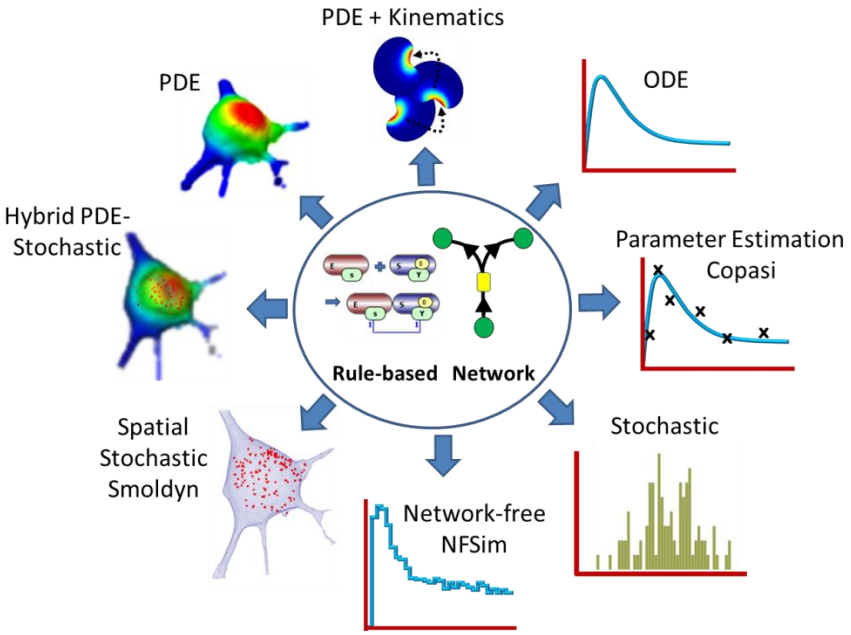
VCell

A modeling environment for the simulation of cellular events. Download at vcell.org .



Virtual Cell is developed by the Center for Cell Analysis and Modeling at the University of Connecticut Health Center. It is funded as a Biomedical Technology Research Resource by the National Institute of General Medical Sciences (NIGMS)

VCell BioModel using the Moving Boundary Solver

Objective

Create a simple Biomodel of a fluorescence photobleaching (FRAP) experiment in a moving cell; learn how to specify kinematics in a VCell Biomodel and utilize the Moving Boundary solver.

Goals

- Create a Biomodel Physiology that recreates a fluoresence photobleaching experiment and a spatial deterministic application of the Physiology using a 2D geometry created from analytic expressions for a simple circle
- Specify kinematics (i.e. velocities) of structures and the molecules contained within the structures
- Define initial conditions that vary in x and y using Boolean expressions.
- Create a simulation using the VCell Moving Boundary solver, specifying time course and computational mesh.
- Run the simulation, view and export results.

Notes on the VCell Moving Boundary Solver

Moving Boundary Applications in VCell allow for PDE (spatial) simulations to occur within a geometry where the boundaries of compartments can change in shape and position within the overall computational space. There are some important things to keep in mind when you create this type of application.

- The current implementation of the moving boundary solver only works with 2D geometries. We hope in the future to enable problems with 3D geometries.
- Creating an application with a moving boundary solver follows the same steps used for fixed domains, except that a velocity is assigned to points on the cell membrane (and optionally for species residing with the volume) by defining Kinematics for surface and volume objects as part of the description of the Geometry.
- Species will have both diffusion terms (which can be 0) and velocity terms defined by the kinematics. Because displacement terms will be different in different compartments, species in different compartments will not necessarily move together. This tutorial provides an example of different types of kinematics for membranes and volumes.
- Currently, VCell tools for analyzing spatial results are not available for results of moving boundary simulations, so it is necessary to export your results to other image processing software to analyze the results of simulations.

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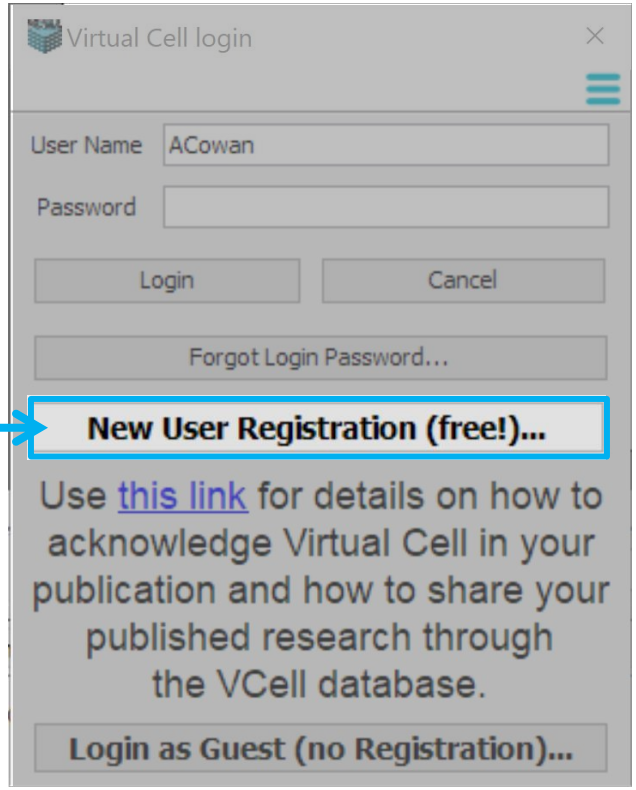
You need to register as a New User if you want to run simulations on the VCell compute resources, or use the VCell database to store models that can be shared with collaborators.



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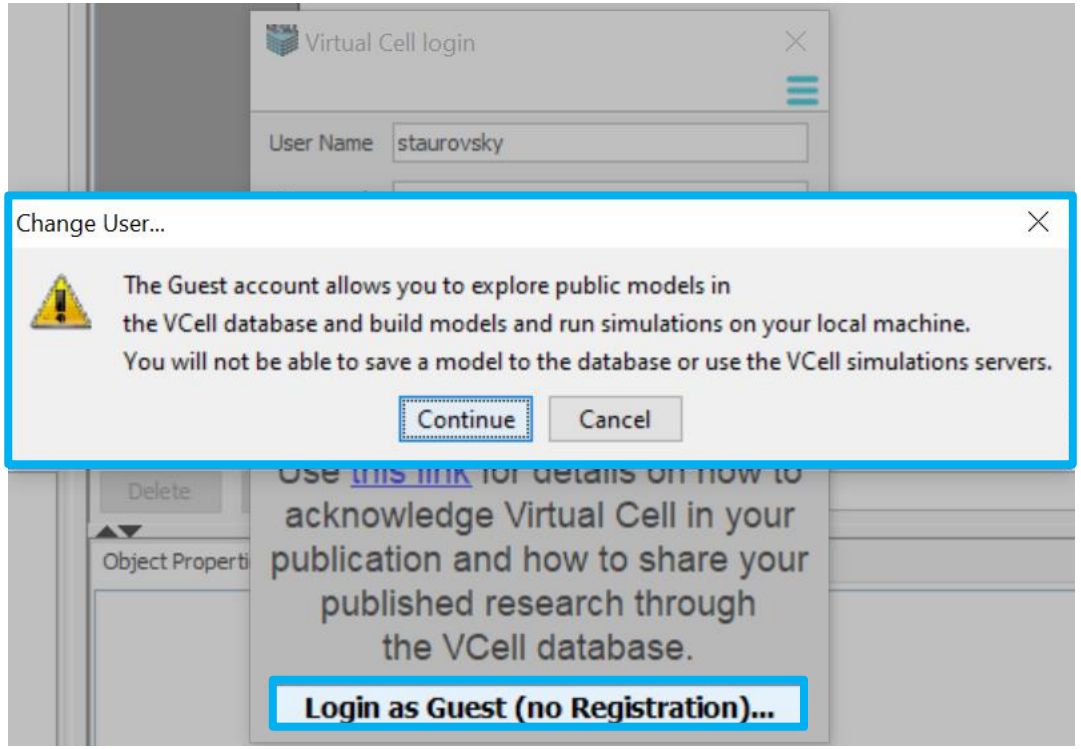
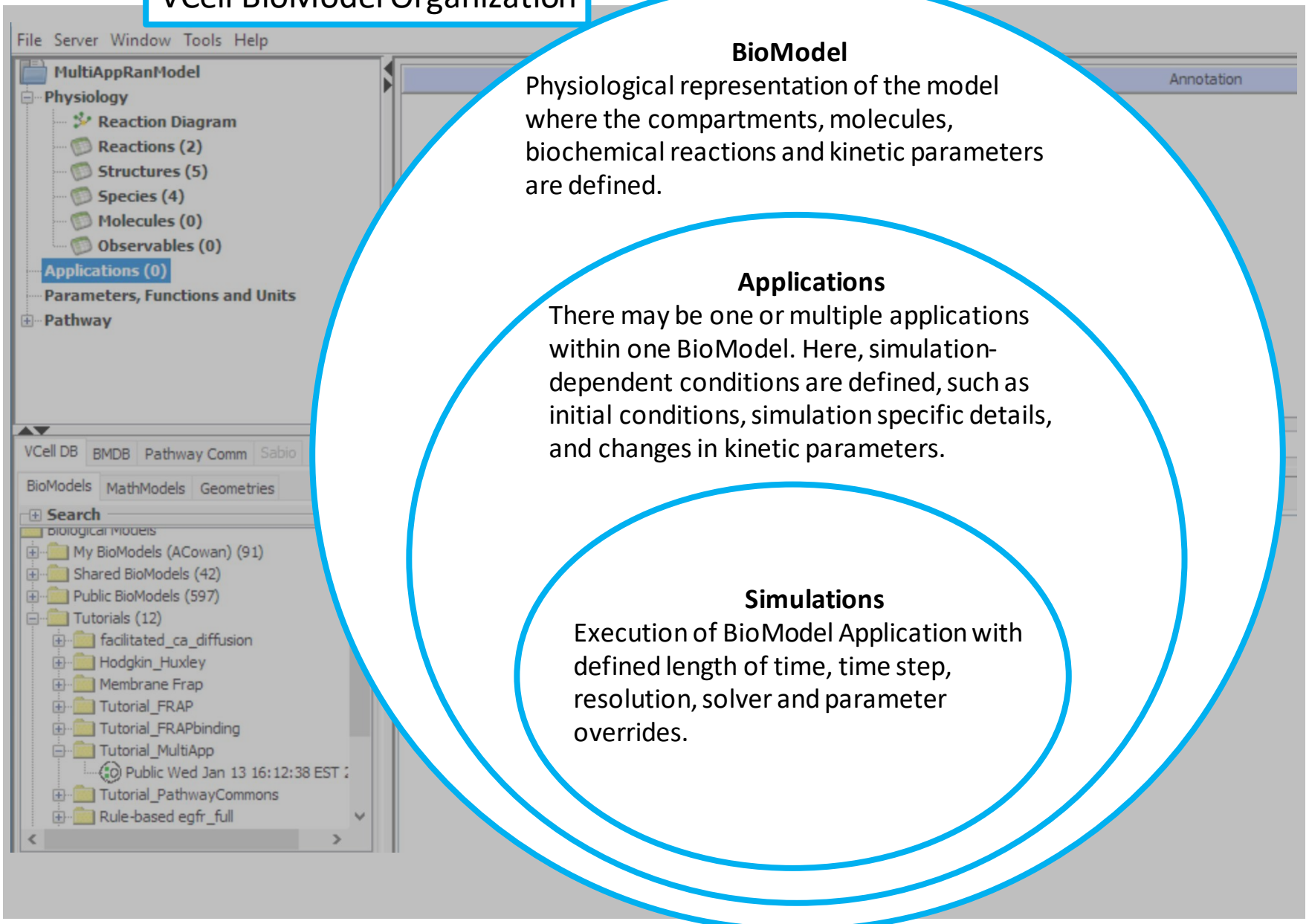


VCell BioModel Organization



BioModel

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

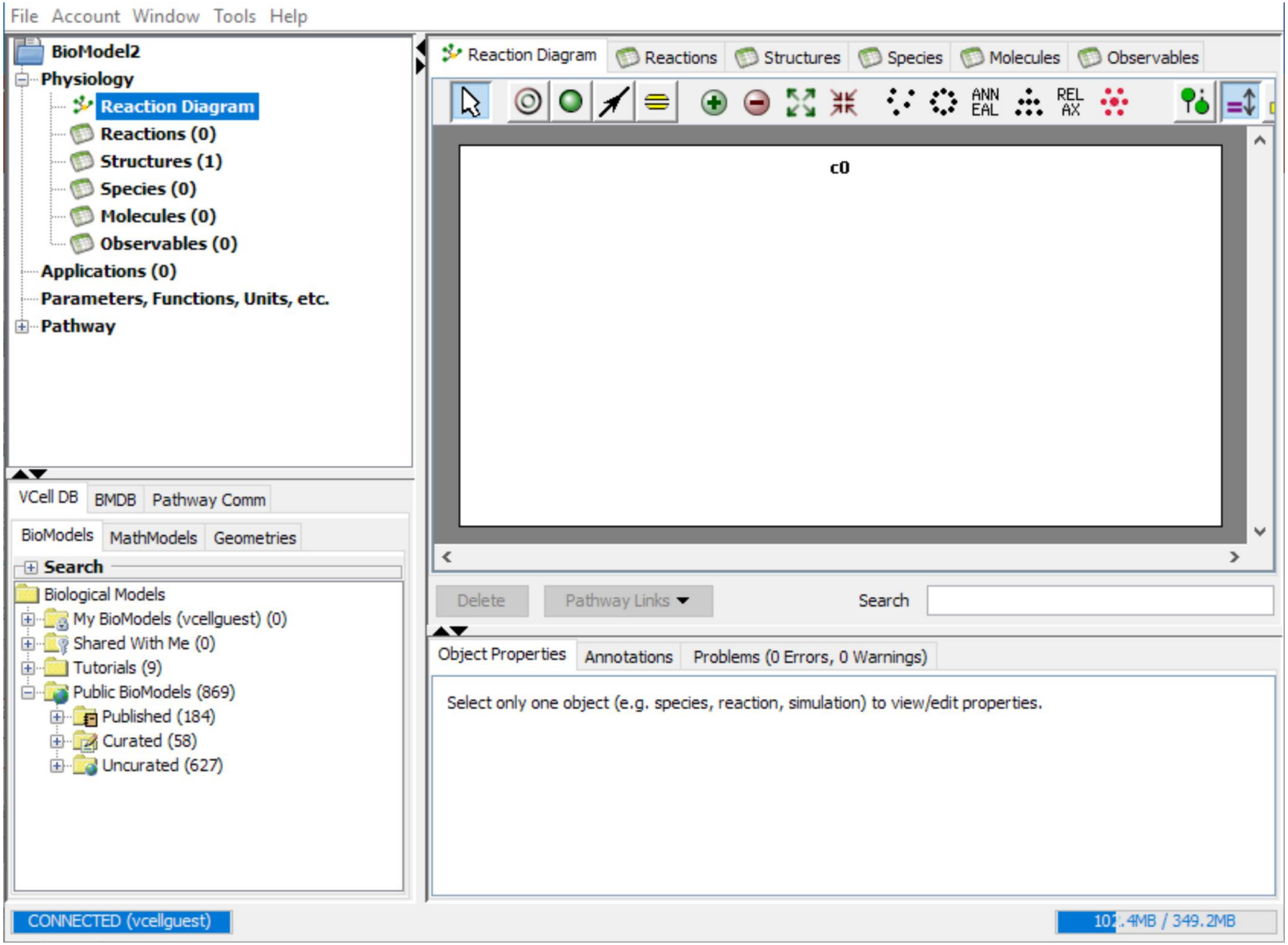
Applications

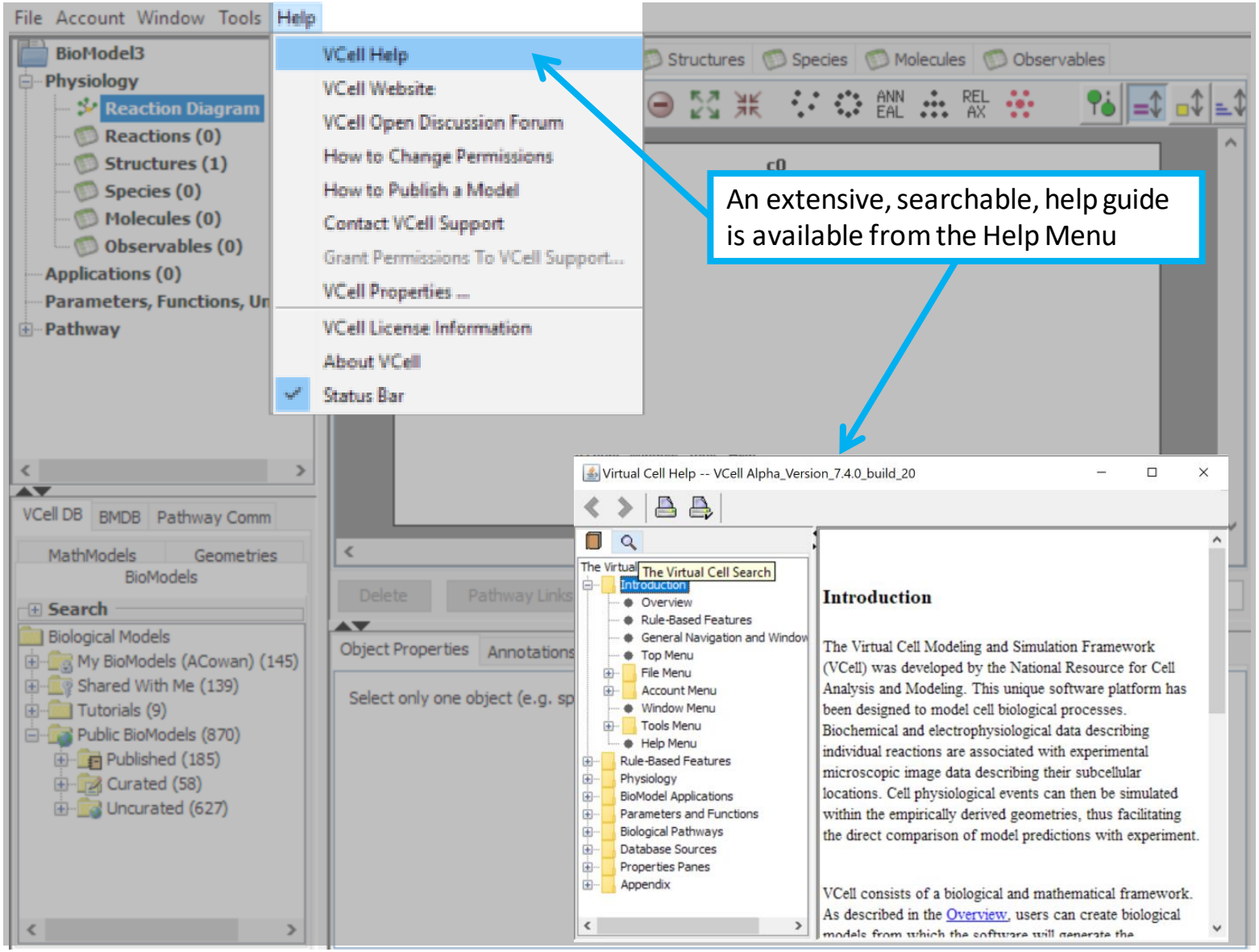
There may be one or multiple applications within one BioModel. Here, simulation-dependent conditions are defined, such as initial conditions, simulation specific details, and changes in kinetic parameters.

Simulations

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

The VCell Interface

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Introduction
The Virtual Cell Modeling and Simulation Framework (VCell) was developed by the National Resource for Cell Analysis and Modeling. This unique software platform has been designed to model cell biological processes. Biochemical and electrophysiological data describing individual reactions are associated with experimental microscopic image data describing their subcellular locations. Cell physiological events can then be simulated within the empirically derived geometries, thus facilitating the direct comparison of model predictions with experiment.
VCell consists of a biological and mathematical framework. As described in the Overview, users can create biological
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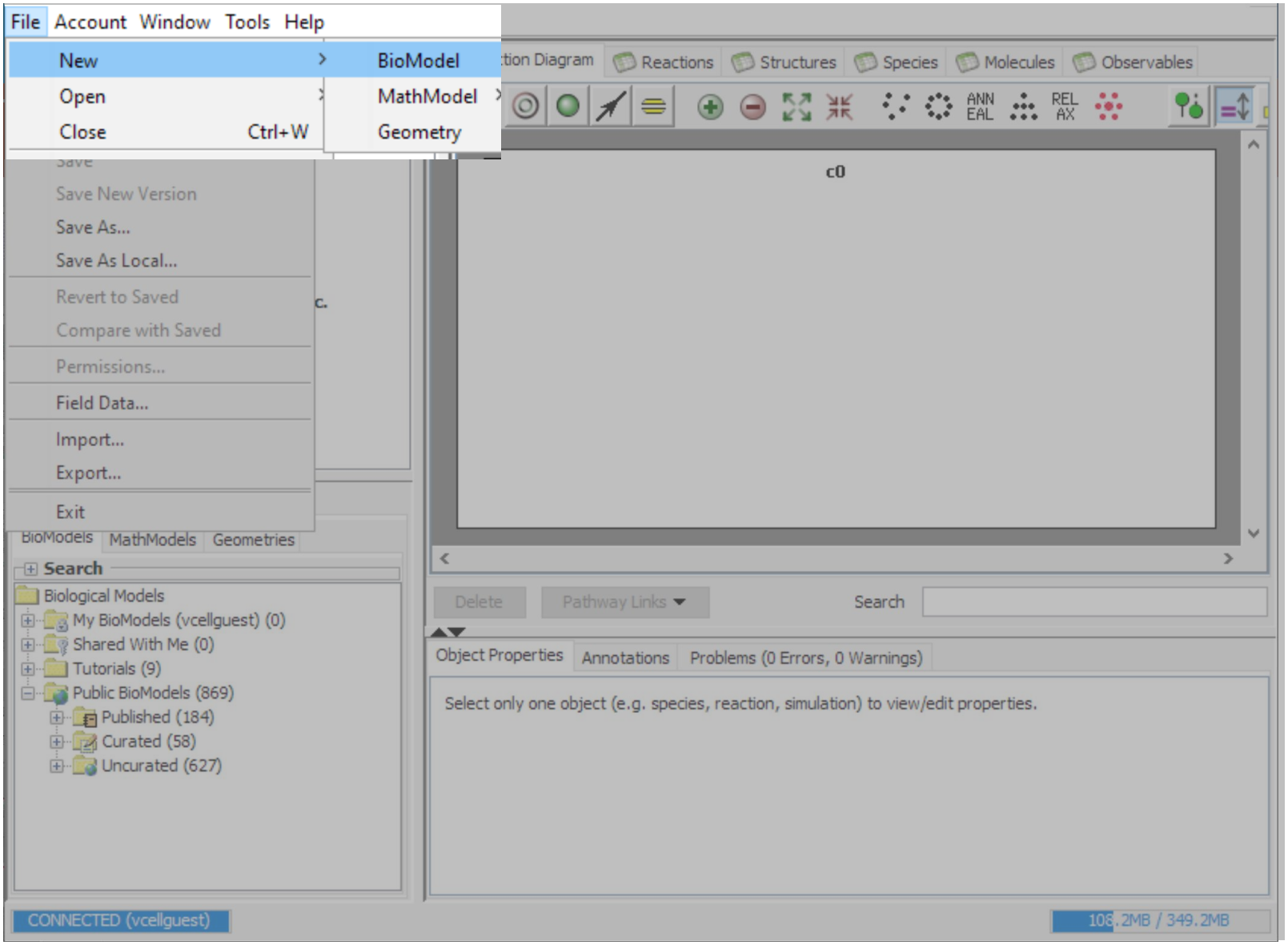
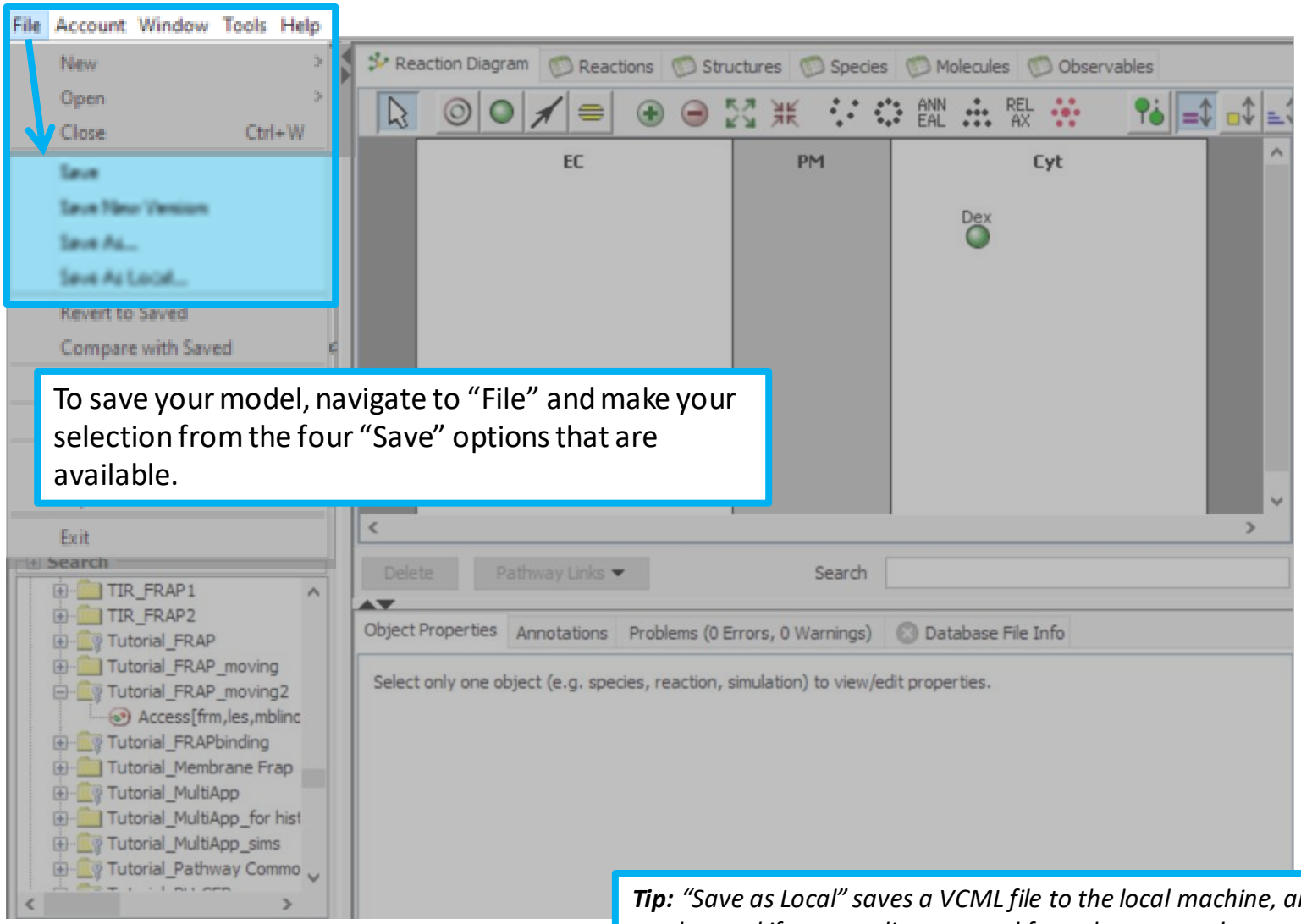
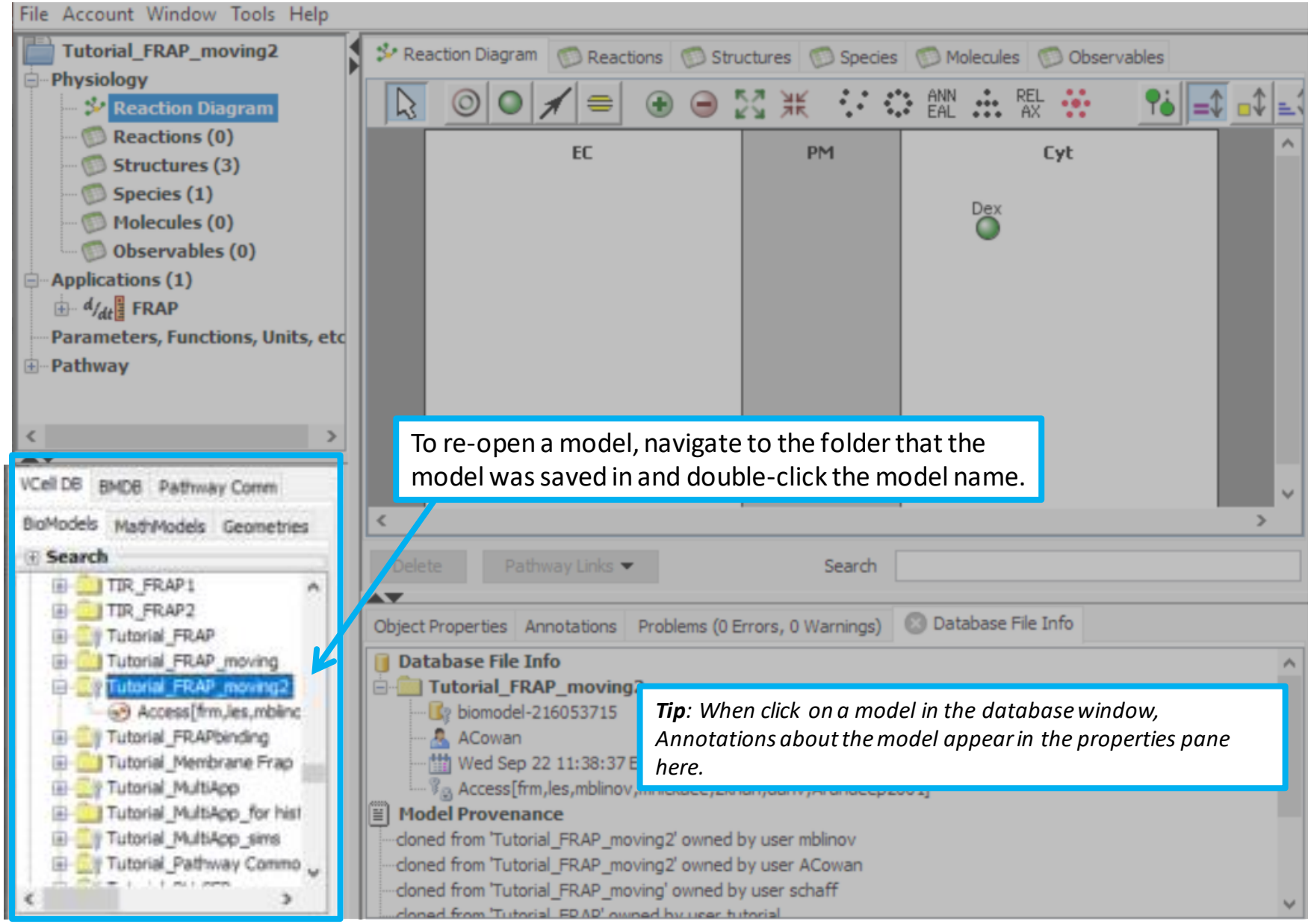
To create a new VCell model, click “File” > “New” > “BioModel”





To save your model, navigate to "File" and make your selection from the four "Save" options that are available.

