

VCell Tutorial

BioModel with Multiple Applications

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

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

The Multi-App Tutorial

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

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

- Part 2: Additional Applications

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

In Part 1 of this tutorial...

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

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First time opening VCell



Virtual Cell login

User Name

Password

Login Cancel

Forgot Login Password...

New User Registration...

Use [this link](#) for details on how to acknowledge Virtual Cell in your publication and how to share your published research through the VCell database.

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

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

New BioModel
Open MathModel
Close Ctrl+W Geometry
Save
Save New Version
Save As...
Revert to Saved
Compare with Saved
Permissions...
Model Annotation ...
Edit Annotation...
Field Data...
Import... m Sabio
Export...
Exit

Reaction Diagram Reactions Structures Species

c0

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 (tanyamiller1221) 99.9MB / 131.6MB

To create a new VCell model, click "File" > "New" > "BioModel".

The screenshot displays the VCell software interface. On the left, a tree view shows the project structure under 'BioModel1', including 'Physiology', 'Reaction Diagram', 'Reactions (0)', 'Structures (1)', 'Species (0)', 'Applications (0)', 'Parameters and Functions', and 'Pathway'. Below this is a search bar and a list of biological models. The main workspace is titled 'Reaction Diagram' and contains a toolbar with various tools. A red box highlights the 'Add Compartment' tool (a circle with a dot). A yellow text box explains: 'To create a new compartment, click on compartment tool. Two dashed vertical lines will appear that will let you to specify membranes surrounding this compartment.' The workspace shows two vertical dashed lines. A red arrow points from the 'Add Membrane' button in a floating menu to one of these dashed lines. A second yellow text box explains: 'To create a new membrane, right click on one of the black lines so that they turn green. Select "add membrane".' The bottom of the interface shows 'CONNECTED (tanyamiller1221)' and a memory usage indicator '42.3MB / 130.5MB'.

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (1)
 - Species (0)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

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

Add Compartment
Add Membrane

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

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

CONNECTED (tanyamiller1221) 42.3MB / 130.5MB

The screenshot displays the VCell software interface for a model named 'BioModel1'. The main workspace shows a reaction diagram with two compartments: 'c0' (a volumetric compartment) and 'm0' (a membrane compartment). The membrane is represented by a vertical dotted black line. A context menu is open over the membrane, with 'Add Compartment' and 'Add Membrane' options highlighted by a red box. A red arrow points from the text box to the 'Add Compartment' option.

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

The interface includes a left sidebar with a tree view of the model's structure (Physiology, Reactions, Structures, Species, Applications, Parameters and Functions, Pathway) and a search bar. The bottom status bar shows 'CONNECTED (tanyamiller1221)' and '75.4MB / 130.5MB'.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (5)
 - Species (0)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

c0 m0 c1 m1

To rearrange compartments and membranes, click selection mode and drag the compartments by their label.

VCeCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

- My BioModels (tanyamiller1221) (3)
- Shared BioModels (0)
- Public BioModels (519)
- Tutorials (5)
- Education (33)

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one structure to edit properties

Structure Name c1

Size Variable Name c1 [μm^3]

Annotation

Continue creating compartments and membranes until you have reached your desired model. This model has extracellular, cytosol, and nucleus as compartments separated by membranes (pm and nm)

CONNECTED (tanyamiller1221) 83.3MB / 130.5MB

To name compartments and membranes, click selection mode.

To change the structure name, double click on the structure's label, or type in the desired name under "Object Properties" > "Structure Name".

To annotate compartments, type notes under "Object Properties" > "Annotation".

The screenshot shows the BioModeler interface with the following components:

- Left Panel:** A tree view showing the model structure: BioModel1 > Physiology > Reaction Diagram (selected), Reactions (0), Structures (5), Species (0), Applications (0), Parameters and Functions, and Pathway.
- Top Panel:** A toolbar with icons for Reaction Diagram, Reactions, Structures, and Species. A red box highlights the selection mode icon (a mouse cursor).
- Center Panel:** A 3D view of a compartment labeled 'EC'. A red box highlights the label 'EC'.
- Bottom Panel:** The 'Object Properties' panel for the selected structure. It contains the following fields:
 - Structure Name:** EC
 - Size Variable Name:** EC [μm^3]
 - Annotation:** Extra Cellular

The screenshot displays the VCell software interface for a model named 'BioModel1'. The main workspace shows a compartment diagram with three regions: 'PM' (Plasma Membrane), 'Cyt' (Cytosol), and 'NM' (Nucleus Membrane). A red box highlights the 'FluxReaction' tool in the toolbar, and another red box highlights the tool being placed on the 'NM' membrane. A yellow text box with a red border provides instructions: 'To create a flux reaction, click on the FluxReaction tool, then click in a membrane you want to place a flux.'

The 'Object Properties' panel at the bottom right is active for the selected 'NM' structure. It shows the following configuration:

- Structure Name:** NM
- Size Variable Name:** NM [μm^2]
- Electrophysiology:**
 - Voltage Variable Name:** Voltage_NM [mV]
 - Positive (inside feature):** (dropdown menu)
 - Negative (outside feature):** (dropdown menu)
- membrane voltage:** "Voltage_NM" = voltage(inside (+) compartment) - voltage(outside (-) compartment)
- inward currents:** from compartment "outside (-) compartment" into compartment "inside (+) compartment"
- Note: VCell reactions and fluxes specify inward currents (- to +) rather than conventional currents (+ to -).*
- Annotation:** (text input field)

At the bottom left, the status bar indicates 'CONNECTED (tanyamiller1221)'. At the bottom right, the memory usage is shown as '31.8MB / 133.2MB'.

The screenshot displays the VCell software interface for a BioModel1. The main workspace shows a reaction diagram with compartments labeled PM, Cyt, NM, and Nuc. A reaction node labeled 'Flux0' is located in the Cyt compartment. A reactant species 's0' is shown in the Cyt compartment, and a product species is indicated by '<<PRODUCT>>' in the Nuc compartment. A red box highlights the reaction tool icon in the toolbar, and another red box highlights the 'Flux0' node. A red arrow points from the reaction tool to the 'Flux0' node, and another red arrow points from the 'Flux0' node to the product species. A yellow text box explains the process of connecting a reactant species to a flux reaction.

To connect a reactant species to a flux reaction, click on the reaction tool, click on a reaction node, and keeping the left button pressed drag a line to the flux symbol.

To create a product of flux reaction, use the reaction tool to drag a line from the flux to a point inside a compartment where a product species will be located.

CONNECTED (tanyamiller1221) 62.3MB / 133.2MB

To create a reaction, select the reaction tool. If you click then on a species, it will become marked <<REACTANT>>, and you drag a line from it to a point inside the compartment where you will create a reaction node.

flux0

include molecular flux include electric current (into inside structure "undefined")

Kinetic Type: General Flux Density ($\mu\text{M}\cdot\mu\text{m}/\text{s}$) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	0.0	$\mu\text{M}\cdot\mu\text{m}\cdot\text{s}^{-1}$
I	inward current density	<input type="checkbox"/>	0.0	$\text{pA}\cdot\mu\text{m}^{-2}$
netValence	net charge valence	<input type="checkbox"/>	1.0	1

DISCONNECTED

90.3MB / 133.2MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (2)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

r0

s0 s1

Drop your mouse, and a reaction symbol will be created for you.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

not connected

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot s_0$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M}\cdot\text{s}^{-1}$
s0	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

72.4MB / 130MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (2)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram

PM Cyt NM Nuc

<<PRODUCT>>

r0

s0

s1

Pathway Links Search

Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot s_0$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M}\cdot\text{s}^{-1}$
s0	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

72.4MB / 130MB

To create a product species, use the reaction tool to drag from the reaction symbol to a point inside the compartment where your product species will be located.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1
Physiology
Reaction Diagram
Reactions (2)

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

s2 s3 s0 s1

VCeCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search
not connected

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name s0

Linked Pathway Object(s)

Annotation

NOT CONNECTED 93.1MB / 116.4MB

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

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

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

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

RanC_Cyt

RanC_Nuc

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name RanC_Nuc

Linked Pathway Object(s)

Annotation

NOT CONNECTED 49.1MB / 124.8MB

To rename species, click on a species and type in a case-sensitive name under "Object Properties" > "Species Name".

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

not connected

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

RanC_Cyt

flux0

RanC_Nuc

Delete Pathway L

Object Properties Problem

Reaction Name flux0

Electrical Properties include molecular flux include electric current (into inside structure "undefined")

Kinetic Type General Flux Density ($\mu\text{M}\cdot\mu\text{m}/\text{s}$) Convert to [molecules. s^{-1}]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$\{K_{\text{flux}} * (\text{RanC_Cyt} - \text{RanC_Nuc})\}$	$\mu\text{M}\cdot\mu\text{m}\cdot\text{s}^{-1}$
I	inward current density	<input type="checkbox"/>	0.0	$\text{pA}\cdot\mu\text{m}^{-2}$
netValence	net charge valence	<input type="checkbox"/>	1.0	1
Kflux	user defined	<input type="checkbox"/>	0.0	$\mu\text{m}\cdot\text{s}^{-1}$
RanC_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

34.1MB / 121.1MB

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.

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

not connected

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

RanC_Cyt

flux0

RanC_Nuc

Delete Pathway Links Search

Object Properties Problems (0)

Reaction Name flux0

Electrical Properties include

Kinetic Type General Flux Density ($\mu\text{M}\cdot\mu\text{m}/\text{s}$) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$Kflux \cdot (RanC_Cyt - RanC_Nuc)$	$\mu\text{M}\cdot\mu\text{m}\cdot\text{s}^{-1}$
I	inward current density	<input type="checkbox"/>	0.0	pA. μm^{-2}
netValence	net charge valence	<input type="checkbox"/>	1.0	1
Kflux	user defined	<input type="checkbox"/>	2.0	$\mu\text{m}\cdot\text{s}^{-1}$
RanC_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

44.1 MB / 121.1 MB

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

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

Reaction Diagram

Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

r0

RanC_Cyt

RanC_Nuc

To change the forward rate constant of a reaction, click on a reaction and under "Object Properties", in the "forward rate constant" row and "Expression" column, type in the desired value.

Reaction Name: r0

Kinetic Type: Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot \text{RanC_Cyt} - K_r \cdot \text{C_Cyt} \cdot \text{Ran_Cyt})$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	1.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
RanC_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
C_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Ran_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

60.5MB / 122.7MB

BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

not connected

Reaction Diagram Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

RanC_Cyt

RanC_Nuc

To change the reverse rate constant of a reaction, click on a reaction and under "Object Properties", in the "reverse rate constant" row and "Expression" column, type in the desired value.

Kinetic Type: Mass Action [$\mu\text{M}/\text{s}$] (recommended for stochastic application) Convert to [$\text{molecules}\cdot\text{s}^{-1}$]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot \text{RanC_Cyt} - K_r \cdot \text{C_Cyt} \cdot \text{Ran_Cyt})$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	1.0	s^{-1}
Kr	reverse rate constant	<input type="checkbox"/>	1000.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
RanC_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
C_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Ran_Cyt	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

NOT CONNECTED

69.8MB / 122.7MB

The screenshot displays the VCell 5.3 (build 4) interface for a model named "BioModel1". The main window shows a reaction diagram with compartments: PM, Cyt, NM, and Nuc. The diagram includes species C_Cyt, Ran_Cyt, and RanC_Cyt in the Cyt compartment, and RanC_Nuc in the Nuc compartment. A reaction arrow connects RanC_Cyt to RanC_Nuc. A yellow box highlights the "Reactions", "Structures", and "Species" tabs in the top toolbar, with a red arrow pointing to them from a text box. Another text box at the bottom right states "The Physiology of your model is now complete." The interface also shows a left sidebar with a tree view of the model's components, a search bar, and a status bar at the bottom indicating "NOT CONNECTED" and "82.3MB / 122.7MB".

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (0)
- Parameters and Functions
- Pathway

Reactions Structures Species

PM Cyt NM Nuc

C_Cyt Ran_Cyt

RanC_Cyt RanC_Nuc

Use the "Reactions", "Structures" and "Species" tabs to look up specific details of the physiology, which are useful when working with large and complicated models.

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

The Physiology of your model is now complete.

NOT CONNECTED 82.3MB / 122.7MB

The screenshot displays the VCell software interface. The main window title is "BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 5.3 (build 4)". The interface includes a menu bar (File, View, Server, Tools, Help), a left-hand tree view, a central workspace, and a bottom panel.

The left-hand tree view shows the following structure:

- BioModel1
 - Physiology
 - Reaction Diagram
 - Reactions (0)
 - Structures (1)
 - Species (0)
 - Applications (0)
 - Parameters and Functions
 - Pathway

The bottom panel shows a search for "BioModels" with the following results:

- My BioModels (tanyamiller 12/1)
- Private Thu Jun 25 16:...
- Tutorial
- Tutorial_MultiApp
- Shared BioModels (0)
- Public BioModels (519)
- Tutorials (5)
- Education (33)

The "Private Thu Jun 25 16:..." entry is highlighted with a red box. A red arrow points from this entry to the "Reaction Diagram" folder in the left-hand tree view. Another red arrow points from the "Reaction Diagram" folder to the "Reaction Diagram" tab in the central workspace. A yellow callout box with a red border contains the text: "To re-open a model, click on the folder that the model was saved in and double-click on the model."

The central workspace shows a reaction diagram with the species "c0". The bottom panel also displays "Object Properties" for the selected model, showing a list of properties such as "DetSpatial", "Deterministic", "geom_20150625_105028 (3D)", "Simulation0", "NonSpatialStoch", "Stochastic", "(copied from Application spatial deterministic)", "Compartmental", "Simulation1", "NonSpatialDet", and "Deterministic (copied from DetSpatial)".

The status bar at the bottom indicates "CONNECTED (tanyamiller 1221)" and "74.4MB / 12.1MB".

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 (1)
 - Applications (0)**
 - Parameters and Functions
- Pathway

VCell DB BioModels.net Path...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller 1221)
 - Tutorial
 - BioModel2
 - Private Thu Jun 25 16:00
 - Tutorial_MultiApp
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Name	Math Type	Annotation
------	-----------	------------

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 (tanyamiller 1221) 356.5MB / 514.8MB

To create a new deterministic model, click "Applications" > "Add New" > "Deterministic".

VCell User Guides

User Guide

Release version now has online help from within the VCell interface. From the Help top menu select "Help" to open the guide.

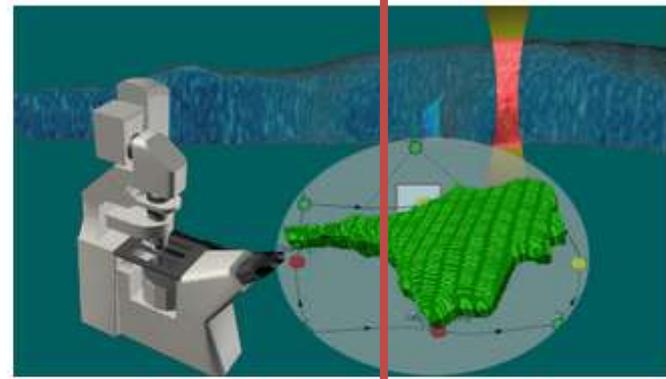
[Click here](#) for a Quick Start guide for Release.

html version of [VCell help program](#) (also available from Help menu of VCell software)

Tutorials

The tutorials have been provided to work in conjunction with the users guide for the release version of Virtual Cell. The tutorials lead the user step by step through the construction of the BioModel, Application and Simulation. There are public versions of the BioModels, Applications and Simulations available in the Tutorial folder. Go to File Open BioModel Model Neighborhood Tutorial folder.

