VCell Tutorial

BioModel with Multiple Applications

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

In 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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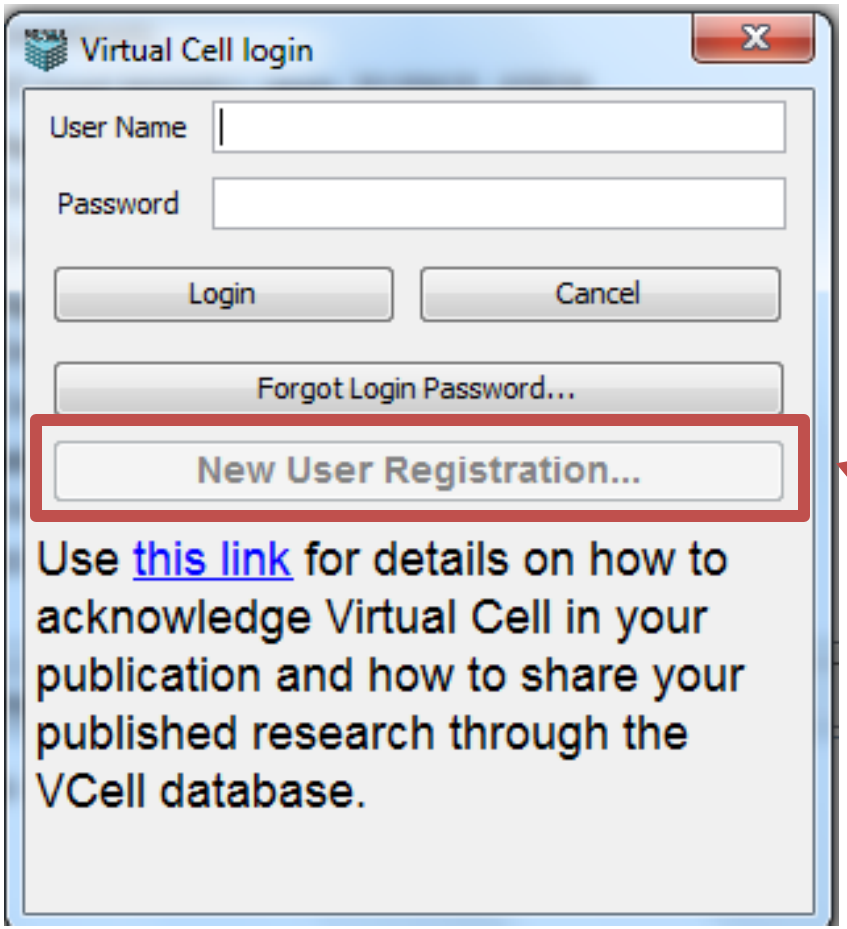
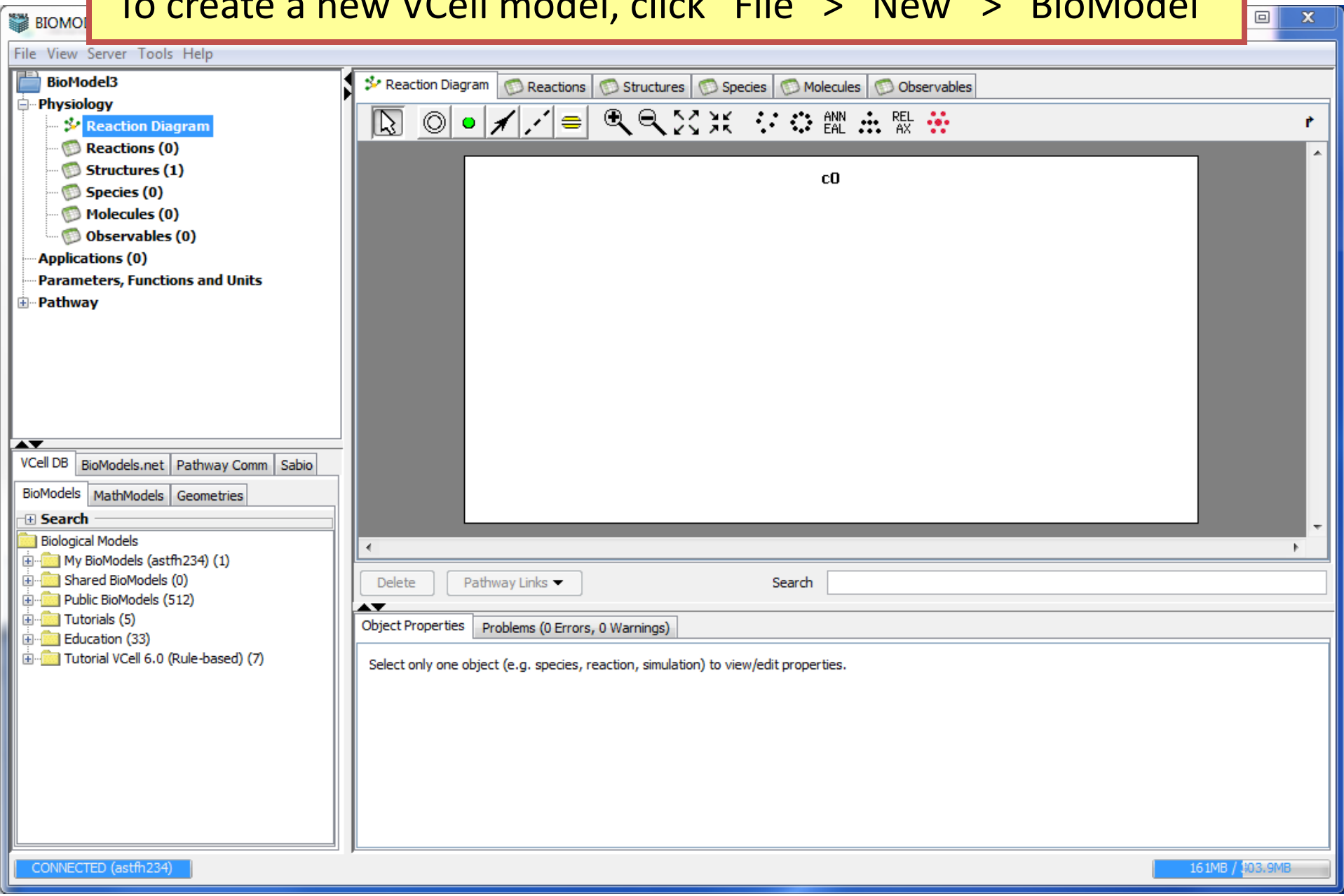
First time opening VCell

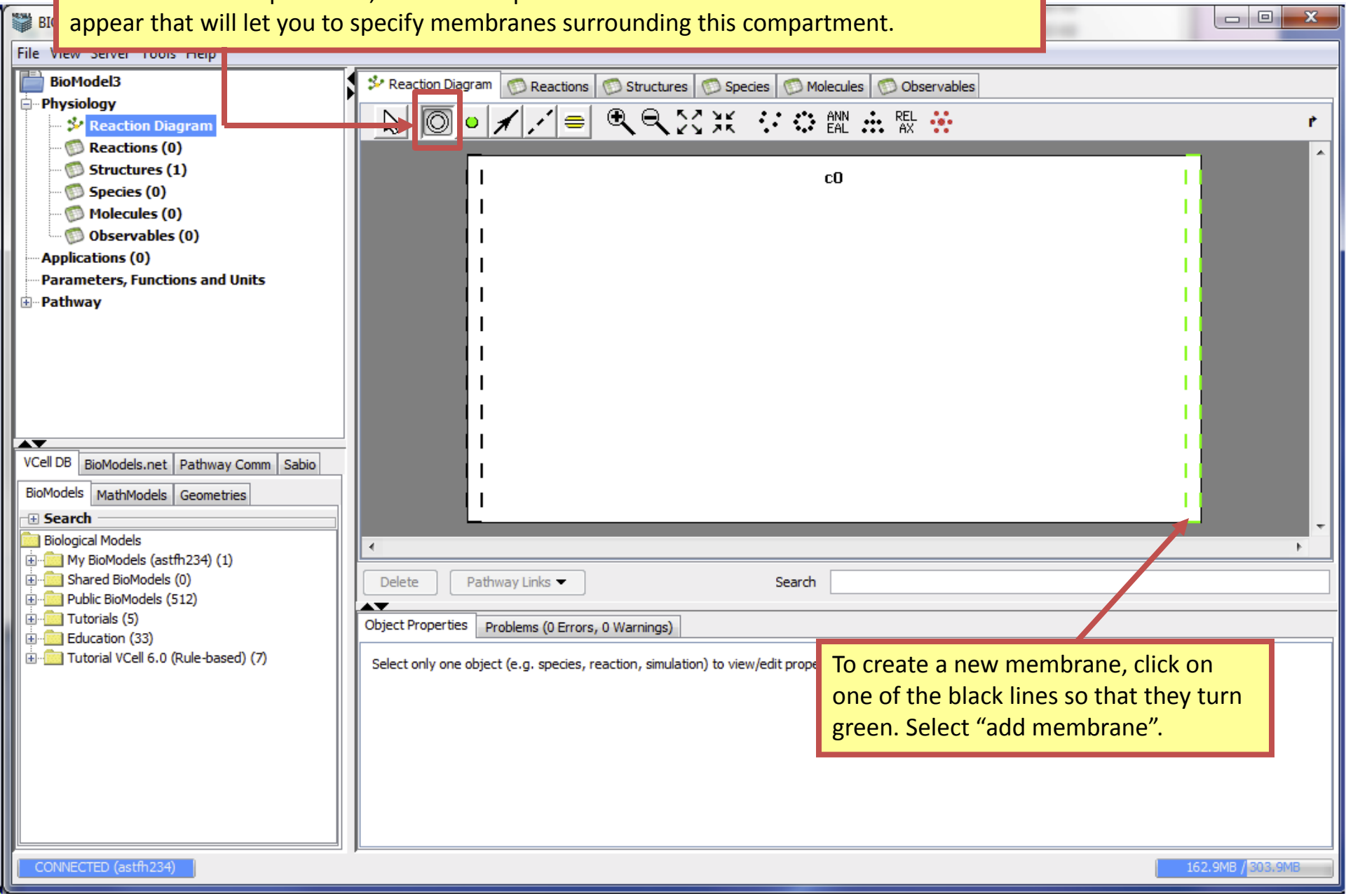


You need to register as a new user if you want to run simulations on VCell compute resources, or use the VCell database to store models that can be shared with collaborators.

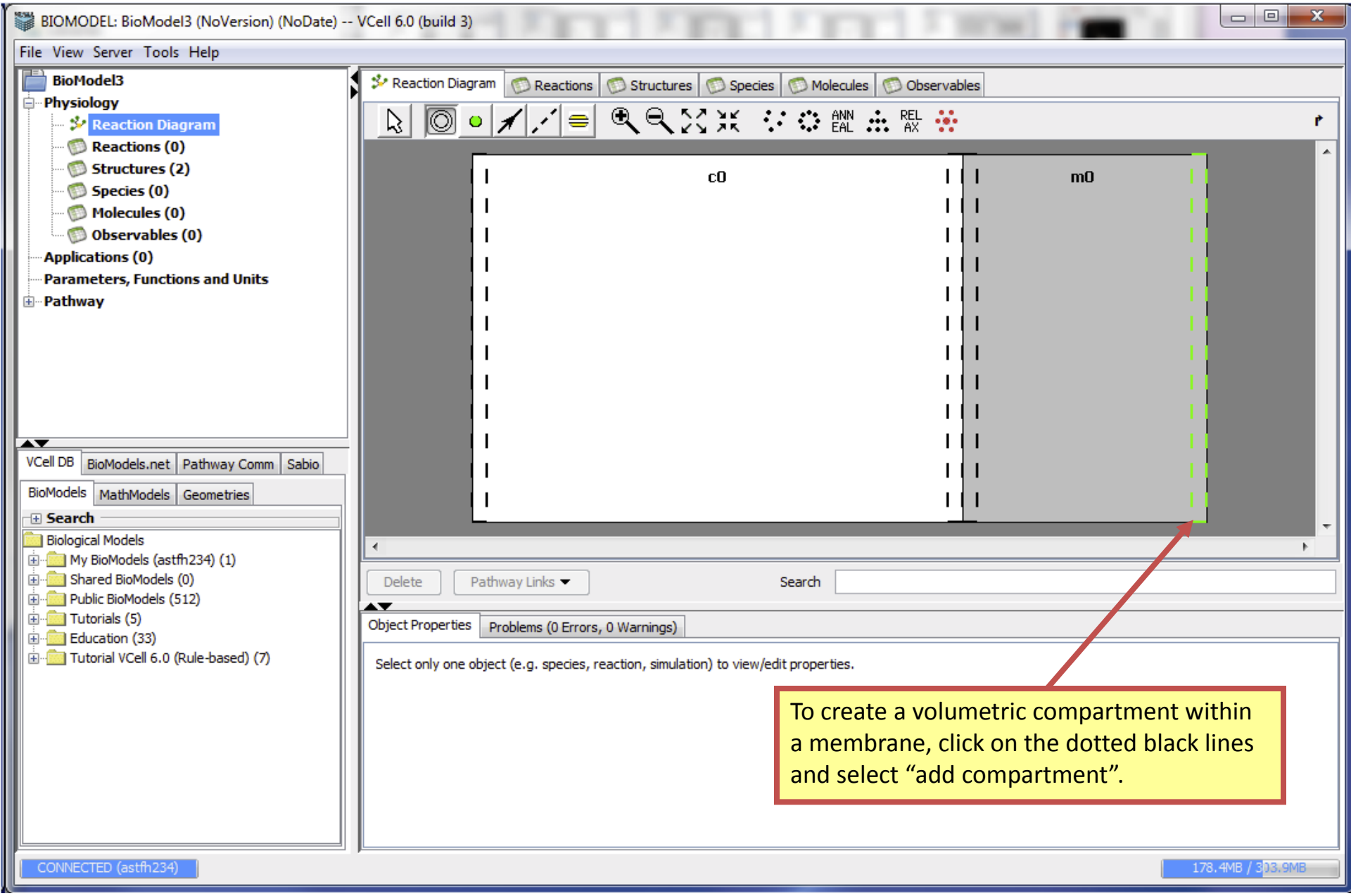
To create a new VCell model, click “File” > “New” > “BioModel”



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



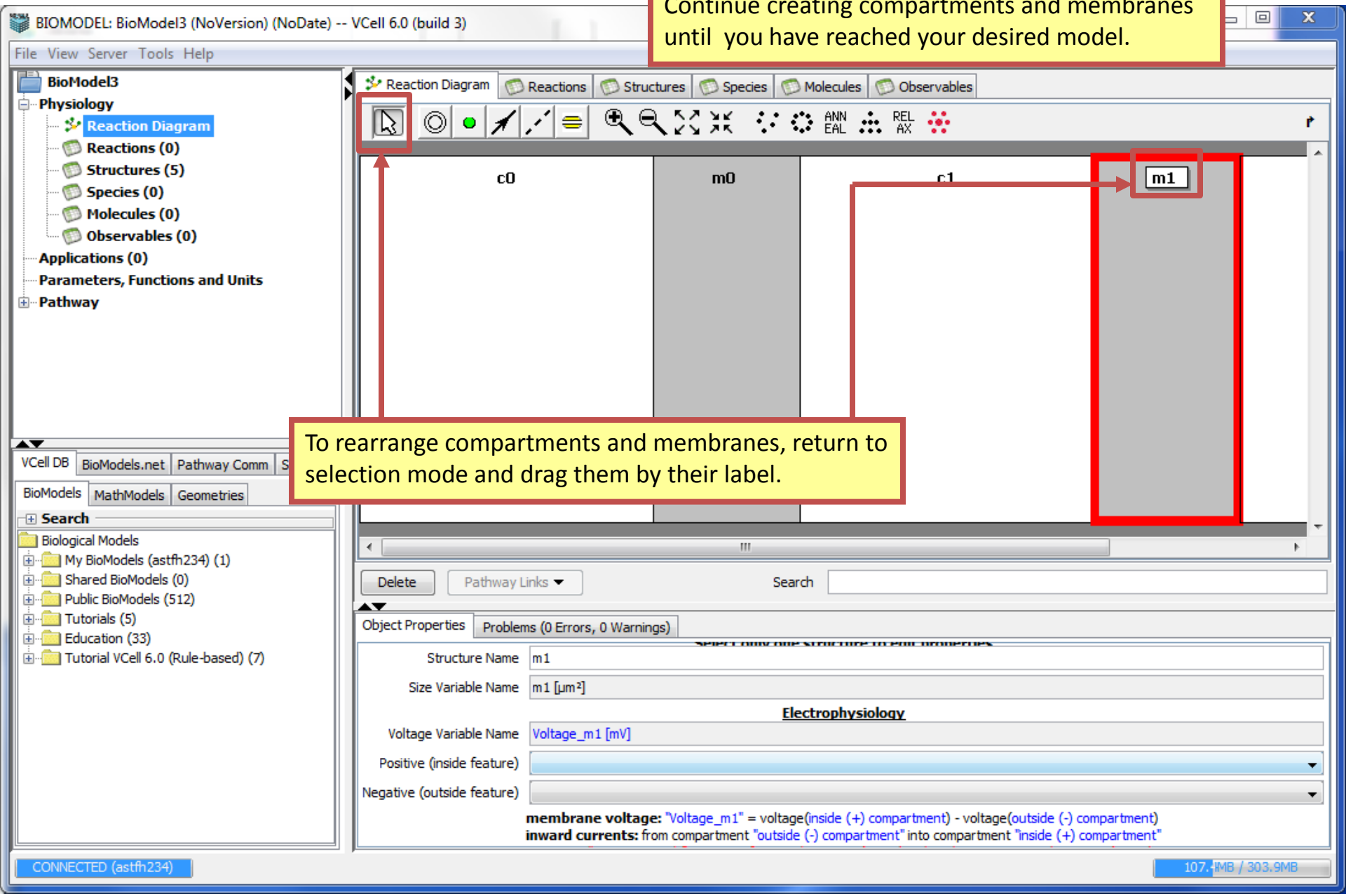
To create a new membrane, click on one of the black lines so that they turn green. Select “add membrane”.

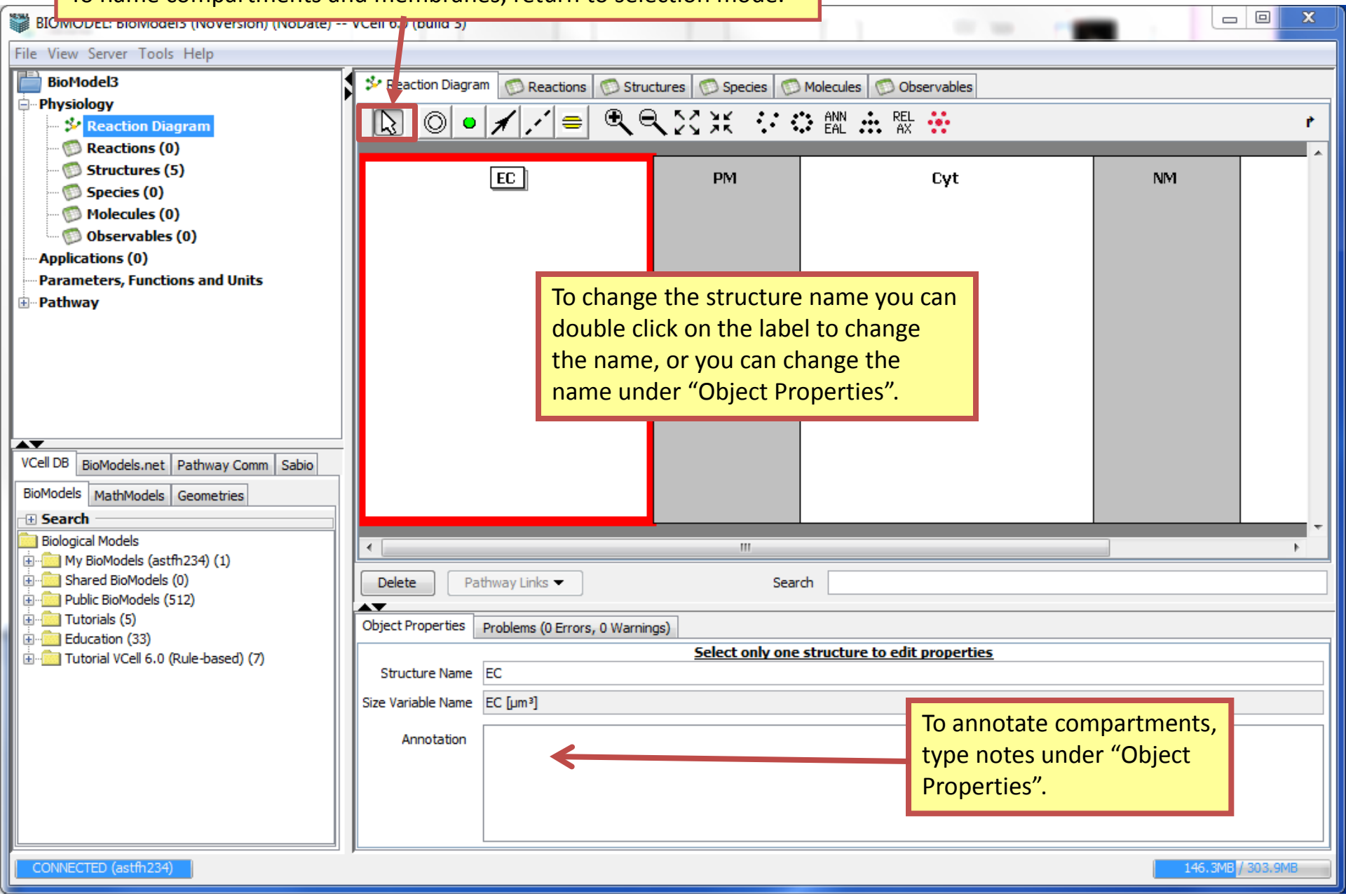


To create a volumetric compartment within a membrane, click on the dotted black lines and select “add compartment”.

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
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Reactions
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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”.
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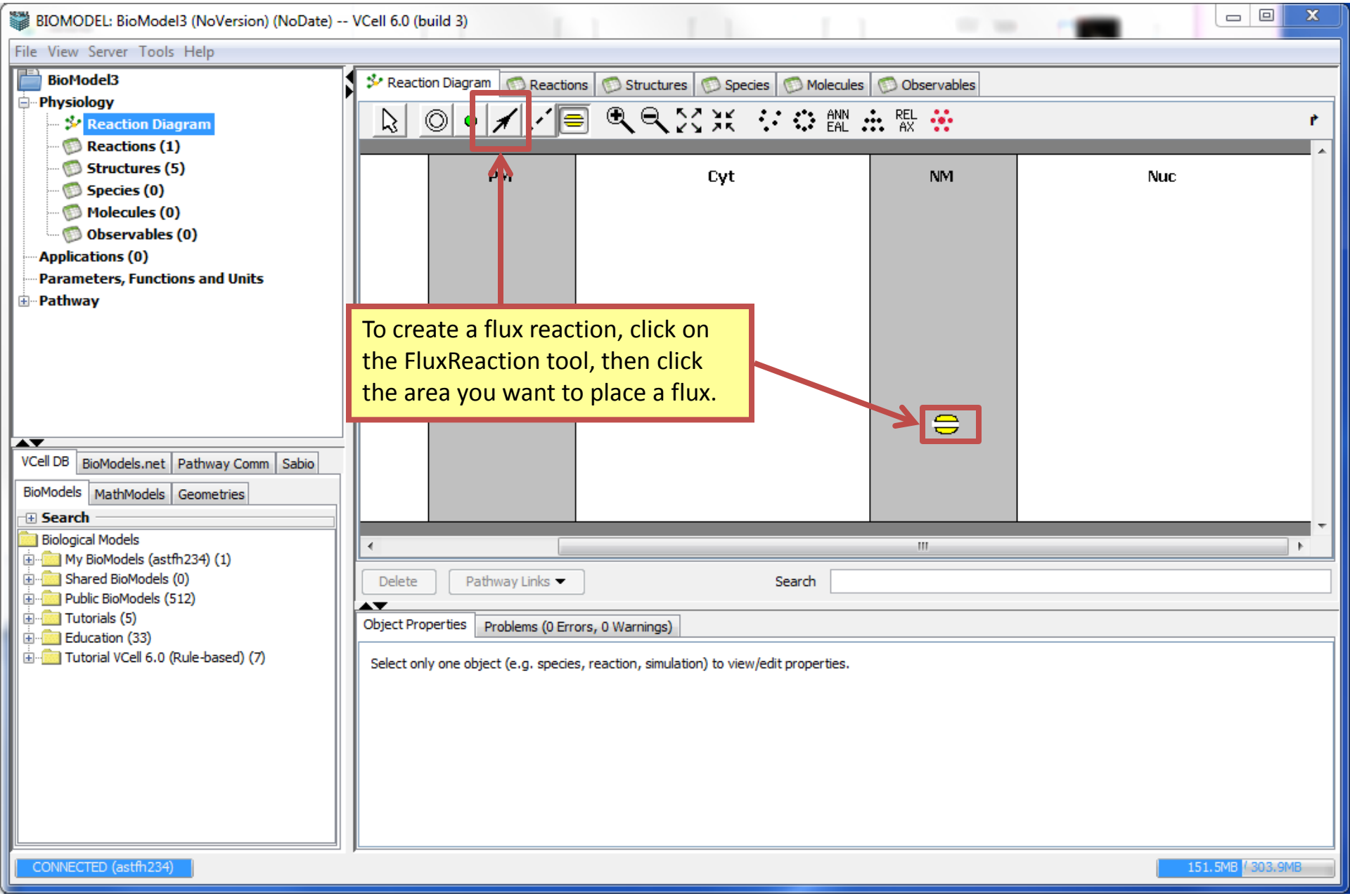
CONNECTED (astfh234)
146.3MB / 303.9MB


BIOMODEL: BioModel3 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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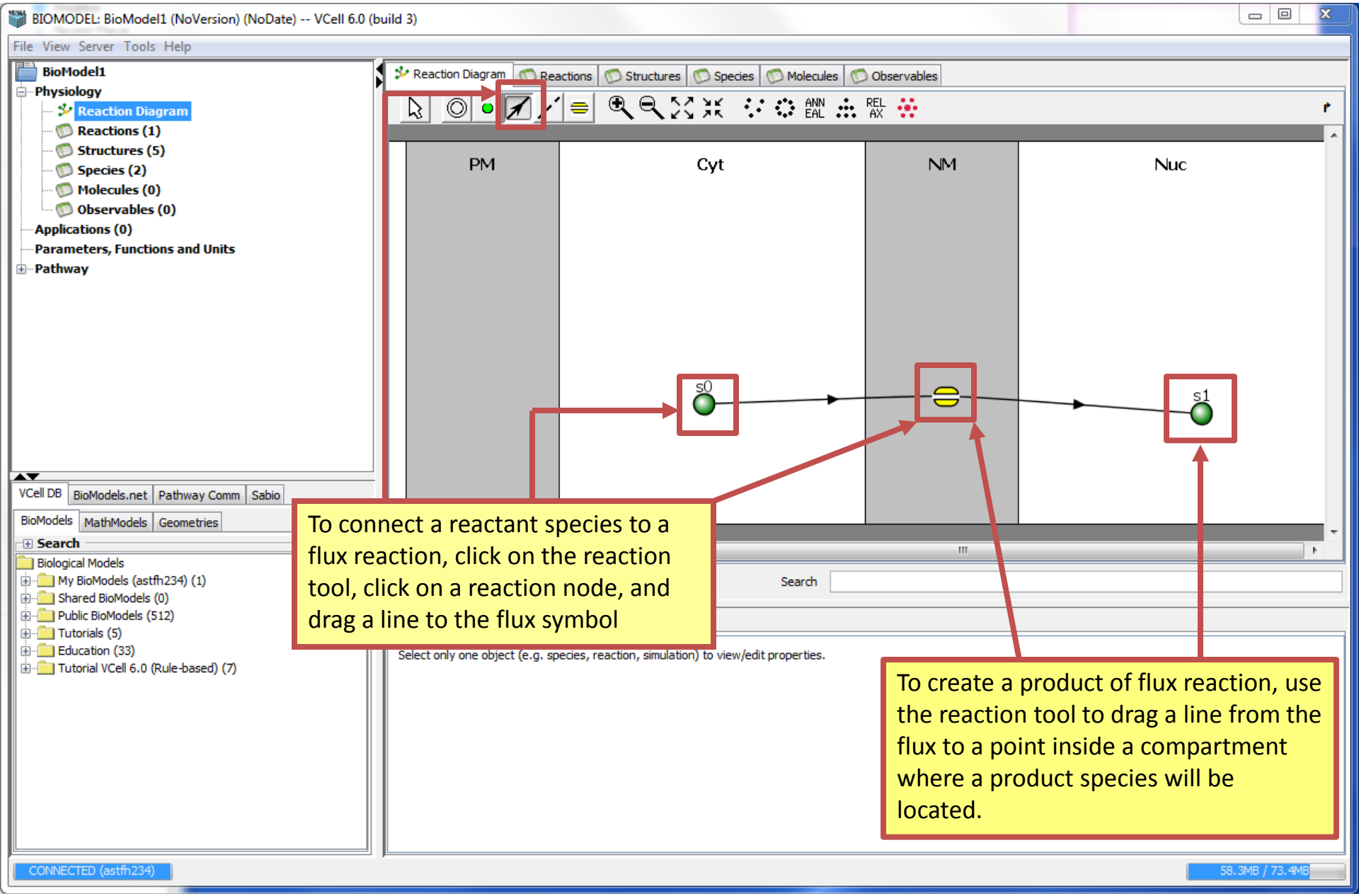
To create a flux reaction, click on the FluxReaction tool, then click the area you want to place a flux.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
151.5MB
303.9MB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Cyt
NM
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

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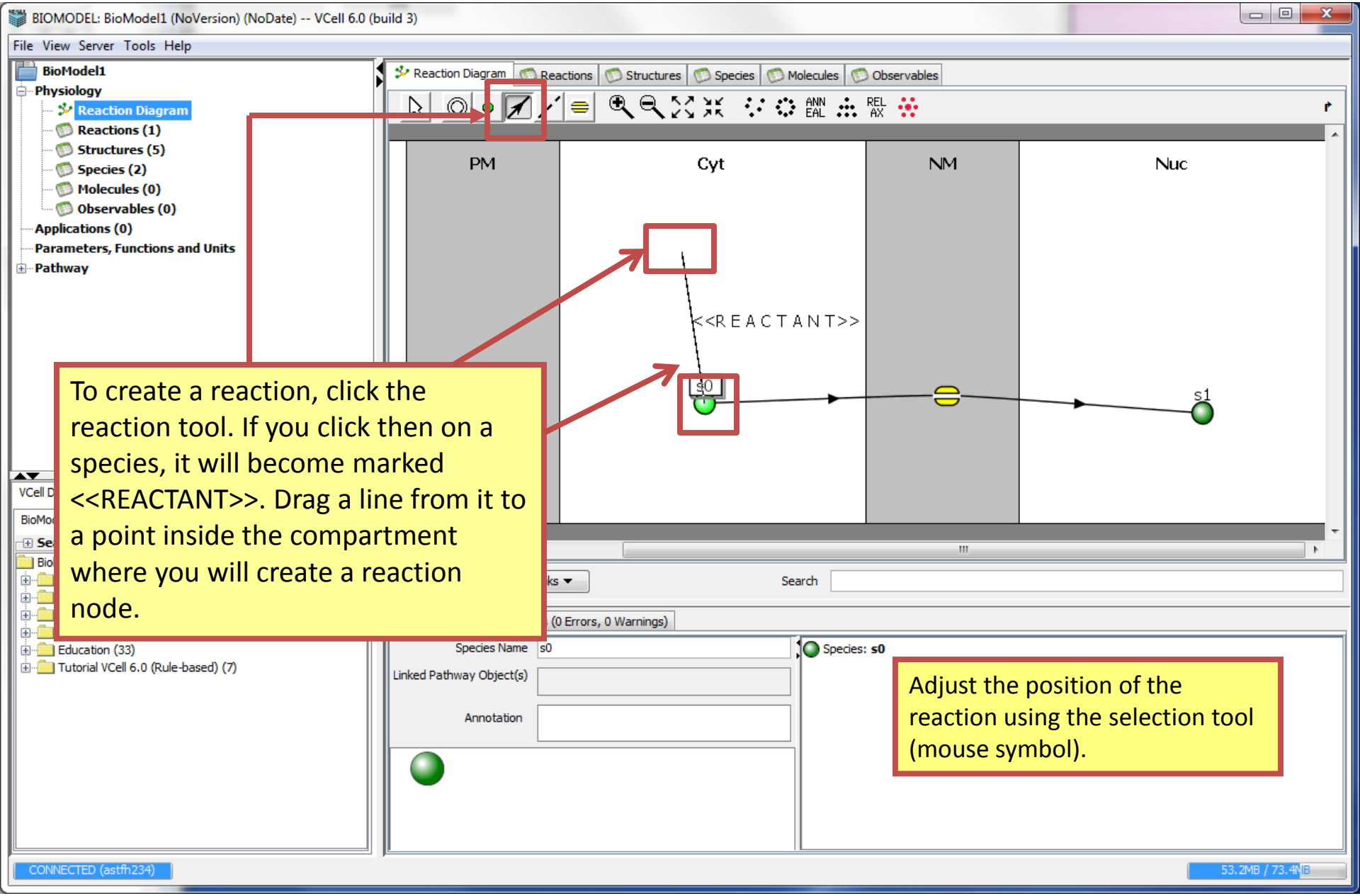
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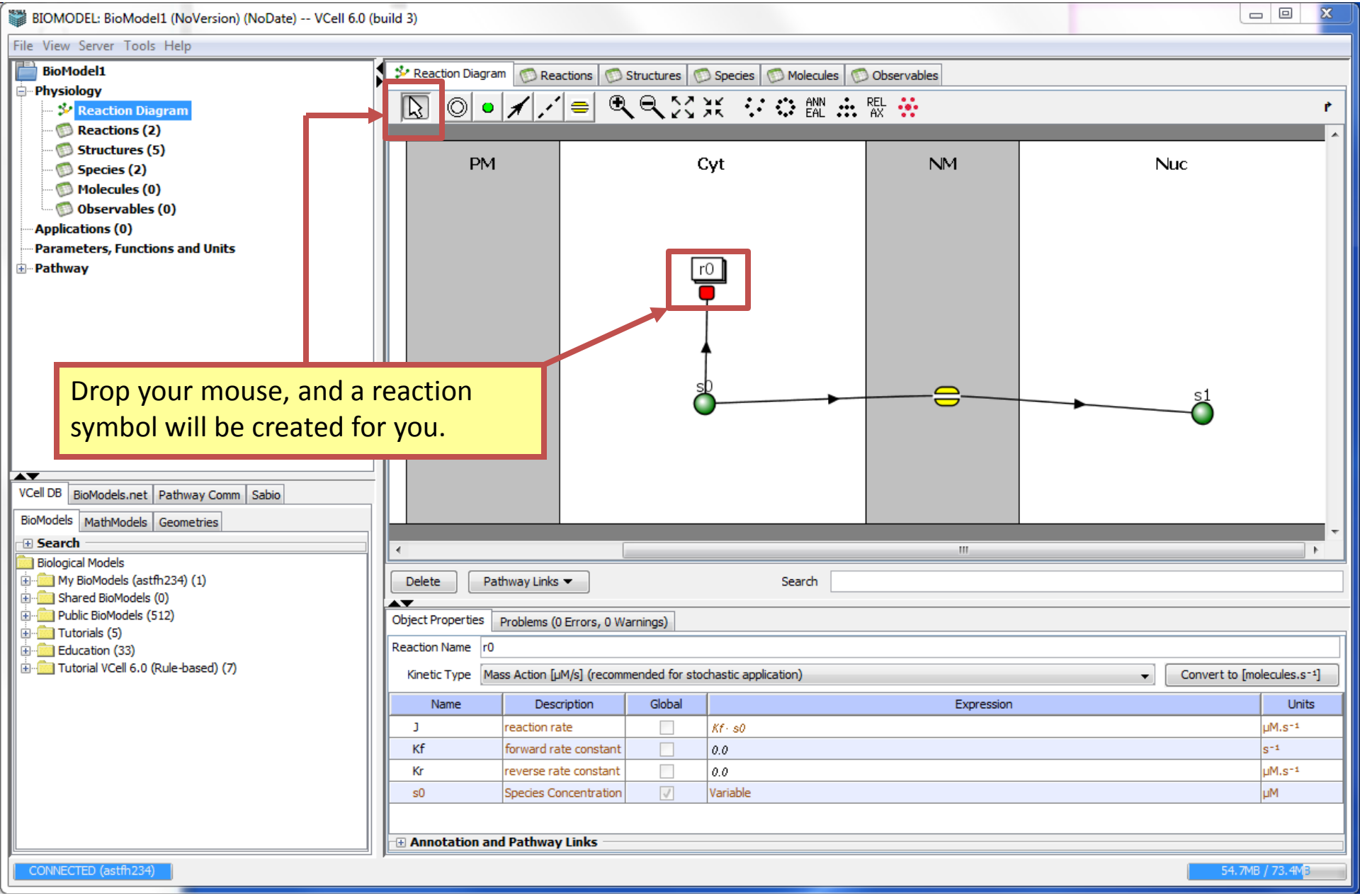
<<REACTANT>>
s0
s1
To create a reaction, click the reaction tool. If you click then on a species, it will become marked <<REACTANT>>. Drag a line from it to a point inside the compartment where you will create a reaction node.
Search
(0 Errors, 0 Warnings)
Species Name
s0
Linked Pathway Object(s)
Annotation
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)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s0
s1
Drop your mouse, and a reaction symbol will be created for you.
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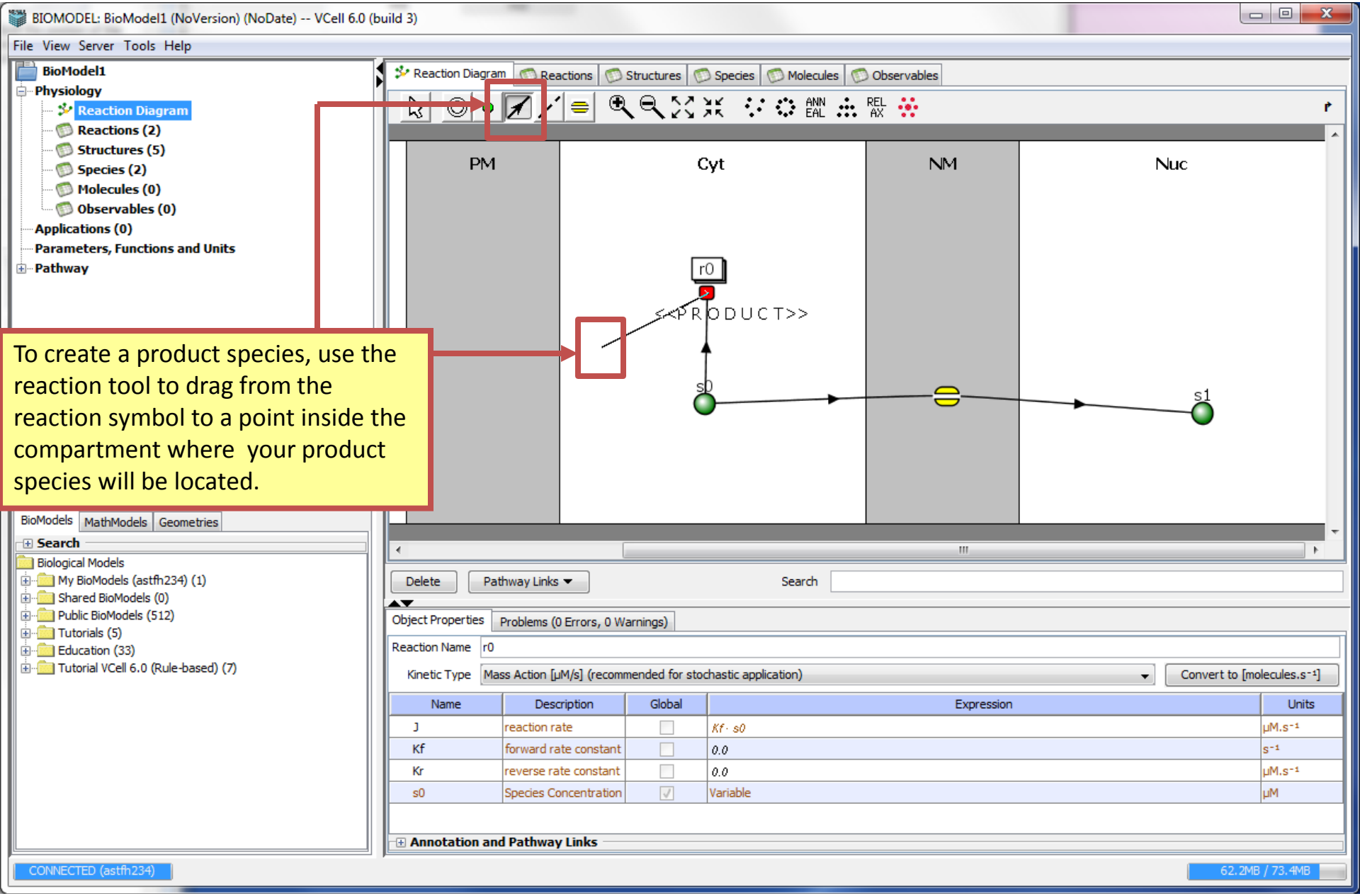
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Reaction Name
r0
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kf· s0
μM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹
Kr
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)
Applications (0)
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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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Pathway Links
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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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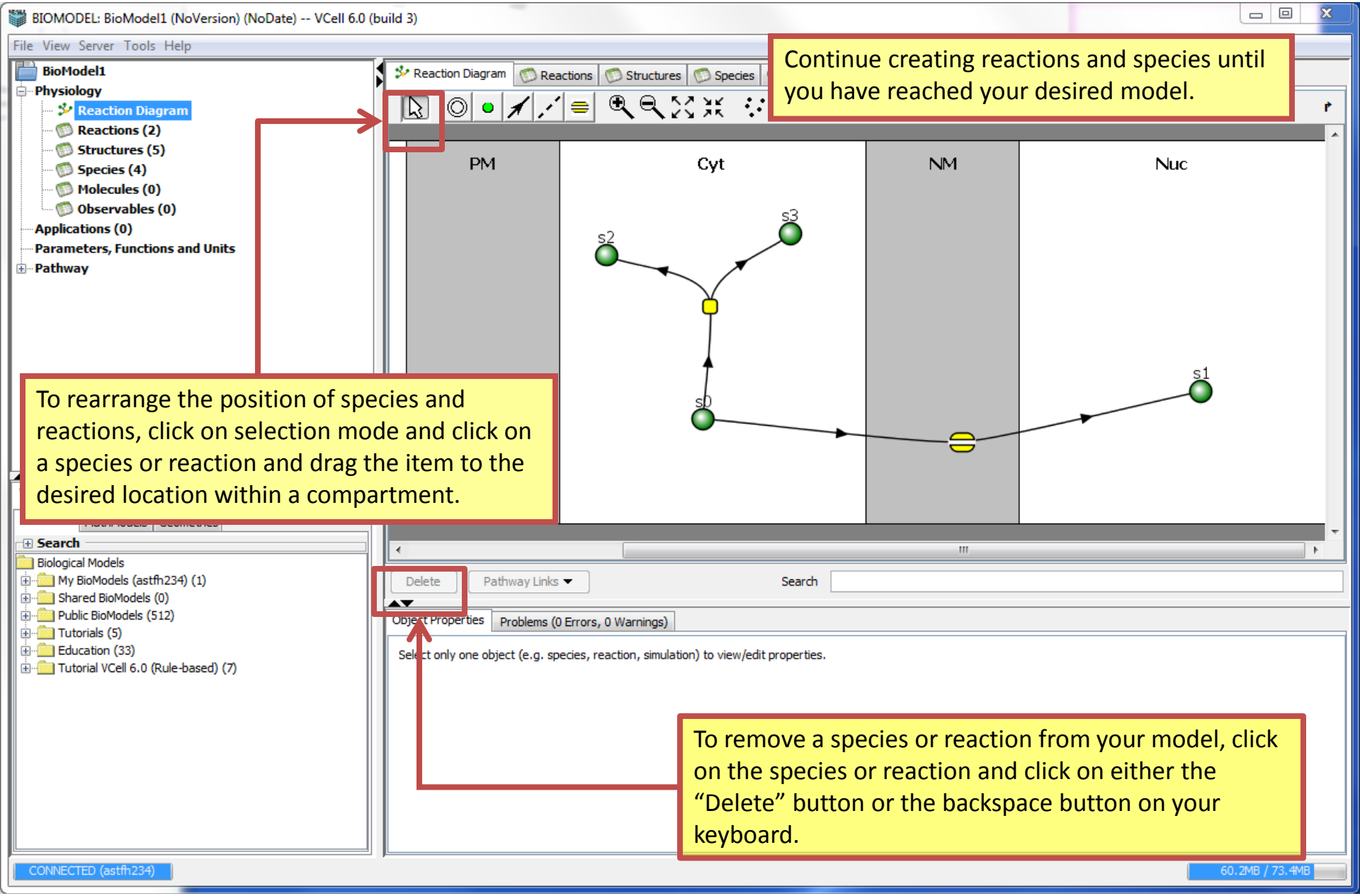
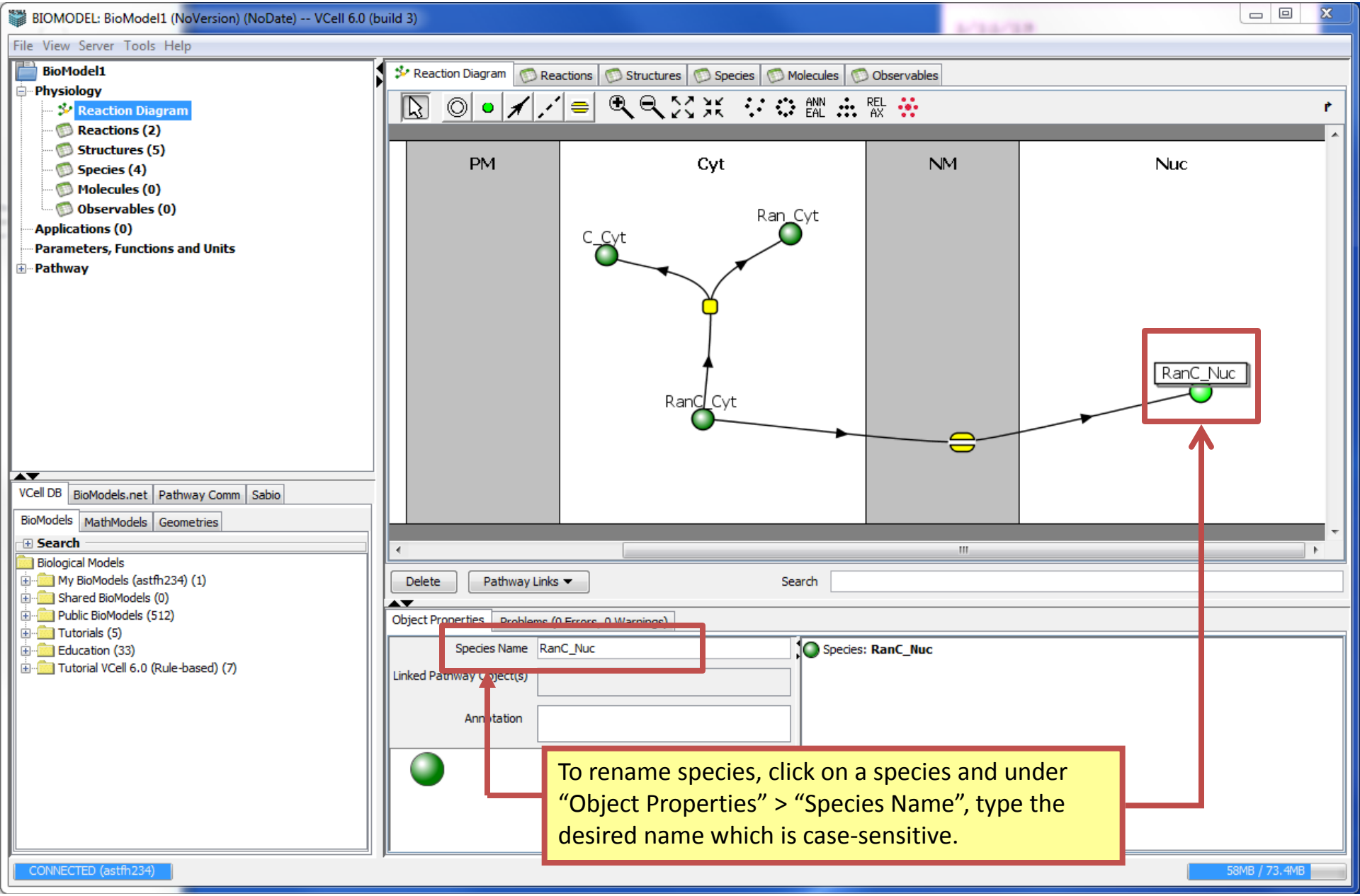


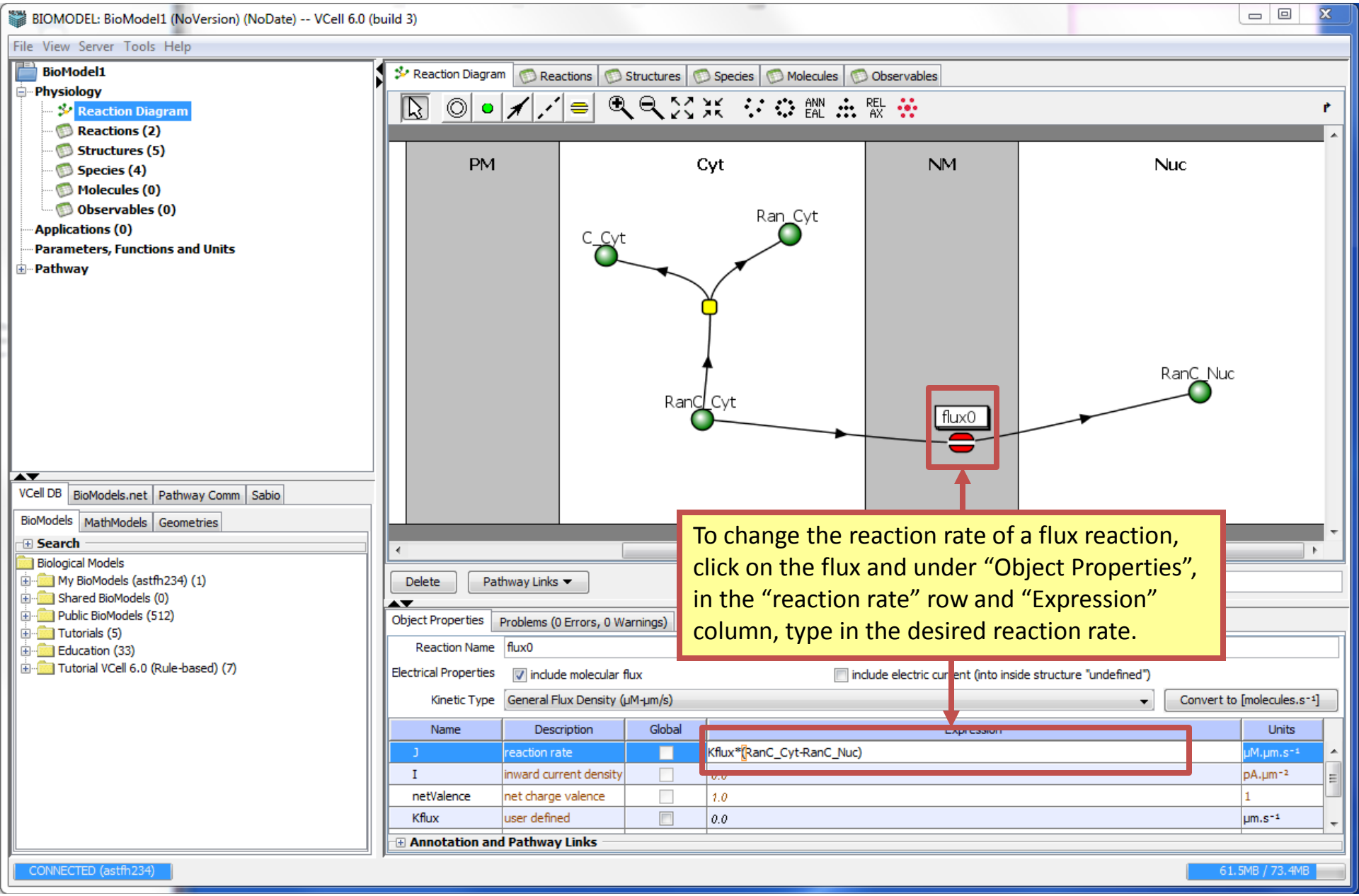
Continue creating reactions and species until you have reached your desired model.

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.