Tip: *"Save as Local" saves a VCML file to the local machine, and can be used if you are disconnected from the server when building a model*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To re-open a model, navigate to the folder that the model was saved in and double-click the model name.
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Access[frm,les,mblinov
Tip: When click on a model in the database window, Annotations about the model appear in the properties pane here.
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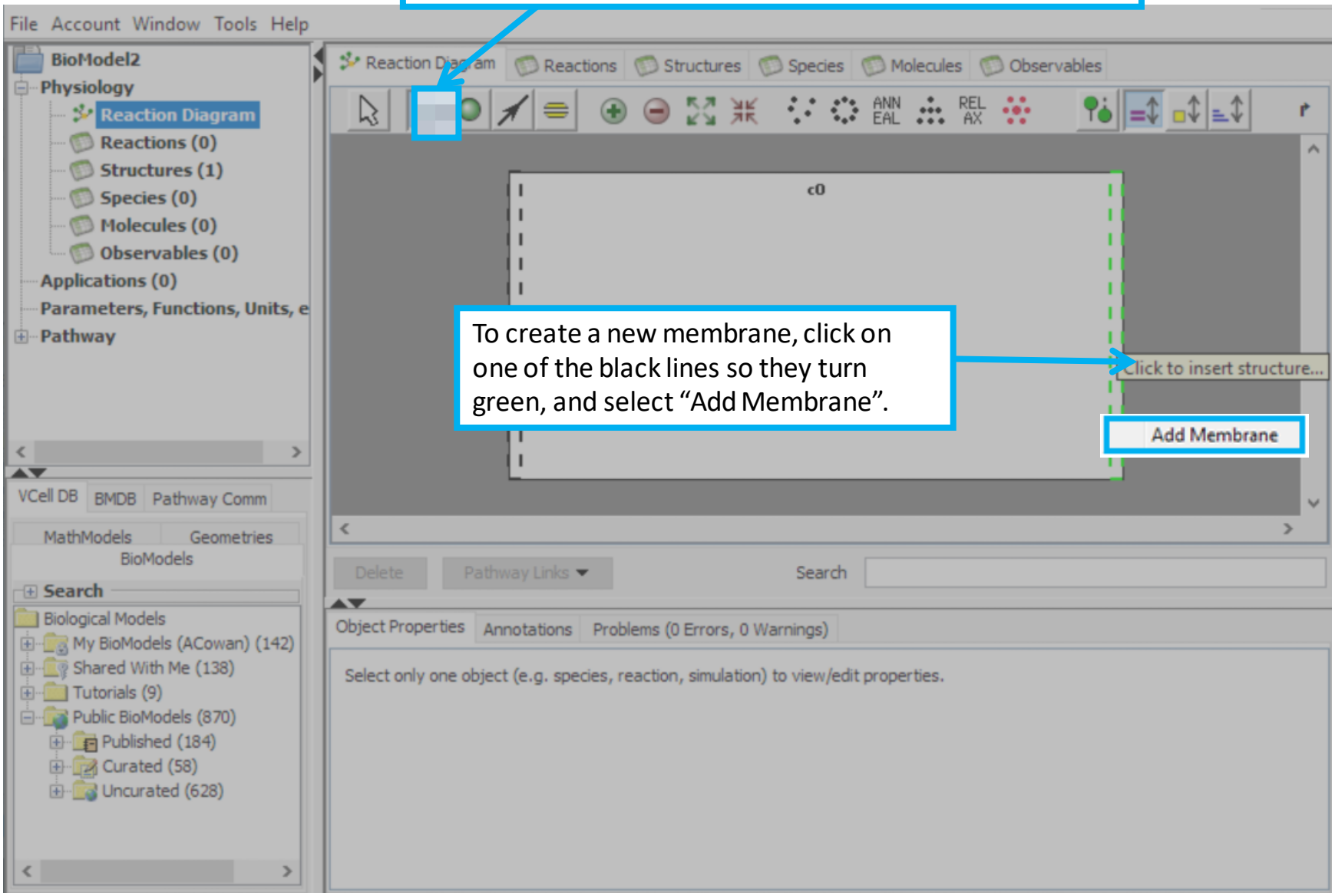
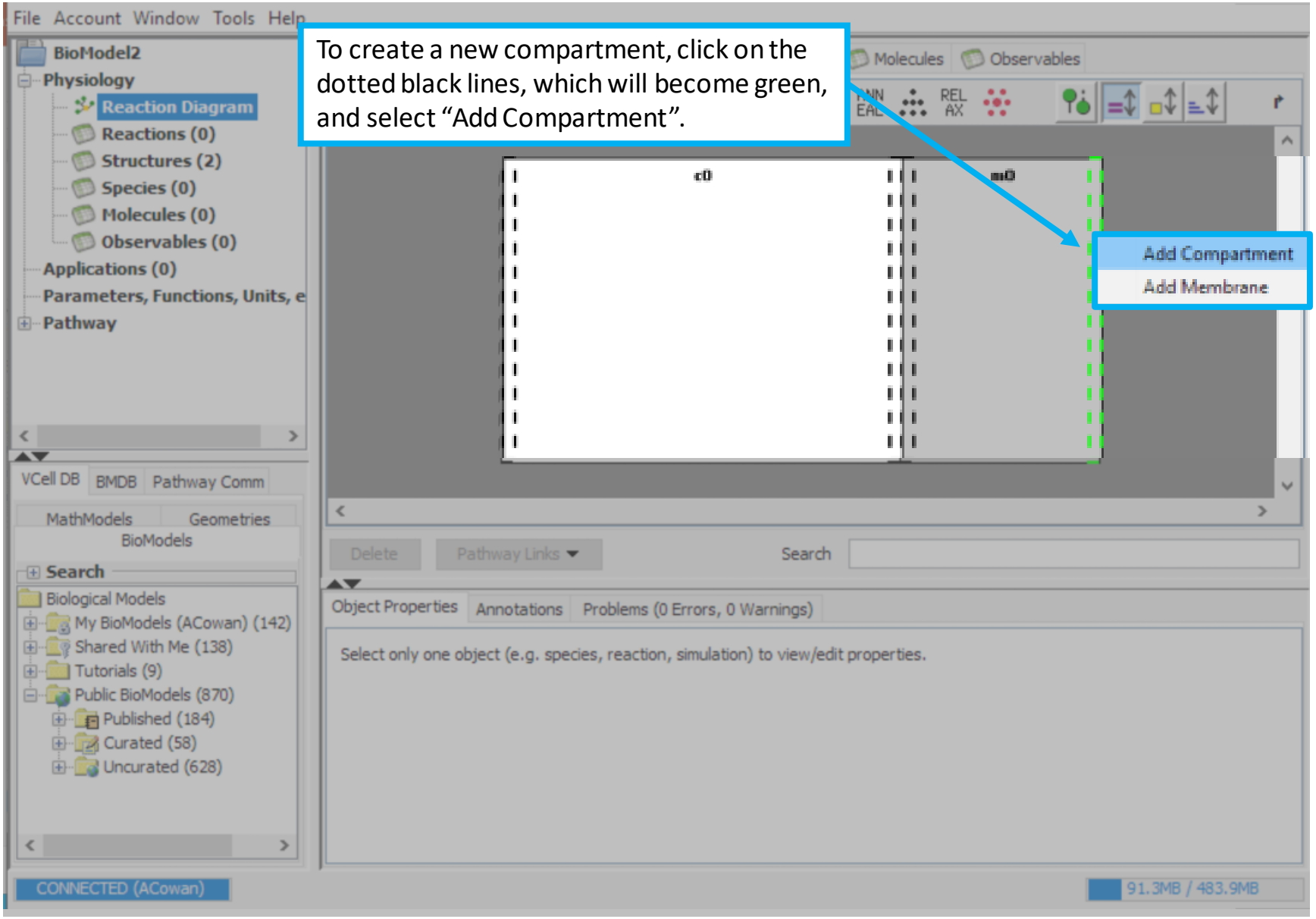
cloned from 'Tutorial_FRAP_moving2' owned by user mblinov
cloned from 'Tutorial_FRAP_moving2' owned by user ACowan
cloned from 'Tutorial_FRAP_moving' owned by user schaff

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



To create a new membrane, click on one of the black lines so they turn green, and select “Add Membrane”.


To create a new compartment, click on the dotted black lines, which will become green, and select “Add Compartment”.
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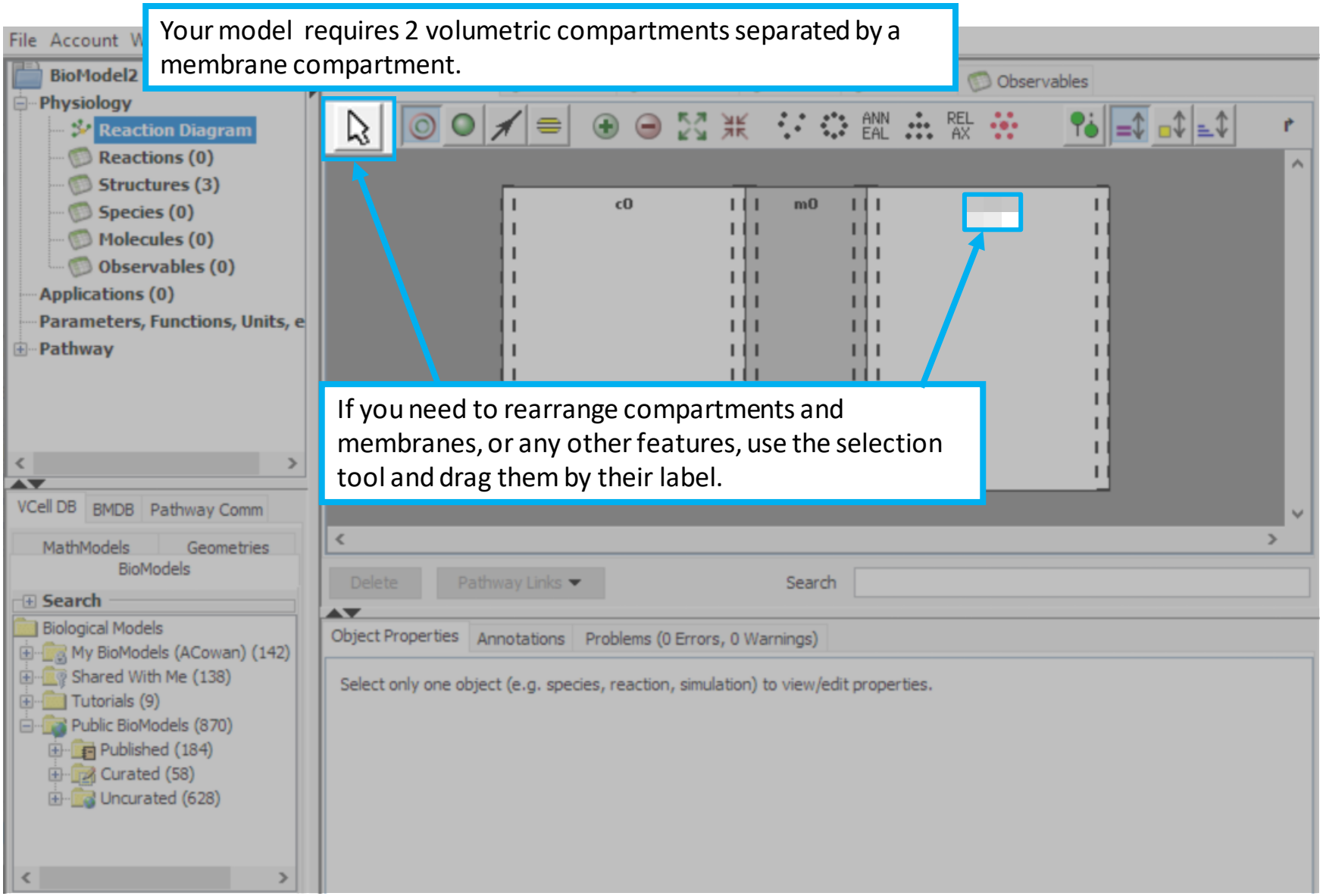
Your model requires 2 volumetric compartments separated by a membrane compartment.
If you need to rearrange compartments and membranes, or any other features, use the selection tool and drag them by their label.
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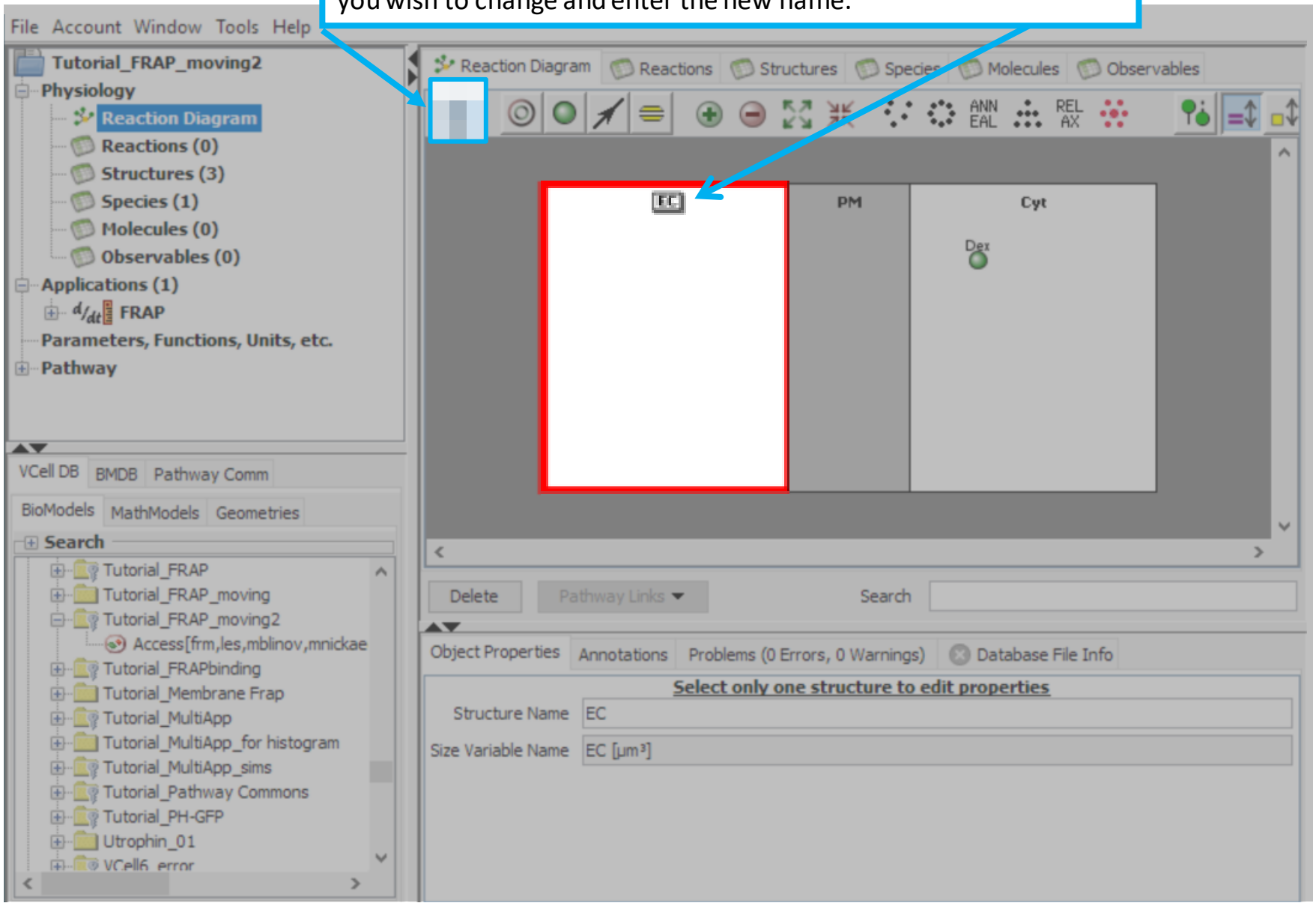
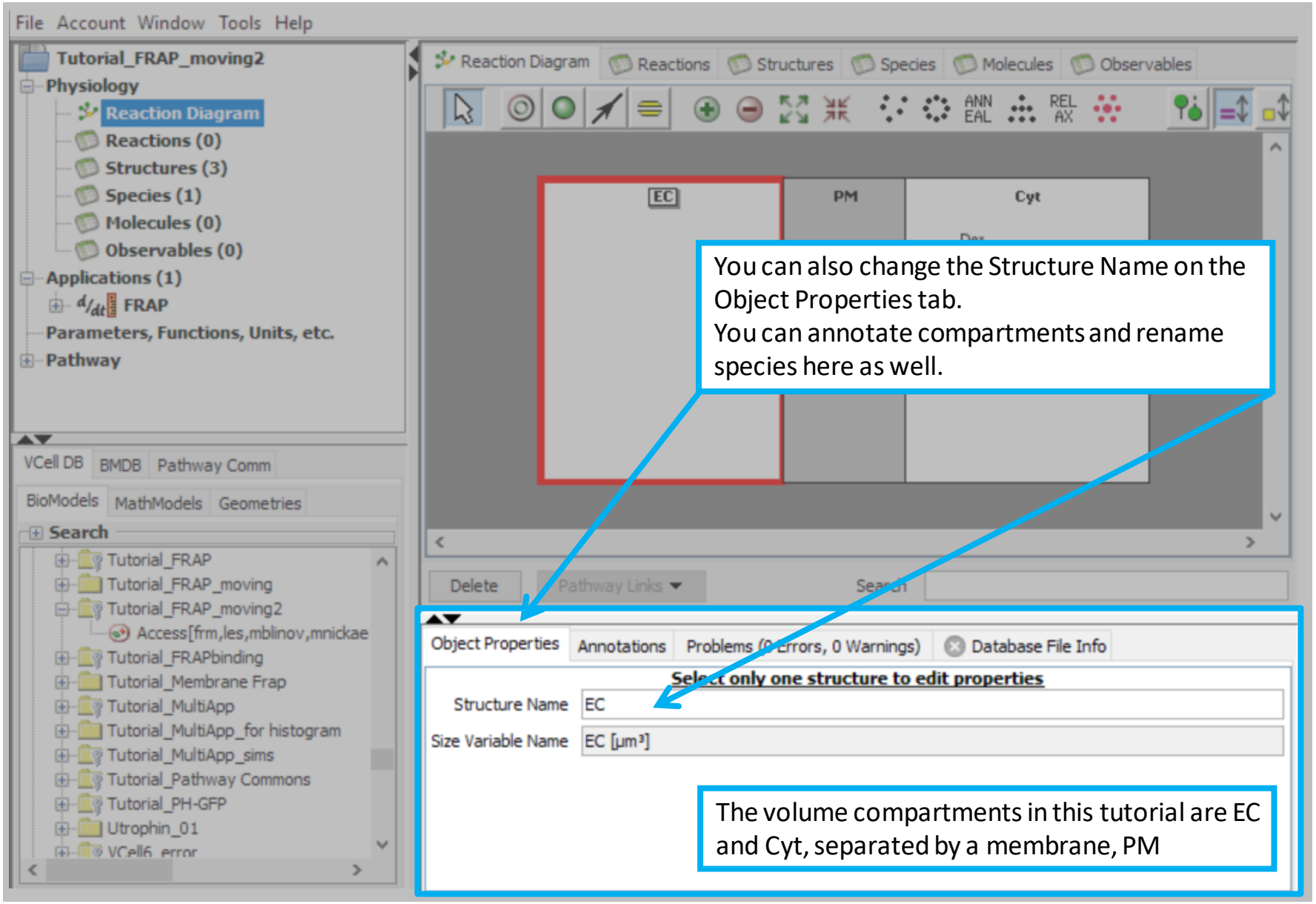
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