Tutorial Guides (pdf)	
simple FRAP	
FRAP with binding	
PH-GFP Translocation	
Multiple Application of a Nuclear Transport Biomodel	
Using Pathway Commons	
Video Tutorials	
VCell Education YouTube Channel	
VCell MultiApp Tutorial: Part 1. Creating Physiology	
VCell MultiApp Tutorial: Part 2. Creating Geometry for tutorial	3D images for tutorial
VCell MultiApp Tutorial: Part 3. Deterministic Spatial Simulation	



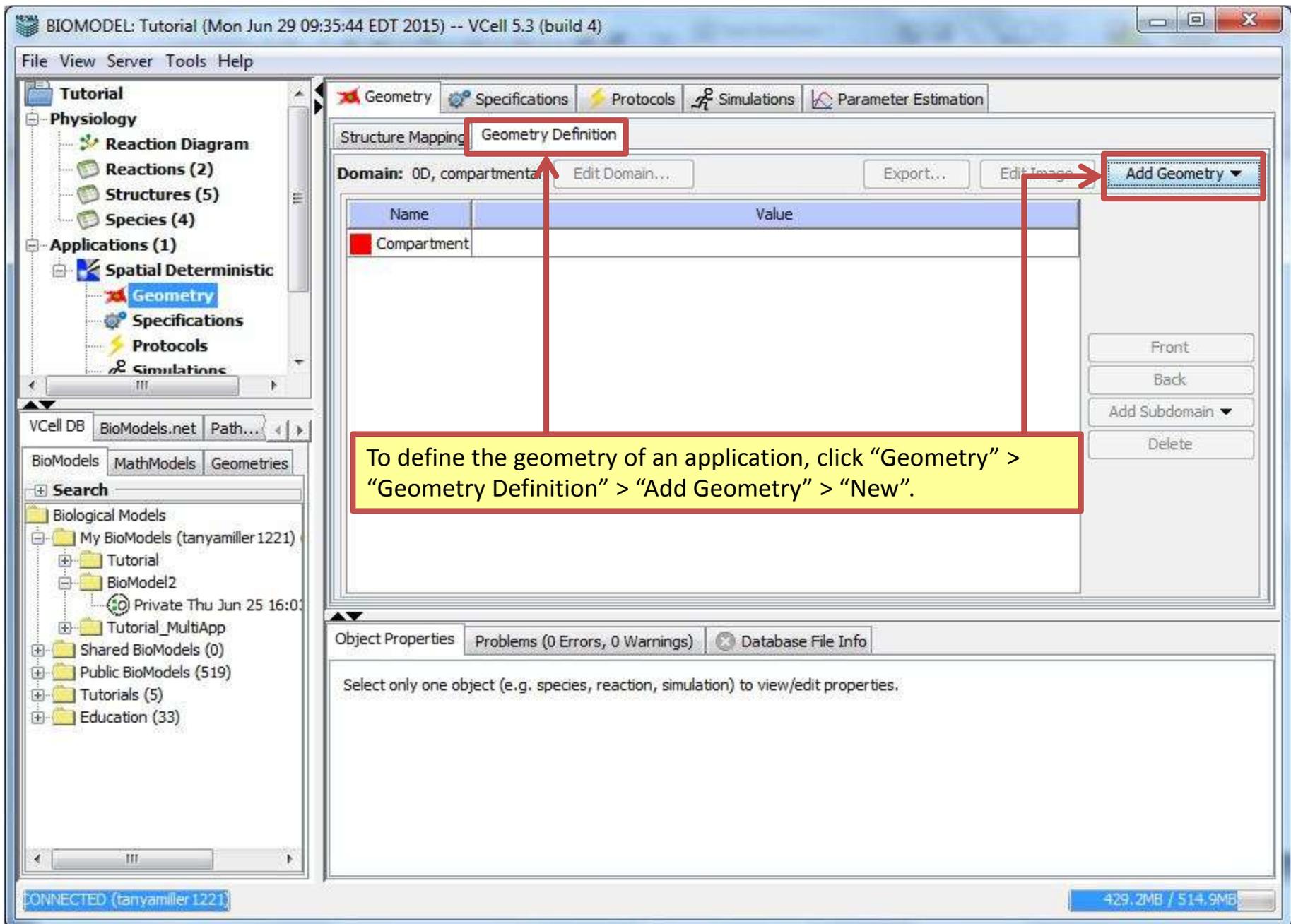
Share your published VCell Models

Modeling/Database Links

Software Support
vcell_support@ucho.edu
VCell Discussion Forum

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.

[3D images for tutorial](#)



BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping **Geometry Definition**

Domain: OD, 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 (tanyamiller 1221) 429.2MB / 514.9MB

The screenshot shows the VCell software interface. The main window is titled "BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)". The left sidebar shows a tree view of the project structure, including "Physiology", "Applications (1)", and "Spatial Deterministic". The "Geometry" application is selected. The main panel shows the "Geometry Definition" tab with a table for defining geometry. A dialog box titled "Choose new geometry type to create" is open, listing several options. The "Image based (import from file, zip or directory)" option is highlighted in blue. The "OK" button is also highlighted. A red box and arrows point to these elements, with a text box below explaining the steps.

Choose new geometry type to create

Geometry Type
Analytic Equations (1D)
Analytic Equations (2D)
Analytic Equations (3D)
Image based (import from file, zip or directory)
Mesh based (import from STL file)
New Blank Image Canvas
Constructed Solid Geometry (3D)

OK Cancel

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

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

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

File name: neuroblastoma_3D_images

Files of type:

Open

Cancel

To select images to import, click on the folder containing the images and click "Open".

CONNECTED (tanyamiller1221)

164.6MB / 586.7MB

The screenshot shows the VCell software interface. The main window is titled "BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)". The interface includes a menu bar (File, View, Server, Tools, Help) and a toolbar with icons for Geometry, Specifications, Protocols, Simulations, and Parameter Estimation. A left sidebar shows a tree view of the model structure, including Physiology (Reaction Diagram, Reactions (2), Structures (5), Species (4)), Applications (1), and Spatial Deterministic (Geometry, Specifications, Protocols, Simulations). The main workspace is divided into tabs for Structure Mapping and Geometry Definition. The Geometry Definition tab is active, showing a table with columns "Name" and "Value". The table contains one entry: "Compartment" with a red square icon. Below the table are buttons for "Front", "Back", "Add Subdomain", and "Delete".

A dialog box is overlaid on the main workspace. The dialog box has a yellow warning icon and contains the following text:

To import everything as Z-sections, click "Import Z-Sections".

**Import all files in directory
'C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images' as Z-Sections**

The dialog box has two buttons: "Import Z-Sections" and "Cancel". A red arrow points from the text in the dialog box to the "Import Z-Sections" button.

At the bottom of the VCell window, there is a status bar showing "CONNECTED (tanyamiller1221)" on the left and "243MB / 536.7MB" on the right.

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition

Domain: 0D, compartmental Edit Domain... Export... Edit Image Add Geometry ▾

Name	Value
Compartment	

Optionally convert imported images.

Image Name: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_ima...

Original Size (x,y,z): (512,512,34)

Changed Size 256,256,34
(x,y,z):

Move slider to change X,Y proportional scale factor.

.1 .2 .3 .4 .5 .6 .7 .8 .9 1x 2x 3x 4x 5x 6x 7x 8x 9x 10x

Channel Count: (1) Merge All Channels to One?

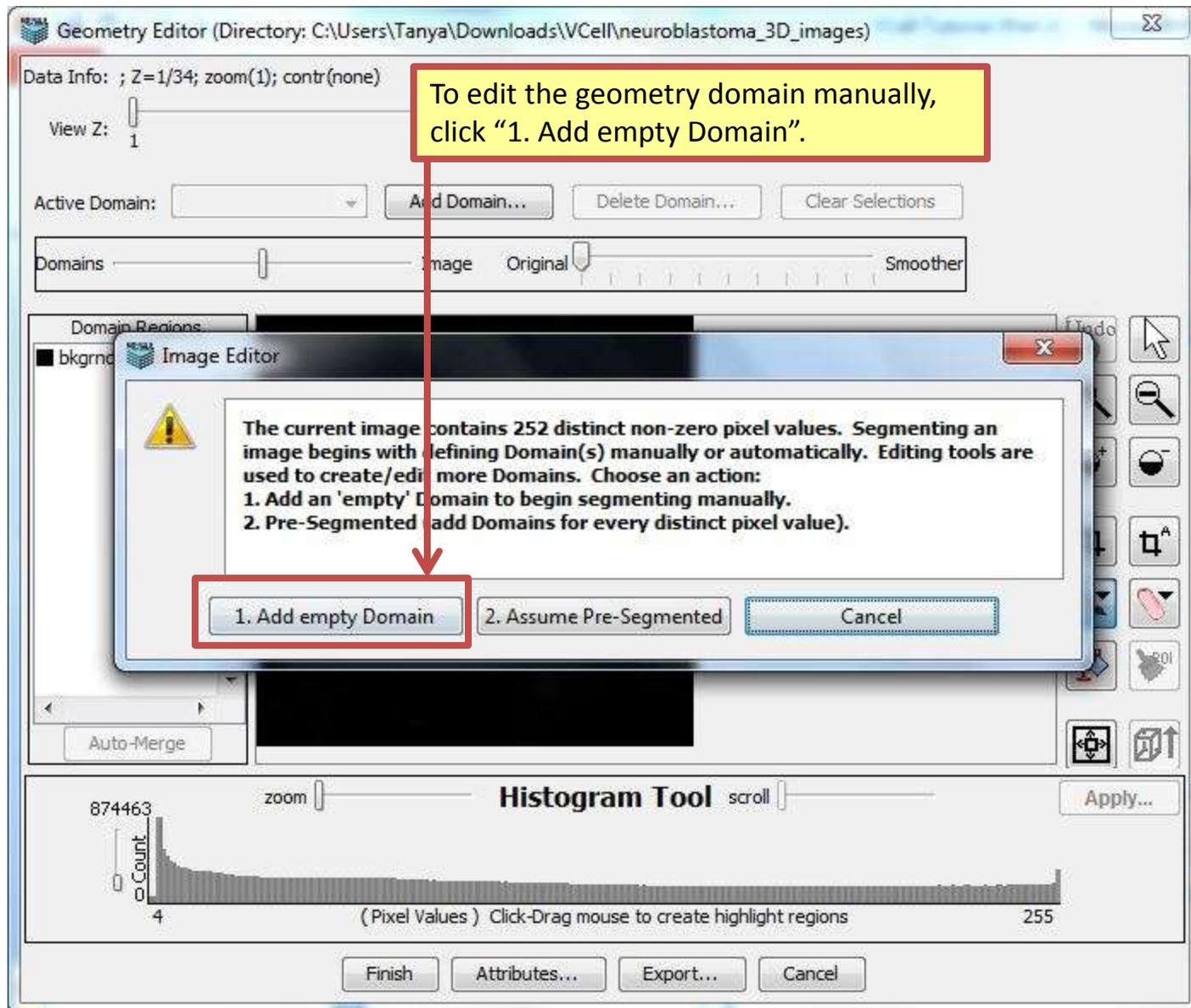
TimePoints: 0.0 Select a TimePoint to import

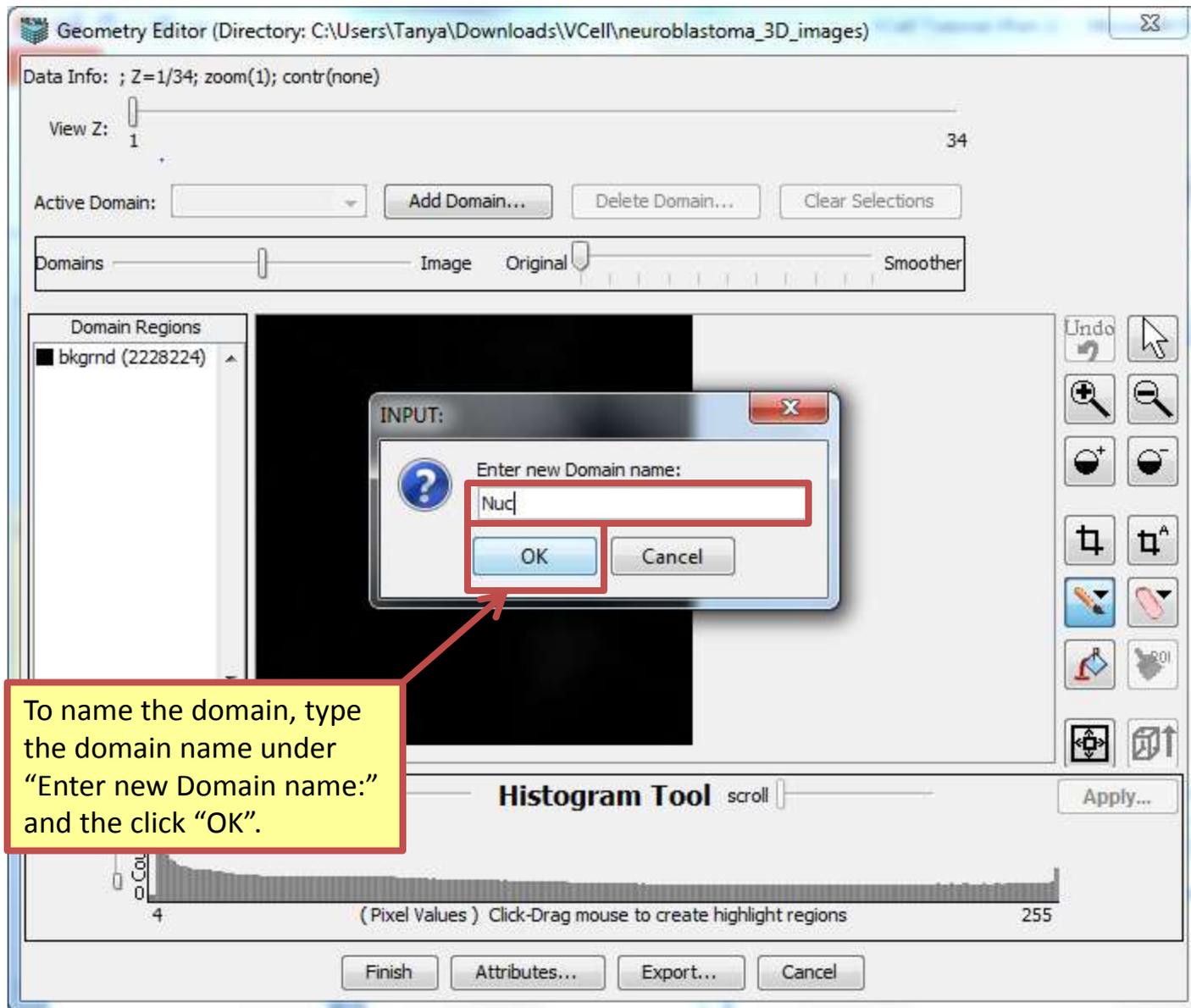
OK Cancel

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

CONNECTED (tanyamiller.1221) 268.3MB / 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".