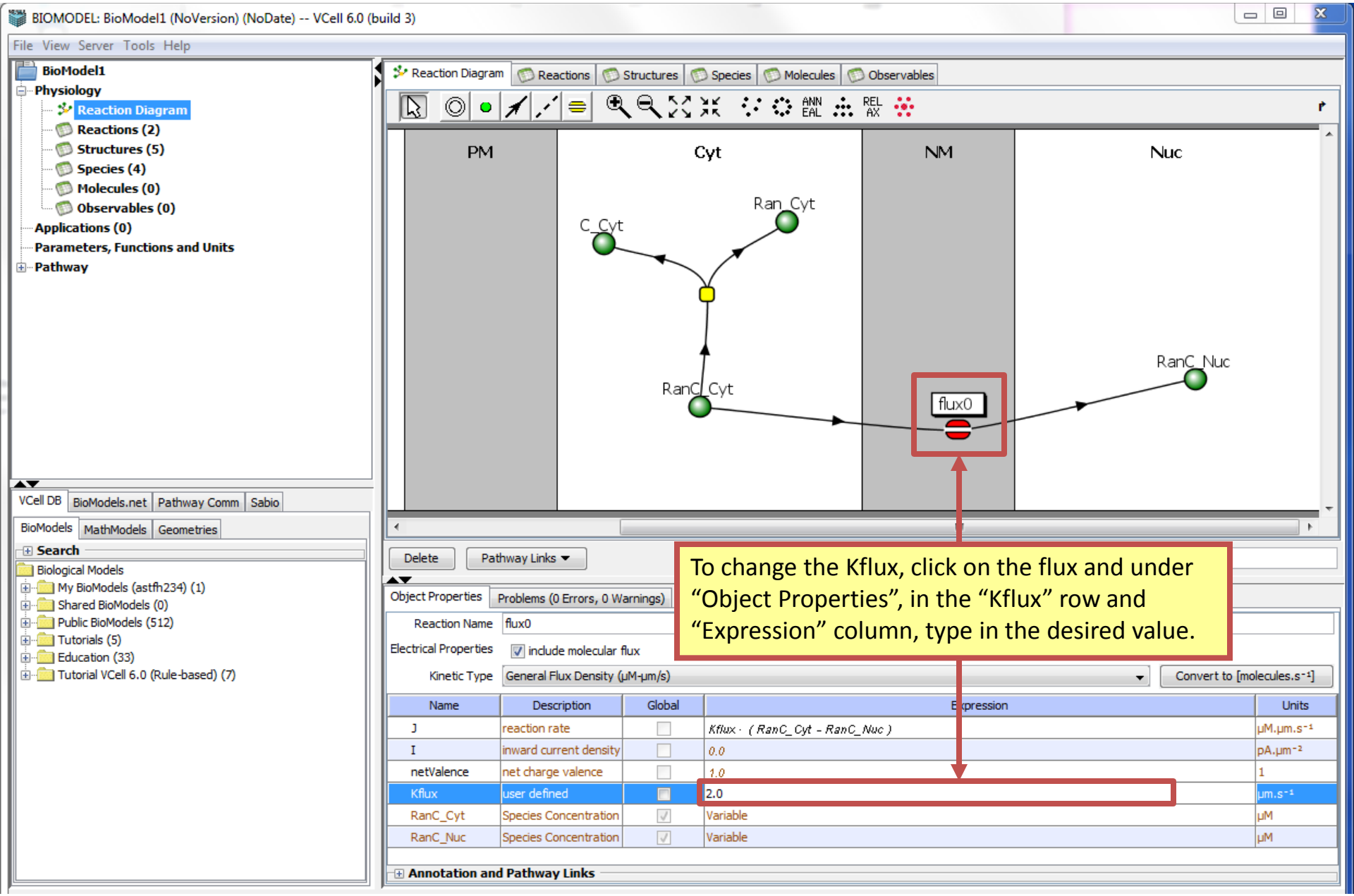
To remove a species or reaction from your model, click on the species or reaction and click on either the “Delete” button or the backspace button on your keyboard.



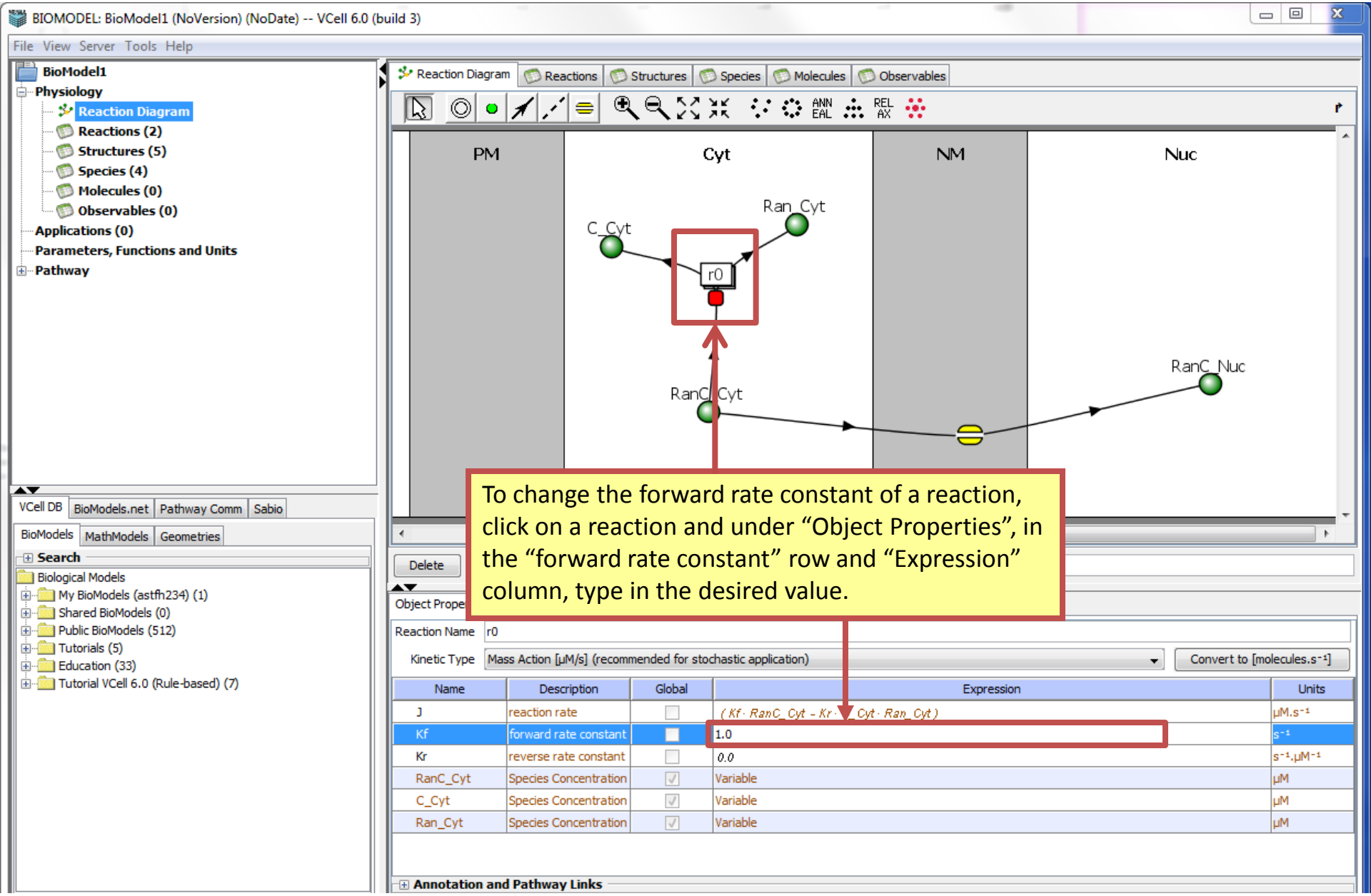
To rename species, click on a species and under “Object Properties” > “Species Name”, type the desired name which is case-sensitive.



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.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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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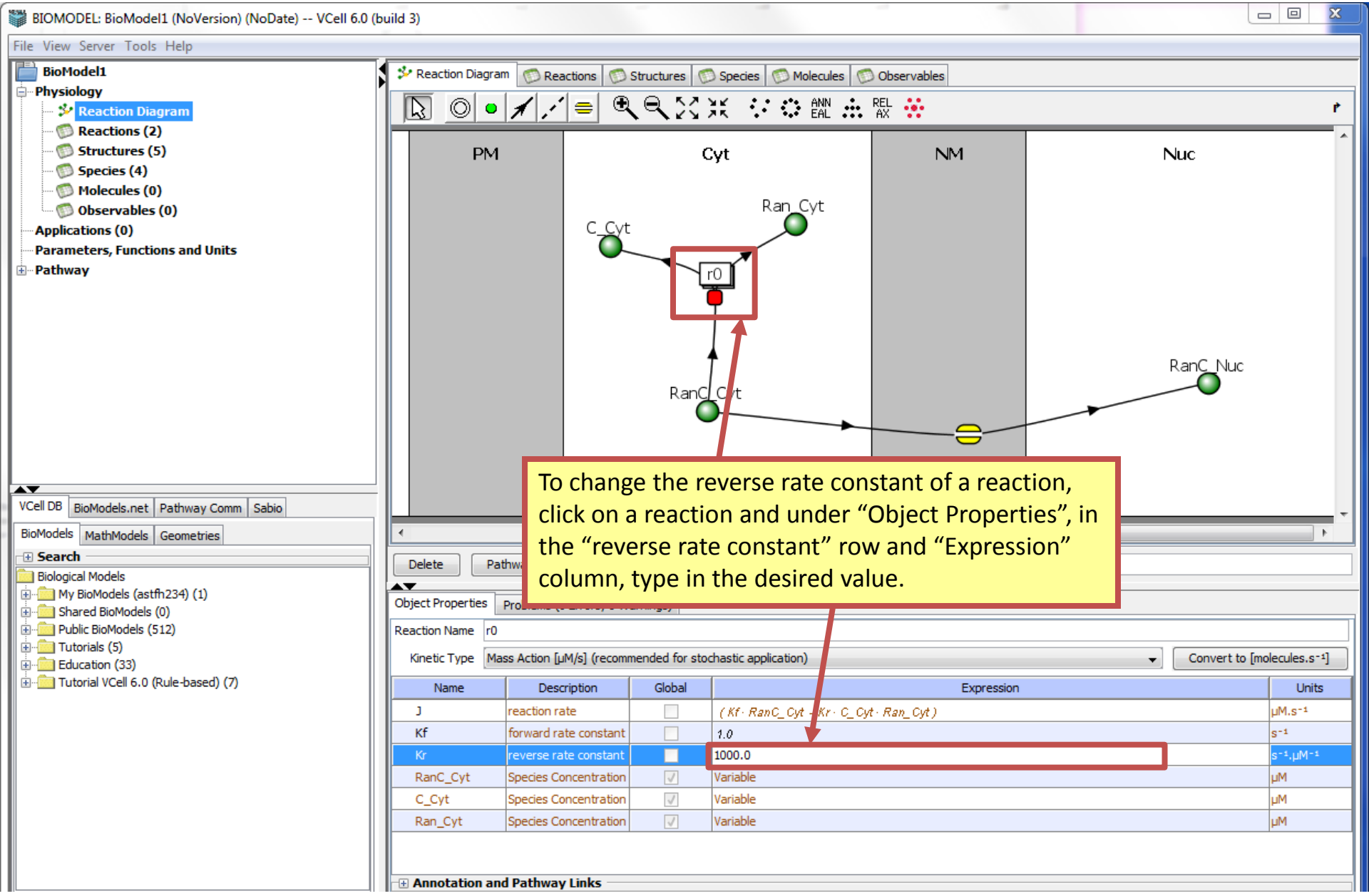
Reaction Name
r0
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
(Kf · RanC_Cyt - Kr · C_Cyt · Ran_Cyt)
μM.s-1
Kf
forward rate constant
1.0
s-1
Kr
reverse rate constant
0.0
s-1.μM-1
RanC_Cyt
Species 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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Structures
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.
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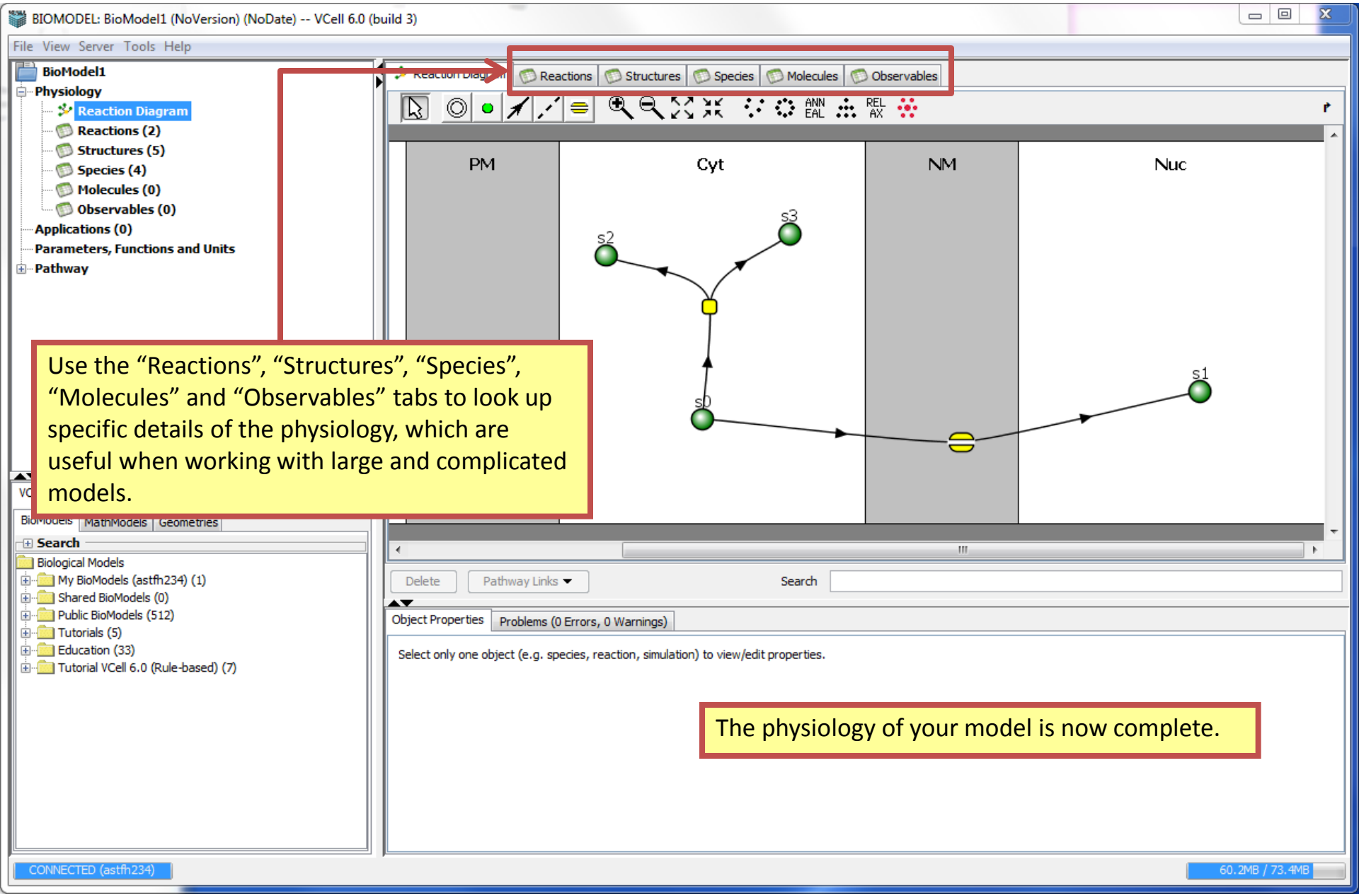
Delete
Object Properties
Reaction Name r0
Kinetic Type Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Name Description Global Expression Units
J reaction rate (Kf · RanC_Cyt - Kr · C_Cyt · Ran_Cyt) μM.s-1
Kf forward rate constant 1.0 s-1
Kr reverse rate constant 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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Nuc
s0
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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
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Public BioModels (512)
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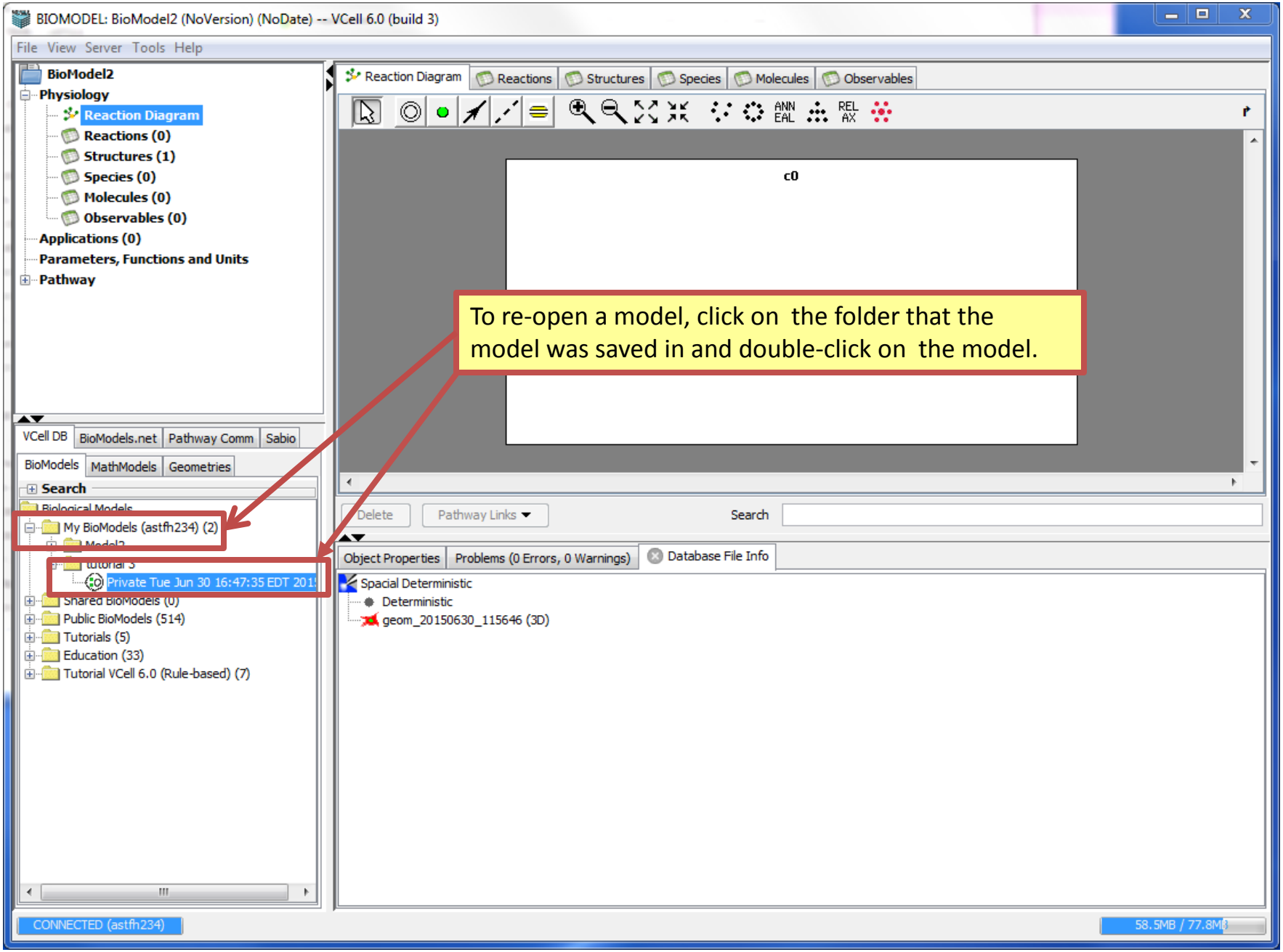
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
The physiology of your model is now complete.
CONNECTED (astfh234)
60.2MB / 73.4MB


BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
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Structures (1)
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Molecules (0)
Observables (0)
Applications (0)
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Reaction Diagram
Reactions
Structures
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Molecules
Observables
c0
To re-open a model, click on the folder that the model was saved in and double-click on the model.
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Private Tue Jun 30 16:47:35 EDT 201
Shared BioModels (0)
Public BioModels (514)
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Delete
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Search
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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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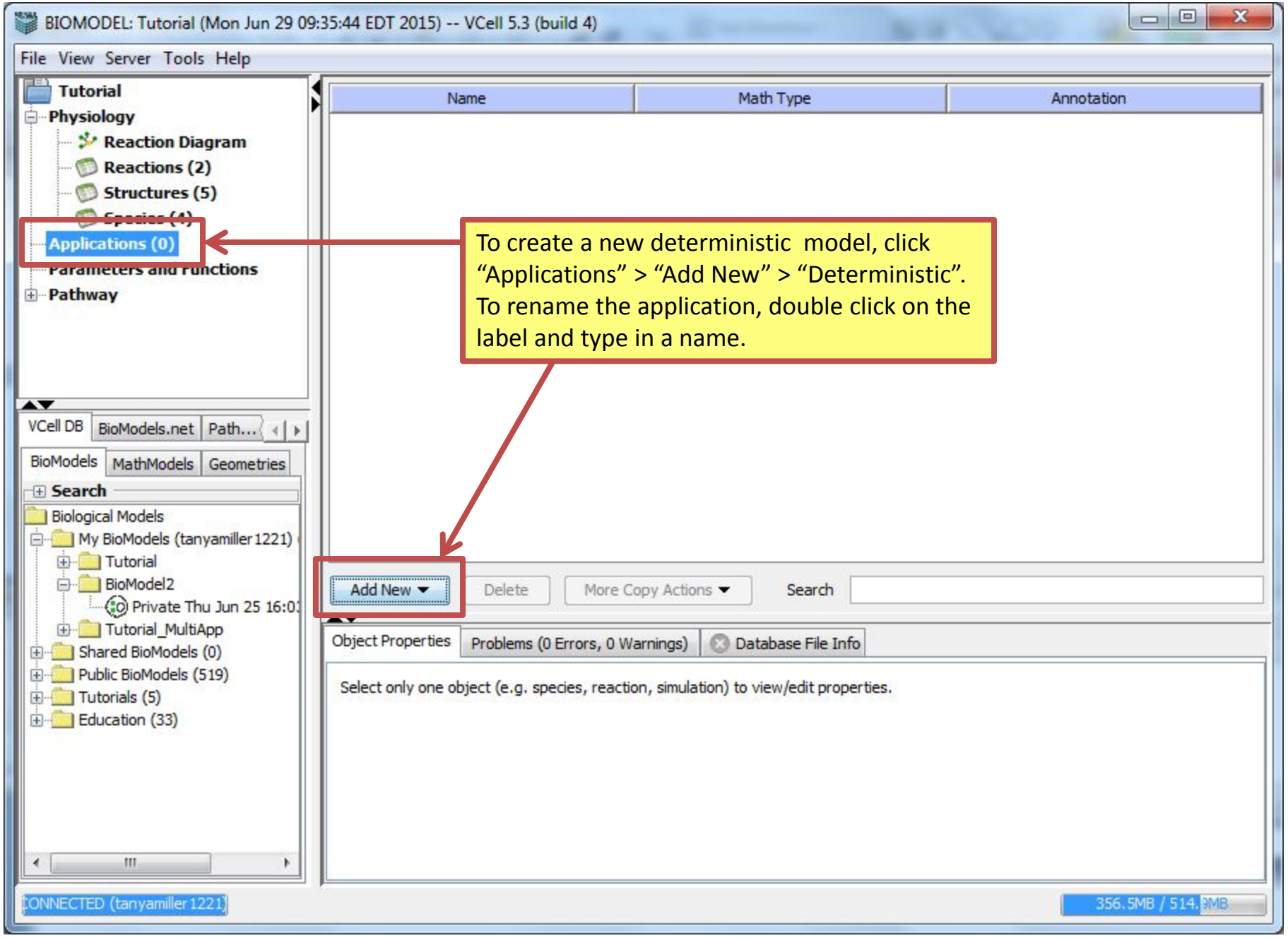
BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
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Applications (0)
Pathway
Name
Math Type
Annotation
To create a new deterministic model, click "Applications" > "Add New" > "Deterministic". To rename the application, double click on the label and type in a name.
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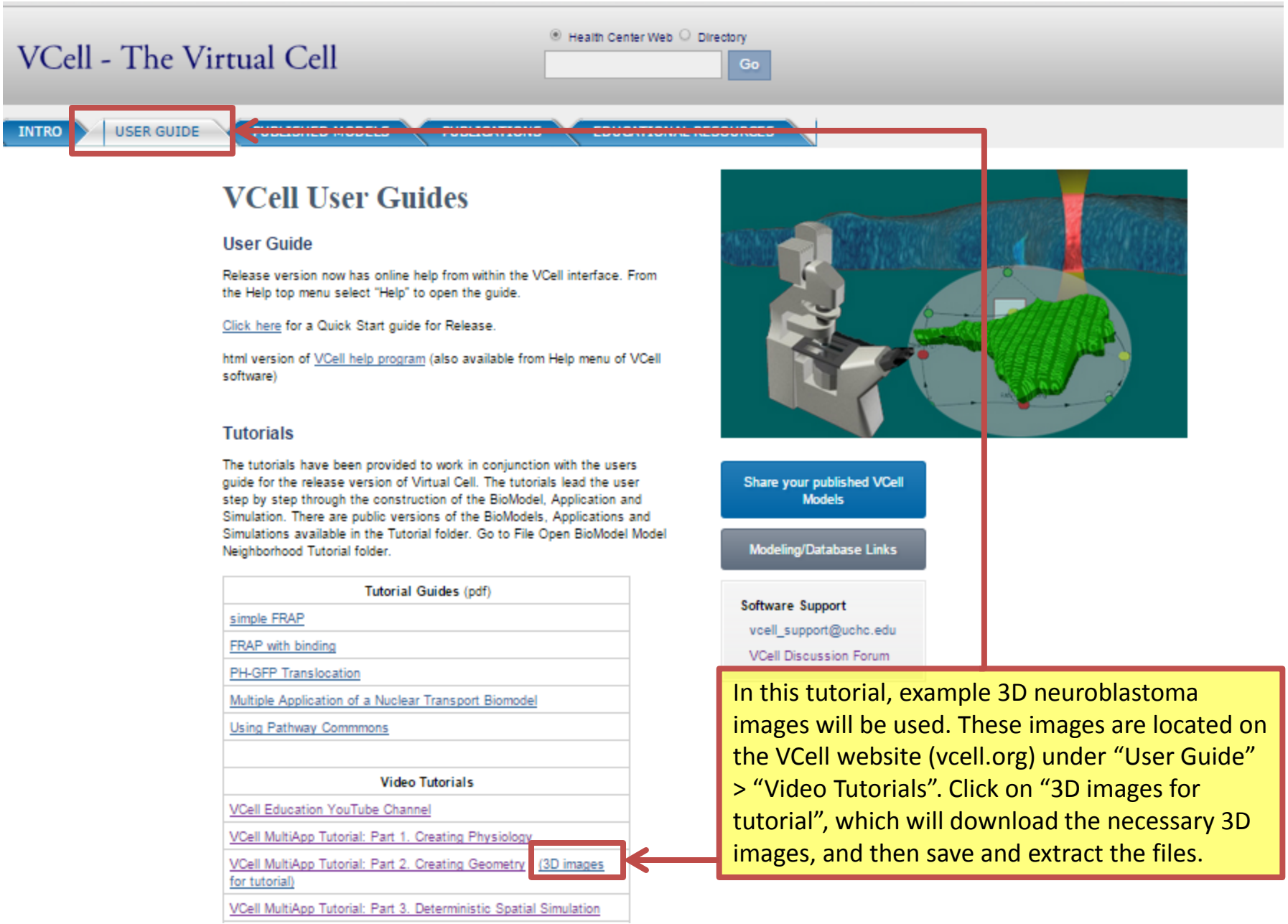
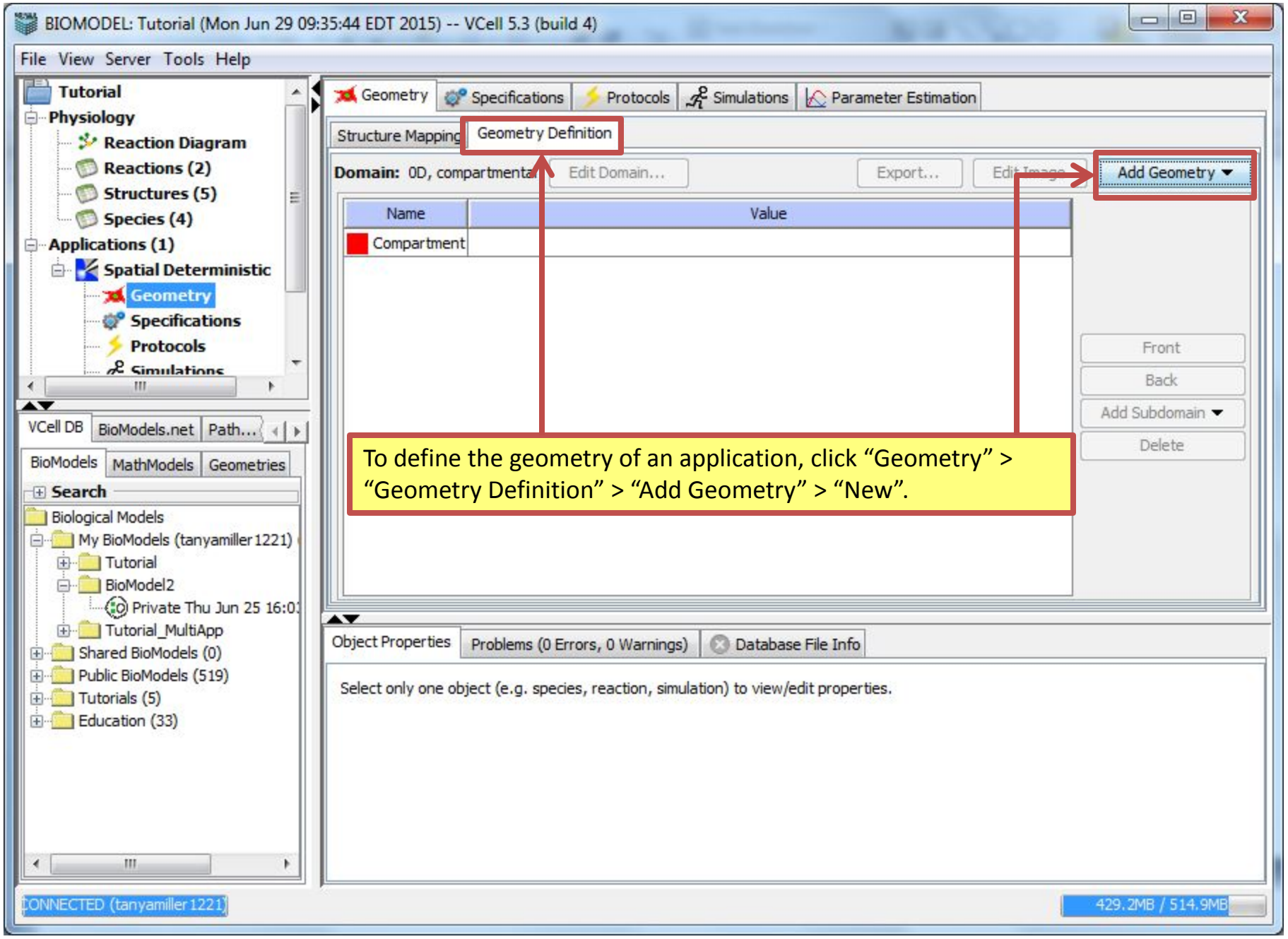
Add New
Delete
More Copy Actions
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
356.5MB / 514.3MB



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)
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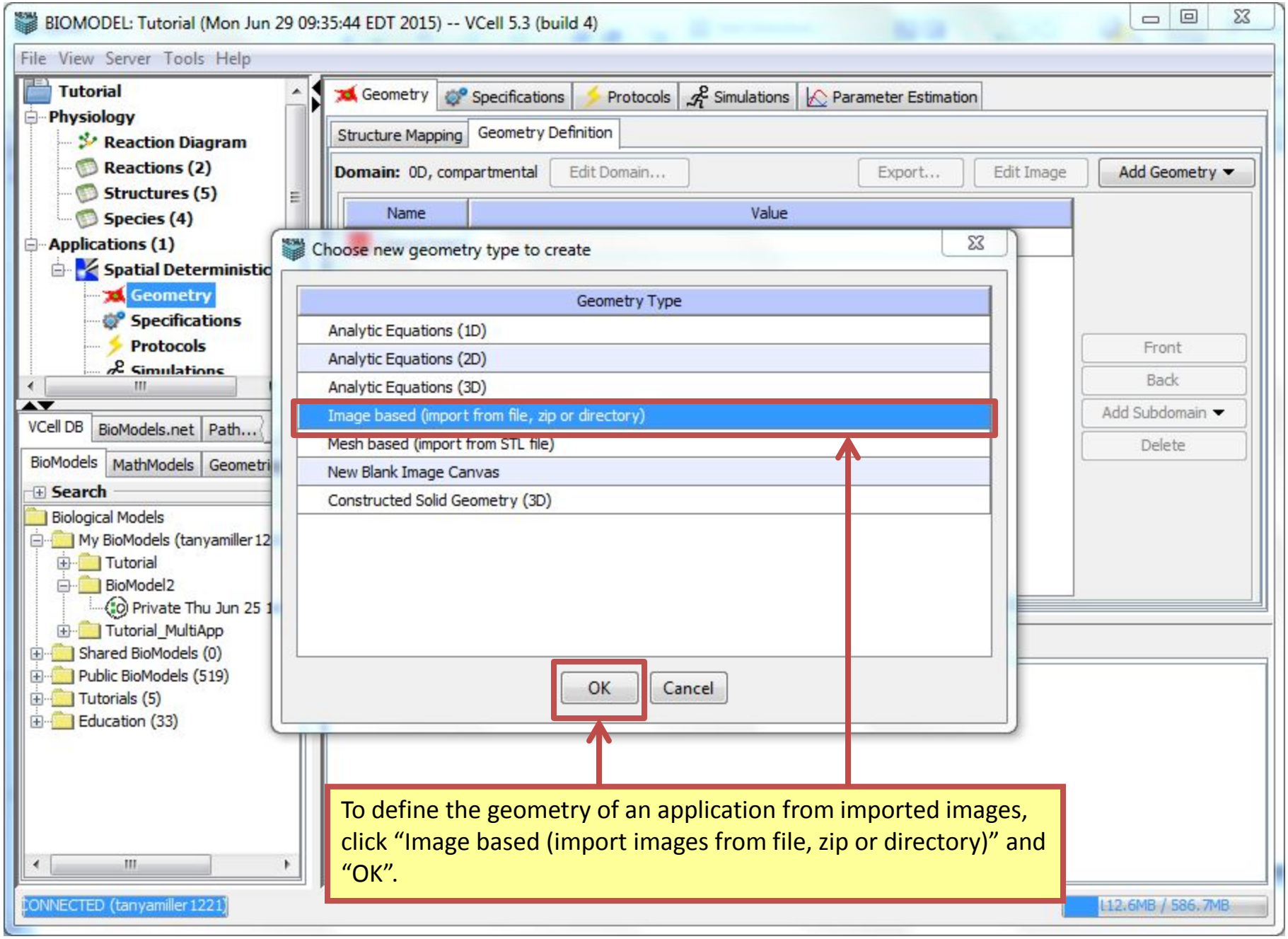
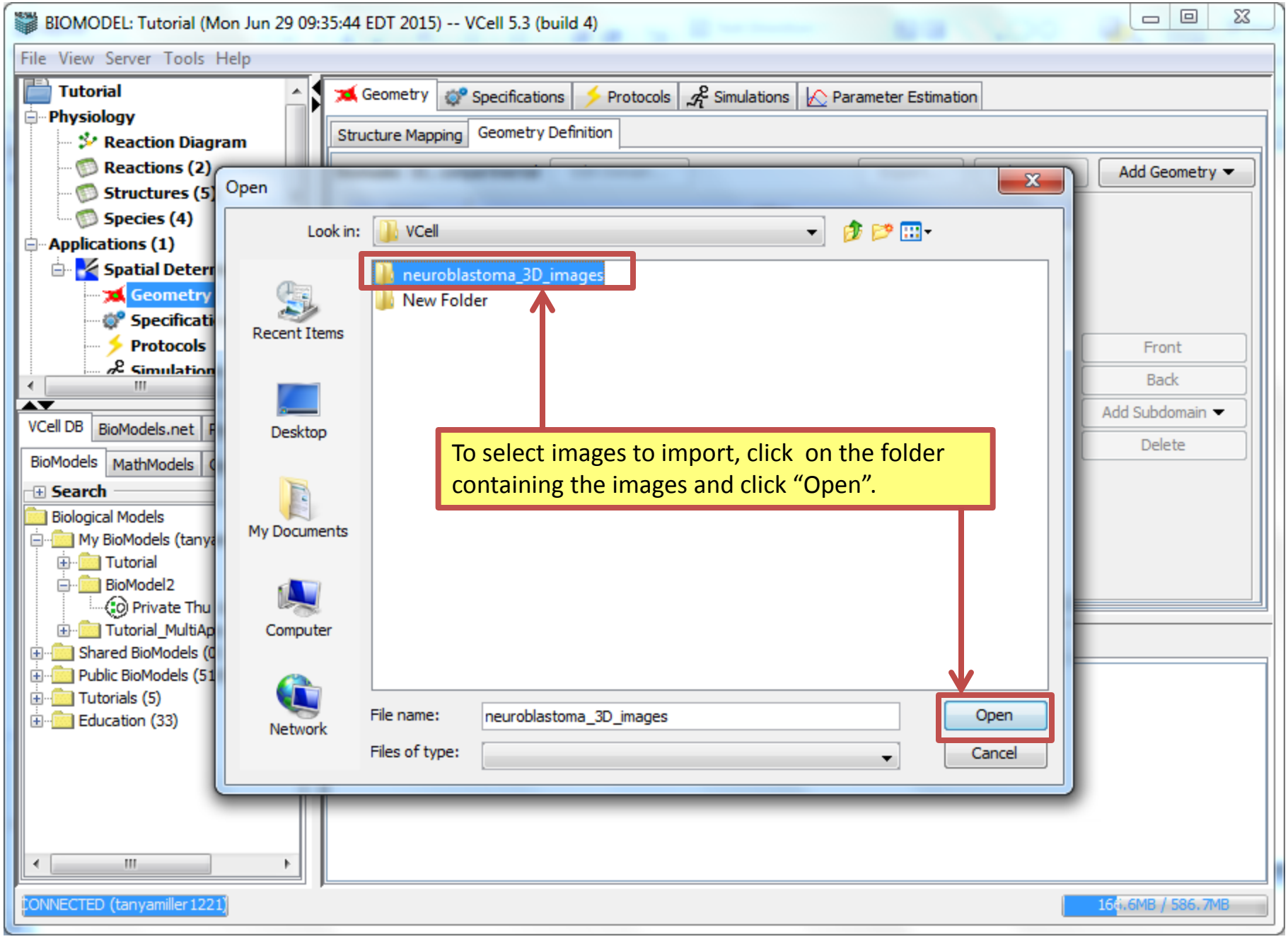
Parameter Estimation
Structure Mapping
Geometry Definition
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image...
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
To define the geometry of an application, click “Geometry” > “Geometry Definition” > “Add Geometry” > “New”.
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

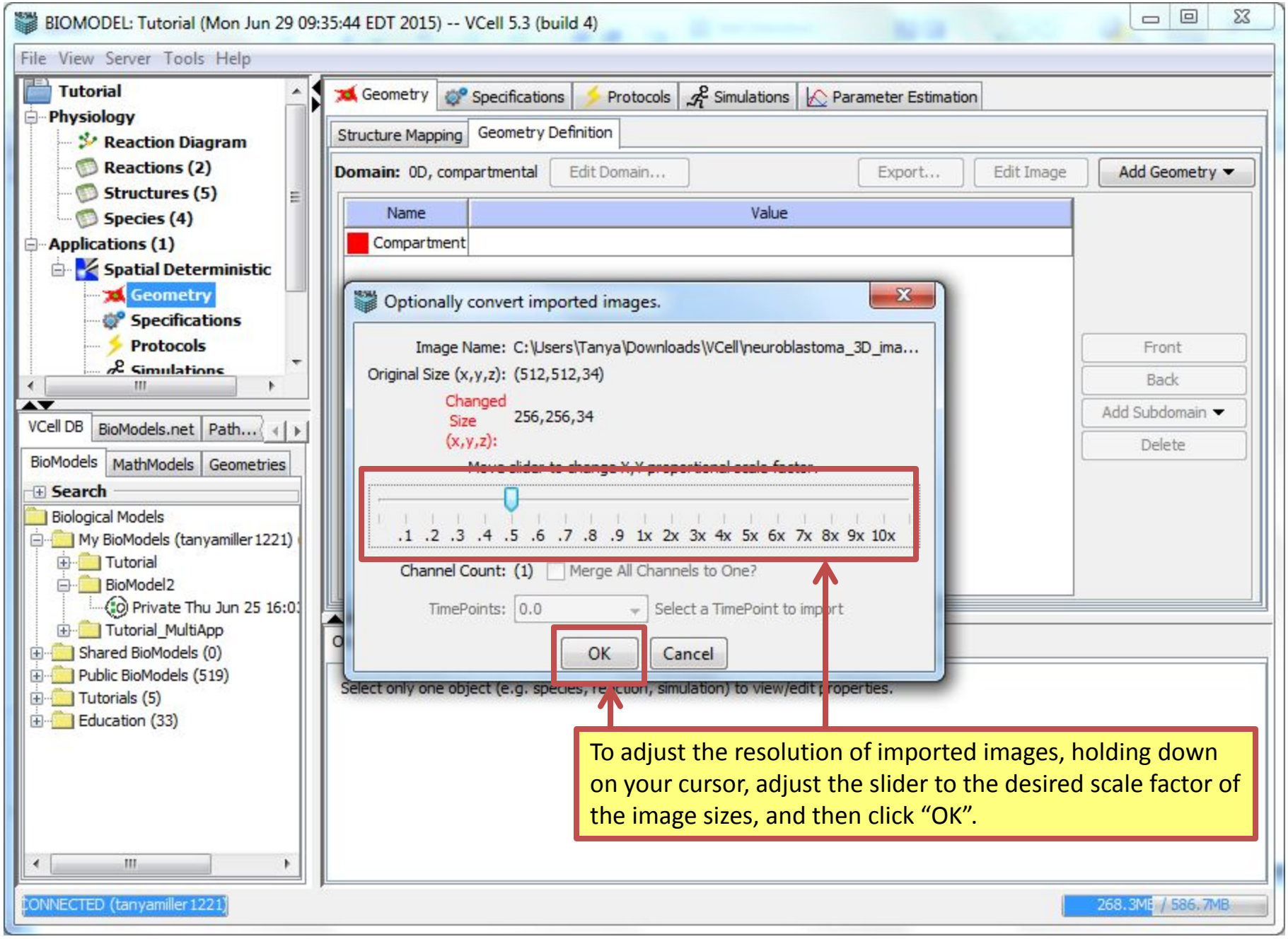
Contents



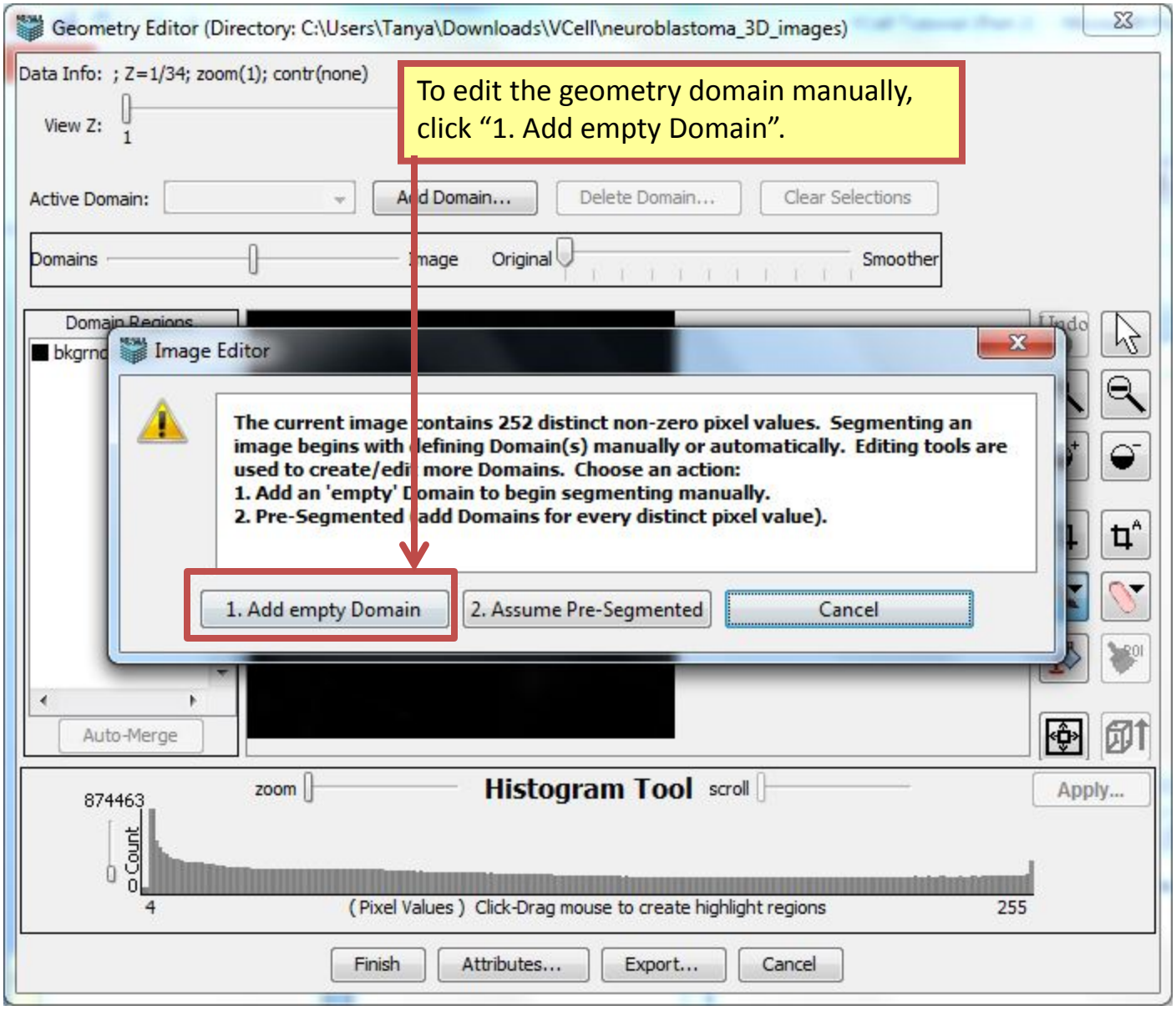
To define the geometry of an application from imported images, click “Image based (import images from file, zip or directory)” and “OK”.

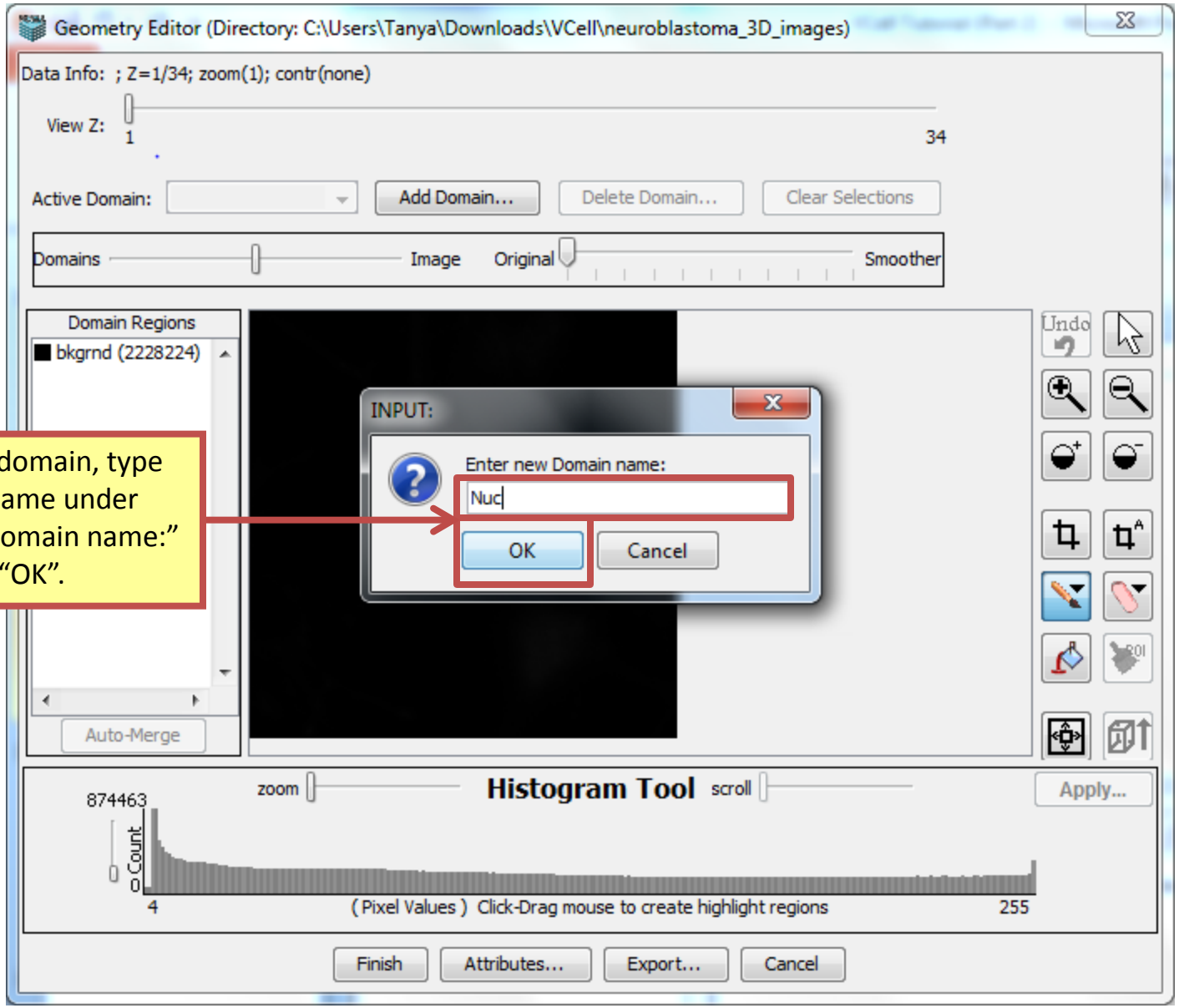
Contents


BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)
File View Server Tools Help
Tutorial
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Applications (1)
Spatial Deterr
Geometry
Specificati
Protocols
Simulation
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)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
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

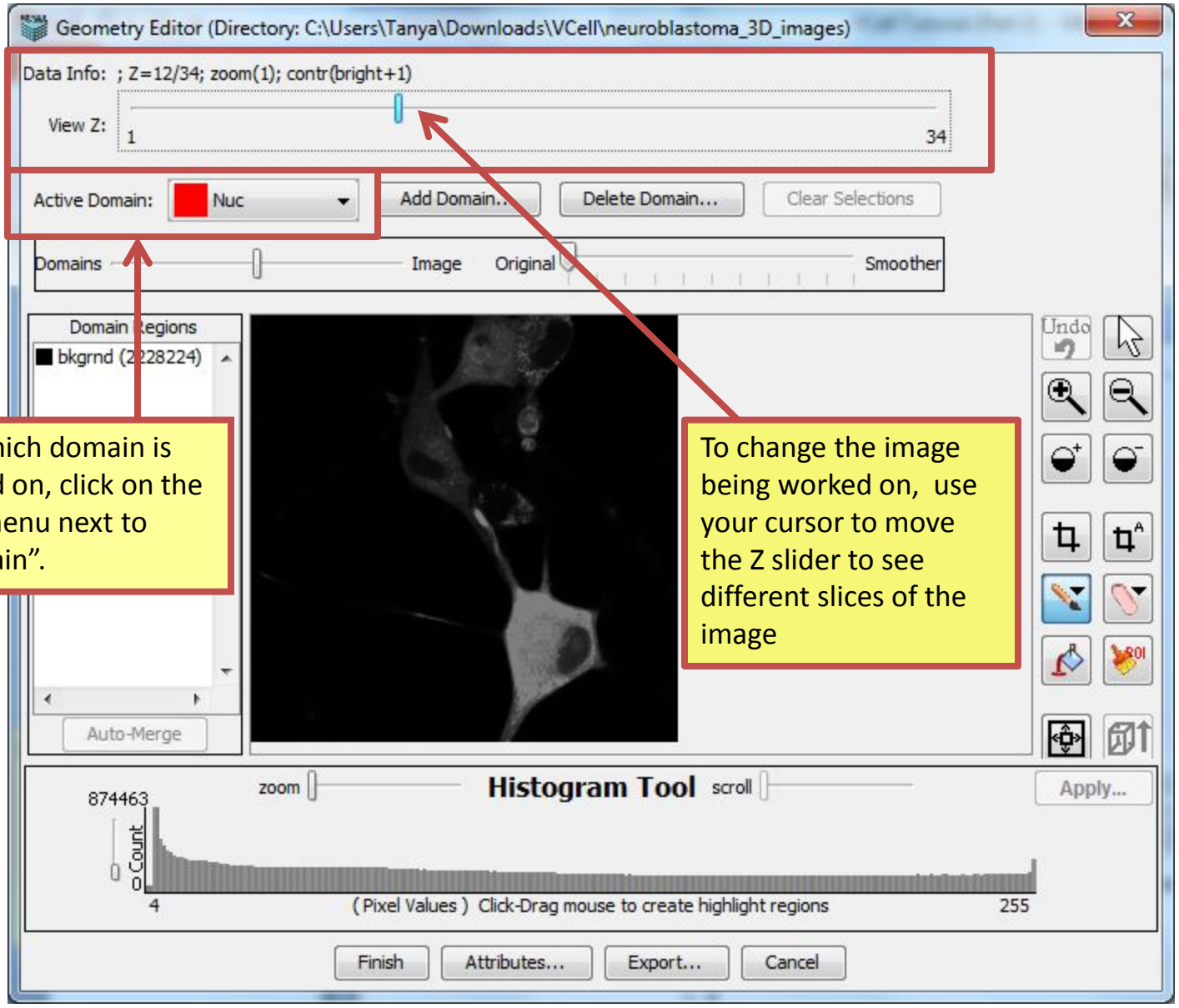


To adjust the resolution of imported images, holding down on your cursor, adjust the slider to the desired scale factor of the image sizes, and then click “OK”.


