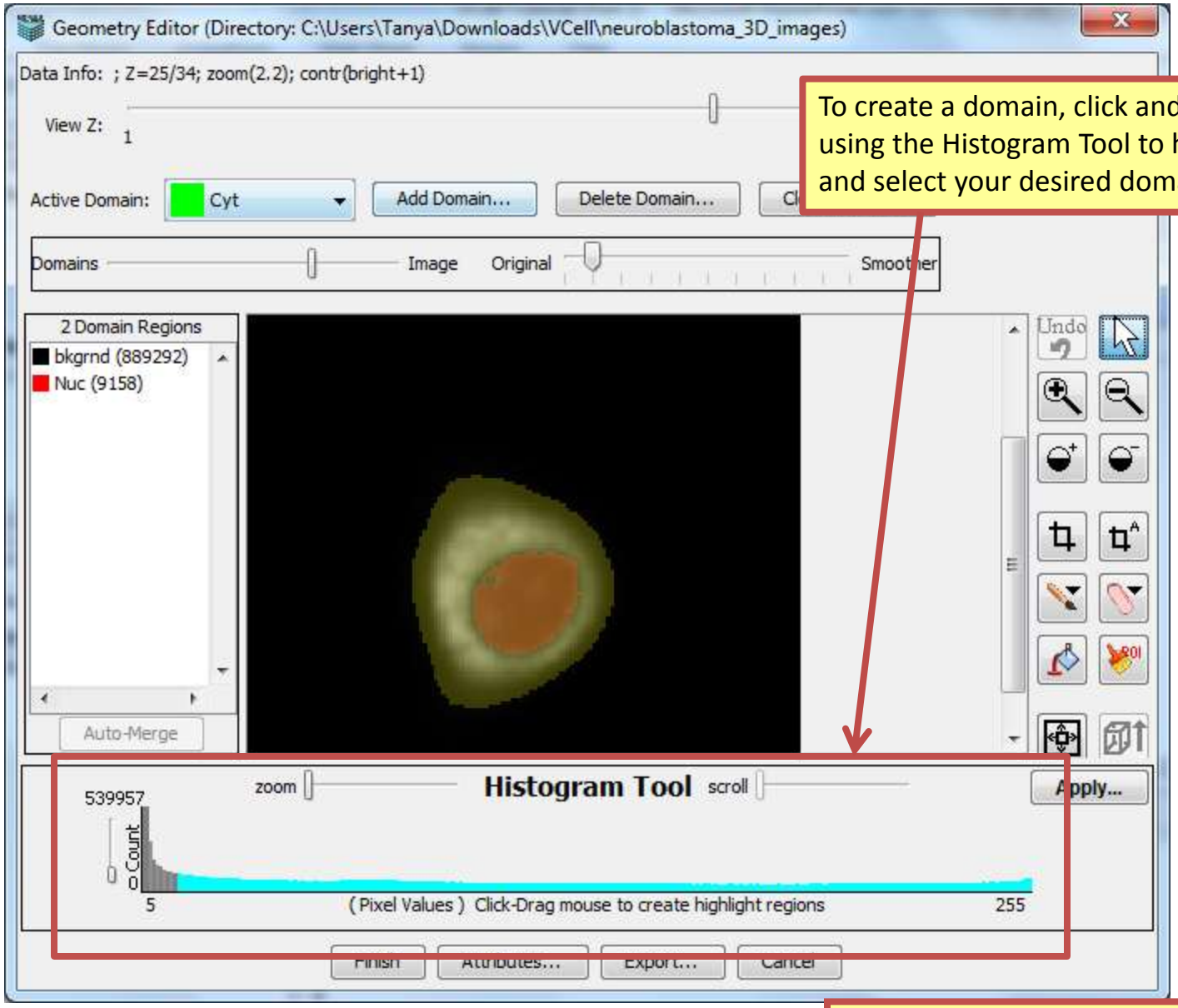
Scroll through the Z slider to view more slices in which the nucleus and membrane are in close proximity

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


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
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.
34
Selections
Domains
Smoother
619 Domain Regions
Nuc (13722)
Nuc (2387)
Nuc (1123)
Nuc (1065)
Nuc (545)
Nuc (432)
Nuc (377)
Nuc (372)
Nuc (253)
Nuc (188)
Nuc (171)
Auto-Merge
Undo
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel

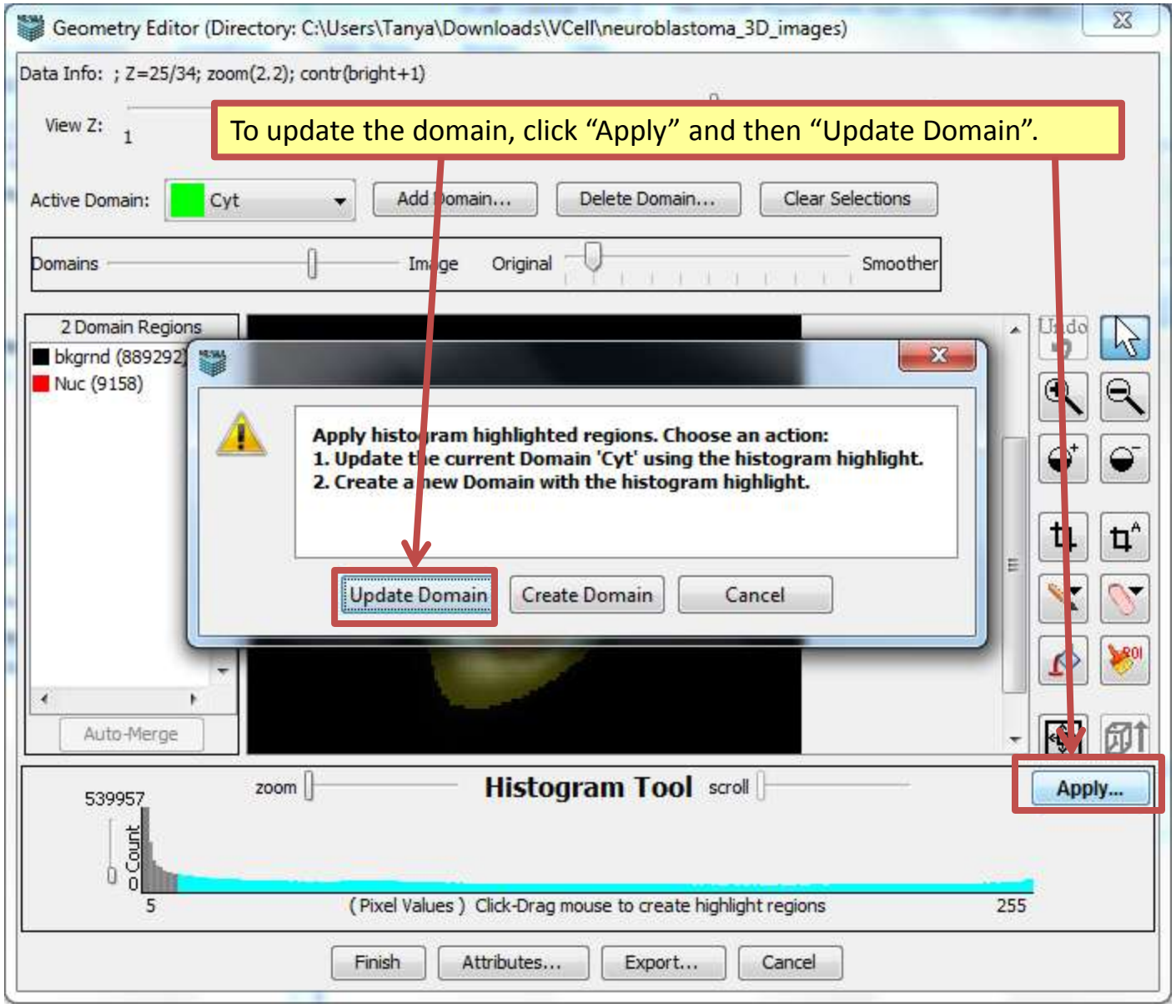

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=28/34; zoom(3.71); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Domains
Image
Original
381 Domain Regions
bkgrnd (882988)
Nuc (9079)
Nuc (1611)
Nuc (1562)
Nuc (486)
Nuc (251)
Nuc (151)
Nuc (137)
Nuc (102)
Nuc (78)
Nuc (75)
Nuc (71)
bkgrnd (58)
Auto-Merge
Undo
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel
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” to deselect them. Next, click “Auto-Merge”.


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=18/34; zoom(3.71); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Delete Domain...
Domains
Image
Original
Smoother
2 Domain Regions
bkgrnd (889292)
Nuc (9158)
Auto-Merge
INPUT:
Enter new Domain name:
Cyt
OK
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
To add a domain, click “Add Domain”, type in the name of the additional domain, and click “OK”.