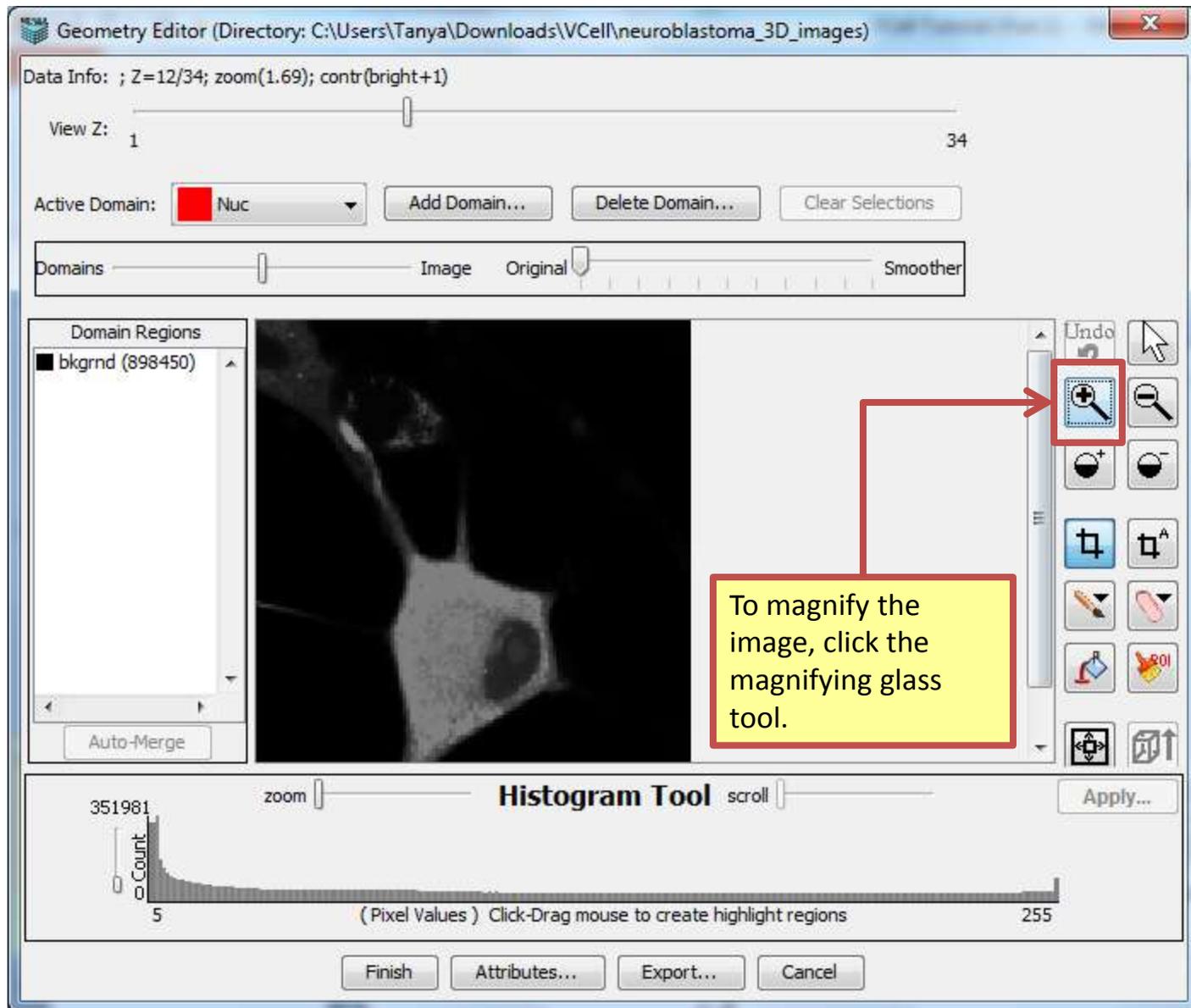
The screenshot shows the Geometry Editor window with the following components:

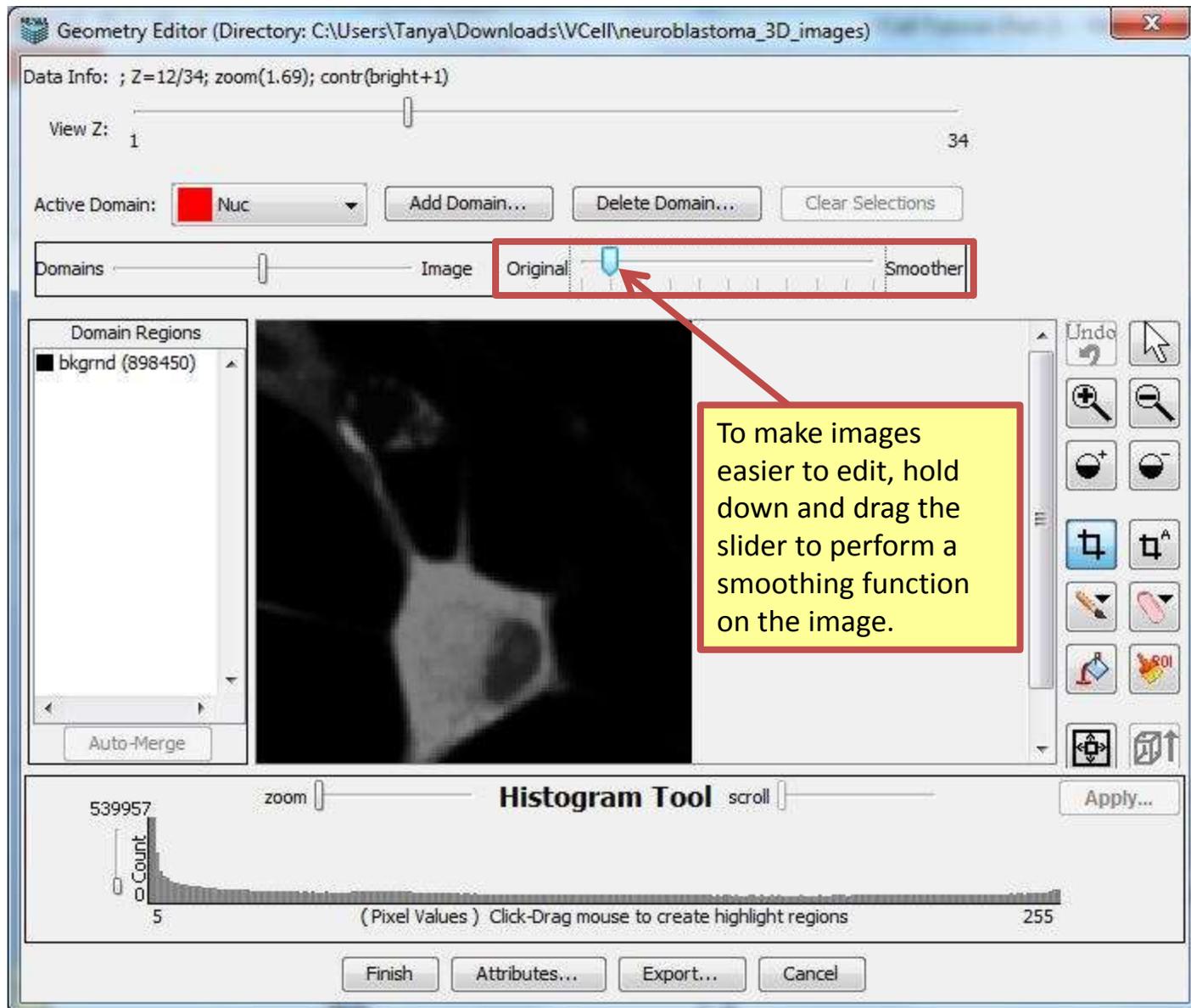
- Data Info:** ; Z=12/34; zoom(1); contr(bright+1)
- View Z:** A slider ranging from 1 to 34, with a blue cursor at 12.
- Active Domain:** A dropdown menu currently set to "Nuc" with a red square icon.
- Domains:** A slider and a list of domains including "bkgnd (2228224)".
- Image:** A central grayscale image of a cell.
- Right Panel:** A toolbar with icons for Undo, mouse cursor, zoom in/out, contrast, and other image manipulation tools.
- Histogram Tool:** A histogram showing pixel value distribution from 4 to 255, with a count of 874463.
- Bottom Panel:** Buttons for "Finish", "Attributes...", "Export...", and "Cancel".

Two red callout boxes provide instructions:

- Left Callout:** To change which domain is being worked on, click on the drop down menu next to "Active Domain".
- Right Callout:** To change the image being worked on, use your cursor to move the Z slider to see different slices of the image.

The screenshot displays the Geometry Editor software interface. At the top, the title bar reads "Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)". Below the title bar, the "Data Info" section shows parameters: "; Z=12/34; zoom(1); contr(bright+1)". A "View Z" slider is set to 1, with a range from 1 to 34. The "Active Domain" is set to "Nuc" with a red color swatch. A "Domains" slider is visible below. On the left, the "Domain Regions" list contains "bkgnd (2228224)". The central image shows a grayscale micrograph of a cell with a green rectangular crop box. A dialog box titled "Confirm Crop Data to new boundaries." is overlaid on the image, asking "Crop data to new bounds?: (105,81) to (255,255)". The "OK" button in the dialog is highlighted with a red box. A yellow text box with a red border contains the instruction: "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'." The crop tool icon, which is a blue square with a white crop symbol, is also highlighted with a red box. At the bottom, the "Histogram Tool" is visible, showing a histogram of pixel values from 4 to 255, with a peak count of 874463. The histogram has a "zoom" slider and an "Apply..." button. At the very bottom, there are buttons for "Finish", "Attributes...", "Export...", and "Cancel".





The screenshot shows the Geometry Editor window with the following components:

- Title Bar:** Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCeell\neuroblastoma_3D_images)
- Data Info:** ; Z=12/34; zoom(1.69); contr(bright+1)
- View Z:** Slider from 1 to 34.
- Active Domain:** Nuc (with a red square icon), Add Domain..., Delete Domain..., Clear Selections.
- Domains:** Image Original (with a blue highlight) Smoother.
- Domain Regions Panel:** bkgnd (898450), Auto-Merge.
- Main View:** A grayscale image of a cell with a yellow highlight on a specific region.
- Right Panel:** Undo, mouse cursor, zoom in/out, crop, and other tools.
- Histogram Tool:** A histogram showing pixel counts. The x-axis is labeled '(Pixel Values) Click-Drag mouse to create highlight regions' with values 5 and 255. The y-axis is labeled 'Count' with a value of 539957. A red box highlights the histogram, and a red arrow points from a text box to it.
- Buttons:** Apply..., Finish, Attributes..., Export..., Cancel.

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.

The screenshot shows the Geometry Editor window with the following components:

- Header:** Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCeCell\neuroblastoma_3D_images)
- Data Info:** ; Z=21/34; zoom(1.69); contr(bright+1)
- View Z:** A slider ranging from 1 to 34, with a blue vertical marker at approximately 21. A red box highlights this slider and a yellow callout box points to it with the text: "To view how well the Histogram Tool highlighted, hold down and drag the Z slider."
- Active Domain:** Nuc (with a red square icon)
- Buttons:** Add Domain..., Delete Domain..., Clear Selections
- Domains:** Image Original Smoother (with a slider)
- Domain Regions:** A list containing "bkgnd (898450)" with a black square icon and an "Auto-Merge" button below it.
- Central View:** A 3D visualization of a cell with a green nucleus and a grey cytoplasm.
- Right Panel:** A vertical toolbar with icons for Undo, mouse cursor, zoom in/out, and other tools. A red box highlights the "Apply..." button at the bottom of this panel, with a yellow callout box pointing to it: "To finalize the selected pixels, click 'Apply'".
- Histogram Tool:** A histogram showing pixel counts. The y-axis is labeled "Count" with a value of 539957. The x-axis is labeled "(Pixel Values)" with a range from 5 to 255. A blue highlight is visible on the histogram. A "scroll" slider is positioned above the histogram.
- Bottom Buttons:** Finish, Attributes..., Export..., Cancel

The screenshot displays the Geometry Editor application window. At the top, the title bar reads "Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCe\neuroblastoma_3D_images)". Below the title bar, the "Data Info" section shows parameters: "; Z=21/34; zoom(1.69); contr(bright+1)". A "View Z:" slider is set to 1, with a range from 1 to 34. The "Active Domain" is set to "Nuc" with a red square icon. Buttons for "Add Domain...", "Delete Domain...", and "Clear Selections" are visible. A "Domains" slider is positioned between "Image" and "Smoother".

The central part of the window shows a 3D visualization of a cell with a highlighted region. A dialog box is overlaid on this visualization, containing the following text:

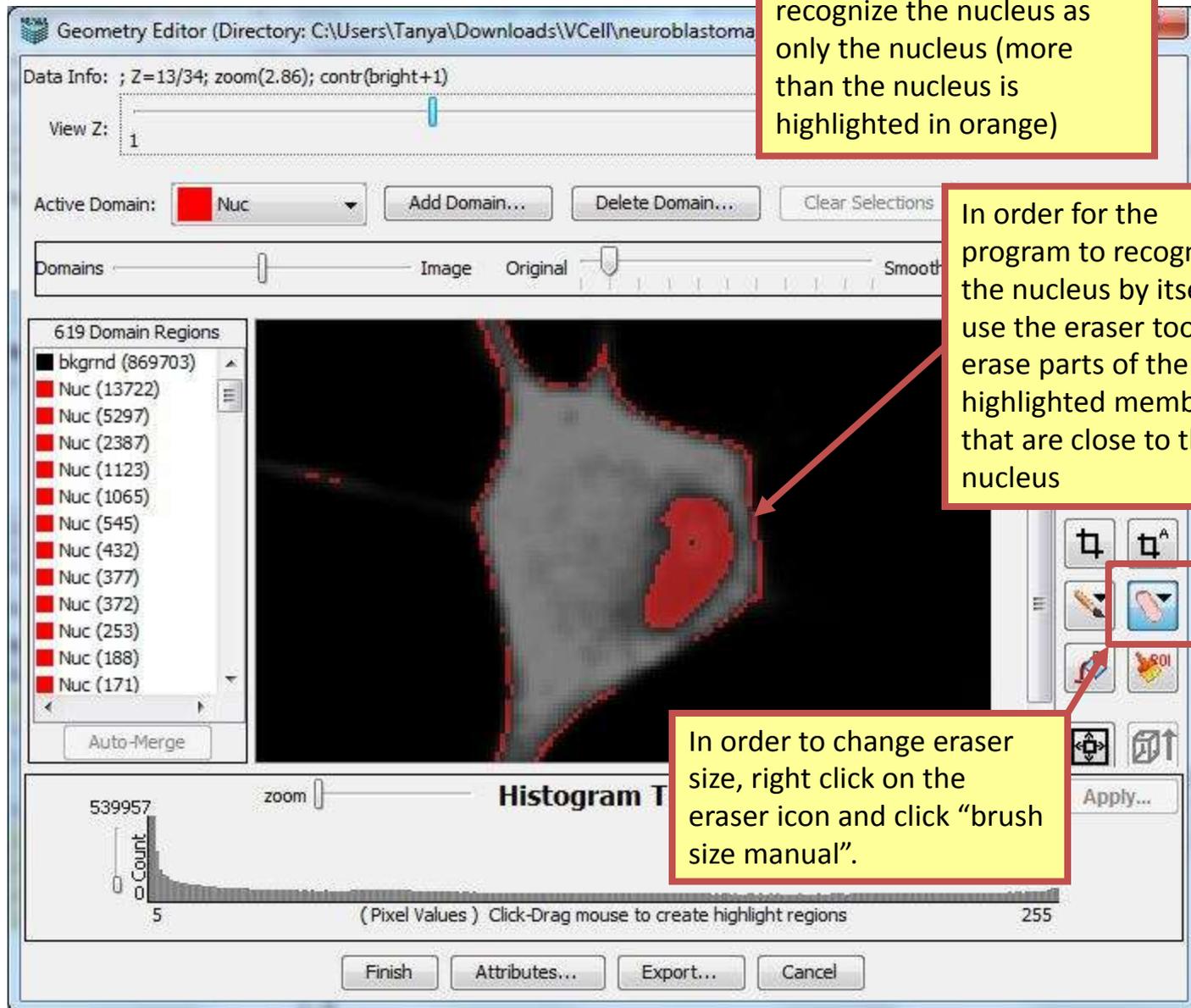
To update the domain, click "Update Domain".