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

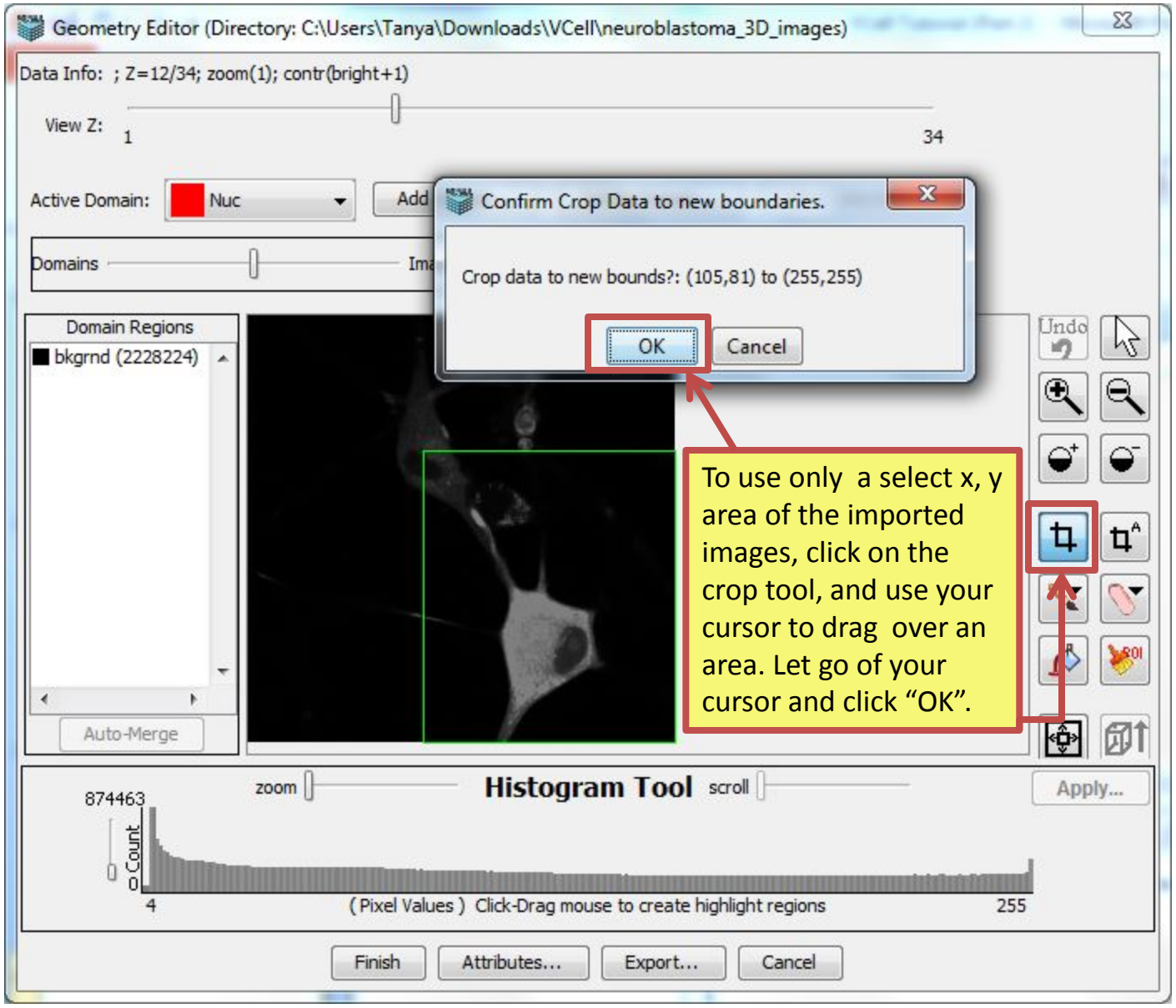


To name the domain, type the domain name under "Enter new Domain name:" and the click "OK".

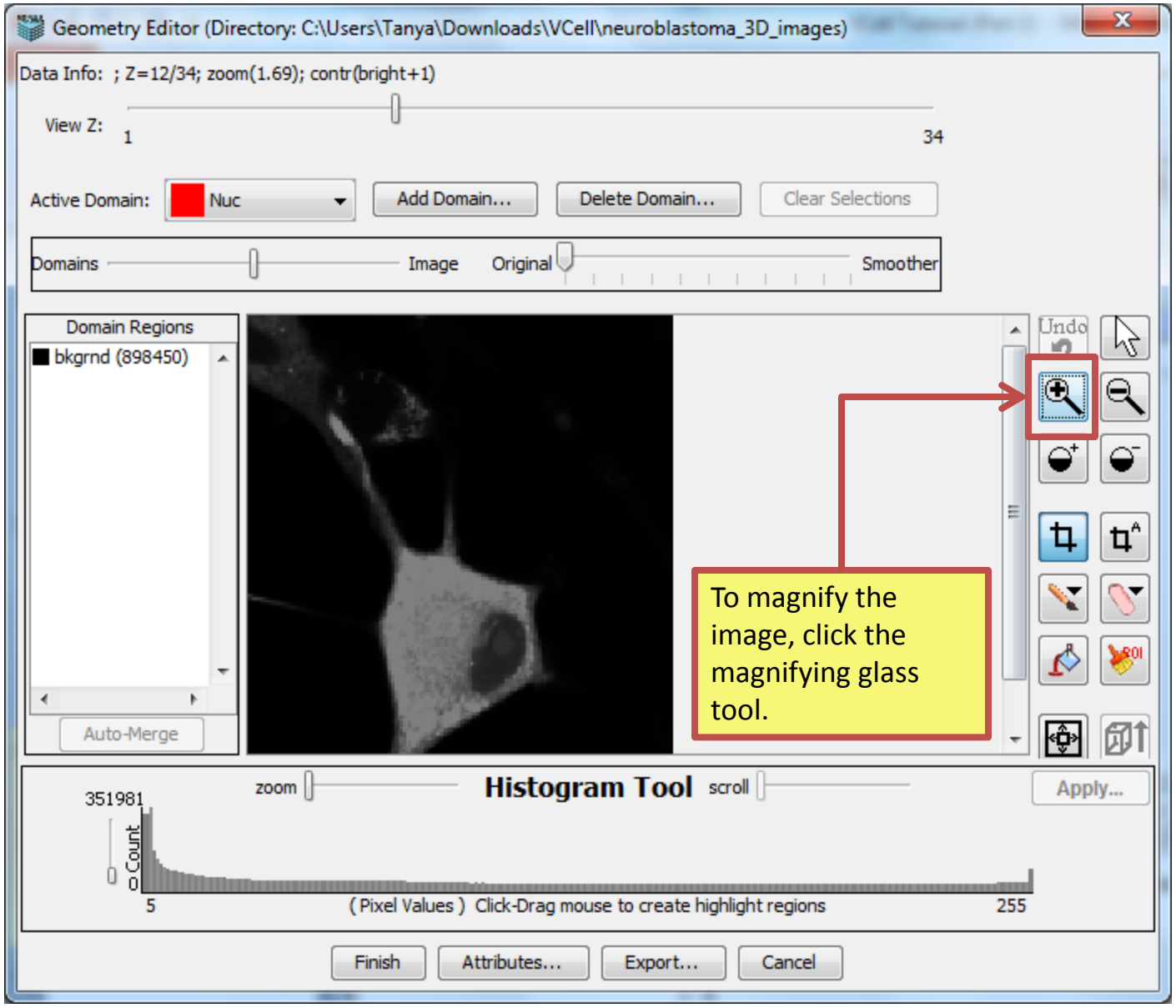


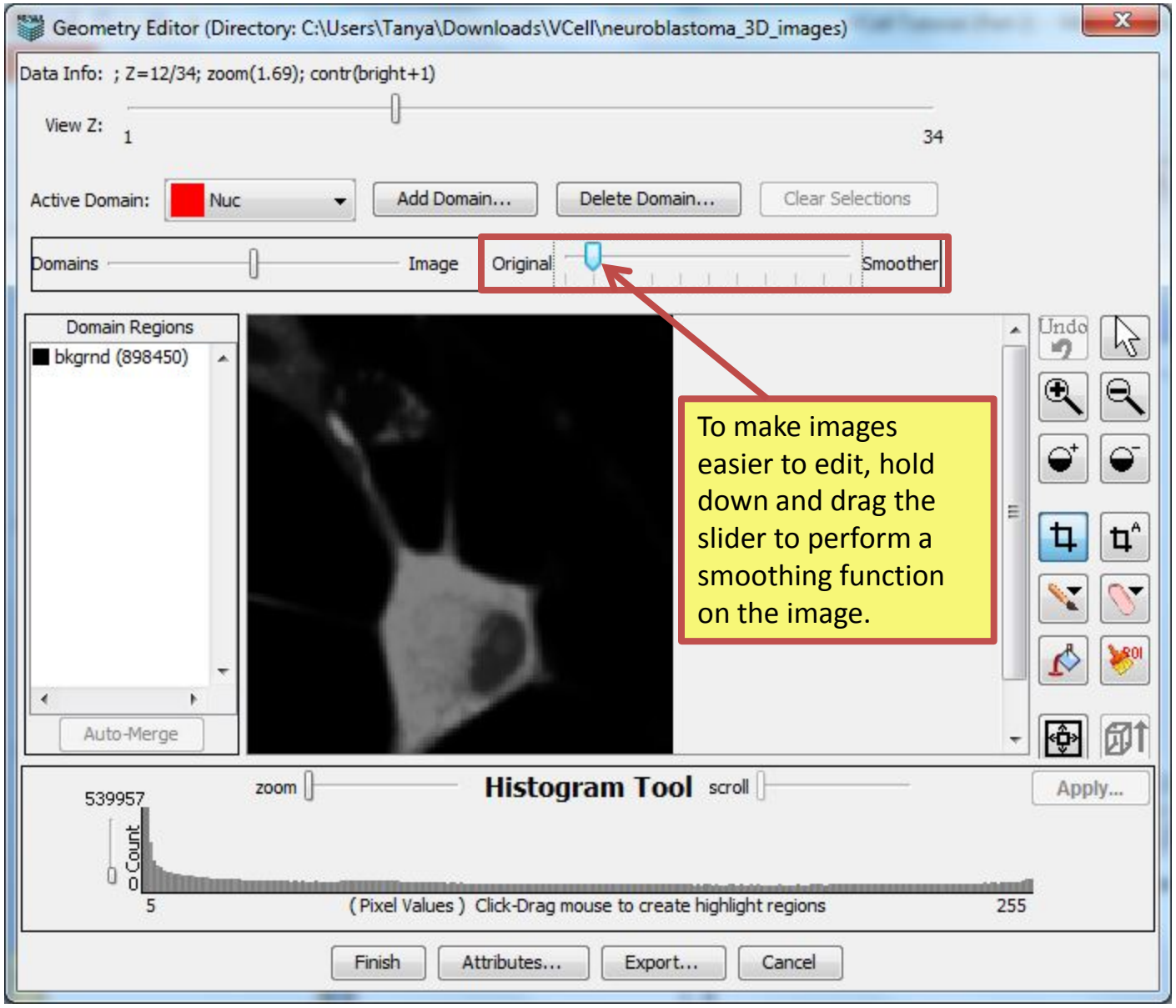
To change which domain is being worked on, click on the drop down menu next to "Active Domain".

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

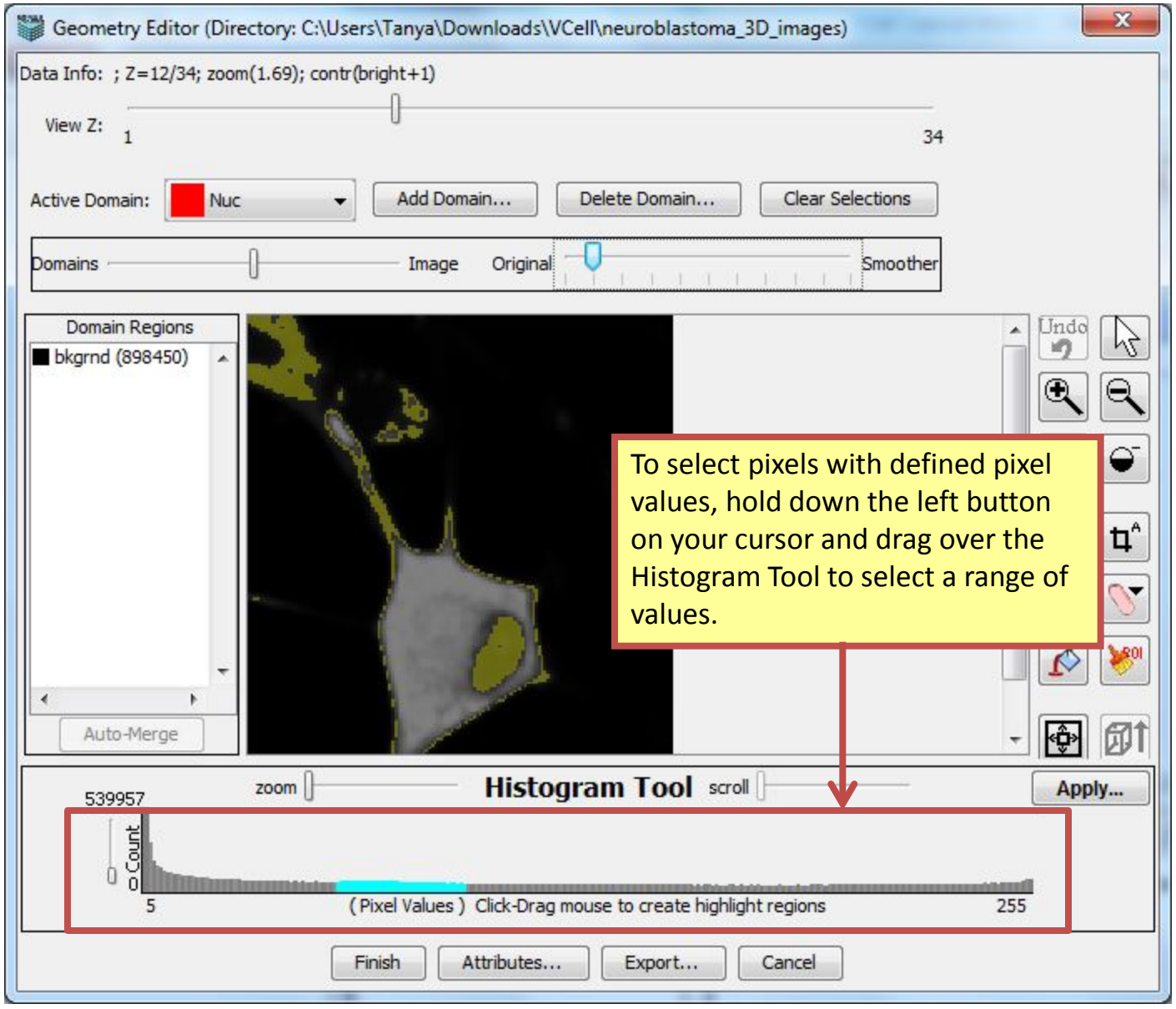

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add
Domains
Confirm Crop Data to new boundaries.
Crop data to new bounds?: (105,81) to (255,255)
OK
Cancel
Domain Regions
bkgrnd (2228224)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

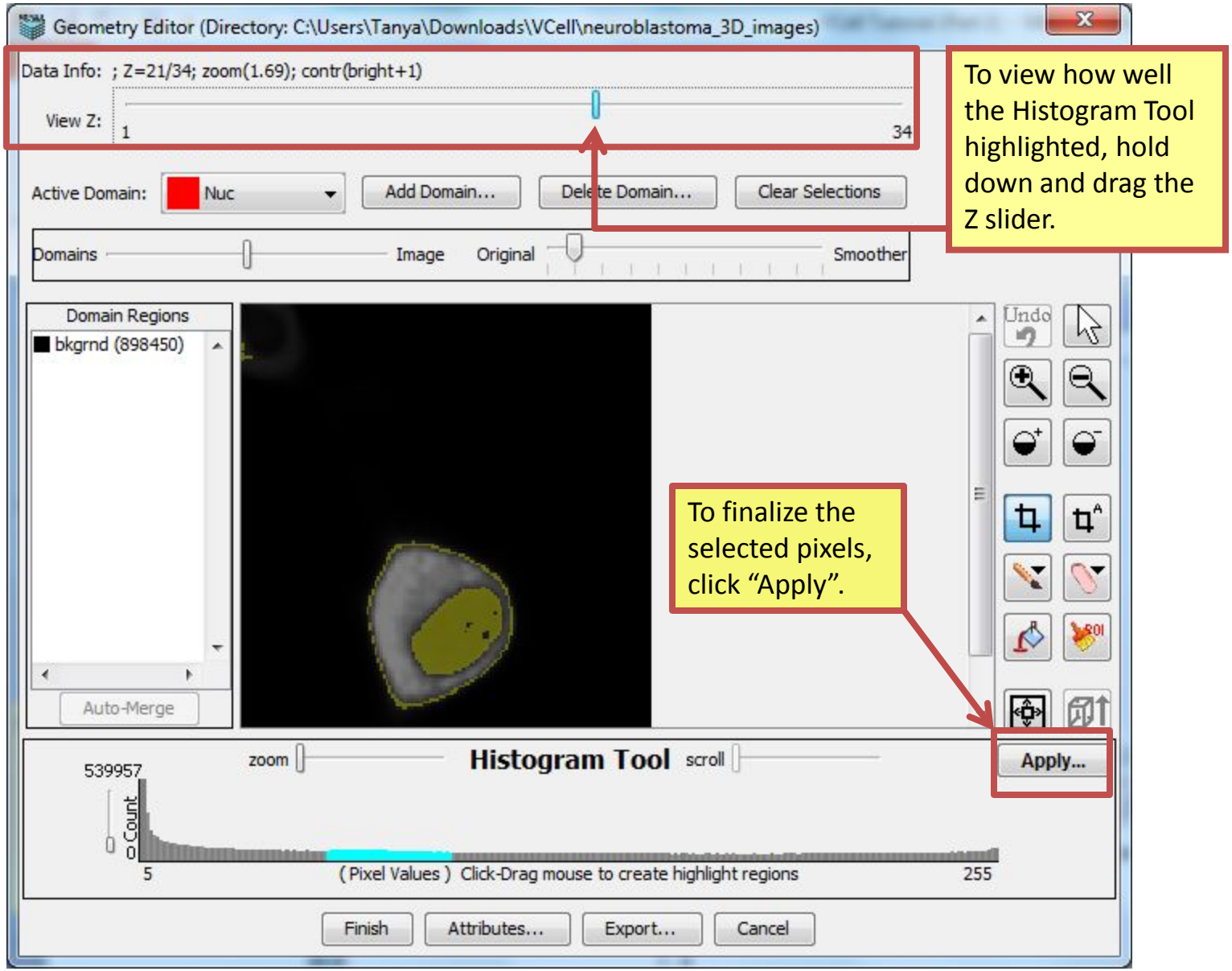

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To magnify 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

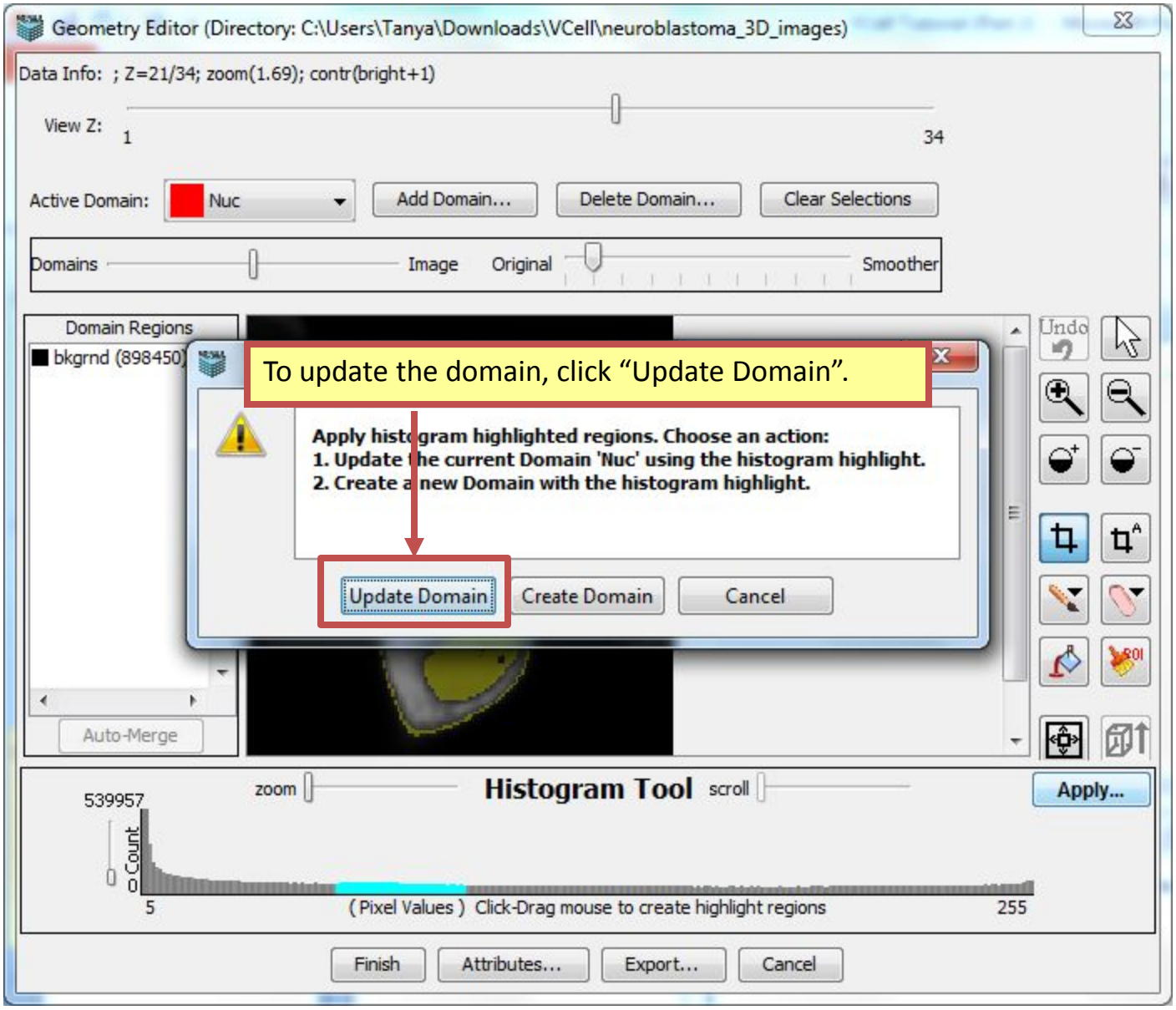

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To make 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

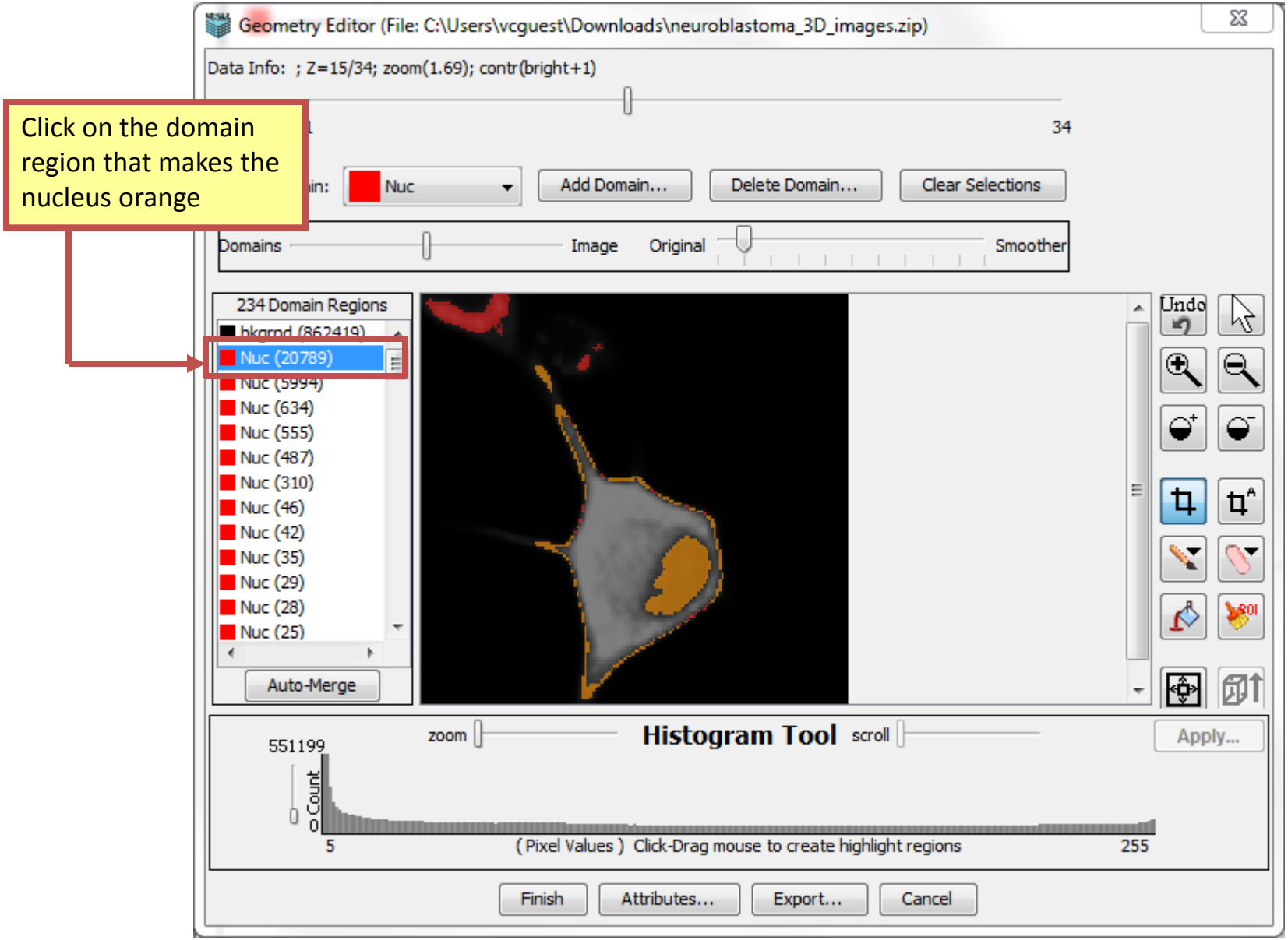
Contents

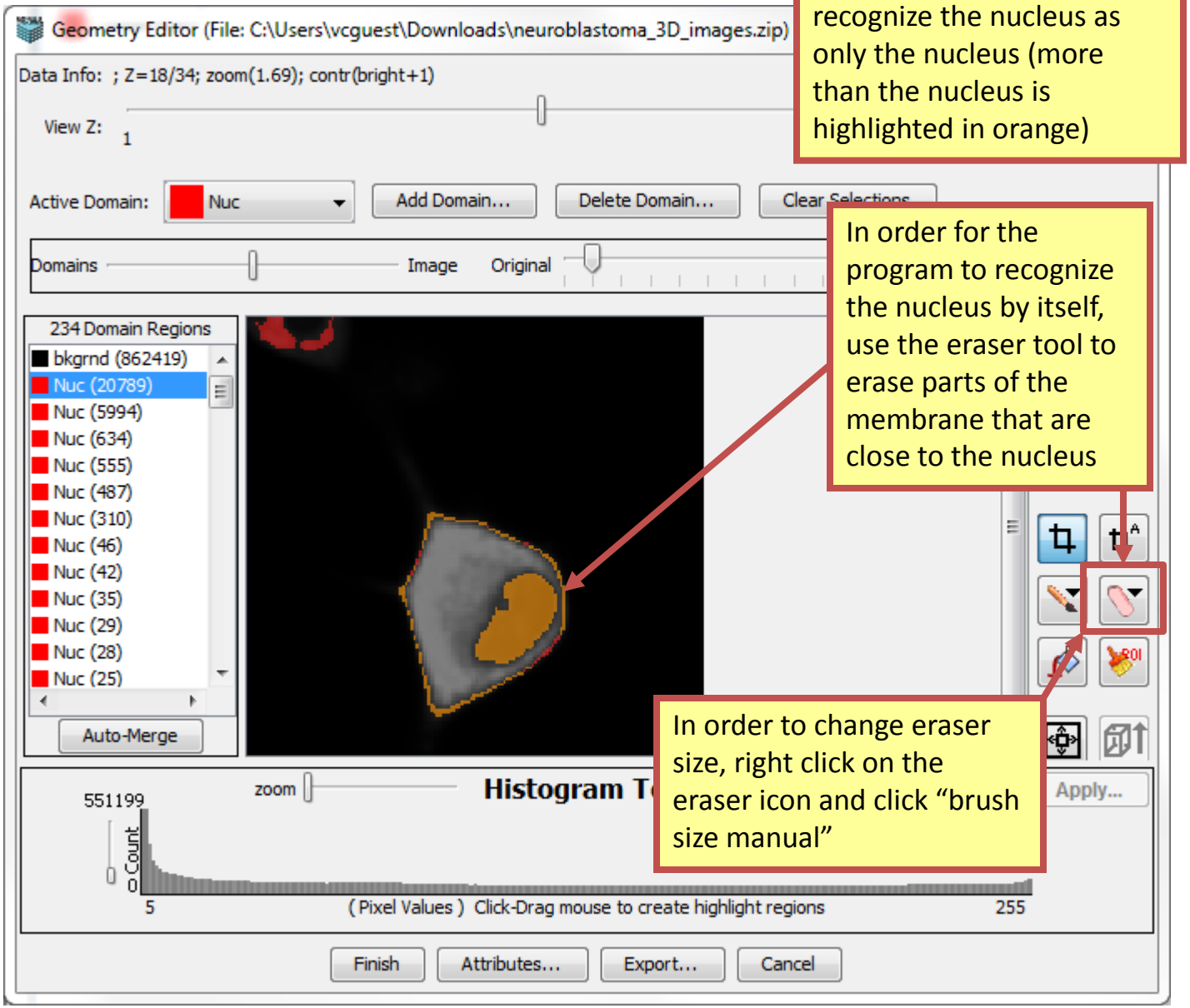

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=12/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
Domain Regions
bkgrnd (898450)
Auto-Merge
Undo
To select 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

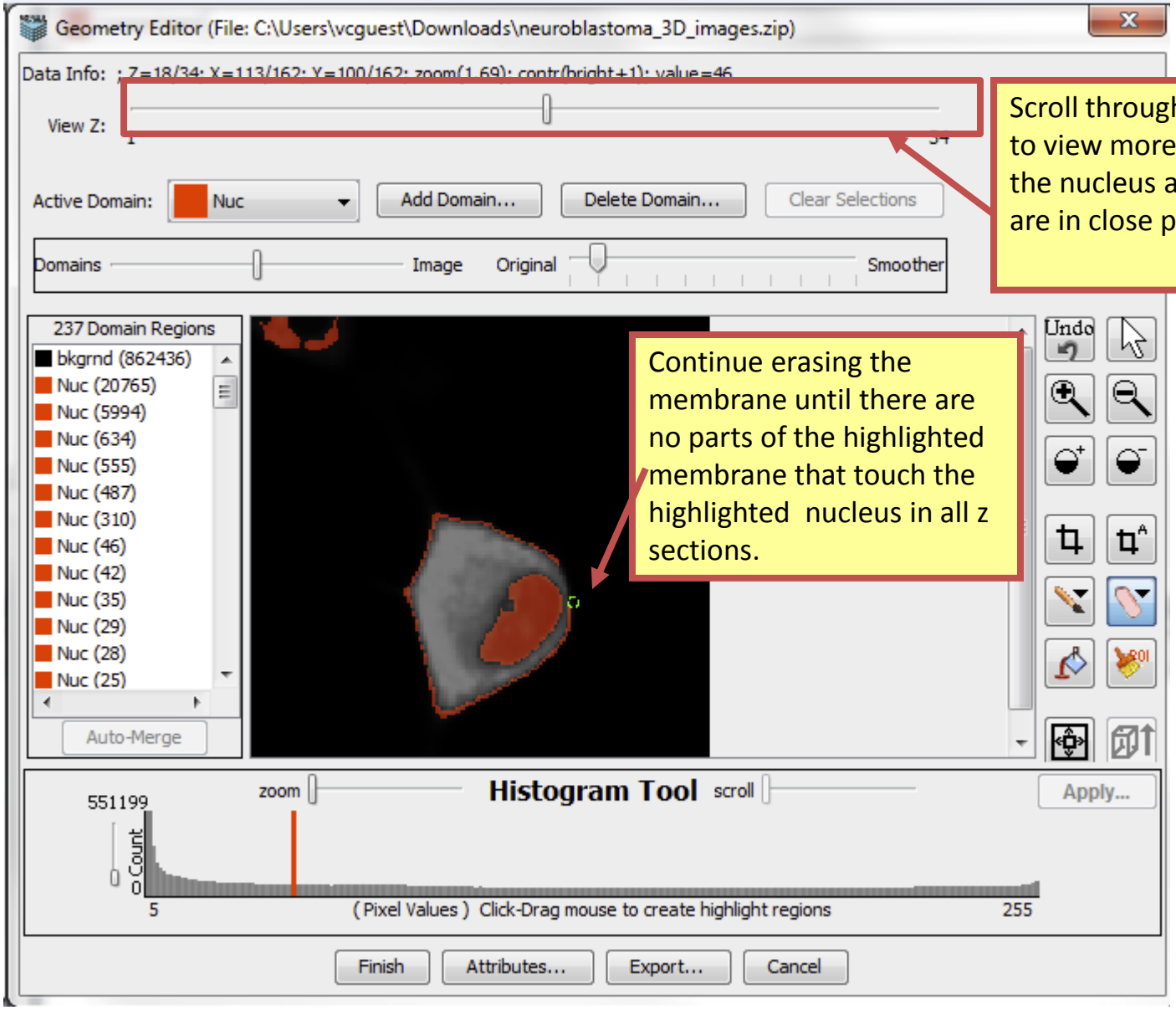
Contents


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

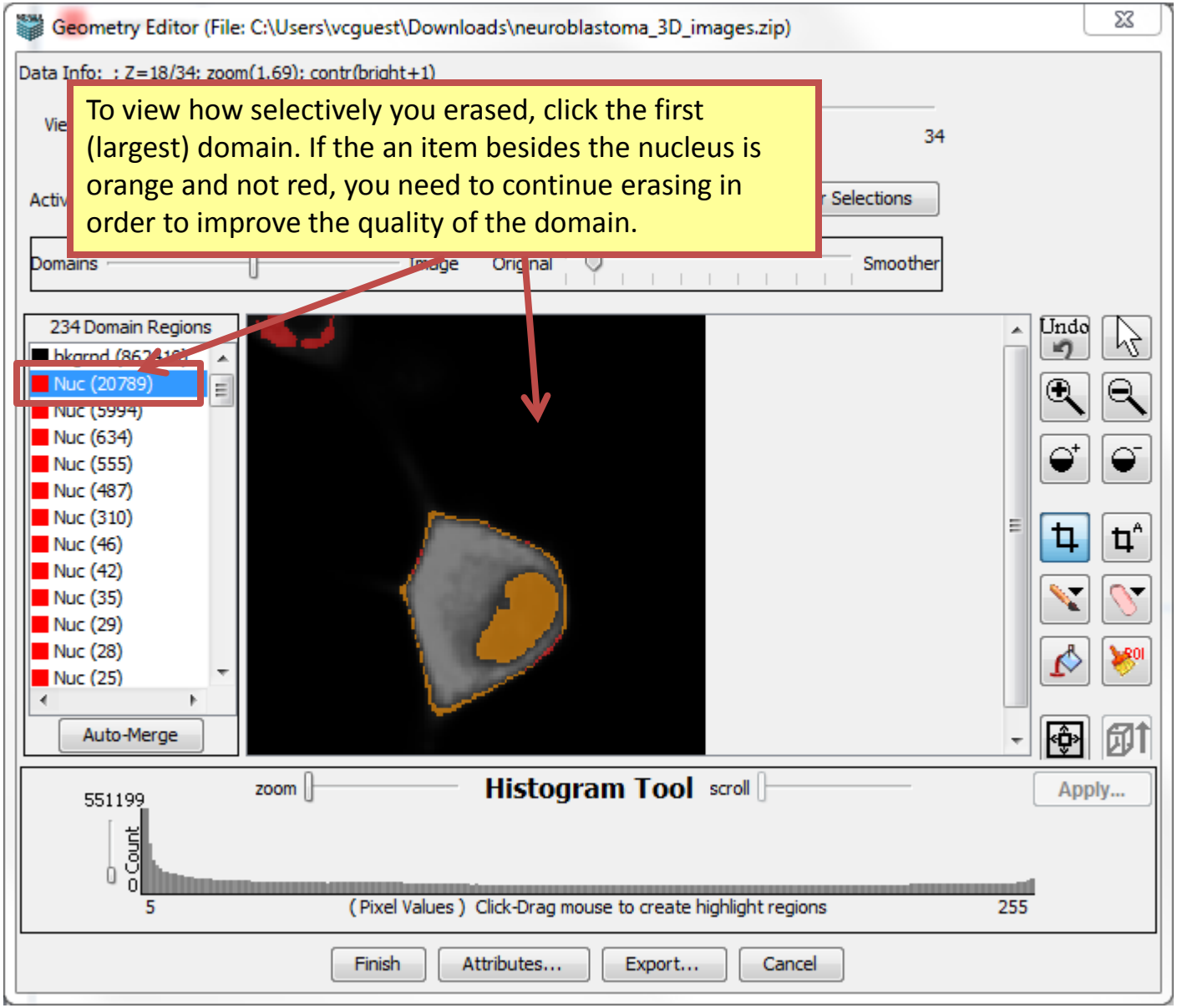

Click on the domain region that makes the nucleus orange
Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=15/34; zoom(1.69); contr(bright+1)
34
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
234 Domain Regions
Nuc (20789)
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

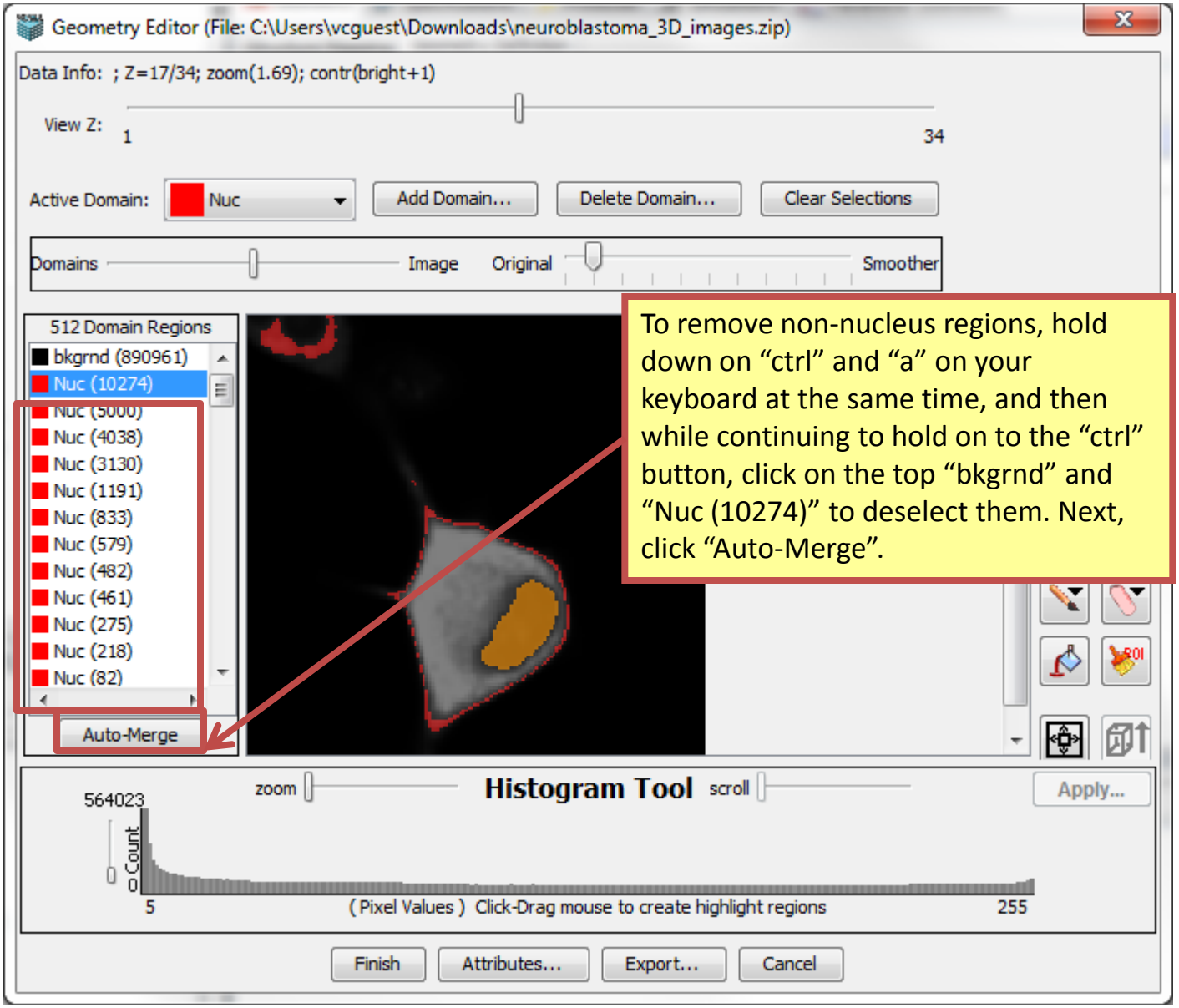

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=18/34; zoom(1.69); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
234 Domain Regions
bkgrnd (862419)
Nuc (20789)
Nuc (5994)
Nuc (634)
Nuc (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”

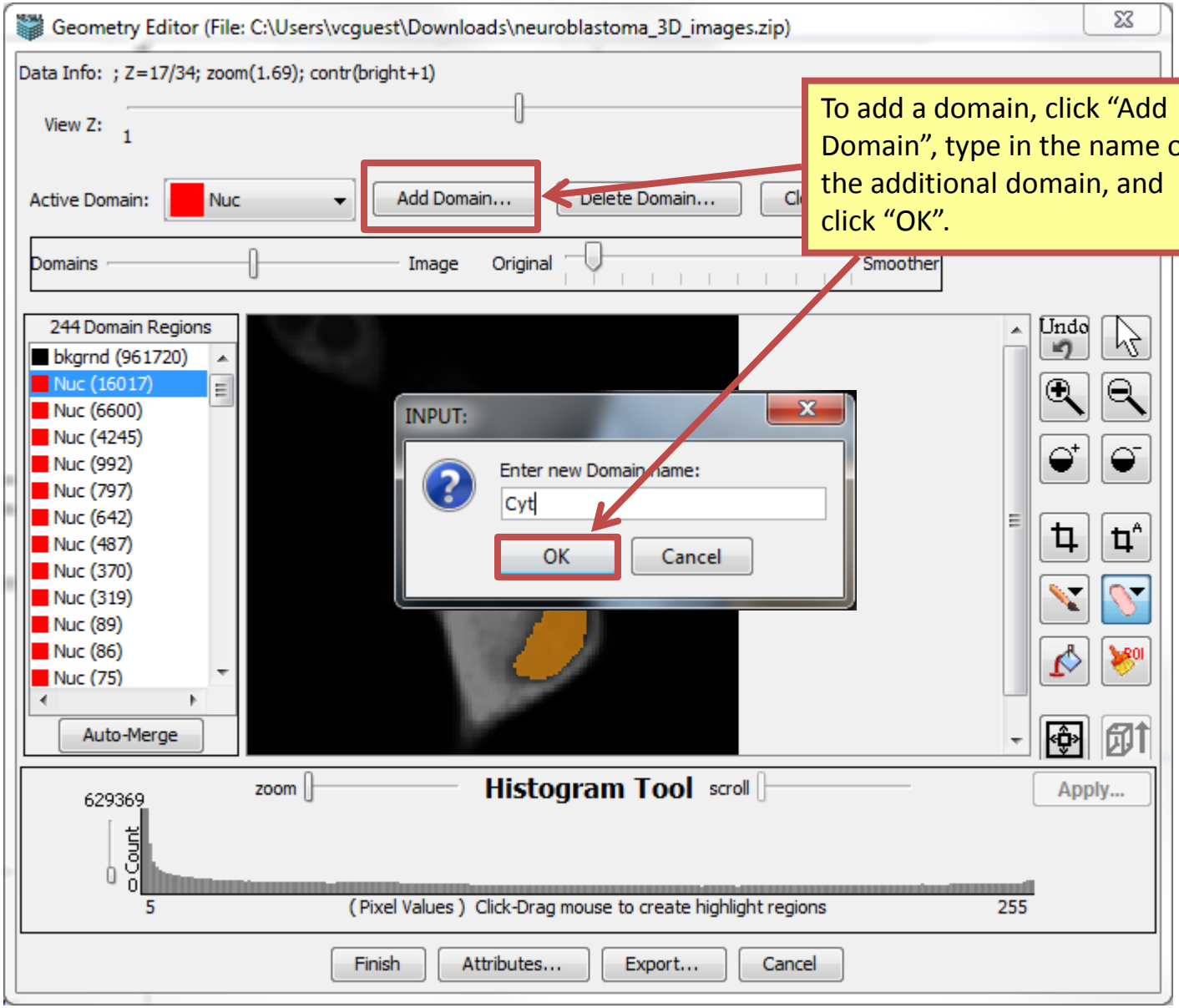


Scroll through the Z slider to view more slices in which the nucleus and membrane are in close proximity

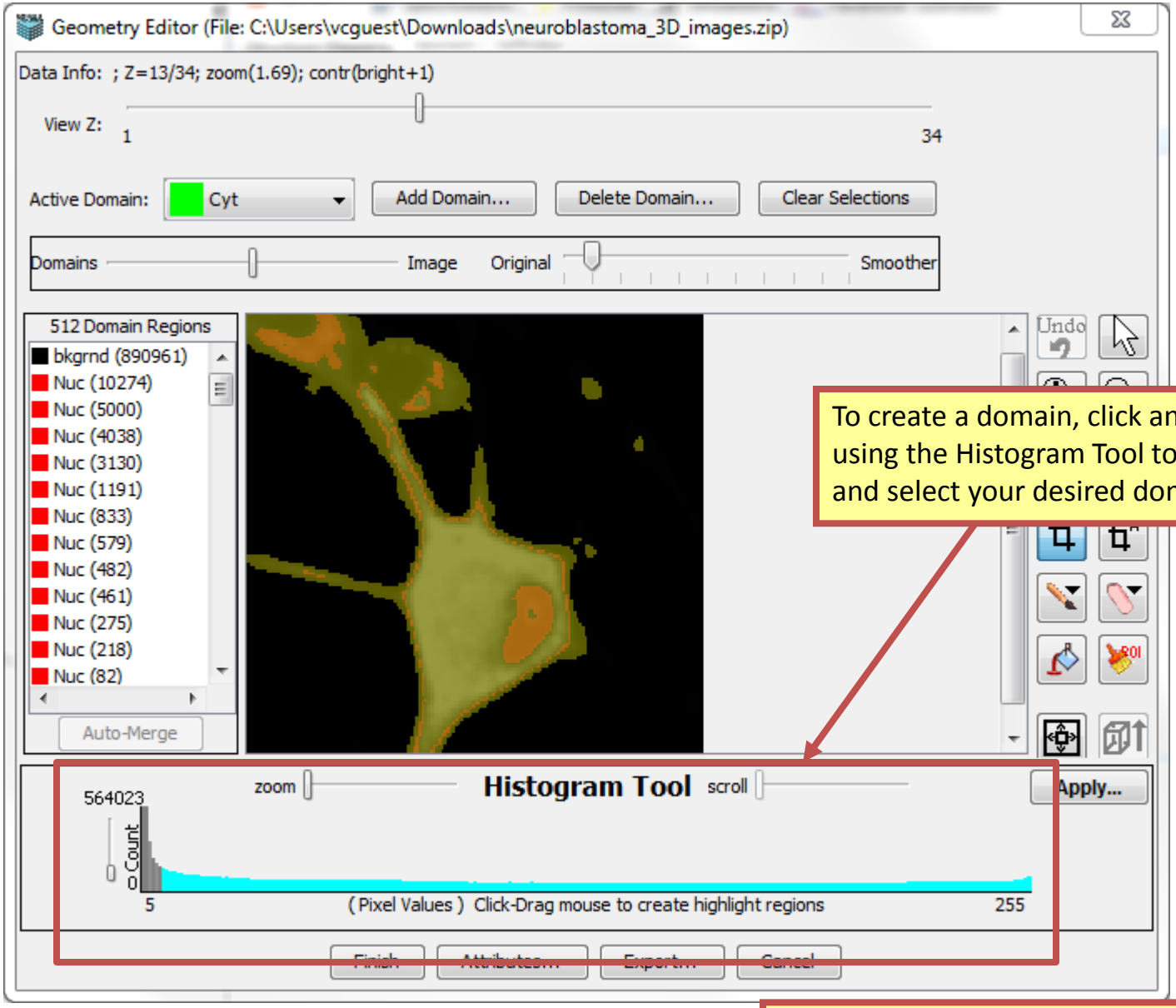
Continue erasing the membrane until there are no parts of the highlighted membrane that touch the highlighted nucleus in all z sections.