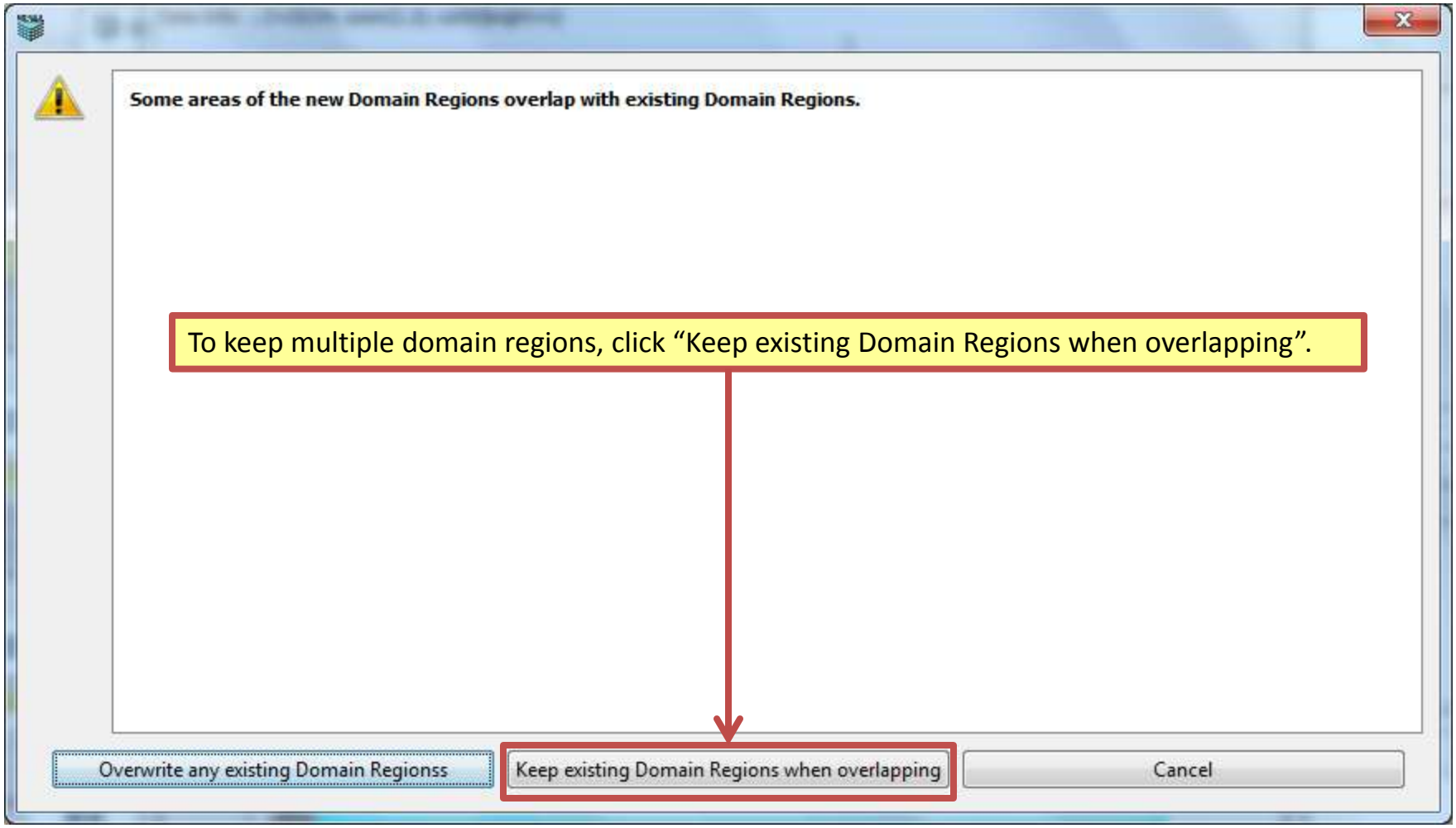


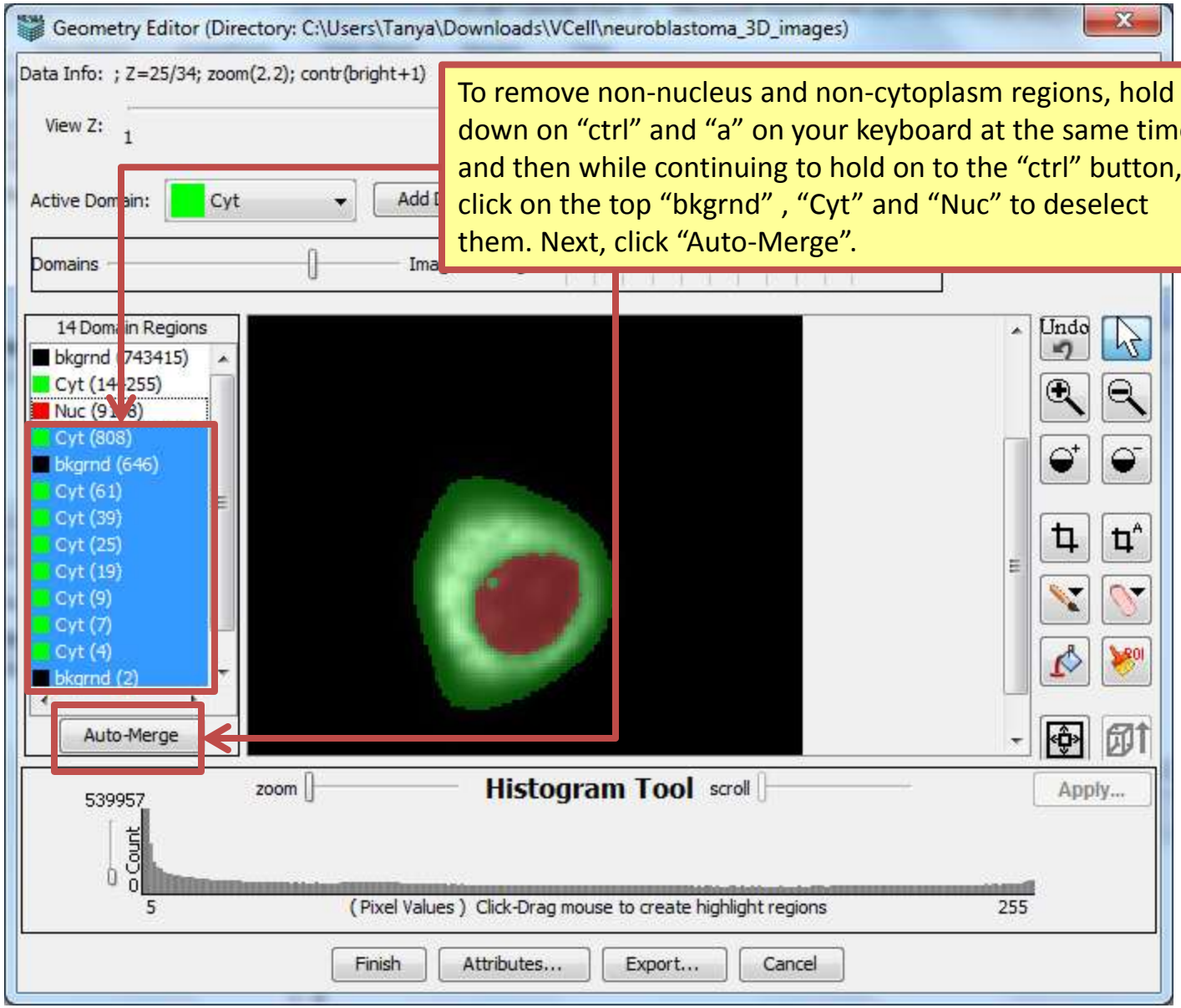
To create a domain, click and drag using the Histogram Tool to highlight and select your desired domain region.

Use the Z slider to make sure all parts of the cytoplasm are highlighted

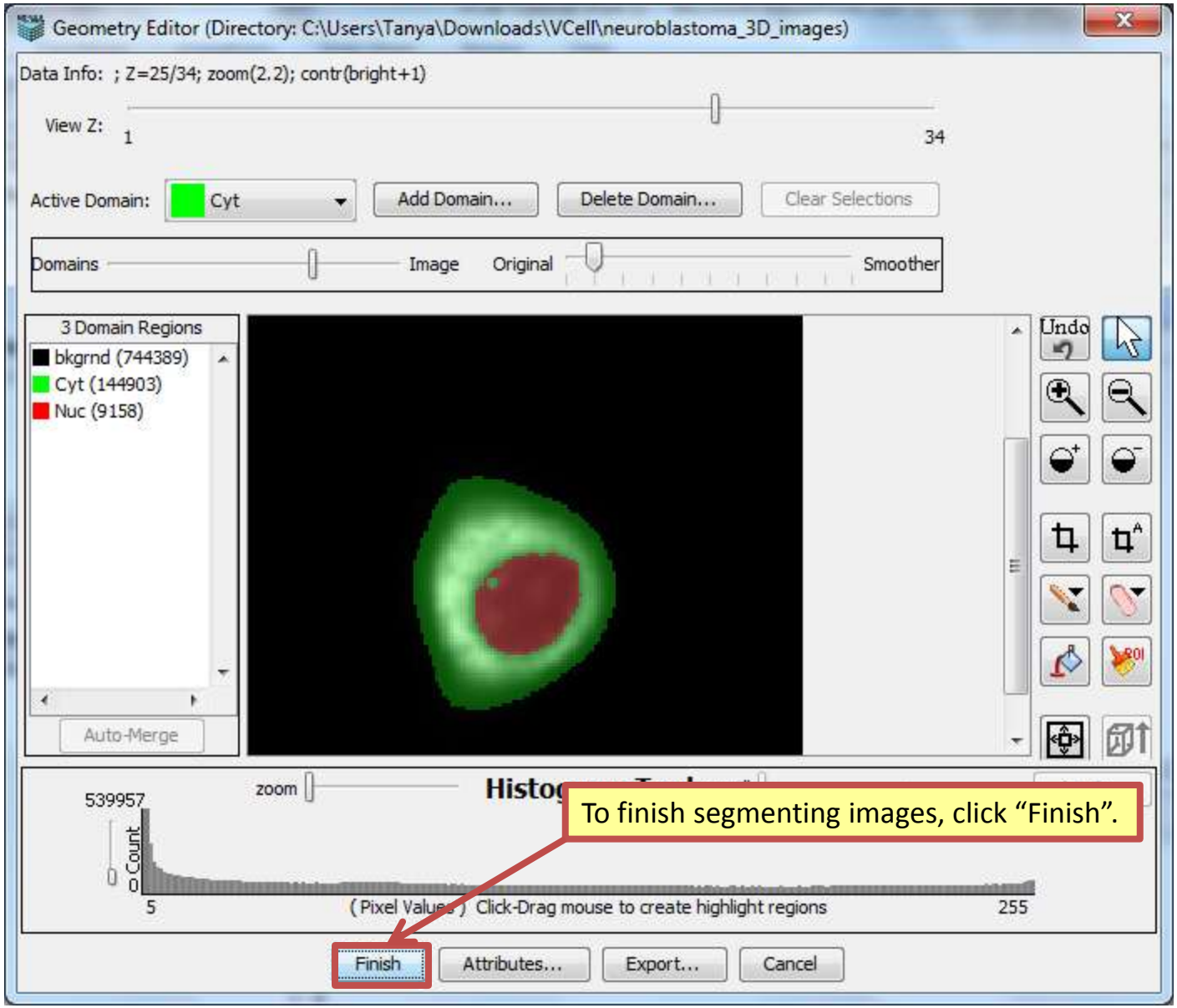

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=25/34; zoom(2.2); contr(bright+1)
View Z:
1
To update the domain, click “Apply” and then “Update Domain”.
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother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

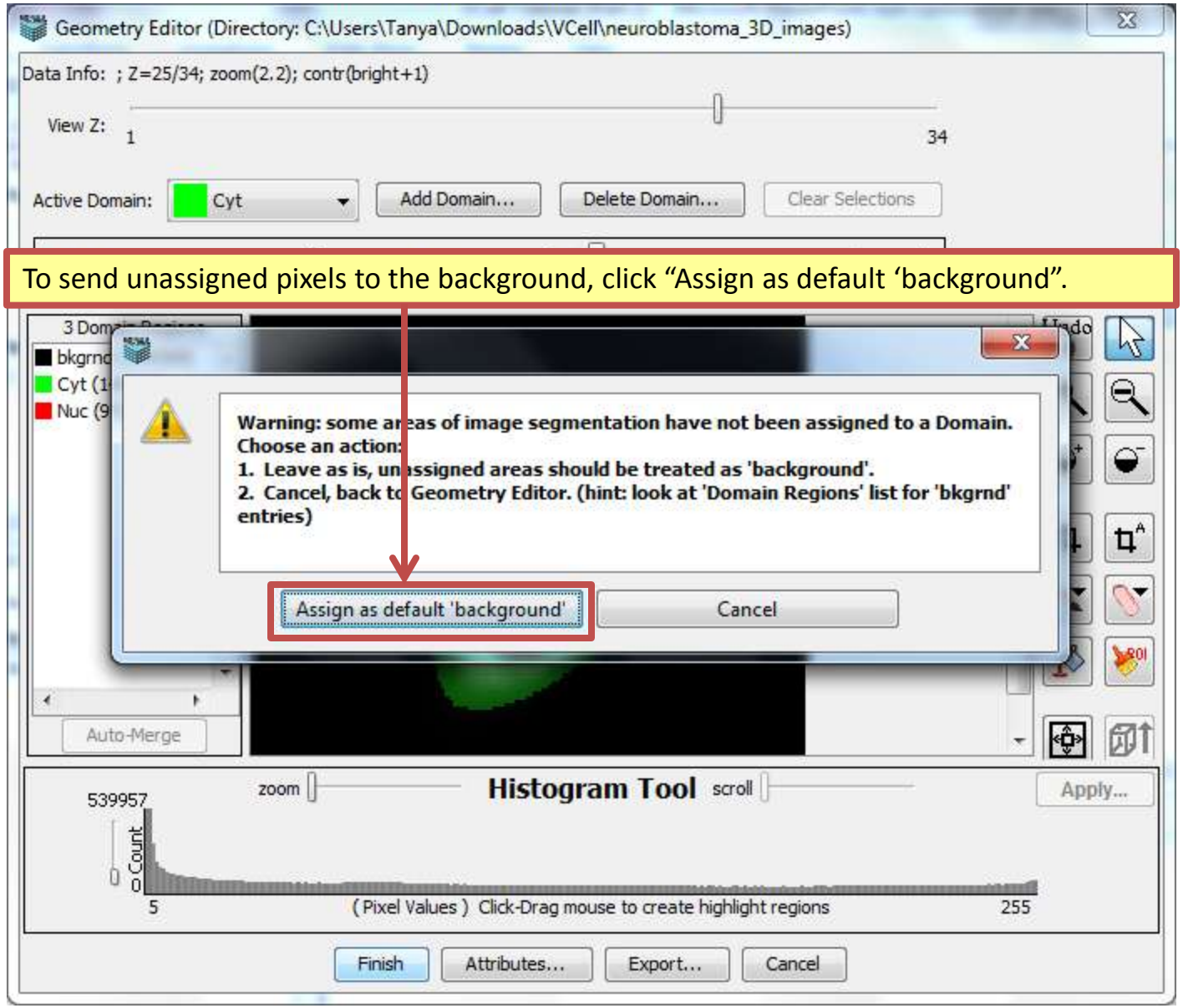
Contents

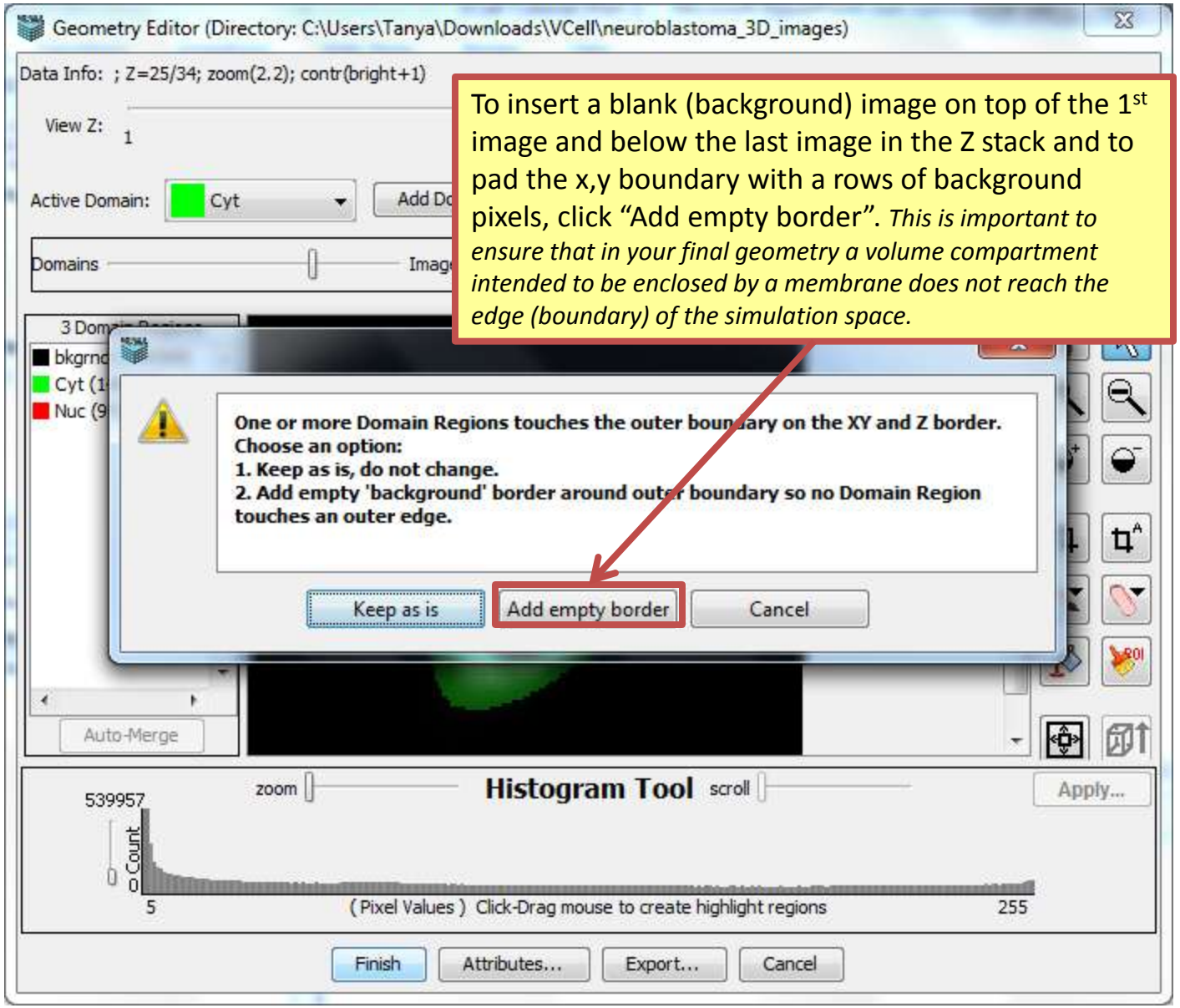

Some areas of the new Domain Regions overlap with existing Domain Regions.
To keep multiple domain regions, click “Keep existing Domain Regions when overlapping”.
Overwrite any existing Domain Regionss
Keep existing Domain Regions when overlapping
Cancel