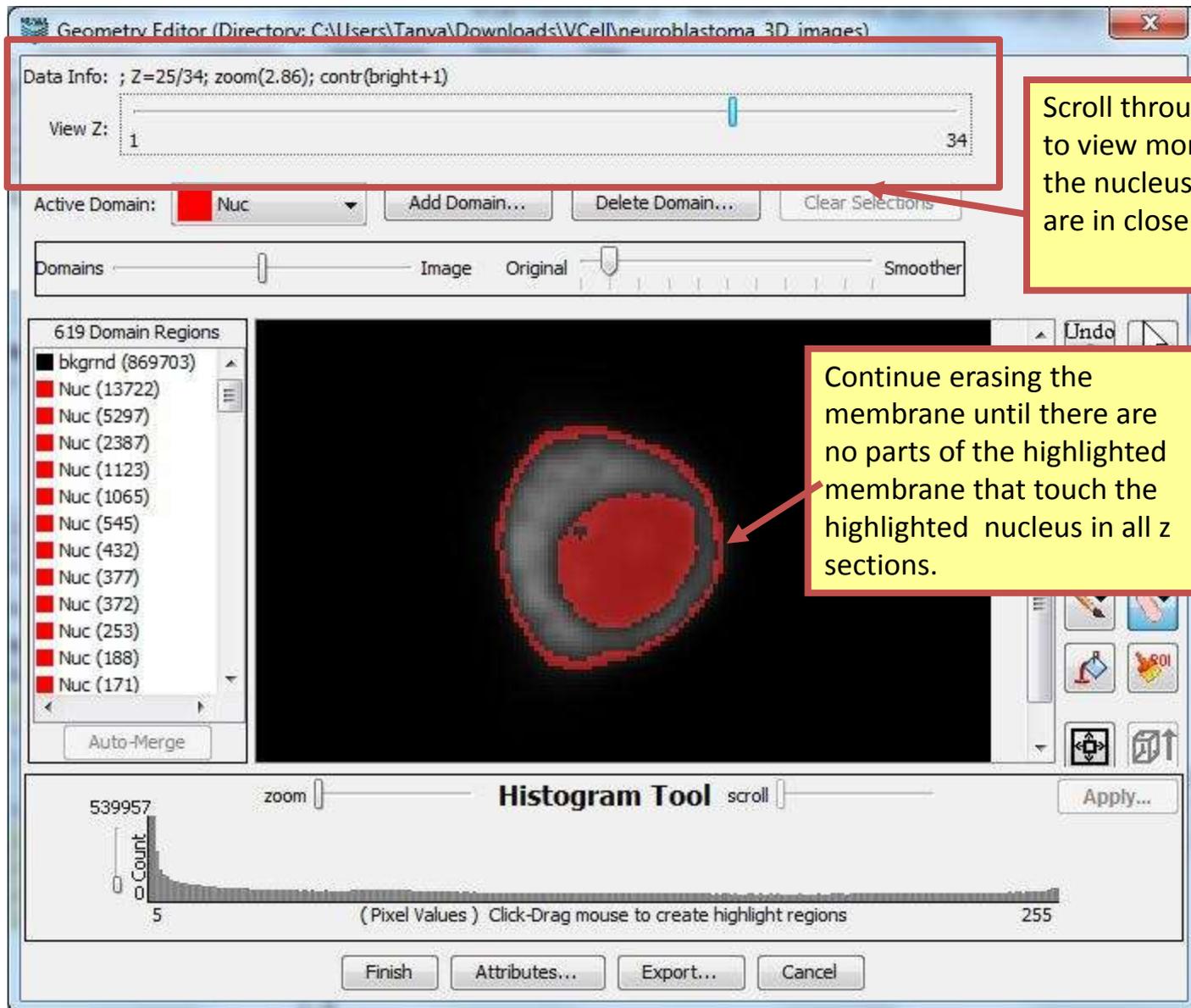
Apply histogram highlighted regions. Choose an action:

1. Update the current Domain 'Nuc' using the histogram highlight.
2. Create a new Domain with the histogram highlight.

The dialog box has three buttons: "Update Domain", "Create Domain", and "Cancel". A red arrow points from the text in the dialog box to the "Update Domain" button.

At the bottom of the window, the "Histogram Tool" is active, showing a histogram with a count of 539957 and a range from 5 to 255. The histogram has a highlighted region. The "Histogram Tool" section includes a "zoom" slider and a "scroll" slider. An "Apply..." button is located to the right of the histogram. At the very bottom of the window, there are buttons for "Finish", "Attributes...", "Export...", and "Cancel".





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.

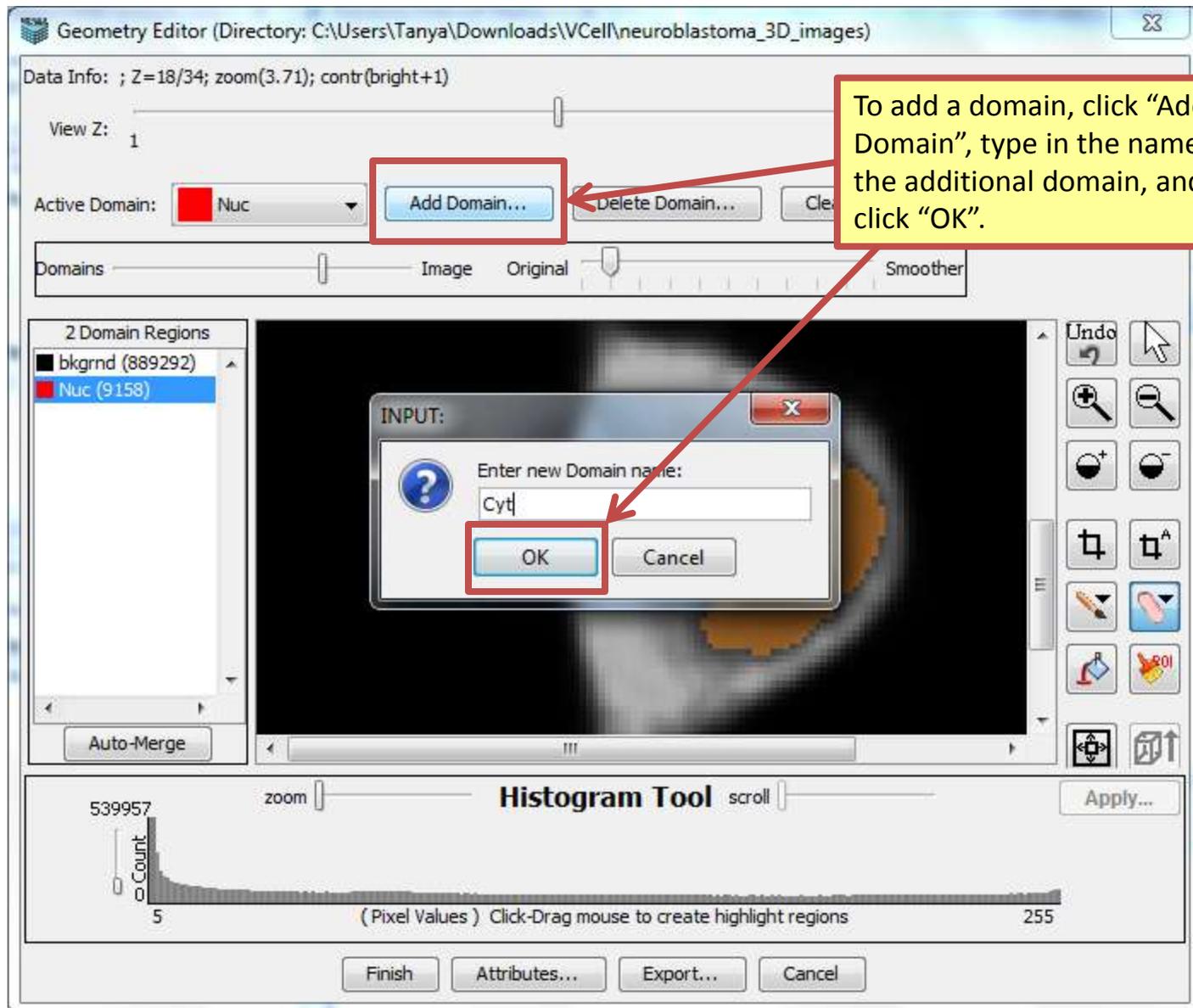
The screenshot shows the Geometry Editor interface. At the top, the window title is "Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)". Below the title bar, there are several panels and controls:

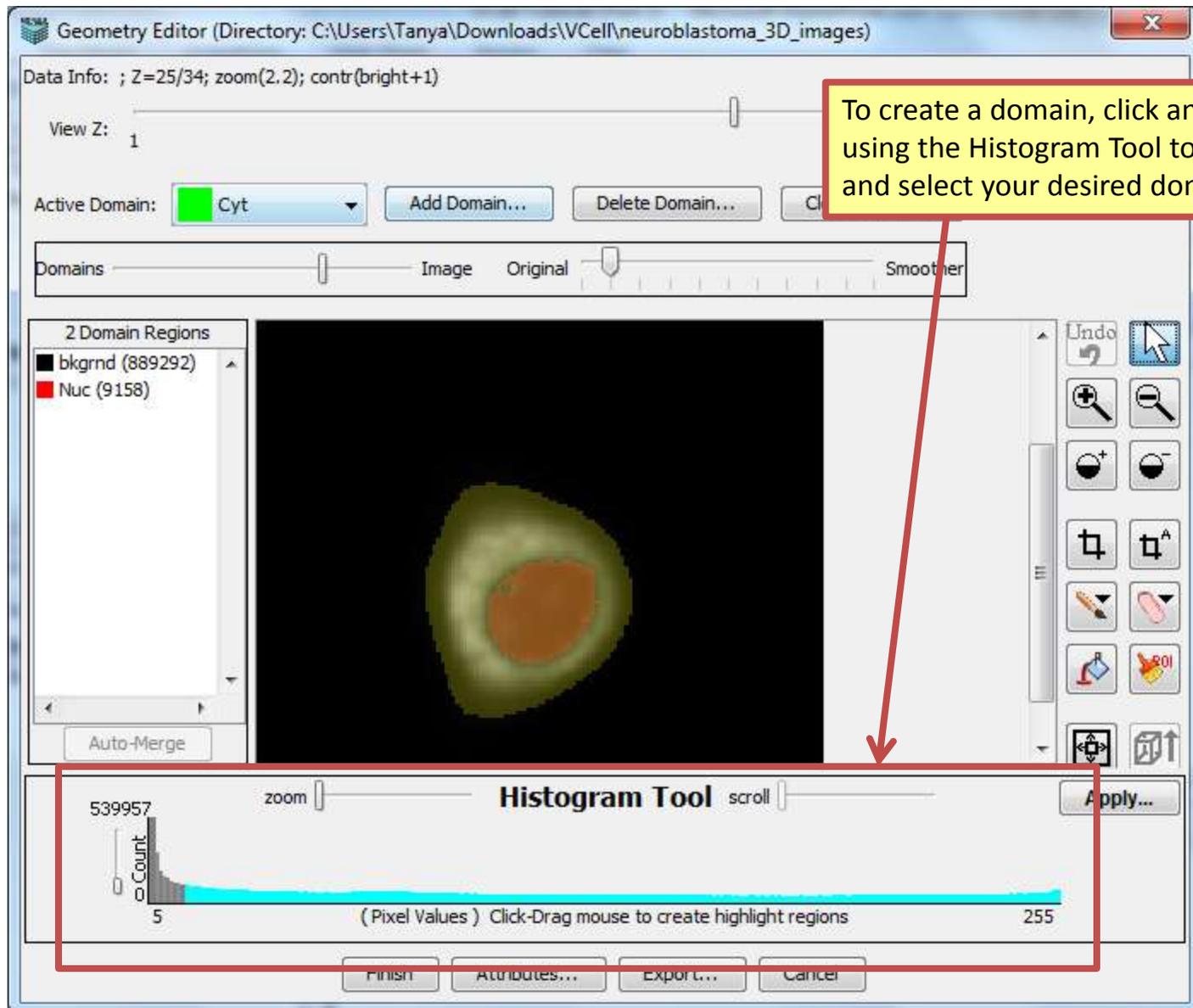
- Data Info:** Shows "7-25/34; zoom(2.86); cont(bright+1)".
- View:** A slider set to "34".
- Active:** A button labeled "Selections".
- Domains:** A slider between "Image" and "Original", with a "Smoother" button to the right.
- 619 Domain Regions:** A list of regions with checkboxes and labels: "Bg (869789)", "Nuc (13722)", "Nuc (5297)", "Nuc (2387)", "Nuc (1123)", "Nuc (1065)", "Nuc (545)", "Nuc (432)", "Nuc (377)", "Nuc (372)", "Nuc (253)", "Nuc (188)", "Nuc (171)". The "Nuc (13722)" item is highlighted with a blue selection bar.
- Auto-Merge:** A button below the domain list.
- Main View:** A central image of a cell with a large orange nucleus and a surrounding greyish-brown cytoplasm. A red arrow points from the text box to the orange nucleus.
- Tools:** A vertical toolbar on the right with icons for Undo, zoom in/out, selection, and other editing tools.
- Histogram Tool:** A panel at the bottom showing a histogram of pixel values. The y-axis is labeled "Count" and the x-axis is labeled "(Pixel Values)". The histogram shows a sharp peak at 5 and a long tail extending to 255. A "zoom" slider is positioned above the histogram, and a "scroll" slider is to the right. An "Apply..." button is at the bottom right of the histogram panel.
- Buttons:** "Finish", "Attributes...", "Export...", and "Cancel" buttons are located at the bottom of the window.

A yellow text box with a red border is overlaid on the top part of the window, containing the following text:

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.