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

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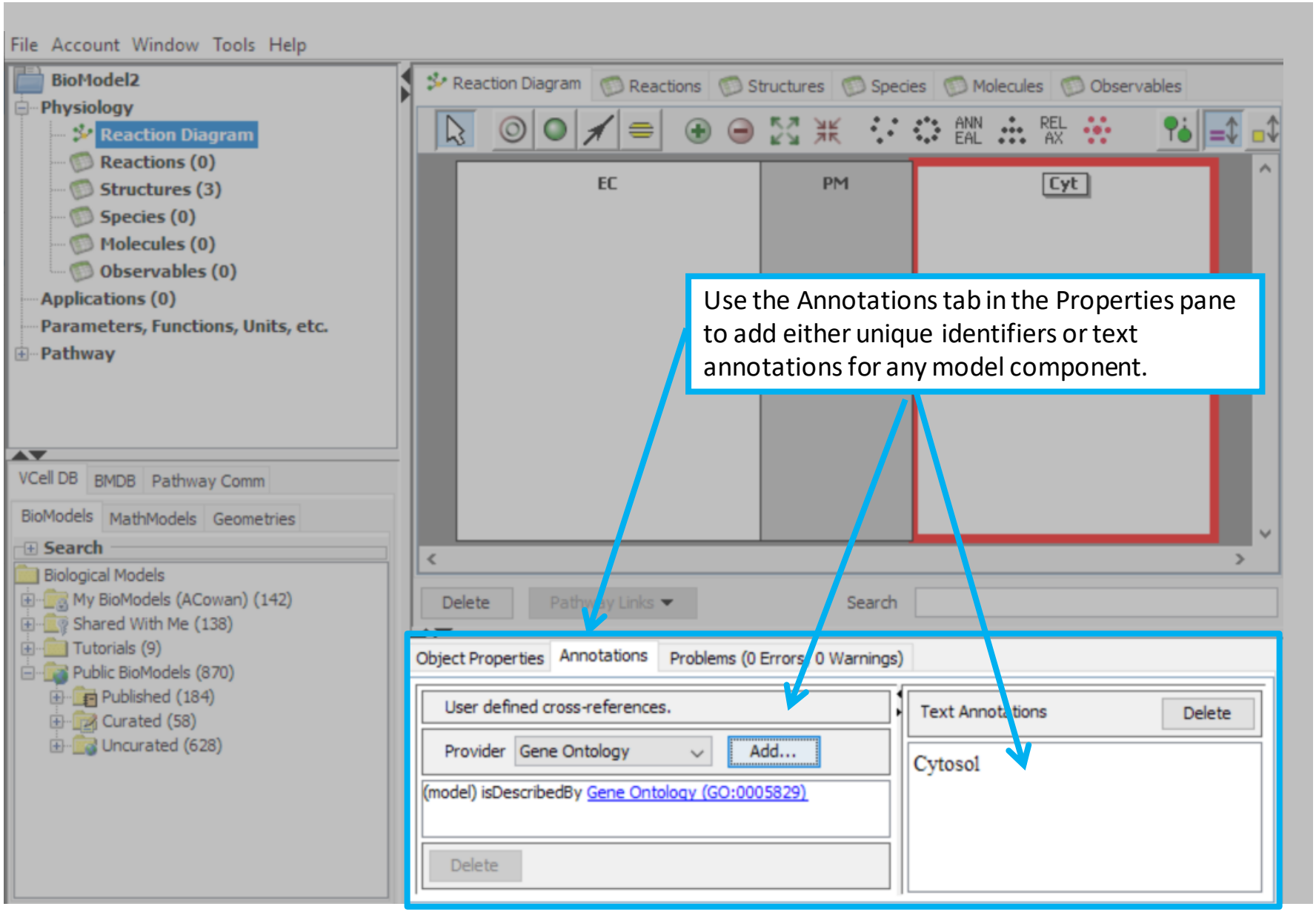
Select only one structure to edit properties
Structure Name
EC
Size Variable Name
EC [µm³]
You can also change the Structure Name on the Object Properties tab.
You can annotate compartments and rename species here as well.
The volume compartments in this tutorial are EC and Cyt, separated by a membrane, PM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Use the Annotations tab in the Properties pane to add either unique identifiers or text annotations for any model component.
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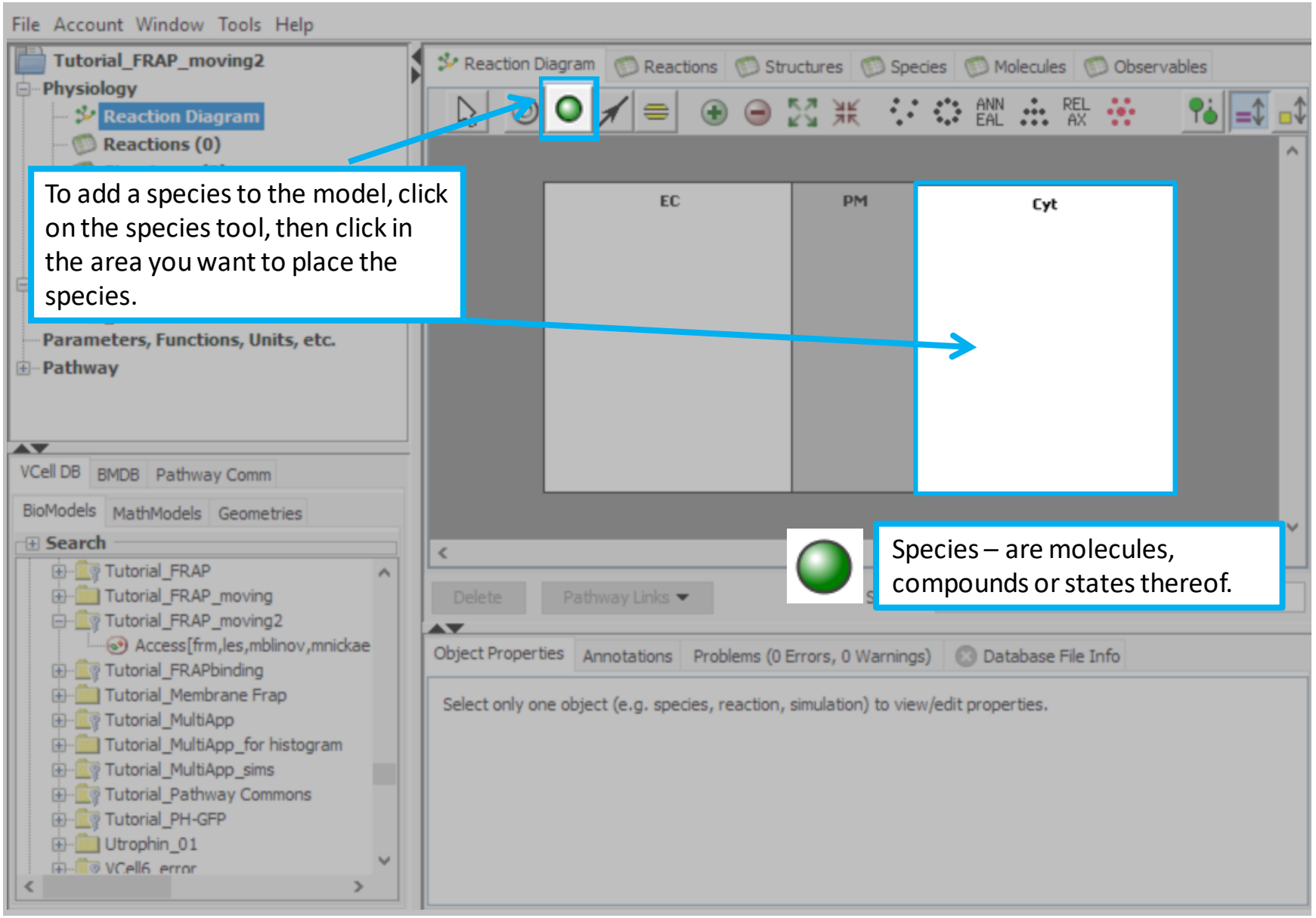
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To add a species to the model, click on the species tool, then click in the area you want to place the species.
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Species – are molecules, compounds or states thereof.
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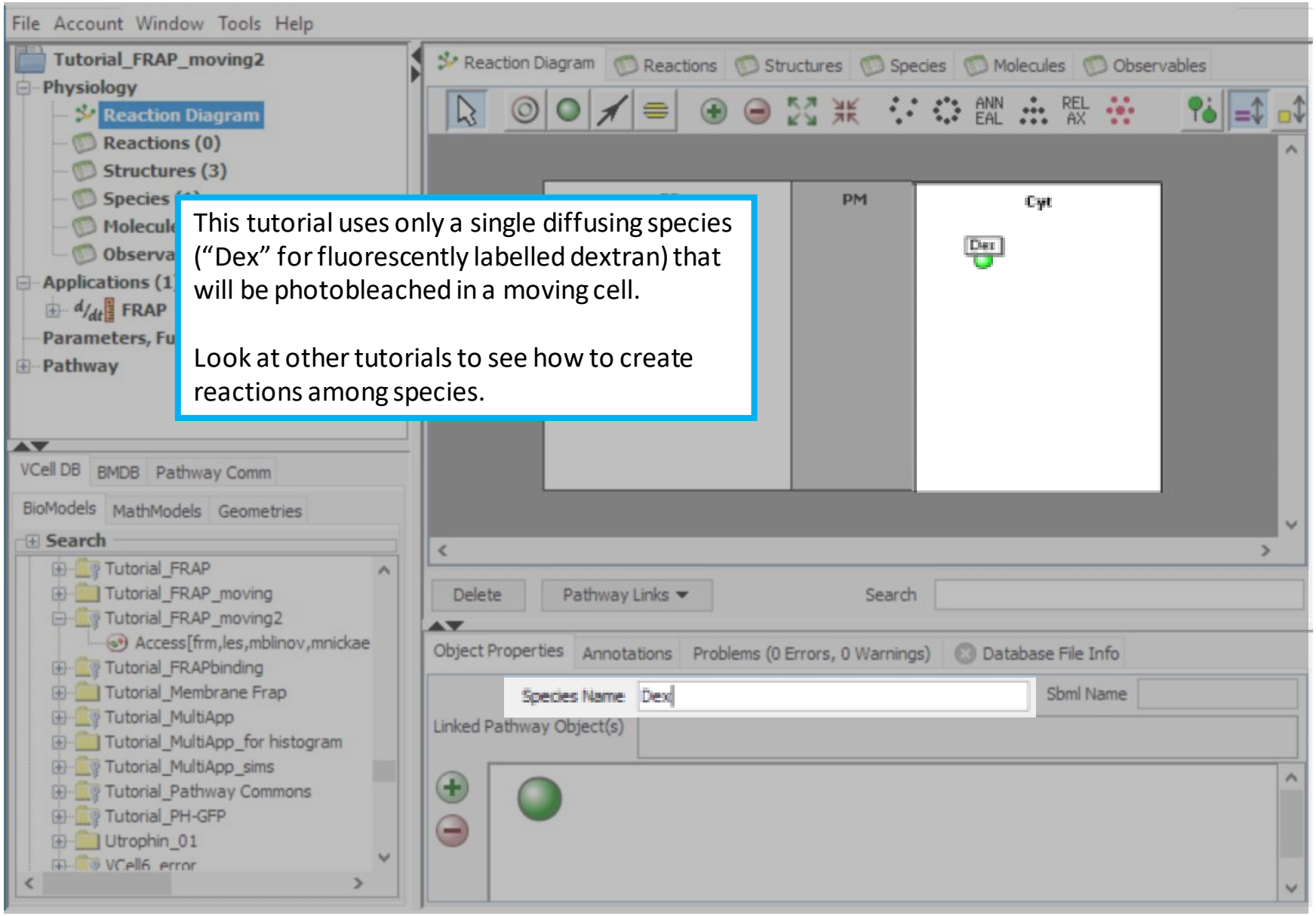
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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This tutorial uses only a single diffusing species ("Dex" for fluorescently labelled dextran) that will be photobleached in a moving cell.
Look at other tutorials to see how to create reactions among species.
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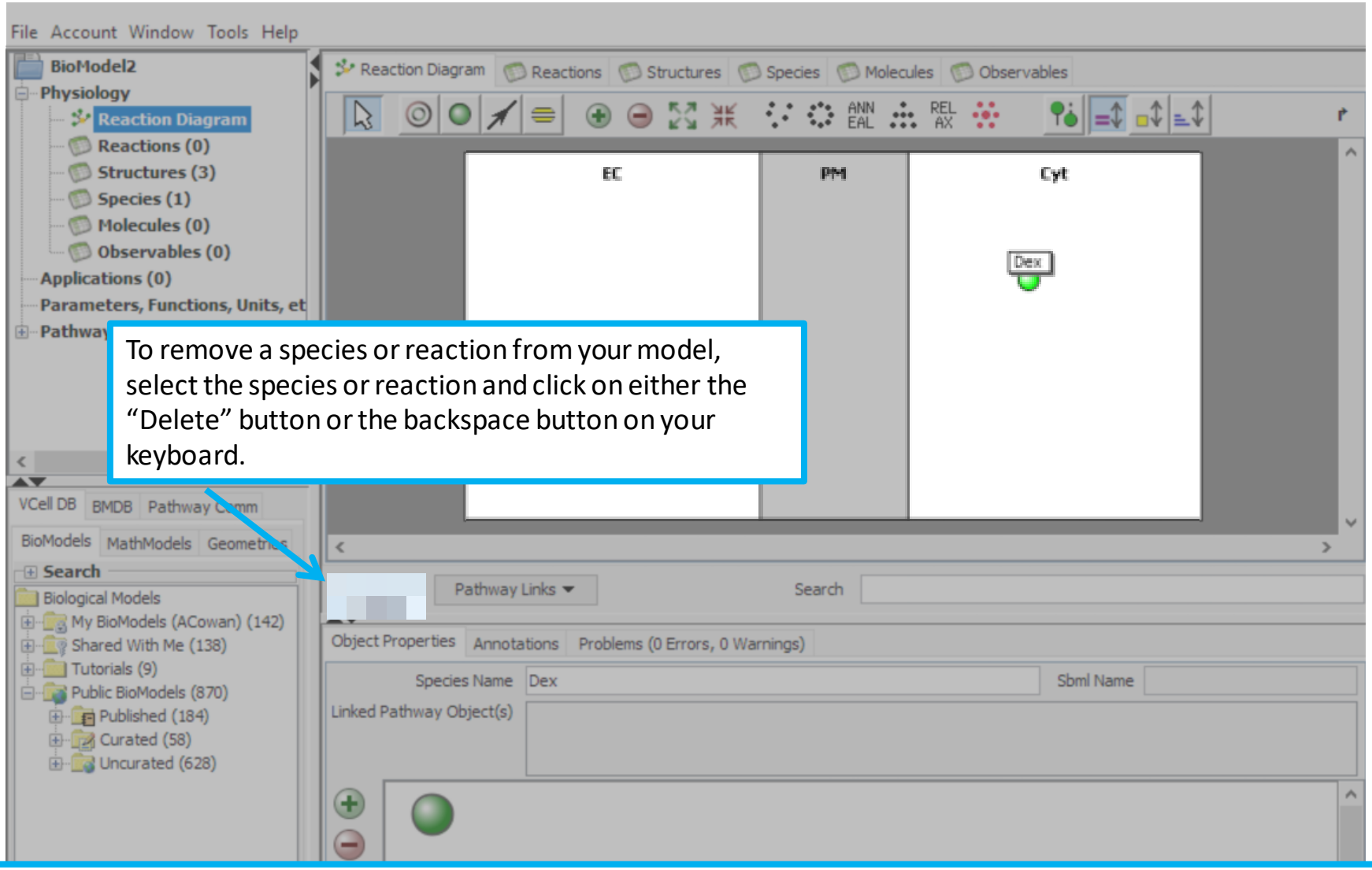
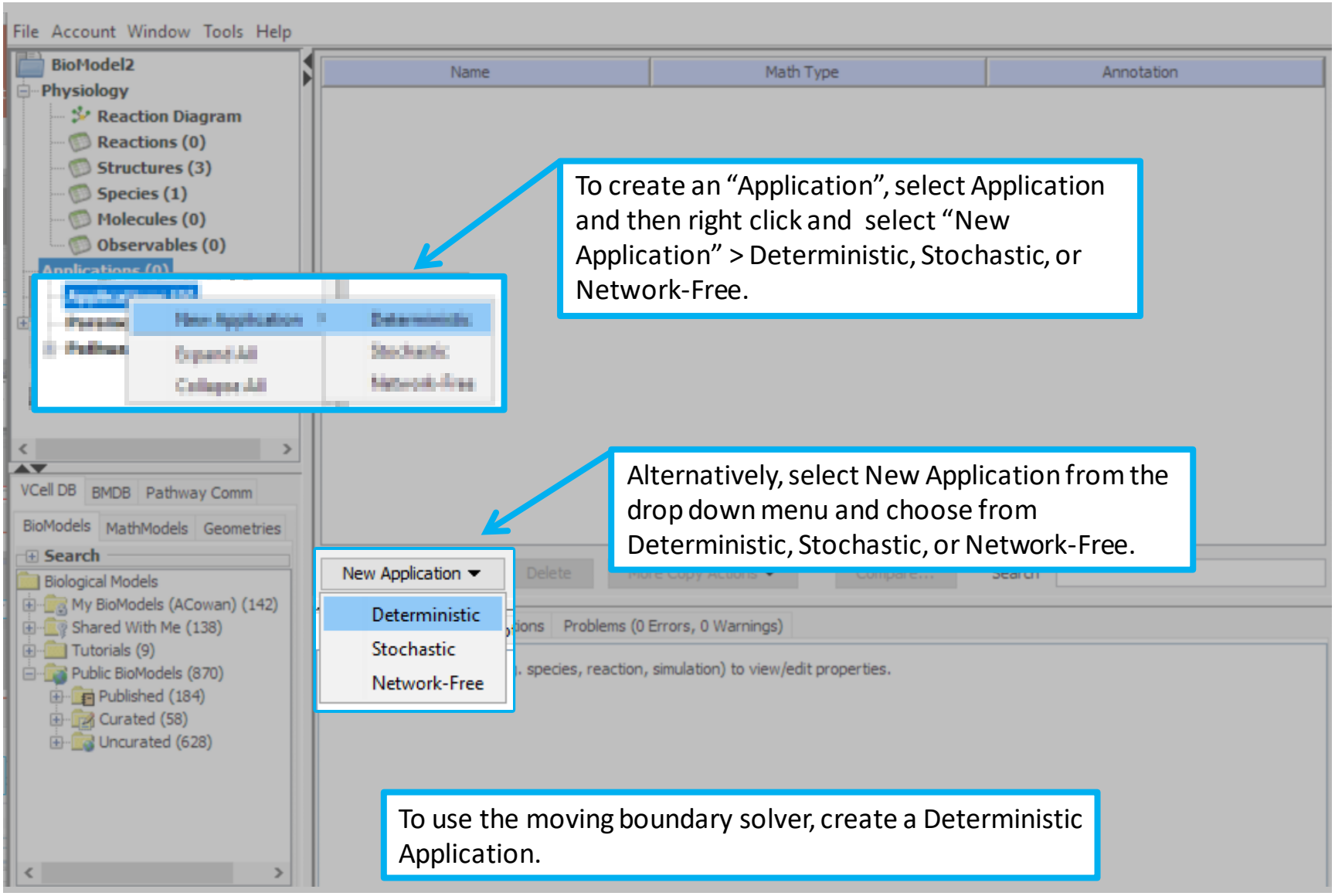


Note that you cannot move species, reactions, or fluxes from one compartment to another. You must delete a species, flux, or reaction from one compartment and then create it in another compartment.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To create an "Application", select Application and then right click and select "New Application" > Deterministic, Stochastic, or Network-Free.
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Alternatively, select New Application from the drop down menu and choose from Deterministic, Stochastic, or Network-Free.
New Application
Deterministic
Stochastic
Network-Free
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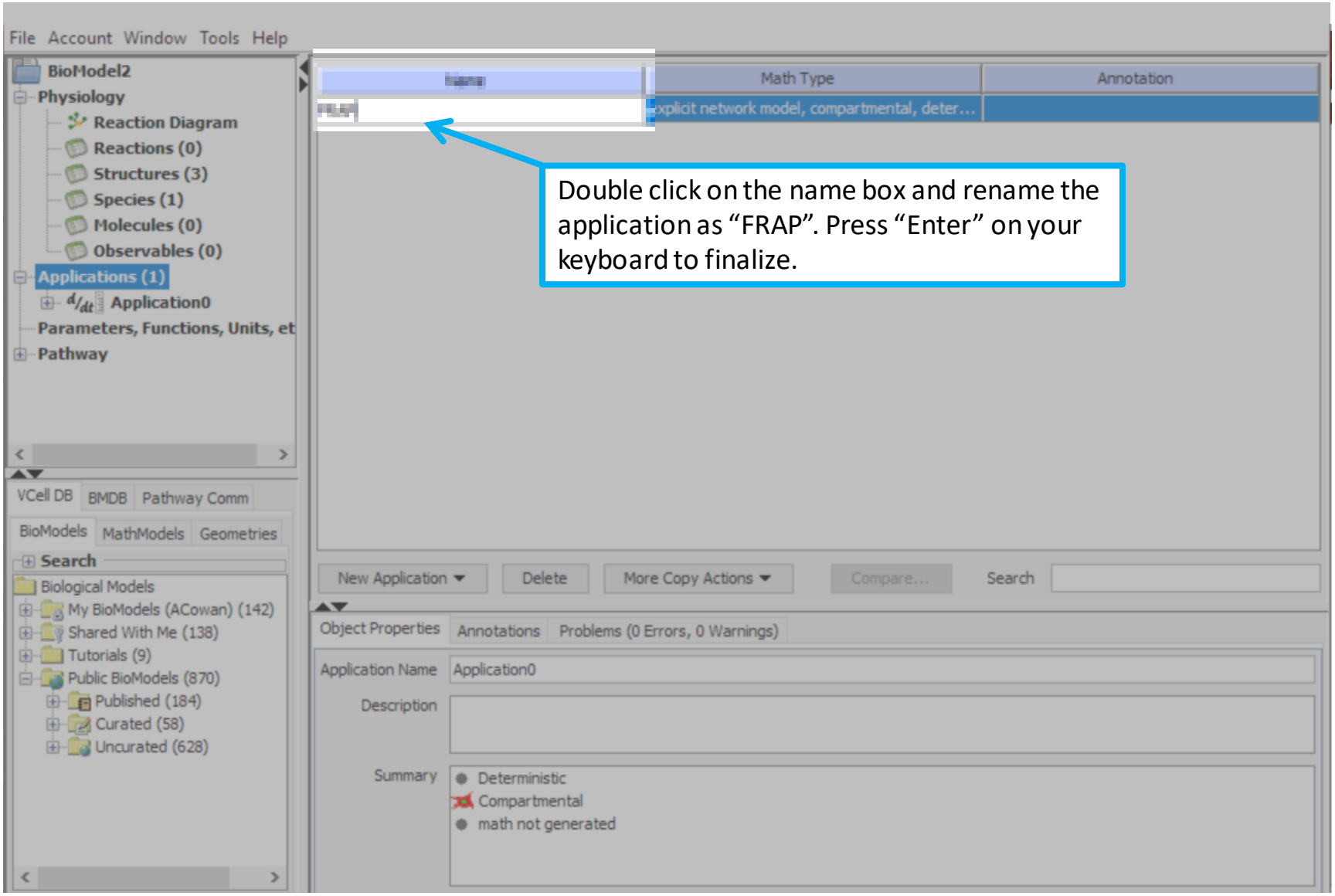
species, reaction, simulation) to view/edit properties.
To use the moving boundary solver, create a Deterministic Application.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Double click on the name box and rename the application as “FRAP”. Press “Enter” on your keyboard to finalize.
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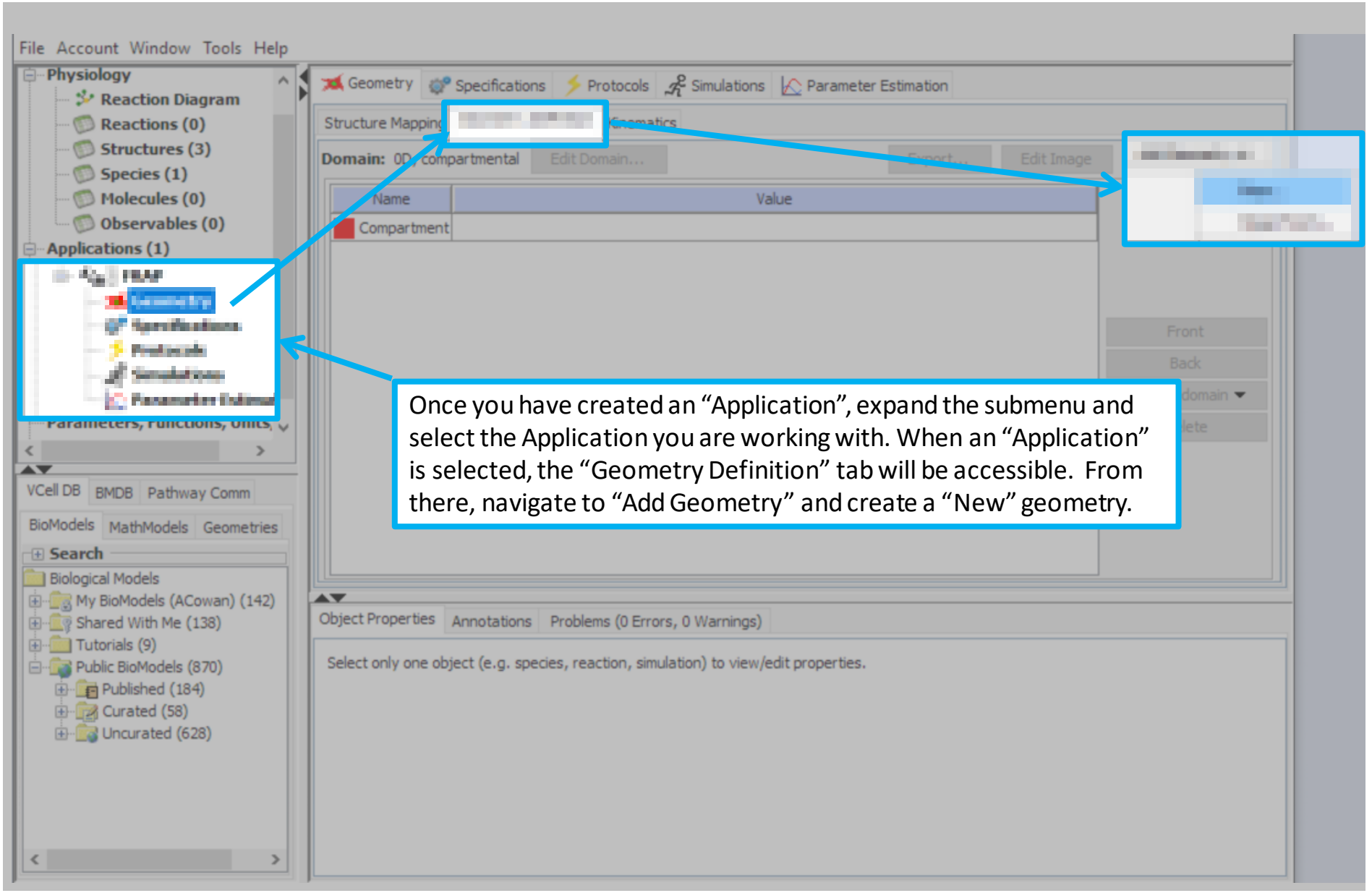
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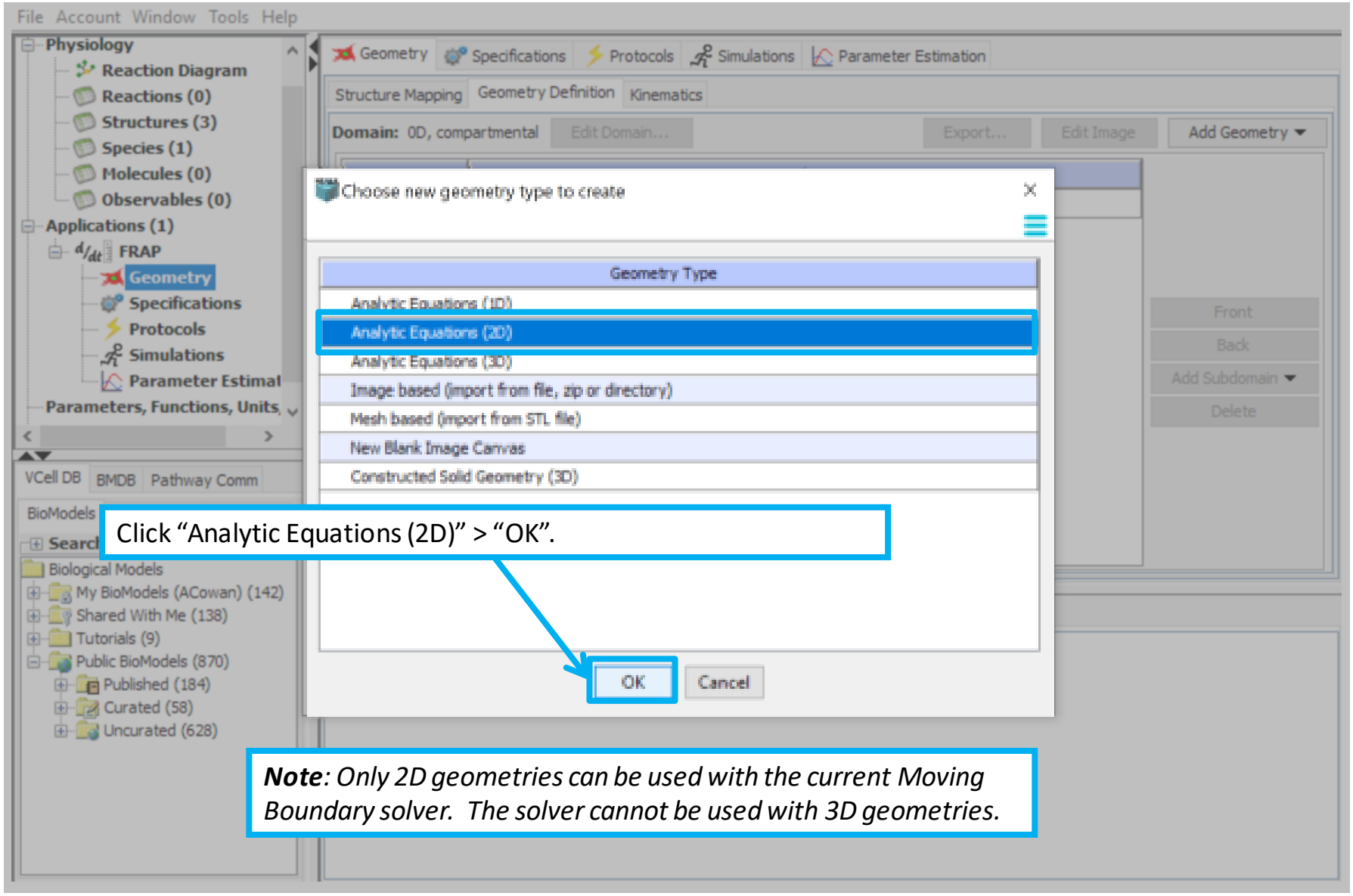
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
Once you have created an “Application”, expand the submenu and select the Application you are working with. When an “Application” is selected, the “Geometry Definition” tab will be accessible. From there, navigate to “Add Geometry” and create a “New” geometry.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Analytic Equations (3D)
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Mesh based (import from STL file)
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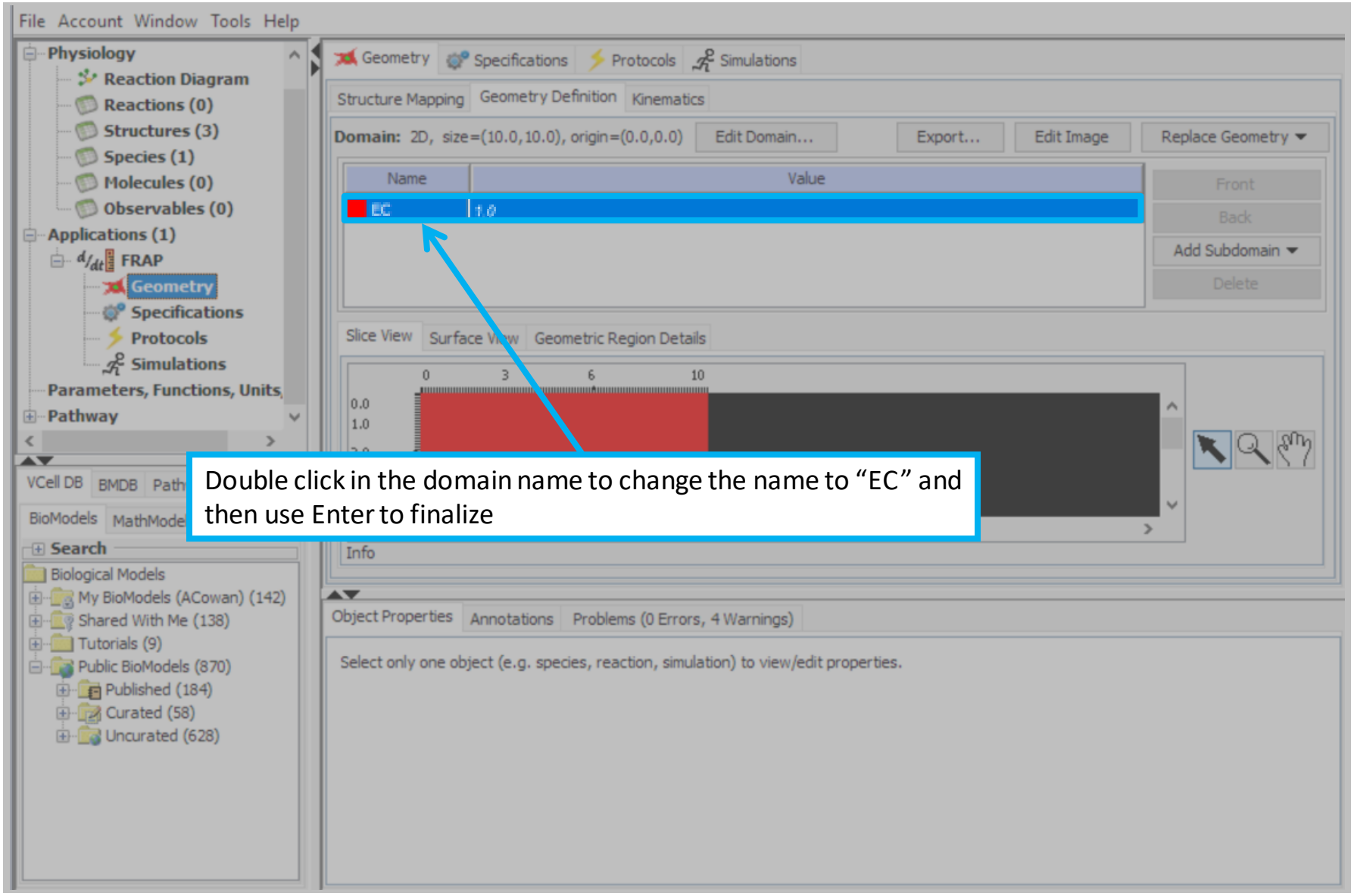
Click “Analytic Equations (2D)” > “OK”.
Note: Only 2D geometries can be used with the current Moving Boundary solver. The solver cannot be used with 3D geometries.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Geometry Definition
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
Info
Double click in the domain name to change the name to "EC" and then use Enter to finalize
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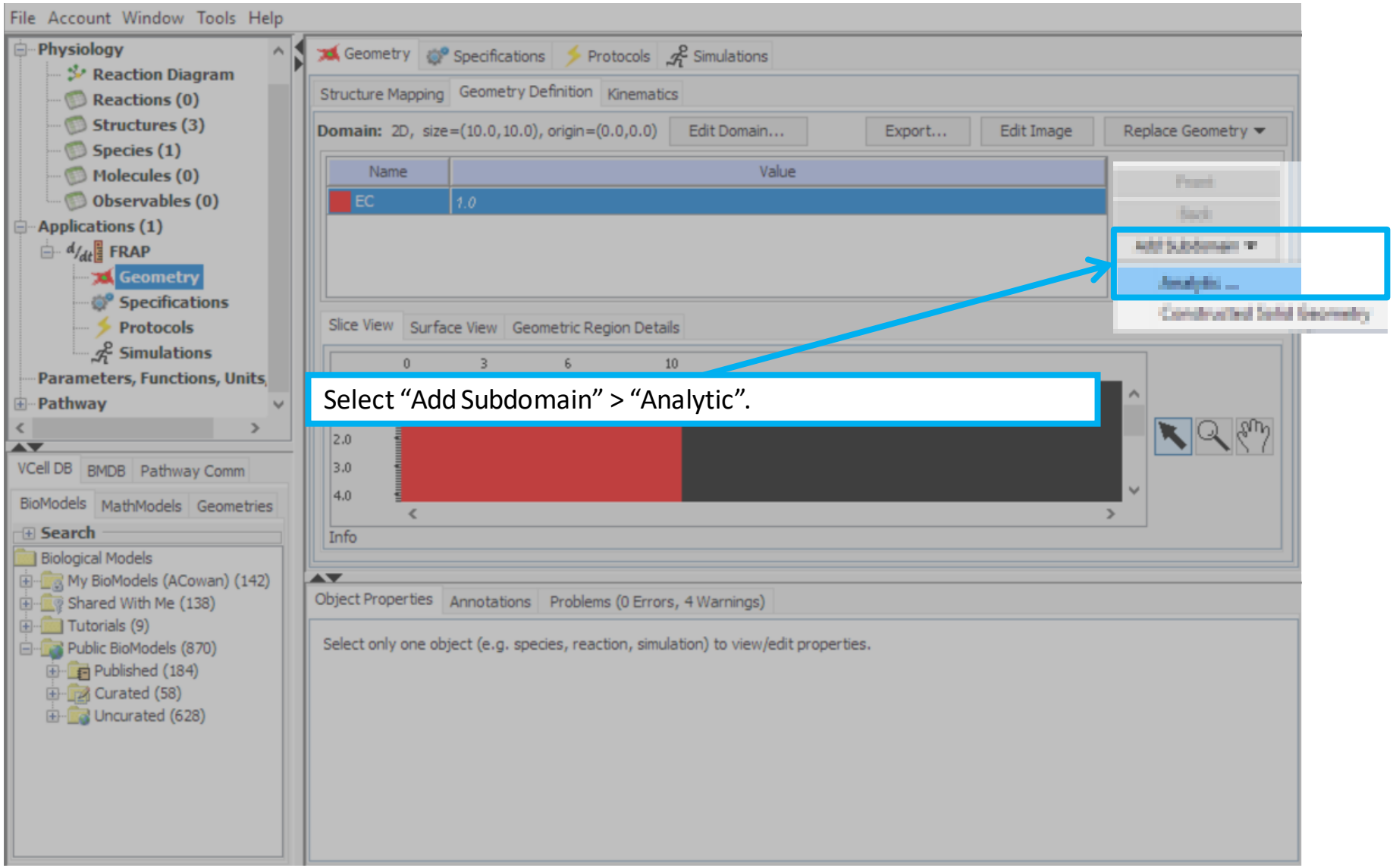
Object Properties
Annotations
Problems (0 Errors, 4 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
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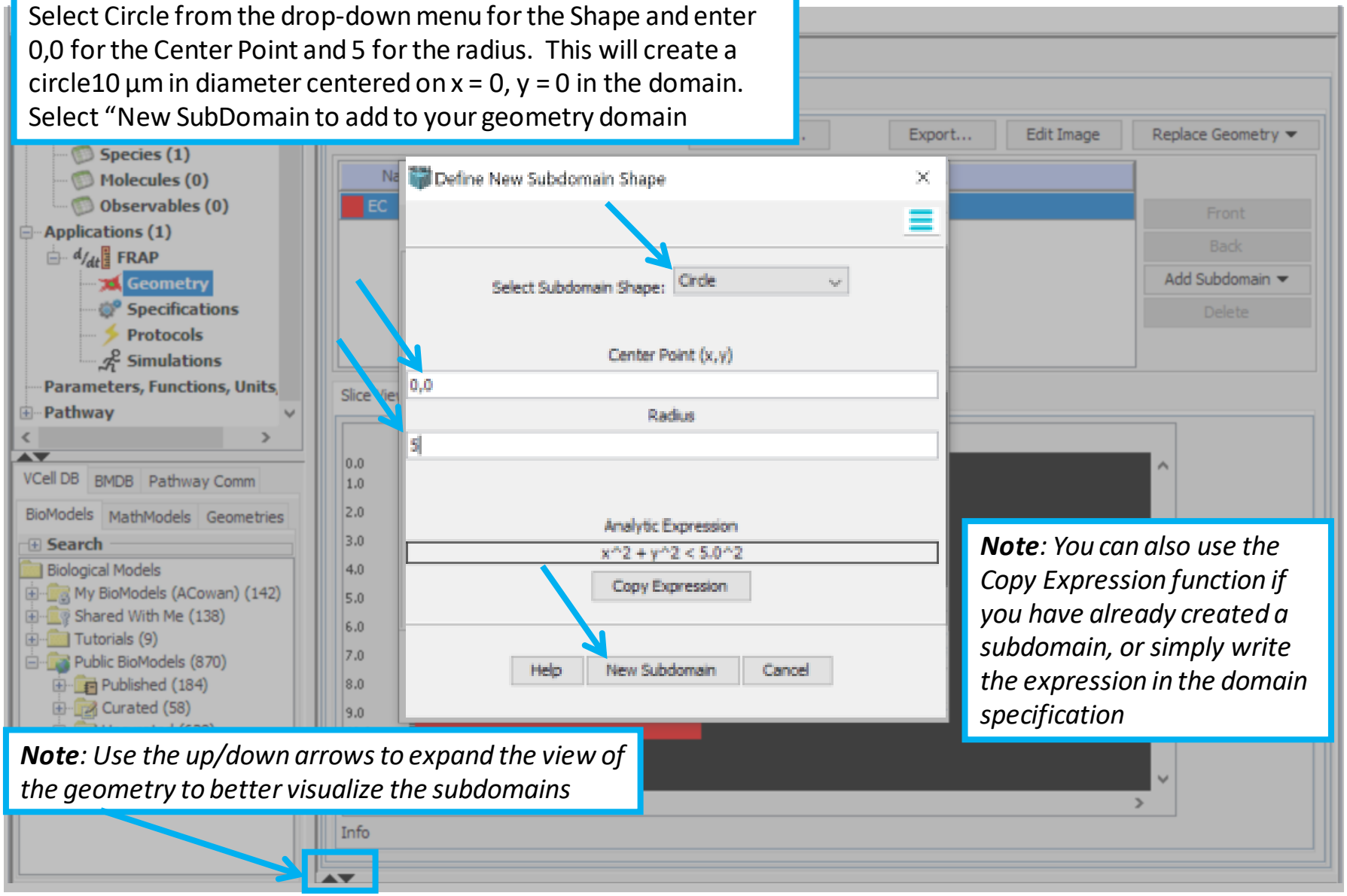
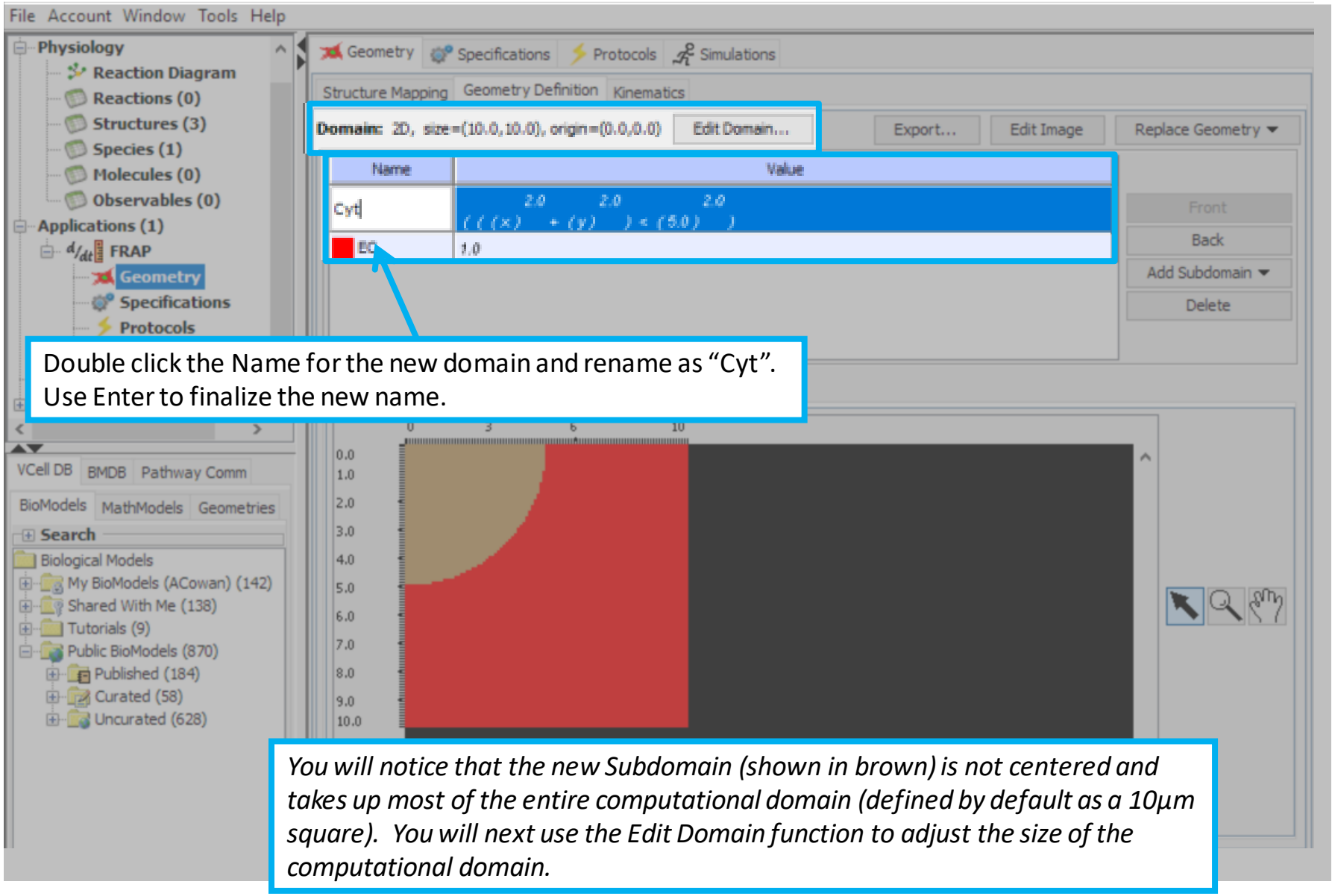
EC
1.0
Slice View
Surface View
Geometric Region Details
0
3
6
10
2.0
3.0
4.0
Info
Select “Add Subdomain” > “Analytic”.
Object Properties
Annotations
Problems (0 Errors, 4 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Select Circle from the drop-down menu for the Shape and enter 0,0 for the Center Point and 5 for the radius. This will create a circle10 µm in diameter centered on x = 0, y = 0 in the domain. Select "New SubDomain to add to your geometry domain