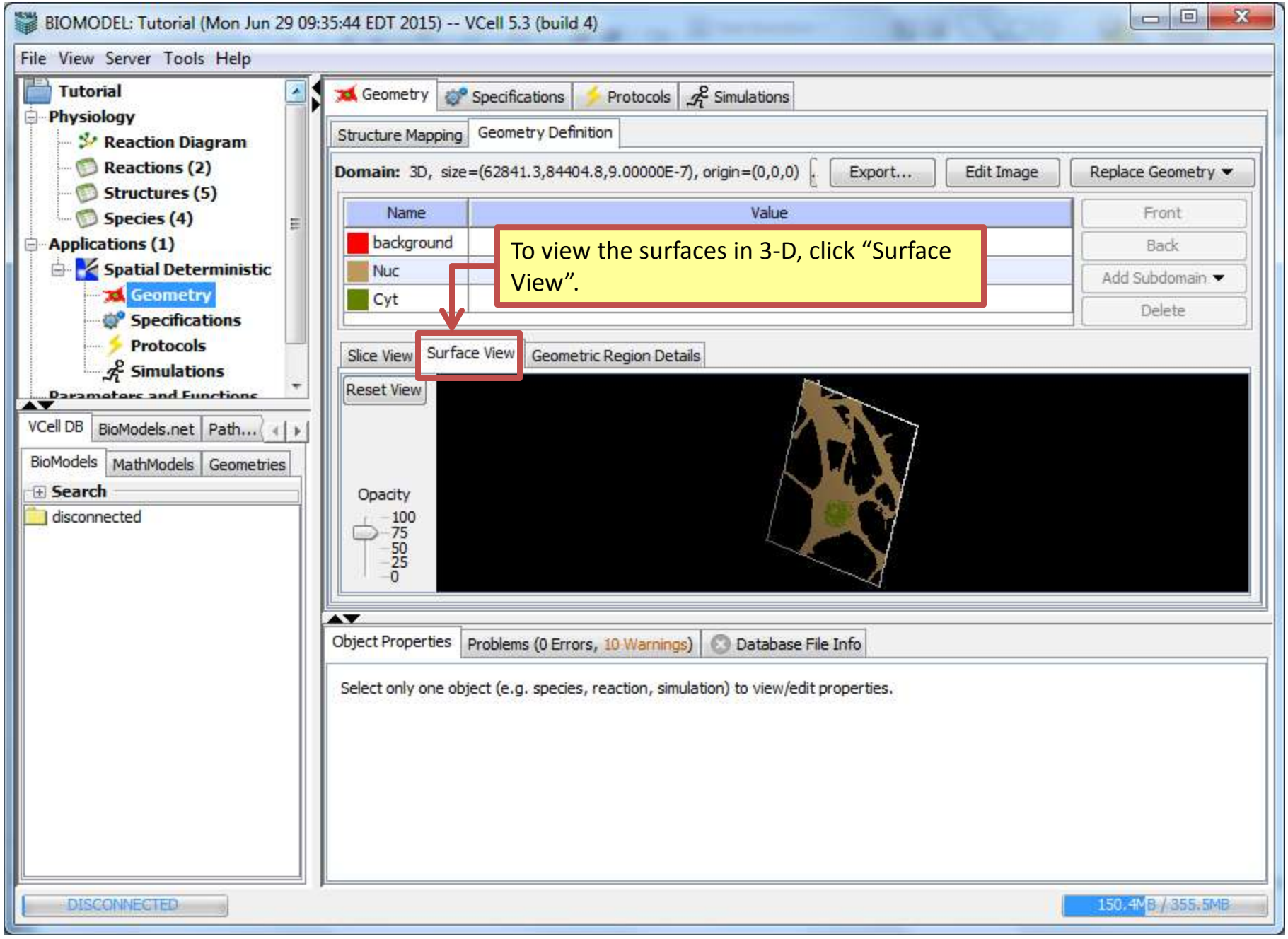
To remove non-nucleus and non-cytoplasm regions, hold down on “ctrl” and “a” on your keyboard at the same time, and then while continuing to hold on to the “ctrl” button, click on the top “bkgrnd” , “Cyt” and “Nuc” to deselect them. Next, click “Auto-Merge”.


Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=25/34; zoom(2.2); contr(bright+1)
View Z:
1
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
3 Domain Regions
bkgrnd (744389)
Cyt (144903)
Nuc (9158)
Auto-Merge
Undo
zoom
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
To finish segmenting images, click “Finish”.
Finish
Attributes...
Export...
Cancel


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
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
To send unassigned pixels to the background, click “Assign as default ‘background”.
Warning: some areas of image segmentation have not been assigned to a Domain.
Choose an action:
1. Leave as is, unassigned areas should be treated as 'background'.
2. Cancel, back to Geometry Editor. (hint: look at 'Domain Regions' list for 'bkgrnd' entries)
Assign as default 'background'
Cancel
bkgrnd
Cyt (1
Nuc (9
Auto-Merge
zoom
Histogram Tool
scroll
Apply...
539957
Count
0
5
(Pixel Values) Click-Drag mouse to create highlight regions
255
Finish
Attributes...
Export...
Cancel