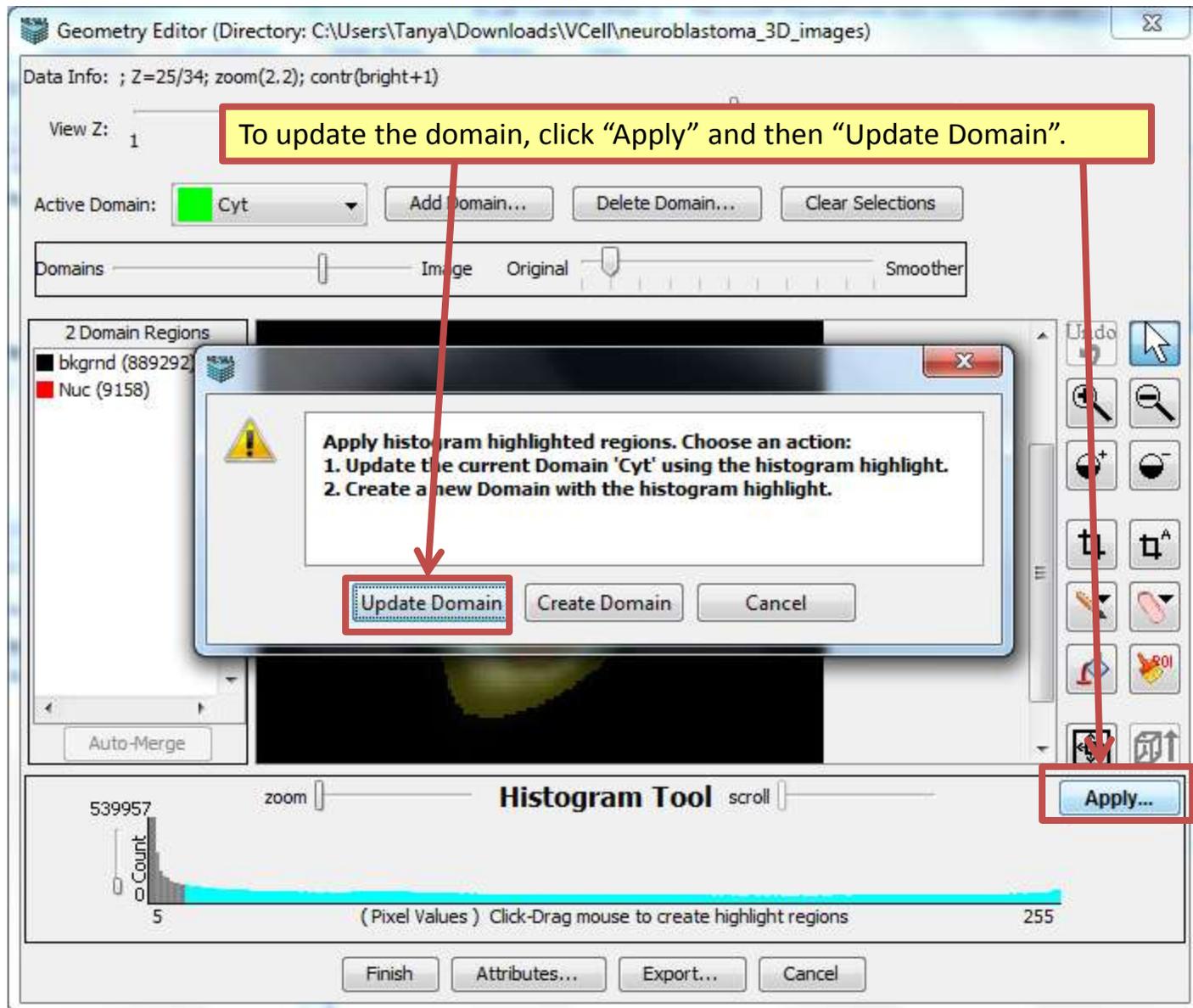
Two red arrows originate from this text box: one points to the "Nuc (13722)" item in the domain list, and the other points to the orange nucleus in the main view.

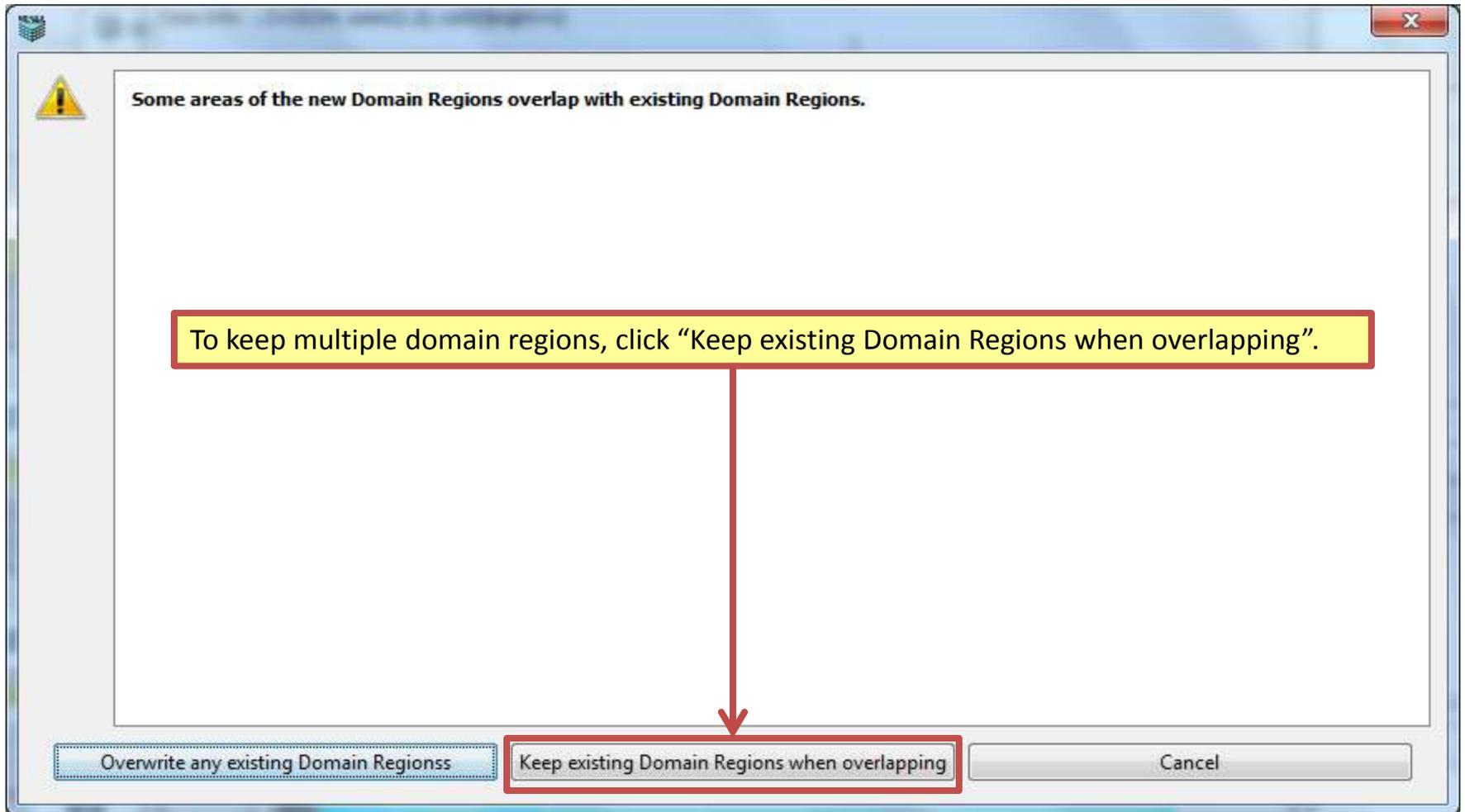


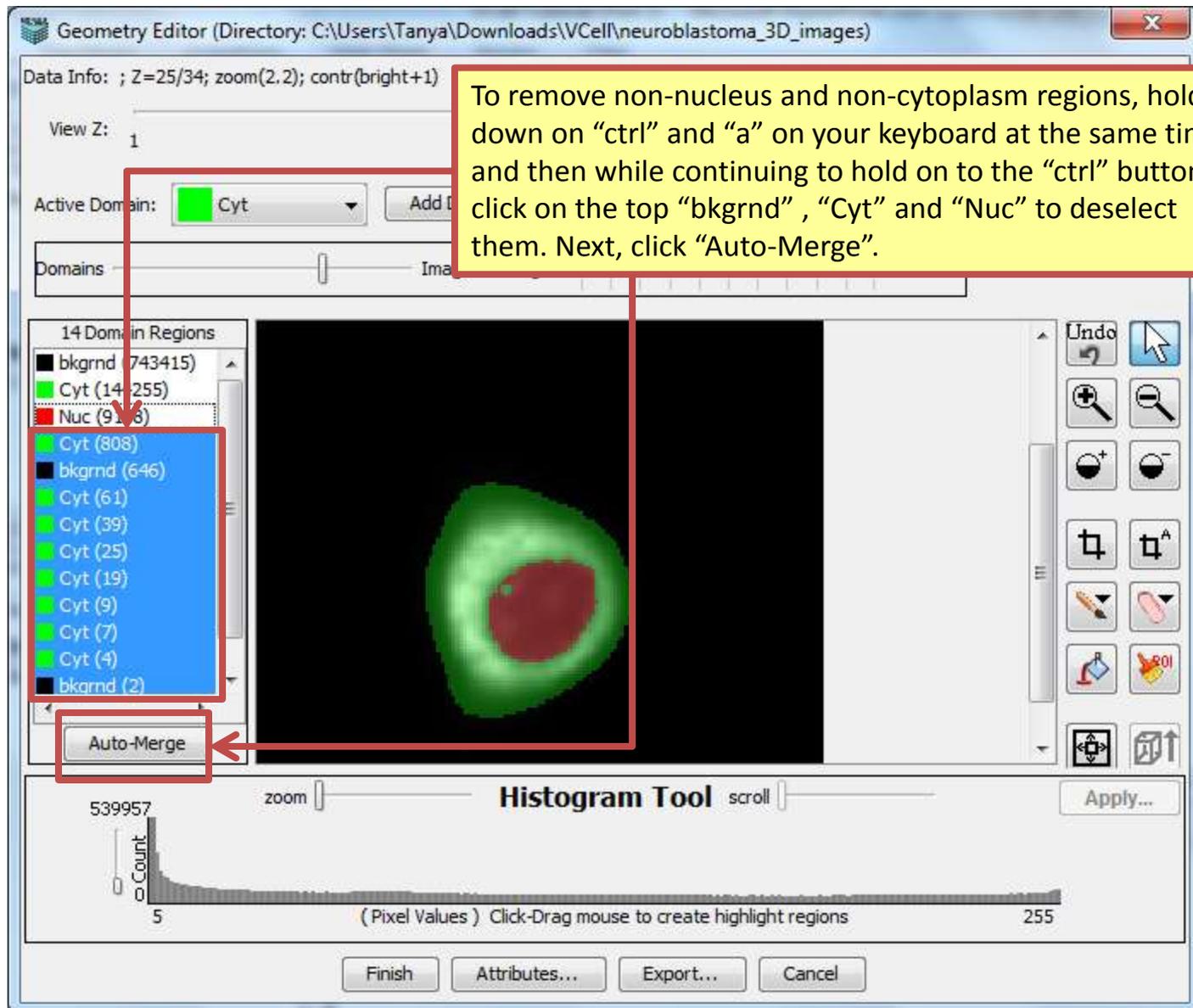


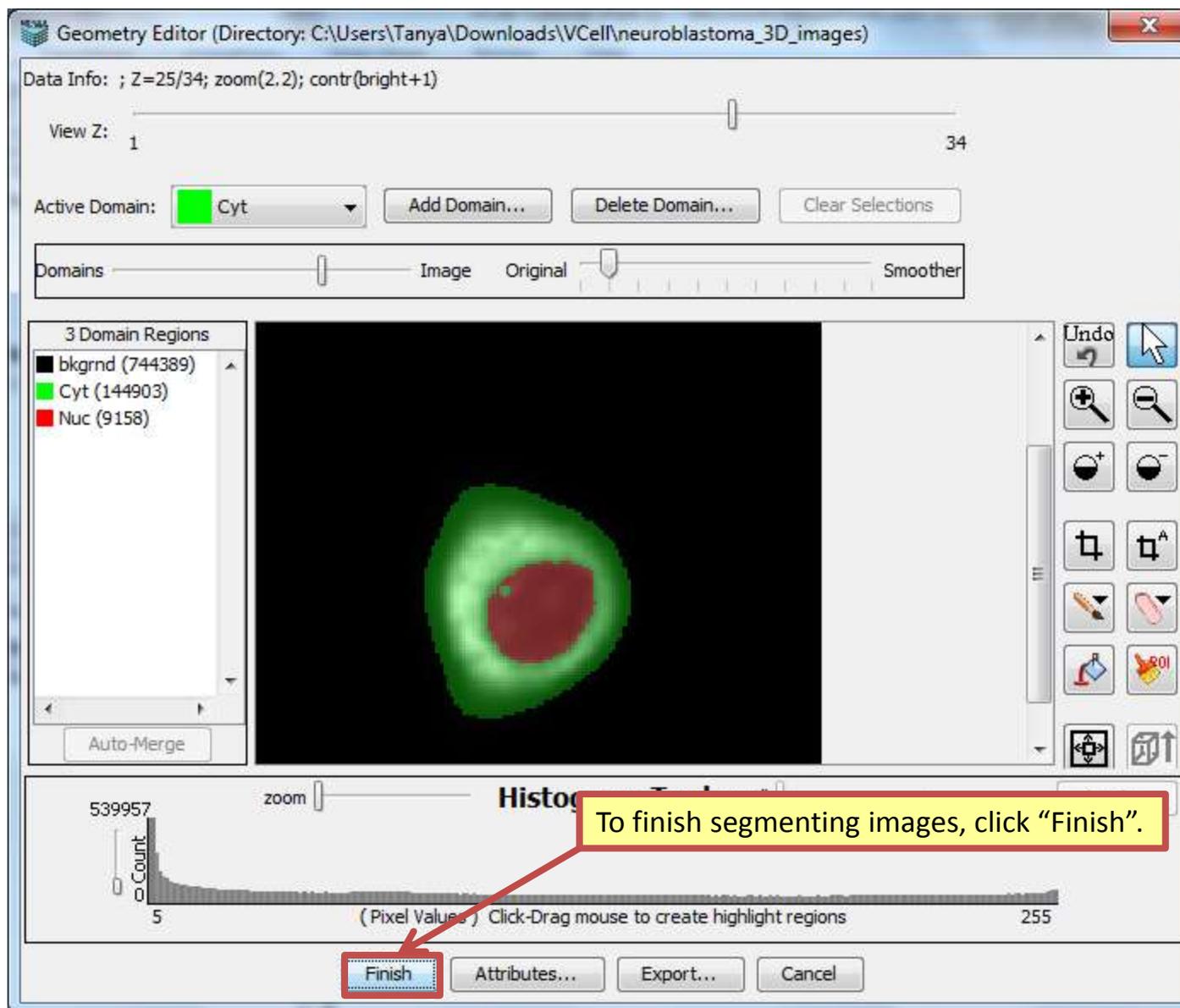
To create a domain, click and drag using the Histogram Tool to highlight and select your desired domain region.