***Note**: You can also use the Copy Expression function if you have already created a subdomain, or simply write the expression in the domain specification*

***Note**: Use the up/down arrows to expand the view of the geometry to better visualize the subdomains*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Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
EC
1.0
Front
Back
Add Subdomain
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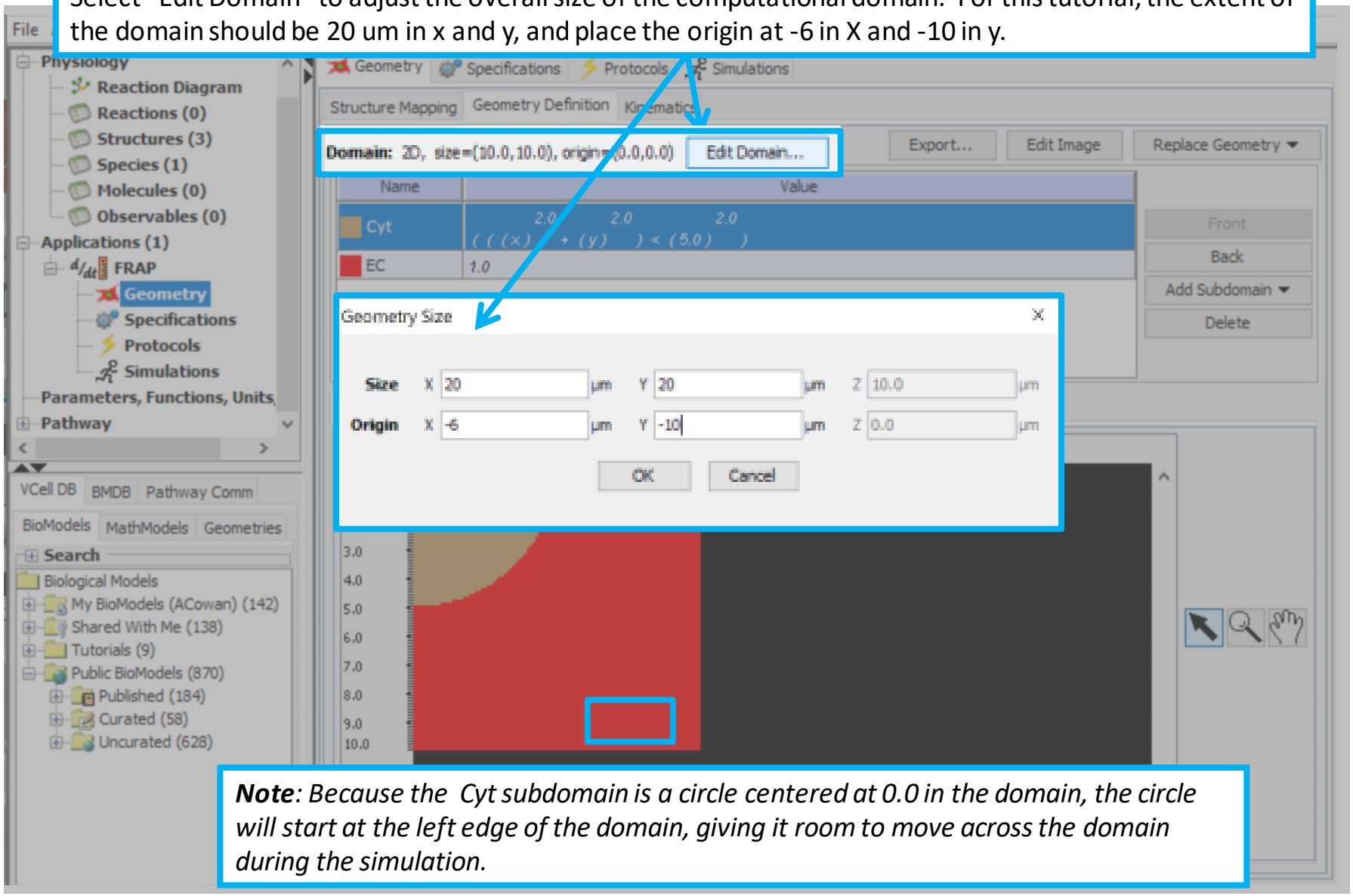
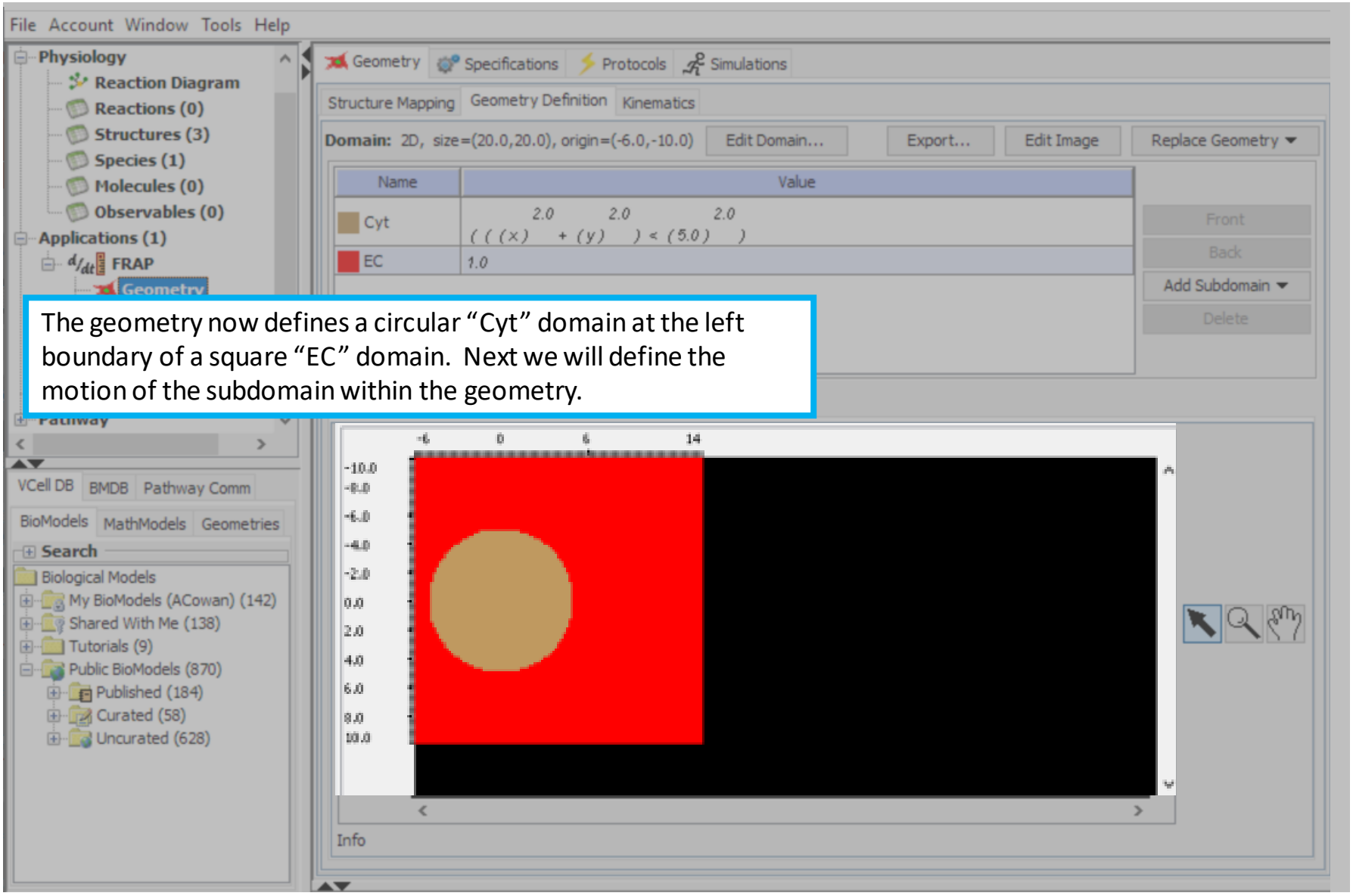
Double click the Name for the new domain and rename as “Cyt”.
Use Enter to finalize the new name.
You will notice that the new Subdomain (shown in brown) is not centered and takes up most of the entire computational domain (defined by default as a 10µm square). You will next use the Edit Domain function to adjust the size of the computational domain.

Select "Edit Domain" to adjust the overall size of the computational domain. For this tutorial, the extent of the domain should be 20 um in x and y, and place the origin at -6 in X and -10 in y.



***Note**: Because the Cyt subdomain is a circle centered at 0.0 in the domain, the circle will start at the left edge of the domain, giving it room to move across the domain during the simulation.*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Geometry Definition
Kinematics
Domain: 2D, size=(20.0,20.0), origin=(-6.0,-10.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
(((x) 2.0 + (y) 2.0) < (5.0) 2.0)
EC
1.0
Front
Back
Add Subdomain
Delete
The geometry now defines a circular "Cyt" domain at the left boundary of a square "EC" domain. Next we will define the motion of the subdomain within the geometry.
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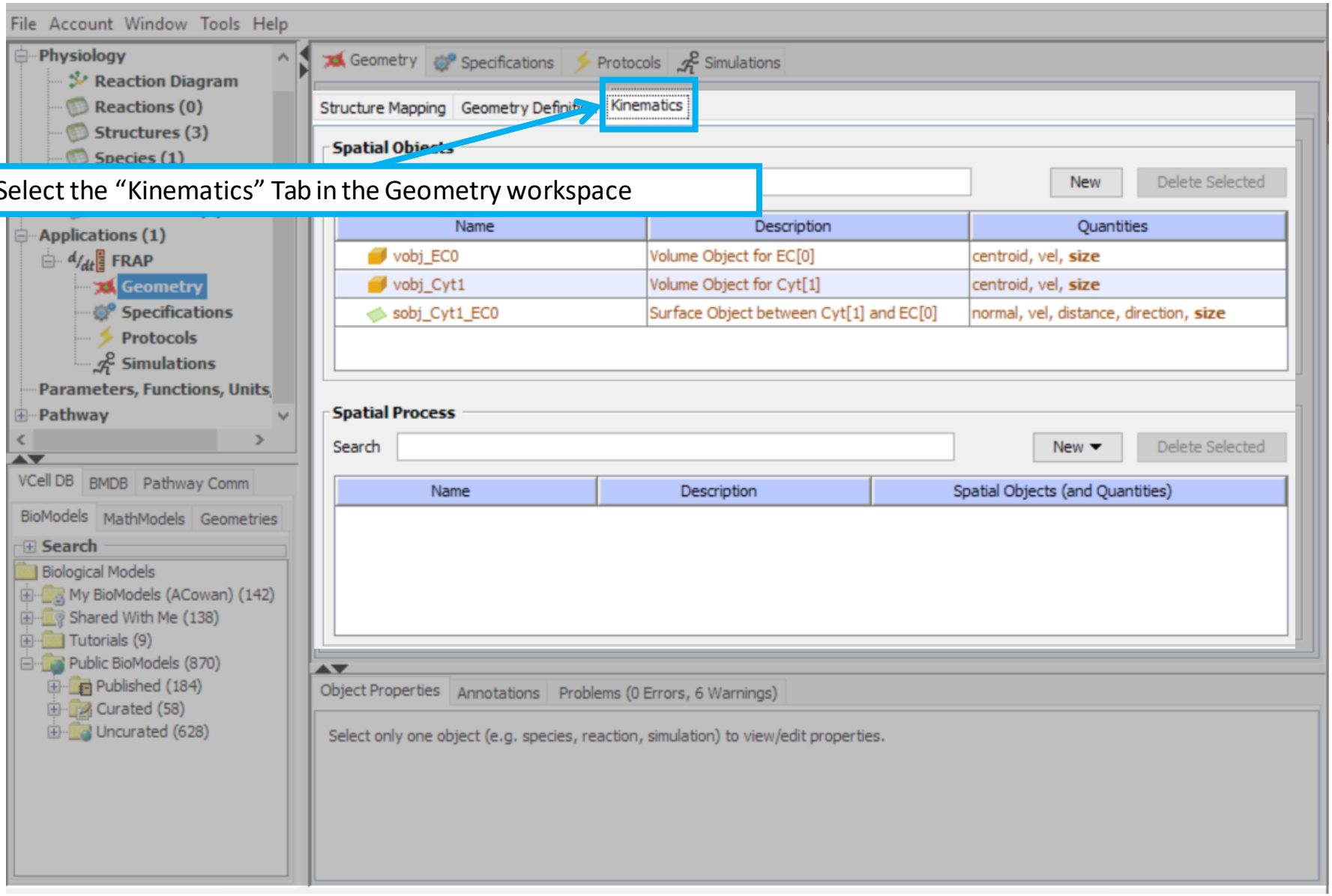
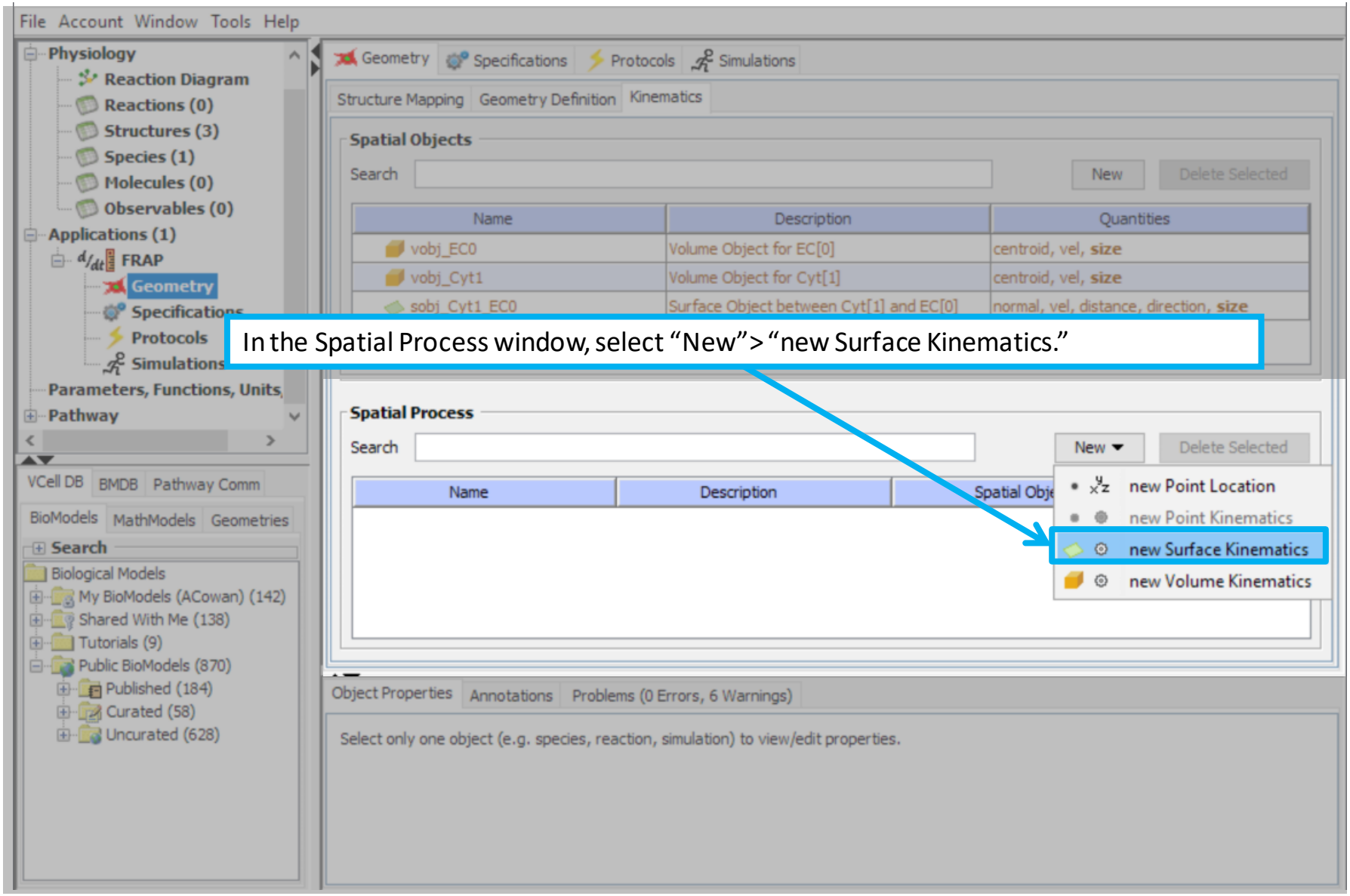