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.*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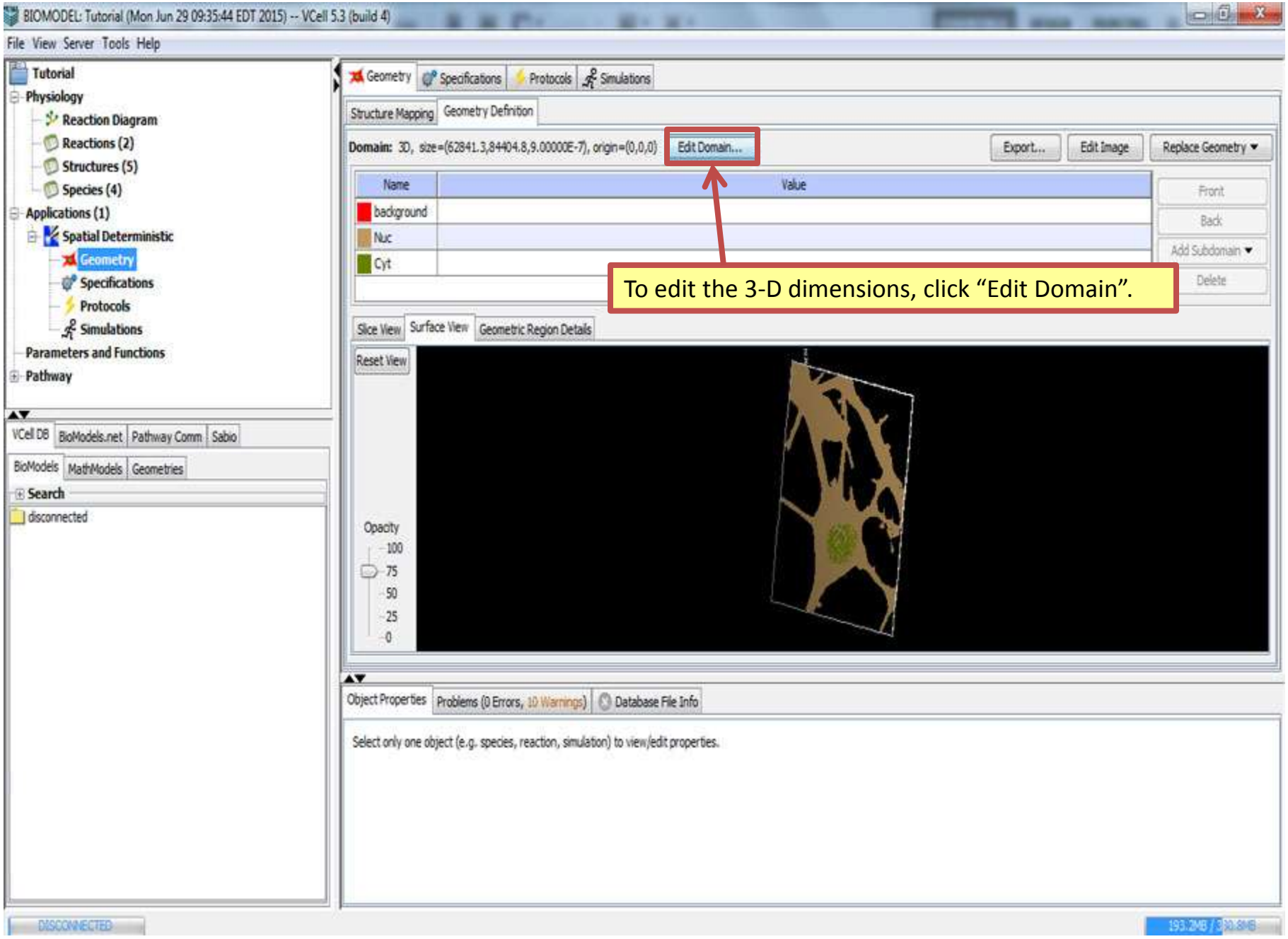
Geometry Definition
Domain: 3D, size=(62841.3,84404.8,9.00000E-7), origin=(0,0,0)
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To view the surfaces in 3-D, click “Surface View”.
Slice View
Surface View
Geometric Region Details
Reset View
Opacity
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: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
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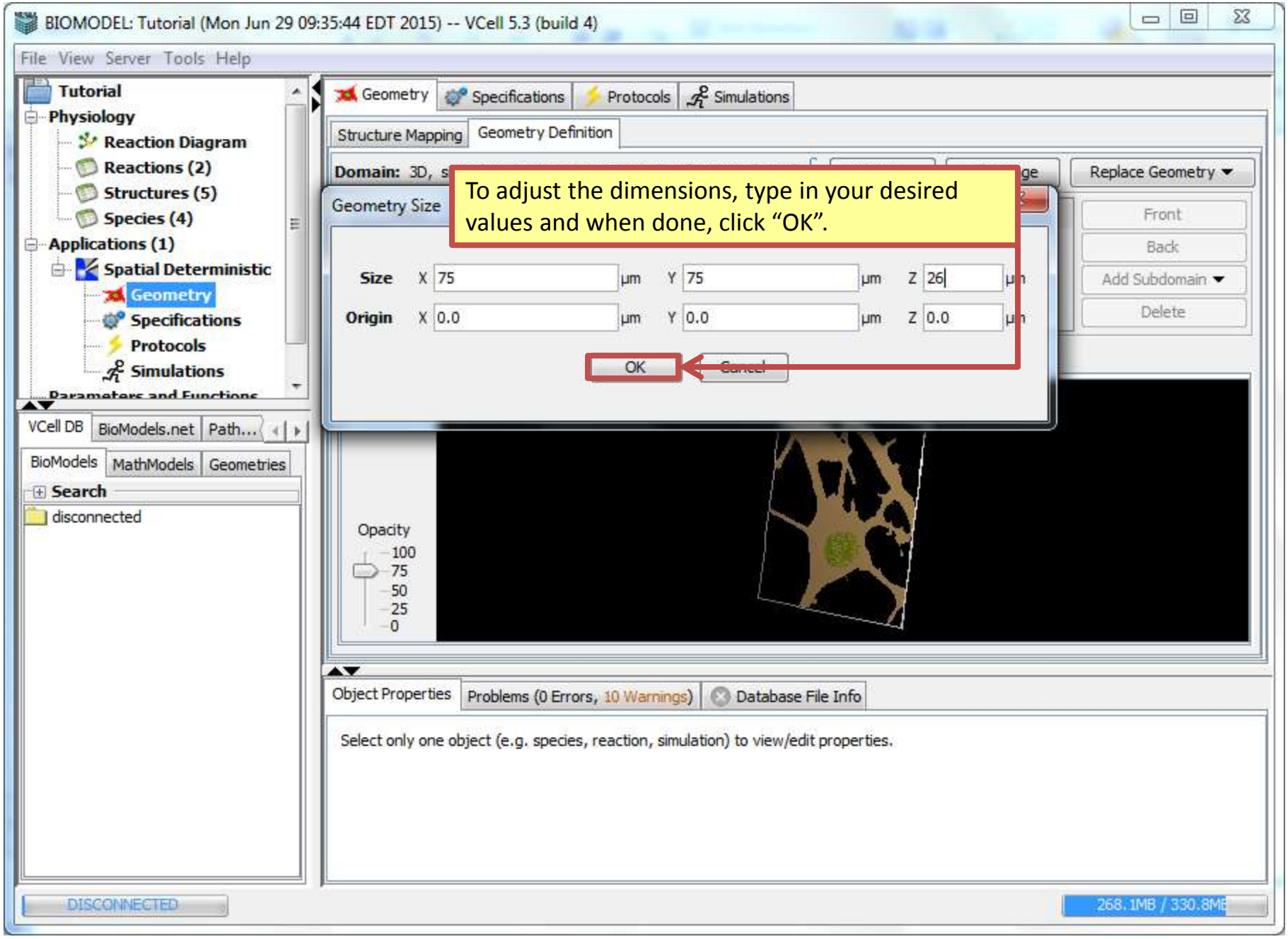
Geometry Definition
Domain: 3D, size=(62841.3,84404.8,9.00000E-7), origin=(0,0,0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To edit the 3-D dimensions, click “Edit Domain”.
Slice View
Surface View
Geometric Region Details
Reset 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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Geometry Definition
Domain: 3D, s
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
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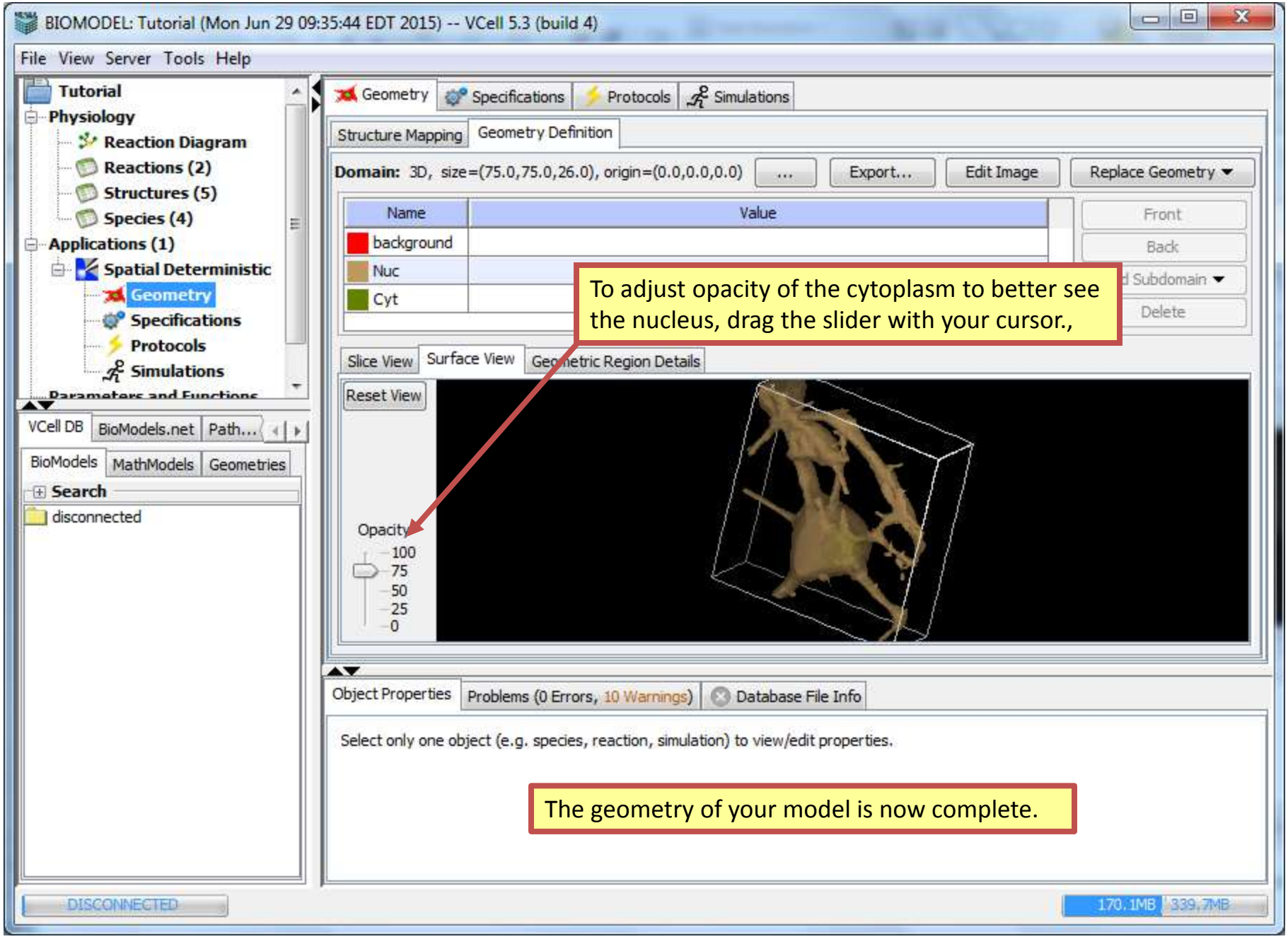
disconnected
Object Properties
Problems (0 Errors, 10 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
DISCONNECTED
268.1MB / 330.8MB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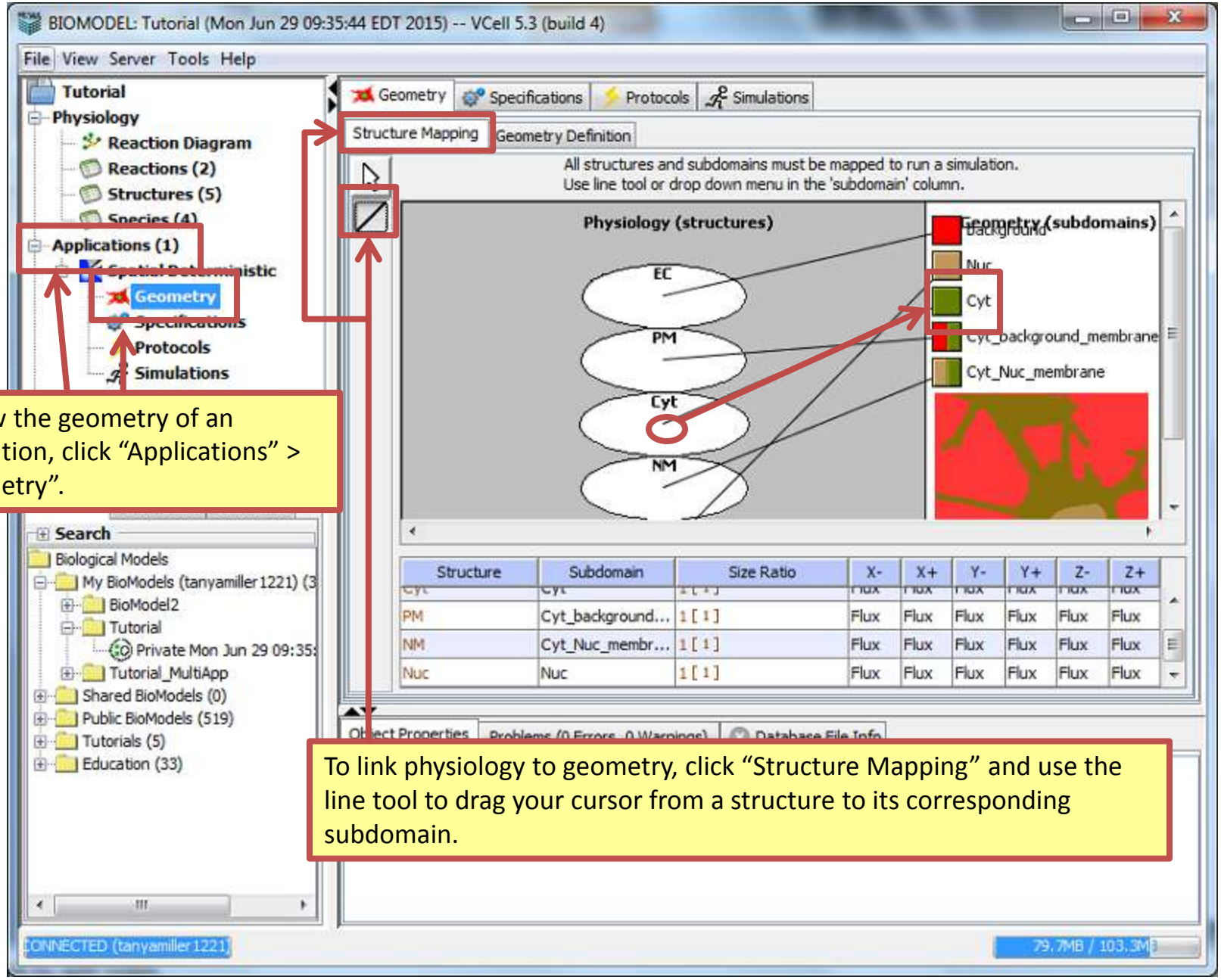
Structure Mapping
Geometry Definition
Domain: 3D, size=(75.0,75.0,26.0), origin=(0.0,0.0,0.0)
...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Subdomain
Delete
To adjust opacity of the cytoplasm to better see the nucleus, drag the slider with your cursor.,
Slice View
Surface View
Geometric Region Details
Reset View
Opacity
100
75
50
25
0
Object Properties
Problems (0 Errors, 10 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
The geometry of your model is now complete.
DISCONNECTED
170.1MB
339.7MB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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)
EC
PM
Cyt
NM
Geometry (subdomains)