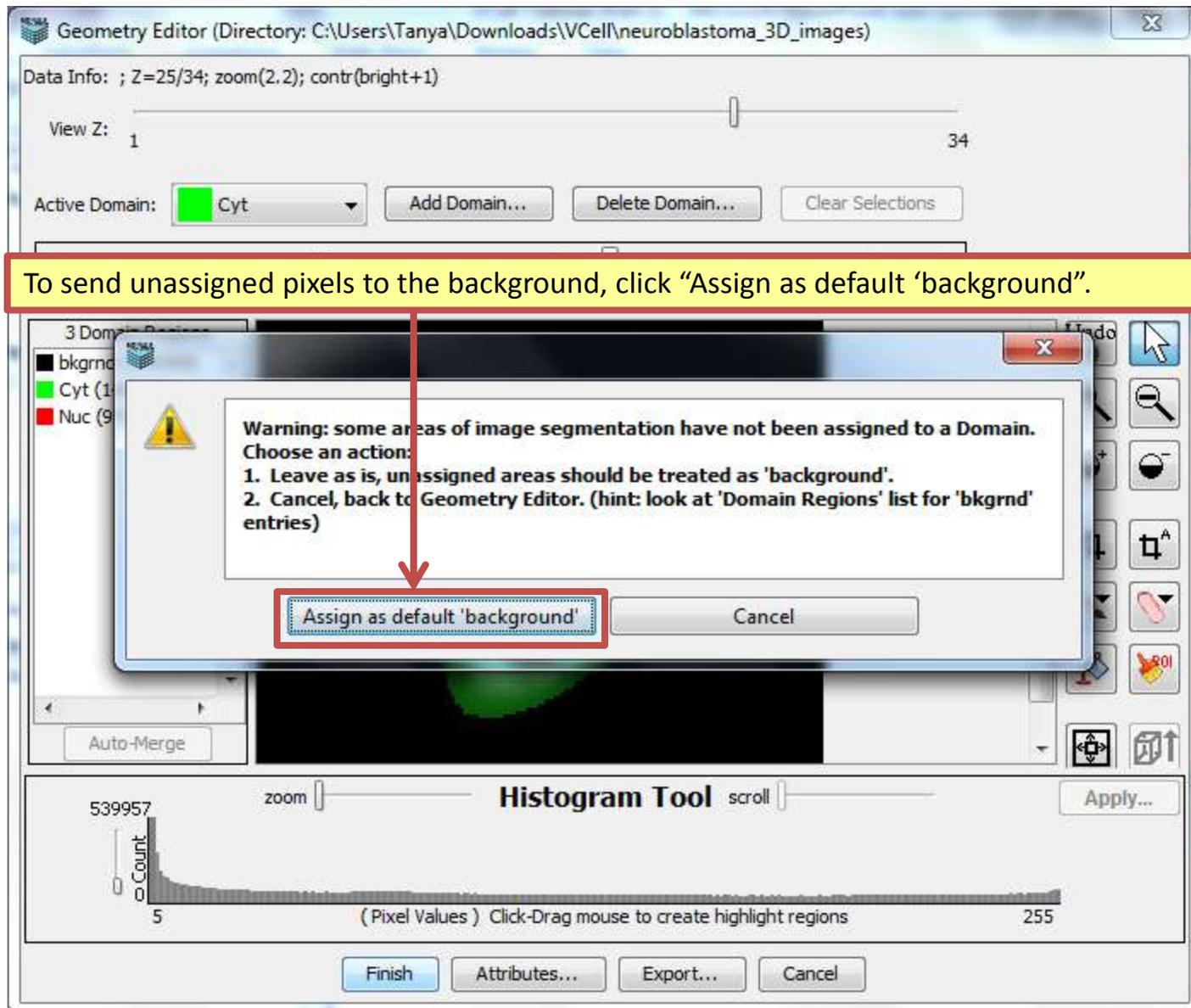
Use the Z slider to make sure all parts of the cytoplasm are highlighted











The screenshot shows the Geometry Editor interface. At the top, the title bar reads "Geometry Editor (Directory: C:\Users\Tanya\Downloads\VCell\neuroblastoma_3D_images)". Below the title bar, the "Data Info" section shows "Z=25/34; zoom(2.2); contr(bright+1)". The "View Z" is set to 1. The "Active Domain" is "Cyt" (green). A warning dialog box is open in the center, with a red arrow pointing to the "Add empty border" button. The dialog box contains the following text:

One or more Domain Regions touches the outer boundary on the XY and Z border.
Choose an option:
1. Keep as is, do not change.
2. Add empty 'background' border around outer boundary so no Domain Region touches an outer edge.

Below the dialog box, the "Histogram Tool" is visible, showing a histogram of pixel values from 5 to 255. The histogram has a peak at 539957. The "Histogram Tool" section includes a "zoom" slider and an "Apply..." button. At the bottom of the window, there are buttons for "Finish", "Attributes...", "Export...", and "Cancel".

To insert a blank (background) image on top of the 1st image and below the last image in the Z stack and to pad the x,y boundary with a rows of background pixels, click "Add empty border". This is important to ensure that in your final geometry a volume compartment intended to be enclosed by a membrane does not reach the edge (boundary) of the simulation space.

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Geometry Specifications 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

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

To view the surfaces in 3-D, click "Surface View".

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Tutorial

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (1)
 - Spatial Deterministic**
 - Geometry**
 - Specifications
 - Protocols
 - Simulations
- Parameters and Functions
- Pathway

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disconnected

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 3D, size=(62841.3,84404.8,9.000000E-7), origin=(0,0,0) **Edit Domain...** Export... Edit Image Replace Geometry ▾

Name	Value
background	
Nuc	
Cyt	

Front
Back
Add Subdomain ▾
Delete

To edit the 3-D dimensions, click "Edit Domain".

Slice View Surface View Geometric Region Details

Reset View

Opacity
100
75
50
25
0

Object Properties Problems (0 Errors, 10 Warnings) Database File Info

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

DISCONNECTED 193.2MB / 330.6MB

The screenshot displays the VCell 5.3 (build 4) interface. The main window title is "BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)". The menu bar includes "File", "View", "Server", "Tools", and "Help".

The left sidebar shows a tree view with the following structure:

- Tutorial
 - Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
 - Applications (1)
 - Spatial Deterministic
 - Geometry**
 - Specifications
 - Protocols
 - Simulations
 - Parameters and Functions

The main workspace is divided into several panels:

- Geometry Definition Panel:** Shows "Domain: 3D, s" and "Geometry Size" settings. The "Size" fields are X: 75 μm , Y: 75 μm , and Z: 26 μm . The "Origin" fields are X: 0.0 μm , Y: 0.0 μm , and Z: 0.0 μm . Buttons for "Replace Geometry", "Front", "Back", "Add Subdomain", and "Delete" are visible.
- Geometry Size Dialog Box:** A yellow callout box with a red border contains the text: "To adjust the dimensions, type in your desired values and when done, click 'OK'". The "OK" button is highlighted with a red box and an arrow pointing to it.
- 3D Viewport:** Displays a 3D model of a cell structure with a green nucleus. An "Opacity" slider is on the left, ranging from 0 to 100.
- Object Properties Panel:** Shows "Problems (0 Errors, 10 Warnings)" and "Database File Info". A message reads: "Select only one object (e.g. species, reaction, simulation) to view/edit properties."

At the bottom of the window, there is a "DISCONNECTED" button on the left and a memory usage indicator "268.1MB / 330.8MB" on the right.

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 3D, size=(75.0,75.0,26.0), origin=(0.0,0.0,0.0) ... Export... Edit Image Replace Geometry ▾

Name	Value
background	
Nuc	
Cyt	

Front Back Add Subdomain ▾ Delete

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 170.1MB 339.7MB

To adjust opacity of the cytoplasm to better see the nucleus, drag the slider with your cursor,

The geometry of your model is now complete.

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Tutorial

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
 - Applications (1)
 - Spatial Deterministic
 - Geometry
 - Specifications
 - Protocols
 - Simulations

Structure Mapping Geometry Definition

All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.

Physiology (structures)

Geometry (subdomains)

- background
- Nuc
- Cyt
- Cyt_background_membrane
- Cyt_Nuc_membrane

EC

PM

Cyt

NM

Structure	Subdomain	Size Ratio	X-	X+	Y-	Y+	Z-	Z+
Cyt	Cyt	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
PM	Cyt_background...	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
NM	Cyt_Nuc_membr...	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
Nuc	Nuc	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux

Object Properties Problems (0 Errors, 0 Warnings) Database File Info

CONNECTED (tanyamiller.1221) 79.7MB / 103.3MB

To view the geometry of an application, click "Applications" > "Geometry".

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

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Tutorial

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (1)
 - Spatial Deterministic
 - Geometry
 - Specifications
 - Protocols
 - Simulations
- Parameters and Functions
- Pathway

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CONNECTED (tanyamiller1221)

76.9MB / 105.9MB

Specifications

Species	Structure	Clamped	Initial Condi...	Well Mixed	Diffusion Co...
RanC_Cyt	Cyt	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
Ran_Cyt	Cyt	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
C_Cyt	Cyt	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
RanC_Nuc	Nuc	<input type="checkbox"/>	4.5E-4	<input type="checkbox"/>	10.0

Object Properties Problems (0 Errors, 0 Warnings) Database File Info

Description	Parameter	Expression	Units
initial concentration for RanC_Nuc	initConc	0.0	μM
diffusion constant for RanC_Nuc	diff	10.0	$\mu\text{m}^2 \cdot \text{s}^{-1}$
Boundary Condition X- for RanC_Nuc	BC_Xm	<zero flux>	$\mu\text{M} \cdot \mu\text{m} \cdot \text{s}^{-1}$
Boundary Condition X+ for RanC_Nuc	BC_Xp	<zero flux>	$\mu\text{M} \cdot \mu\text{m} \cdot \text{s}^{-1}$
Boundary Condition Y- for RanC_Nuc	BC_Ym	<zero flux>	$\mu\text{M} \cdot \mu\text{m} \cdot \text{s}^{-1}$

To change the concentration of a species, click "Specifications" and type in a value under the "Initial Condition" column.

The screenshot shows the VCell 5.3 software interface. The main window is titled "BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the model structure. Under "Applications (1)", "Spatial Deterministic" is expanded, showing "Geometry", "Specifications", "Protocols", and "Simulations" (highlighted in blue).
- Top Panel:** A tabbed interface with "Simulations" selected. Below the tabs are icons for "Simulations", "Output Functions", and "Generated Math". A red box highlights the "Simulations" icon.
- Table:** A table with the following columns: Name, End Time, Output Option, Solver, Running Status, and Results. The table contains one row: "Simulation0", "1.0", "every 0.05", "fully-implicit", "not saved", and "no".
- Bottom Panel:** "Object Properties" for the selected simulation. It shows settings for "max timestep" (0.1s), "output" (every 0.05), "rel tol" (1.0E-7), and "abs tol" (1.0E-9). It also shows "Mesh: 72x72x25 = 129600 elements" and "Geometry size: (75.0,75.0,26.0) microns".

A red box highlights the "Simulations" tab and the "Simulations" icon. A red arrow points from the icon to the "Simulations" tab. A yellow box with a red border contains the text: "To create a new simulation, click 'Simulations' and the new simulation icon."

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	every 0.05	fully-implicit	not saved	no

The screenshot shows the VCell 5.3 (build 4) interface. The main window displays a table of simulations. A red box highlights the edit simulation icon (a pencil) in the toolbar above the table. A red arrow points from this icon to a yellow callout box containing the text: "To edit a simulation, click the edit simulation icon."

The Simulations table is as follows:

Name	End Time	Output Option	Solver	Running Status	Results
Simulation	1.0	every 0.05	Fully-Implicit	not saved	no

The Object Properties panel at the bottom shows the following settings:

Annotation:

Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.05	1.0E-7	1.0E-9

Mesh: 72x72x25 = 129600 elements Geometry size: (75.0,75.0,26.0) microns

CONNECTED (tanyamiller1221) 58.7MB / 103.6MB

Parameters Mesh

Mesh Size

Geometry Size (um) (75.0, 75.0, 26.0)

Mesh Size (elements) Lock aspect ratio

X 101

Y 101

Z 36

Total Size (elements) 101 x 101 x 36 = 367236

Spatial Step (um) Δx 0.75

Δy 0.75

Δz 0.7428571428571429

OK Cancel

CONNECTED (tanyamiller 1221) 70.8MB / 103.1MB

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".

To maintain the resolution ratio of the simulation, check off "Lock aspect ratio".

BIOMODEL: Tutorial

Edit: Simulation0

Parameters Mesh **Solver**

Choose solver algorithm and fine-tune its parameters

Integrator Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)

General

Time Bounds

Starting 0.0

Ending 15.0

Time Step

Minimum

Default

Maximum 0.1

Error Tolerance

Absolute 1.0E-9

Relative 1.0E-7

Output Options

Keep Every [] time samples and at most [] time samples

Output Interval 0.5 secs

Miscellaneous

OK Cancel

VCCell DB BioModels.net

BioModels MathModels

Search

Biological Models

My BioModels (ta)

BioModel2

Tutorial

Private M

Tutorial_Mult

Shared BioModels

Public BioModels

Tutorials (5)

Education (33)

CONNECTED (tanyamiller 1221)

71.8MB / 103.4MB

To edit the simulation solver, click the "Solver" tab, type in values and click "OK".

The screenshot shows the VCell 5.3 interface. The left sidebar contains a tree view with categories: Tutorial, Physiology (Reaction Diagram, Reactions (2), Structures (5), Species (4)), Applications (1) (Spatial Deterministic: Geometry, Specifications, Protocols, Simulations), Parameters and Functions, and Pathway. The main window has tabs for Geometry, Specifications, Protocols, and Simulations. The Simulations tab is active, showing a table with one entry: Simulation0, End Time 1.0, Output Option every 0.05, Solver Fully-Implicit, Running Status not saved, and Results no. A warning dialog box is displayed in the center, with a yellow warning icon and the following text: "Warnings from Simulation: 'Simulation0!' The simulation has large result dataset (352MB), suggested size limits are: 50 MB for compartmental ODE simulations, 200 MB for spatial simulations, 100 MB for compartmental stochastic simulations. Try saving fewer timepoints or using a coarser mesh if spatial. Do you want to continue anyway?". The "OK" button is highlighted with a red box and an arrow pointing to it. Below the dialog box, a yellow text box contains the instruction: "To create a large simulation, click 'OK'. (VCell will warn you before you create a large simulation.)". The bottom of the interface shows the Object Properties panel with settings for max timestep (0.1s), output (every 0.05), rel tol (1.0E-7), abs tol (1.0E-9), Mesh (72x72x25 = 129600 elements), and Geometry size (75.0, 75.0, 26.0) microns. The status bar at the bottom indicates "CONNECTED (tanyamiller1221)" and "77.2MB / 103.8MB".

BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)

File View Server Tools Help

Tutorial

- Physiology
 - Reaction Diagram
 - Reactions (2)
 - Structures (5)
 - Species (4)
- Applications (1)
 - Spatial Deterministic
 - Geometry
 - Specifications
 - Protocols
 - Simulations
- Parameters and Functions
- Pathway

VCell DB BioModels.net Pathw...