Select the “Kinematics” Tab in the Geometry workspace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Spatial Objects
Search
New
Delete Selected
Name
Description
Quantities
vobj_EC0
Volume Object for EC[0]
centroid, vel, size
vobj_Cyt1
Volume Object for Cyt[1]
centroid, vel, size
sobj_Cyt1_EC0
Surface Object between Cyt[1] and EC[0]
normal, vel, distance, direction, size
In the Spatial Process window, select "New"> "new Surface Kinematics."
Spatial Process
Search
New
Delete Selected
Name
Description
new Point Location
new Point Kinematics
new Surface Kinematics
new Volume Kinematics
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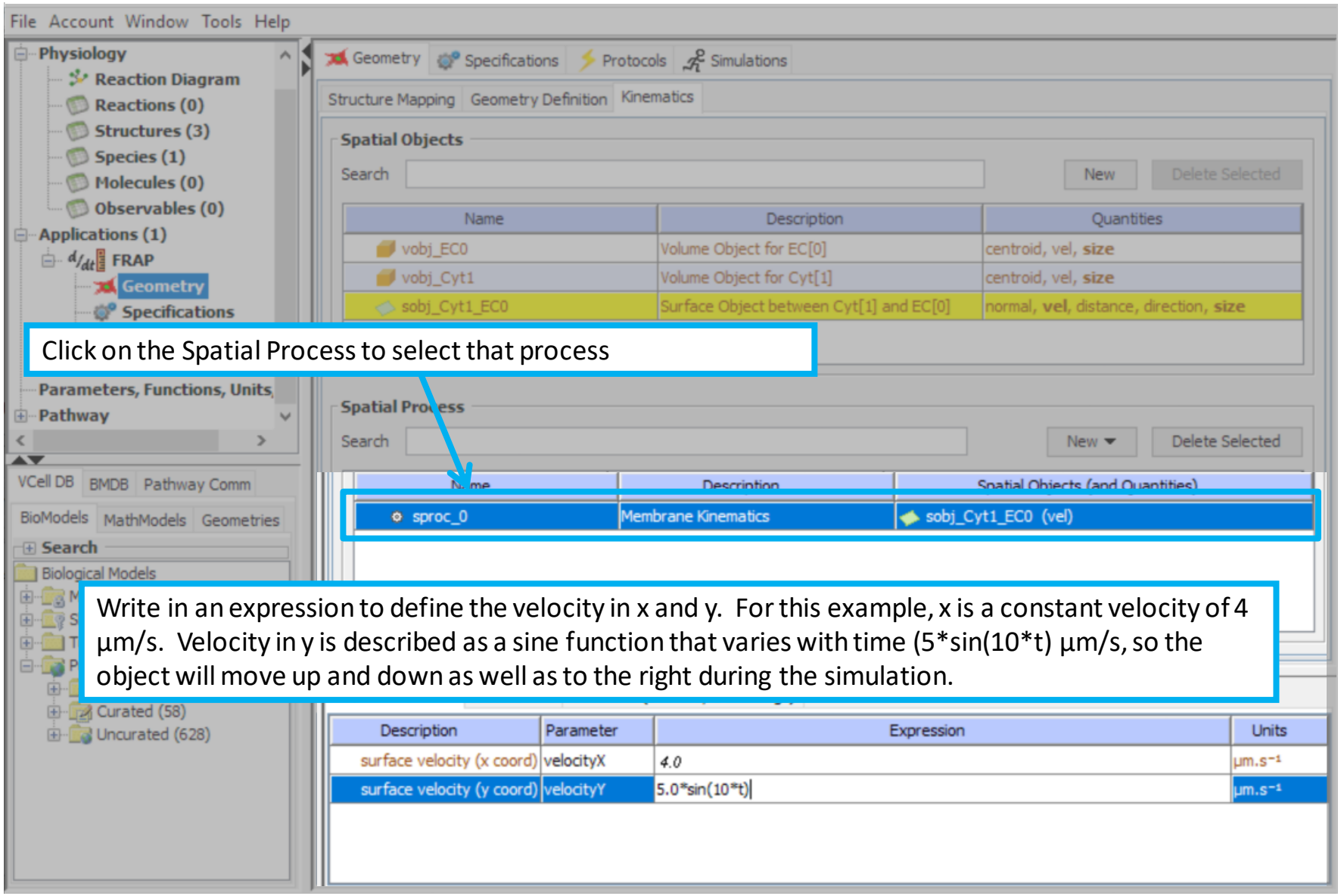
Annotations
Problems (0 Errors, 6 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.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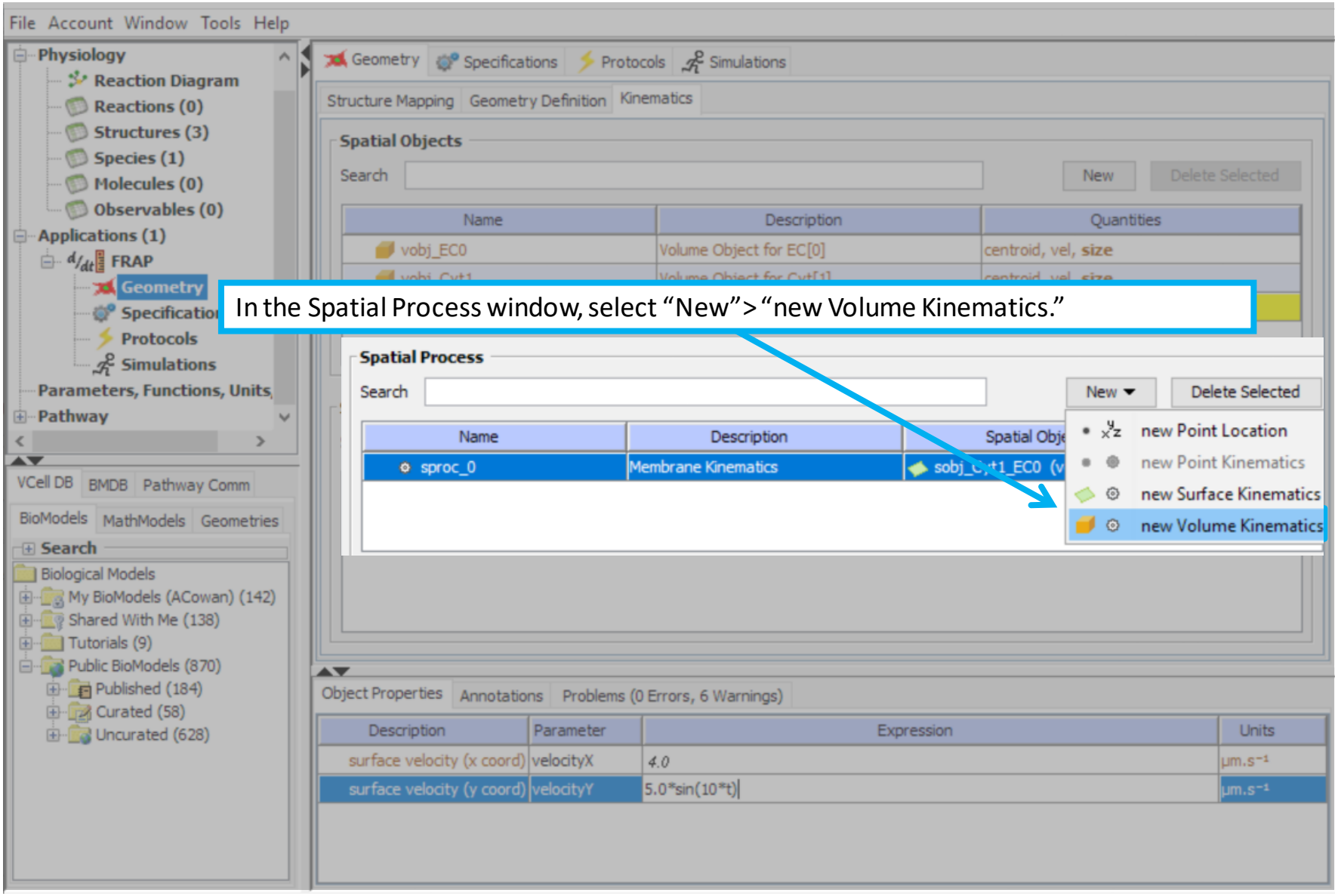
Spatial Objects
Search
New
Delete Selected
Name
Description
Quantities
vobj_EC0
Volume Object for EC[0]
centroid, vel, size
vobj_Cyt1
Volume Object for Cyt[1]
centroid, vel, size
sobj_Cyt1_EC0
Surface Object between Cyt[1] and EC[0]
normal, vel, distance, direction, size
Click on the Spatial Process to select that process
Spatial Process
Search
New
Delete Selected
Name
Description
Spatial Objects (and Quantities)
sproc_0
Membrane Kinematics
sobj_Cyt1_EC0 (vel)
Write in an expression to define the velocity in x and y. For this example, x is a constant velocity of 4 µm/s. Velocity in y is described as a sine function that varies with time (5*sin(10*t) µm/s, so the object will move up and down as well as to the right during the simulation.
Description
Parameter
Expression
Units
surface velocity (x coord)
velocityX
4.0
µm.s⁻¹
surface velocity (y coord)
velocityY
5.0*sin(10*t)
µm.s⁻¹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Spatial Objects
Search
New
Delete Selected
Name
Description
Quantities
vobj_EC0
Volume Object for EC[0]
centroid, vel, size
In the Spatial Process window, select "New" > "new Volume Kinematics."
Spatial Process
Search
New
Delete Selected
Name
Description
sproc_0
Membrane Kinematics
new Point Location
new Point Kinematics
new Surface Kinematics
new Volume Kinematics
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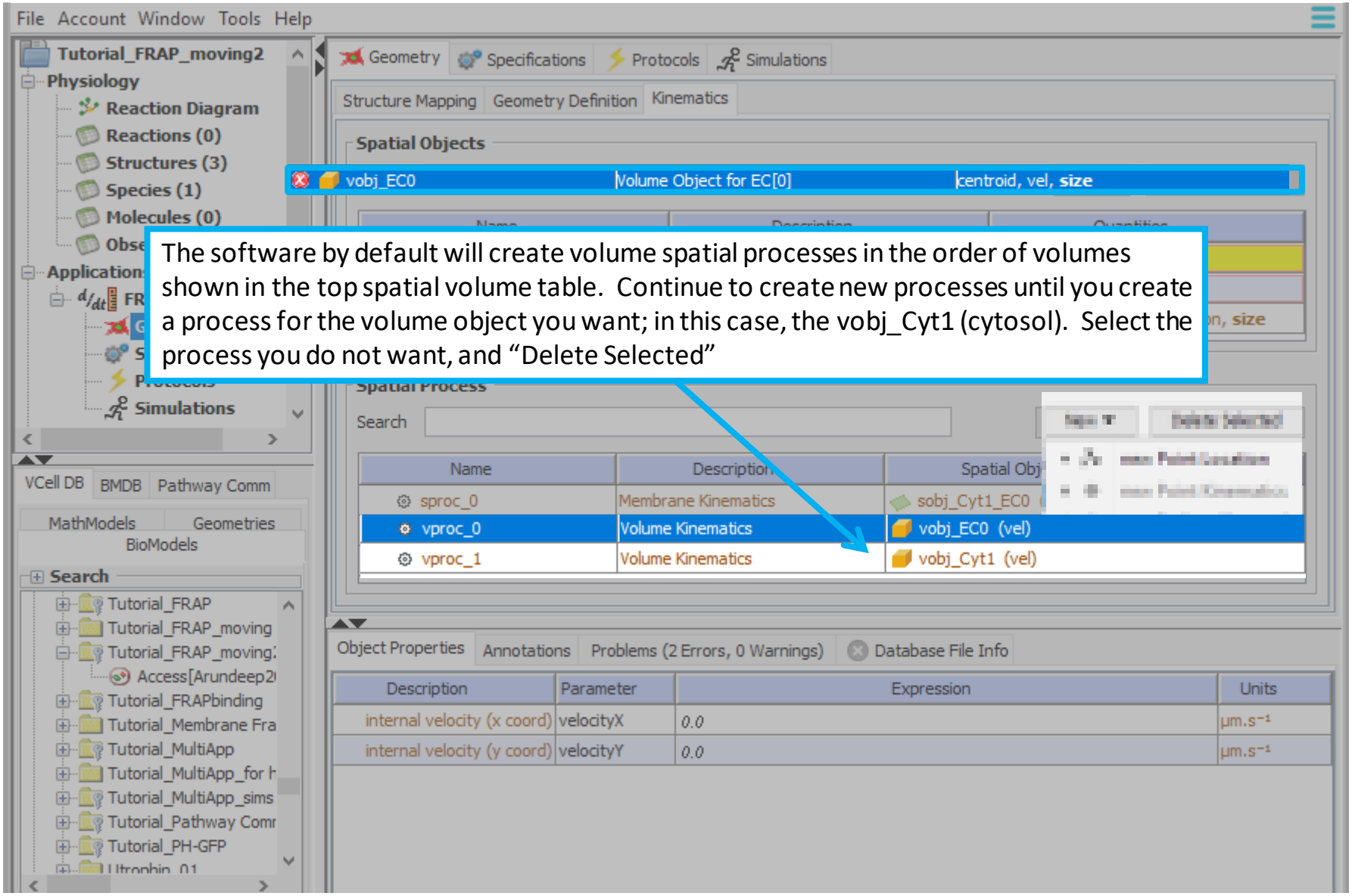
Annotations
Problems (0 Errors, 6 Warnings)
Description
Parameter
Expression
Units
surface velocity (x coord)
velocityX
4.0
μm.s⁻¹
surface velocity (y coord)
velocityY
5.0*sin(10*t)
μm.s⁻¹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Molecules (0)
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Geometry Definition
Kinematics
Spatial Objects
vobj_EC0
Volume Object for EC[0]
centroid, vel, size
The software by default will create volume spatial processes in the order of volumes shown in the top spatial volume table. Continue to create new processes until you create a process for the volume object you want; in this case, the vobj_Cyt1 (cytosol). Select the process you do not want, and "Delete Selected"
Search
Name
Description
Spatial Obj
sproc_0
Membrane Kinematics
sobj_Cyt1_EC0
vproc_0
Volume Kinematics
vobj_EC0 (vel)
vproc_1
Volume Kinematics
vobj_Cyt1 (vel)
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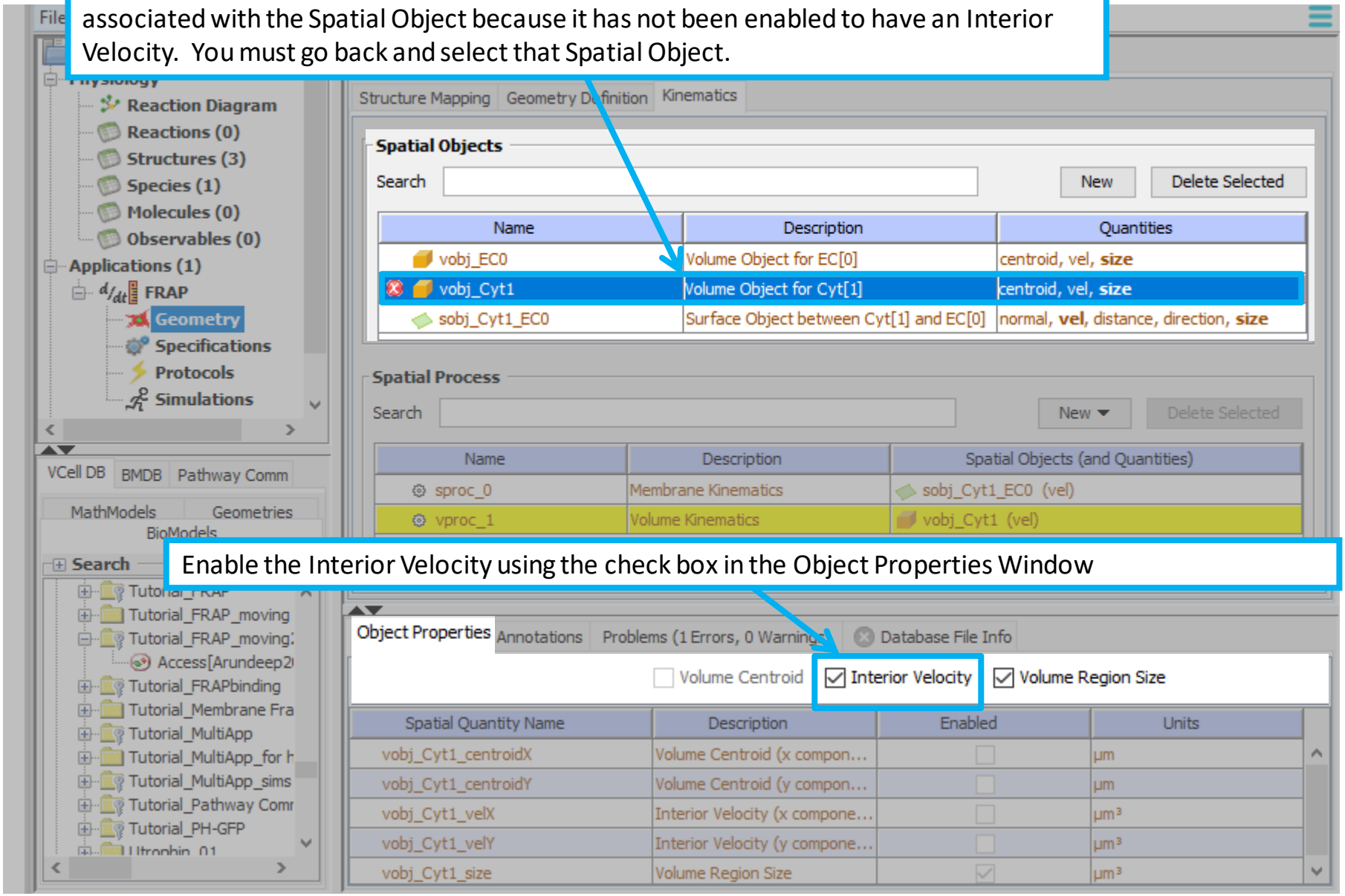
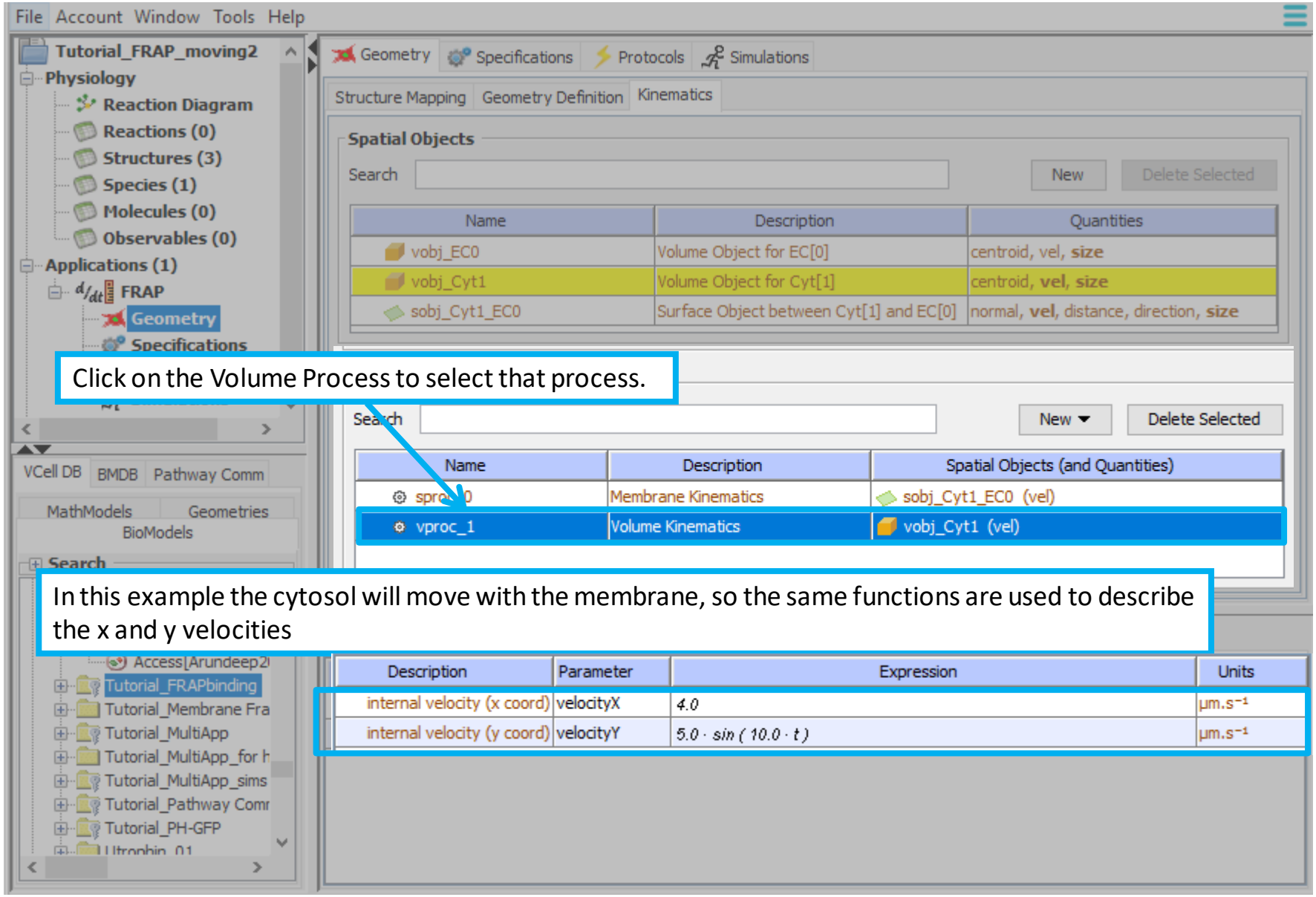
Tutorial_FRAPbinding
Tutorial_MultiApp
Tutorial_Pathway Comm
Tutorial_PH-GFP
Object Properties
Annotations
Problems (2 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
internal velocity (x coord)
velocityX
0.0
μm.s⁻¹
internal velocity (y coord)
velocityY
0.0
μm.s⁻¹

When a new Spatial Process for a volume object is created, an error is created associated with the Spatial Object because it has not been enabled to have an Interior Velocity. You must go back and select that Spatial Object.



Enable the Interior Velocity using the check box in the Object Properties Window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Spatial Objects
Search
New
Delete Selected
Name Description Quantities
vobj_EC0 Volume Object for EC[0] centroid, vel, size
vobj_Cyt1 Volume Object for Cyt[1] centroid, vel, size
sobj_Cyt1_EC0 Surface Object between Cyt[1] and EC[0] normal, vel, distance, direction, size
Click on the Volume Process to select that process.
Search
New
Delete Selected
Name Description Spatial Objects (and Quantities)
Membrane Kinematics sobj_Cyt1_EC0 (vel)
vproc_1 Volume Kinematics vobj_Cyt1 (vel)
In this example the cytosol will move with the membrane, so the same functions are used to describe the x and y velocities
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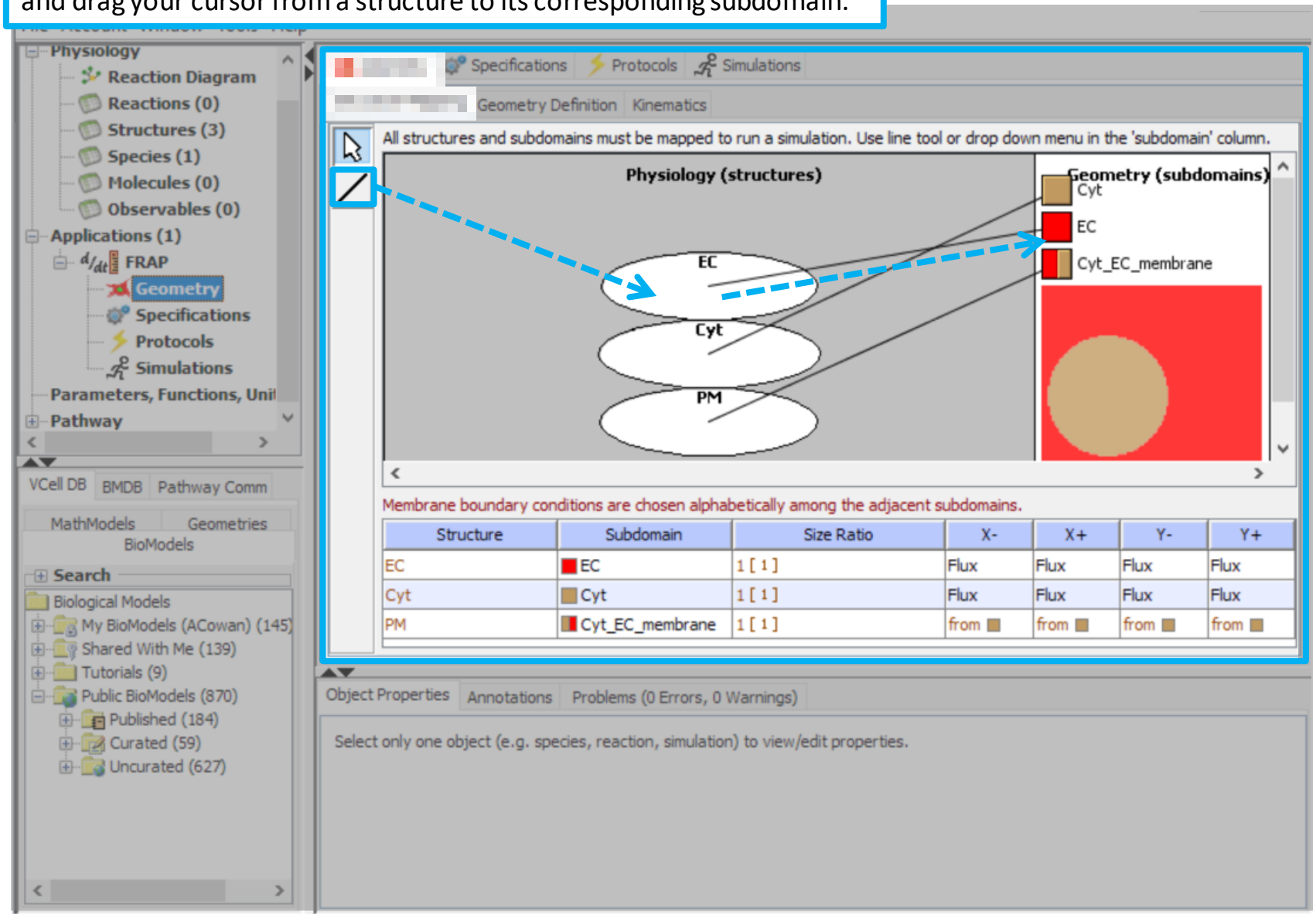
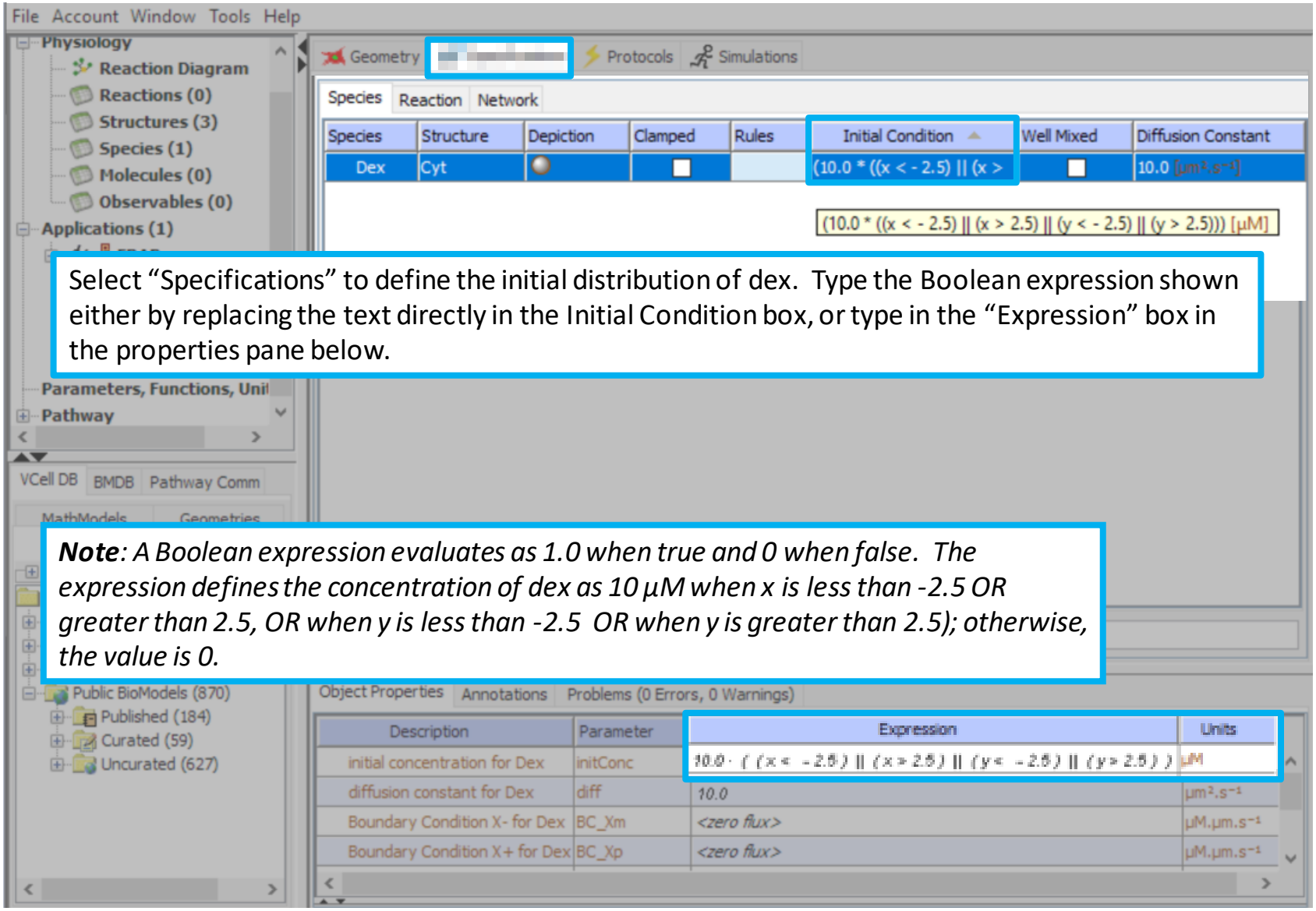
Tutorial_FRAPbinding
Tutorial_Membrane Fra
Tutorial_MultiApp
Tutorial_MultiApp_for h
Tutorial_MultiApp_sims
Tutorial_Pathway Comr
Tutorial_PH-GFP
Description Parameter Expression Units
internal velocity (x coord) velocityX 4.0 µm.s⁻¹
internal velocity (y coord) velocityY 5.0 · sin (10.0 · t) µm.s⁻¹