Nuc
Cyt
Cyt_background_membrane
Cyt_Nuc_membrane
Structure
Subdomain
Size Ratio
X-
X+
Y-
Y+
Z-
Z+
PM
Cyt_background...
1 [1]
Flux
NM
Cyt_Nuc_membr...
Nuc
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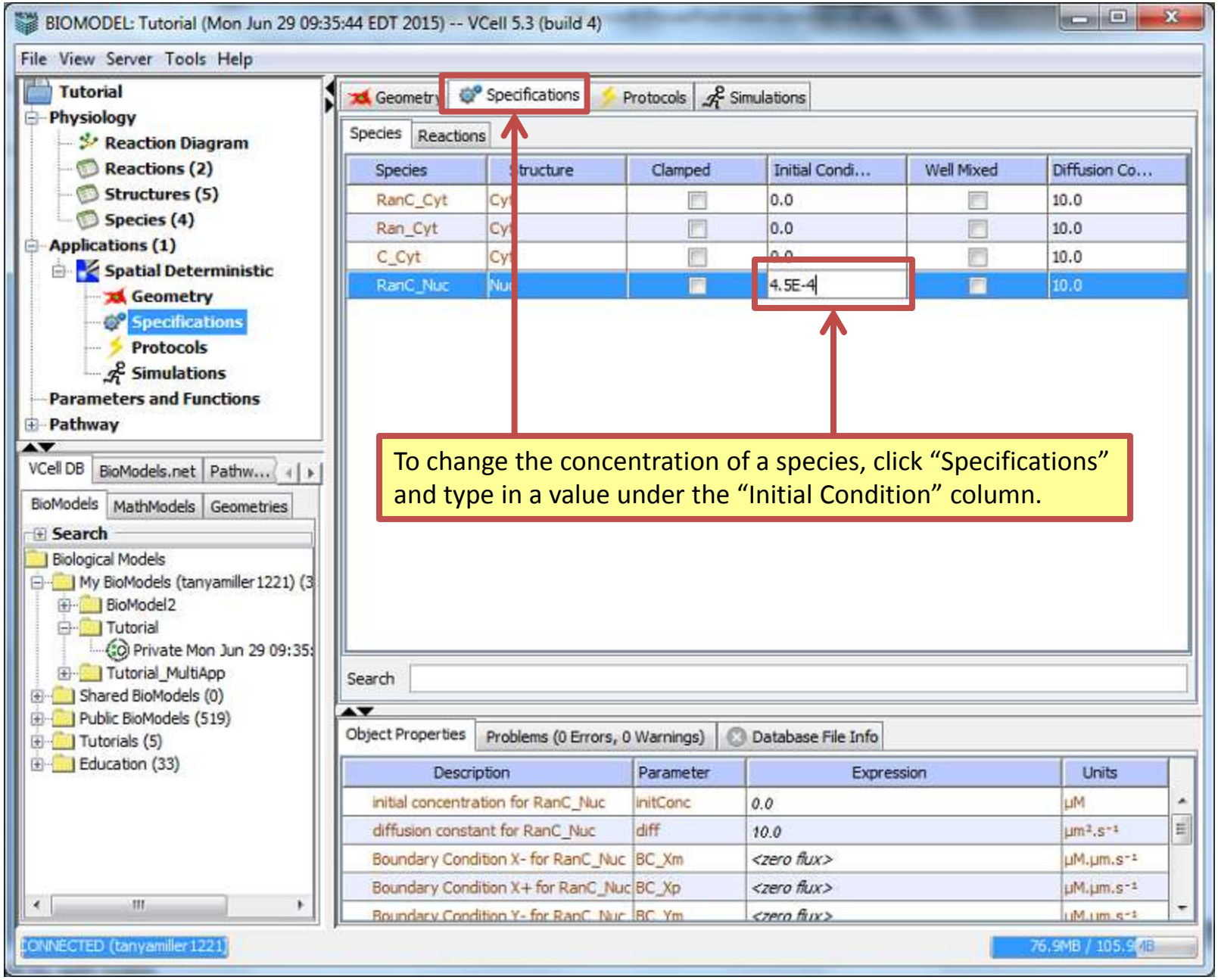
CONNECTED (tanyamiller1221)
79.7MB / 103.3MB
To view the geometry of an application, click “Applications” > “Geometry”.
To link physiology to geometry, click “Structure Mapping” and use the line tool to drag your cursor from a structure to its corresponding subdomain.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Species
Structure
Clamped
Initial Condi...
Well Mixed
Diffusion Co...
RanC_Cyt
Ran_Cyt
C_Cyt
RanC_Nuc
0.0
4.5E-4
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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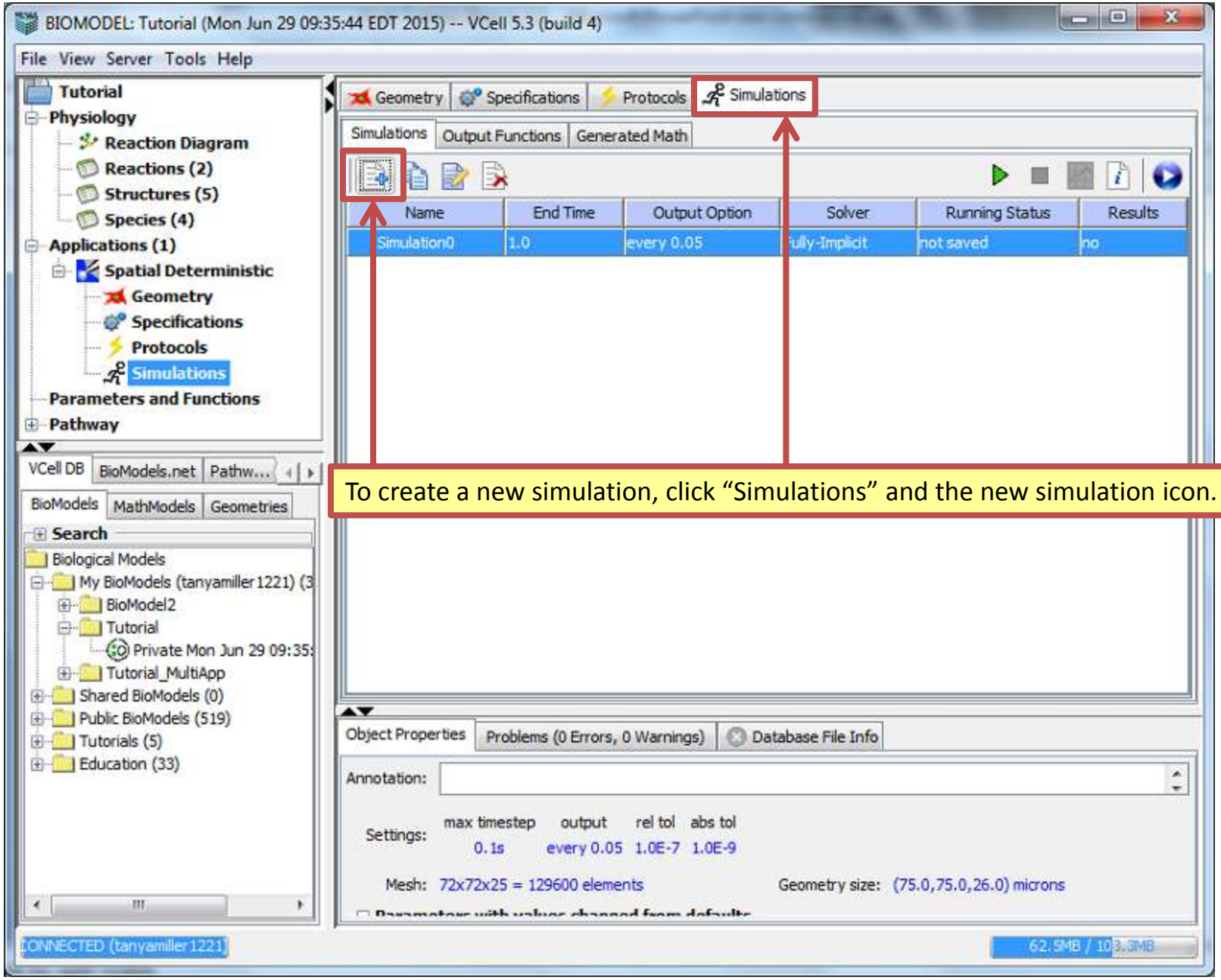
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for RanC_Nuc
initConc
0.0
µM
diffusion constant for RanC_Nuc
diff
10.0
µm².s⁻¹
Boundary Condition X- for RanC_Nuc
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for RanC_Nuc
BC_Xp
<zero flux>
µM.µm.s⁻¹
CONNECTED (tanyamiller1221)
76,9MB / 105,9MB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Simulations
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End Time
Output Option
Solver
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Results
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1.0
every 0.05
not saved
no
To create a new simulation, click “Simulations” and the new simulation icon.
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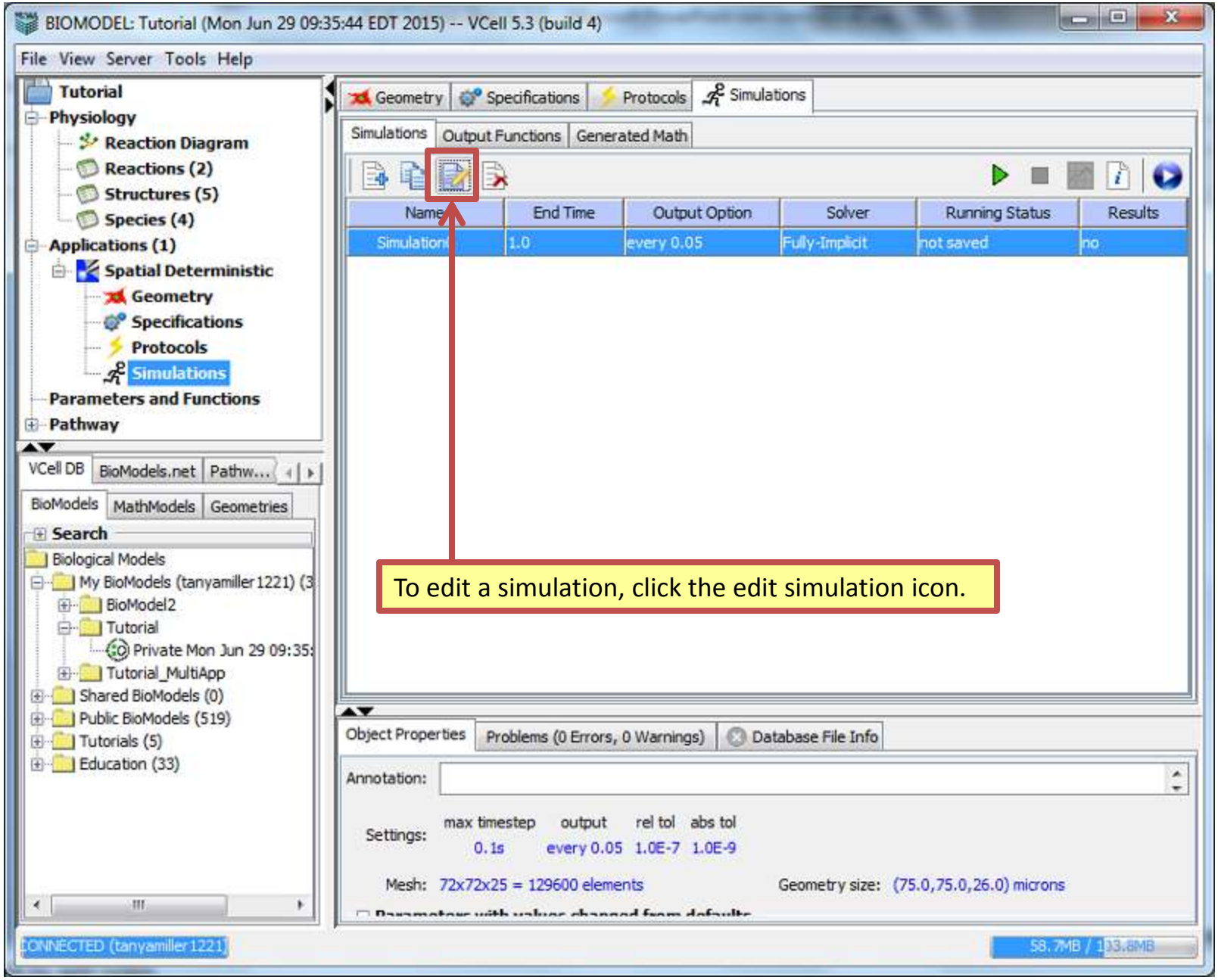
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
CONNECTED (tanyamiller1221)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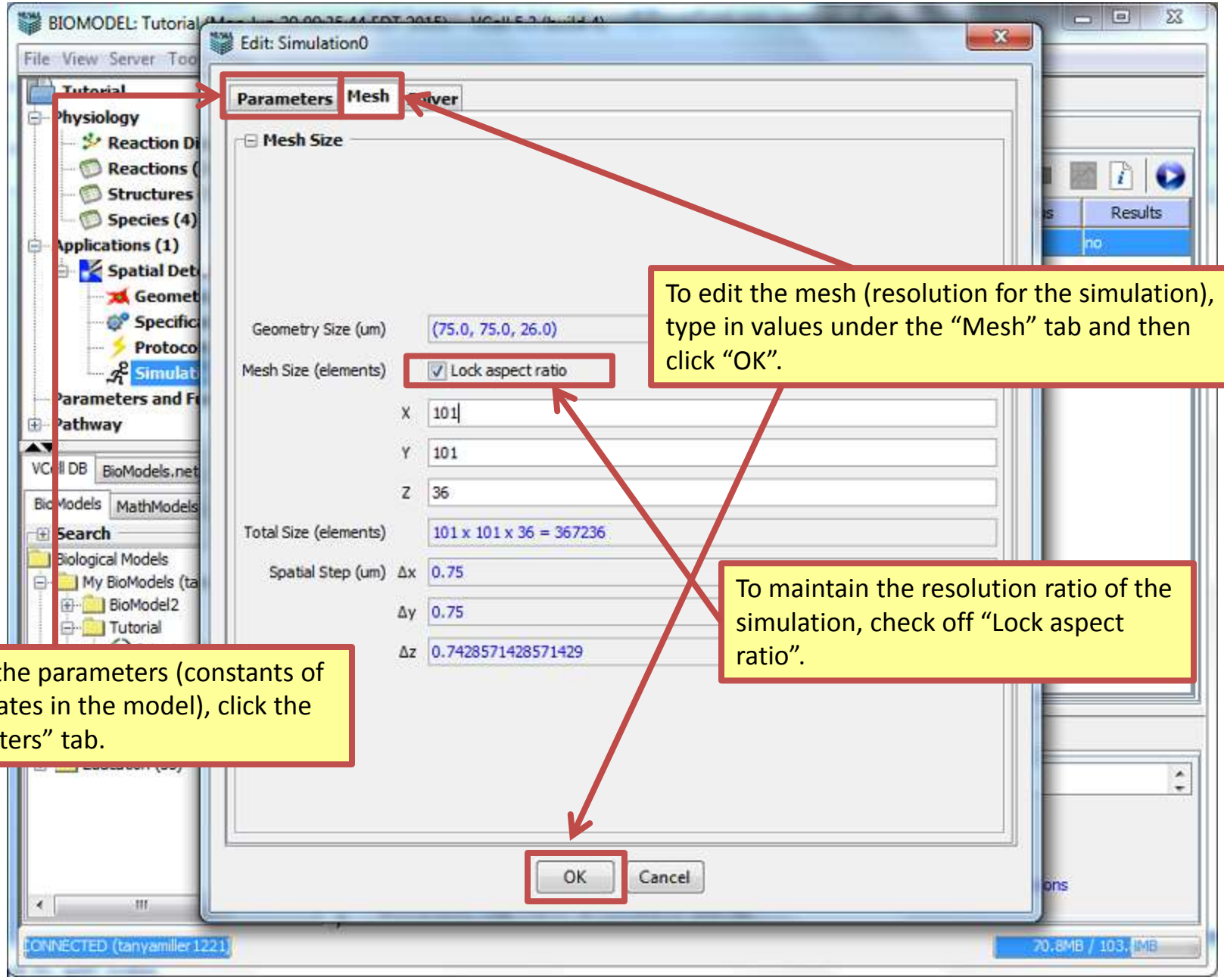
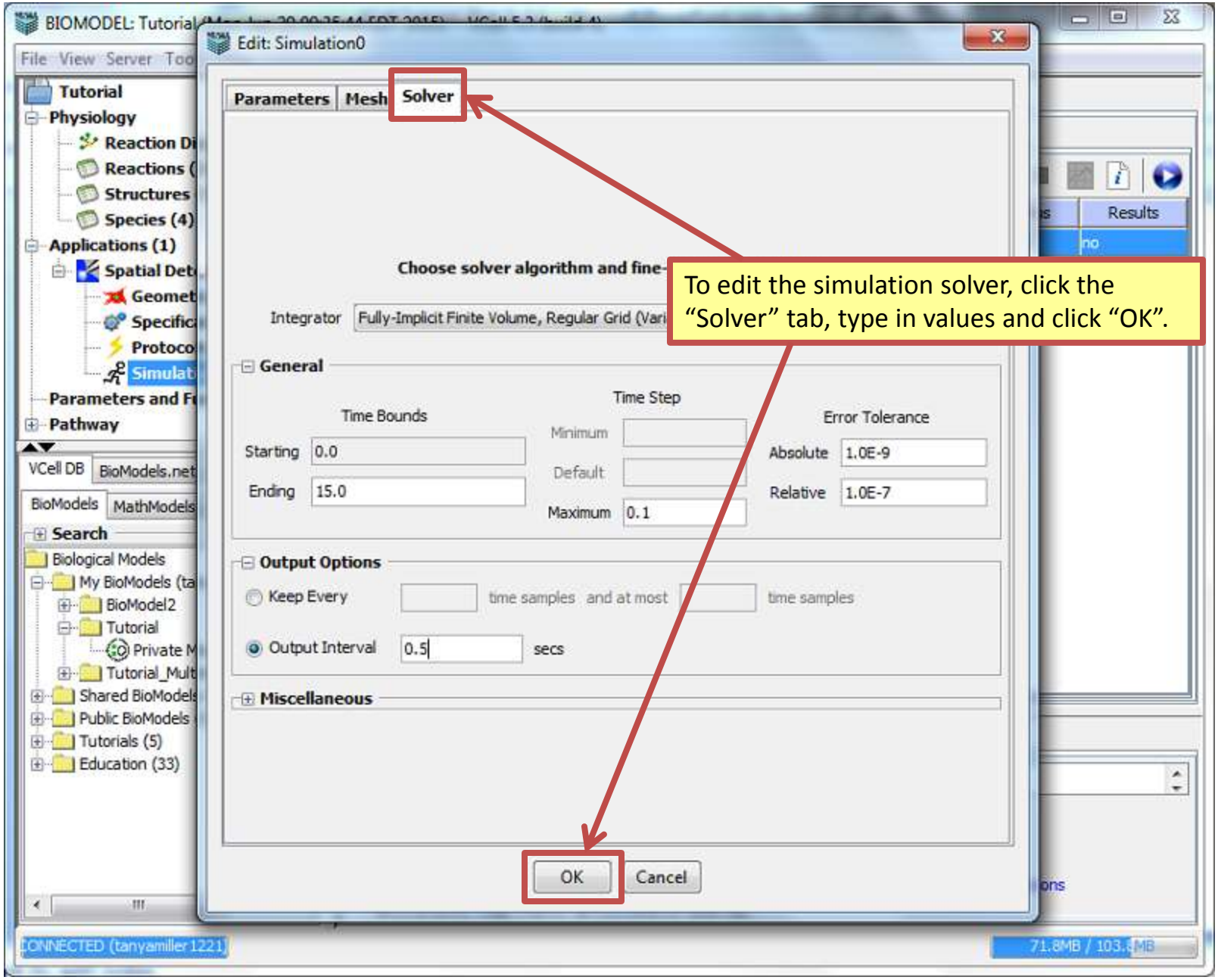
Simulation
1.0
every 0.05
Fully-Implicit
not saved
no
To edit a simulation, click the edit simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
CONNECTED (tanyamiller1221)
58.7MB / 103.8MB