BioModels MathModels Geometries

Search

- Biological Models
 - My BioModels (tanyamiller1221) (3)
 - BioModel2
 - Tutorial
 - Private Mon Jun 29 09:35:...
 - Tutorial_MultiApp
 - Shared BioModels (0)
 - Public BioModels (519)
 - Tutorials (5)
 - Education (33)

Simulations

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	every 0.05	Fully-Implicit	not saved	no

Warnings from Simulation: 'Simulation0'!

The simulation has large result dataset (352MB), suggested size limits are:
50 MB for compartmental ODE simulations
200 MB for spatial simulations
100 MB for compartmental stochastic simulations
Try saving fewer timepoints or using a coarser mesh if spatial.

Do you want to continue anyway?

OK Cancel

To create a large simulation, click "OK".
(VCell will warn you before you create a large simulation.)

Object Prop

Annotation:

Settings:

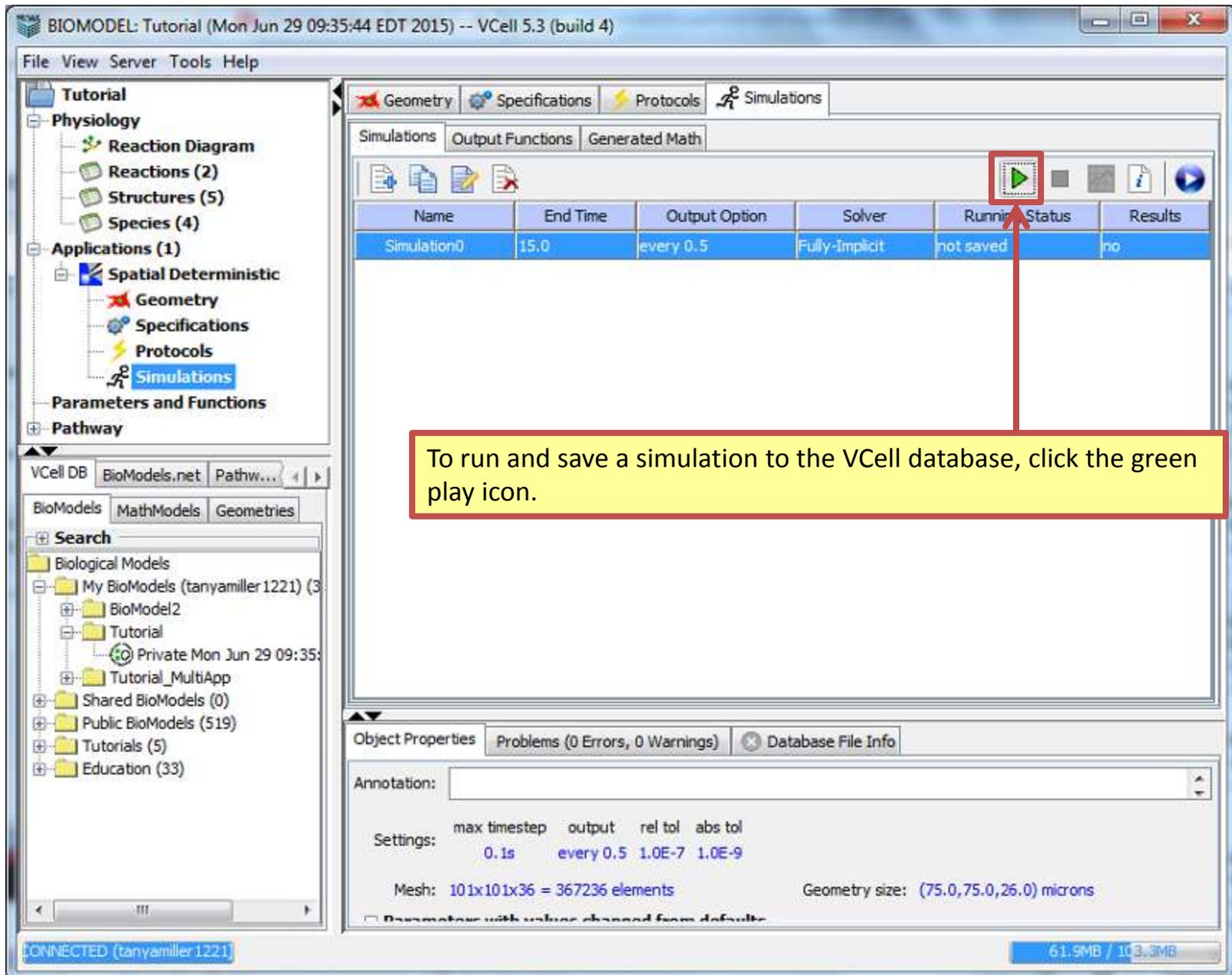
max timestep	output	rel tol	abs tol
0.1s	every 0.05	1.0E-7	1.0E-9

Mesh: 72x72x25 = 129600 elements

Geometry size: (75.0, 75.0, 26.0) microns

CONNECTED (tanyamiller1221)

77.2MB / 103.8MB



The screenshot displays the VCell 5.3 (build 4) interface. The main window title is "BIOMODEL: Tutorial (Mon Jun 29 09:35:44 EDT 2015) -- VCell 5.3 (build 4)". The interface includes a menu bar (File, View, Server, Tools, Help) and a toolbar with icons for Geometry, Specifications, Protocols, and Simulations. A left sidebar shows a tree view of the model structure, including Physiology (Reaction Diagram, Reactions (2), Structures (5), Species (4)), Applications (1) (Spatial Deterministic, Geometry, Specifications, Protocols, Simulations), Parameters and Functions, and Pathway. Below the sidebar is a VCell DB browser showing a search tree with folders like Biological Models, My BioModels (tanyamiller 1221), Tutorial, and Tutorial_MultiApp. The main workspace contains a "Simulations" table with columns: Name, End Time, Output Option, Solver, Run, Status, and Results. A red box highlights the green play icon in the Run column of the first row (Simulation0). A red arrow points from this icon to a yellow callout box. The bottom of the interface shows "Object Properties" and "Database File Info" tabs, with a settings table for simulation parameters.

Name	End Time	Output Option	Solver	Run	Status	Results
Simulation0	15.0	every 0.5	Fully-Implicit	not saved		no

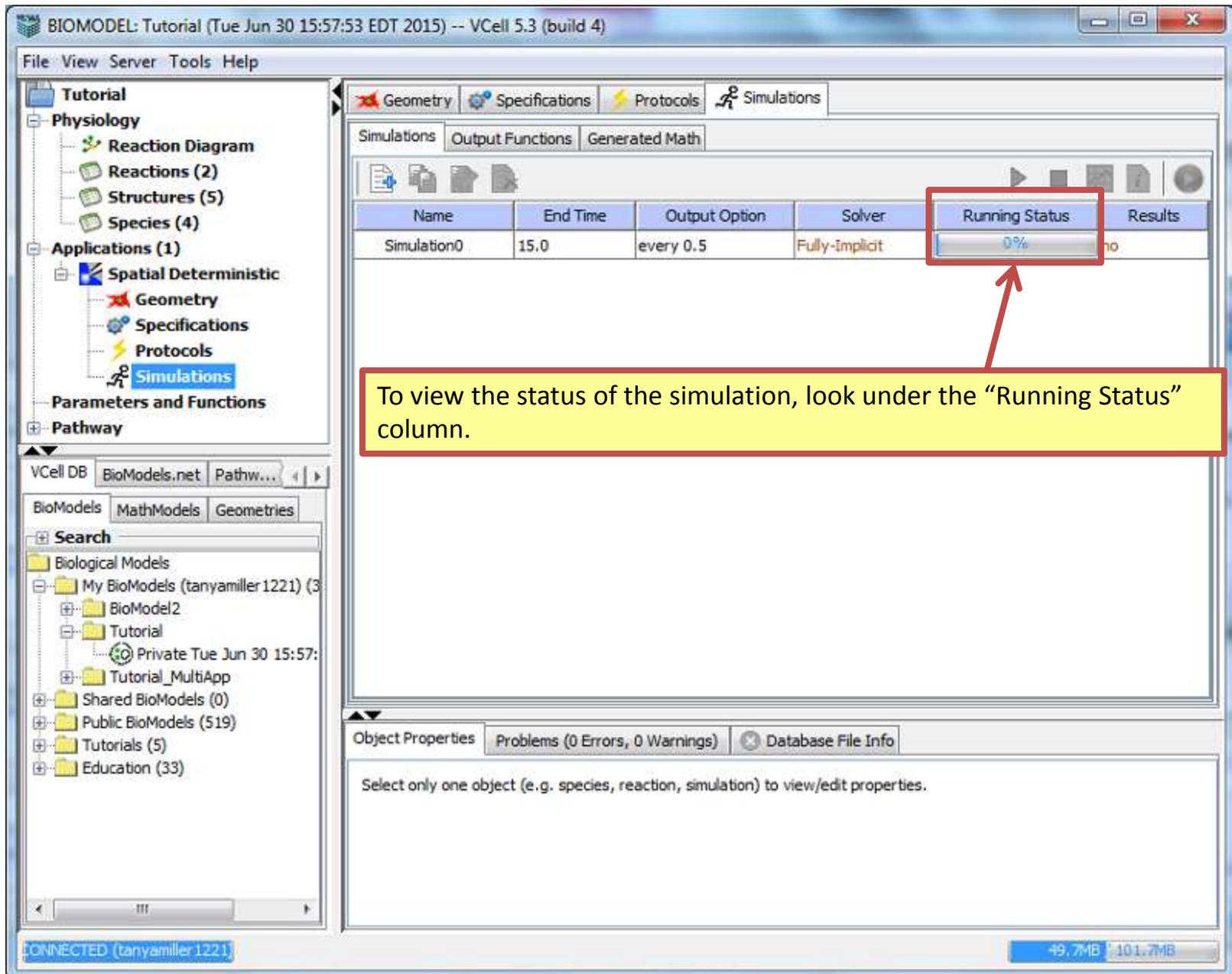
To run and save a simulation to the VCell database, click the green play icon.

Settings:	max timestep	output	rel tol	abs tol
	0.1s	every 0.5	1.0E-7	1.0E-9

Mesh: 101x101x36 = 367236 elements Geometry size: (75.0,75.0,26.0) microns

CONNECTED (tanyamiller 1221)

61.9MB / 103.3MB



The screenshot displays the VCell software interface. The main window title is "BIOMODEL: Tutorial (Tue Jun 30 15:57:53 EDT 2015) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the project structure under "Tutorial". It includes "Physiology" (Reaction Diagram, Reactions (2), Structures (5), Species (4)), "Applications (1)" (Spatial Deterministic, Geometry, Specifications, Protocols, Simulations), "Parameters and Functions", and "Pathway".
- Top Panel:** Tabs for "Geometry", "Specifications", "Protocols", and "Simulations". Below these are sub-tabs for "Simulations", "Output Functions", and "Generated Math".
- Table:** A table with columns: "Name", "End Time", "Output Option", "Solver", "Running Status", and "Results". The table contains one row for "Simulation0" with values: "15.0", "every 0.5", "Fully-implicit", "0%", and "no". The "Running Status" column is highlighted with a red box, and a red arrow points to it from a text box.
- Bottom Panel:** "Object Properties" tab, showing "Problems (0 Errors, 0 Warnings)" and "Database File Info". A message reads: "Select only one object (e.g. species, reaction, simulation) to view/edit properties."

At the bottom of the window, it shows "CONNECTED (tanyamiller1221)" and memory usage: "49.7MB / 101.7MB".

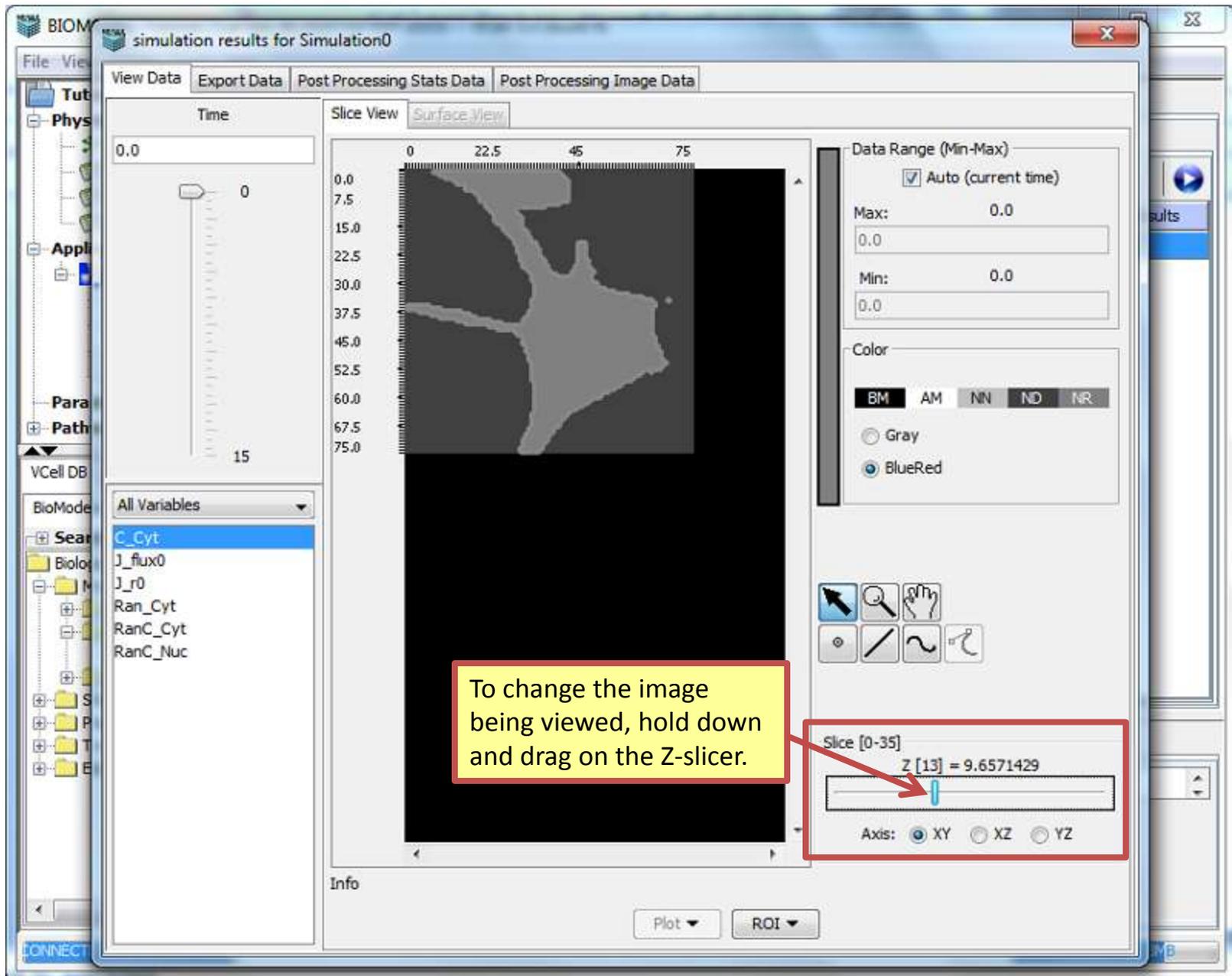
To view the status of the simulation, look under the "Running Status" column.