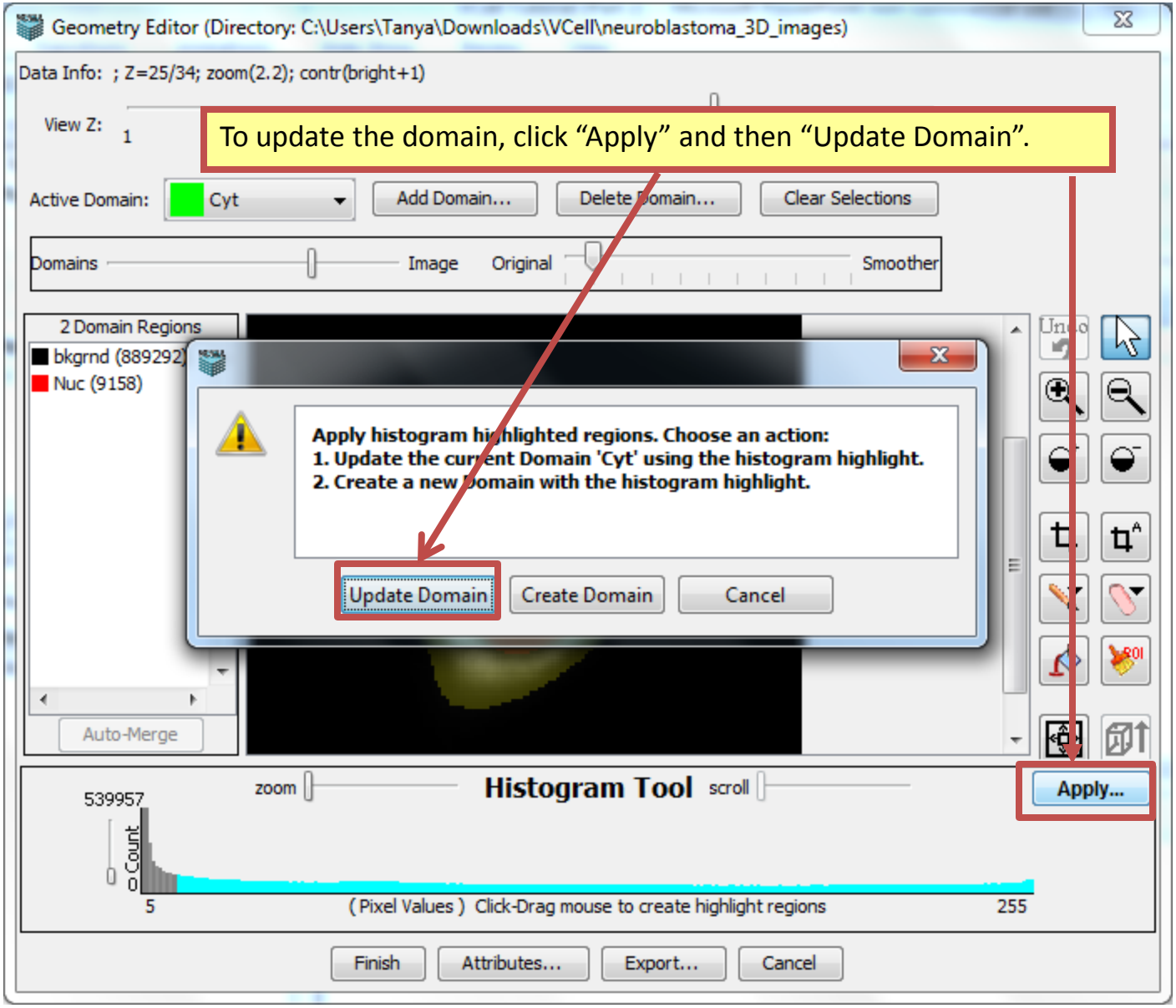

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=18/34; zoom(1.69); contr(bright+1)
34
Selections
Domains
Smoother
To view how selectively you erased, click the first (largest) domain. If the an item besides the nucleus is orange and not red, you need to continue 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

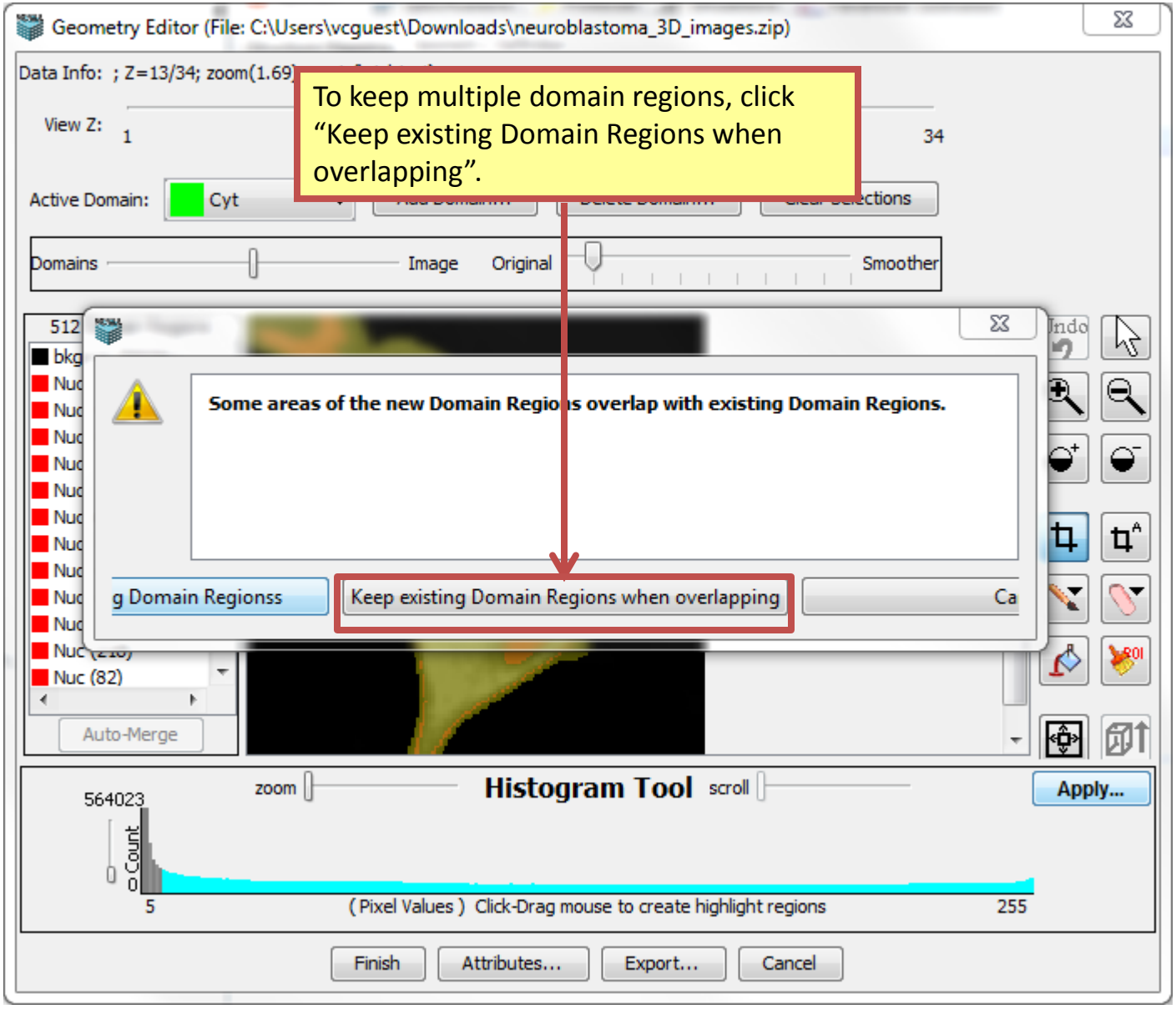

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=17/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Nuc
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
512 Domain Regions
bkgrnd (890961)
Nuc (10274)
Nuc (5000)
Nuc (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

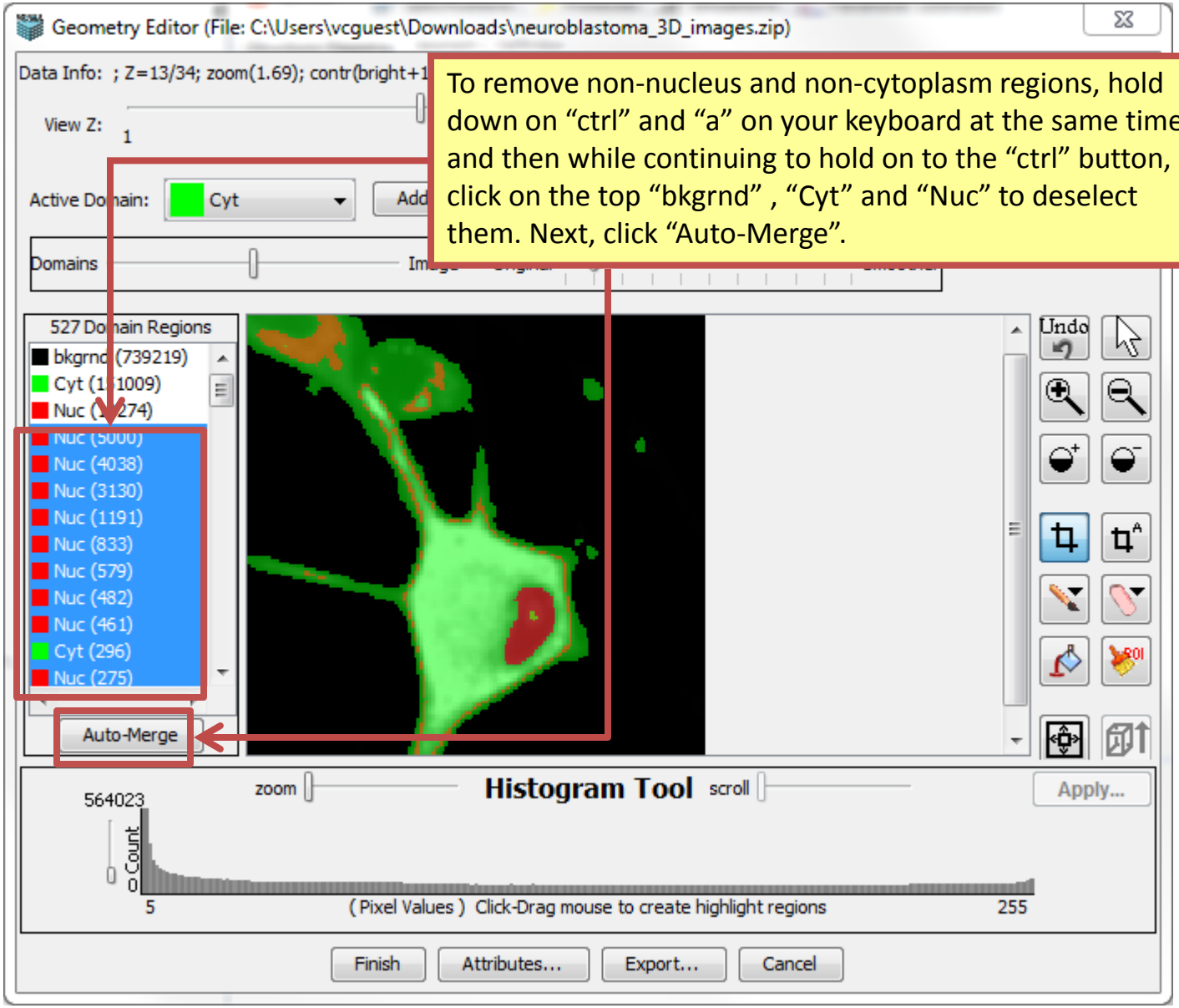

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=17/34; zoom(1.69); contr(bright+1)
View Z:
1
Active Domain:
Nuc
Add Domain...
Delete Domain...
Domains
Image
Original
Smoother
244 Domain Regions
bkgrnd (961720)
Nuc (16017)
Nuc (6600)
Nuc (4245)
Nuc (992)
Nuc (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

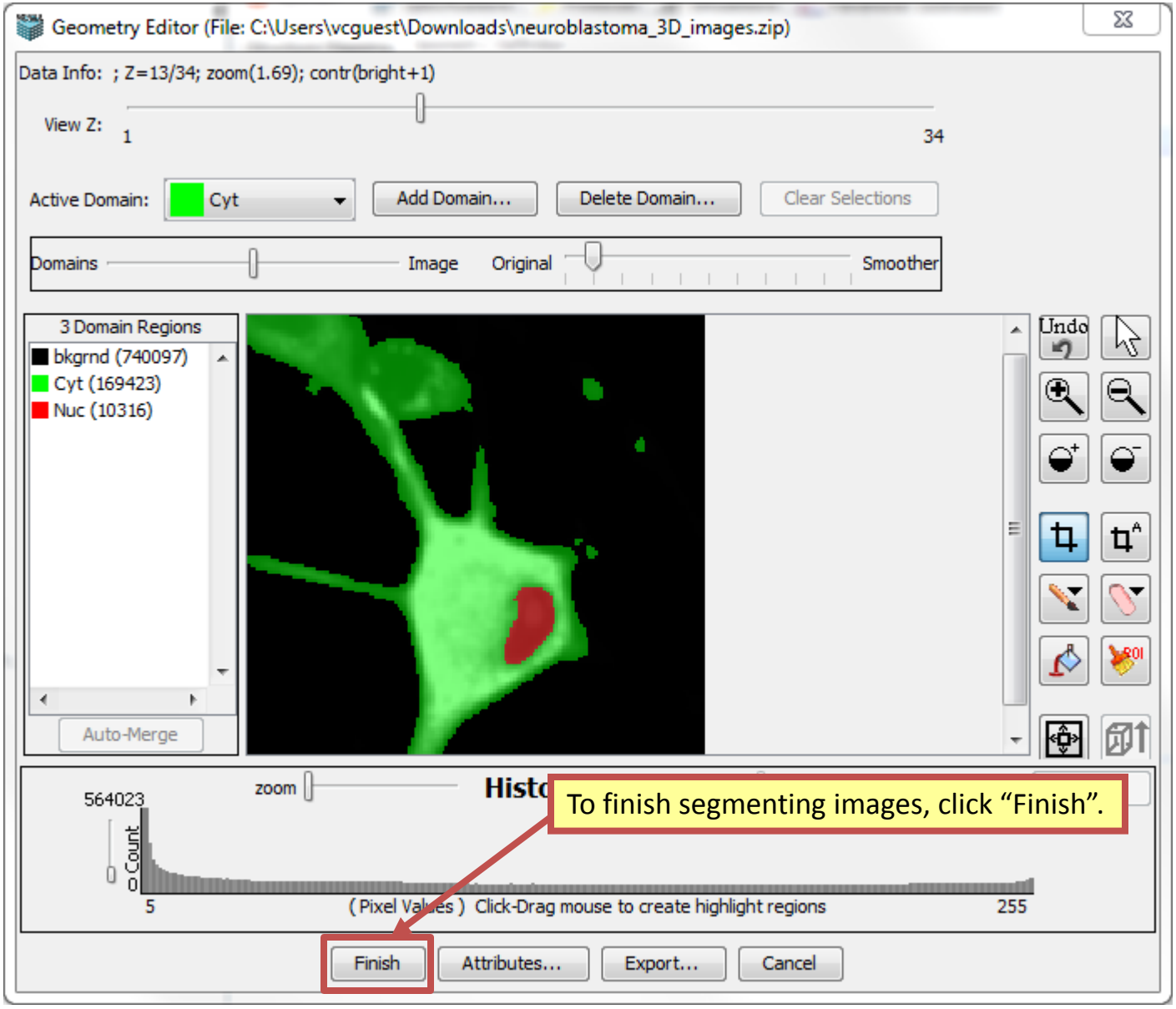

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=13/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
512 Domain Regions
bkgrnd (890961)
Nuc (10274)
Nuc (5000)
Nuc (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

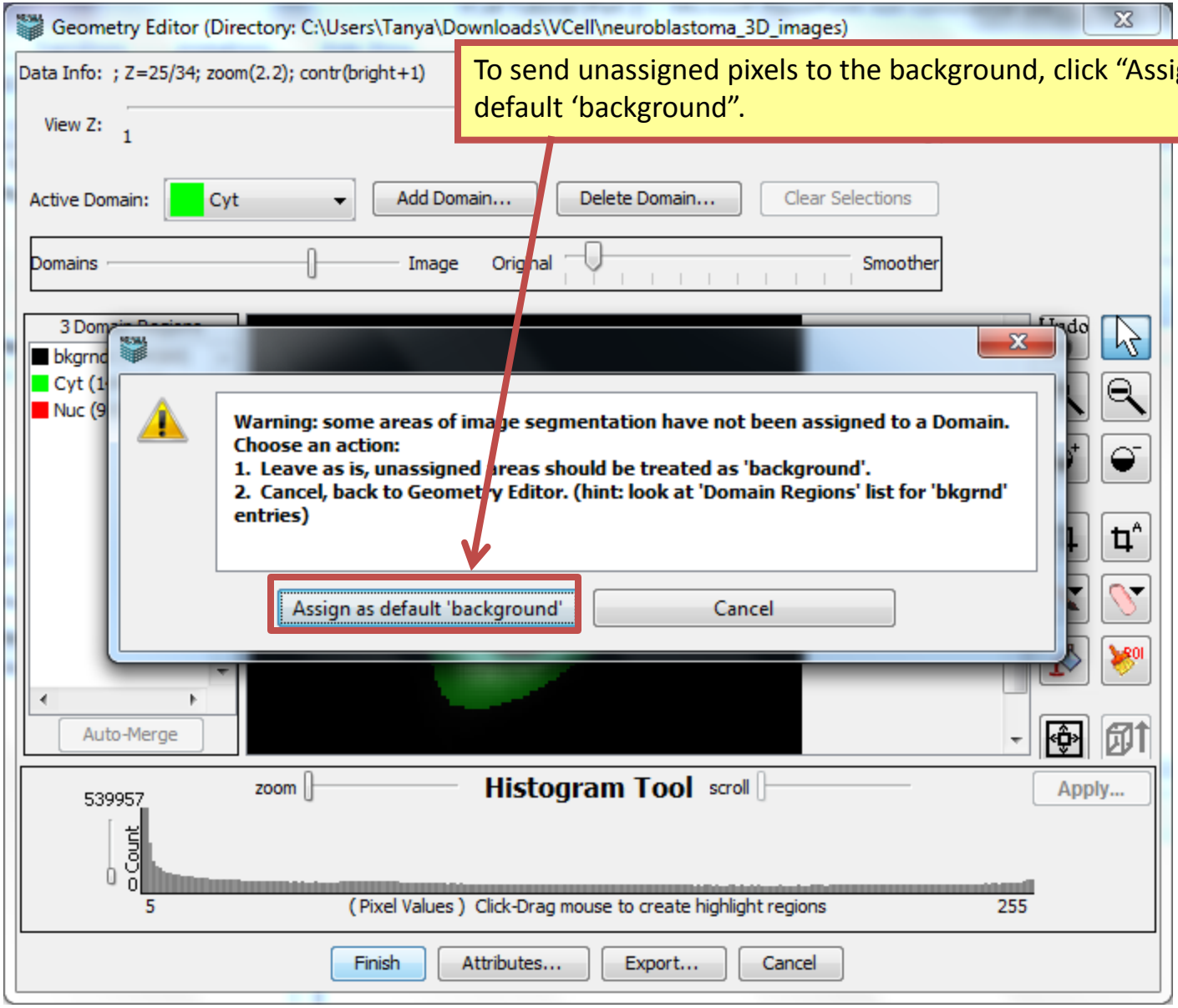

Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)
Data Info: ; Z=25/34; zoom(2.2); contr(bright+1)
View Z:
1
To update the domain, click “Apply” and then “Update Domain”.
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
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

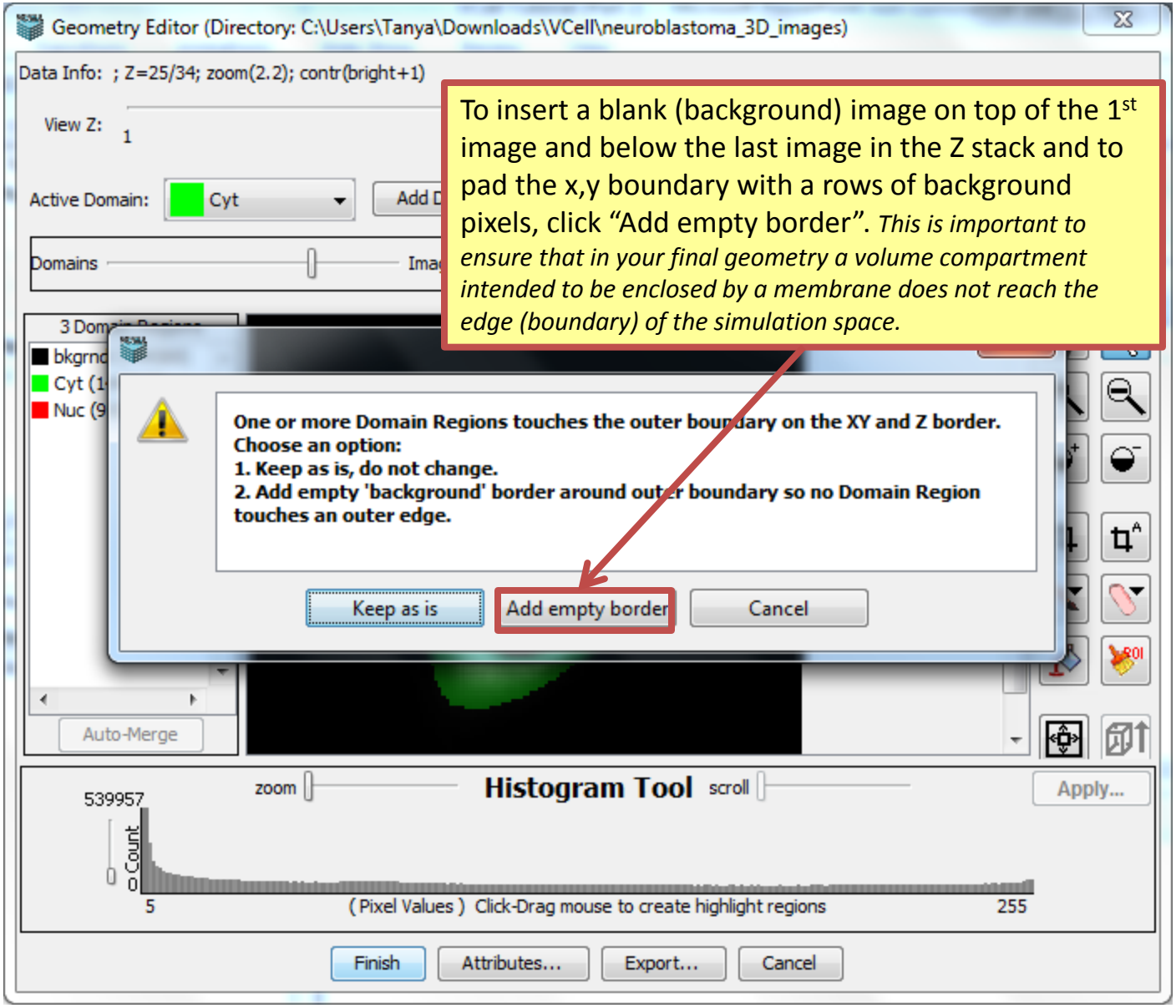


To remove non-nucleus and non-cytoplasm regions, hold down on “ctrl” and “a” on your keyboard at the same time, and then while continuing to hold on to the “ctrl” button, click on the top “bkgrnd” , “Cyt” and “Nuc” to deselect them. Next, click “Auto-Merge”.

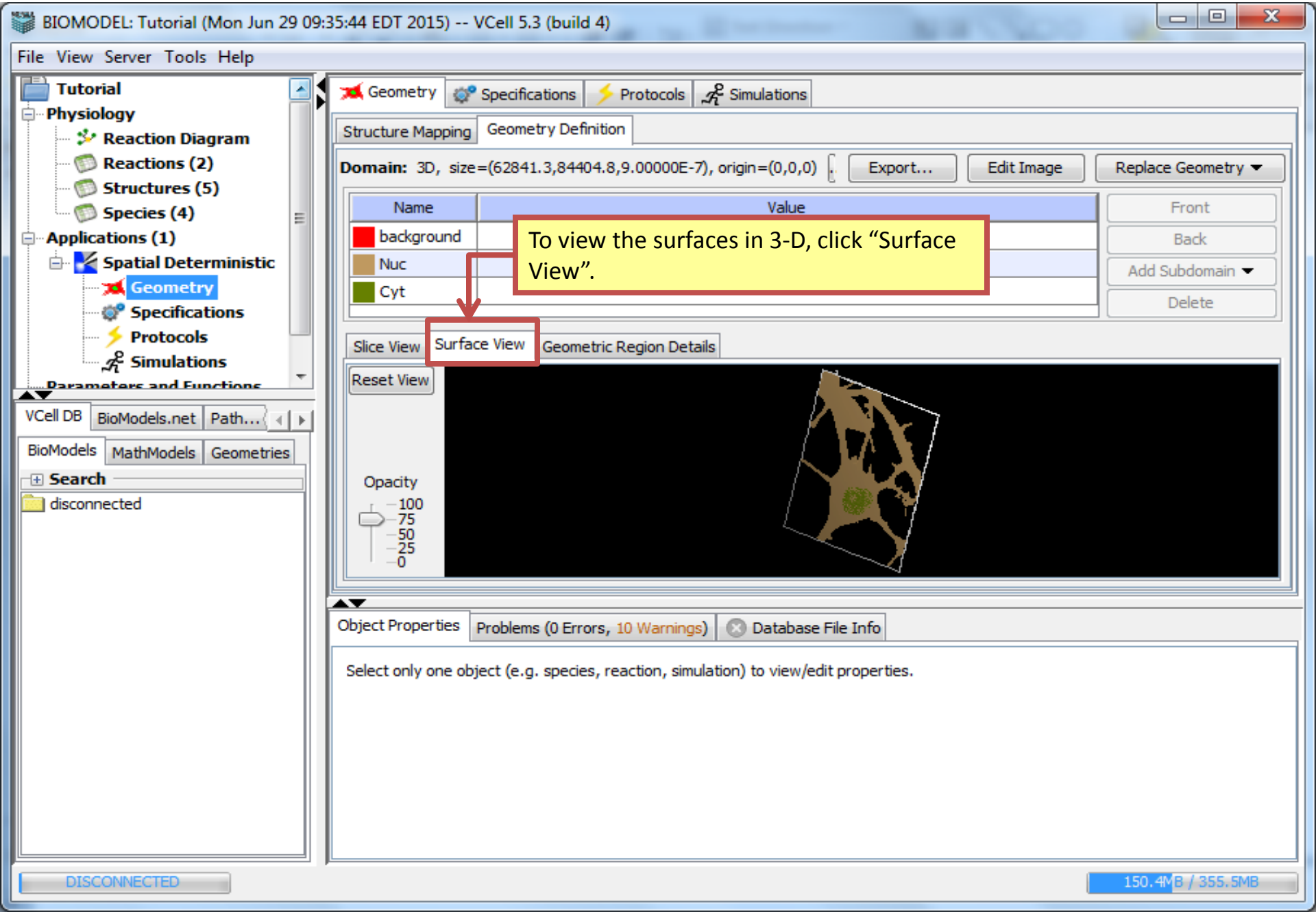

Geometry Editor (File: C:\Users\vcguest\Downloads\neuroblastoma_3D_images.zip)
Data Info: ; Z=13/34; zoom(1.69); contr(bright+1)
View Z:
1
34
Active Domain:
Cyt
Add Domain...
Delete Domain...
Clear Selections
Domains
Image
Original
Smoother
3 Domain Regions
bkgrnd (740097)
Cyt (169423)
Nuc (10316)
Auto-Merge
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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Search
disconnected
Geometry
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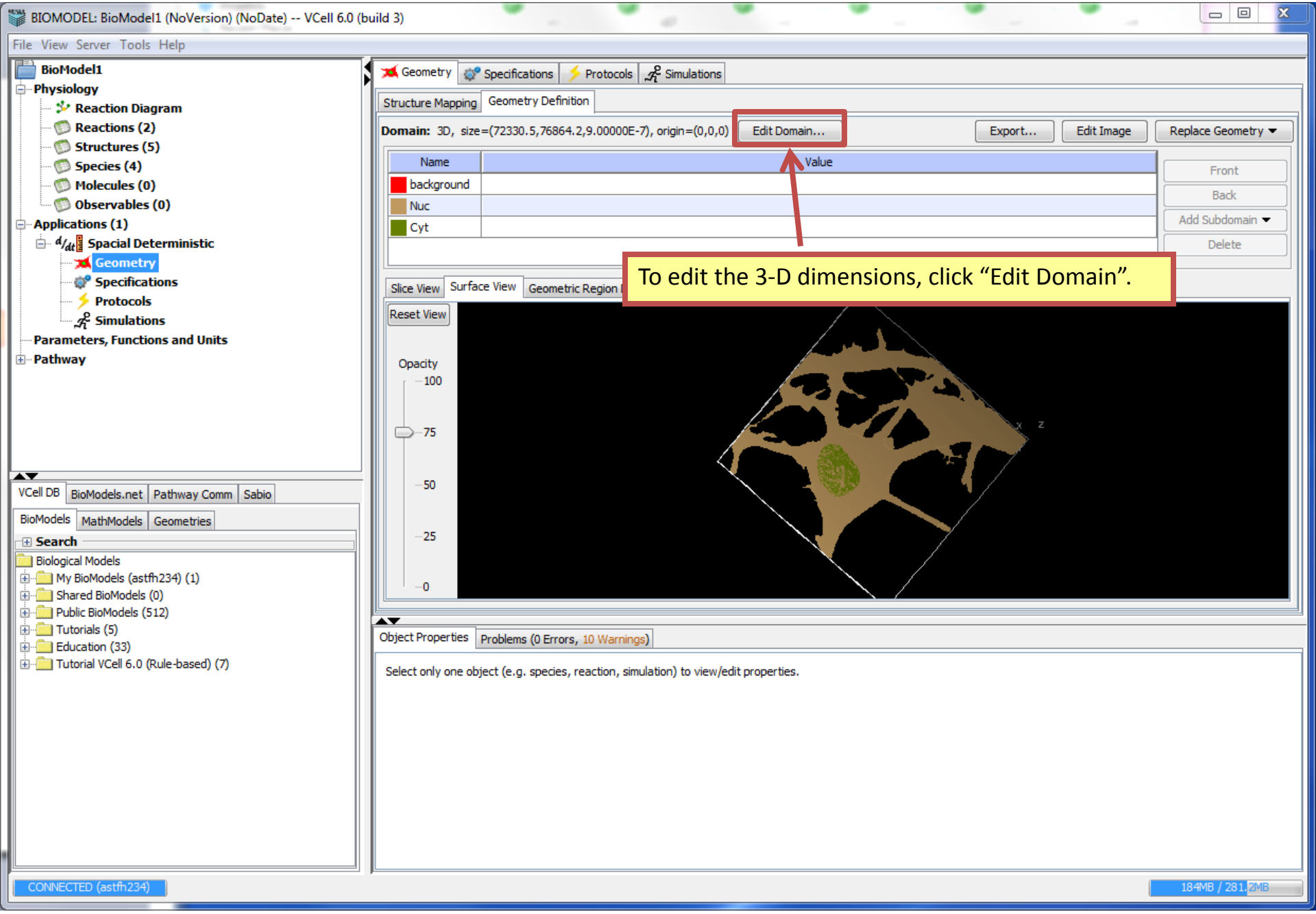
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(62841.3,84404.8,9.00000E-7), origin=(0,0,0)
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To view the surfaces in 3-D, click “Surface View”.
Slice View
Surface View
Geometric 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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Tutorial VCell 6.0 (Rule-based) (7)
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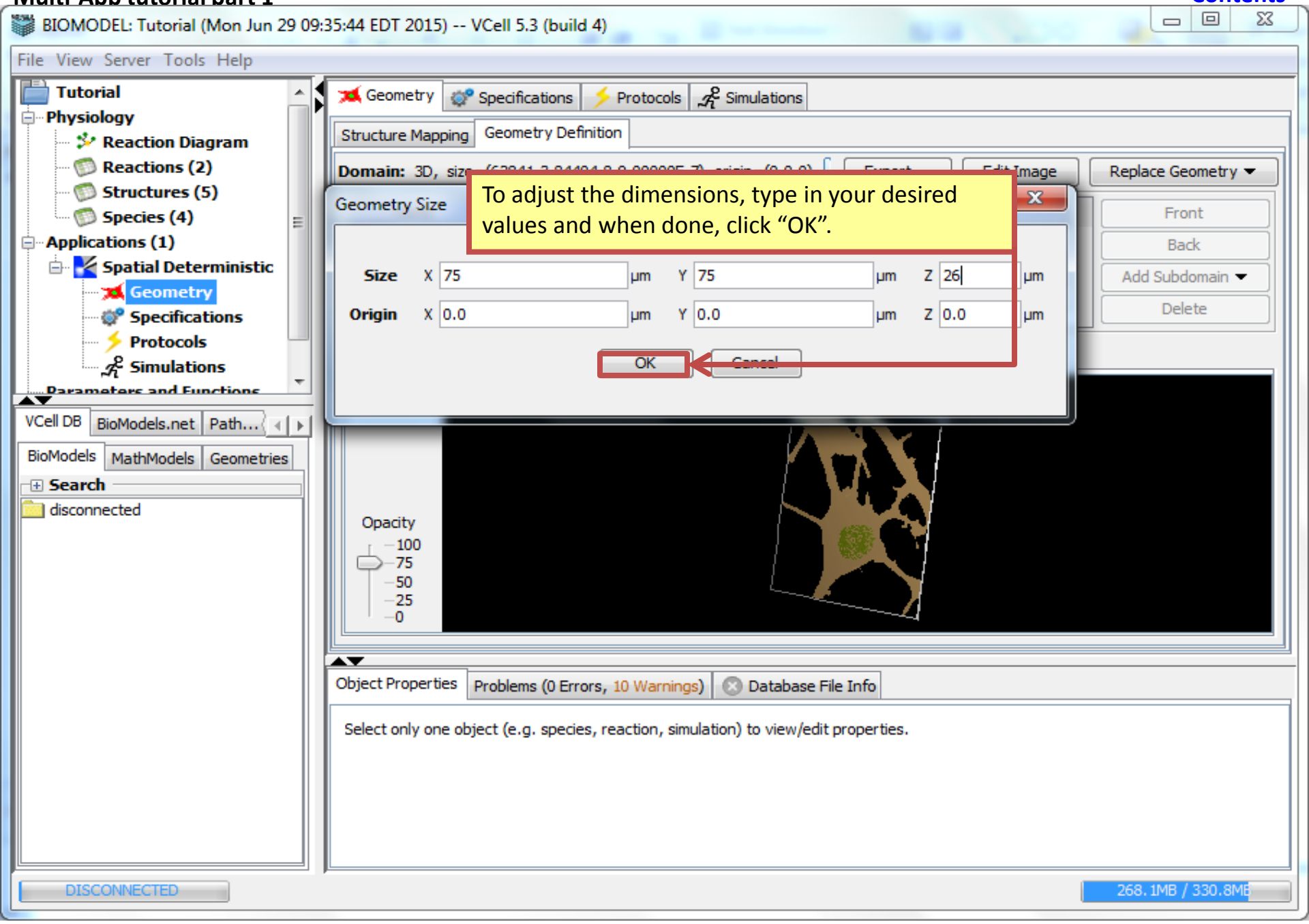
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(72330.5,76864.2,9.00000E-7), origin=(0,0,0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
background
Nuc
Cyt
Front
Back
Add Subdomain
Delete
To edit the 3-D dimensions, click “Edit Domain”.
Slice View
Surface View
Geometric 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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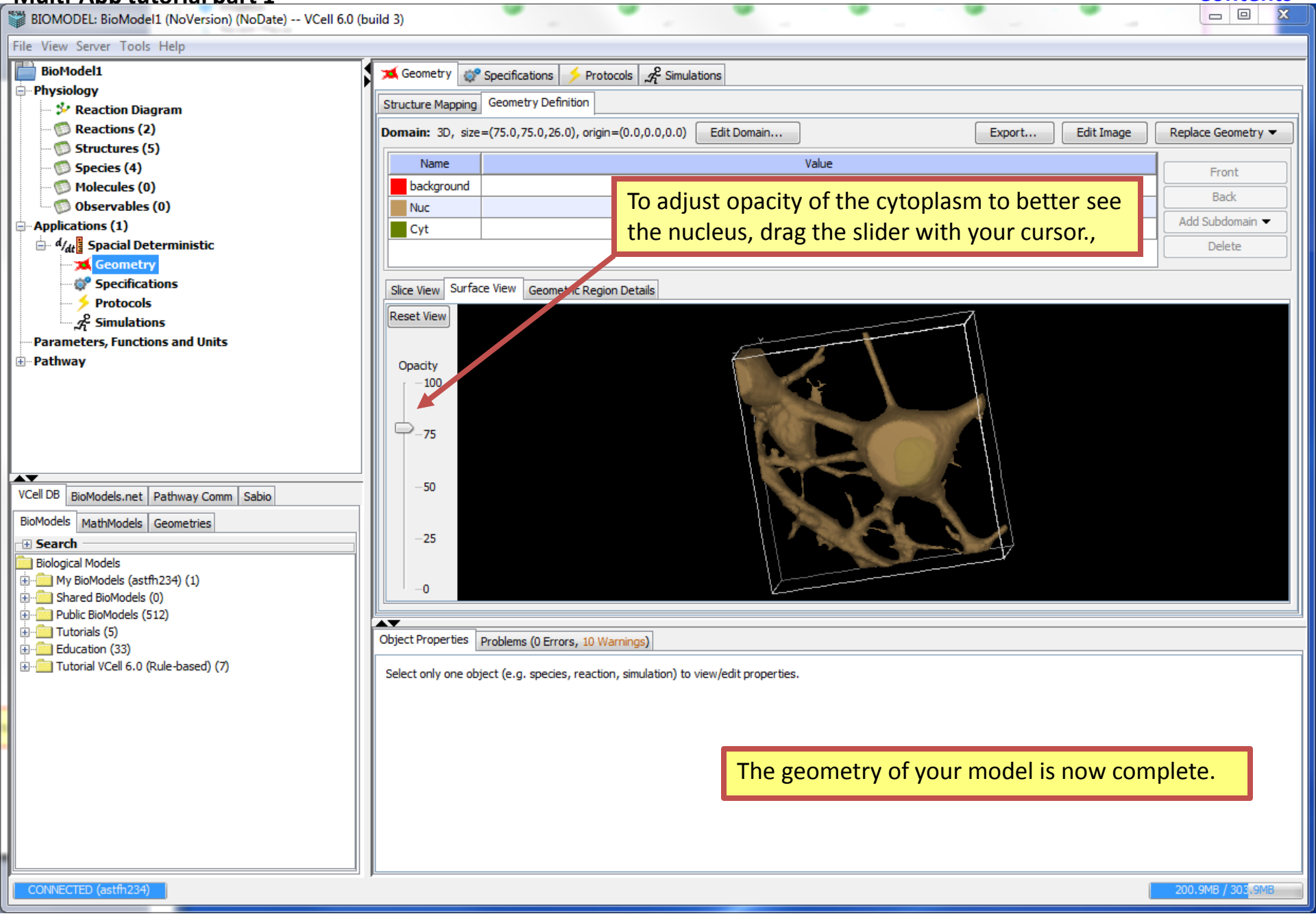
MathModels
Geometries
Search
disconnected
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D,
Export...
Edit Image
Replace Geometry
Front
Back
Add Subdomain
Delete
Geometry Size
To adjust the dimensions, type in your desired values and when done, click "OK".
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)
File View Server Tools Help
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Reactions (2)
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Molecules (0)
Observables (0)
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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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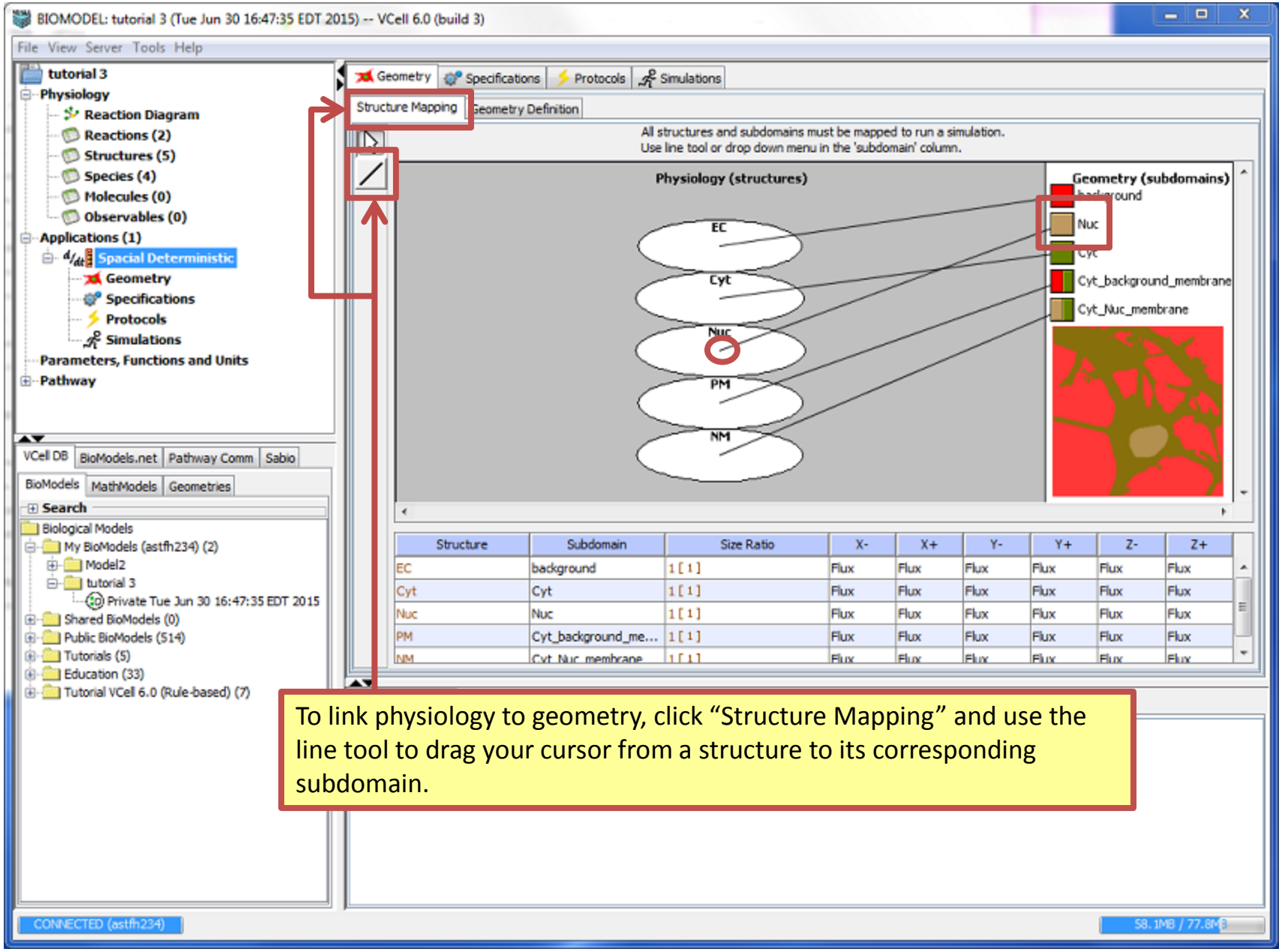
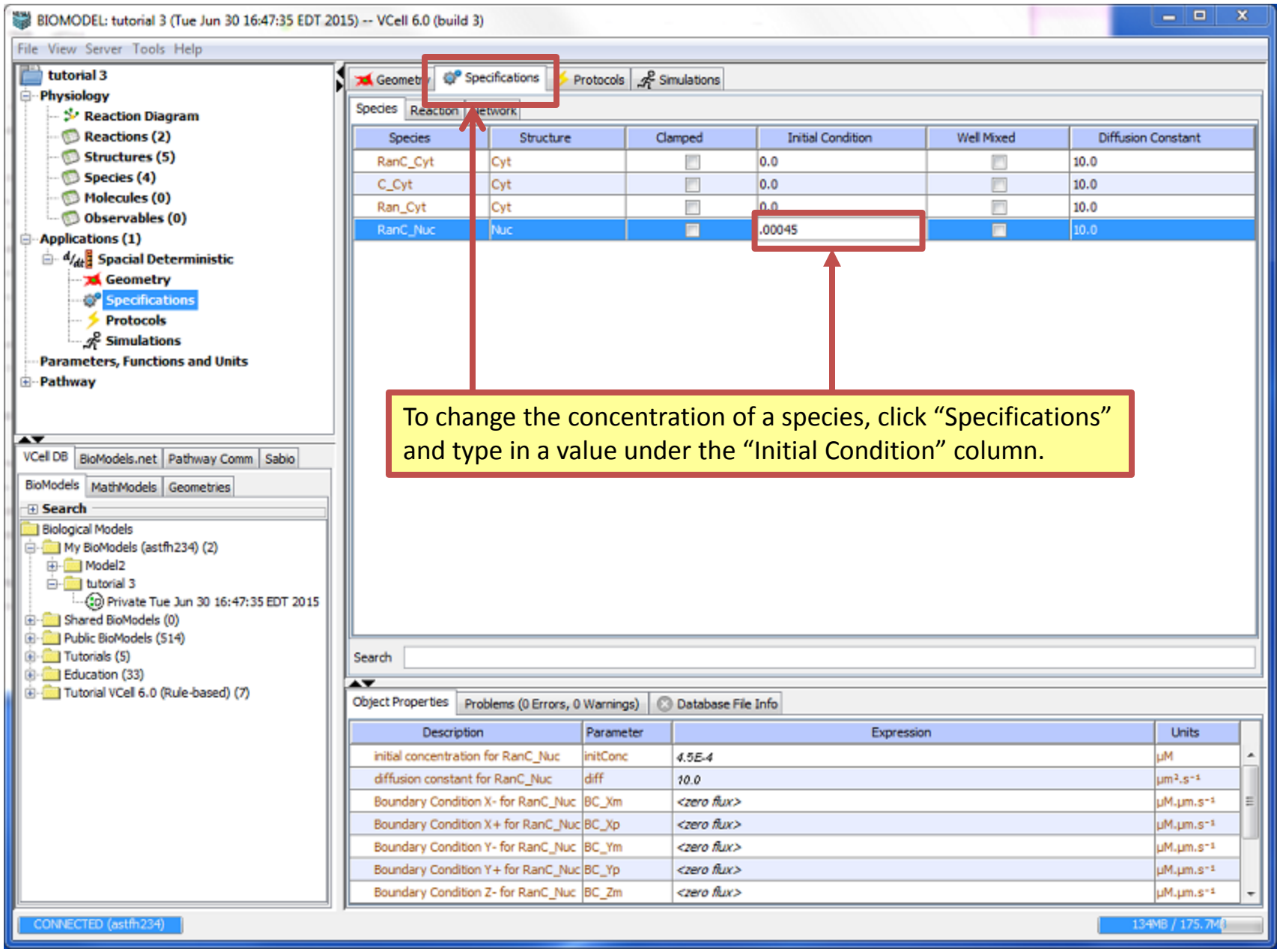
Object Properties
Problems (0 Errors, 10 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
The geometry of your model is now complete.
CONNECTED (astfh234)
200.9MB / 303.9MB

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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Species
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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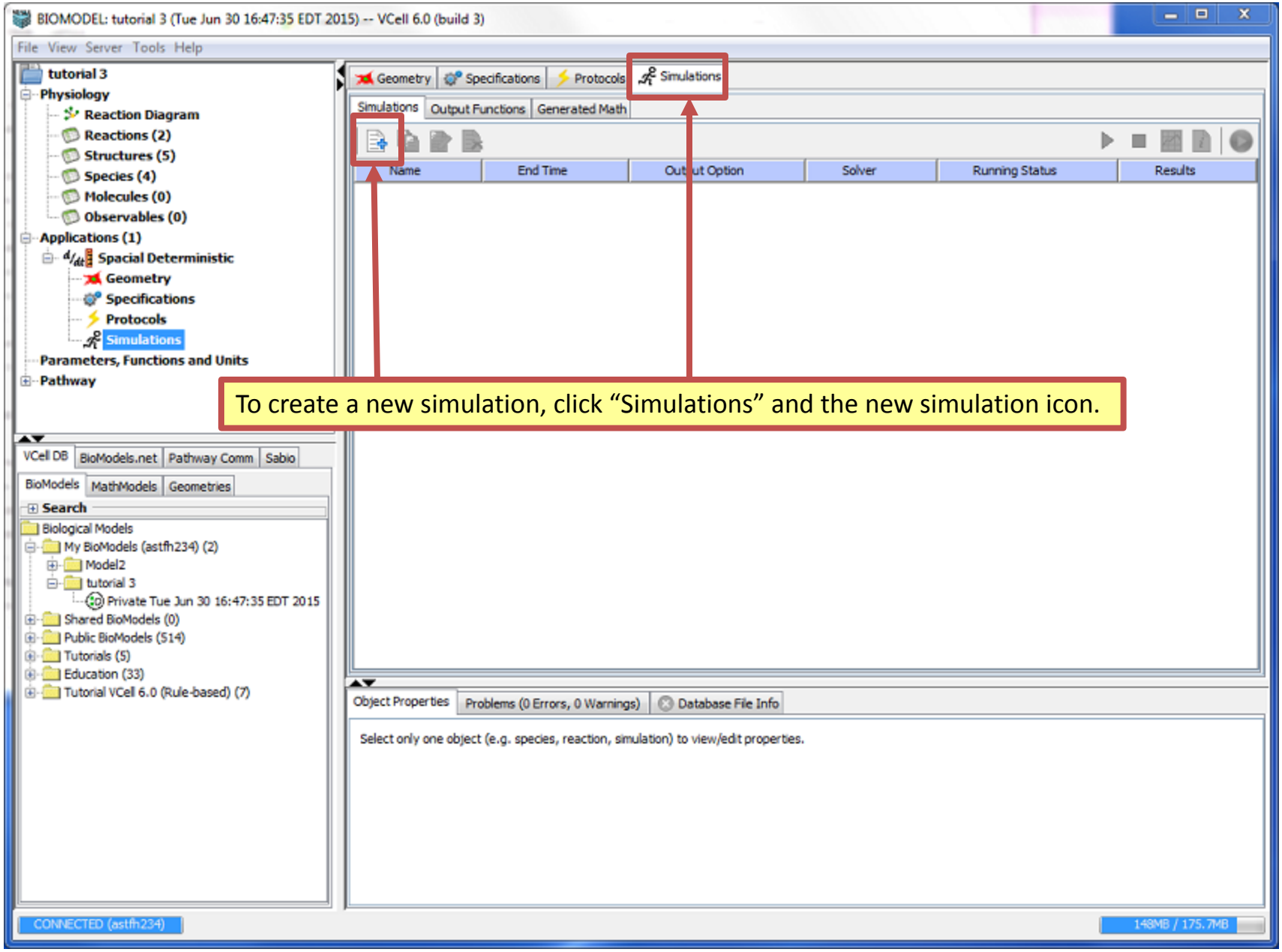
Tutorial VCell 6.0 (Rule-based) (7)
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for RanC_Nuc
initConc
4.5E-4
μM
diffusion constant for RanC_Nuc
diff
10.0
μm².s⁻¹
Boundary Condition X- for RanC_Nuc
BC_Xm
<zero 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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Observables (0)
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Simulations
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Generated Math
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End Time
Output Option
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Running Status
Results
To create a new simulation, click “Simulations” and the new simulation icon.
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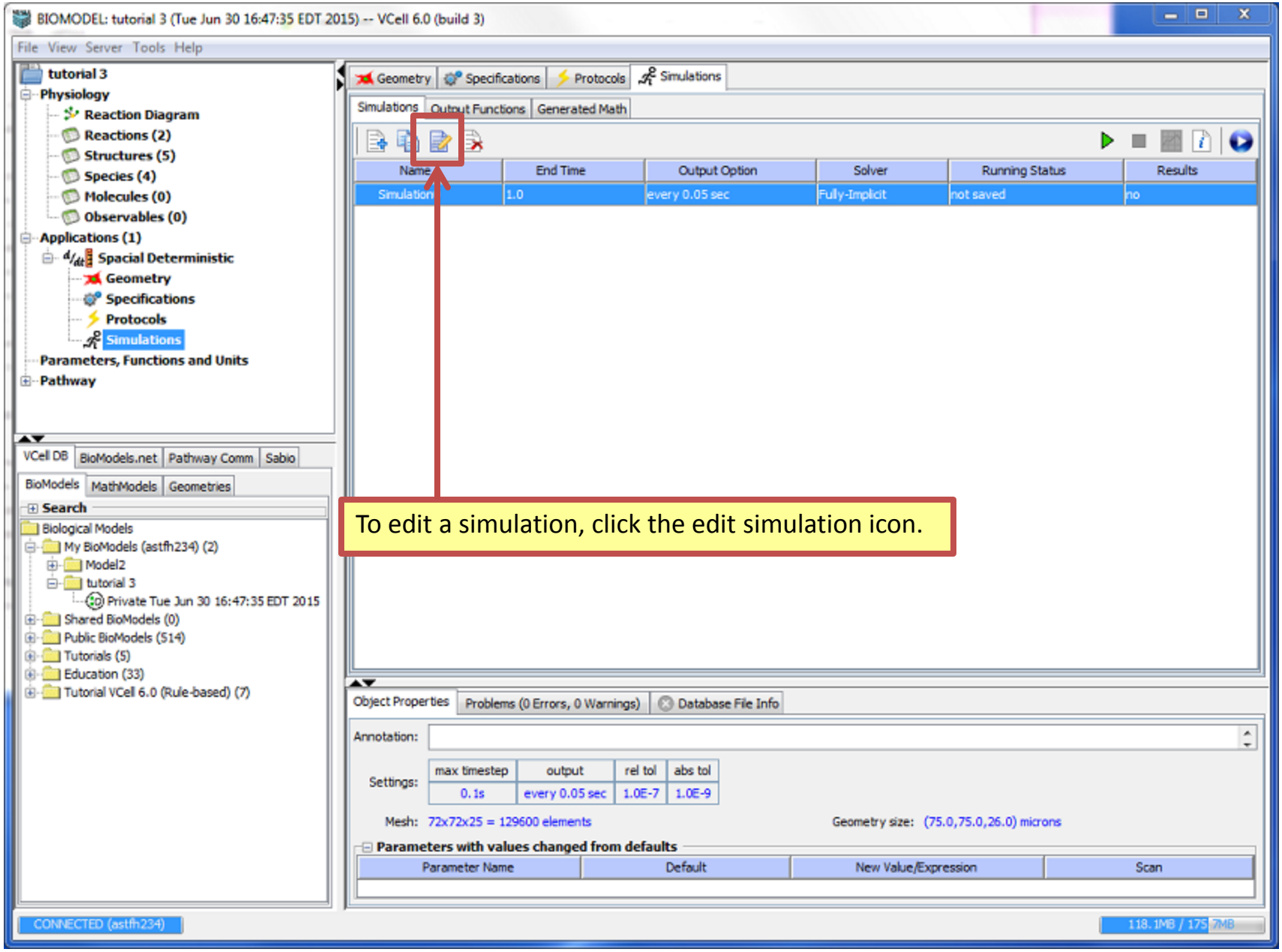
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
148MB / 175.7MB

Contents


BIOMODEL: tutorial 3 (Tue Jun 30 16:47:35 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
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Species (4)
Molecules (0)
Observables (0)
Applications (1)
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Pathway
Geometry
Specifications
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Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
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
BioModels.net
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Sabio
BioModels
MathModels
Geometries
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My BioModels (astfh234) (2)
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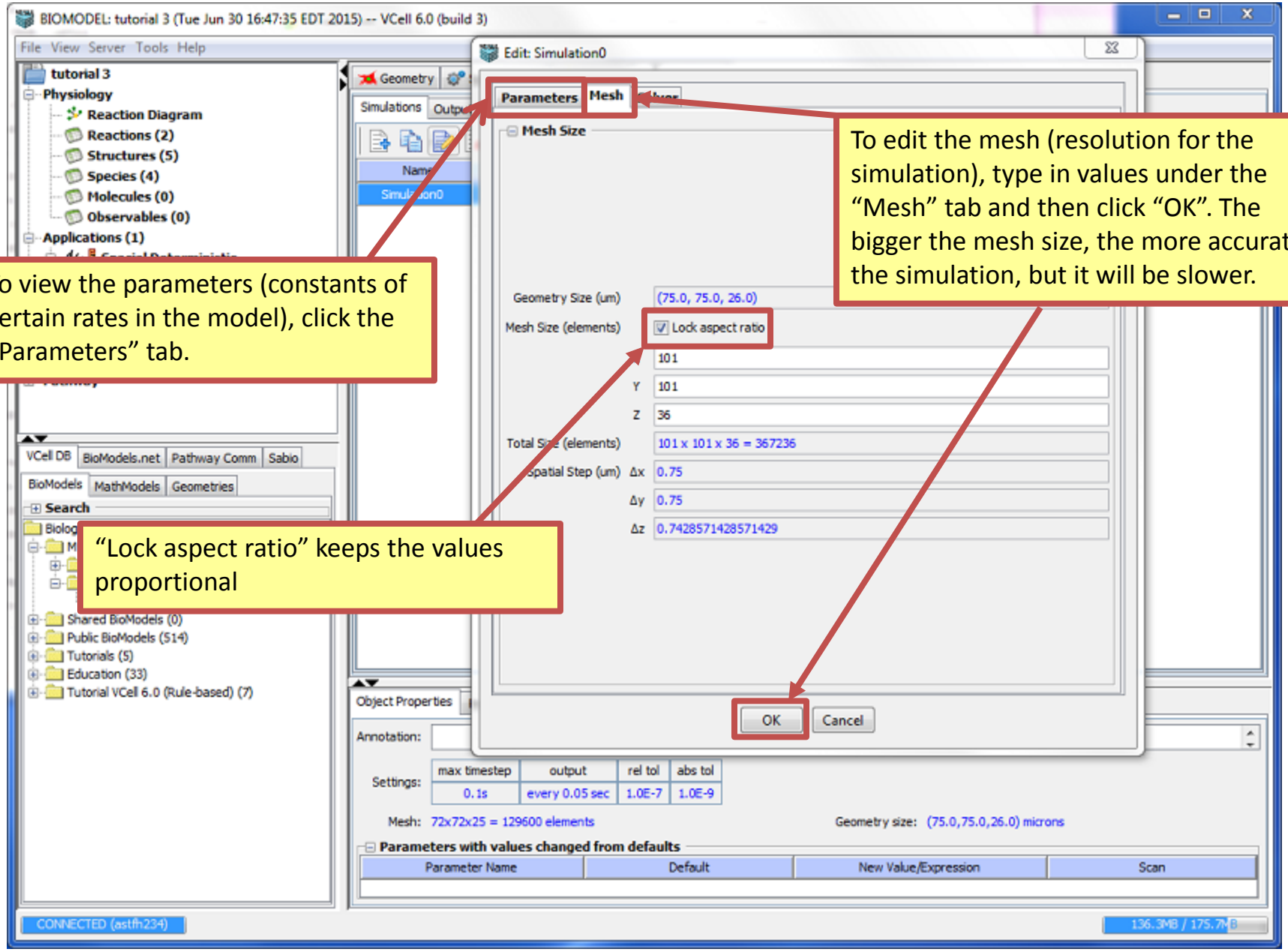
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.05 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
118.1MB / 175.7MB

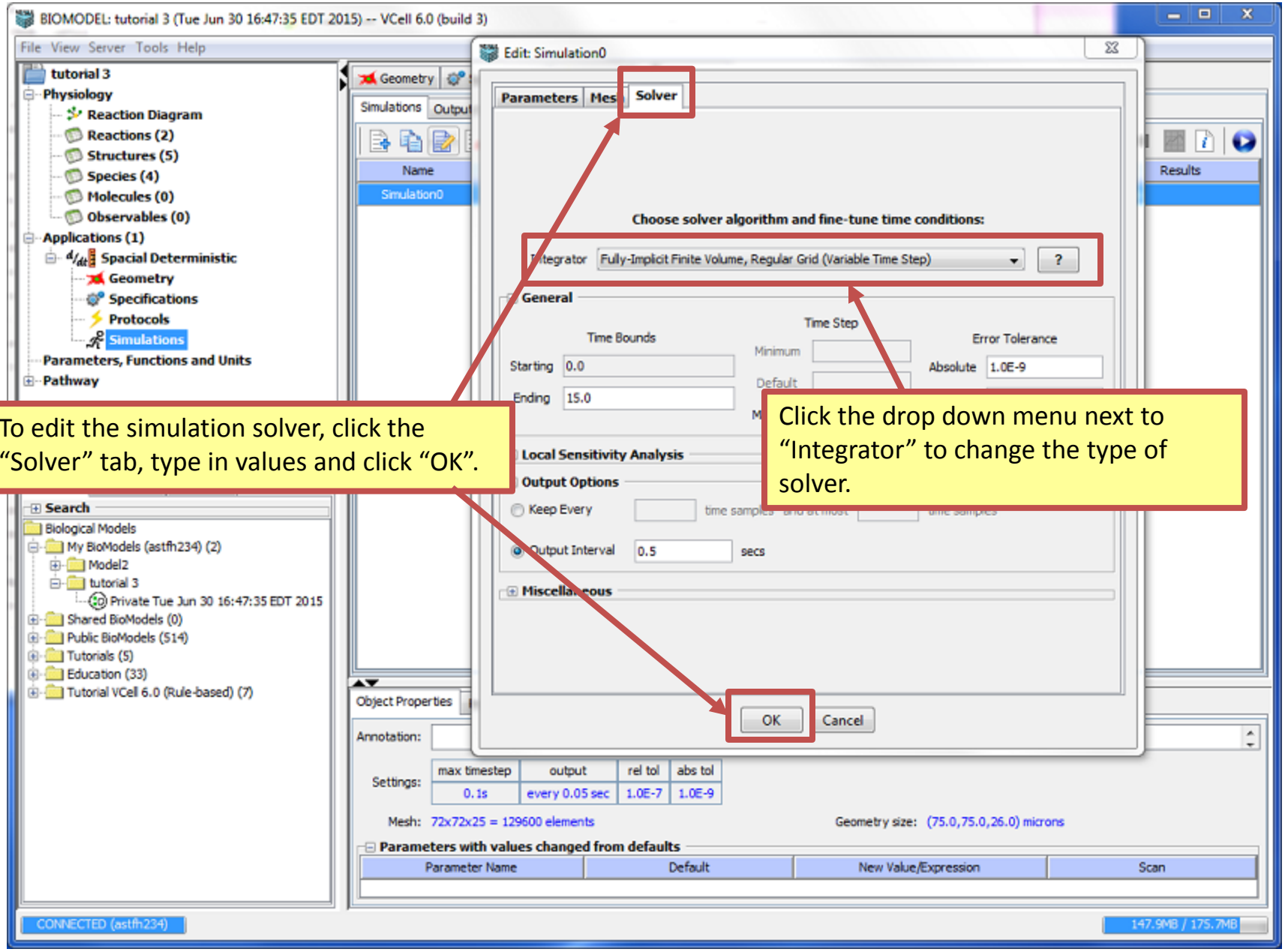


To view the parameters (constants of certain rates in the model), click the "Parameters" tab.