Edit: Simulation0
Parameters
Mesh
Mesh Size
Geometry Size (um)
(75.0, 75.0, 26.0)
Mesh Size (elements)
Lock aspect ratio
X
101
Y
101
Z
36
Total Size (elements)
101 x 101 x 36 = 367236
Spatial Step (um)
Δx
0.75
Δy
0.75
Δz
0.7428571428571429
OK
Cancel
To edit the mesh (resolution for the simulation), type in values under the "Mesh" tab and then click "OK".
To maintain the resolution ratio of the simulation, check off "Lock aspect ratio".
To view the parameters (constants of certain rates in the model), click the "Parameters" tab.


BIOMODEL: Tutorial
Edit: Simulation0
Parameters
Mesh
Solver
Choose solver algorithm and fine-
Integrator
Fully-Implicit Finite Volume, Regular Grid (Vari
General
Time Bounds
Starting
0.0
Ending
15.0
Time Step
Minimum
Default
Maximum
0.1
Error Tolerance
Absolute
1.0E-9
Relative
1.0E-7
Output Options
Keep Every
time samples and at most
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".
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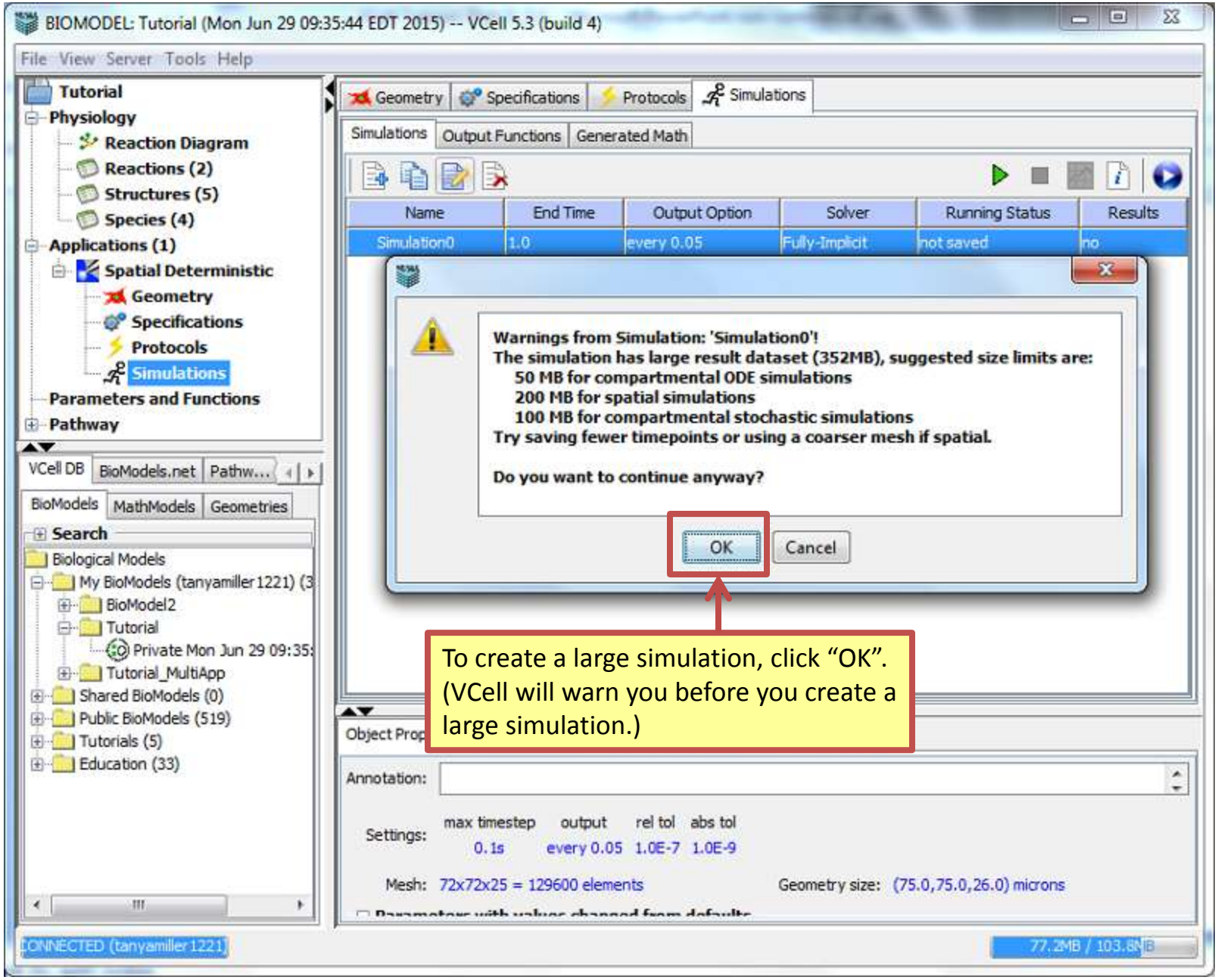
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Name End Time Output Option Solver Running Status Results
Simulation0 1.0 every 0.05 Fully-Implicit not saved no
Warnings from Simulation: 'Simulation0'!
The simulation has large result dataset (352MB), suggested size limits are:
50 MB for compartmental 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”. (VCell will warn you before you create a large simulation.)
VCell DB BioModels.net Pathw...
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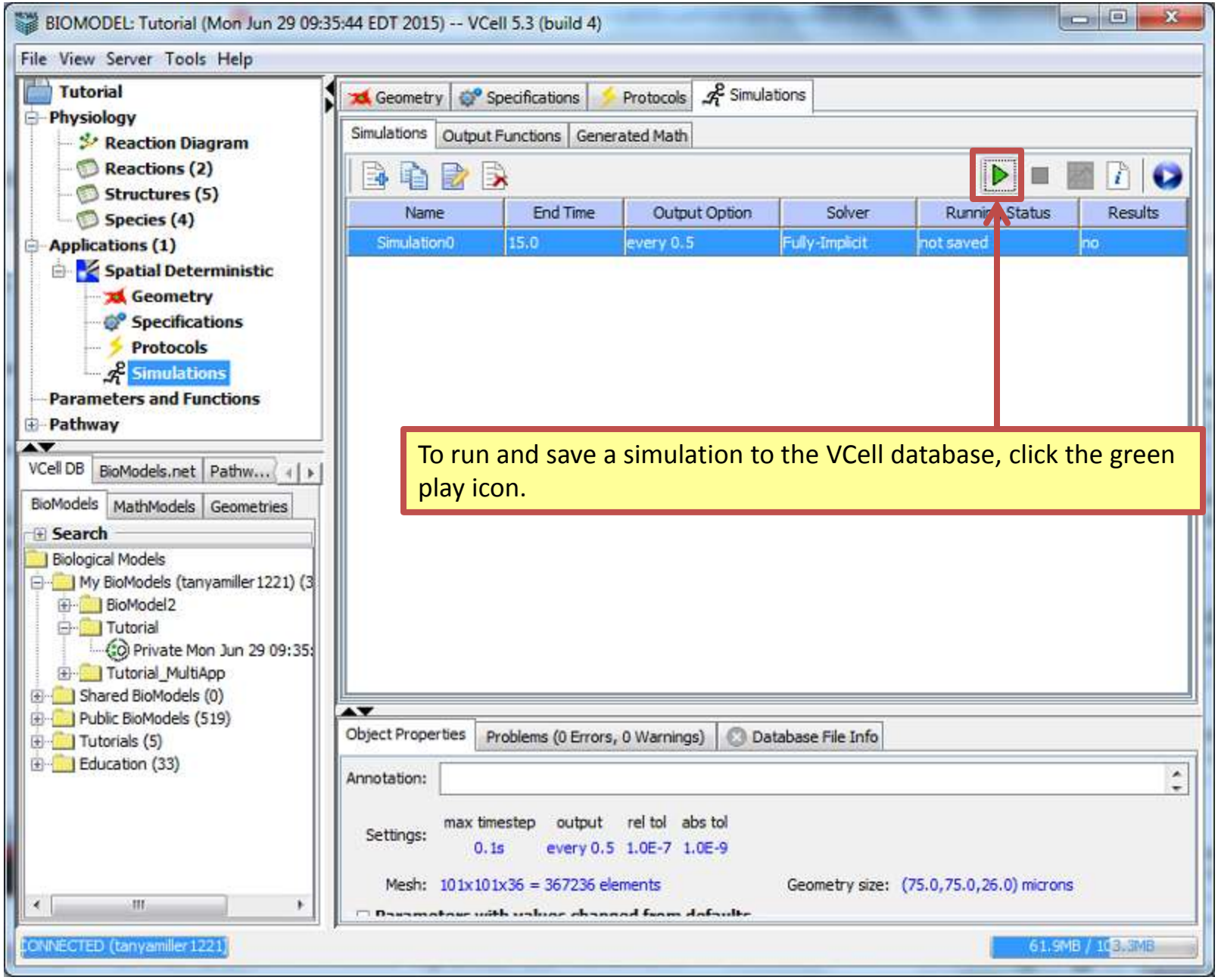
Object Prop
Annotation:
Settings: max timestep 0.1s output every 0.05 rel tol 1.0E-7 abs tol 1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
CONNECTED (tanyamiller1221)
77.2MB / 103.8MB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Geometry Specifications Protocols Simulations
Simulations Output Functions Generated Math
Name End Time Output Option Solver Runni Status Results
Simulation0 15.0 every 0.5 Fully-Implicit not saved no
To run and save a simulation to the VCell database, click the green play icon.
VCell DB BioModels.net Pathw...
BioModels MathModels Geometries
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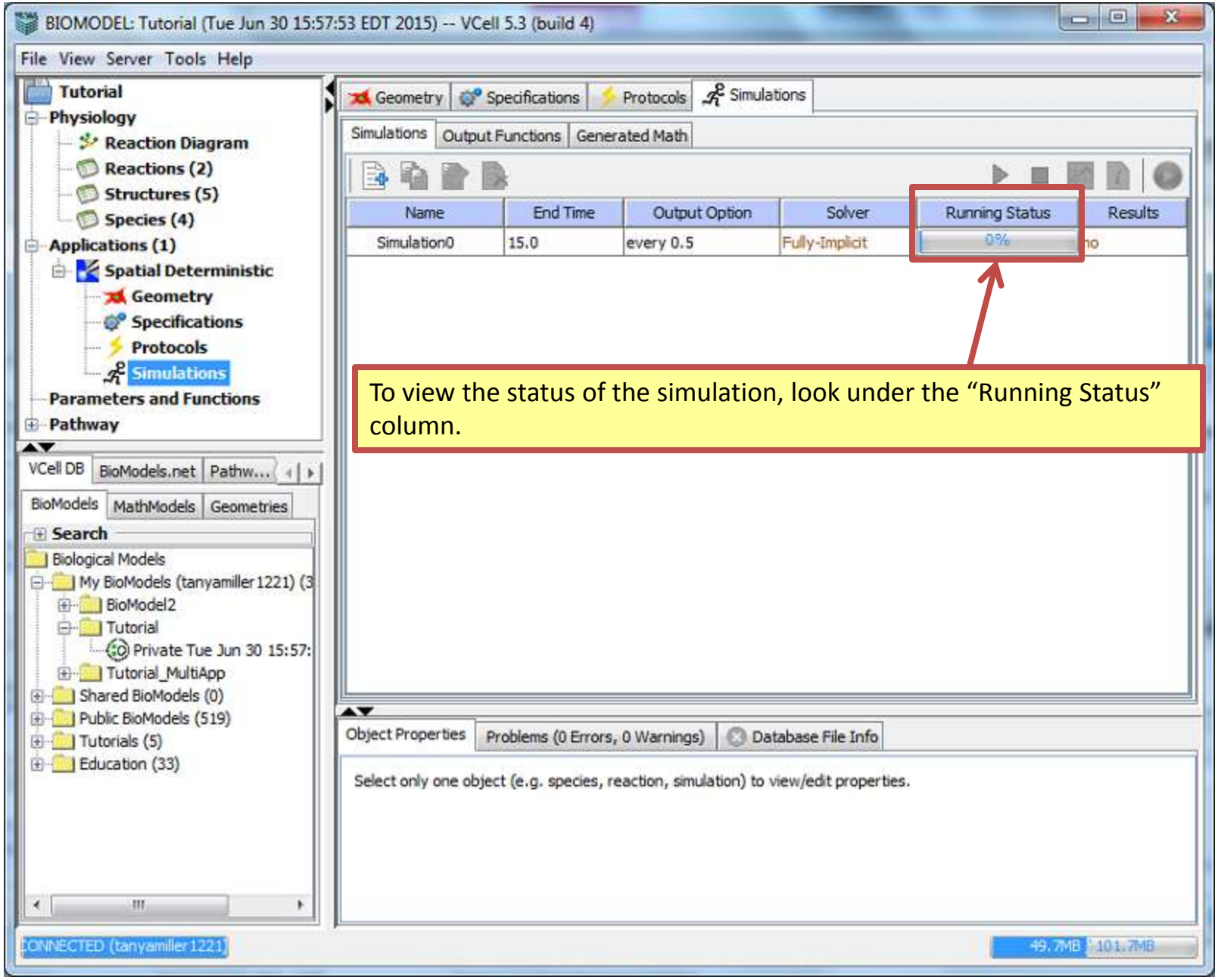
Public BioModels (519)
Tutorials (5)
Education (33)
Object Properties Problems (0 Errors, 0 Warnings) Database File Info
Annotation:
Settings: max timestep output rel tol abs tol
0.1s every 0.5 1.0E-7 1.0E-9
Mesh: 101x101x36 = 367236 elements
Geometry size: (75.0,75.0,26.0) microns
CONNECTED (tanyamiller1221)
61.9MB / 103.3MB