The screenshot displays the VCell software interface. The main window title is "BIOMODEL: Tutorial (Tue Jun 30 15:57:53 EDT 2015) -- VCell 5.3 (build 4)". The interface is divided into several panels:

- Left Panel:** A tree view showing the project structure under "Tutorial". It includes "Physiology" (Reaction Diagram, Reactions (2), Structures (5), Species (4)), "Applications (1)" (Spatial Deterministic, Geometry, Specifications, Protocols, Simulations), "Parameters and Functions", and "Pathway".
- Top Panel:** Tabs for "Geometry", "Specifications", "Protocols", and "Simulations". Below these are sub-tabs for "Simulations", "Output Functions", and "Generated Math".
- Table:** A table listing simulation results. A red box highlights the "Results" column for "Simulation0".
- Callout Box:** A yellow box with a red border and an arrow pointing to the "Results" icon in the table, containing the text: "To view simulation results, click the results icon."
- Bottom Panel:** "Object Properties" section showing "Database File Info" and "Settings" (max timestep: 0.1s, output: every 0.5, rel tol: 1.0E-7, abs tol: 1.0E-9). It also displays "Mesh: 101x101x36 = 367236 elements" and "Geometry size: (75.0,75.0,26.0) microns".

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	15.0	every 0.5	Fully-Implicit	completed	yes

CONNECTED (tanyamiller1221) 62.9MB / 105.9MB



The screenshot displays the 'simulation results for Simulation0' window. The 'Time' control is highlighted with a red box, showing a text input field with the value '8.5' and a vertical slider below it. The slider has a blue handle and is marked with '15' at the bottom. A yellow callout box with a red border contains the text: 'To change the time frame being viewed, input a value under "Time" or hold down and drag the slider under "Time".' The main visualization area shows a 'Surface View' of a biological structure with a color scale from blue to red. The 'Data Range (Min-Max)' section is visible, with 'Auto (current time)' checked. The 'Color' section shows 'BlueRed' selected. The 'Slice [0-35]' section shows 'Z [13] = 9.6571429' and 'Axis: XY' selected.

simulation results for Simulation0

View Data Export Data Post Processing Stats Data Post Processing Image Data

Time

8.5

15

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: 4.8229429939463156E-5
4.8229429939463156E-5

Min: 4.010434082978926E-14
4.010434082978926E-14

Color

BM AM NN ND NR

Gray

BlueRed

Slice [0-35]

Z [13] = 9.6571429

Axis: XY XZ YZ

Plot ROI

The screenshot displays the BIOM simulation results for Simulation0. The interface includes a menu bar (File, View), tabs for View Data, Export Data, Post Processing Stats Data, and Post Processing Image Data. A central plot area shows a heatmap with axes ranging from 0.0 to 75.0. To the right of the plot is a color gradient control panel with a vertical color bar and a legend. The legend includes radio buttons for Gray and BlueRed, with BlueRed selected. A red box highlights these options, and a red arrow points from a text box to them. The text box contains the instruction: "To change the color gradient, click either 'Gray' or 'BlueRed'." Below the plot, there are controls for Z [13] = 9.6571429 and Axis selection (XY, XZ, YZ).

simulation results for Simulation0

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data

Time: 8.5

0

15

0.0 7.5 15.0 22.5 30.0 37.5 45.0 52.5 60.0 67.5 75.0

0 22.5 45 75

Data Range (Min-Max)

Auto (current time)

Max: 4.8229429939463156E-5
4.8229429939463156E-5

Min: 4.010434082978926E-14
4.010434082978926E-14

Color

BM AM NN ND NR

Gray

BlueRed

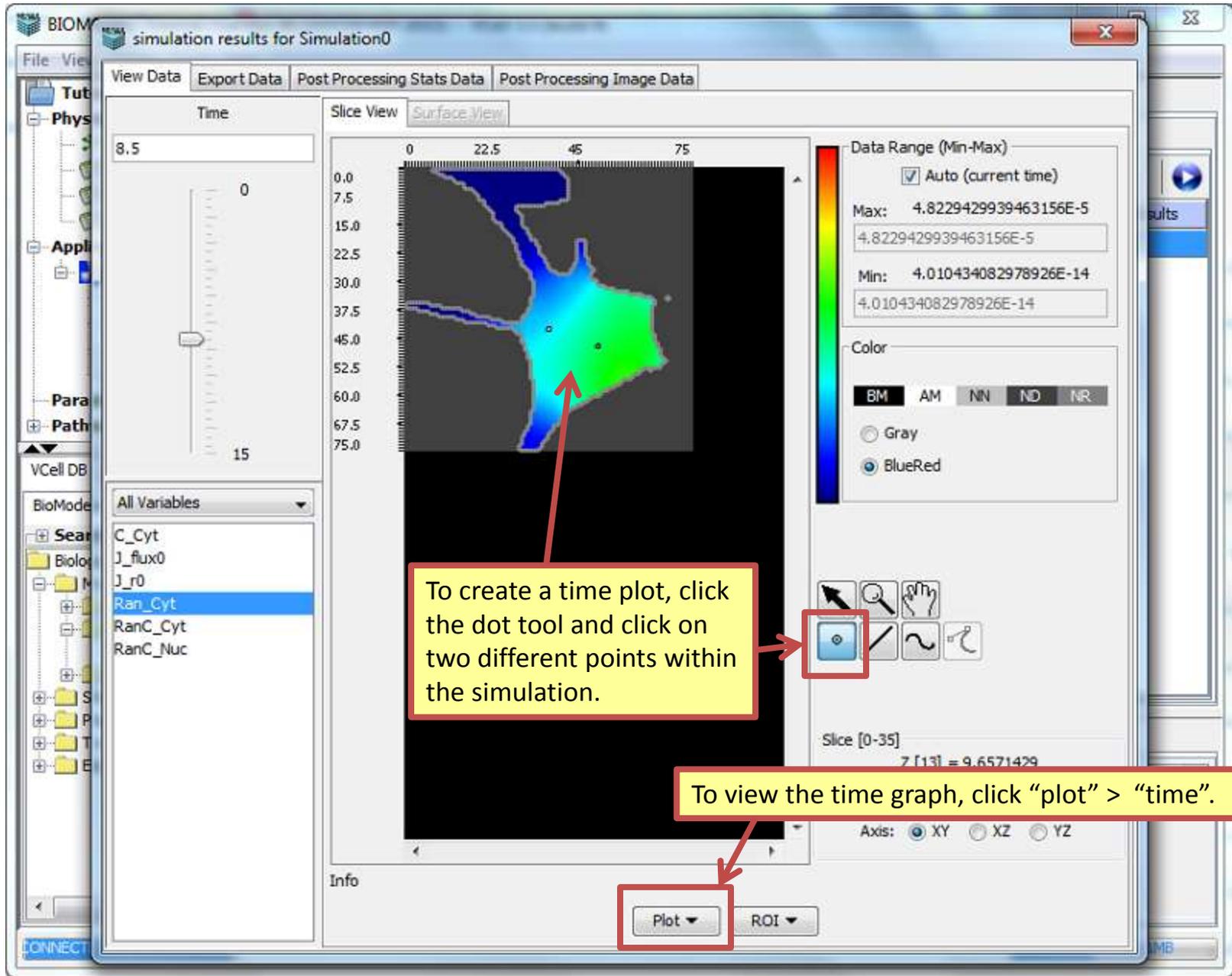
To change the color gradient, click either "Gray" or "BlueRed".

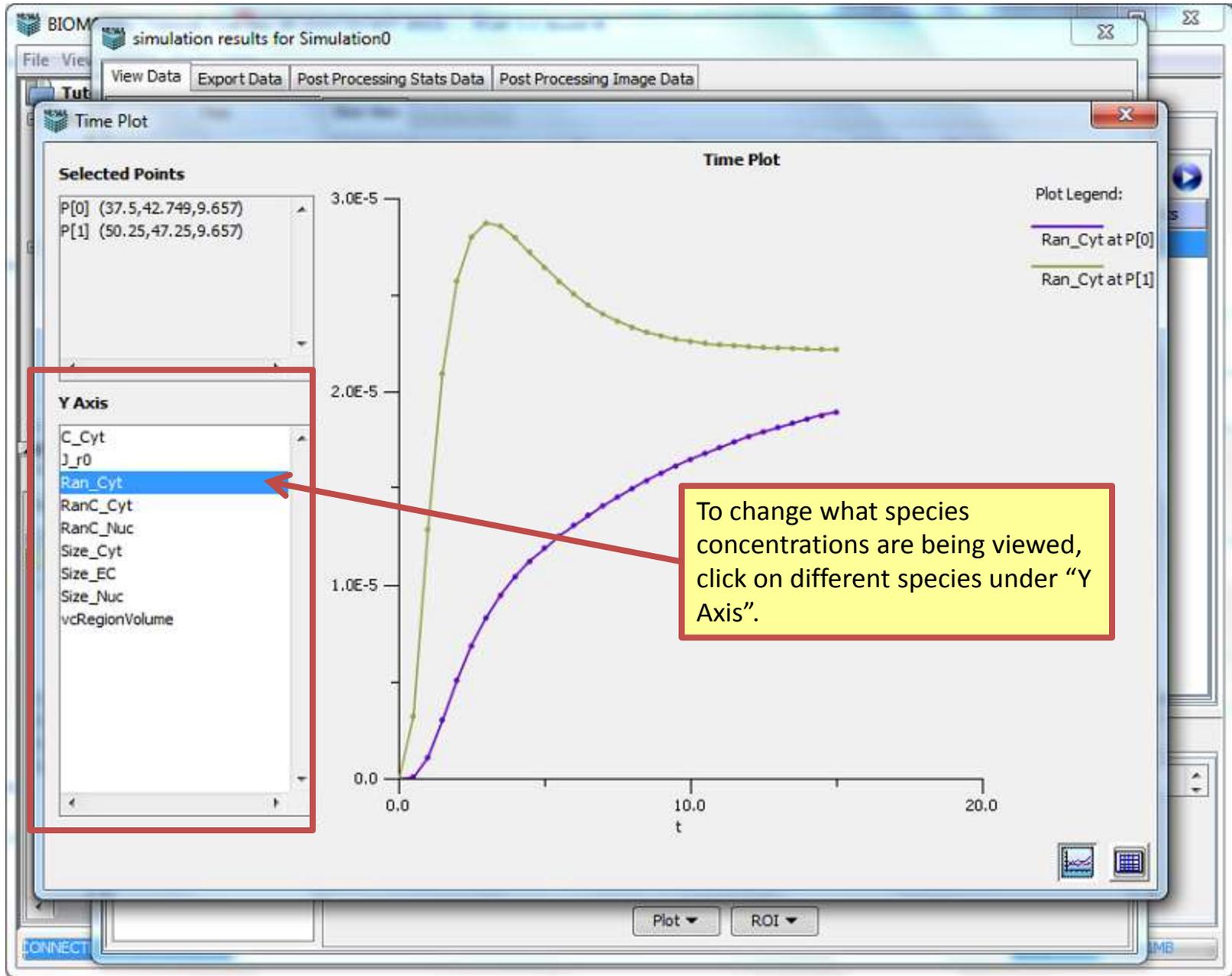
Slice [0-35]

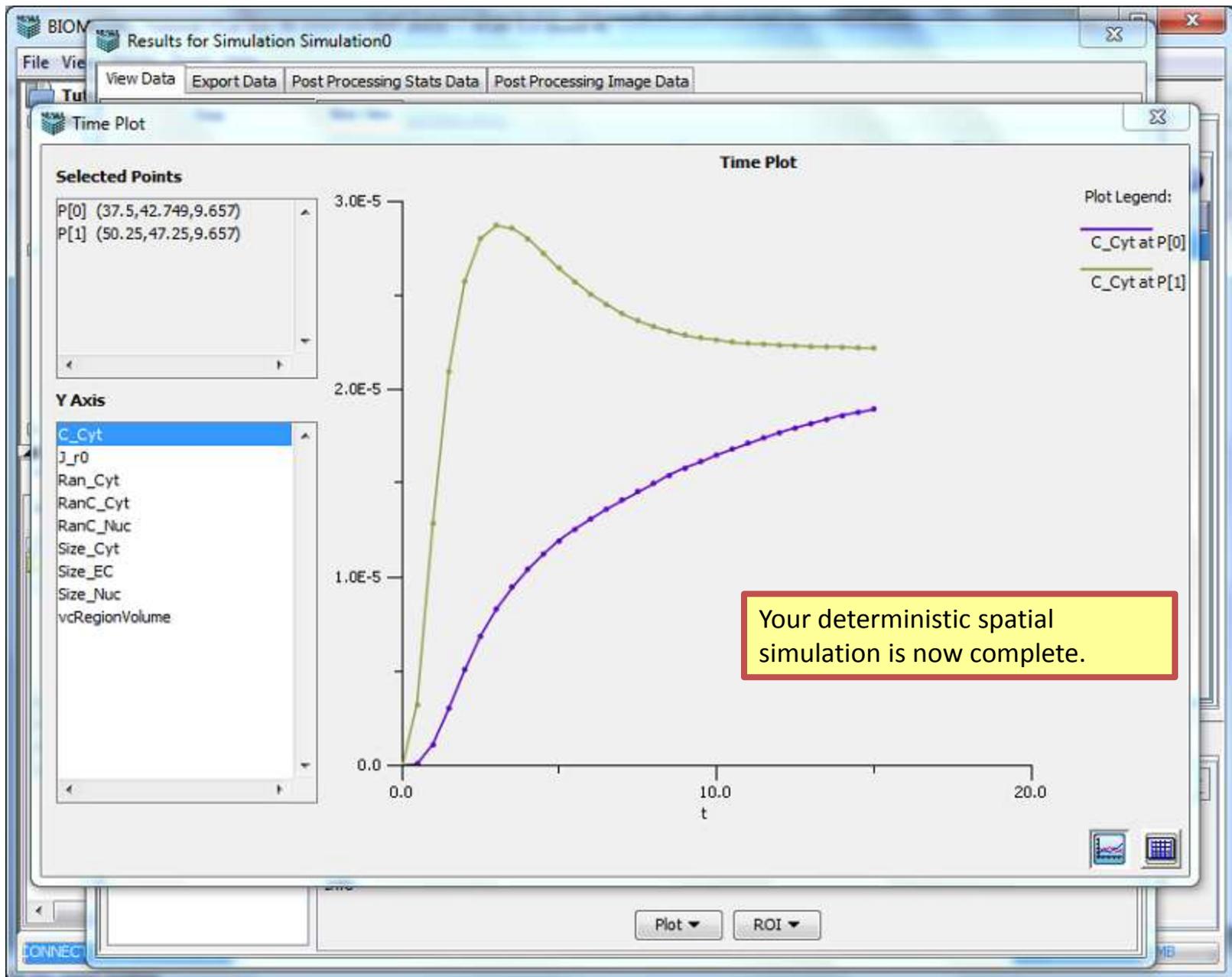
Z [13] = 9.6571429

Axis: XY XZ YZ

Plot ROI







Next: VCell Tutorial
BioModel with Multiple Applications

Part 2 Compartmental Applications and
Parameter Estimation