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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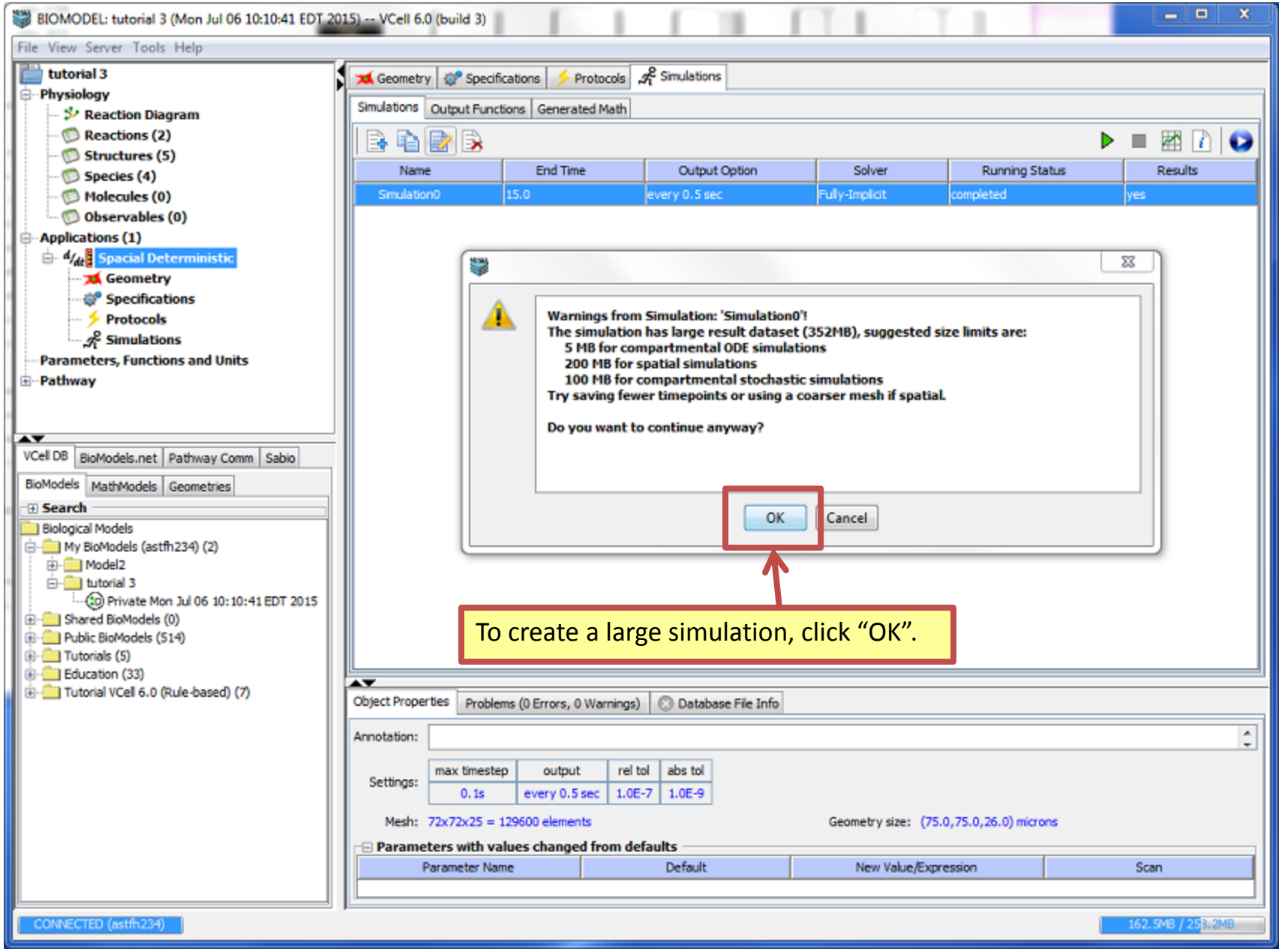
Tutorial VCell 6.0 (Rule-based) (7)
Geometry
Simulations
Output
Name
Simulation0
Results
Edit: Simulation0
Parameters
Mes
Solver
Choose solver algorithm and fine-tune time conditions:
Integrator
Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)
?
General
Time Bounds
Starting
0.0
Ending
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)
File View Server Tools Help
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Observables (0)
Applications (1)
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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
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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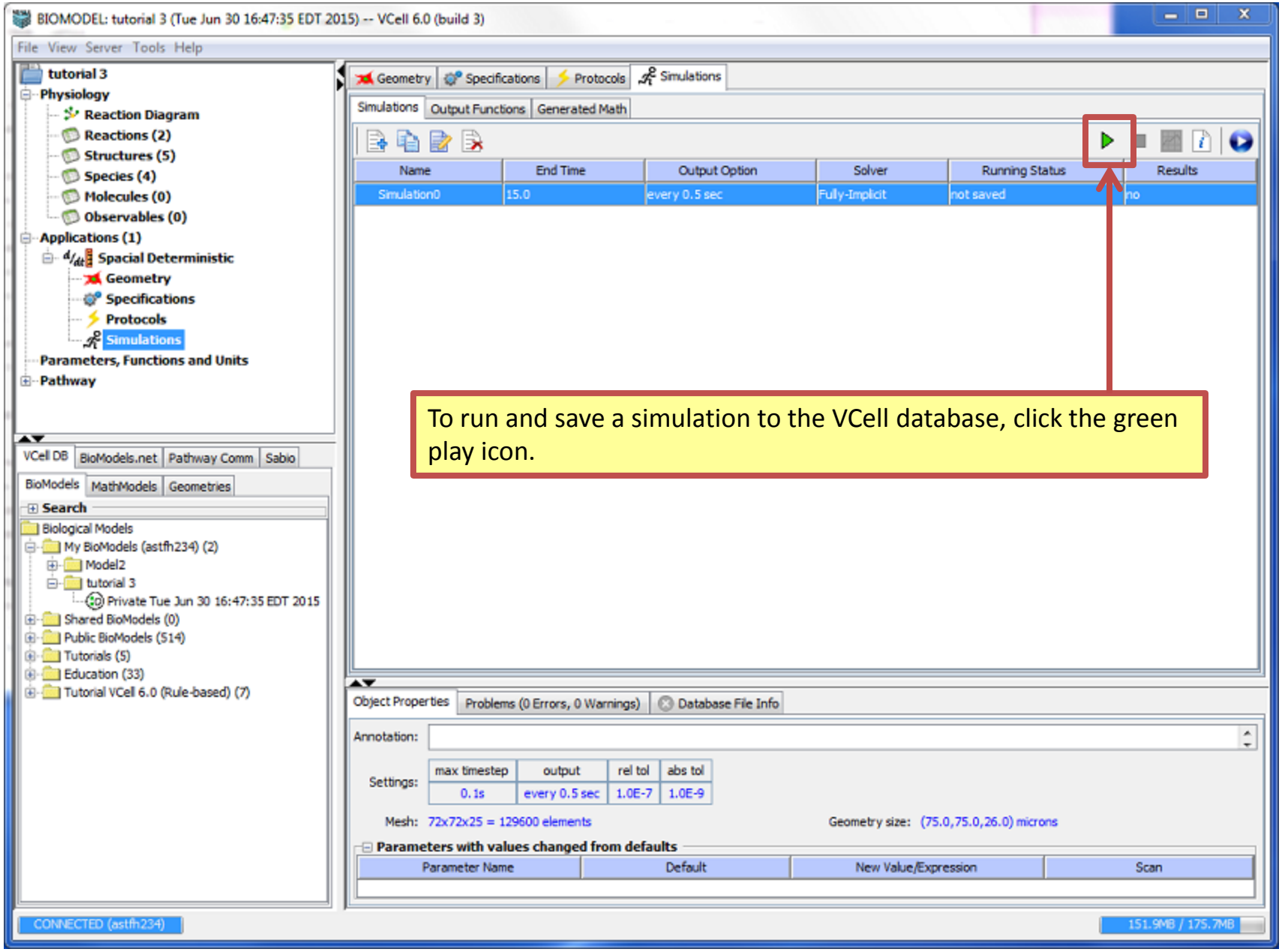
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
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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Simulations
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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.
VCell DB
BioModels.net
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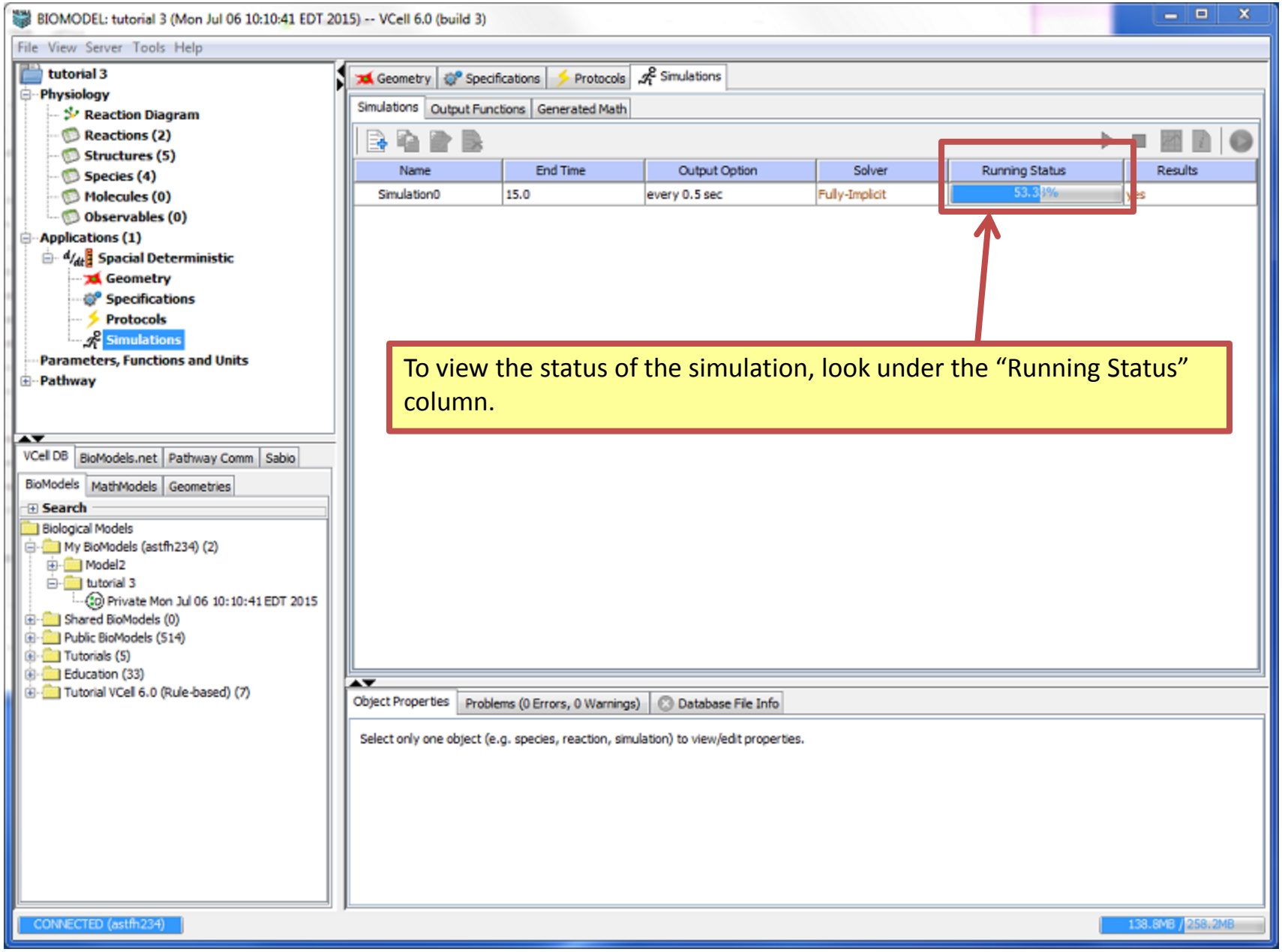
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from 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.
VCell DB
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Public BioModels (514)
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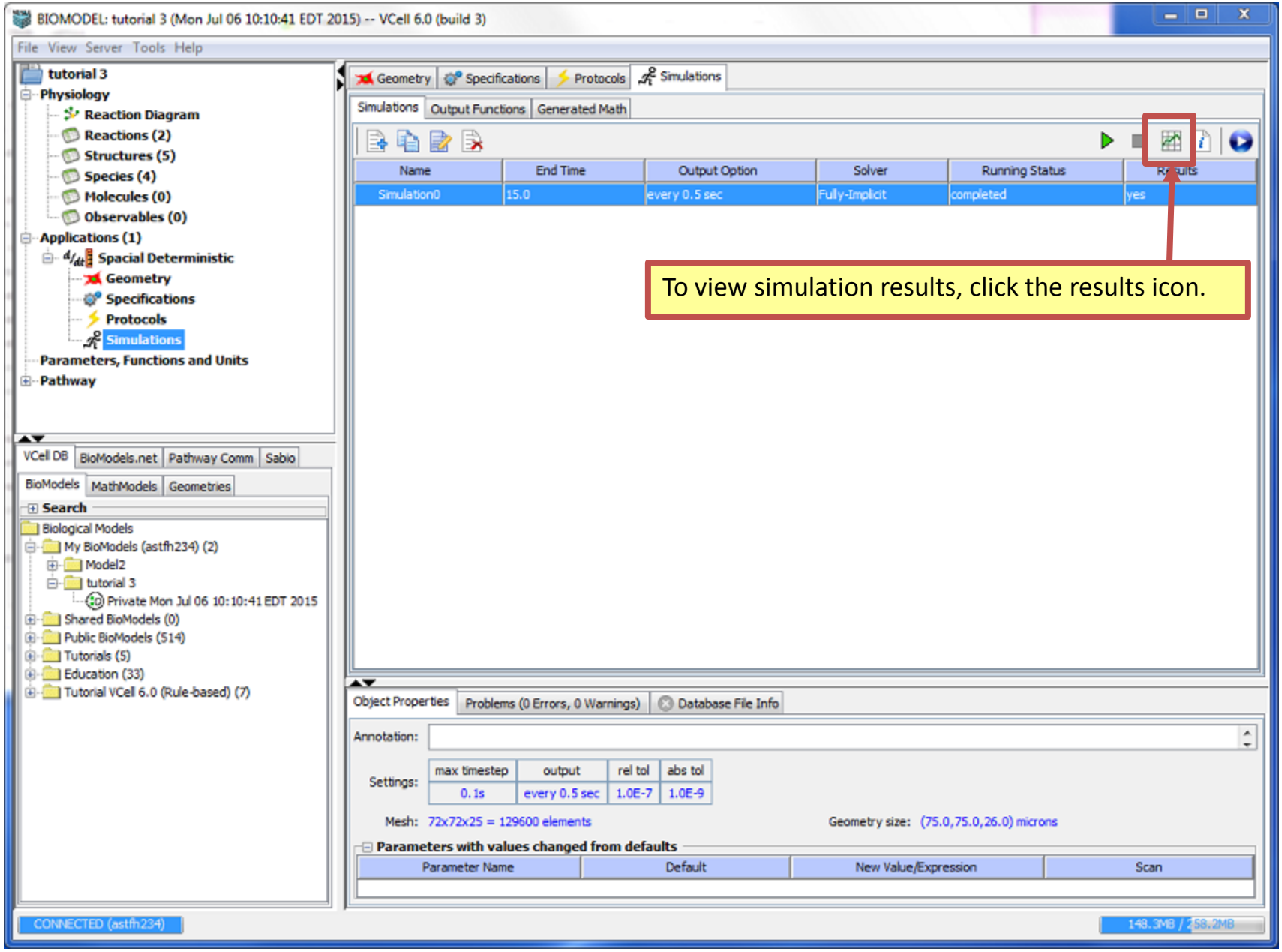
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
138.8MB / 258.2MB


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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Observables (0)
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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
BioModels.net
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Sabio
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MathModels
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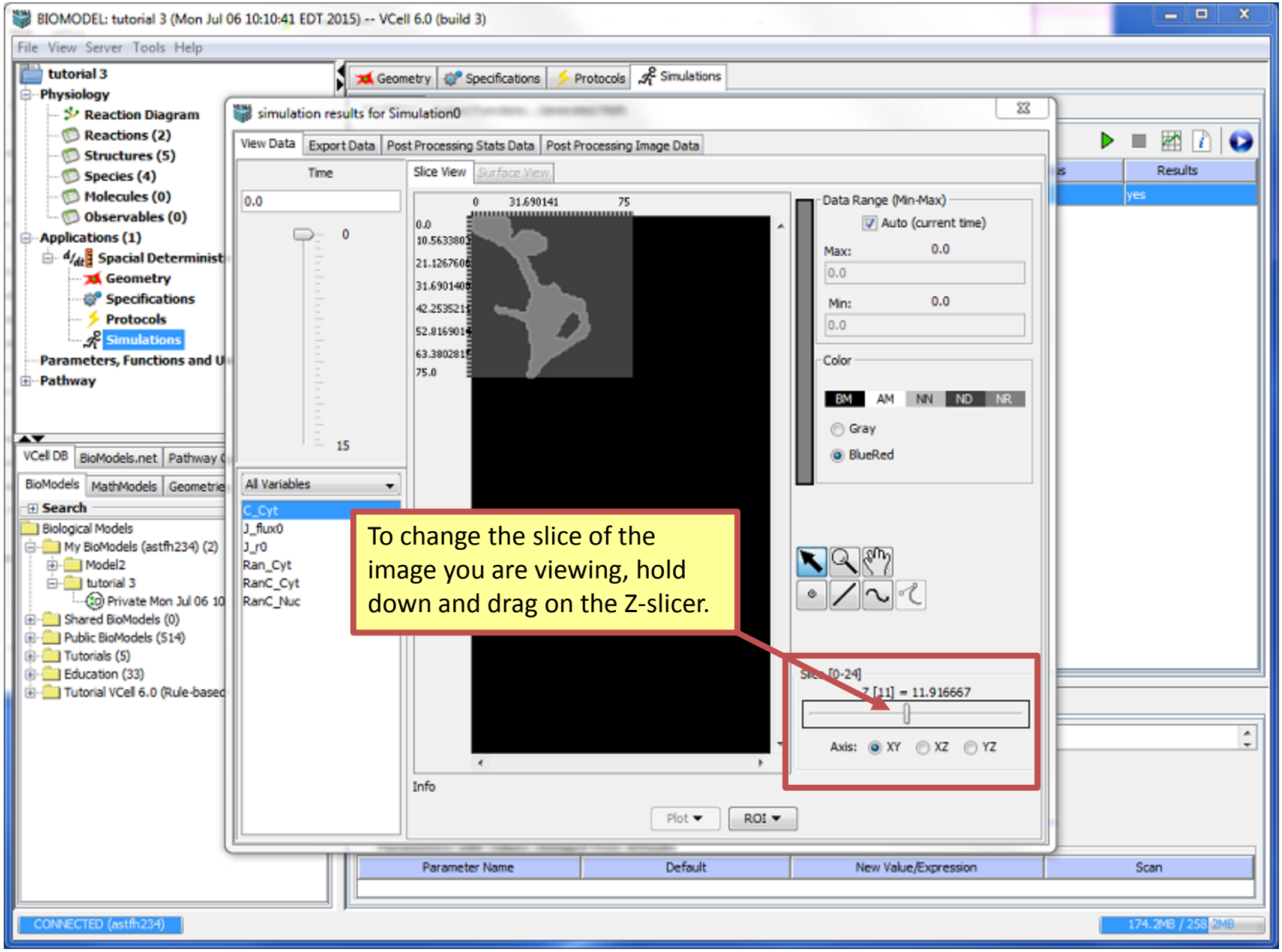
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
max timestep
output
rel tol
abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
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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Reactions (2)
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Specifications
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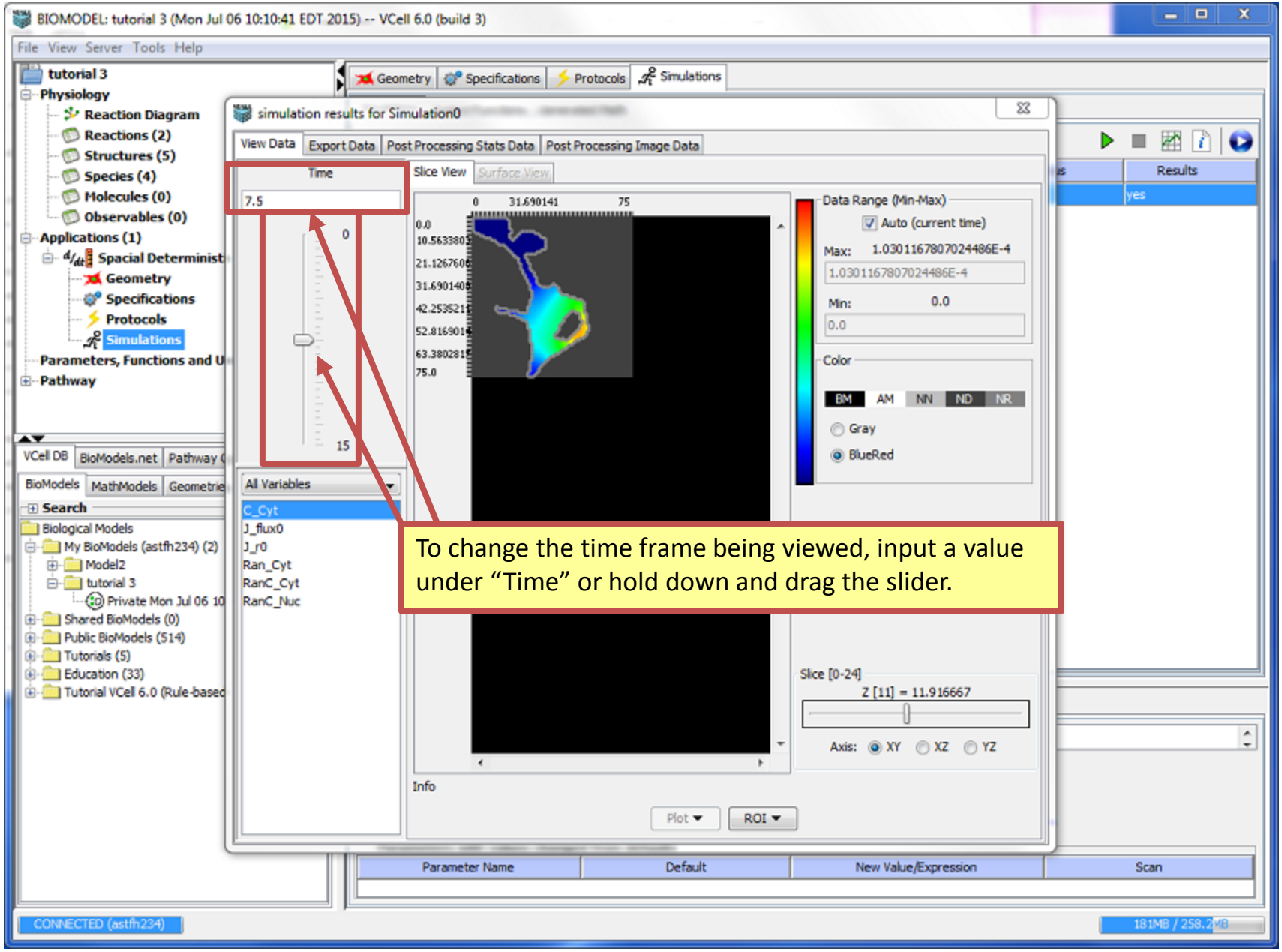
Simulations
simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
0.0
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max:
0.0
Min:
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
C_Cyt
J_flux0
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
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
Default
New Value/Expression
Scan
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (astfh234) (2)
Model2
tutorial 3
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based
CONNECTED (astfh234)
Results
yes

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (1)
Spacial Determinist
Geometry
Specifications
Protocols
Simulations
Parameters, Functions and U
Pathway
Geometry
Specifications
Protocols
Simulations
simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
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
Info
Plot
ROI
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (astfh234) (2)
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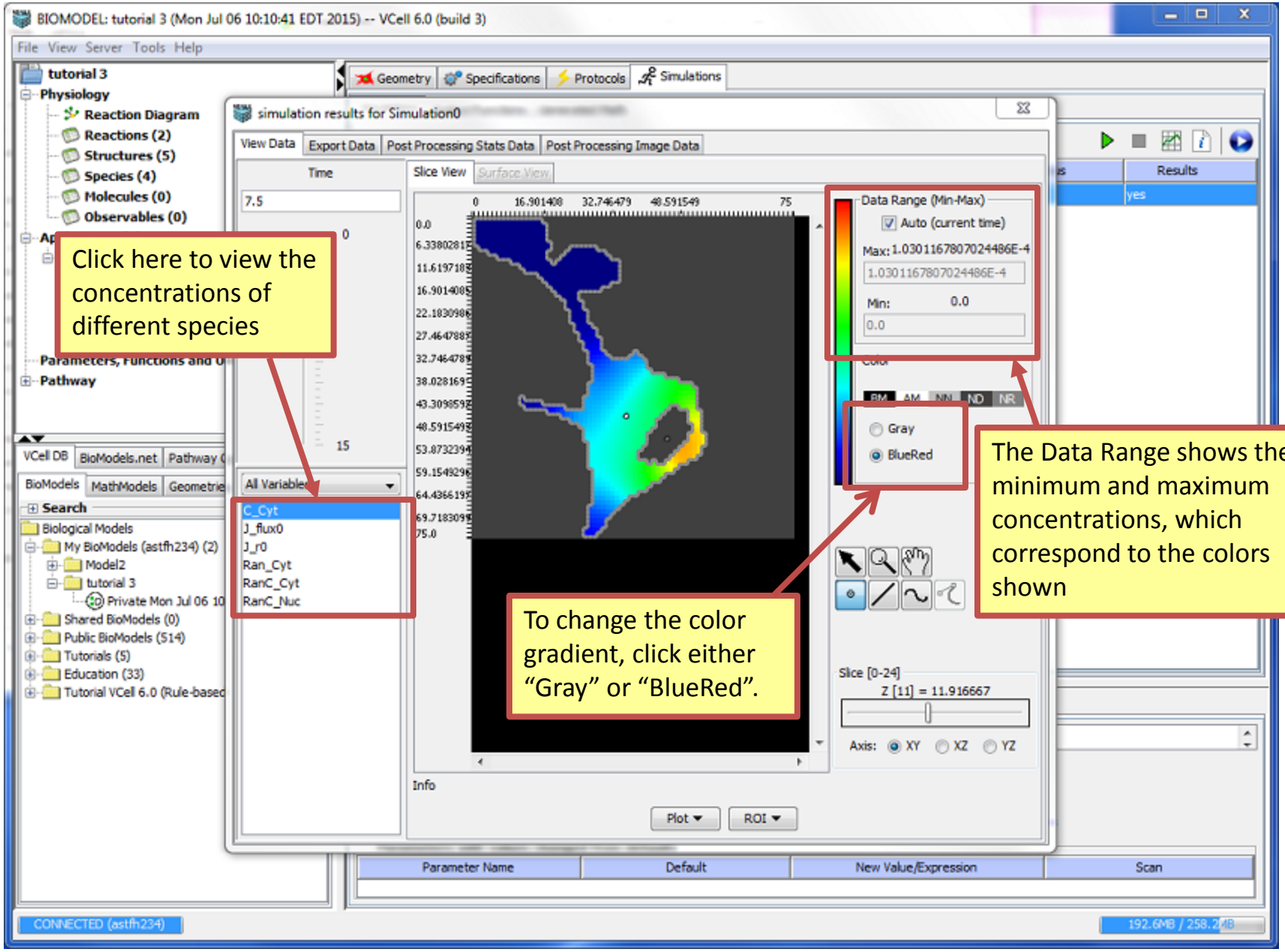
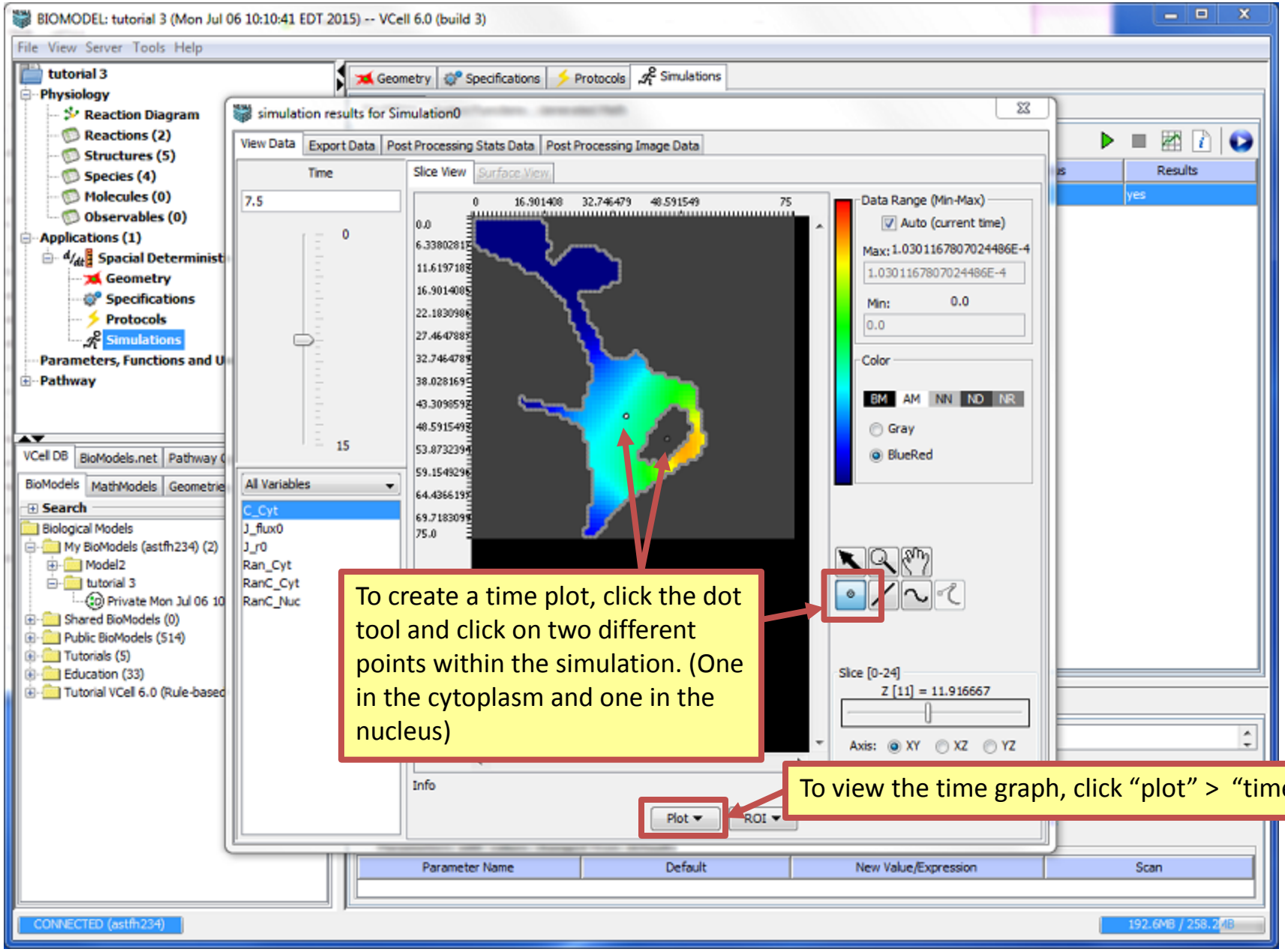
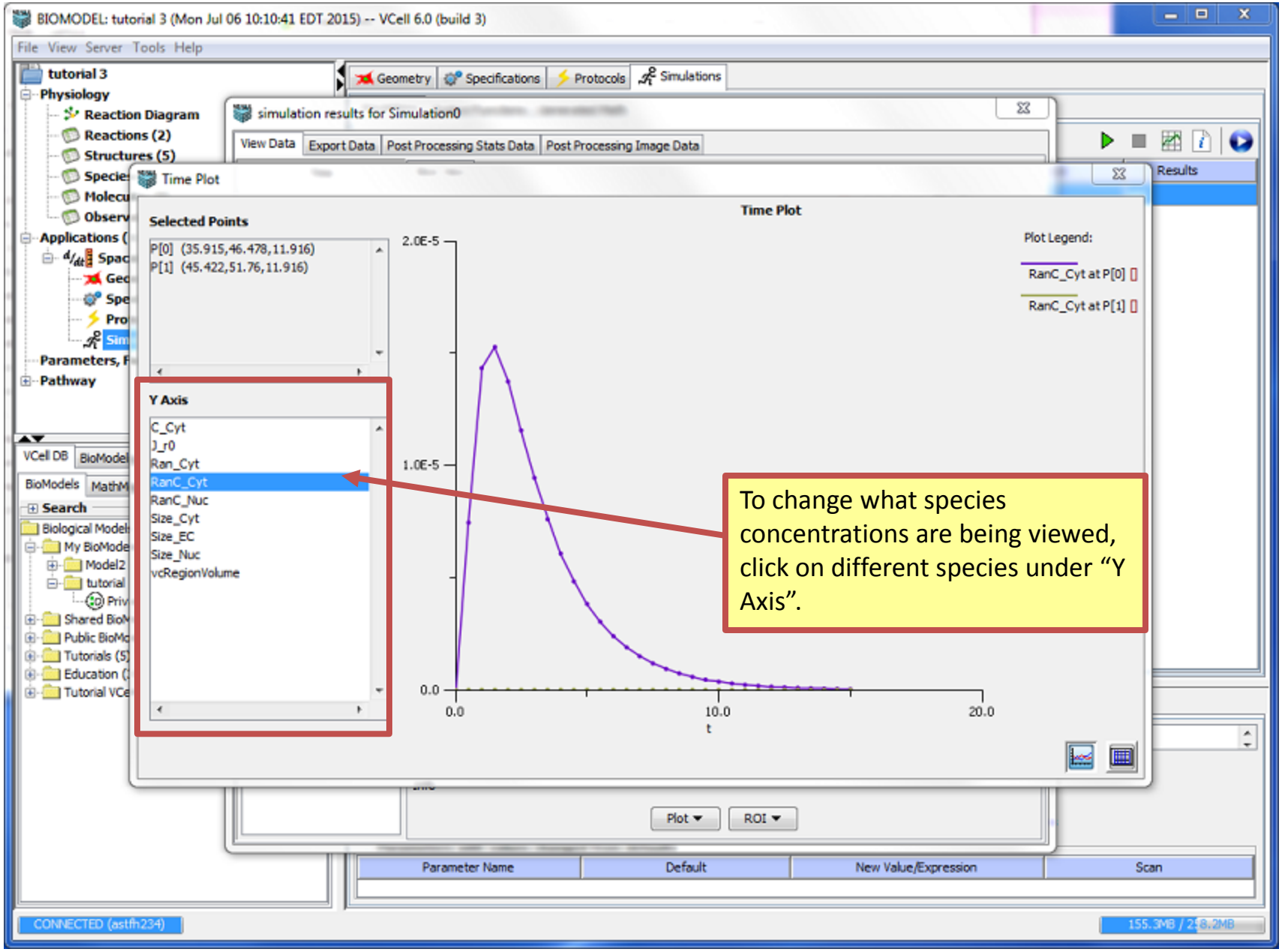
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based
Results
yes
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
181MB / 258.2MB
To change the time frame being viewed, input a value under “Time” or hold down and drag the slider.

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


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
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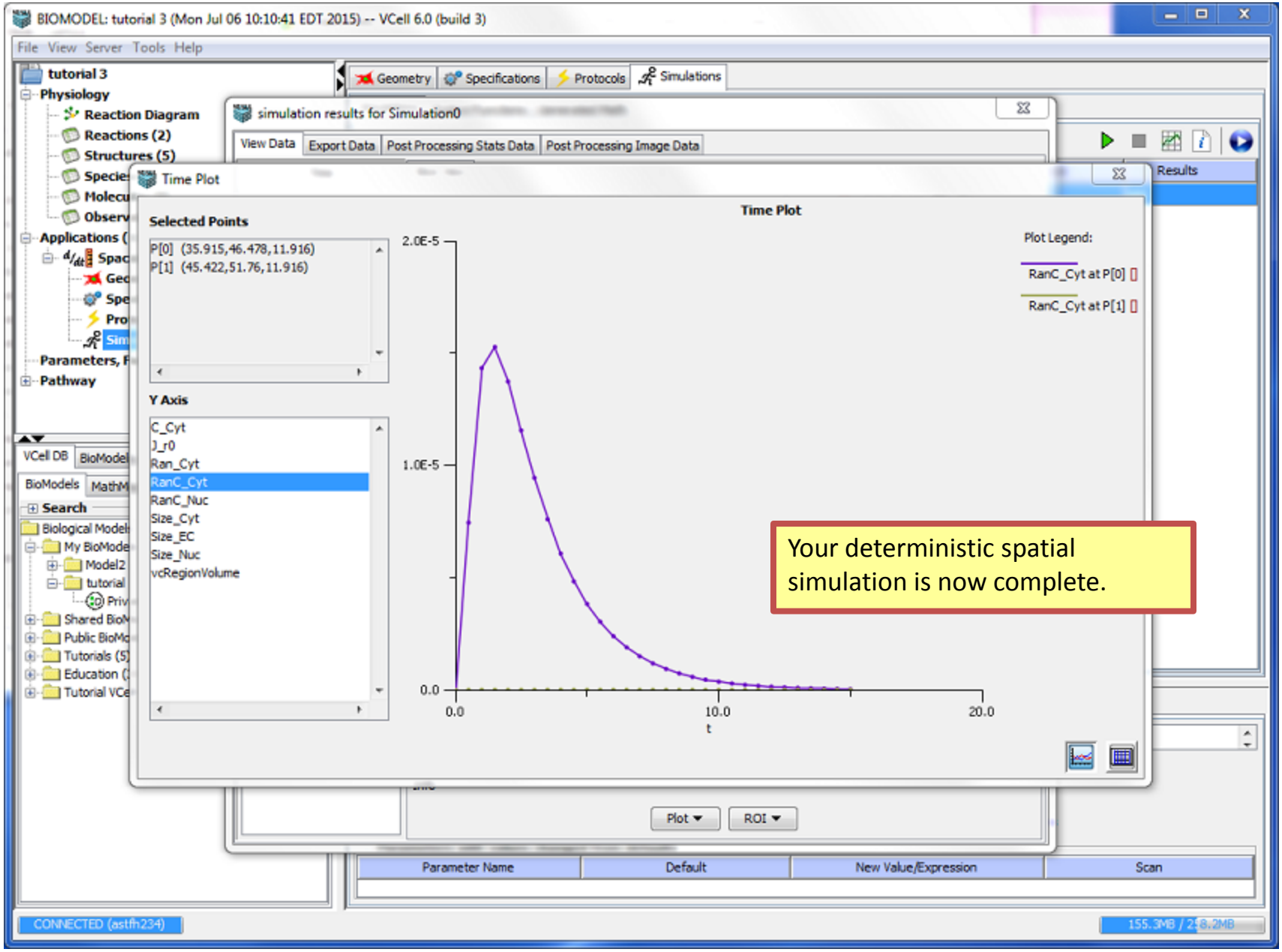
Protocols
Simulations
simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Results
Time Plot
Selected Points
P[0] (35.915,46.478,11.916)
P[1] (45.422,51.76,11.916)
Time Plot
Plot Legend:
RanC_Cyt at P[0]
RanC_Cyt at P[1]
2.0E-5
1.0E-5
0.0
0.0
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
ROI
Parameter Name
Default
New Value/Expression
Scan
VCell DB
BioModels
Search
Biological Model
My BioMode
Model2
tutorial
Shared BioM
Public BioMo
Tutorials (5)
Education (
Tutorial VCe
CONNECTED (astfh234)

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 10:10:41 EDT 2015) -- VCell 6.0 (build 3)
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tutorial 3
Physiology
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Reactions (2)
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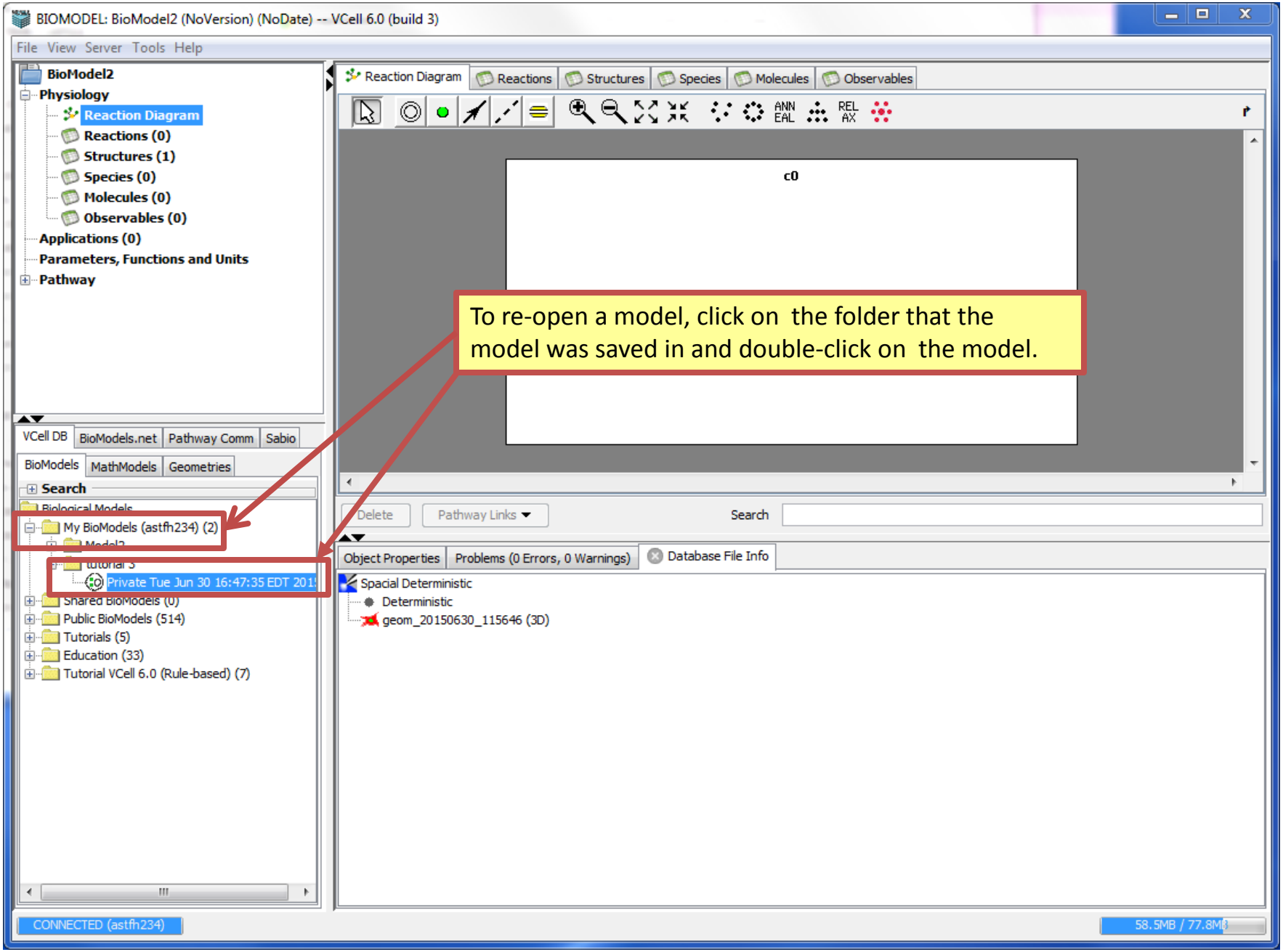
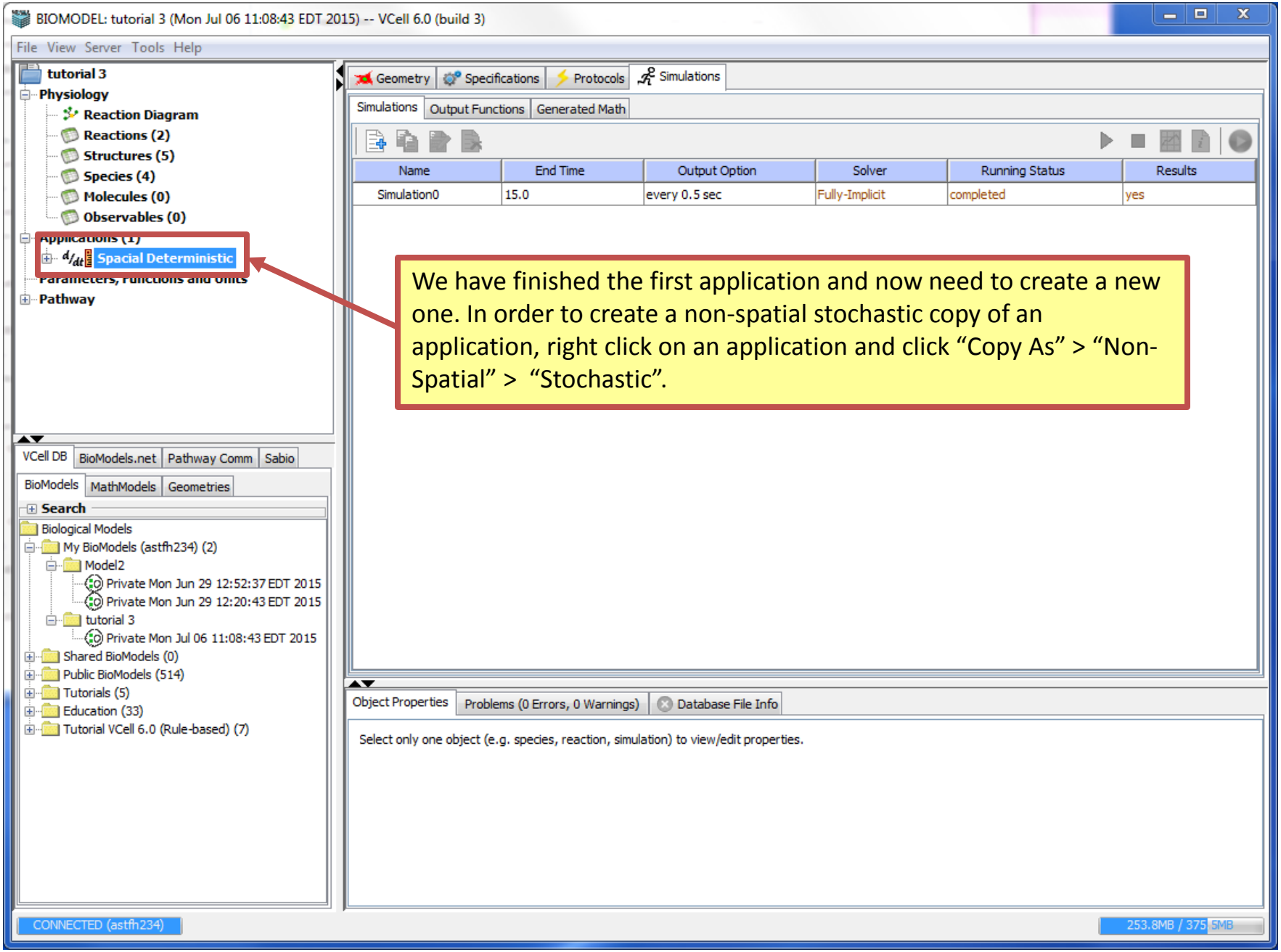
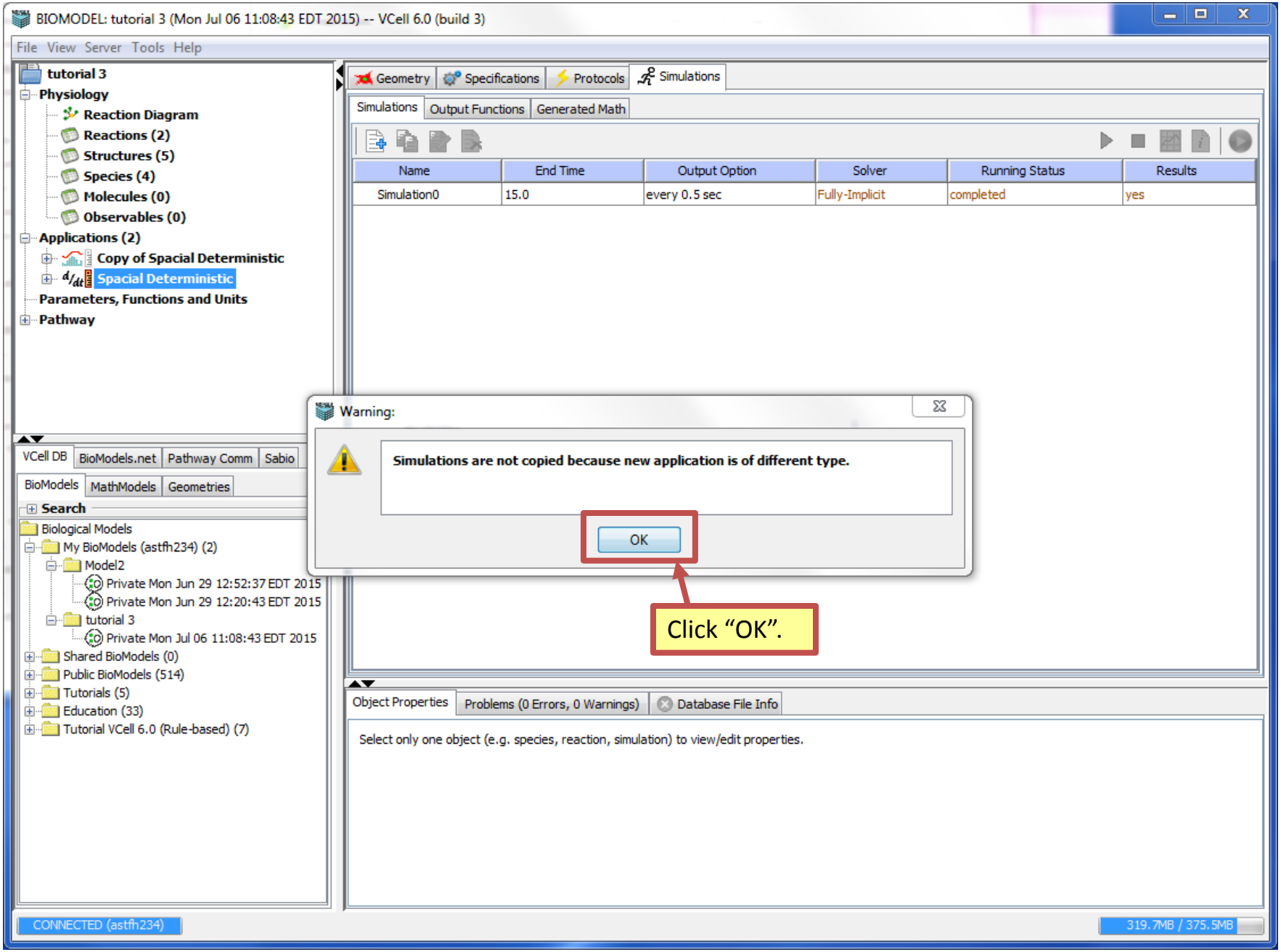
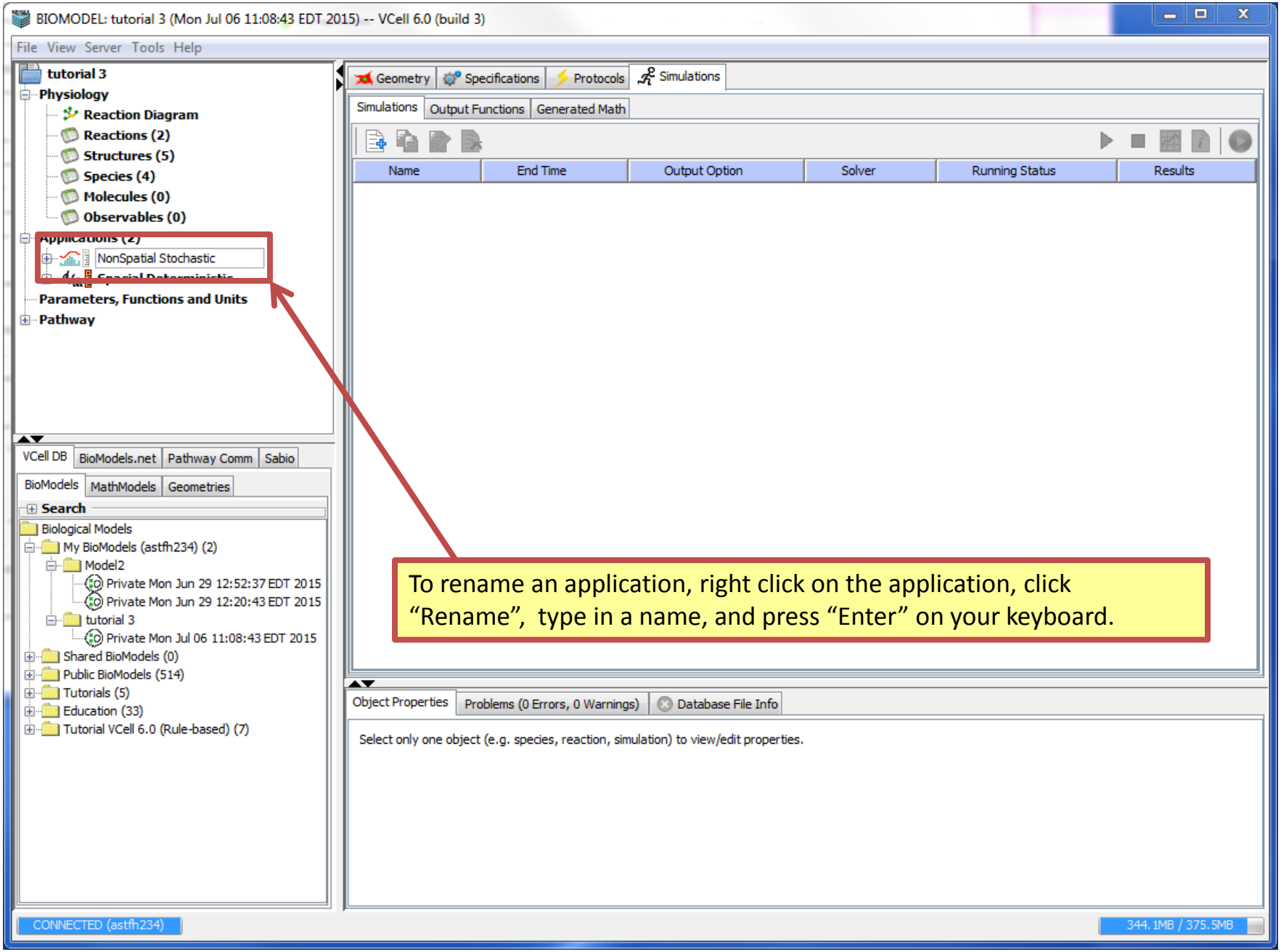
simulation results for Simulation0
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Results
Time Plot
Selected Points
P[0] (35.915,46.478,11.916)
P[1] (45.422,51.76,11.916)
Y Axis
C_Cyt
J_r0
Ran_Cyt
RanC_Cyt
RanC_Nuc
Size_Cyt
Size_EC
Size_Nuc
vcRegionVolume
Time Plot
Plot Legend:
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
Scan
VCell DB
BioModels
Search
CONNECTED (astfh234)