BIOMODEL: Tutorial (Tue Jun 30 15:57:53 EDT 2015) -- VCell 5.3 (build 4)
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Simulations
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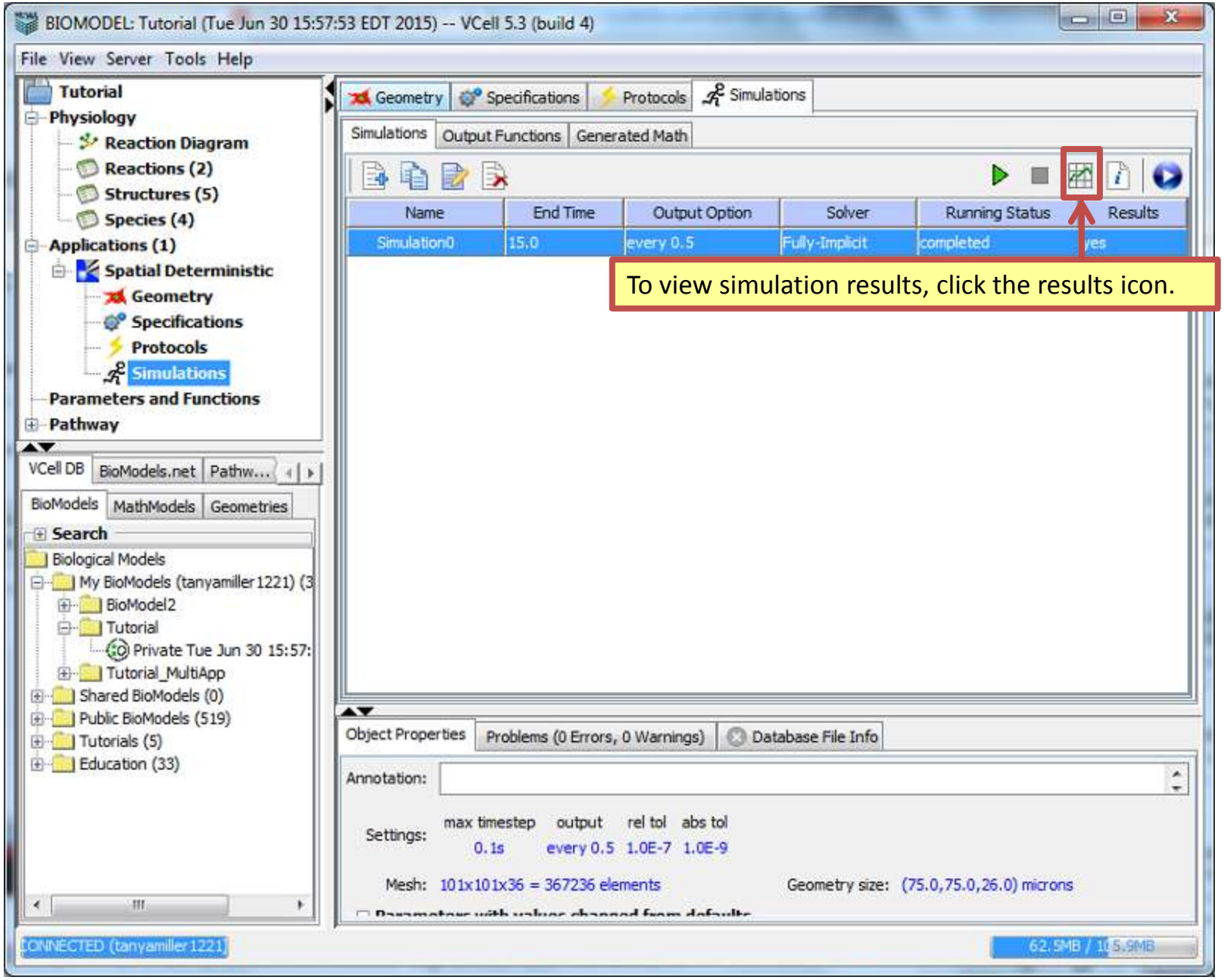
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5
Fully-Implicit
0%
To view the status of the simulation, look under the “Running Status” column.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
49.7MB
101.7MB


BIOMODEL: Tutorial (Tue Jun 30 15:57:53 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
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Physiology
Reaction Diagram
Reactions (2)
Structures (5)
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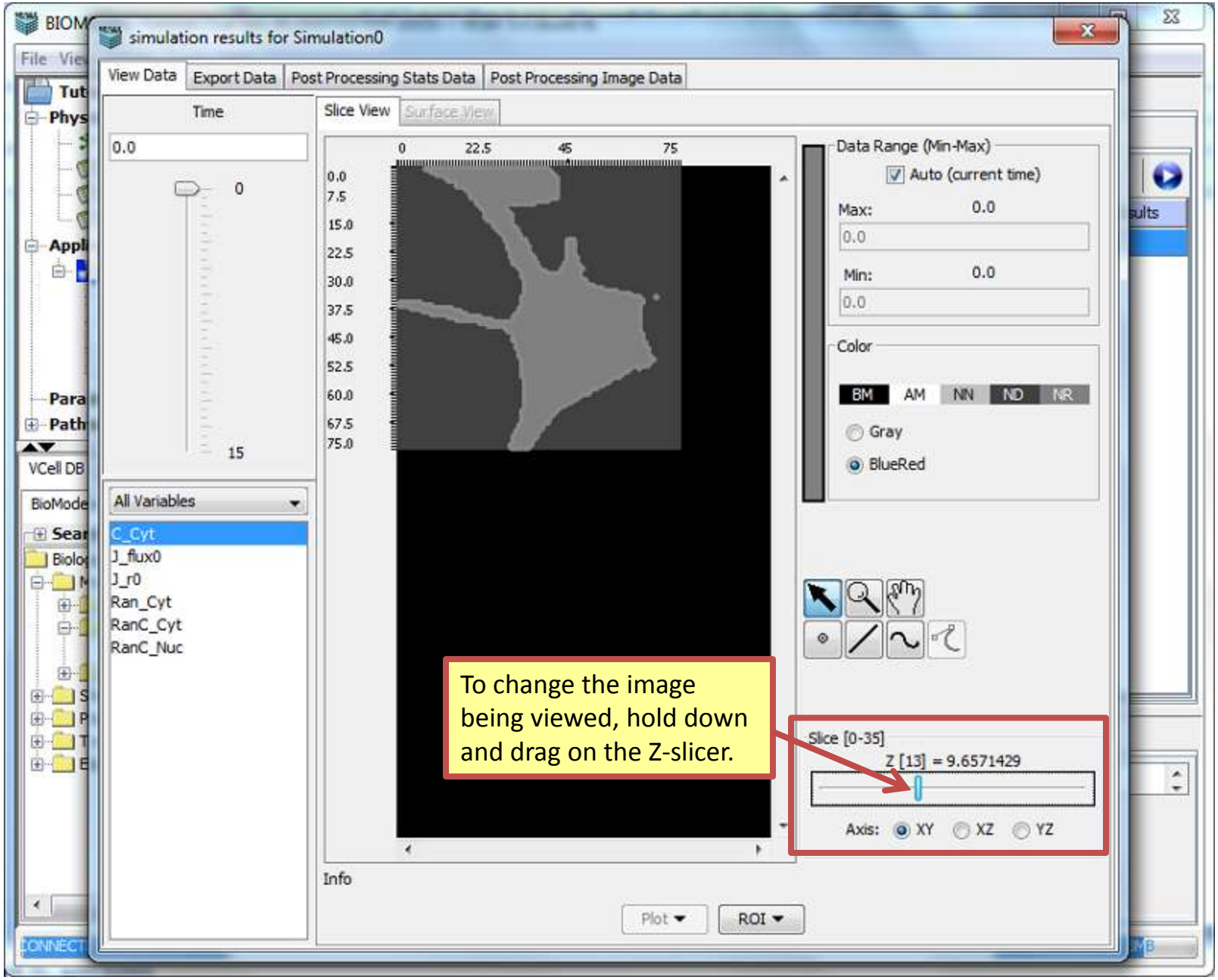
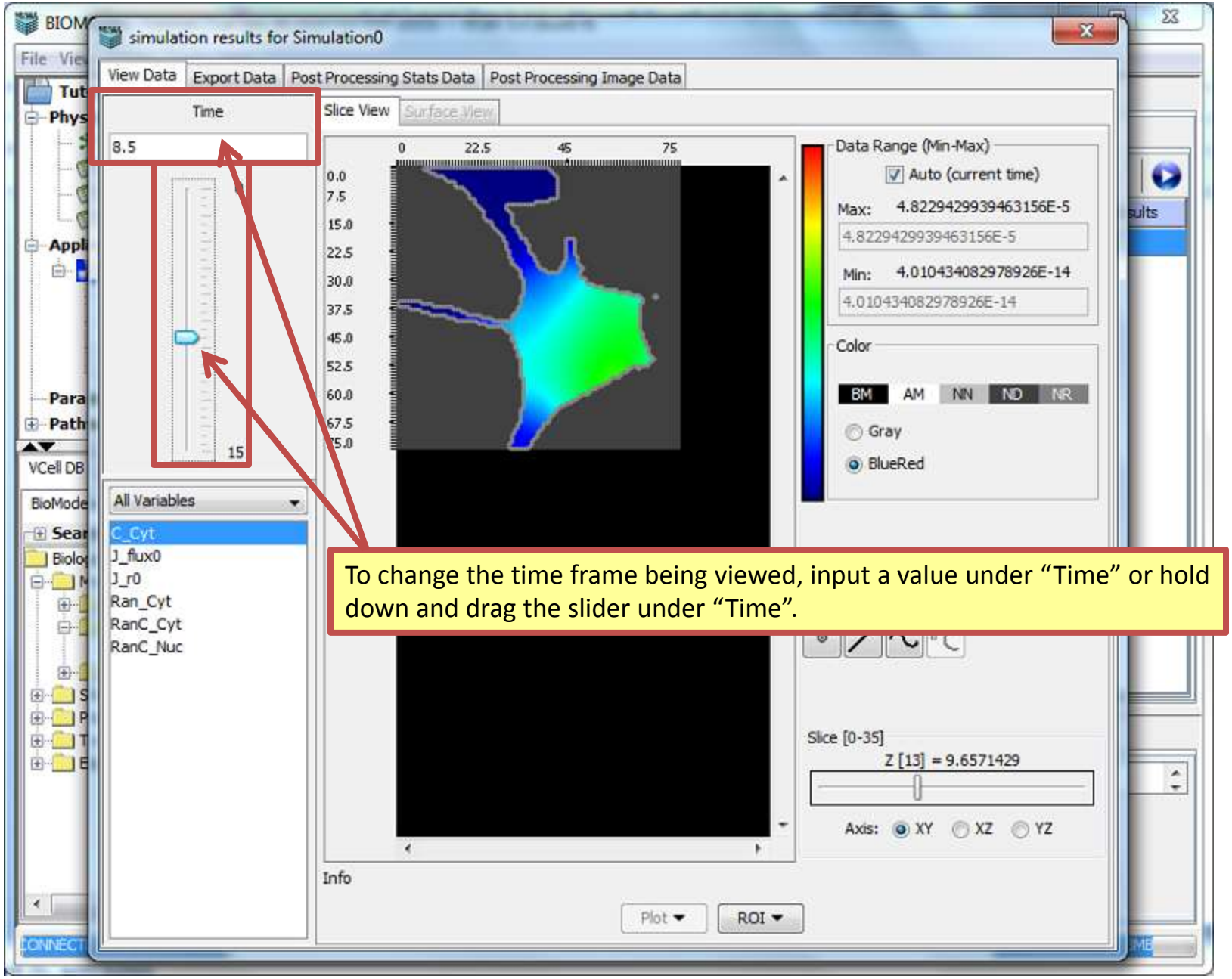
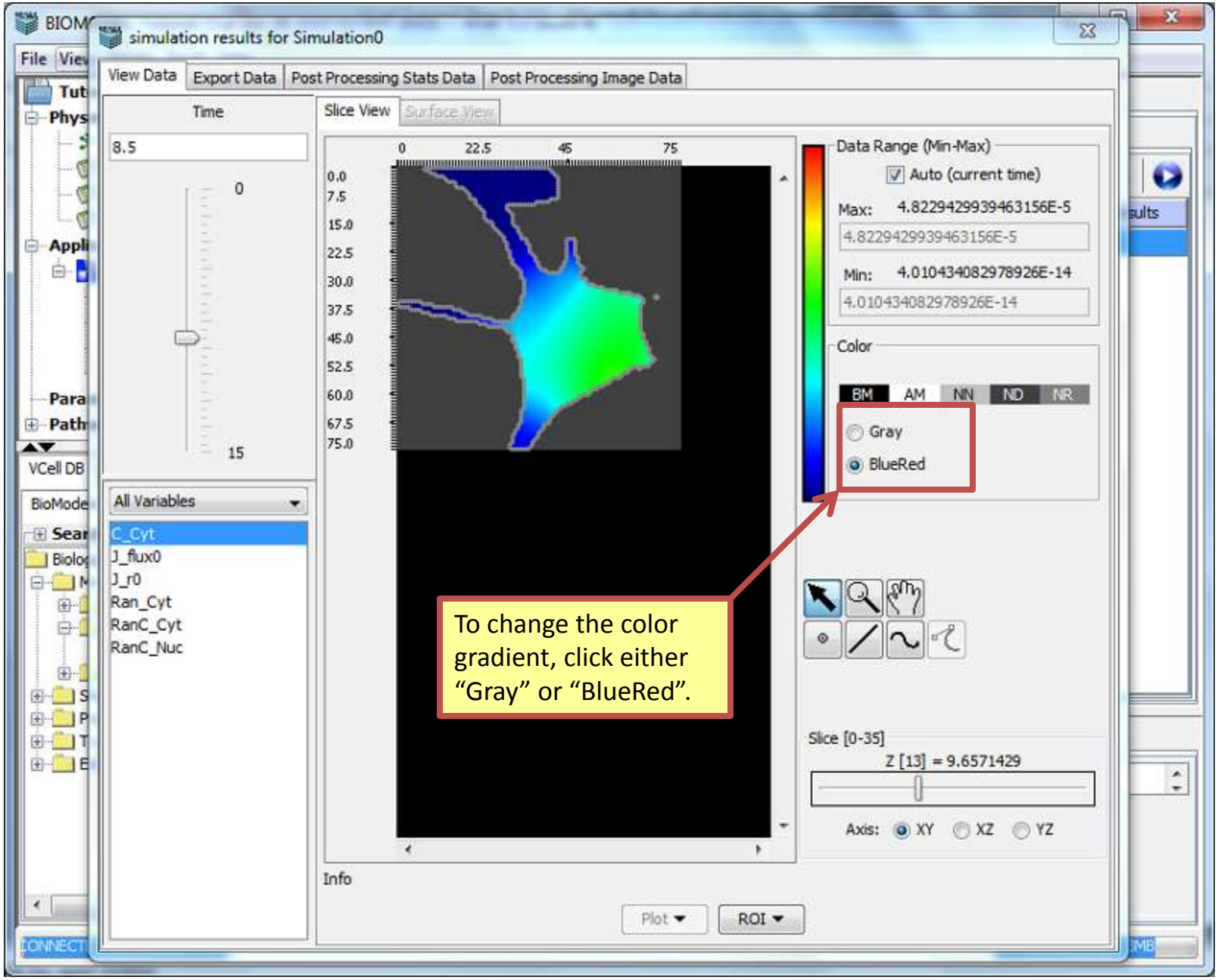
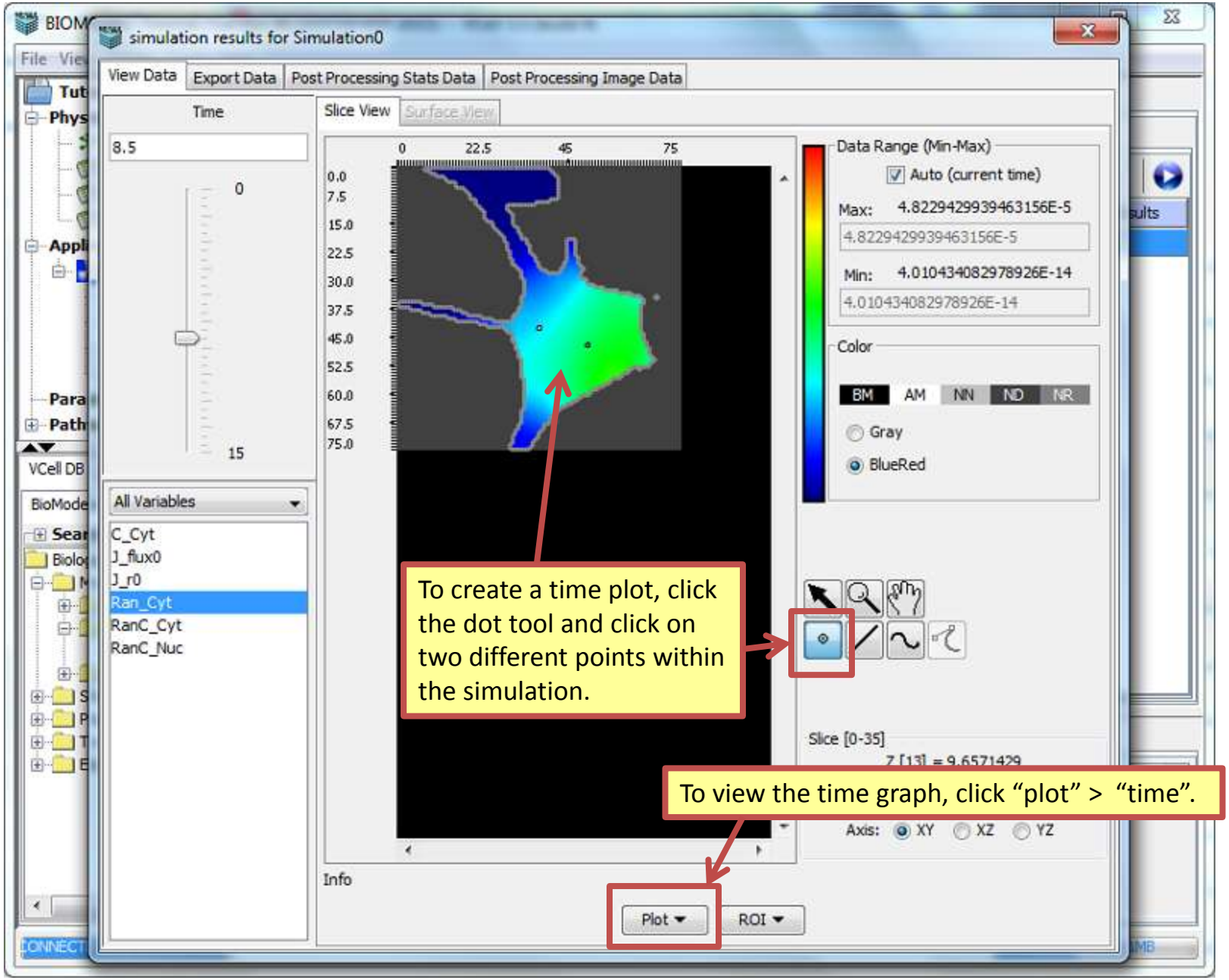
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5
Fully-Implicit
completed
To view simulation results, click the results icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5
1.0E-7
1.0E-9
Mesh: 101x101x36 = 367236 elements
Geometry size: (75.0,75.0,26.0) microns
CONNECTED (tanyamiller1221)
62.5MB / 105.9MB