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

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Structure
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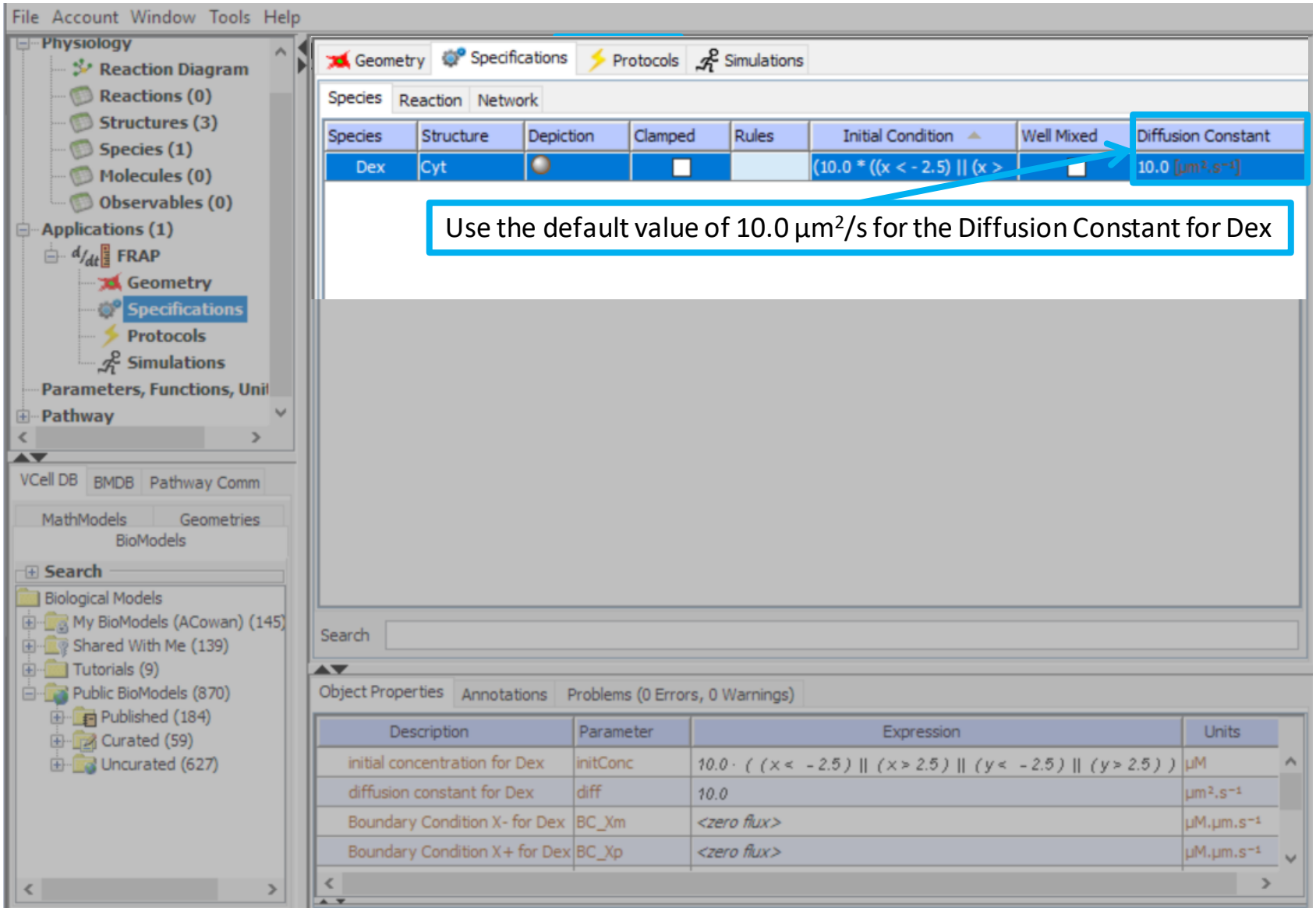
Initial Condition
Well Mixed
Diffusion Constant
Dex
Cyt
(10.0 * ((x < - 2.5) || (x >
10.0 [µm².s⁻¹]
(10.0 * ((x < - 2.5) || (x > 2.5) || (y < - 2.5) || (y > 2.5))) [µM]
Select “Specifications” to define the initial distribution of dex. Type the Boolean expression shown either by replacing the text directly in the Initial Condition box, or type in the “Expression” box in the properties pane below.
Note: A Boolean expression evaluates as 1.0 when true and 0 when false. The expression defines the concentration of dex as 10 µM when x is less than -2.5 OR greater than 2.5, OR when y is less than -2.5 OR when y is greater than 2.5); otherwise, the value is 0.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Description
Parameter
Expression
Units
initial concentration for Dex
initConc
10.0 · ((x < -2.5) || (x > 2.5) || (y < -2.5) || (y > 2.5))
µM
diffusion constant for Dex
diff
10.0
µm².s⁻¹
Boundary Condition X- for Dex
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for Dex
BC_Xp
<zero flux>
µM.µm.s⁻¹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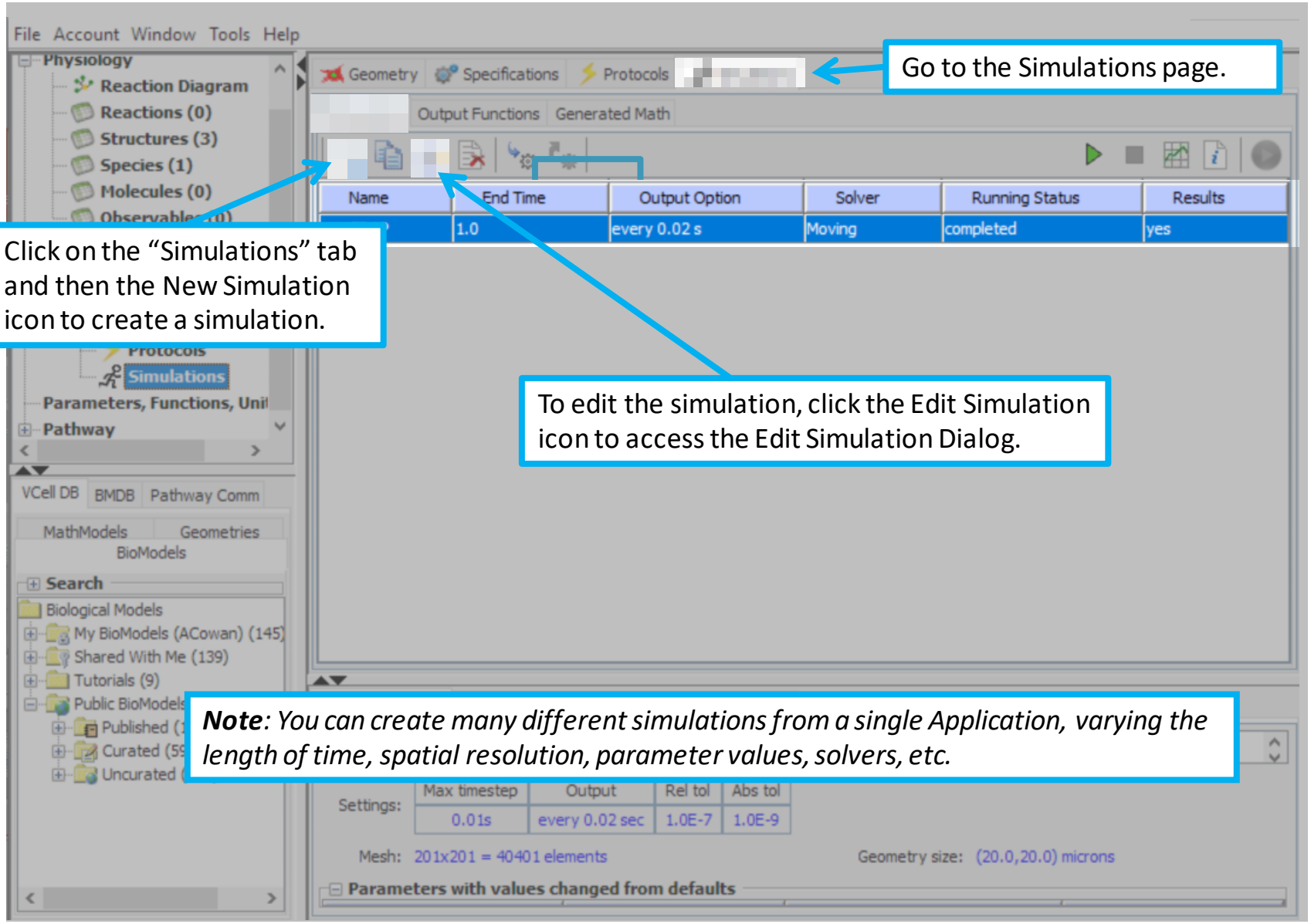
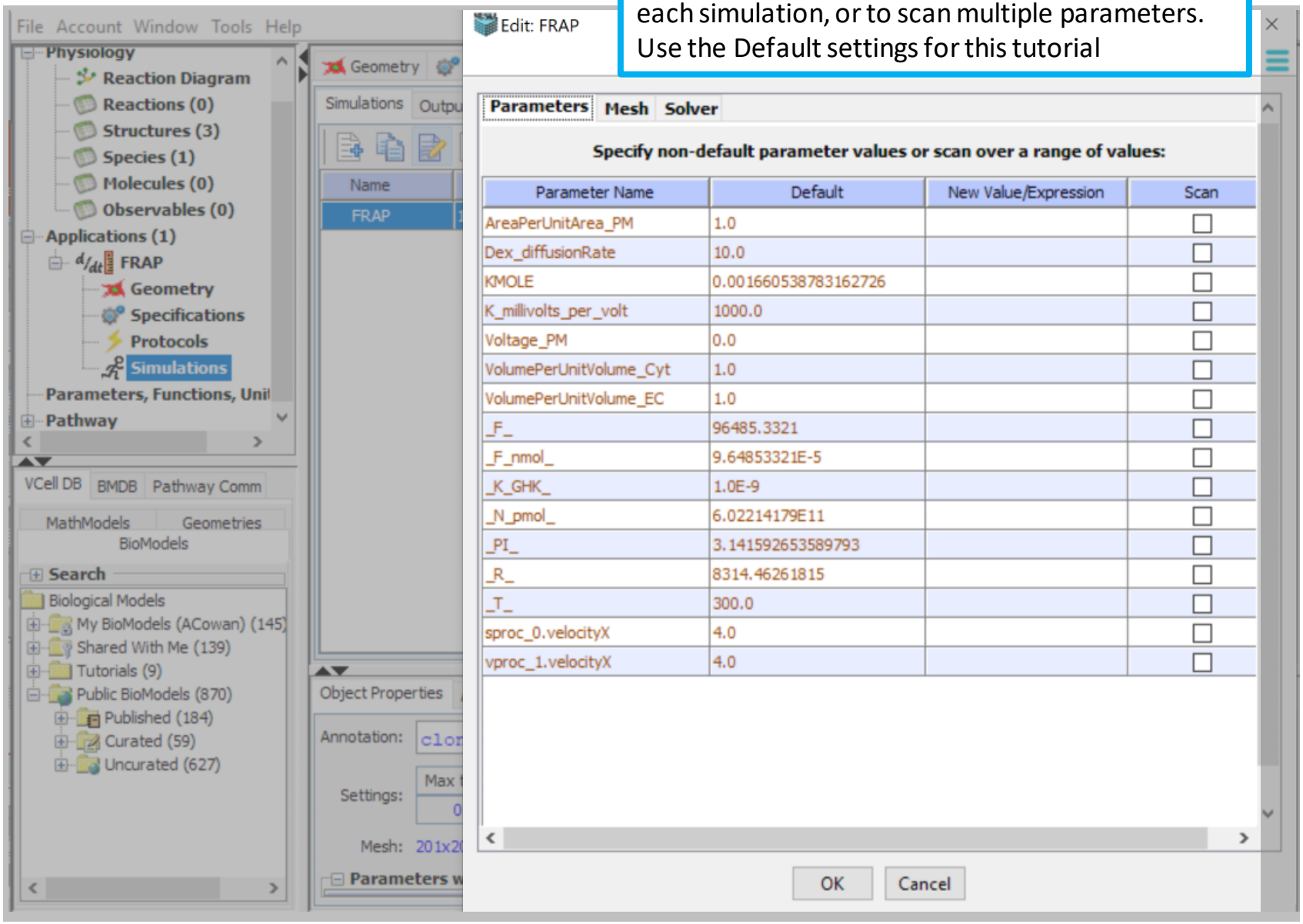
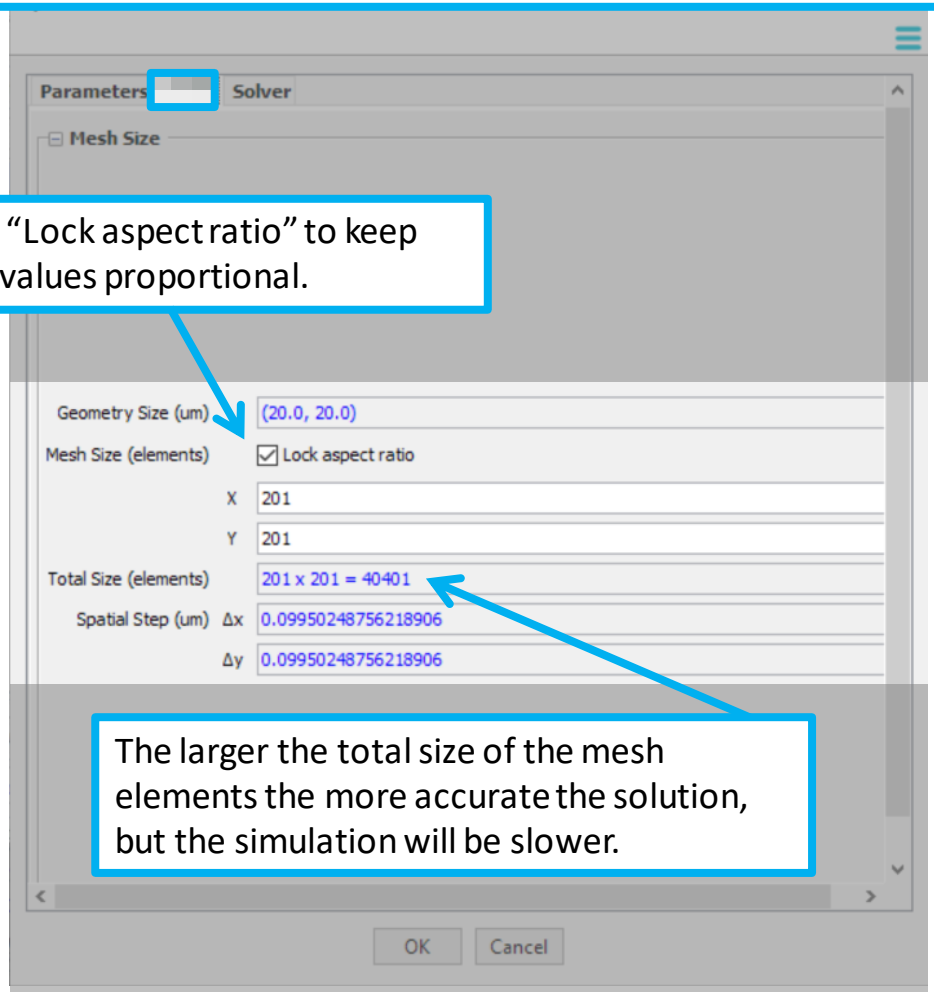
Well Mixed
Diffusion Constant
Dex
Cyt
(10.0 * ((x < - 2.5) || (x >
10.0 [µm².s⁻¹]
Use the default value of 10.0 µm²/s for the Diffusion Constant for Dex
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Description
Parameter
Expression
Units
initial concentration for Dex
initConc
10.0 · ((x < - 2.5) || (x > 2.5) || (y < - 2.5) || (y > 2.5))
µM
diffusion constant for Dex
diff
10.0
µm².s⁻¹
Boundary Condition X- for Dex
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for Dex
BC_Xp
<zero flux>
µM.µm.s⁻¹


Go to the Simulations page.
Click on the "Simulations" tab and then the New Simulation icon to create a simulation.
To edit the simulation, click the Edit Simulation icon to access the Edit Simulation Dialog.
***Note**: You can create many different simulations from a single Application, varying the length of time, spatial resolution, parameter values, solvers, etc.*

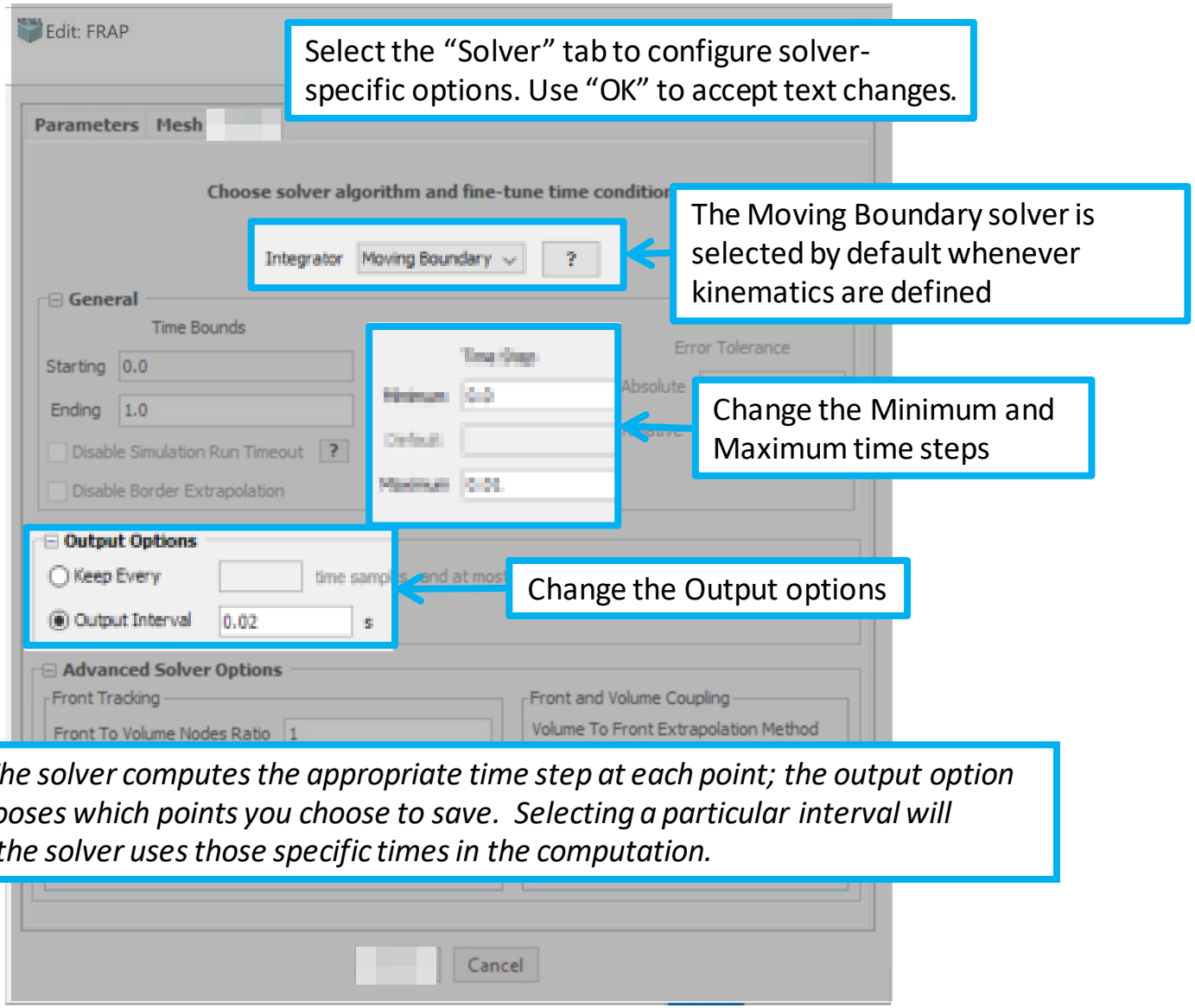
The Edit Simulation Dialog has 3 tabs. The Parameters Tab is used to adjust parameters for each simulation, or to scan multiple parameters. Use the Default settings for this tutorial



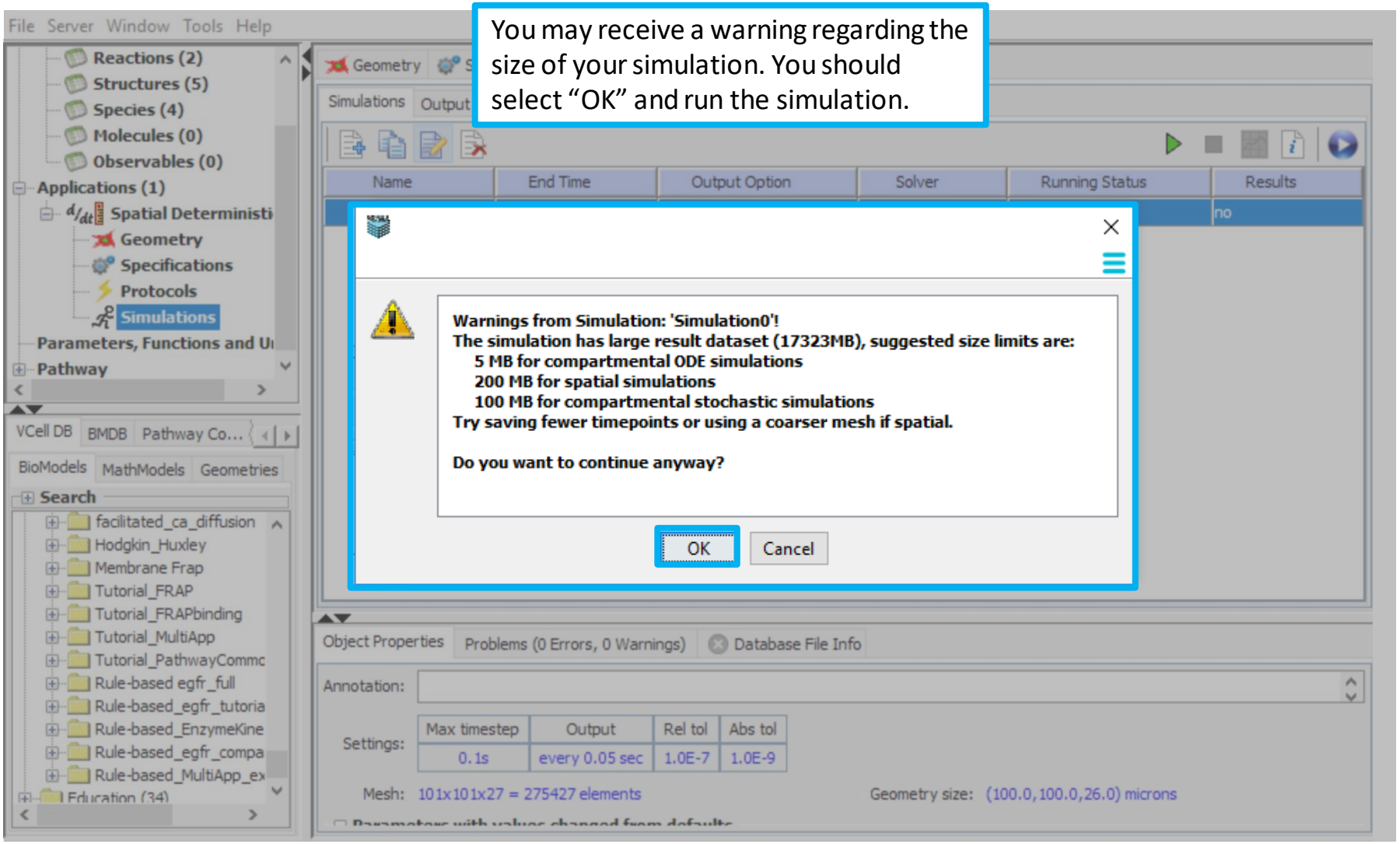
Select the “Mesh” tab to edit the mesh resolution for the simulation in the X and Y planes. Select “OK” to accept any changes.