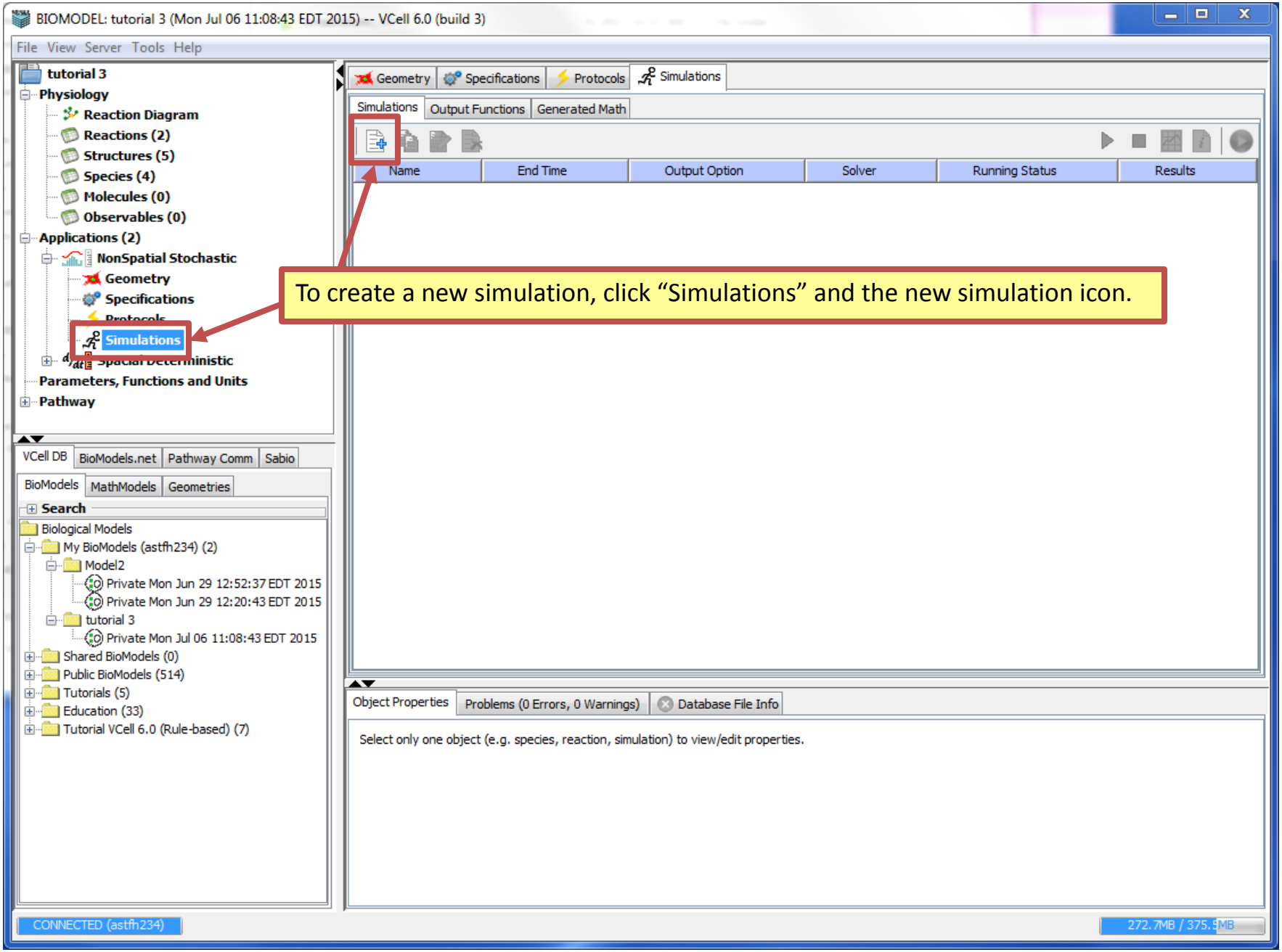

BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
File View Server Tools Help
BioModel2
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
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
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
My BioModels (astfh234) (2)
Private Tue Jun 30 16:47:35 EDT 201
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Spacial Deterministic
Deterministic
geom_20150630_115646 (3D)
CONNECTED (astfh234)
58.5MB / 77.8MB

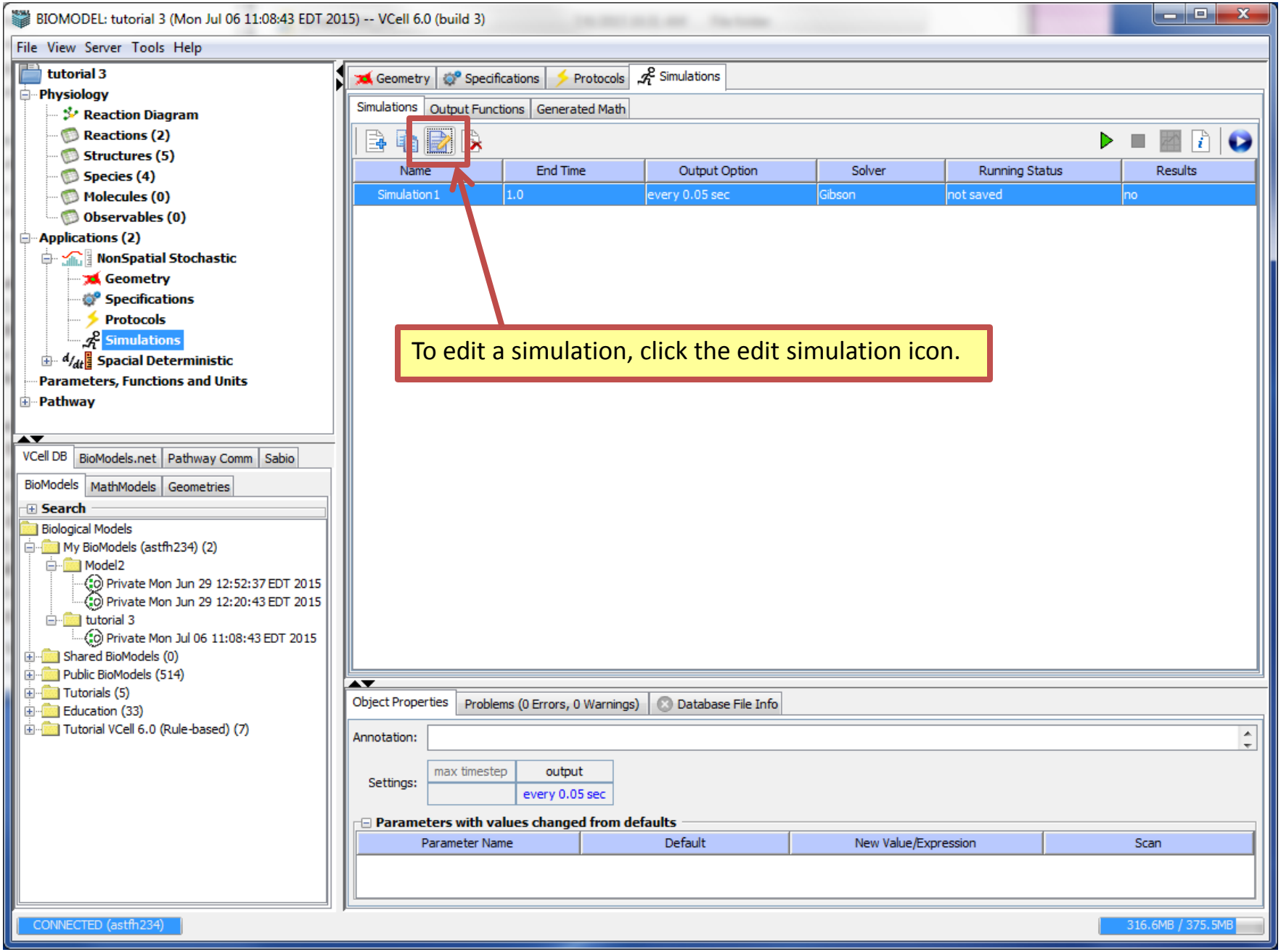

BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Spacial Deterministic
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
15.0
every 0.5 sec
Fully-Implicit
completed
yes
We have finished the first application and now need to create a new one. In order to create a non-spatial stochastic copy of an application, right click on an application and click “Copy As” > “Non-Spatial” > “Stochastic”.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 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
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
253.8MB / 375.5MB

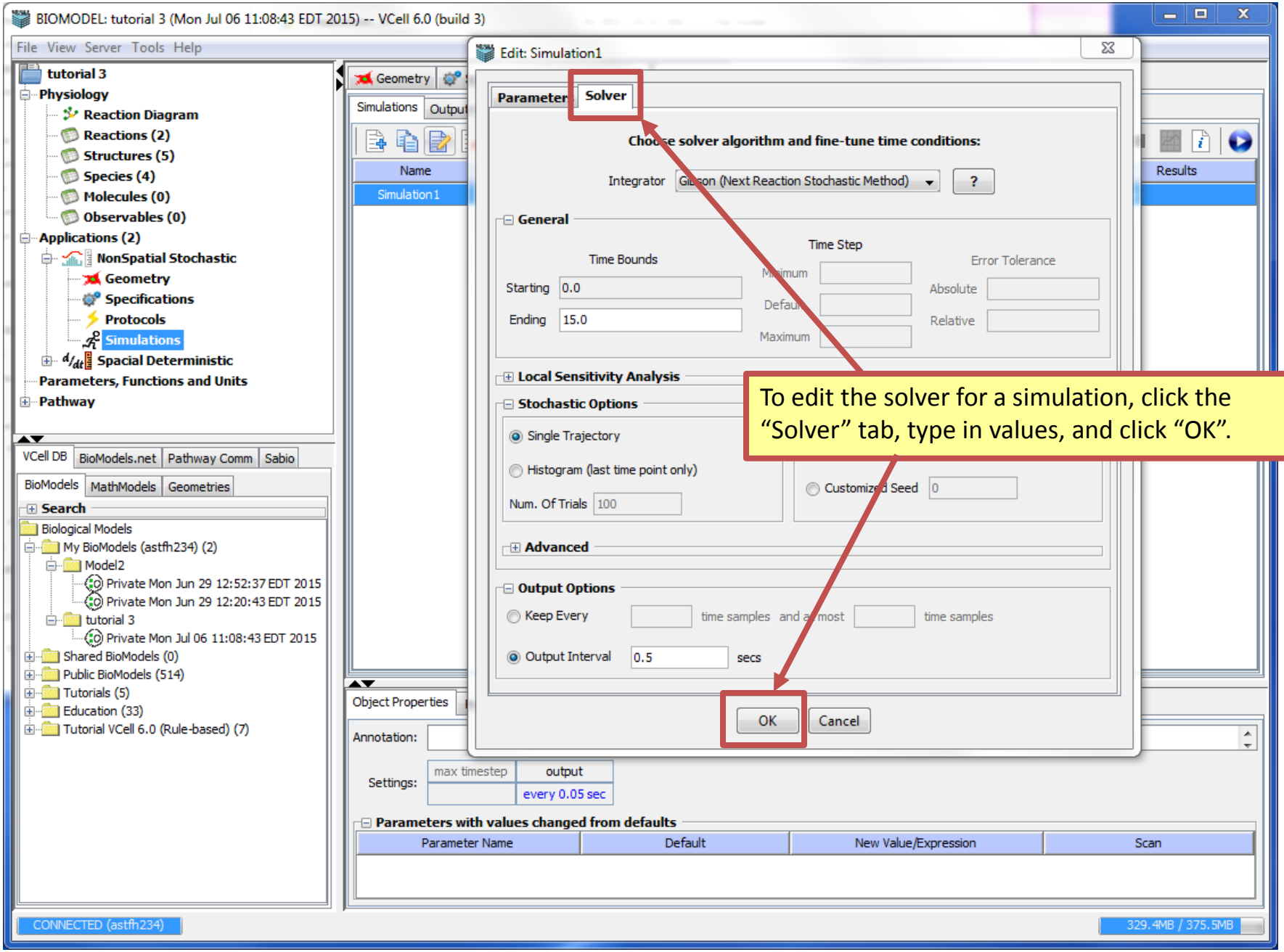

BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
Copy of Spacial Deterministic
Spacial Deterministic
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
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
Warning:
Simulations are not copied because new application is of different type.
OK
Click “OK”.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 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
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
319.7MB / 375.5MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To rename an application, right click on the application, click "Rename", type in a name, and press "Enter" on your keyboard.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 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
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
344.1MB / 375.5MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Geometry
Specifications
Simulations
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To create a new simulation, click “Simulations” and the new simulation icon.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 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
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
272.7MB / 375.5MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Geometry
Specifications
Protocols
Simulations
Spacial Deterministic
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
1.0
every 0.05 sec
Gibson
not saved
no
To edit a simulation, click the edit simulation icon.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 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
every 0.05 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
316.6MB / 375.5MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:08:43 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Geometry
Specifications
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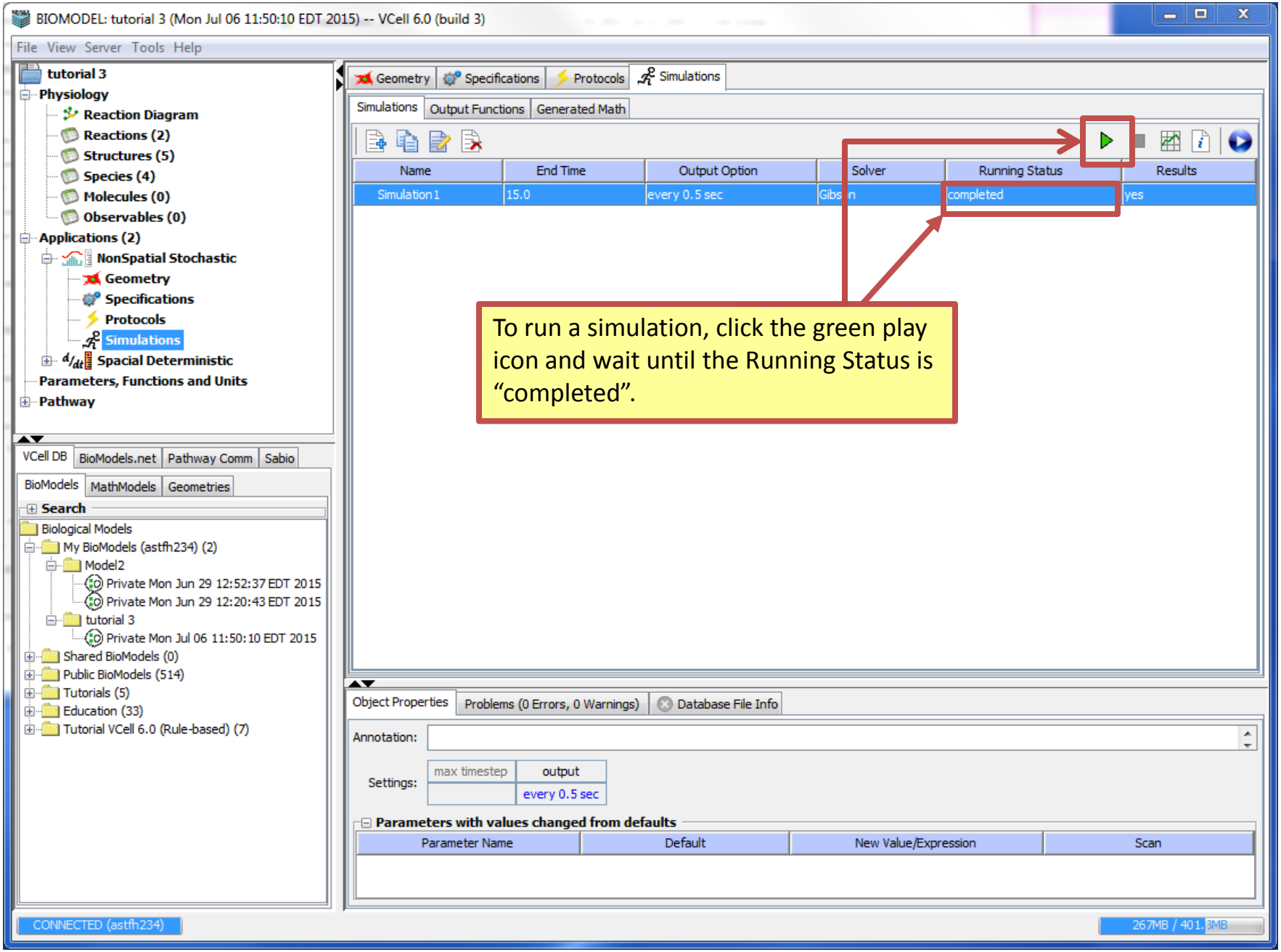
Spacial Deterministic
Parameters, Functions and Units
Pathway
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:08:43 EDT 2015
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Geometry
Simulations
Output
Name
Simulation1
Results
Edit: Simulation1
Parameter
Solver
Choose solver algorithm and fine-tune time conditions:
Integrator
Gibson (Next Reaction Stochastic Method)
?
General
Time Bounds
Starting
0.0
Ending
15.0
Time Step
Minimum
Default
Maximum
Error Tolerance
Absolute
Relative
Local Sensitivity Analysis
Stochastic Options
Single Trajectory
Histogram (last time point only)
Num. Of Trials
100
Customized Seed
0
Advanced
Output Options
Keep Every
time samples and at most
time samples
Output Interval
0.5
secs
OK
Cancel
To edit the solver for a simulation, click the "Solver" tab, type in values, and click "OK".
Object Properties
Annotation:
Settings:
max timestep
output
every 0.05 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
329.4MB / 375.5MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
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Physiology
Reaction Diagram
Reactions (2)
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Molecules (0)
Observables (0)
Applications (2)
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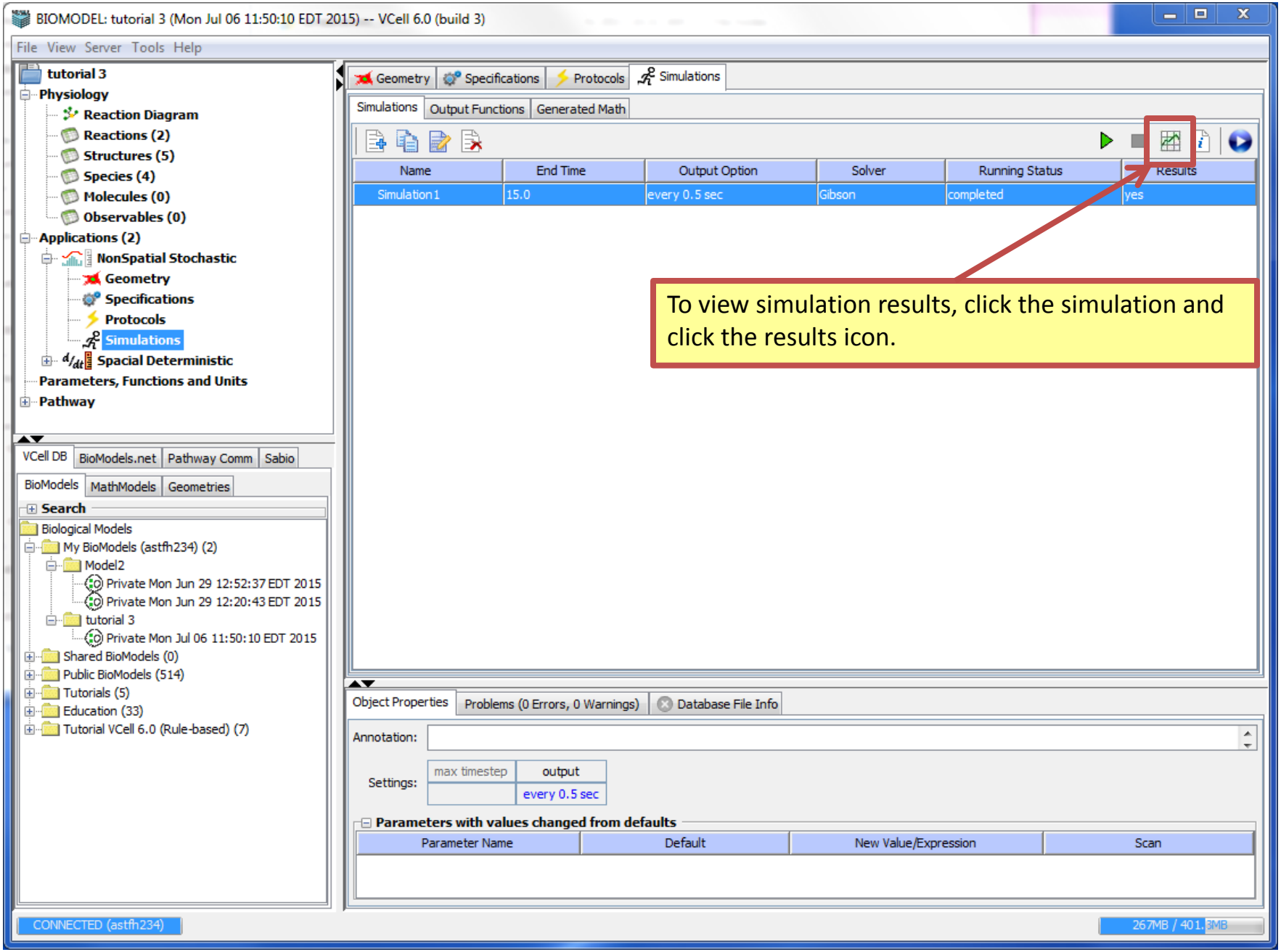
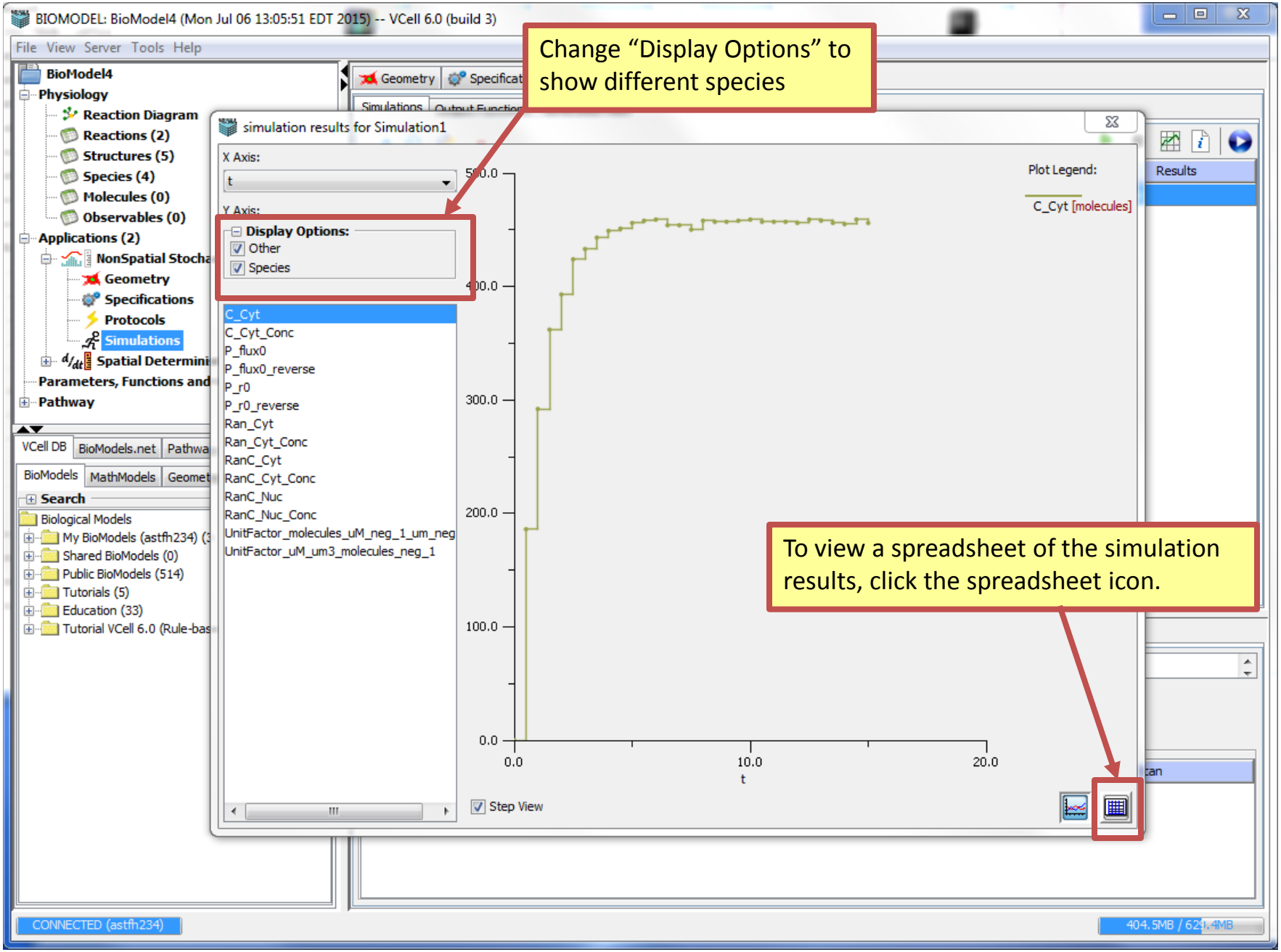
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
15.0
every 0.5 sec
completed
yes
To run a simulation, click the green play icon and wait until the Running Status is "completed".
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:50:10 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
every 0.5 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
267MB / 401.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Geometry
Specifications
Protocols
Simulations
Spacial Deterministic
Parameters, Functions and Units
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
15.0
every 0.5 sec
Gibson
completed
yes
To view simulation results, click the simulation and click the results icon.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:50:10 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
every 0.5 sec
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
267MB / 401.3MB

Contents


Change “Display Options” to show different species
To view a spreadsheet of the simulation results, click the spreadsheet icon.
BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
BioModel4
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
Geometry
Specifications
Protocols
Simulations
Parameters, Functions and
Pathway
simulation results for Simulation1
X Axis:
t
Y Axis:
Display Options:
Other
Species
C_Cyt
C_Cyt_Conc
P_flux0
P_flux0_reverse
P_r0
P_r0_reverse
Ran_Cyt
Ran_Cyt_Conc
RanC_Cyt
RanC_Cyt_Conc
RanC_Nuc
RanC_Nuc_Conc
UnitFactor_molecules_uM_neg_1_um_neg
UnitFactor_uM_um3_molecules_neg_1
Plot Legend:
C_Cyt [molecules]
500.0
400.0
300.0
200.0
100.0
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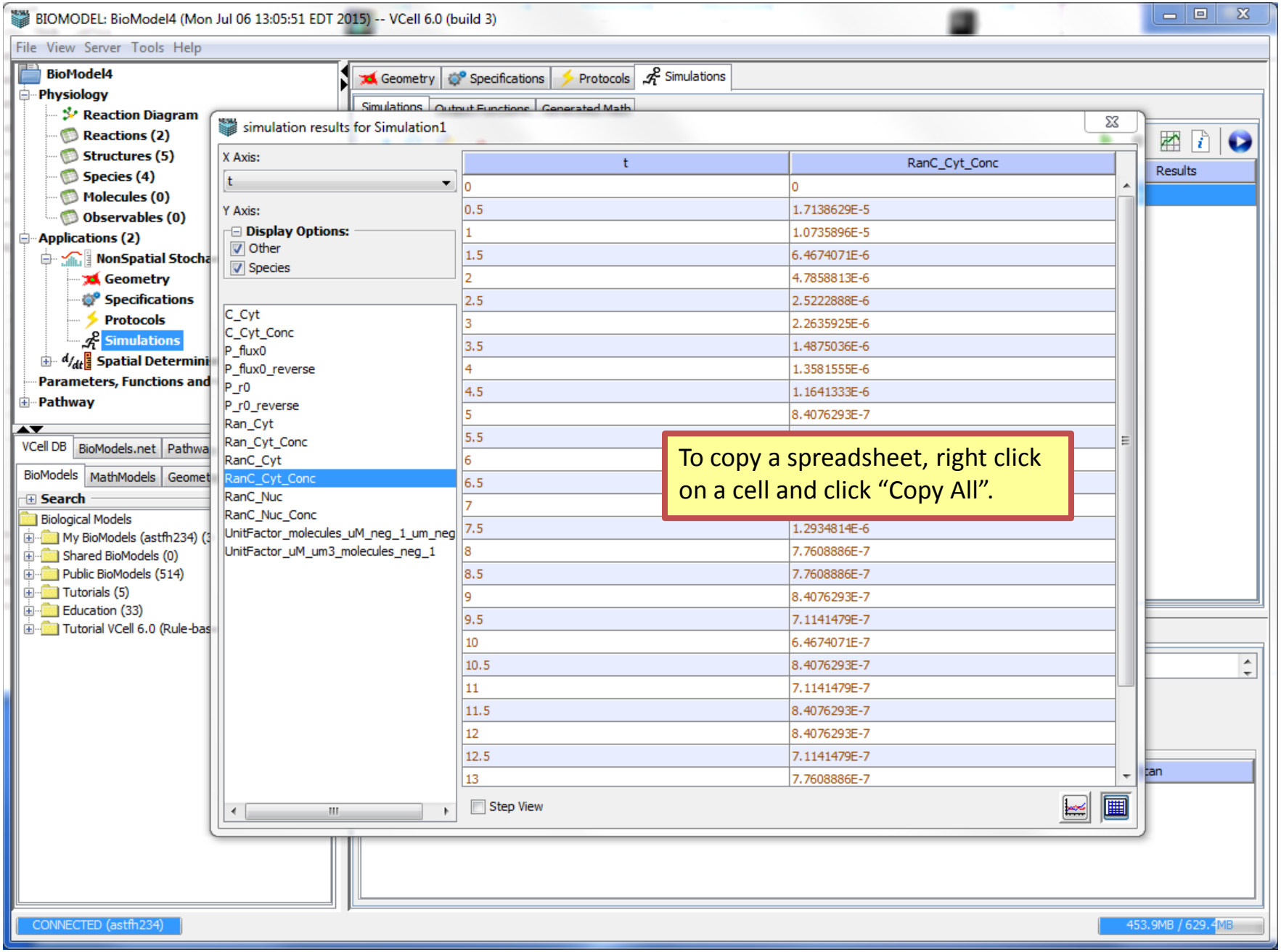
t
Step View
Results
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (astfh234)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-bas
CONNECTED (astfh234)
404.5MB / 621.4MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
BioModel4
Physiology
Reaction Diagram
Reactions (2)
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Species (4)
Molecules (0)
Observables (0)
Applications (2)
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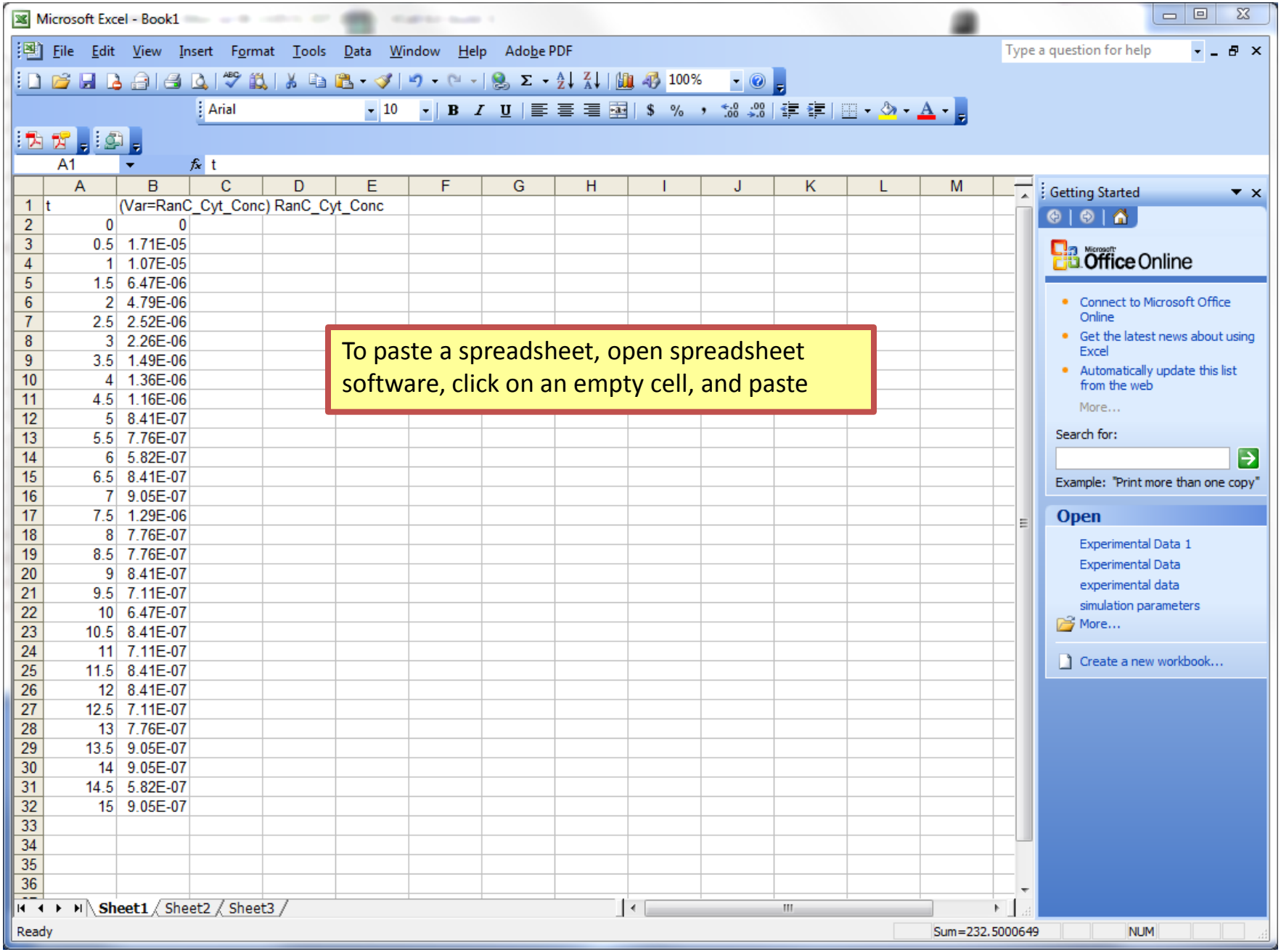
Geometry
Specifications
Protocols
Simulations
Spatial Determini
Parameters, Functions and
Pathway
Geometry
Specifications
Protocols
Simulations
simulation results for Simulation1
X Axis:
t
Y Axis:
Display Options:
Other
Species
C_Cyt
C_Cyt_Conc
P_flux0
P_flux0_reverse
P_r0
P_r0_reverse
Ran_Cyt
Ran_Cyt_Conc
RanC_Cyt
RanC_Cyt_Conc
RanC_Nuc
RanC_Nuc_Conc
UnitFactor_molecules_uM_neg_1_um_neg
UnitFactor_uM_um3_molecules_neg_1
t
RanC_Cyt_Conc
0 0
0.5 1.7138629E-5
1 1.0735896E-5
1.5 6.4674071E-6
2 4.7858813E-6
2.5 2.5222888E-6
3 2.2635925E-6
3.5 1.4875036E-6
4 1.3581555E-6
4.5 1.1641333E-6
5 8.4076293E-7
7.5 1.2934814E-6
8 7.7608886E-7
8.5 7.7608886E-7
9 8.4076293E-7
9.5 7.1141479E-7
10 6.4674071E-7
10.5 8.4076293E-7
11 7.1141479E-7
11.5 8.4076293E-7
12 8.4076293E-7
12.5 7.1141479E-7
13 7.7608886E-7
Step View
To copy a spreadsheet, right click on a cell and click “Copy All”.
Results
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (astfh234)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-bas
CONNECTED (astfh234)
453.9MB / 629.4MB



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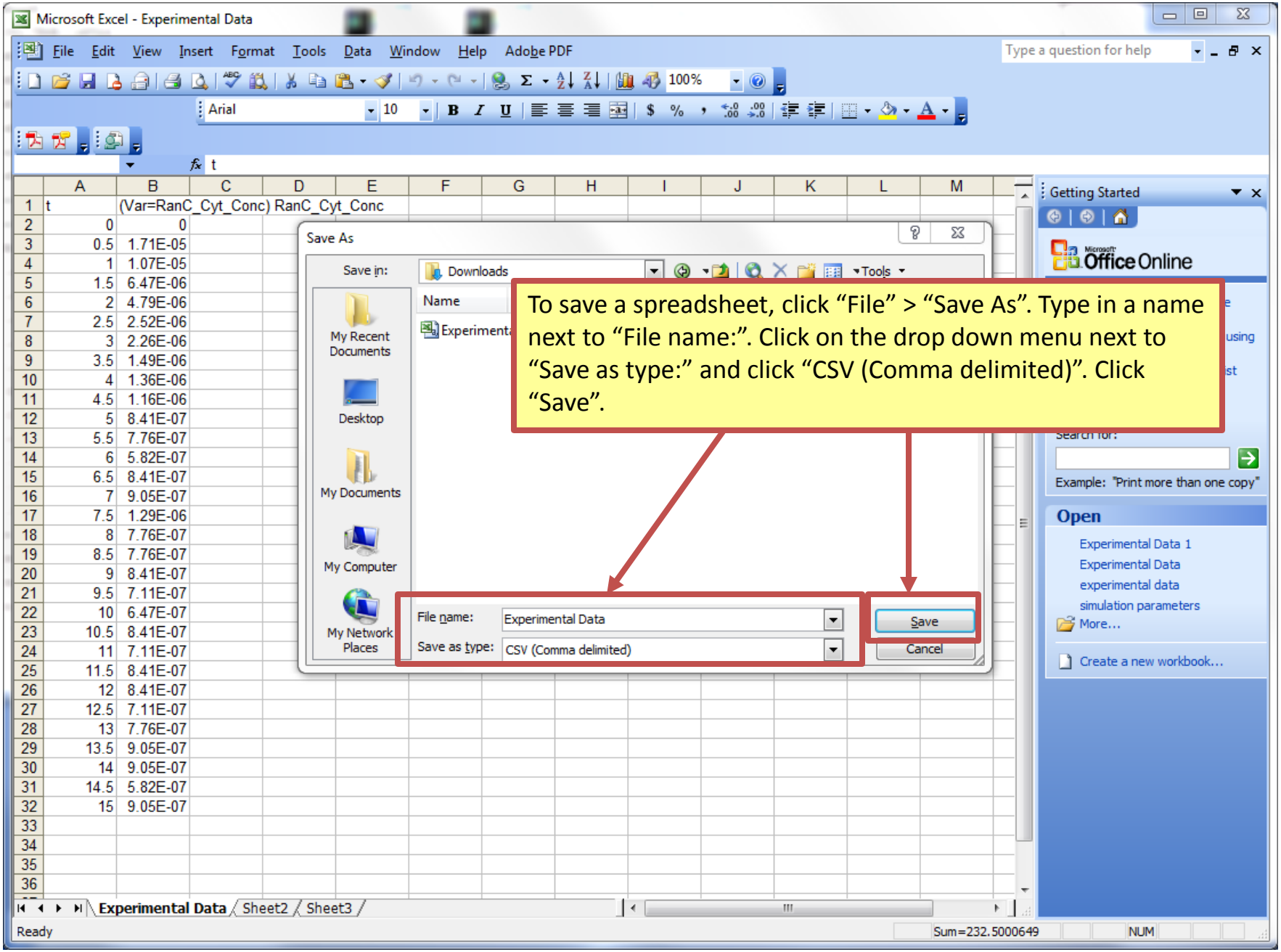

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	t	(Var=RanC_Cyt_Conc)	RanC_Cyt_Conc										
2	0	0											
3	0.5	1.71E-05											
4	1	1.07E-05											
5	1.5	6.47E-06											
6	2	4.79E-06											
7	2.5	2.52E-06											
8	3	2.26E-06											
9	3.5	1.49E-06											
10	4	1.36E-06											
11	4.5	1.16E-06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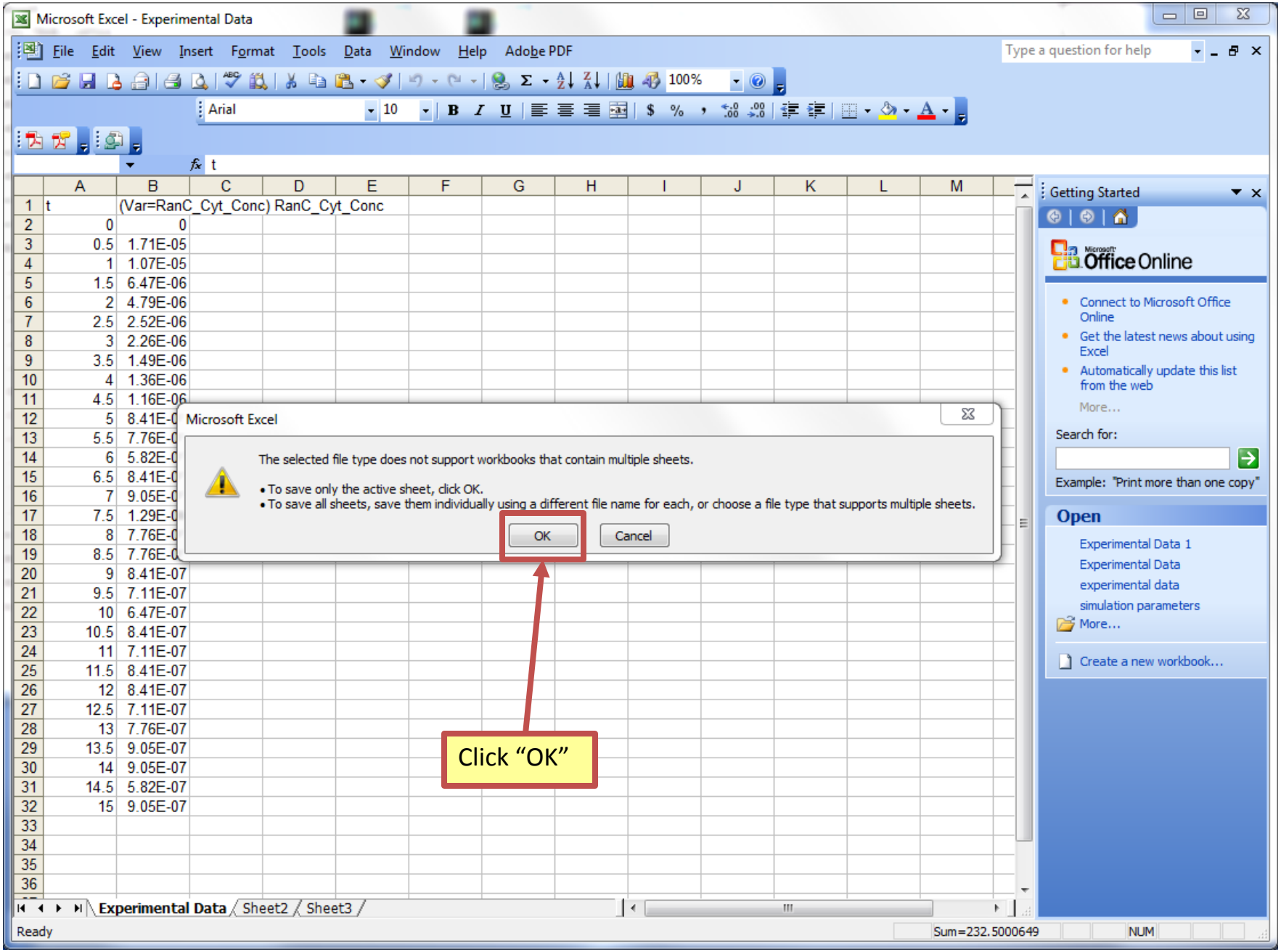
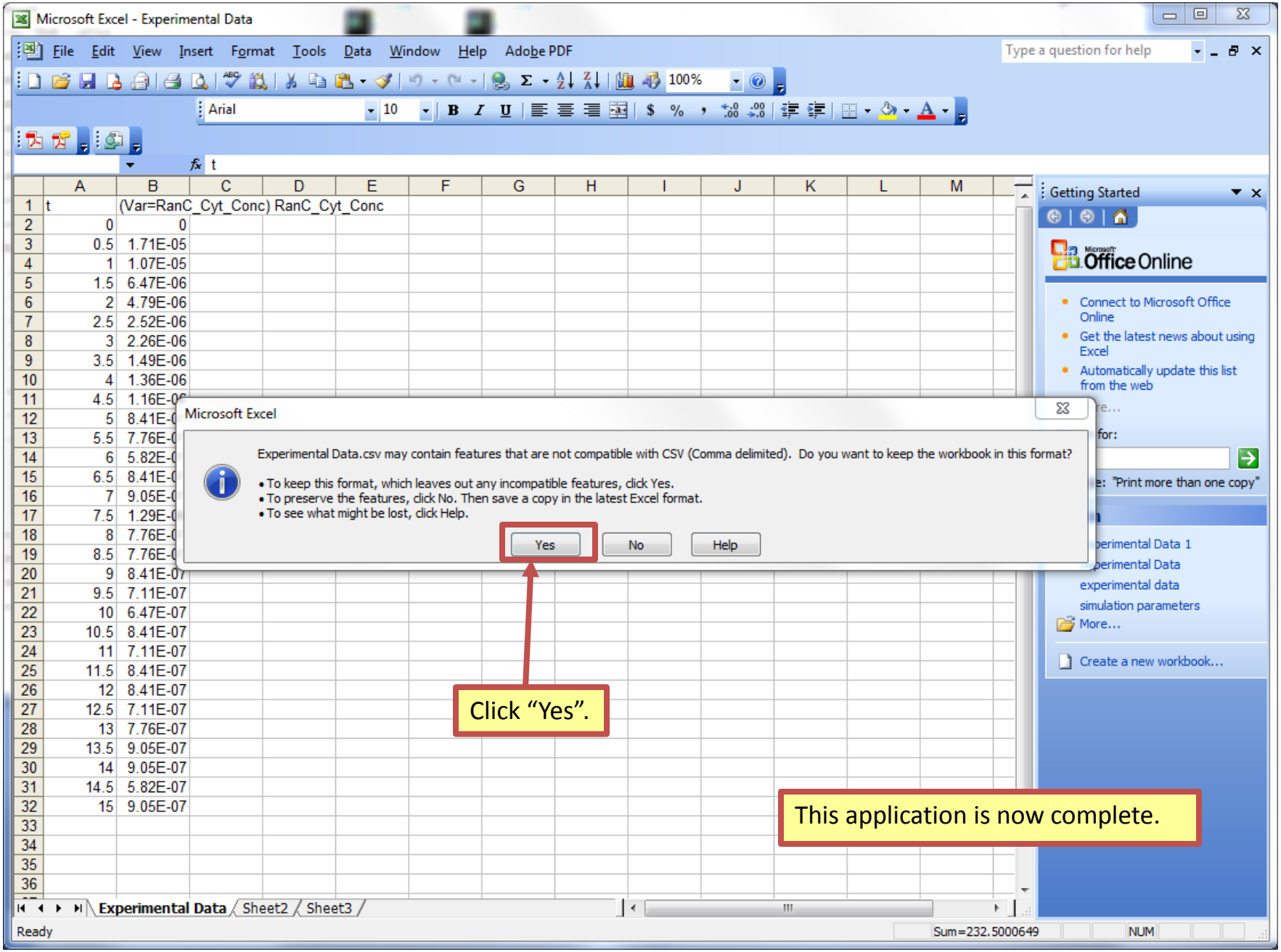


	A	B	C	D	E	F	G	H	I	J	K	L	M
1	t	(Var=RanC_Cyt_Conc) RanC_Cyt_Conc											
2	0	0											
3	0.5	1.71E-05											
4	1	1.07E-05											
5	1.5	6.47E-06											
6	2	4.79E-06											
7	2.5	2.52E-06											
8	3	2.26E-06											
9	3.5	1.49E-06											
10	4	1.36E-06											
11	4.5	1.16E-06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



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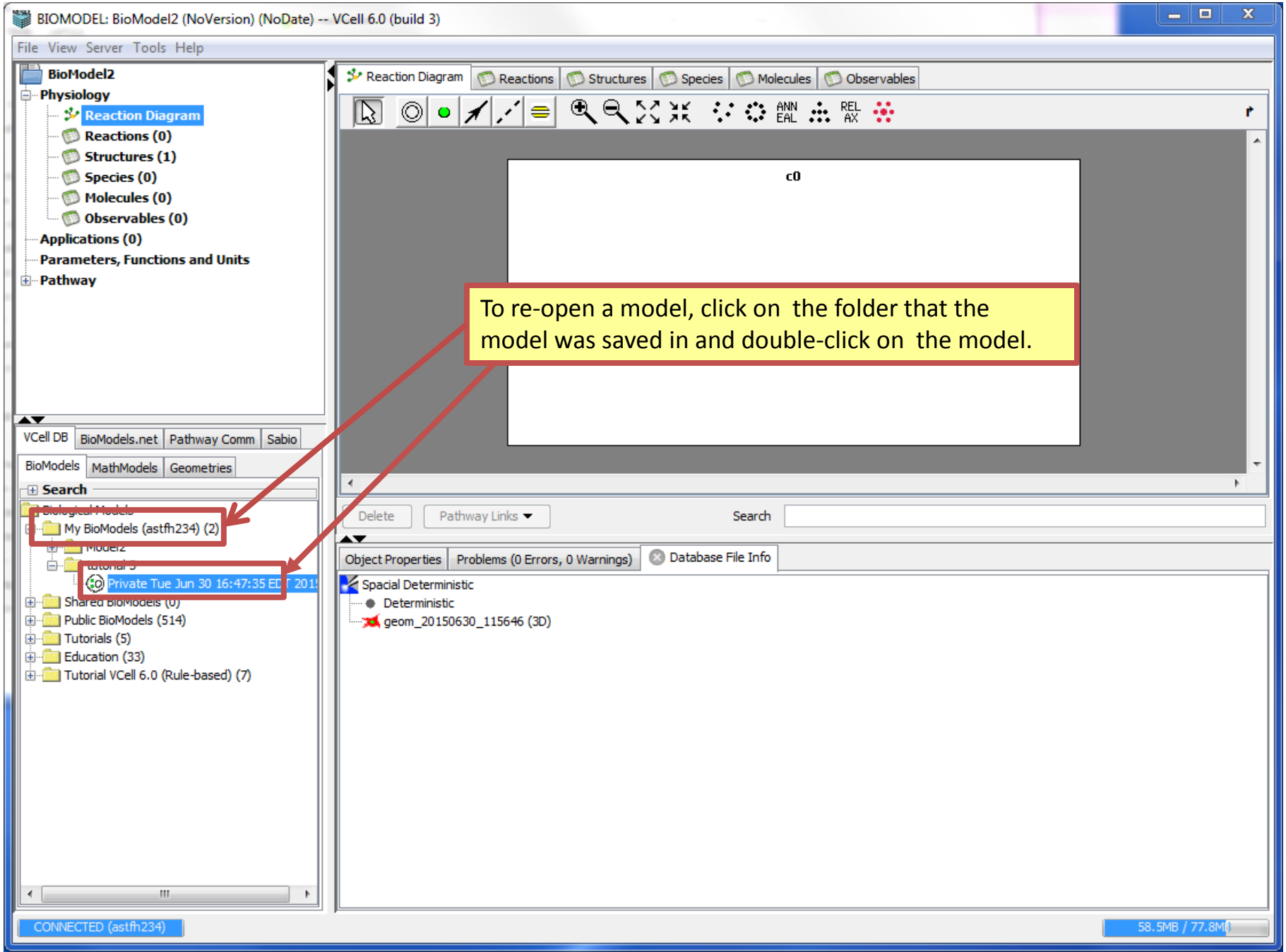
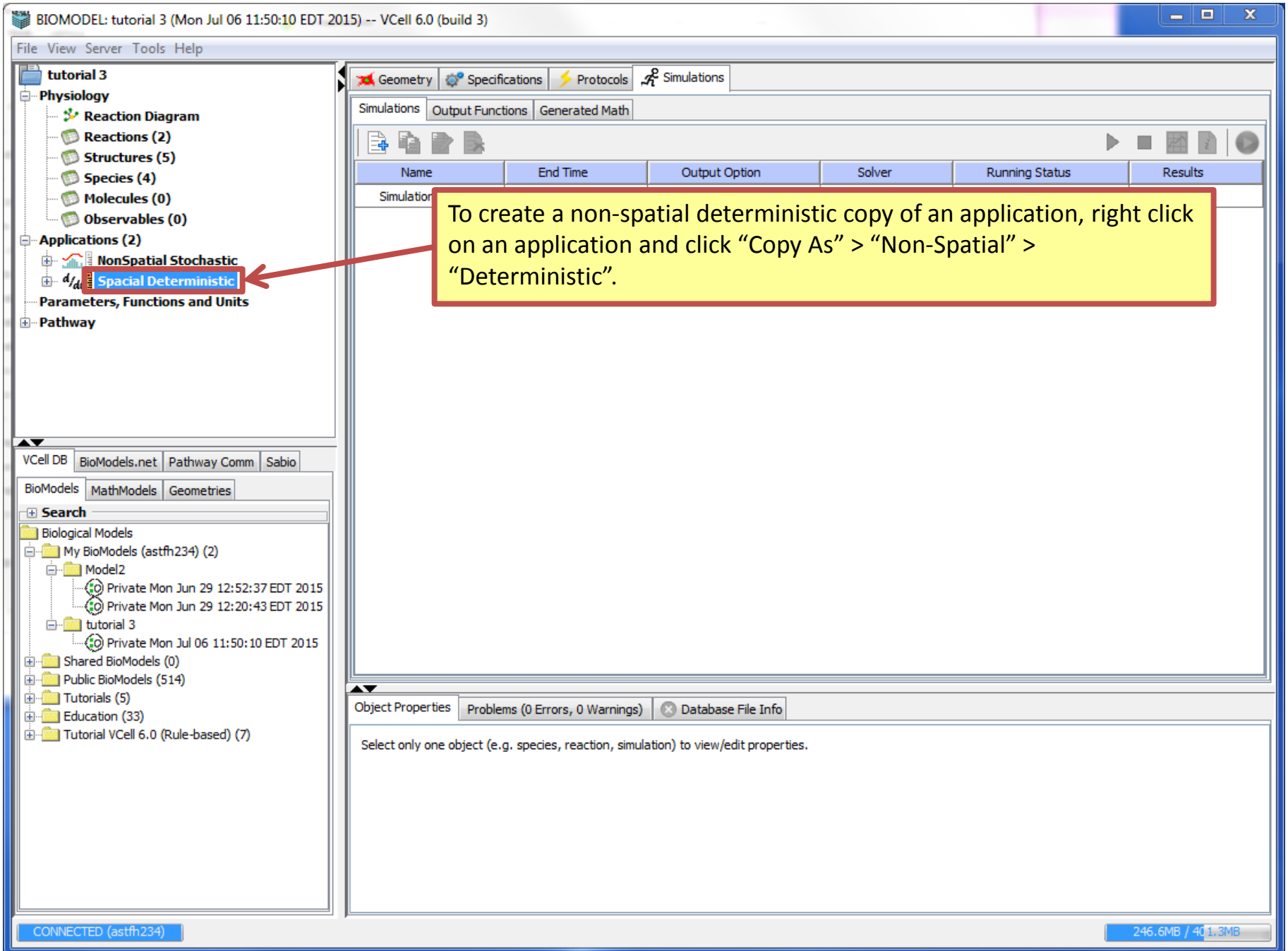

BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 6.0 (build 3)
File View Server Tools Help
BioModel2
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions and Units
Pathway
Reaction Diagram
Reactions
Structures
Species
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
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
My BioModels (astfh234) (2)
Private Tue Jun 30 16:47:35 ED
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Spacial Deterministic
Deterministic
geom_20150630_115646 (3D)
CONNECTED (astfh234)
58.5MB / 77.8MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (2)
NonSpatial Stochastic
Spacial Deterministic
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Pathway
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Protocols
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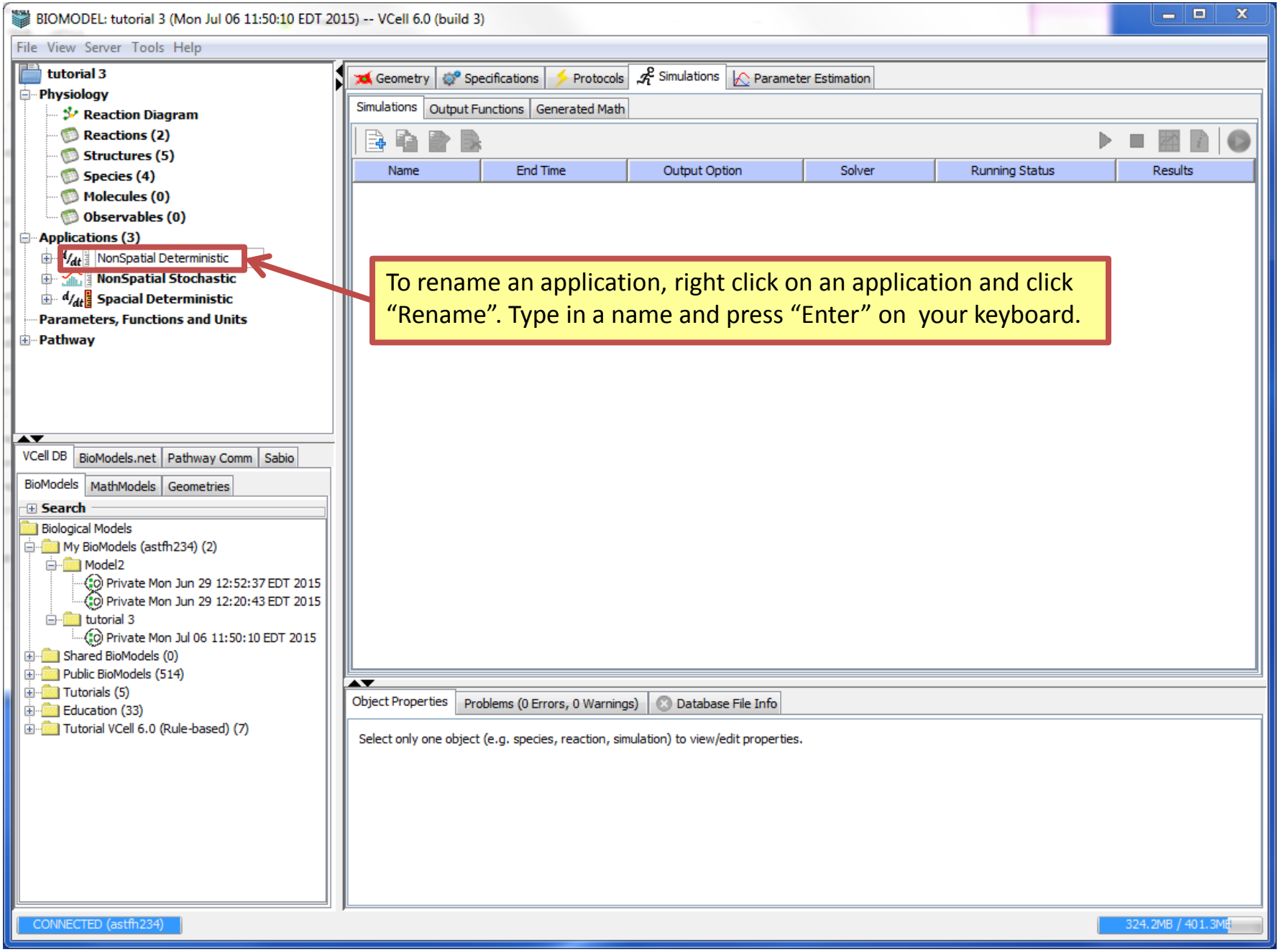
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To create a non-spatial deterministic copy of an application, right click on an application and click “Copy As” > “Non-Spatial” > “Deterministic”.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:50:10 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
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
246.6MB / 40 1.3MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
NonSpatial Stochastic
Spacial Deterministic
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Pathway
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Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To rename an application, right click on an application and click "Rename". Type in a name and press "Enter" on your keyboard.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
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Private Mon Jul 06 11:50:10 EDT 2015
Shared BioModels (0)
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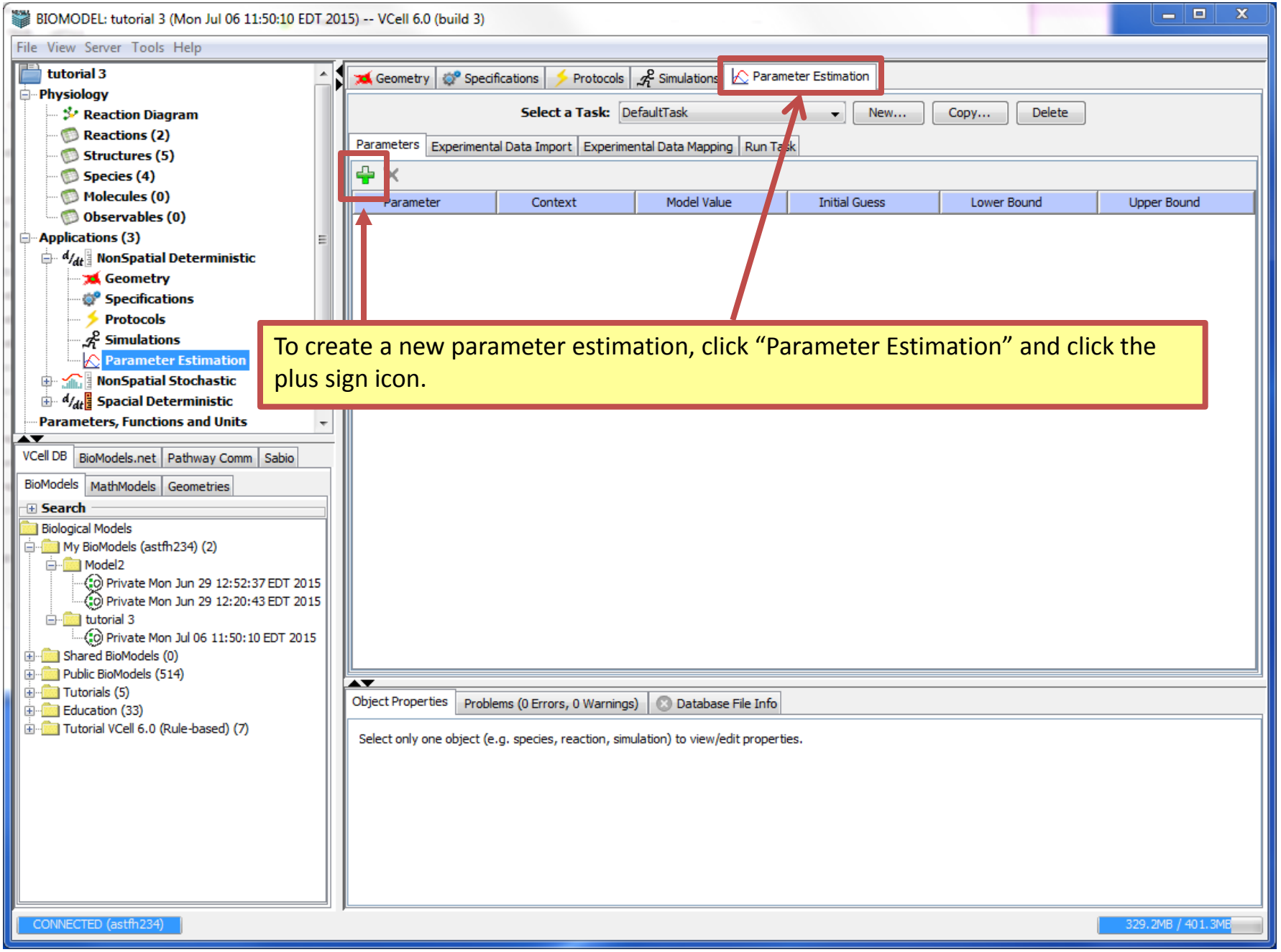
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
324.2MB / 401.3MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
tutorial 3
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Reactions (2)
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Molecules (0)
Observables (0)
Applications (3)
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Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
Private Mon Jul 06 11:50:10 EDT 2015
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Public BioModels (514)
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Geometry
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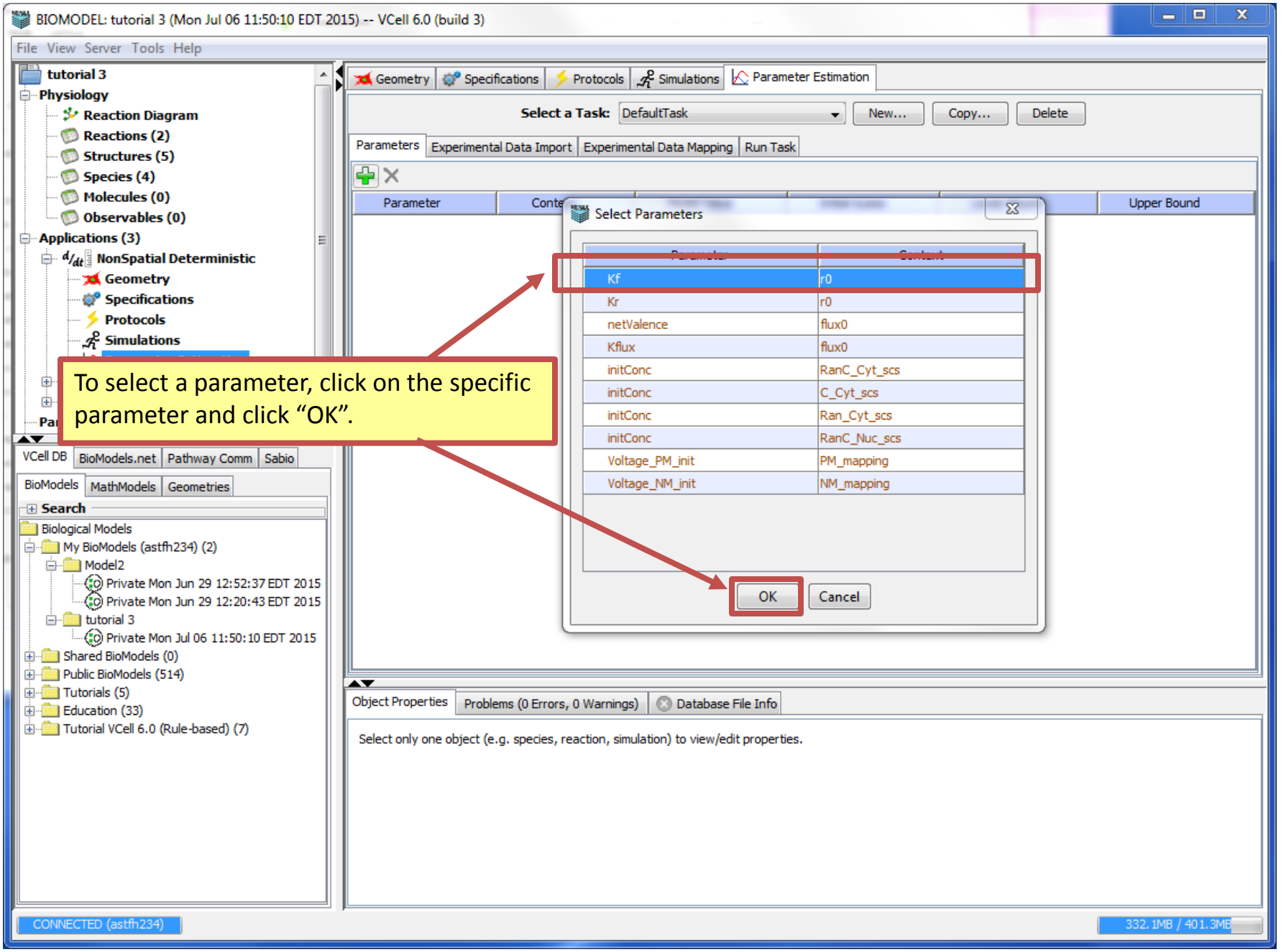
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Parameter
Context
Model Value
Initial Guess
Lower Bound
Upper Bound
To create a new parameter estimation, click “Parameter Estimation” and click the plus sign icon.
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)
329.2MB / 401.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
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Observables (0)
Applications (3)
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Geometry Specifications Protocols Simulations Parameter Estimation
Select a Task: DefaultTask New... Copy... Delete
Parameters Experimental Data Import Experimental Data Mapping Run Task
Parameter
Upper Bound
Select Parameters
Parameter Constant
Kf r0
Kr r0
netValence flux0
Kflux flux0
initConc RanC_Cyt_scs
initConc C_Cyt_scs
initConc Ran_Cyt_scs
initConc RanC_Nuc_scs
Voltage_PM_init PM_mapping
Voltage_NM_init NM_mapping
OK
Cancel
To select a parameter, click on the specific parameter and click “OK”.
VCell DB BioModels.net Pathway Comm Sabio
BioModels MathModels Geometries
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My BioModels (astfh234) (2)
Model2
Private Mon Jun 29 12:52:37 EDT 2015
Private Mon Jun 29 12:20:43 EDT 2015
tutorial 3
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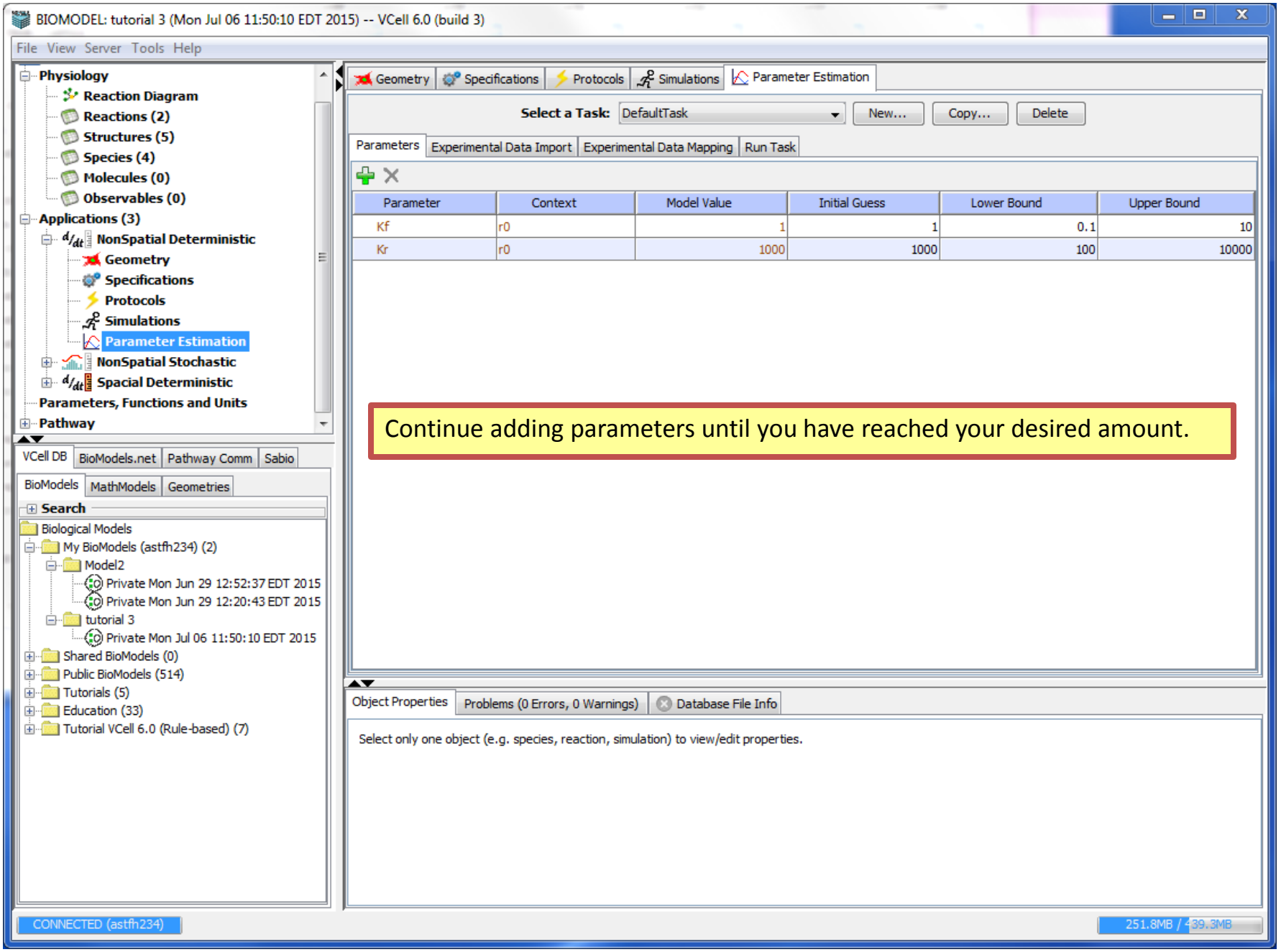
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties Problems (0 Errors, 0 Warnings) Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
332.1MB / 401.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
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Private Mon Jun 29 12:20:43 EDT 2015
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Private Mon Jul 06 11:50:10 EDT 2015
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Public BioModels (514)
Tutorials (5)
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Tutorial VCell 6.0 (Rule-based) (7)
Geometry
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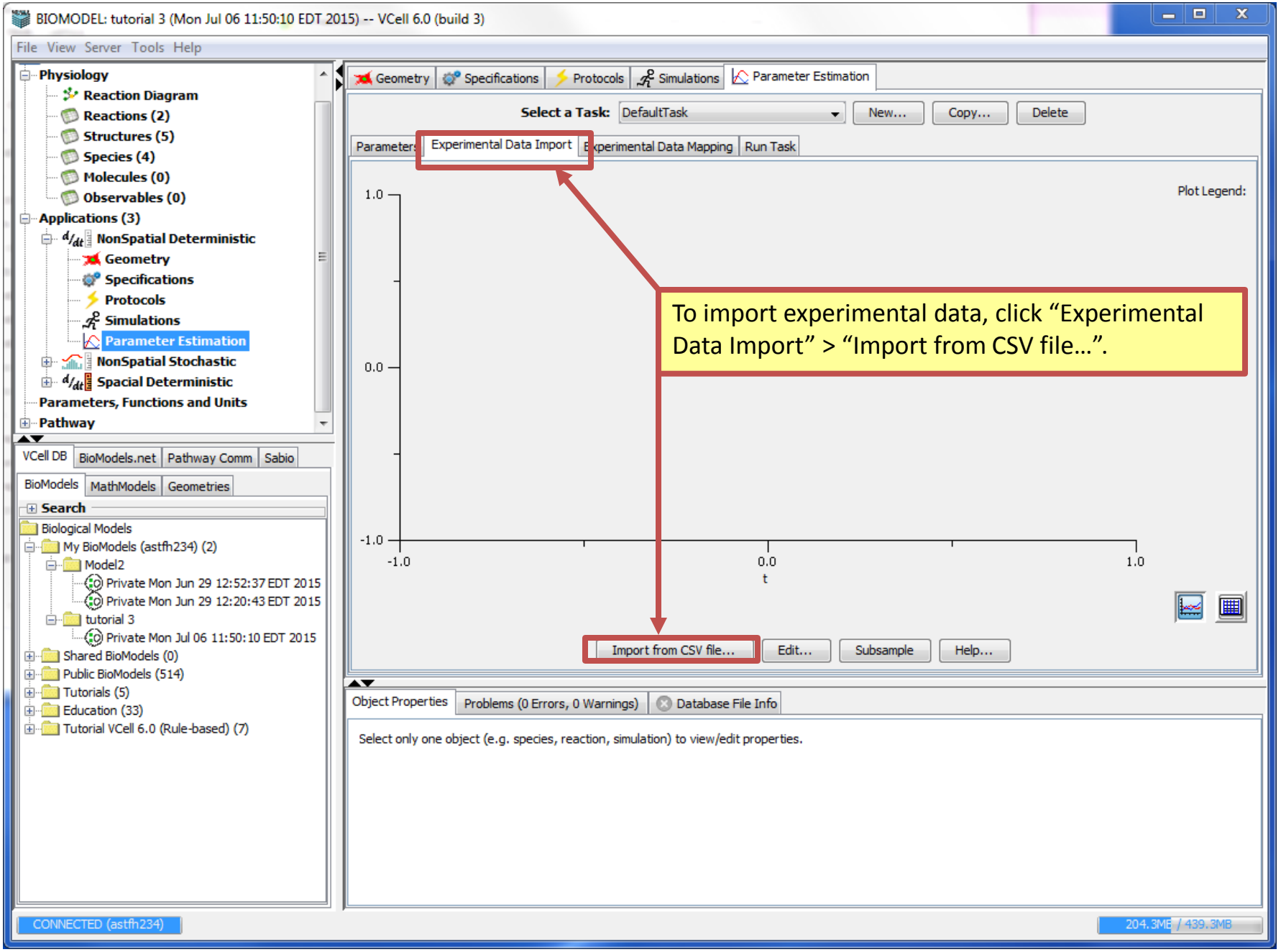
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Parameter
Context
Model Value
Initial Guess
Lower Bound
Upper Bound
Kf
r0
1
1
0.1
10
Kr
r0
1000
1000
100
10000
Continue adding parameters until you have reached your desired amount.
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)
251.8MB / 439.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
Physiology
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New...
Copy...
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Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Plot Legend:
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0.0
-1.0
-1.0
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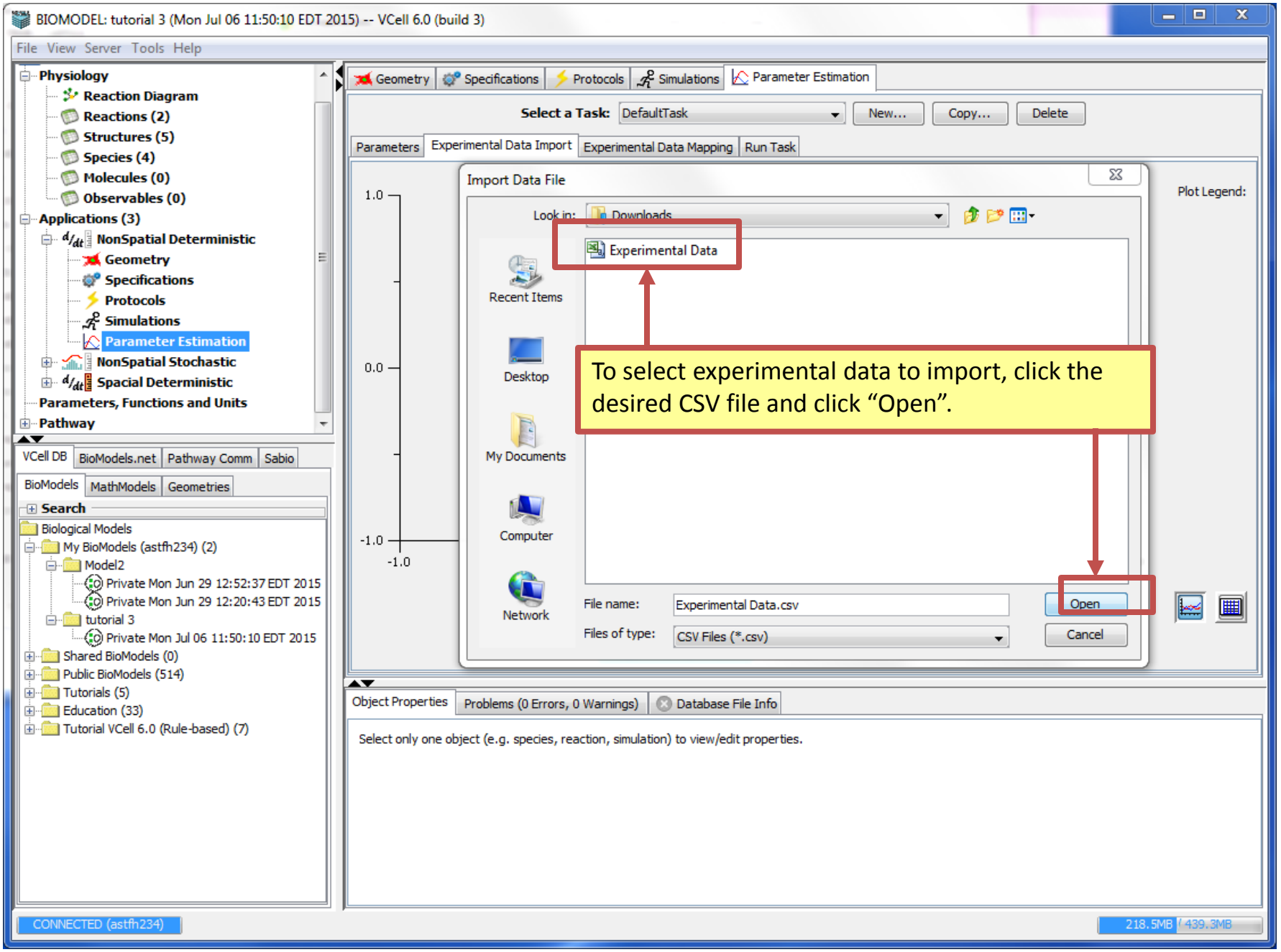
t
To import experimental data, click “Experimental Data Import” > “Import from CSV file…”.
Import from CSV file...
Edit...
Subsample
Help...
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
204.3MB / 439.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
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Observables (0)
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Private Mon Jun 29 12:20:43 EDT 2015
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Public BioModels (514)
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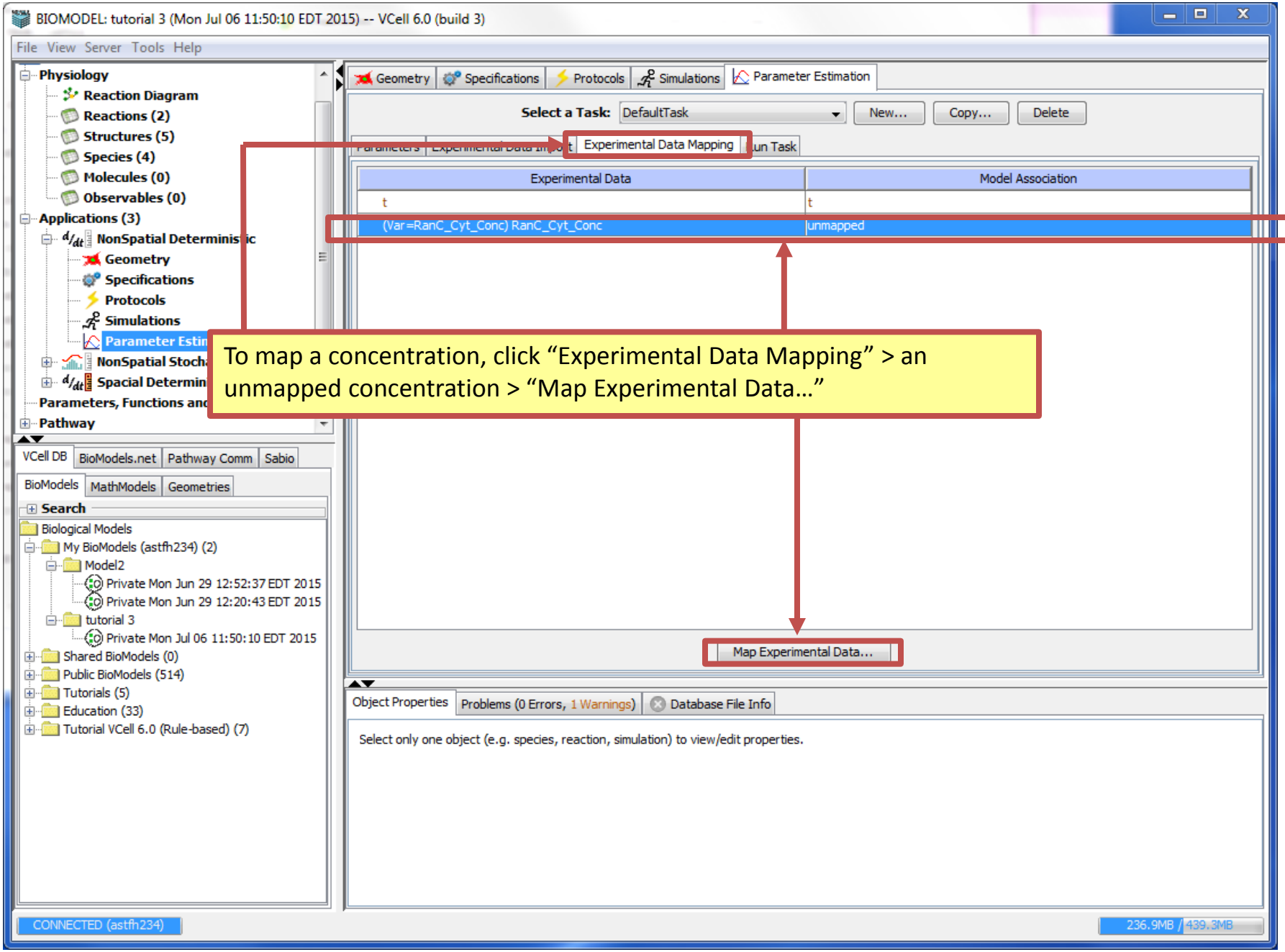
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
1.0
0.0
-1.0
-1.0
Import Data File
Look in:
Downloads
Experimental Data
Recent Items
Desktop
My Documents
Computer
Network
File name:
Experimental Data.csv
Files of type:
CSV Files (*.csv)
Open
Cancel
Plot Legend:
To select experimental data to import, click the desired CSV file and click “Open”.
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)
218.5MB
439.3MB

Contents


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
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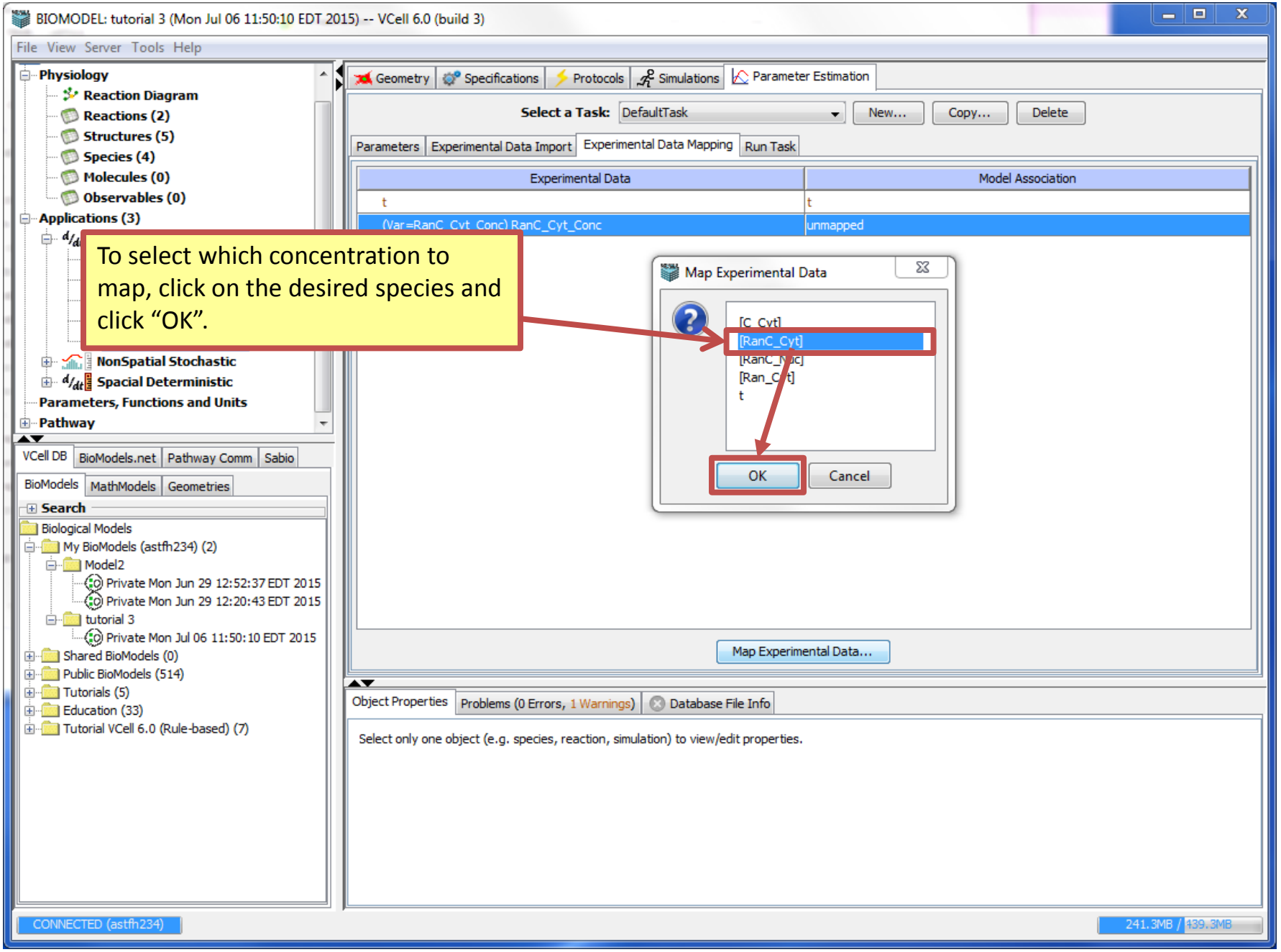
Select a Task:
DefaultTask
New...
Copy...
Delete
Experimental Data Mapping
Run Task
Experimental Data
Model Association
t
t
(Var=RanC_Cyt_Conc) RanC_Cyt_Conc
unmapped
To map a concentration, click “Experimental Data Mapping” > an unmapped concentration > “Map Experimental Data…”
Map Experimental Data...
Object Properties
Problems (0 Errors, 1 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
236.9MB / 439.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
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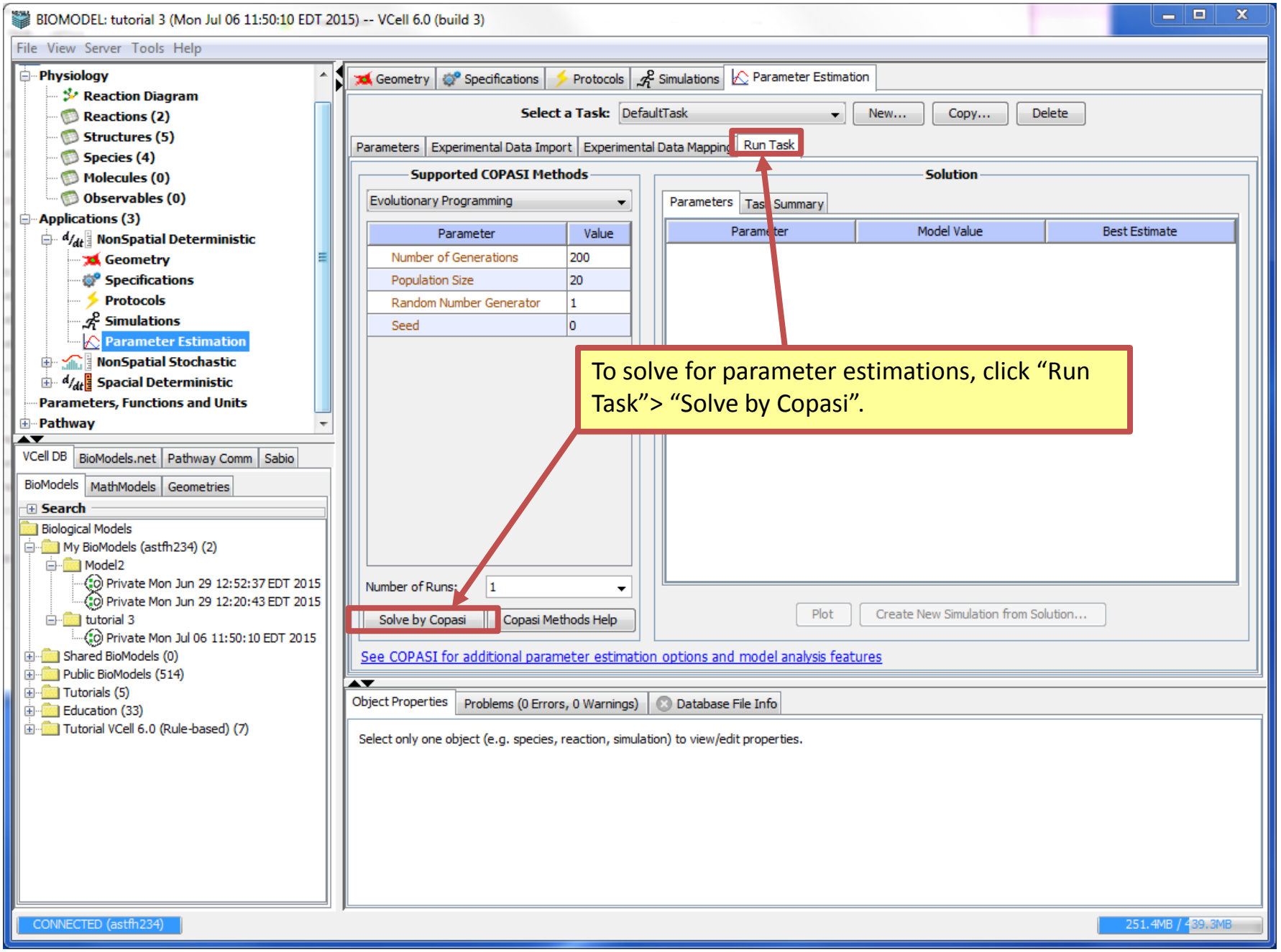
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Experimental Data
Model Association
t
t
(Var=RanC_Cyt_Conc) RanC_Cyt_Conc
unmapped
To select which concentration to map, click on the desired species and click “OK”.
Map Experimental Data
[C_Cyt]
[RanC_Cyt]
[RanC_Nuc]
[Ran_Cyt]
t
OK
Cancel
Map Experimental Data...
Object Properties
Problems (0 Errors, 1 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
241.3MB / 439.3MB


BIOMODEL: tutorial 3 (Mon Jul 06 11:50:10 EDT 2015) -- VCell 6.0 (build 3)
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Select a Task:
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New...
Copy...
Delete
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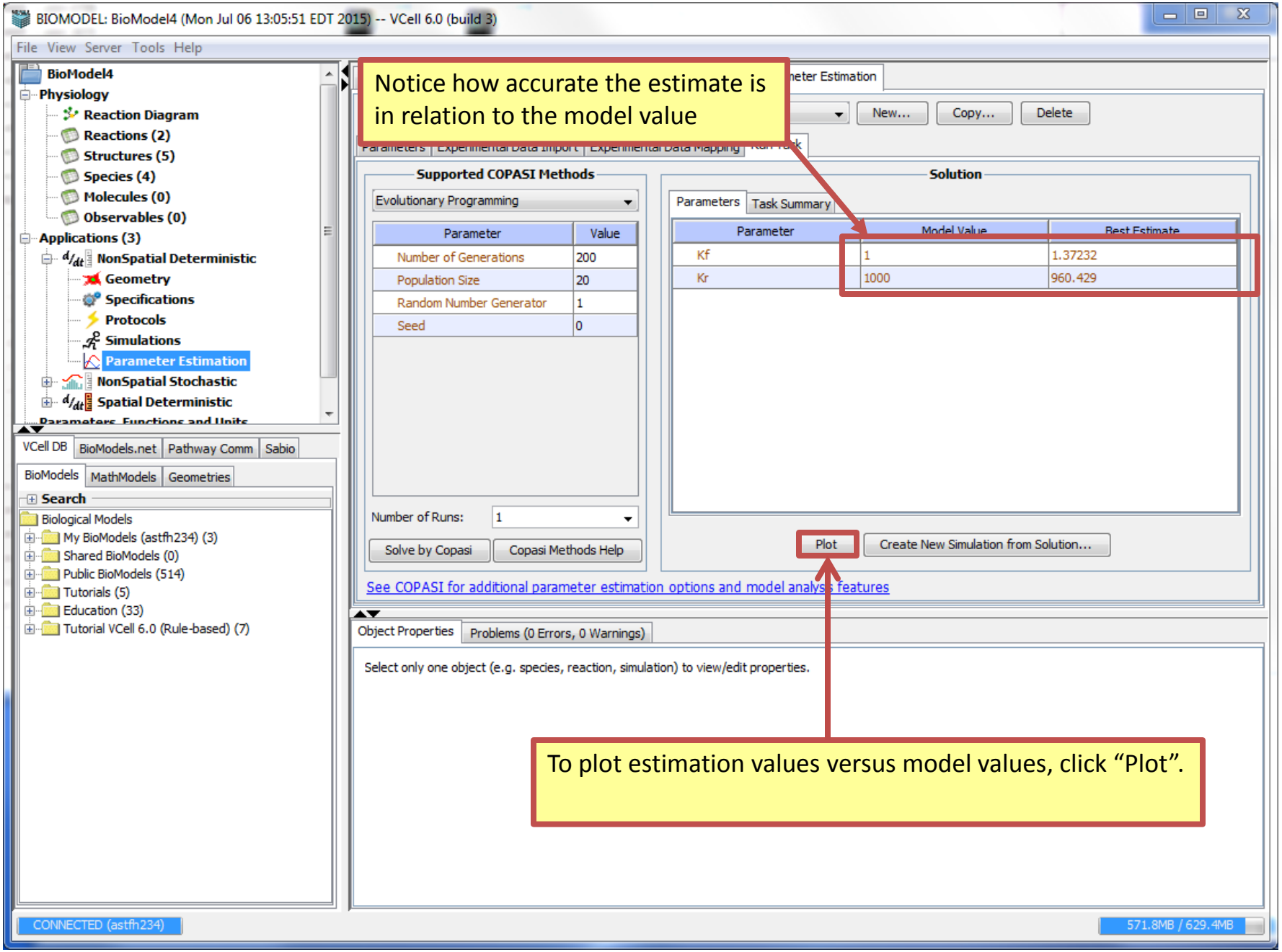
Run Task
Supported COPASI Methods
Evolutionary Programming
Parameter
Value
Number of Generations
200
Population Size
20
Random Number Generator
1
Seed
0
Number of Runs:
1
Solve by Copasi
Copasi Methods Help
Solution
Parameters
Tas
Summary
Parameter
Model Value
Best Estimate
Plot
Create New Simulation from Solution...
See COPASI for additional parameter estimation options and model analysis features
To solve for parameter estimations, click “Run Task”> “Solve by Copasi”.
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)
251.4MB / 439.3MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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Reactions (2)
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Molecules (0)
Observables (0)
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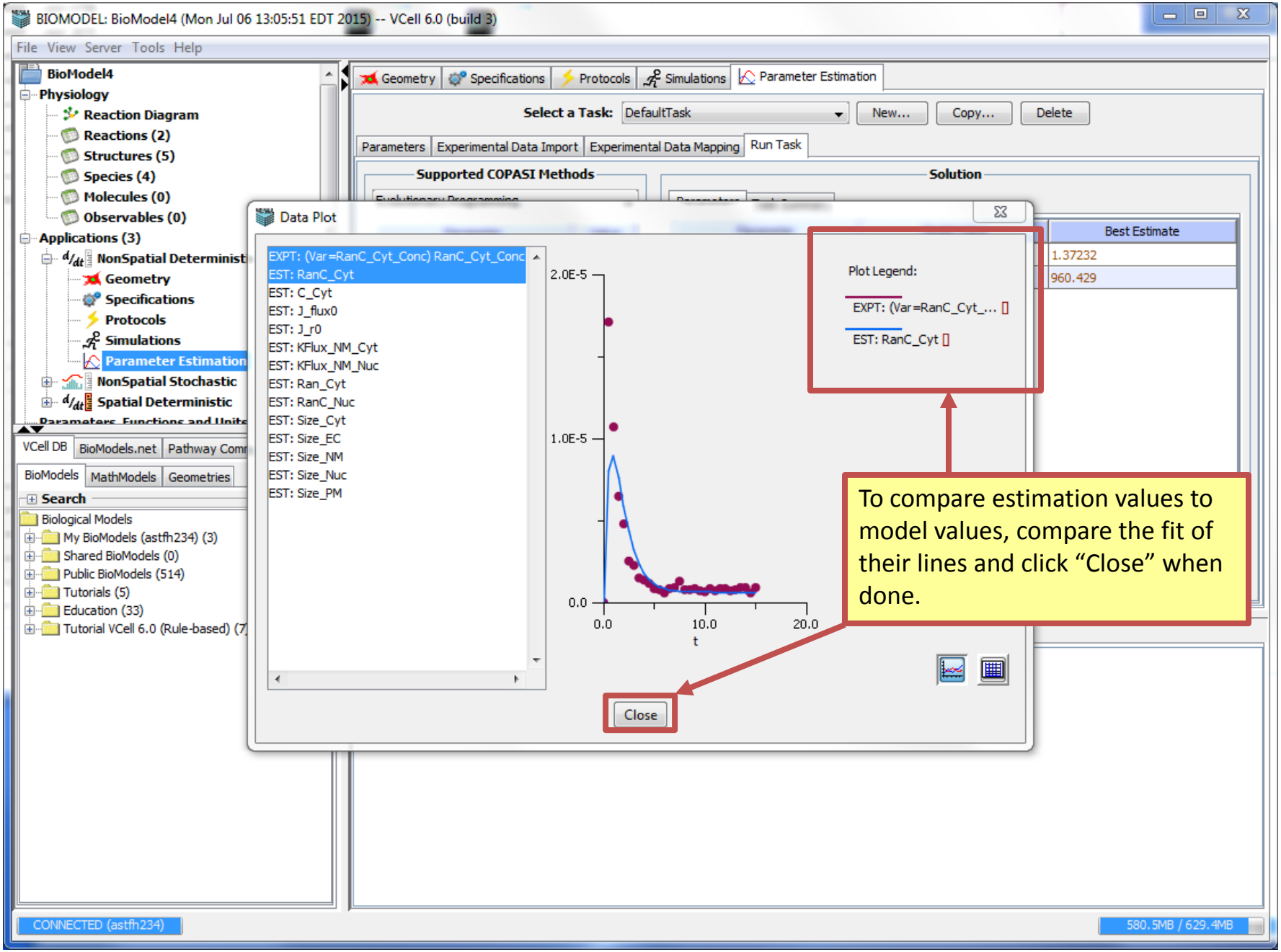
Tutorial VCell 6.0 (Rule-based) (7)
Notice how accurate the estimate is in relation to the model value
New...
Copy...
Delete
Supported COPASI Methods
Evolutionary Programming
Parameter
Value
Number of Generations
200
Population Size
20
Random Number Generator
1
Seed
0
Number of Runs:
1
Solve by Copasi
Copasi Methods Help
Solution
Parameters
Task Summary
Parameter
Model Value
Best Estimate
Kf
1
1.37232
Kr
1000
960.429
Plot
Create New Simulation from Solution...
See COPASI for additional parameter estimation options and model analysis features
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
To plot estimation values versus model values, click “Plot”.
CONNECTED (astfh234)
571.8MB / 629.4MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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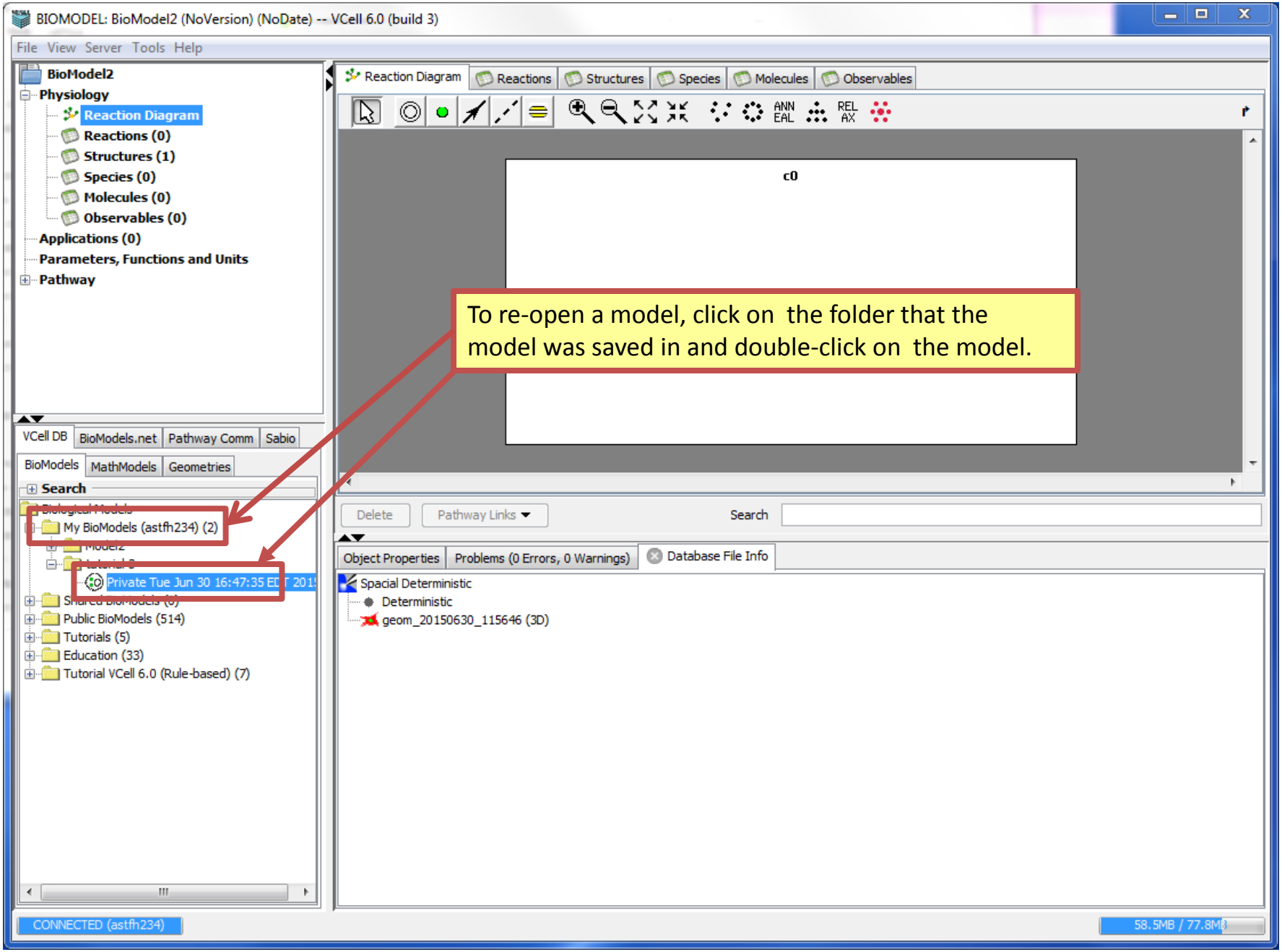
Specifications
Protocols
Simulations
Parameter Estimation
Select a Task:
DefaultTask
New...
Copy...
Delete
Parameters
Experimental Data Import
Experimental Data Mapping
Run Task
Supported COPASI Methods
Solution
Best Estimate
1.37232
960.429
Data Plot
EXPT: (Var=RanC_Cyt_Conc) RanC_Cyt_Conc
EST: RanC_Cyt
EST: C_Cyt
EST: J_flux0
EST: J_r0
EST: KFlux_NM_Cyt
EST: KFlux_NM_Nuc
EST: Ran_Cyt
EST: RanC_Nuc
EST: Size_Cyt
EST: Size_EC
EST: Size_NM
EST: Size_Nuc
EST: Size_PM
2.0E-5
1.0E-5
0.0
0.0
10.0
20.0
t
Plot Legend:
EXPT: (Var=RanC_Cyt_...
EST: RanC_Cyt
Close
To compare estimation values to model values, compare the fit of their lines and click “Close” when done.
CONNECTED (astfh234)
580.5MB / 629.4MB