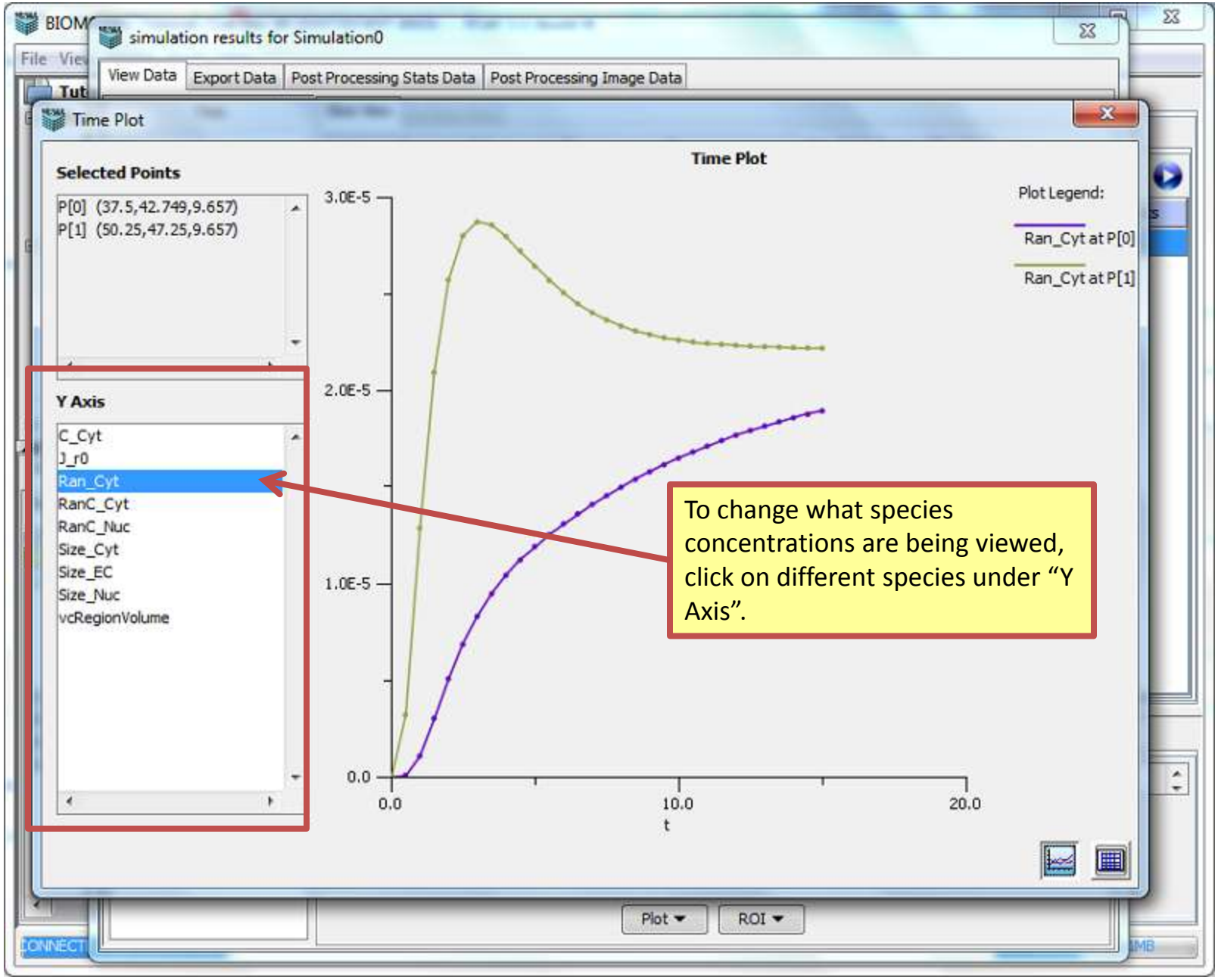

simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
0.0
0
15
Slice View
Surface View
0
22.5
45
75
0.0
7.5
15.0
22.5
30.0
37.5
45.0
52.5
60.0
67.5
75.0
Data Range (Min-Max)
Auto (current time)
Max:
0.0
0.0
Min:
0.0
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
To change the image being viewed, hold down and drag on the Z-slicer.
Slice [0-35]
Z [13] = 9.6571429
Axis:
XY
XZ
YZ
Info
Plot
ROI

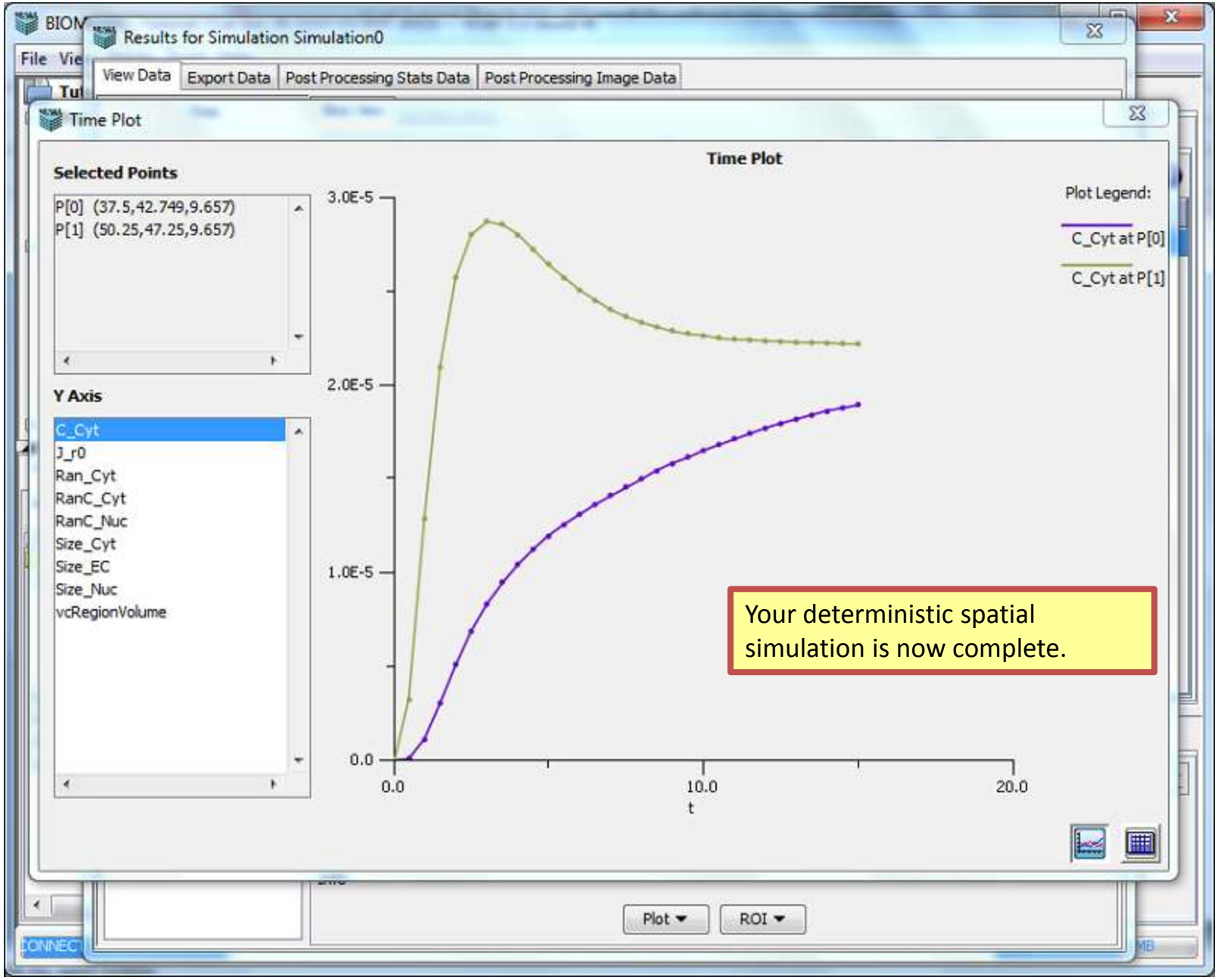

simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
8.5
15
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max: 4.8229429939463156E-5
Min: 4.010434082978926E-14
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Slice [0-35]
Z [13] = 9.6571429
Axis: XY XZ YZ
Info
Plot
ROI
To change the time frame being viewed, input a value under “Time” or hold down and drag the slider under “Time”.


simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
8.5
Slice View
Surface View
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Data Range (Min-Max)
Auto (current time)
Max: 4.8229429939463156E-5
Min: 4.010434082978926E-14
Color
BM
AM
NN
ND
NR
Gray
BlueRed
To change the color gradient, click either "Gray" or "BlueRed".
Slice [0-35]
Z [13] = 9.6571429
Axis: XY XZ YZ
Info
Plot
ROI


simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
8.5
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max: 4.8229429939463156E-5
Min: 4.010434082978926E-14
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
To create a time plot, click the dot tool and click on two different points within the simulation.
Slice [0-35]
To view the time graph, click “plot” > “time”.
Axis: XY XZ YZ
Info
Plot
ROI

Contents


simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time Plot
Selected Points
P[0] (37.5,42.749,9.657)
P[1] (50.25,47.25,9.657)
Y Axis
C_Cyt
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Size_Cyt
Size_EC
Size_Nuc
vcRegionVolume
Time Plot
Plot Legend:
Ran_Cyt at P[0]
Ran_Cyt at P[1]
3.0E-5
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
To change what species concentrations are being viewed, click on different species under "Y Axis".
Plot
ROI


Results for Simulation Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time Plot
Selected Points
P[0] (37.5,42.749,9.657)
P[1] (50.25,47.25,9.657)
Y Axis
C_Cyt
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Size_Cyt
Size_EC
Size_Nuc
vcRegionVolume
Time Plot
Plot Legend:
C_Cyt at P[0]
C_Cyt at P[1]
3.0E-5
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
Your deterministic spatial simulation is now complete.
Plot
ROI

Contents

Next: VCell Tutorial
BioModel with Multiple Applications

Part 2 Compartmental Applications and Parameter Estimation