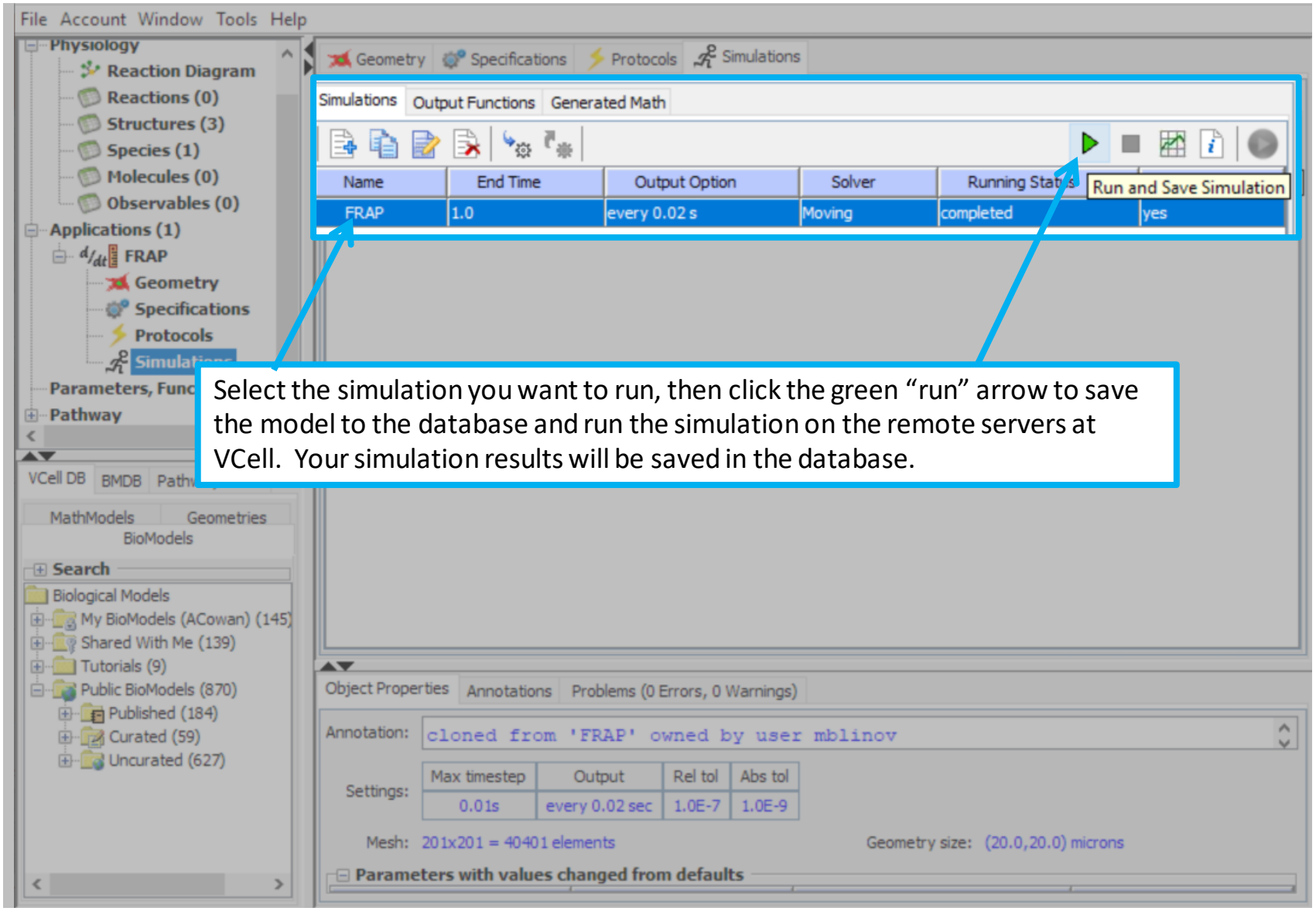


***Note**: Use the smaller mesh size values shown here for the tutorial, or the simulation will take a long time to run.*



***Note**: The solver computes the appropriate time step at each point; the output option only chooses which points you choose to save. Selecting a particular interval will ensure the solver uses those specific times in the computation.*


You may receive a warning regarding the size of your simulation. You should select "OK" and run the simulation.
Warnings from Simulation: 'Simulation0'!
The simulation has large result dataset (17323MB), suggested size limits are:
5 MB for compartmental ODE simulations
200 MB for spatial simulations
100 MB for compartmental stochastic simulations
Try saving fewer timepoints or using a coarser mesh if spatial.
Do you want to continue anyway?
OK
Cancel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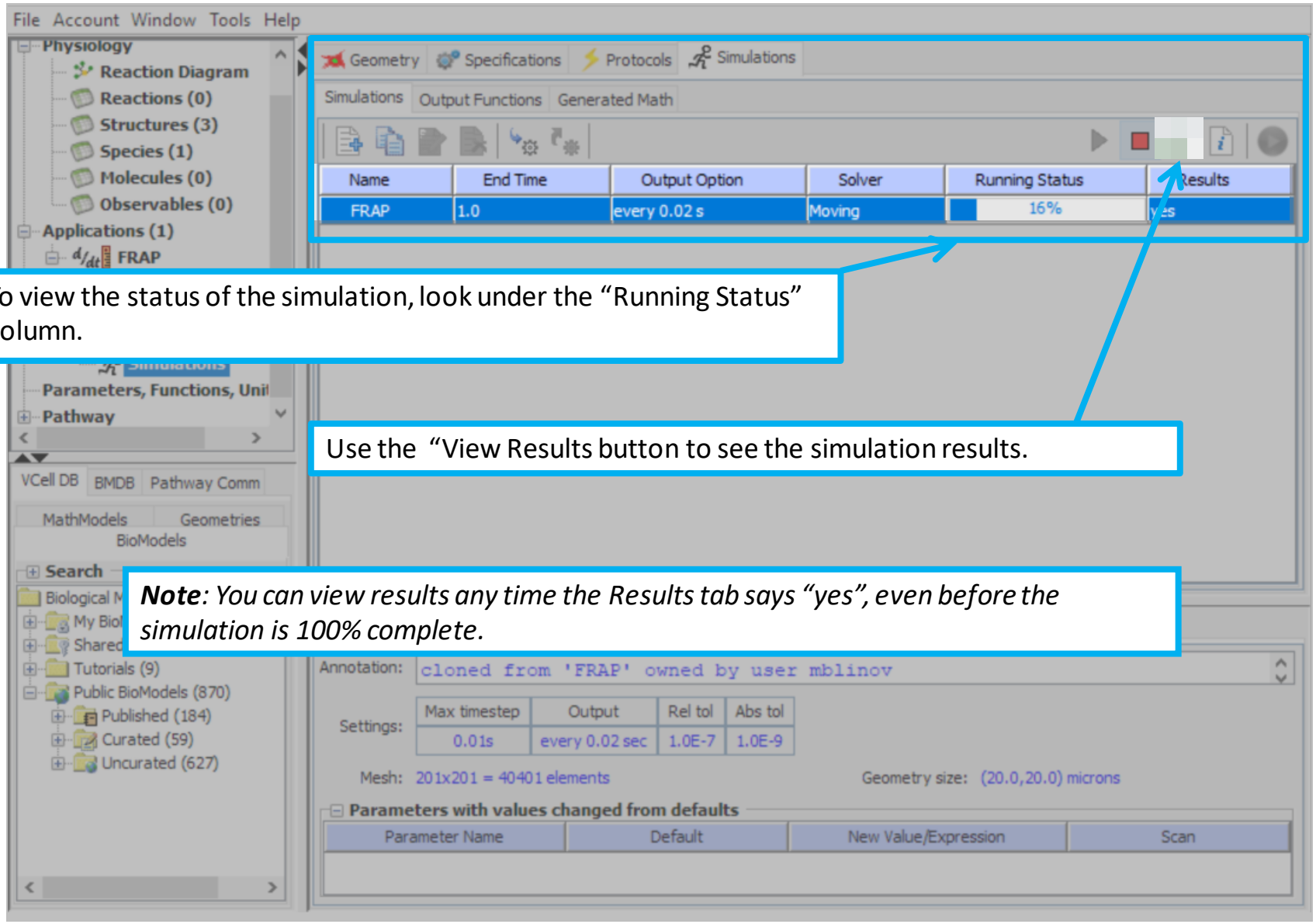
Pathway
Geometry Specifications Protocols Simulations
Simulations Output Functions Generated Math
Name End Time Output Option Solver Running Status
FRAP 1.0 every 0.02 s Moving completed yes
Run and Save Simulation
Select the simulation you want to run, then click the green "run" arrow to save the model to the database and run the simulation on the remote servers at VCell. Your simulation results will be saved in the database.
VCell DB BMDB
MathModels Geometries BioModels
Search
Biological Models
My BioModels (ACowan) (145)
Shared With Me (139)
Tutorials (9)
Public BioModels (870)
Published (184)
Curated (59)
Uncurated (627)
Object Properties Annotations Problems (0 Errors, 0 Warnings)
Annotation: cloned from 'FRAP' owned by user mblinov
Settings:
Max timestep Output Rel tol Abs tol
0.01s every 0.02 sec 1.0E-7 1.0E-9
Mesh: 201x201 = 40401 elements
Geometry size: (20.0,20.0) microns
Parameters with values changed from defaults


File Account Window Tools Help
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (1)
FRAP
Parameters, Functions, Unit
Pathway
VCell DB
BMDB
Pathway Comm
MathModels
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Search
Biological M
My Bio
Shared
Tutorials (9)
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Published (184)
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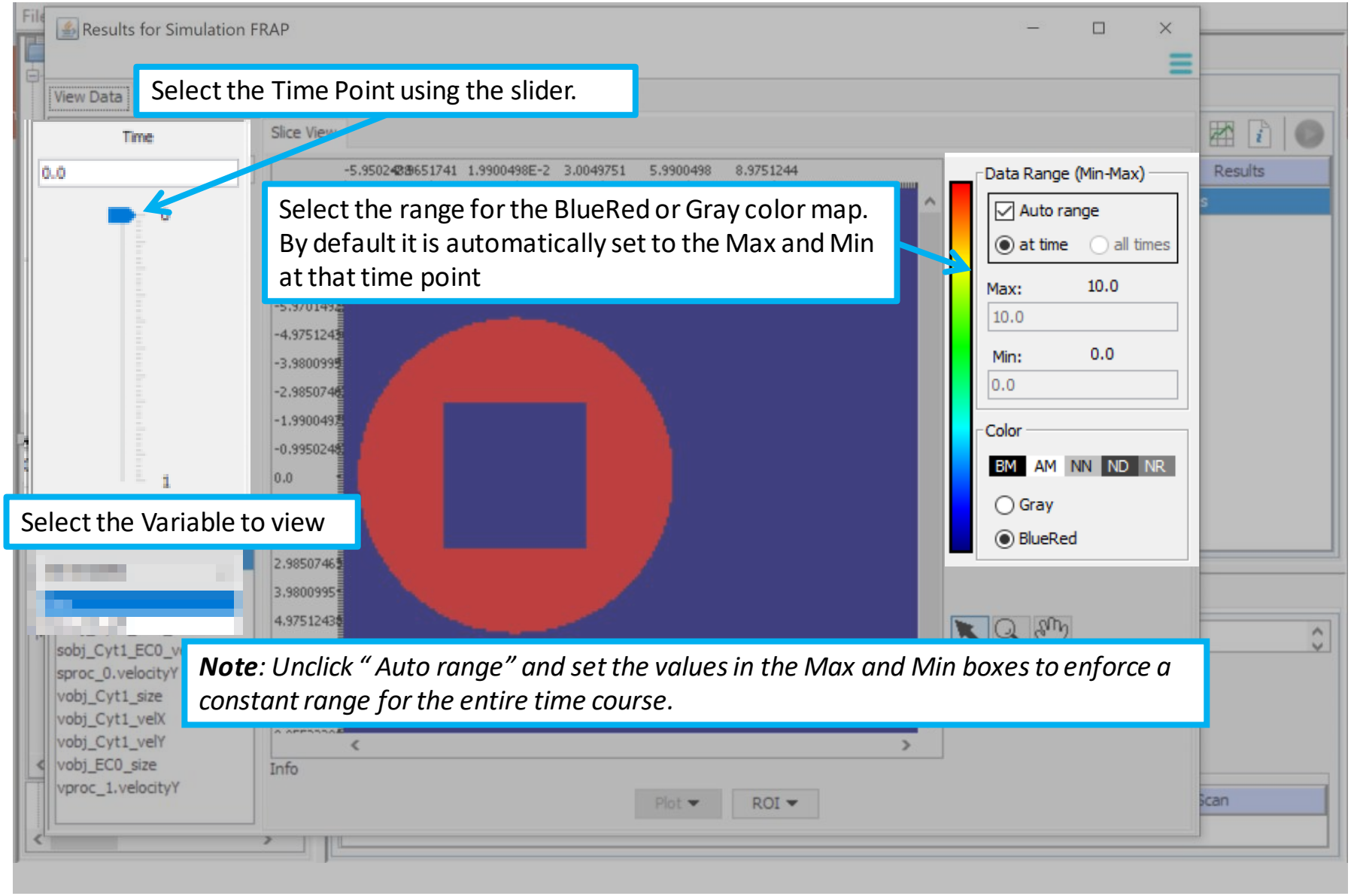
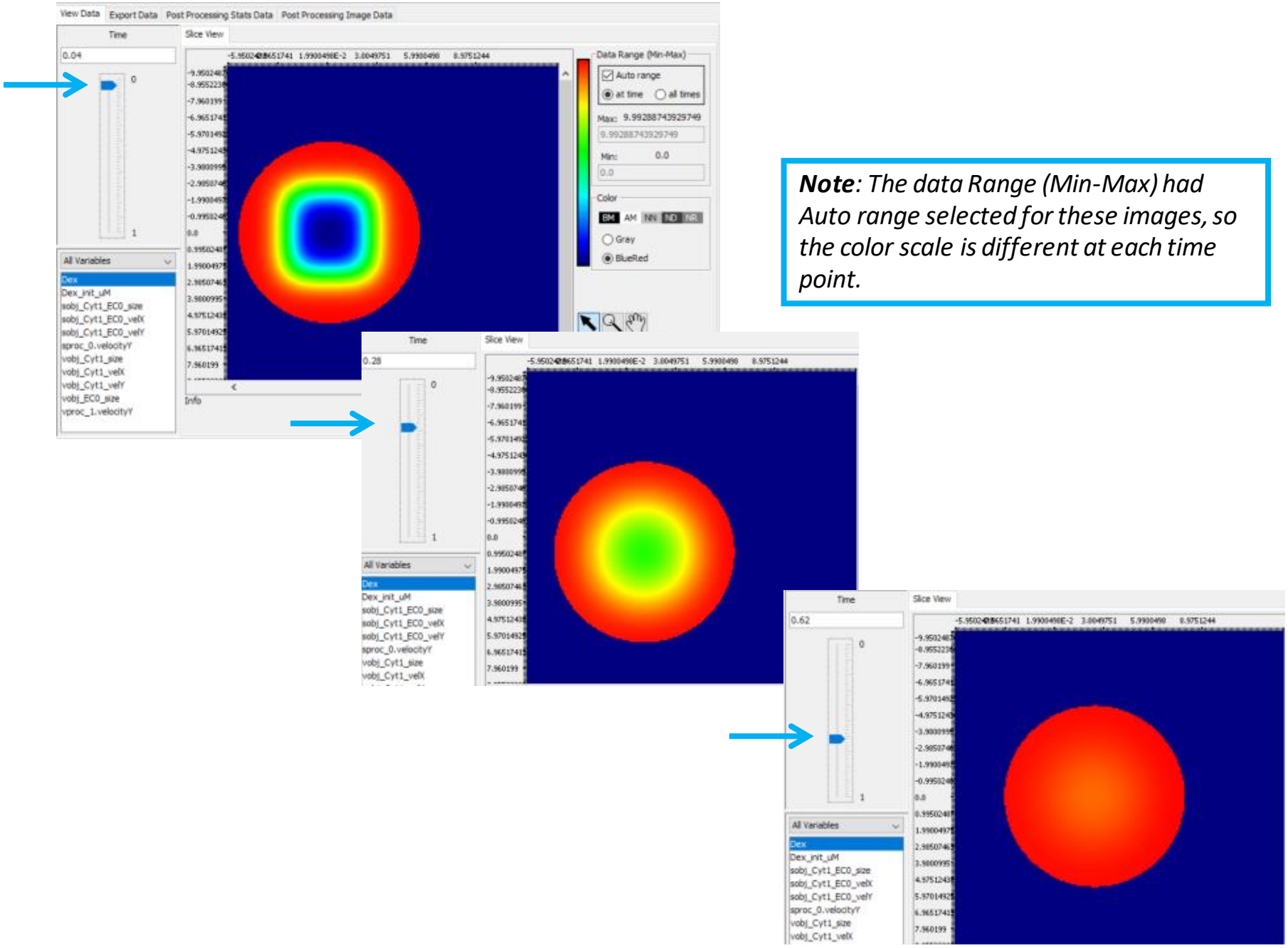
Uncurated (627)
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
FRAP
1.0
every 0.02 s
Moving
16%
yes
To view the status of the simulation, look under the "Running Status" column.
Use the "View Results button to see the simulation results.
Note: You can view results any time the Results tab says "yes", even before the simulation is 100% complete.
Annotation:
cloned from 'FRAP' owned by user mblinov
Settings:
Max timestep
Output
Rel tol
Abs tol
0.01s
every 0.02 sec
1.0E-7
1.0E-9
Mesh: 201x201 = 40401 elements
Geometry size: (20.0,20.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan

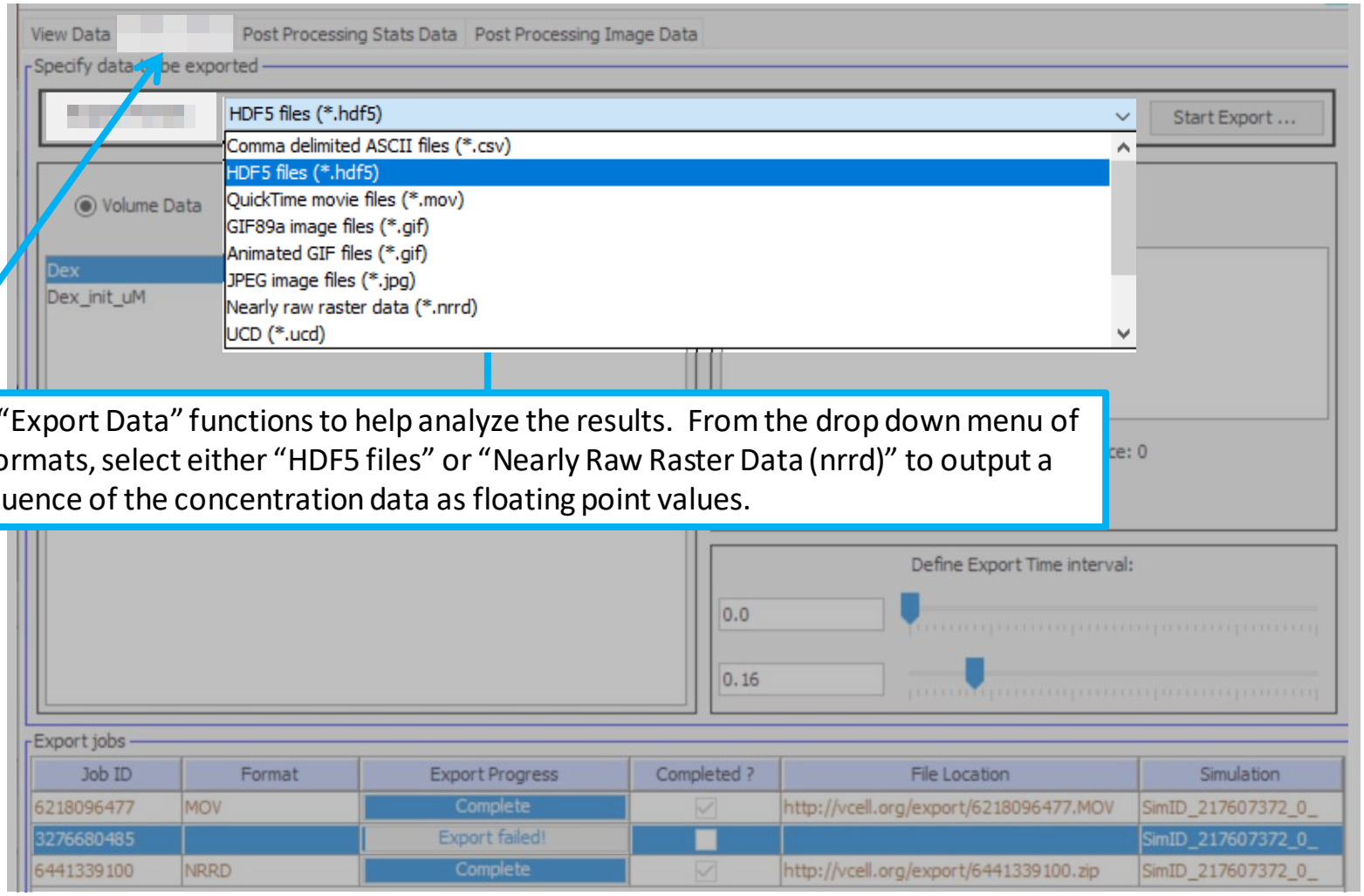


***Note**: Unclick " Auto range" and set the values in the Max and Min boxes to enforce a constant range for the entire time course.*

Contents

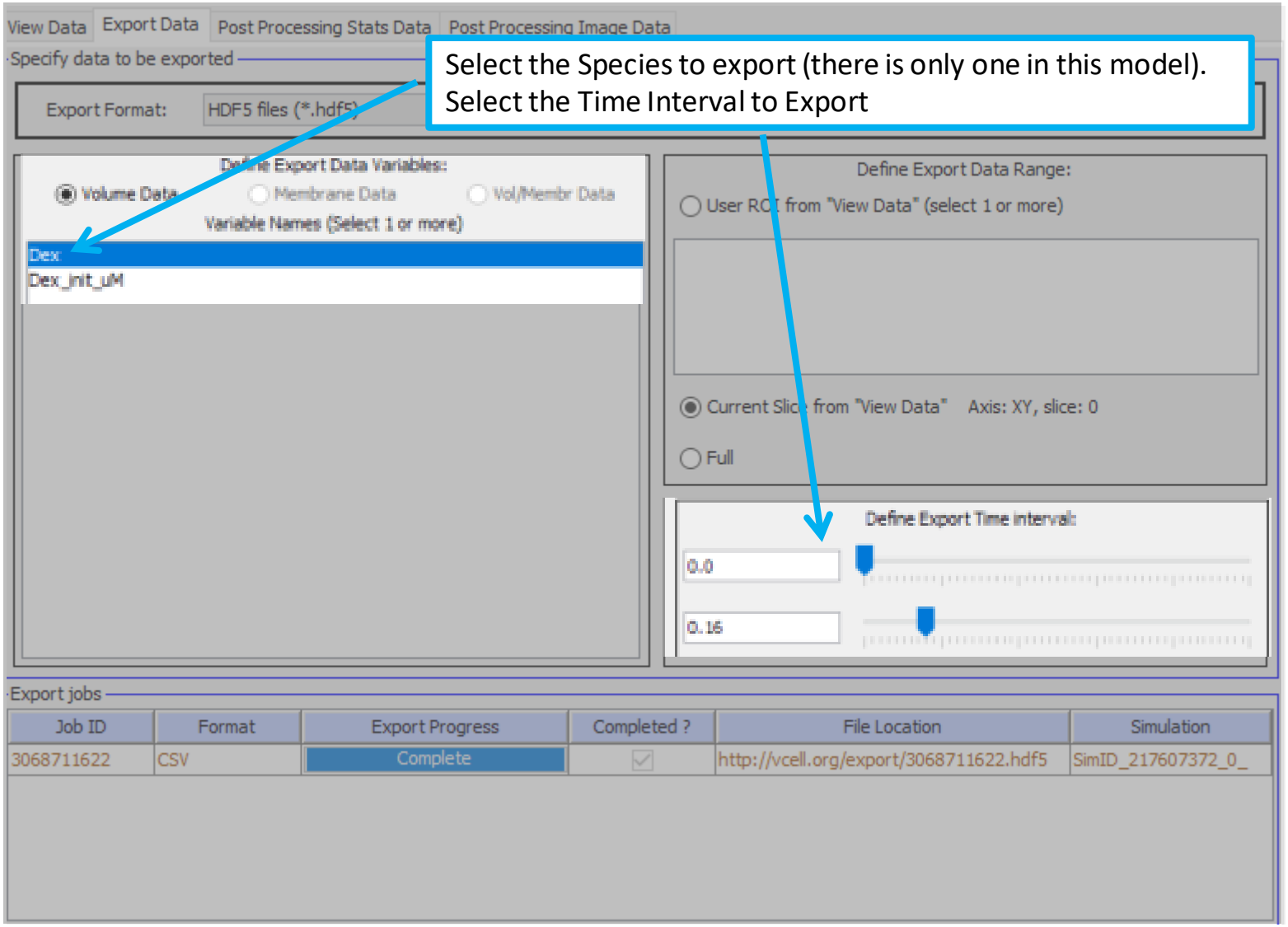


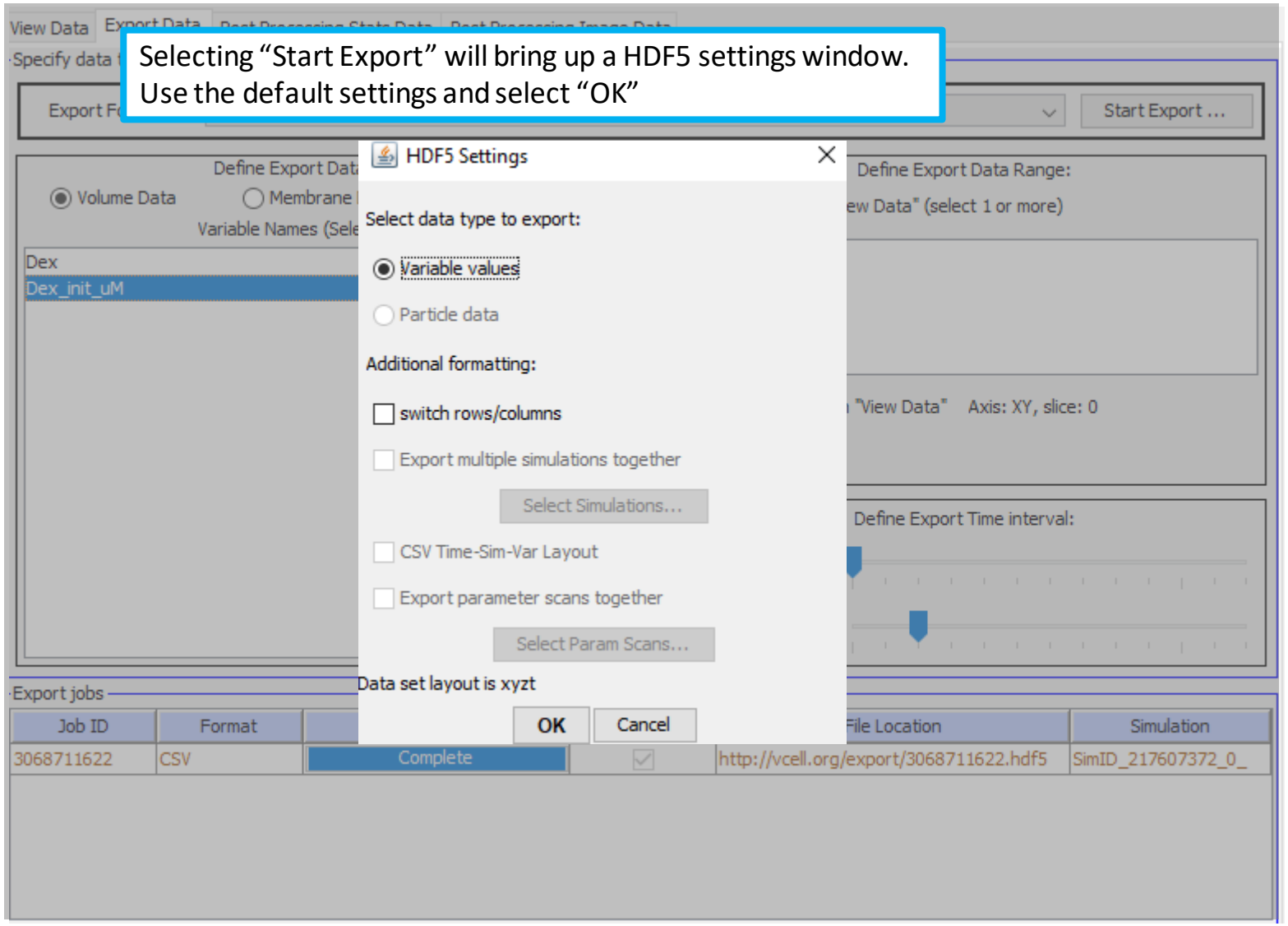
***Note**: The data Range (Min-Max) had Auto range selected for these images, so the color scale is different at each time point.*



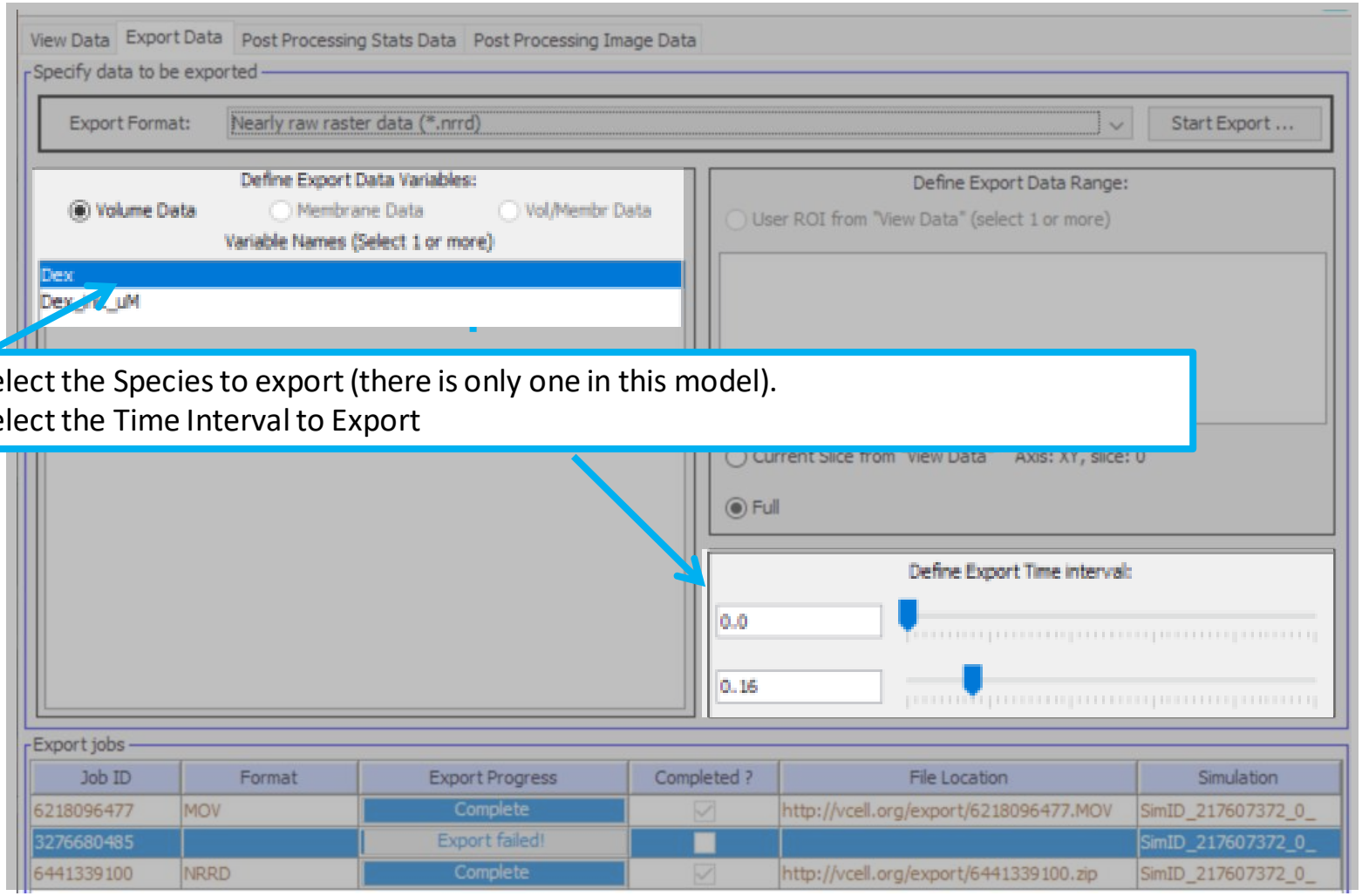
Use the “Export Data” functions to help analyze the results. From the drop down menu of export formats, select either “HDF5 files” or “Nearly Raw Raster Data (nrrd)” to output a time sequence of the concentration data as floating point values.