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
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
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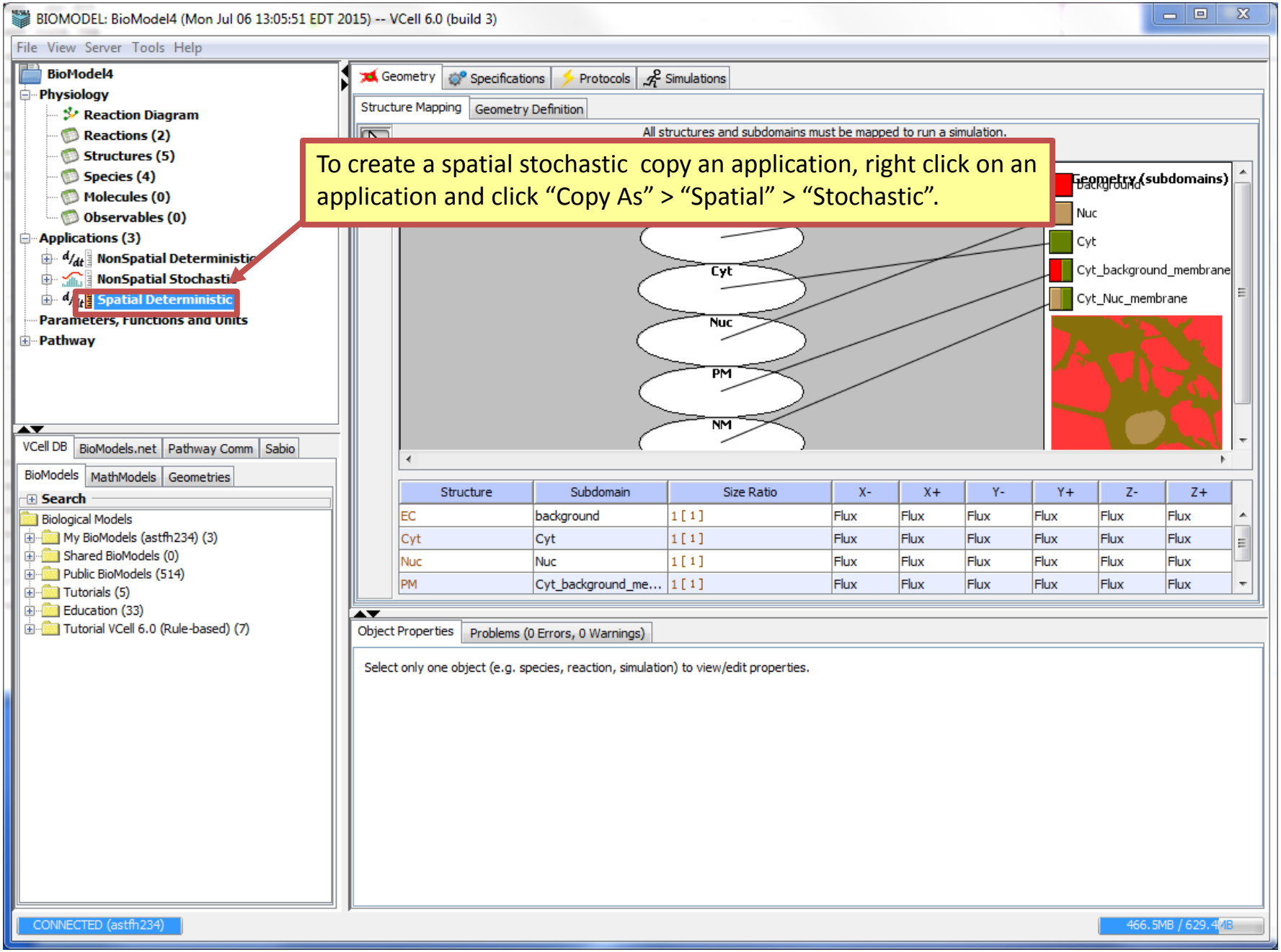
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Spacial Deterministic
Deterministic
geom_20150630_115646 (3D)
CONNECTED (astfh234)


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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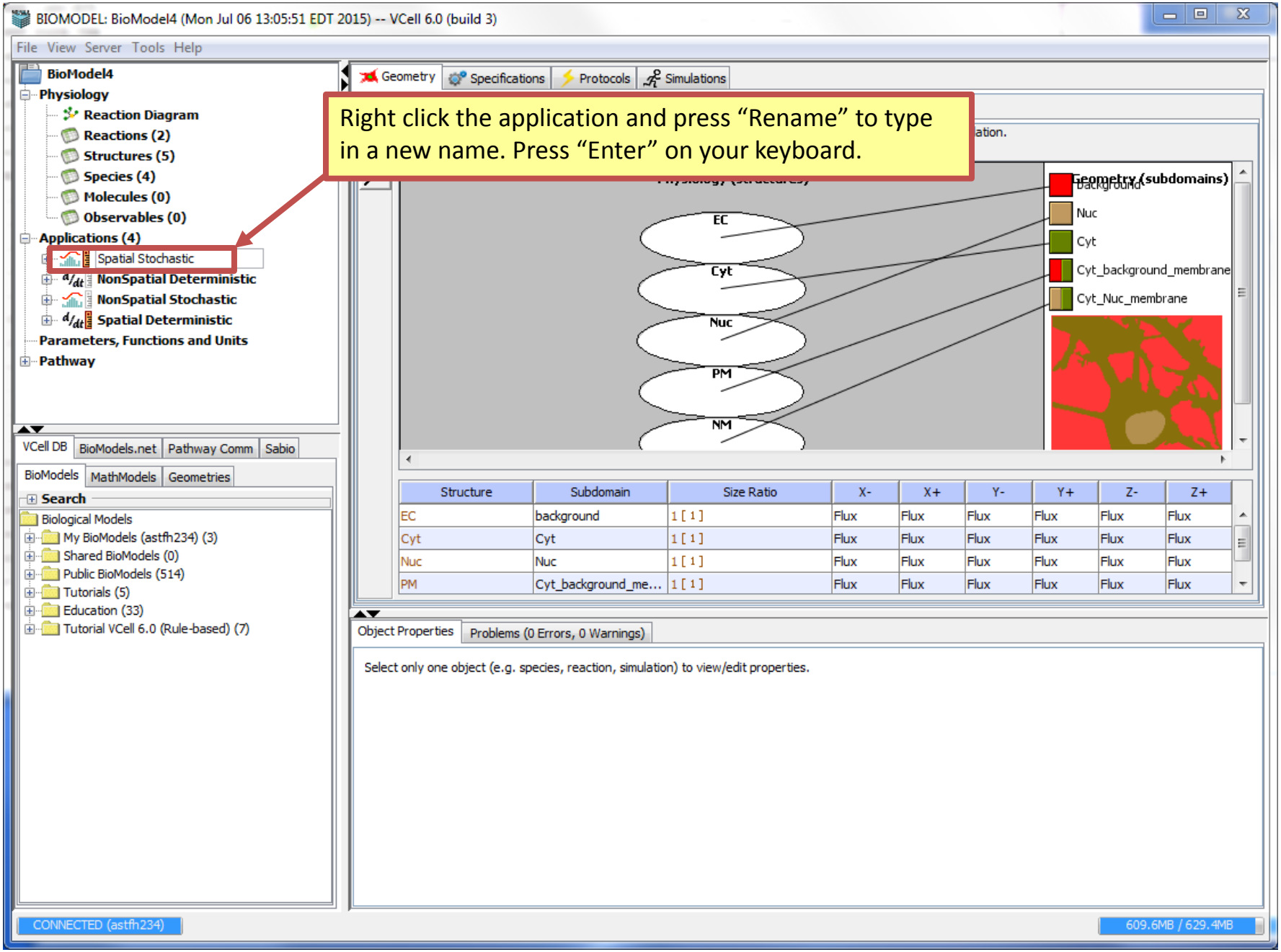
Physiology
Reaction Diagram
Reactions (2)
Structures (5)
Species (4)
Molecules (0)
Observables (0)
Applications (3)
NonSpatial Deterministic
NonSpatial Stochasti
Spatial Deterministic
Parameters, Functions and Units
Pathway
To create a spatial stochastic copy an application, right click on an application and click “Copy As” > “Spatial” > “Stochastic”.
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
All structures and subdomains must be mapped to run a simulation.
Cyt
Nuc
PM
NM
Geometry (subdomains)
Nuc
Cyt
Cyt_background_membrane
Cyt_Nuc_membrane
Structure
Subdomain
Size Ratio
X-
X+
Y-
Y+
Z-
Z+
EC
background
1 [1]
Flux
Cyt
Cyt
1 [1]
Nuc
Nuc
1 [1]
PM
Cyt_background_me...
1 [1]
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (astfh234) (3)
Shared BioModels (0)
Public BioModels (514)
Tutorials (5)
Education (33)
Tutorial VCell 6.0 (Rule-based) (7)
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
466.5MB / 629.4MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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Reactions (2)
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Species (4)
Molecules (0)
Observables (0)
Applications (4)
Spatial Stochastic
NonSpatial Deterministic
NonSpatial Stochastic
Spatial Deterministic
Parameters, Functions and Units
Pathway
Right click the application and press “Rename” to type in a new name. Press “Enter” on your keyboard.
Geometry
Specifications
Protocols
Simulations
EC
Cyt
Nuc
PM
NM
Geometry (subdomains)
Nuc
Cyt
Cyt_background_membrane
Cyt_Nuc_membrane
Structure
Subdomain
Size Ratio
X-
X+
Y-
Y+
Z-
Z+
EC
background
1 [1]
Cyt
Cyt
1 [1]
Nuc
Nuc
1 [1]
PM
Cyt_background_me...
1 [1]
Flux
VCell DB
BioModels.net
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Sabio
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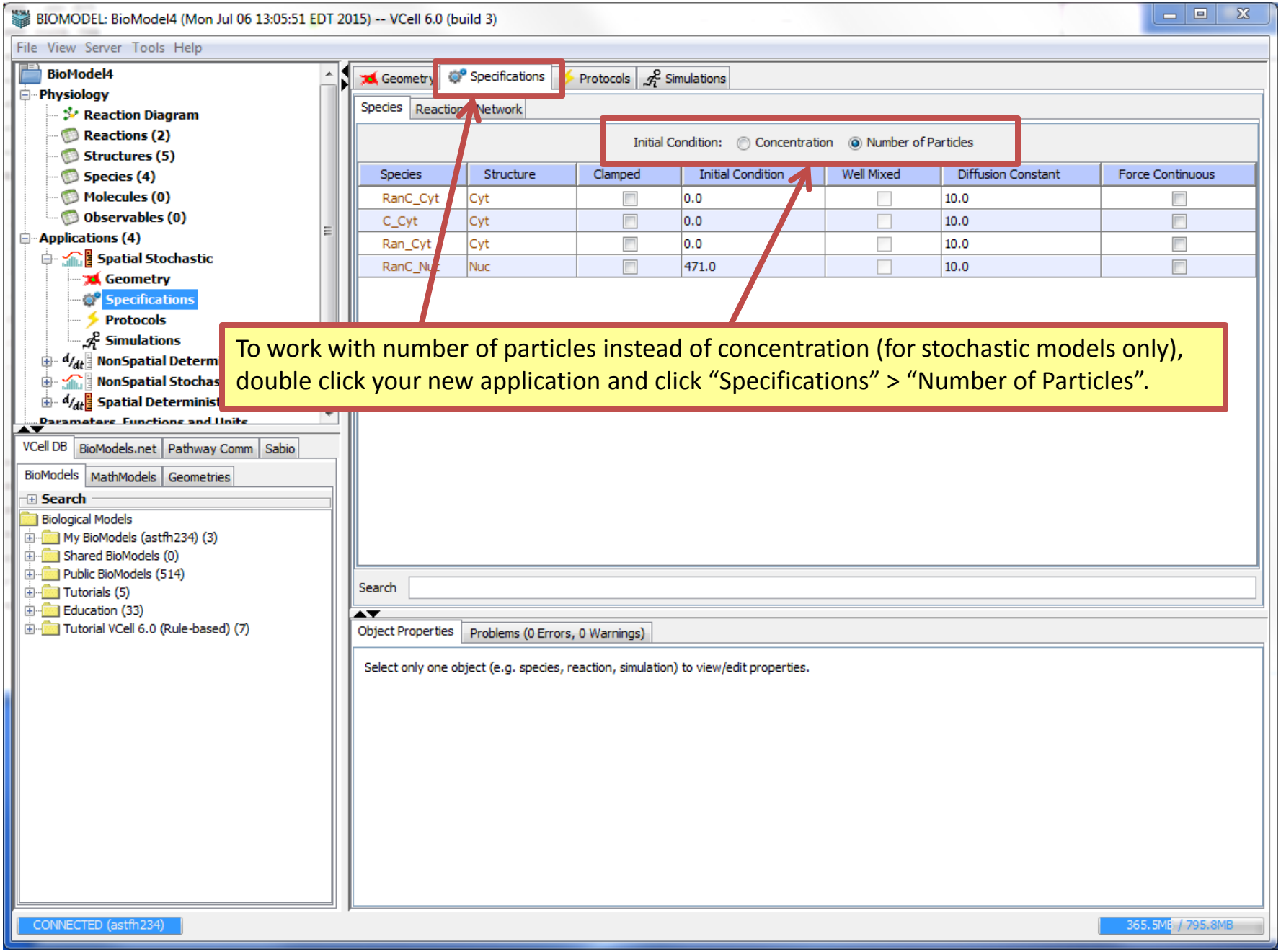
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
609.6MB / 629.4MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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NonSpatial Determ
NonSpatial Stochas
Spatial Determinist
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Network
Initial Condition: Concentration Number of Particles
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Force Continuous
RanC_Cyt
Cyt
0.0
10.0
C_Cyt
Cyt
0.0
10.0
Ran_Cyt
Cyt
0.0
10.0
RanC_Nuc
Nuc
471.0
10.0
To work with number of particles instead of concentration (for stochastic models only), double click your new application and click “Specifications” > “Number of Particles”.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
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Public BioModels (514)
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Education (33)
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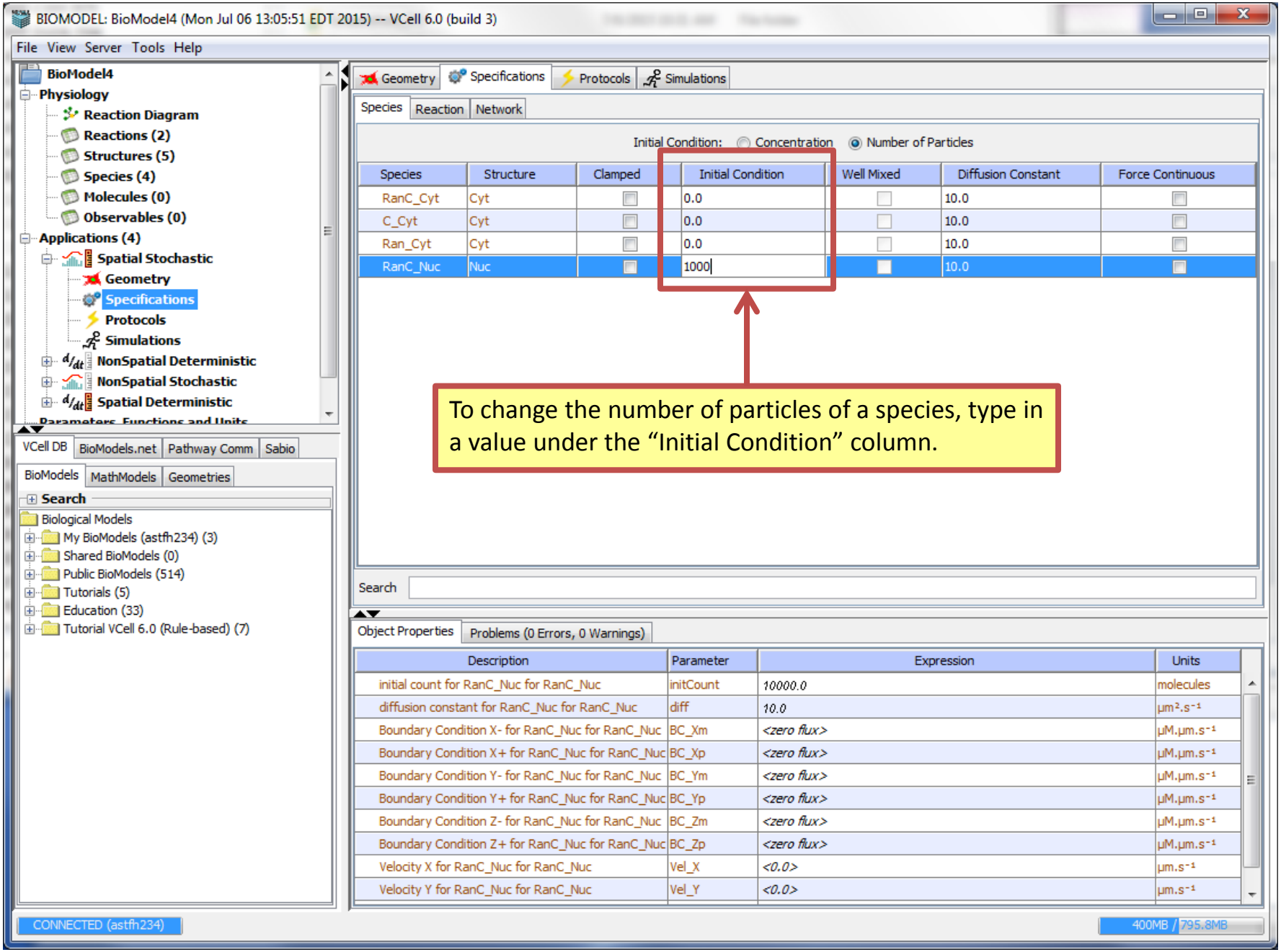
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
365.5MB / 795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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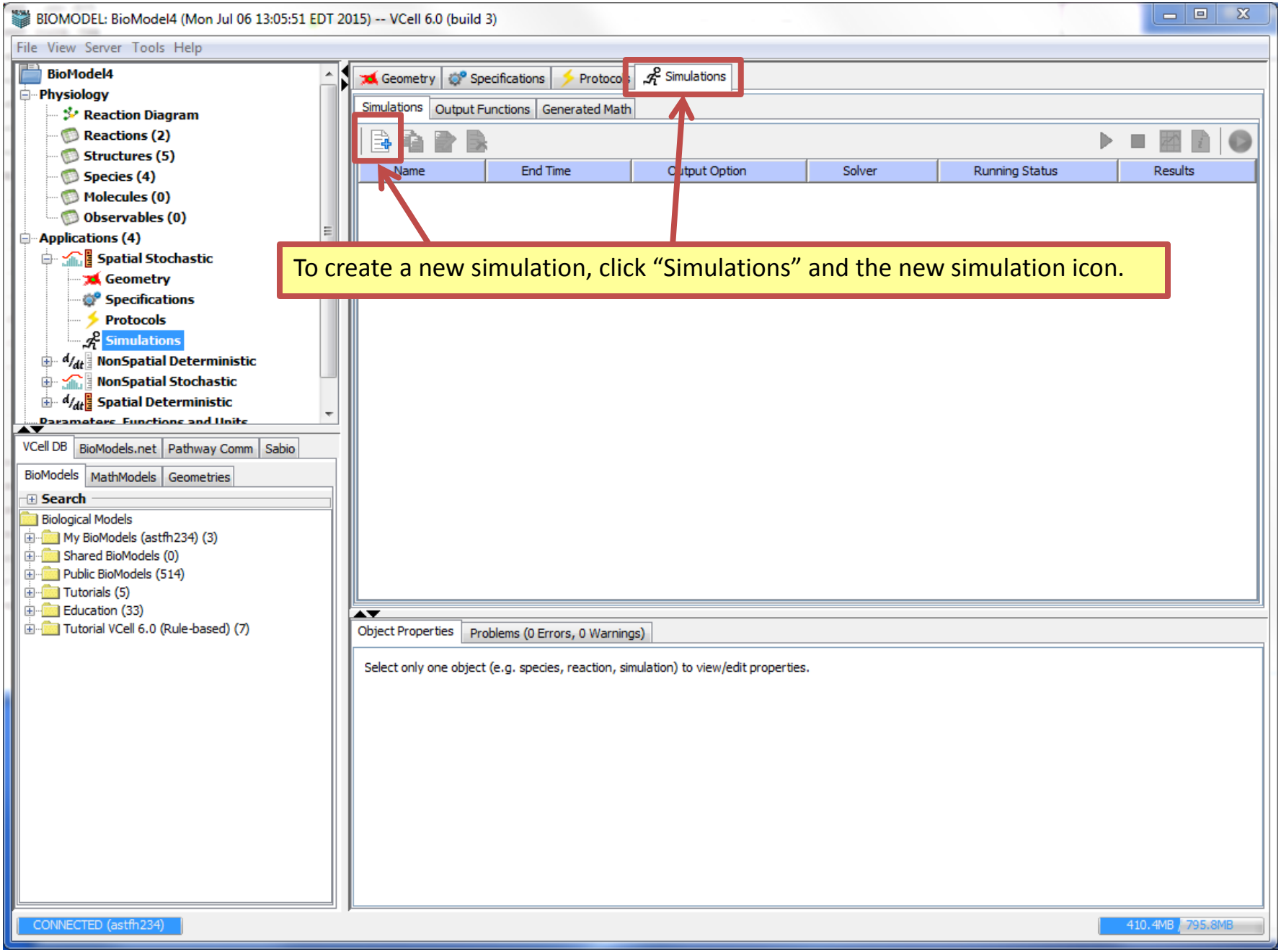
Initial Condition: Concentration Number of Particles
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Force Continuous
RanC_Cyt
Cyt
0.0
10.0
C_Cyt
Cyt
0.0
10.0
Ran_Cyt
Cyt
0.0
10.0
RanC_Nuc
Nuc
1000
10.0
To change the number of particles of a species, type in a value under the “Initial Condition” column.
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Description
Parameter
Expression
Units
initial count for RanC_Nuc for RanC_Nuc
initCount
10000.0
molecules
diffusion constant for RanC_Nuc for RanC_Nuc
diff
10.0
μm².s⁻¹
Boundary Condition X- for RanC_Nuc for RanC_Nuc
BC_Xm
<zero flux>
μM.μm.s⁻¹
Boundary Condition X+ for RanC_Nuc for RanC_Nuc
BC_Xp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y- for RanC_Nuc for RanC_Nuc
BC_Ym
<zero flux>
μM.μm.s⁻¹
Boundary Condition Y+ for RanC_Nuc for RanC_Nuc
BC_Yp
<zero flux>
μM.μm.s⁻¹
Boundary Condition Z- for RanC_Nuc for RanC_Nuc
BC_Zm
<zero flux>
μM.μm.s⁻¹
Boundary Condition Z+ for RanC_Nuc for RanC_Nuc
BC_Zp
<zero flux>
μM.μm.s⁻¹
Velocity X for RanC_Nuc for RanC_Nuc
Vel_X
<0.0>
μm.s⁻¹
Velocity Y for RanC_Nuc for RanC_Nuc
Vel_Y
<0.0>
μm.s⁻¹
CONNECTED (astfh234)
400MB / 795.8MB

Contents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Simulations
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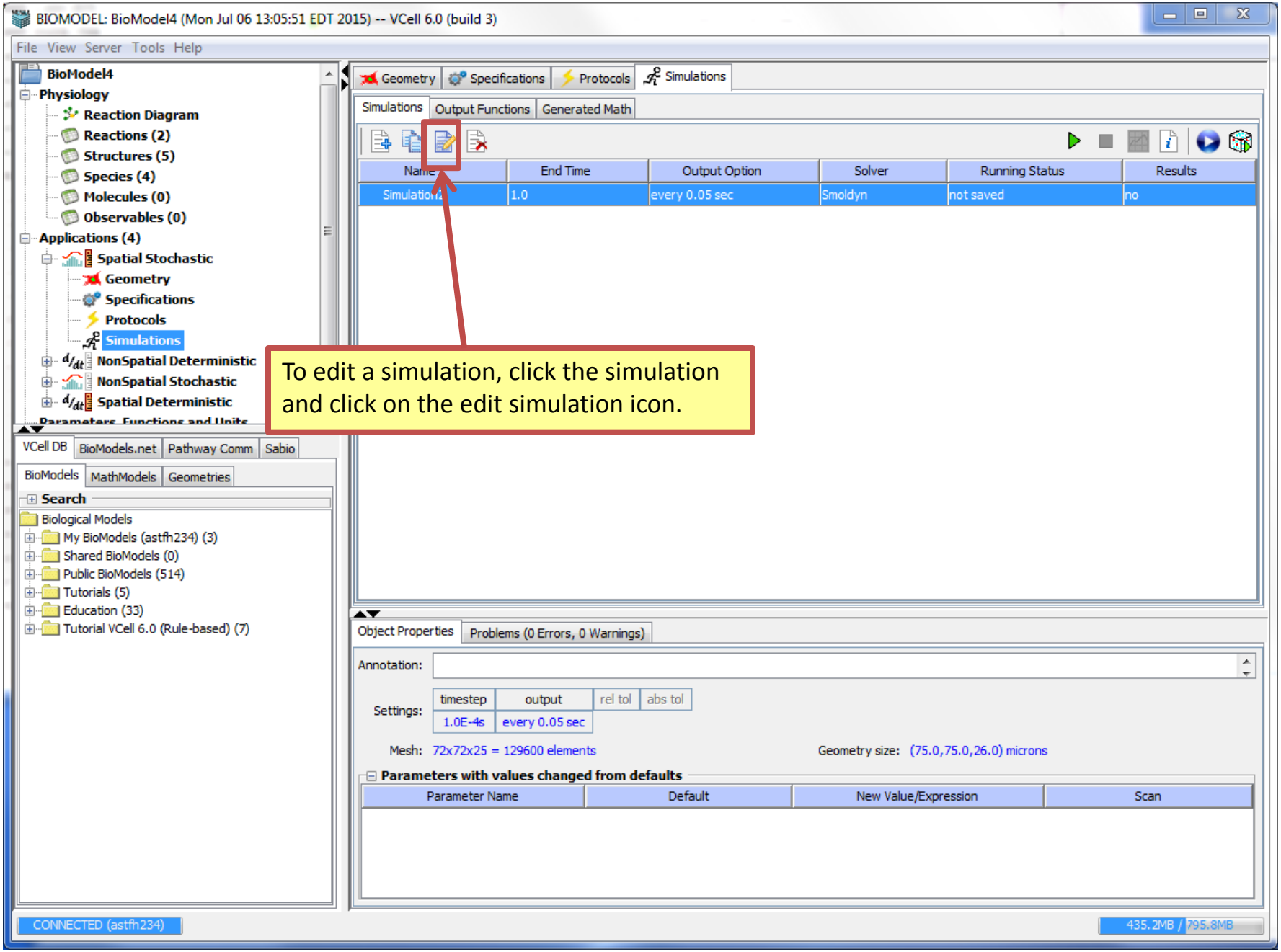
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
To create a new simulation, click “Simulations” and the new simulation icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (astfh234)
410.4MB
795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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NonSpatial Stochastic
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Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
1.0
every 0.05 sec
Smoldyn
not saved
no
To edit a simulation, click the simulation and click on the edit simulation icon.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
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Public BioModels (514)
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Education (33)
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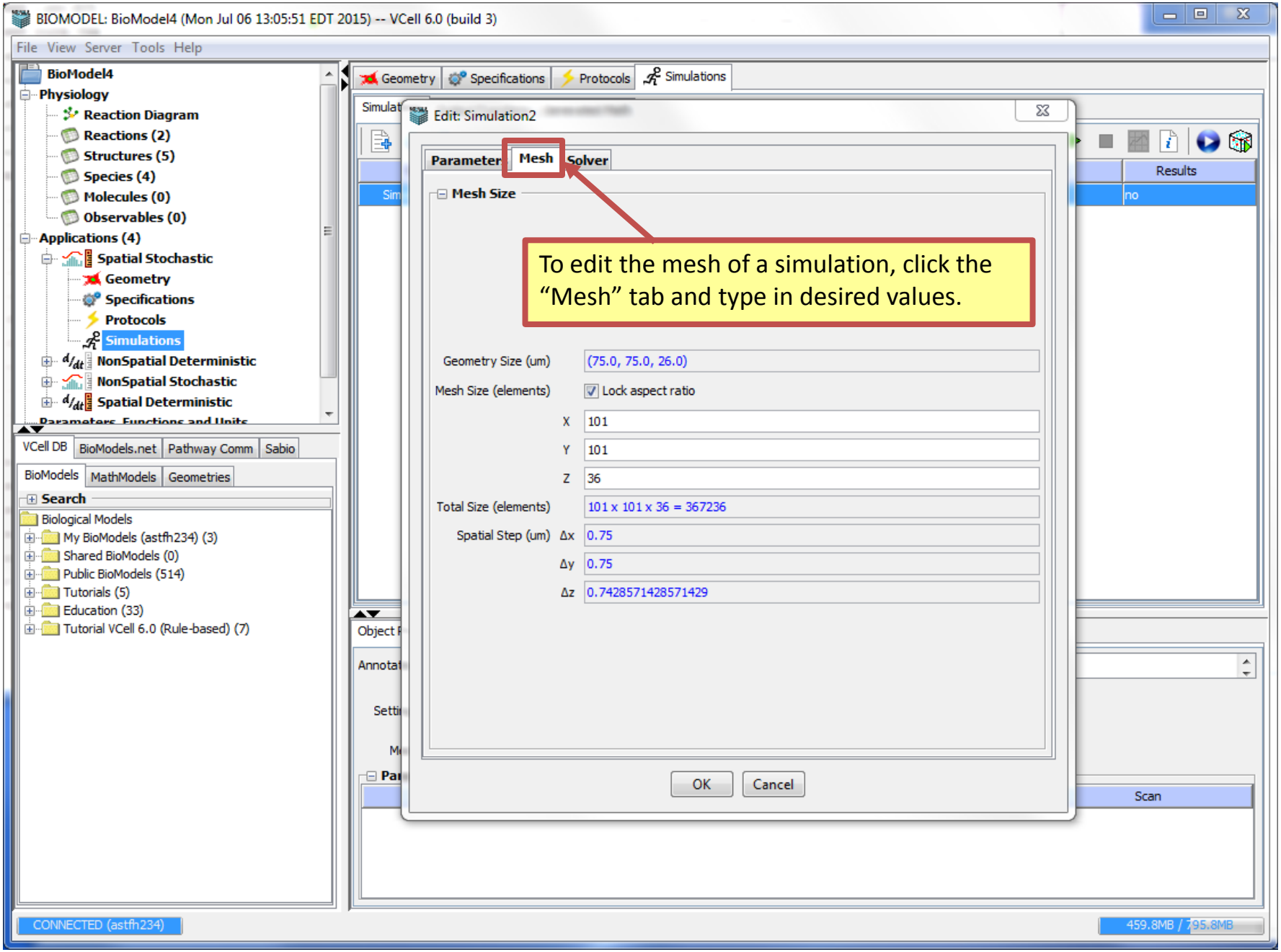
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
timestep
output
rel tol
abs tol
1.0E-4s
every 0.05 sec
Mesh: 72x72x25 = 129600 elements
Geometry size: (75.0,75.0,26.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (astfh234)
435.2MB / 795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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Observables (0)
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NonSpatial Stochastic
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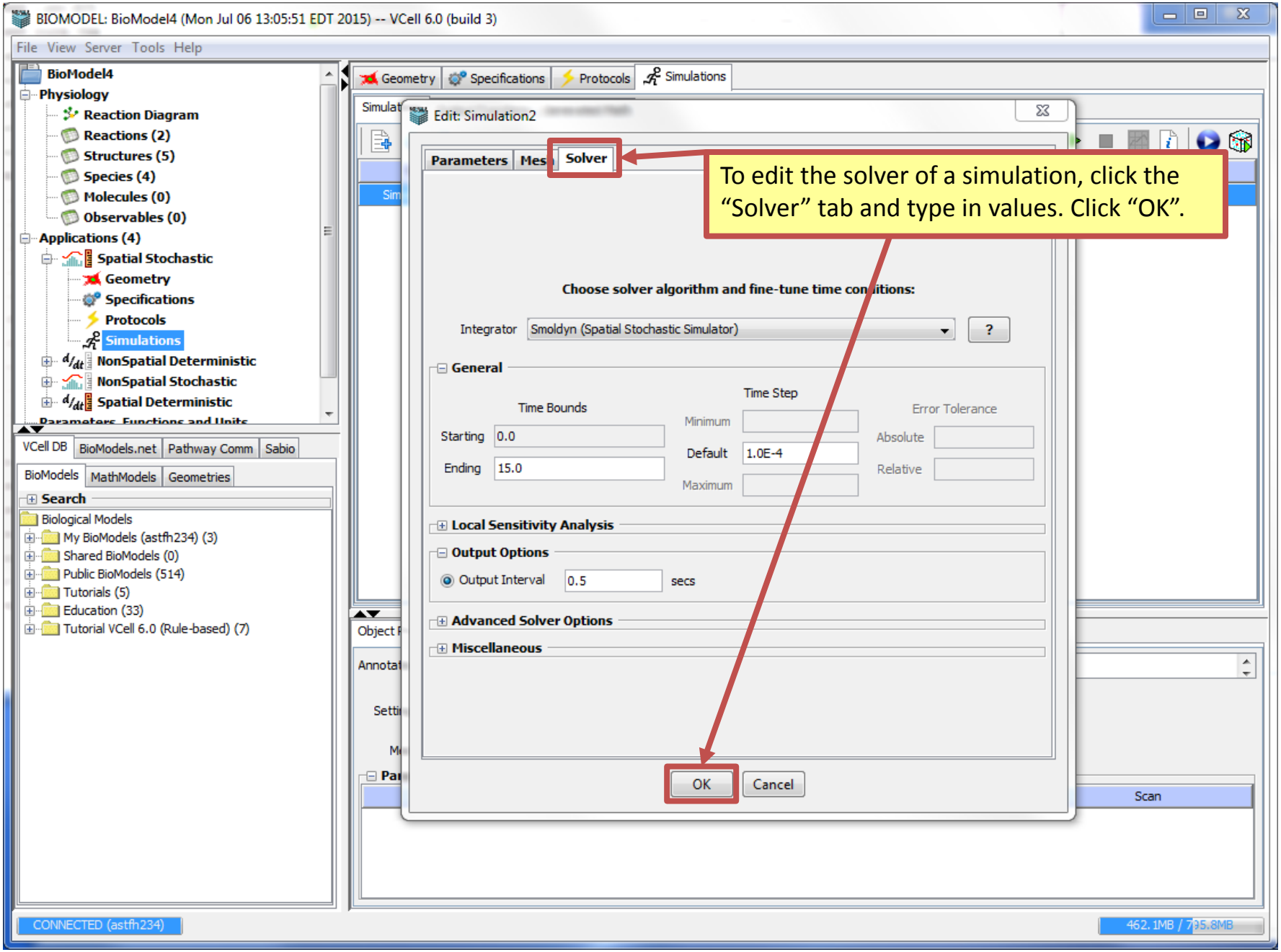
Edit: Simulation2
Parameter
Mesh
Solver
Mesh Size
To edit the mesh of a simulation, click the "Mesh" tab and type in desired values.
Geometry Size (um)
(75.0, 75.0, 26.0)
Mesh Size (elements)
Lock aspect ratio
X
101
Y
101
Z
36
Total Size (elements)
101 x 101 x 36 = 367236
Spatial Step (um)
Δx
0.75
Δy
0.75
Δz
0.7428571428571429
OK
Cancel
Scan
CONNECTED (astfh234)
459.8MB / 795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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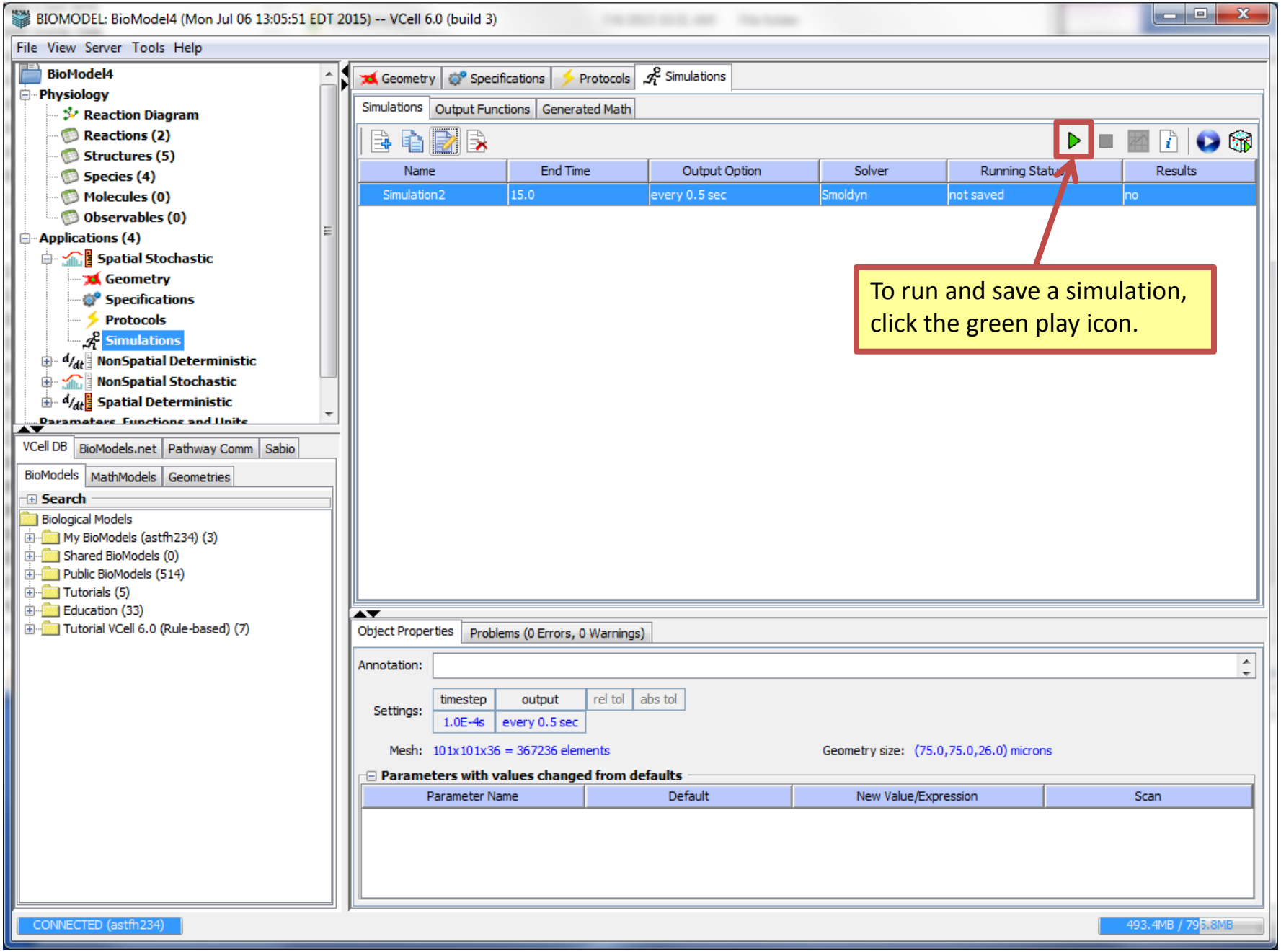
Edit: Simulation2
Parameters
Solver
To edit the solver of a simulation, click the "Solver" tab and type in values. Click "OK".
Choose solver algorithm and fine-tune time conditions:
Integrator
Smoldyn (Spatial Stochastic Simulator)
?
General
Time Bounds
Starting
0.0
Ending
15.0
Time Step
Minimum
Default
1.0E-4
Maximum
Error Tolerance
Absolute
Relative
Local Sensitivity Analysis
Output Options
Output Interval
0.5
secs
Advanced Solver Options
Miscellaneous
OK
Cancel
Scan
CONNECTED (astfh234)
462.1MB / 795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:05:51 EDT 2015) -- VCell 6.0 (build 3)
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Simulations
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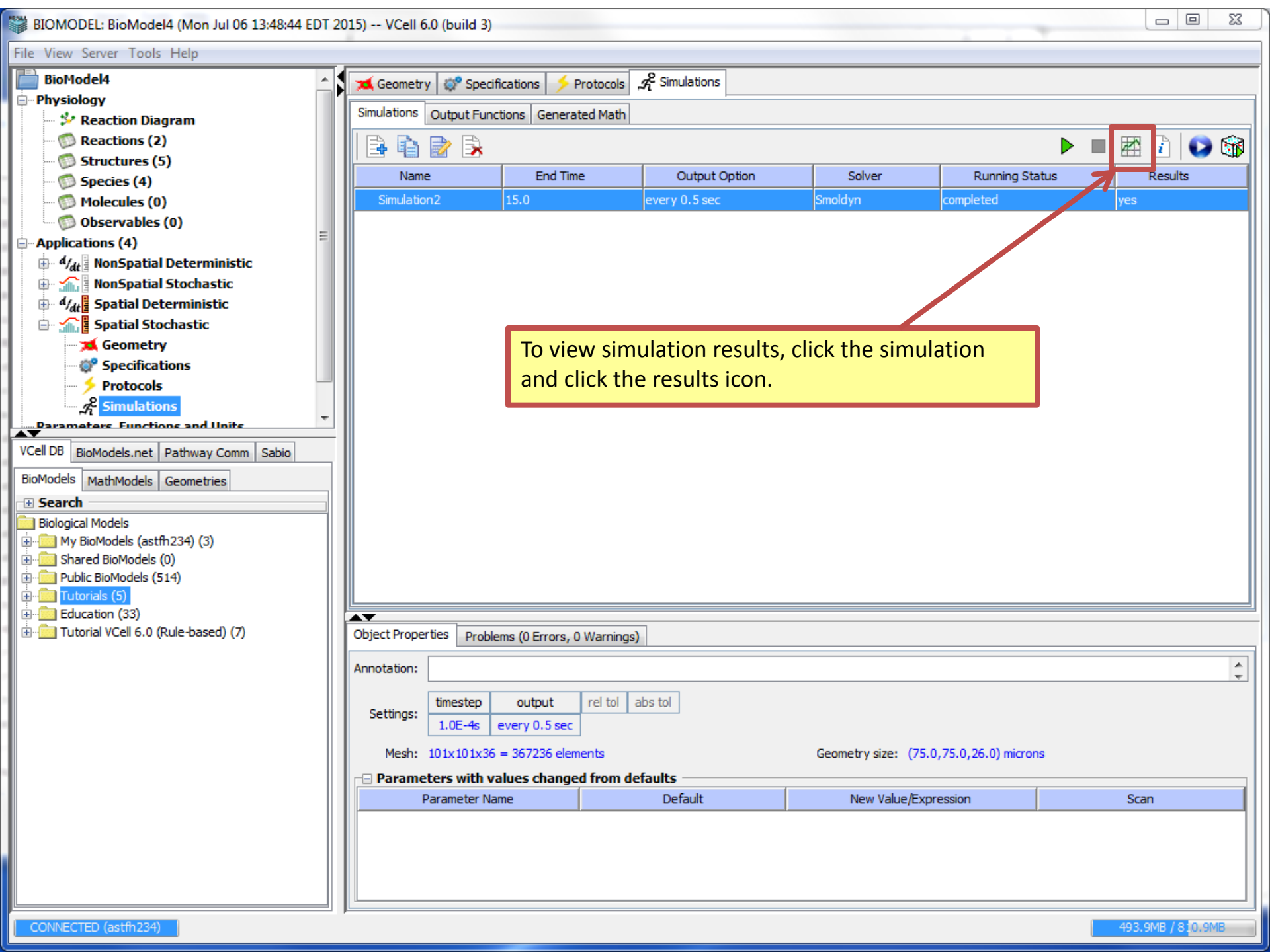
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation2
15.0
every 0.5 sec
Smoldyn
not saved
no
To run and save a simulation, click the green play icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
timestep
output
rel tol
abs tol
1.0E-4s
every 0.5 sec
Mesh: 101x101x36 = 367236 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)
493.4MB / 795.8MB


BIOMODEL: BioModel4 (Mon Jul 06 13:48:44 EDT 2015) -- VCell 6.0 (build 3)
File View Server Tools Help
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Molecules (0)
Observables (0)
Applications (4)
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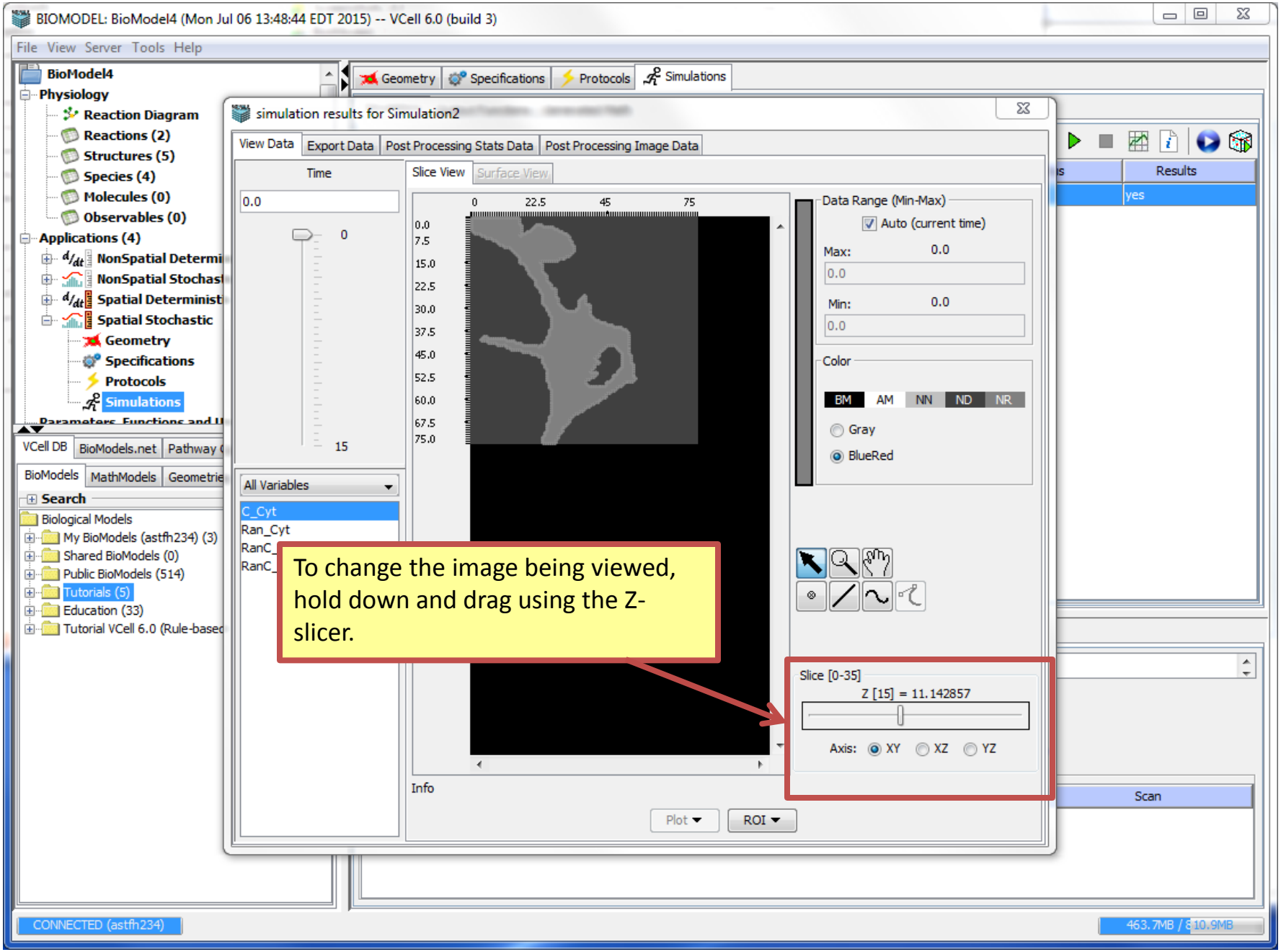
Name
End Time
Output Option
Solver
Running Status
Results
Simulation2
15.0
every 0.5 sec
Smoldyn
completed
yes
To view simulation results, click the simulation and click the results icon.
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation:
Settings:
timestep
output
rel tol
abs tol
1.0E-4s
every 0.5 sec
Mesh: 101x101x36 = 367236 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)
493.9MB / 8


BIOMODEL: BioModel4 (Mon Jul 06 13:48:44 EDT 2015) -- VCell 6.0 (build 3)
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Observables (0)
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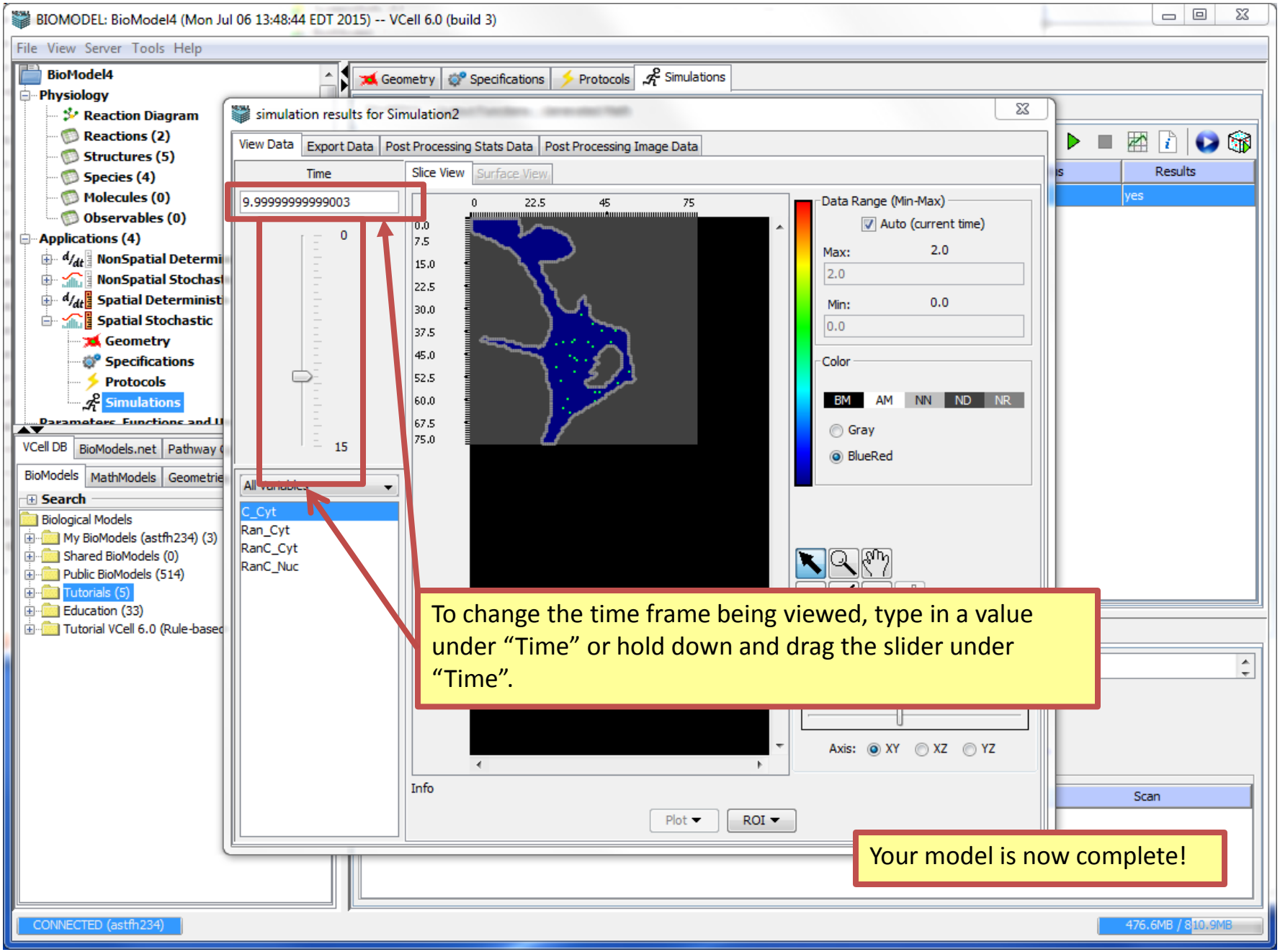
simulation results for Simulation2
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
0.0
0
15
All Variables
C_Cyt
Ran_Cyt
RanC_
RanC_
Slice View
Surface View
0
22.5
45
75
0.0
7.5
15.0
22.5
30.0
37.5
45.0
52.5
60.0
67.5
75.0
Data Range (Min-Max)
Auto (current time)
Max:
0.0
0.0
Min:
0.0
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
Slice [0-35]
Z [15] = 11.142857
Axis:
XY
XZ
YZ
Info
Plot
ROI
Results
yes
Scan
CONNECTED (astfh234)
463.7MB / 810.9MB
To change the image being viewed, hold down and drag using the Z-slicer.


BIOMODEL: BioModel4 (Mon Jul 06 13:48:44 EDT 2015) -- VCell 6.0 (build 3)
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simulation results for Simulation2
View Data
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Post Processing Image Data
Time
9.99999999999003
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max:
2.0
Min:
0.0
Color
BM
AM
NN
ND
NR
Gray
BlueRed
C_Cyt
Ran_Cyt
RanC_Cyt
RanC_Nuc
Axis: XY XZ YZ
Info
Plot
ROI
Results
yes
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CONNECTED (astfh234)
476.6MB / 810.9MB
To change the time frame being viewed, type in a value under “Time” or hold down and drag the slider under “Time”.
Your model is now complete!