To export as HDF5 files:

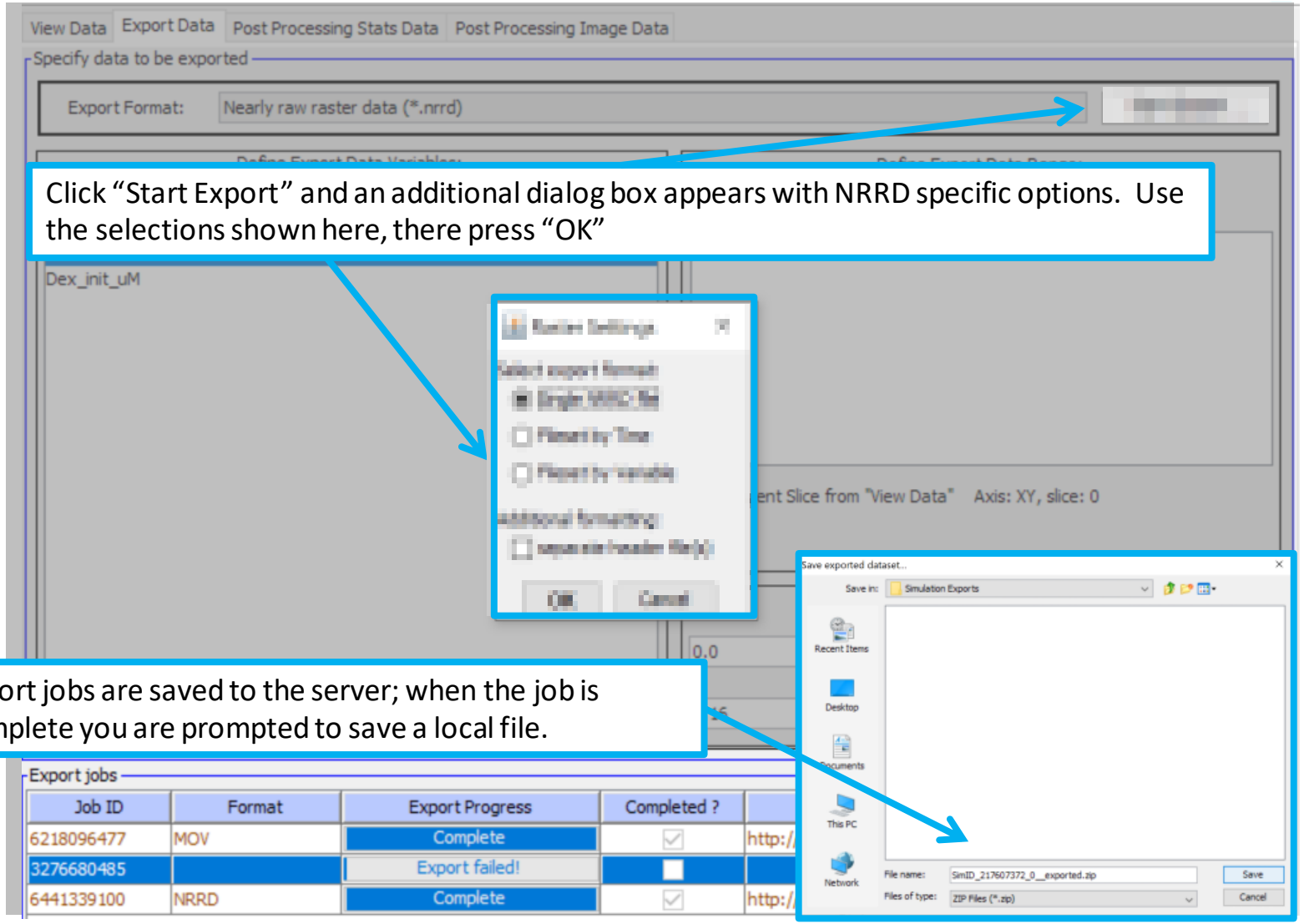



Selecting “Start Export” will bring up a HDF5 settings window.
Use the default settings and select “OK”
View Data
Export Data
Specify data
Export F
Start Export ...
Define Export Data Range:
Volume Data
Membrane
Variable Names (Sele
ew Data" (select 1 or more)
Dex
Dex_init_uM
"View Data" Axis: XY, slice: 0
Define Export Time interval:
HDF5 Settings
Select data type to export:
Variable values
Particle data
Additional formatting:
switch rows/columns
Export multiple simulations together
Select Simulations...
CSV Time-Sim-Var Layout
Export parameter scans together
Select Param Scans...
Data set layout is xyzt
OK
Cancel
Export jobs
Job ID
Format
File Location
Simulation
3068711622
CSV
Complete
http://vcell.org/export/3068711622.hdf5
SimID_217607372_0_

To export as HDF5 files:



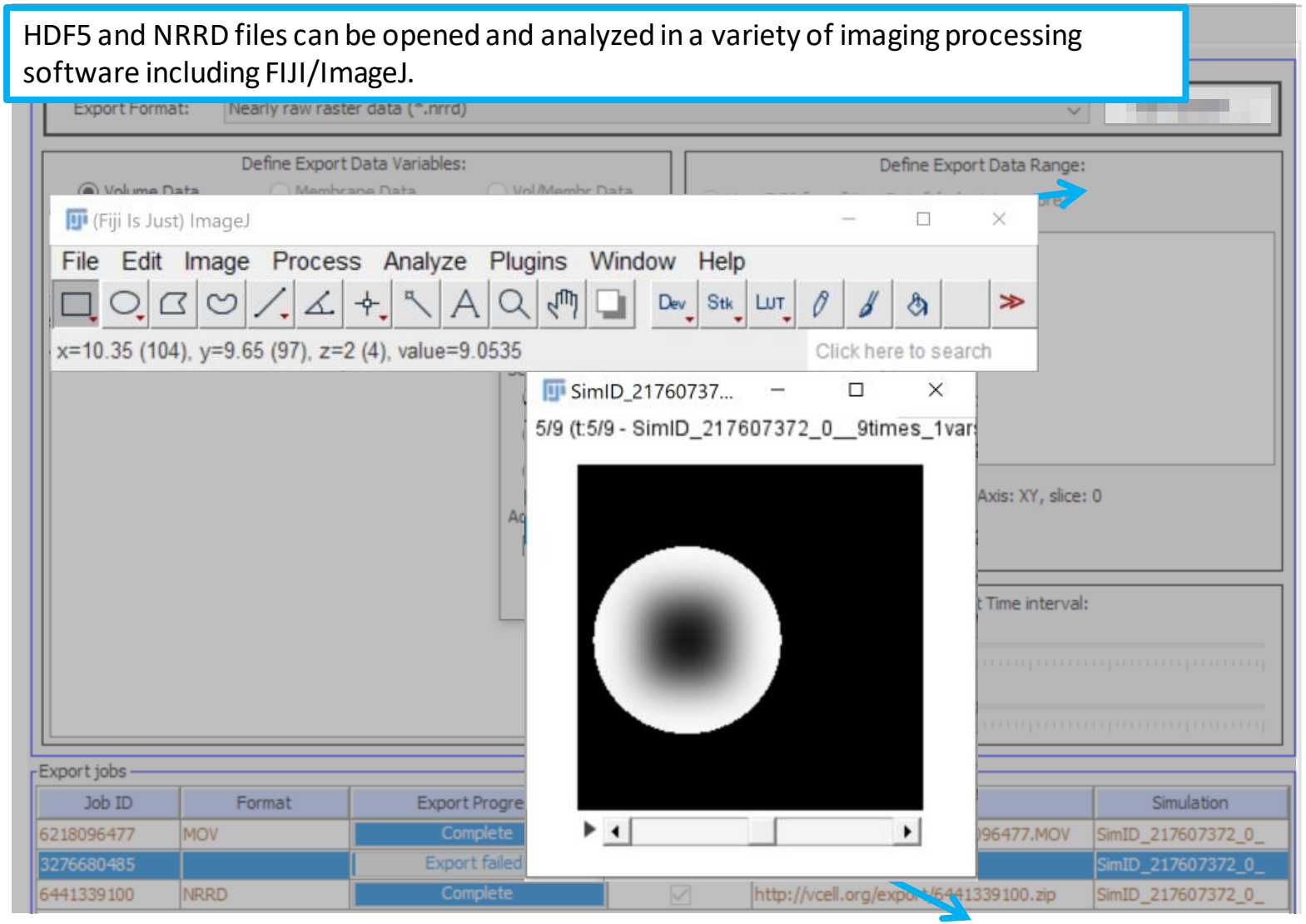
Select the Species to export (there is only one in this model).
Select the Time Interval to Export



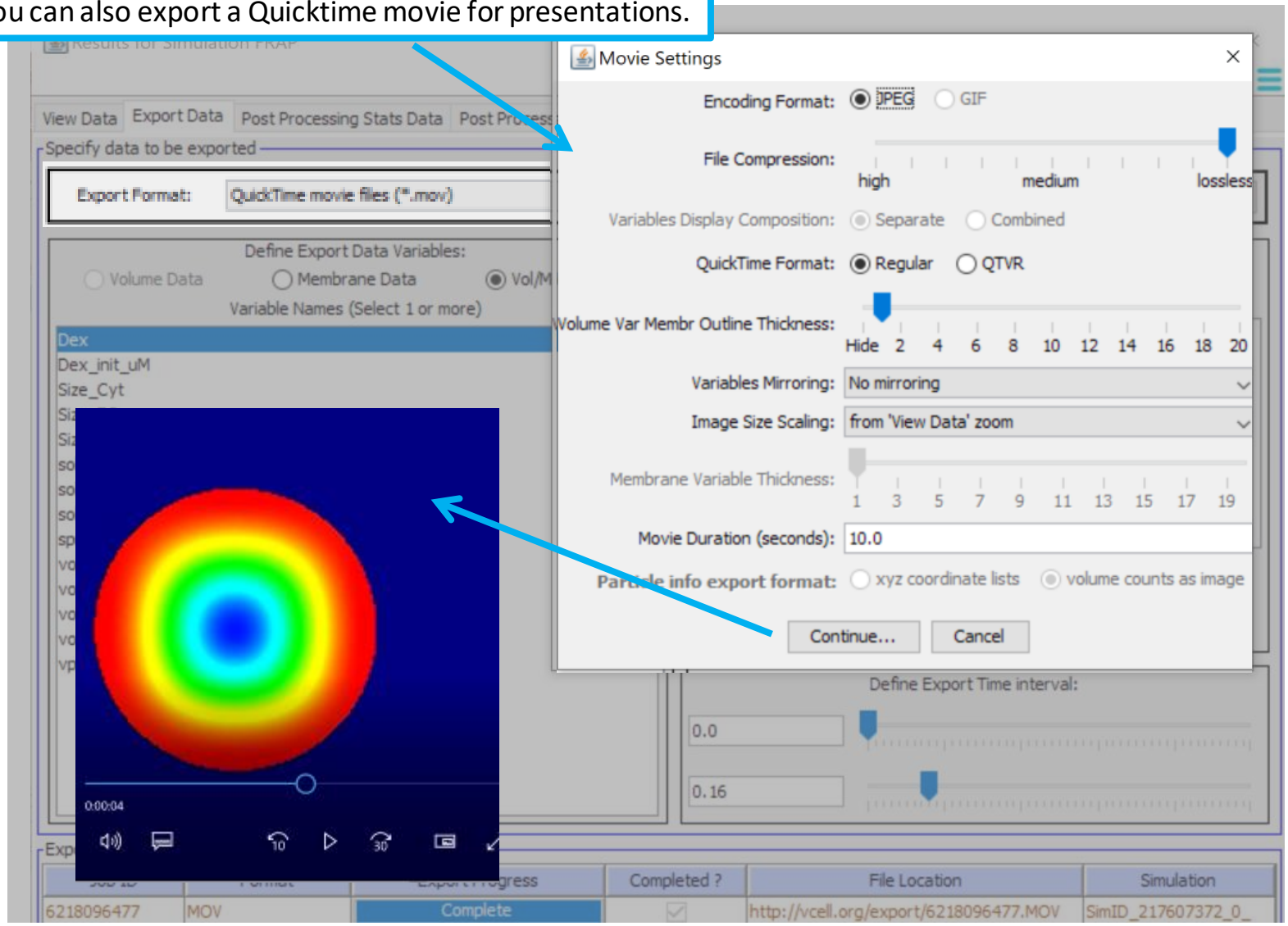
Click “Start Export” and an additional dialog box appears with NRRD specific options. Use the selections shown here, there press “OK”

Export jobs are saved to the server; when the job is complete you are prompted to save a local file.

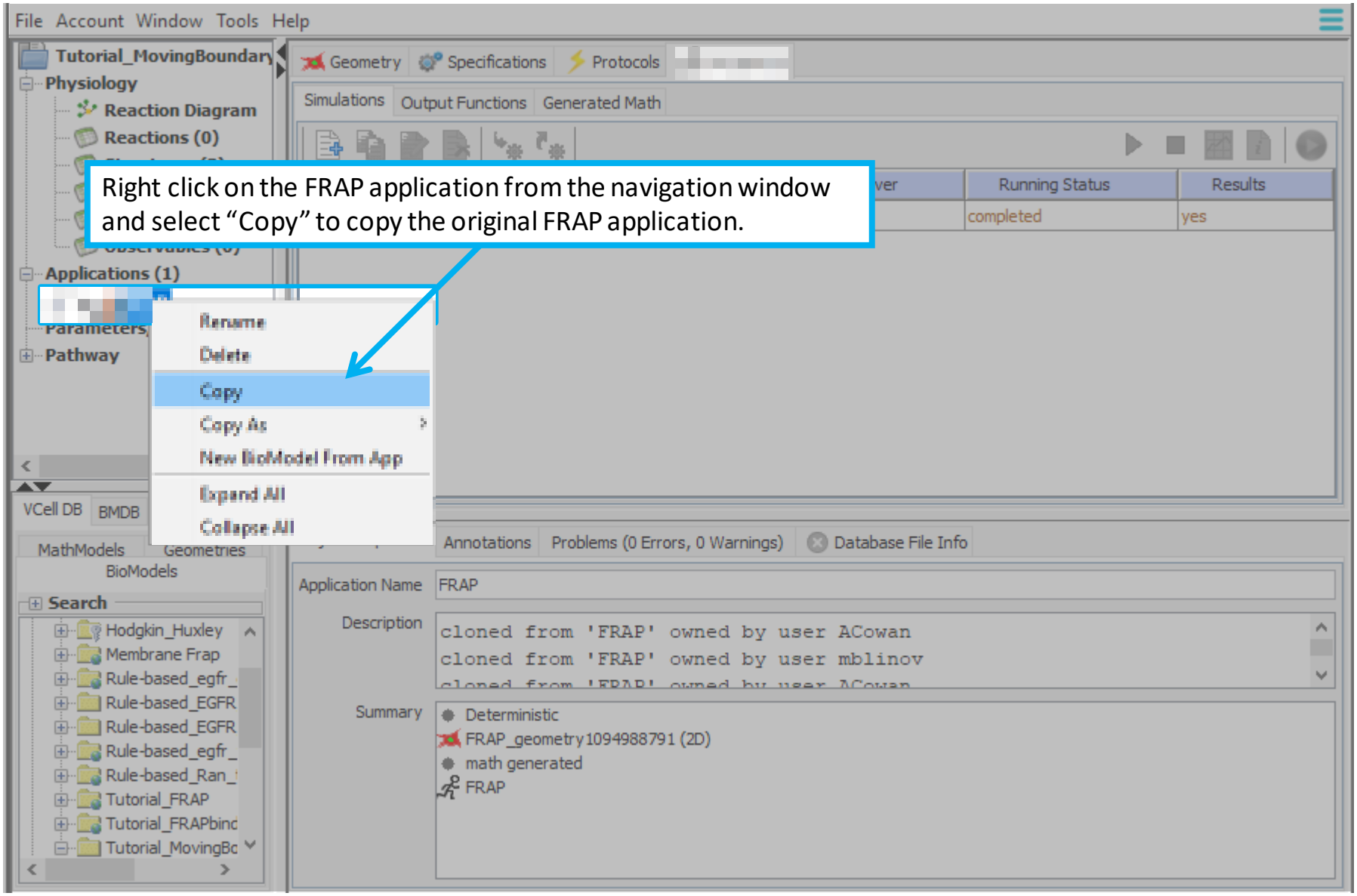
HDF5 and NRRD files can be opened and analyzed in a variety of imaging processing software including FIJI/ImageJ.

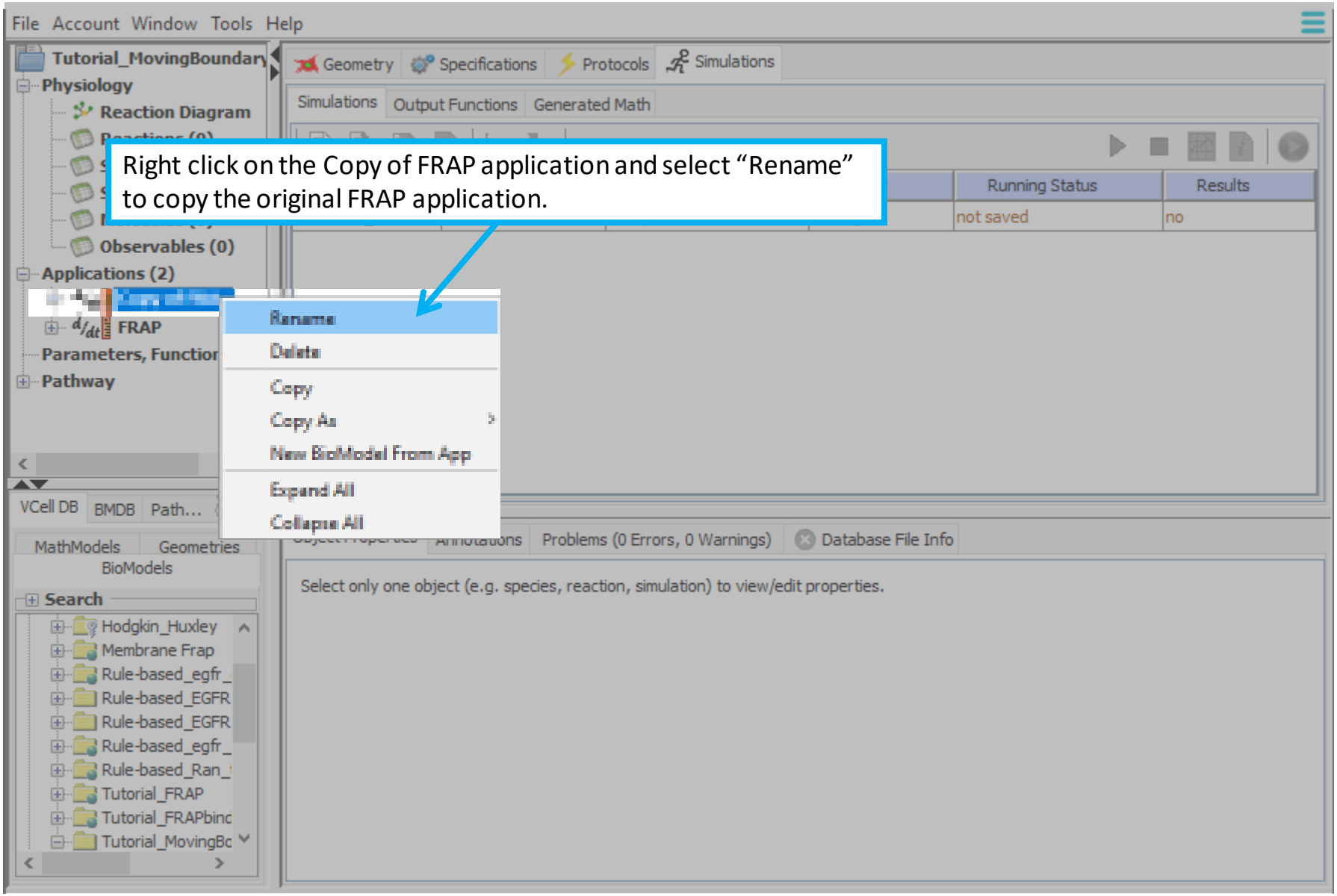


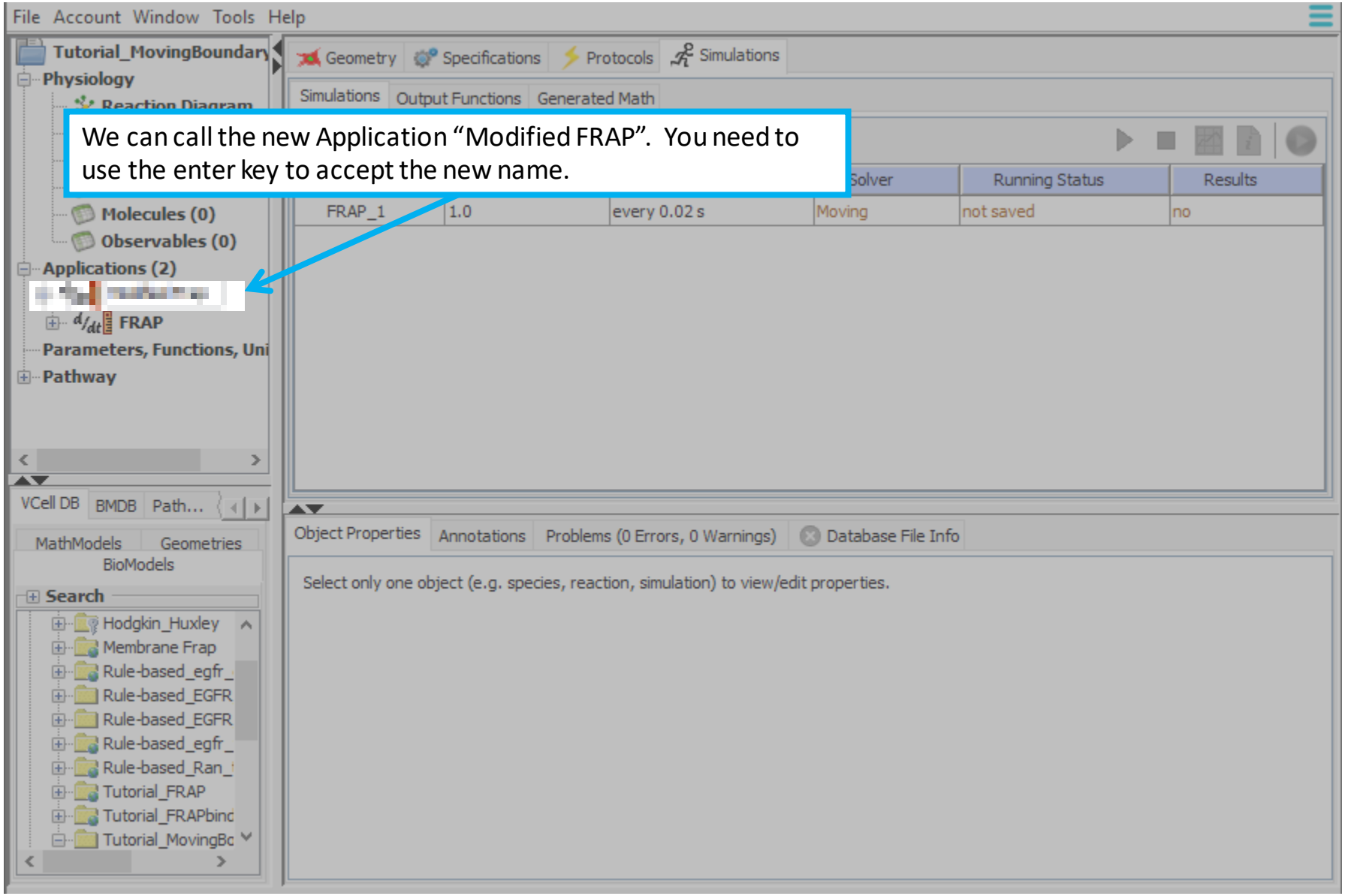
You can also export a Quicktime movie for presentations.



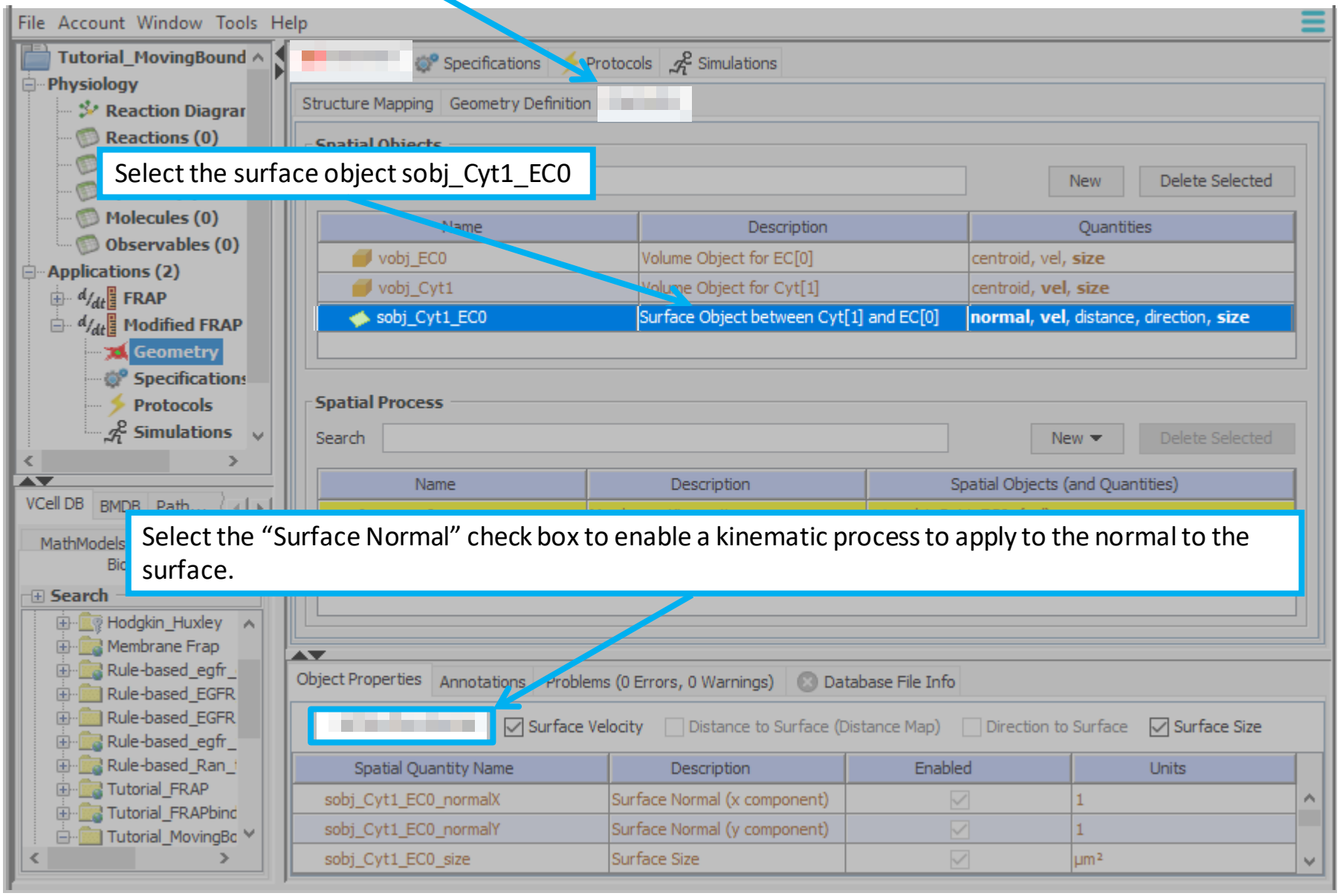
Let's create a second Application to change the parameters for both the kinematics and diffusion coefficient and see how that affects the spatial distribution of the fluorescent probe




File Account Window Tools Help
Tutorial_MovingBoundary
Physiology
Reaction Diagram
Observables (0)
Applications (2)
FRAP
Parameters, Functior
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Running Status
Results
not saved
no
Right click on the Copy of FRAP application and select “Rename” to copy the original FRAP application.
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
VCell DB
BMDB
Path...
MathModels
Geometries
BioModels
Search
Hodgkin_Huxley
Membrane Frap
Rule-based_egfr_
Rule-based_EGFR
Rule-based_EGFR
Rule-based_egfr_
Rule-based_Ran_
Tutorial_FRAP
Tutorial_FRAPbinc
Tutorial_MovingBc
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

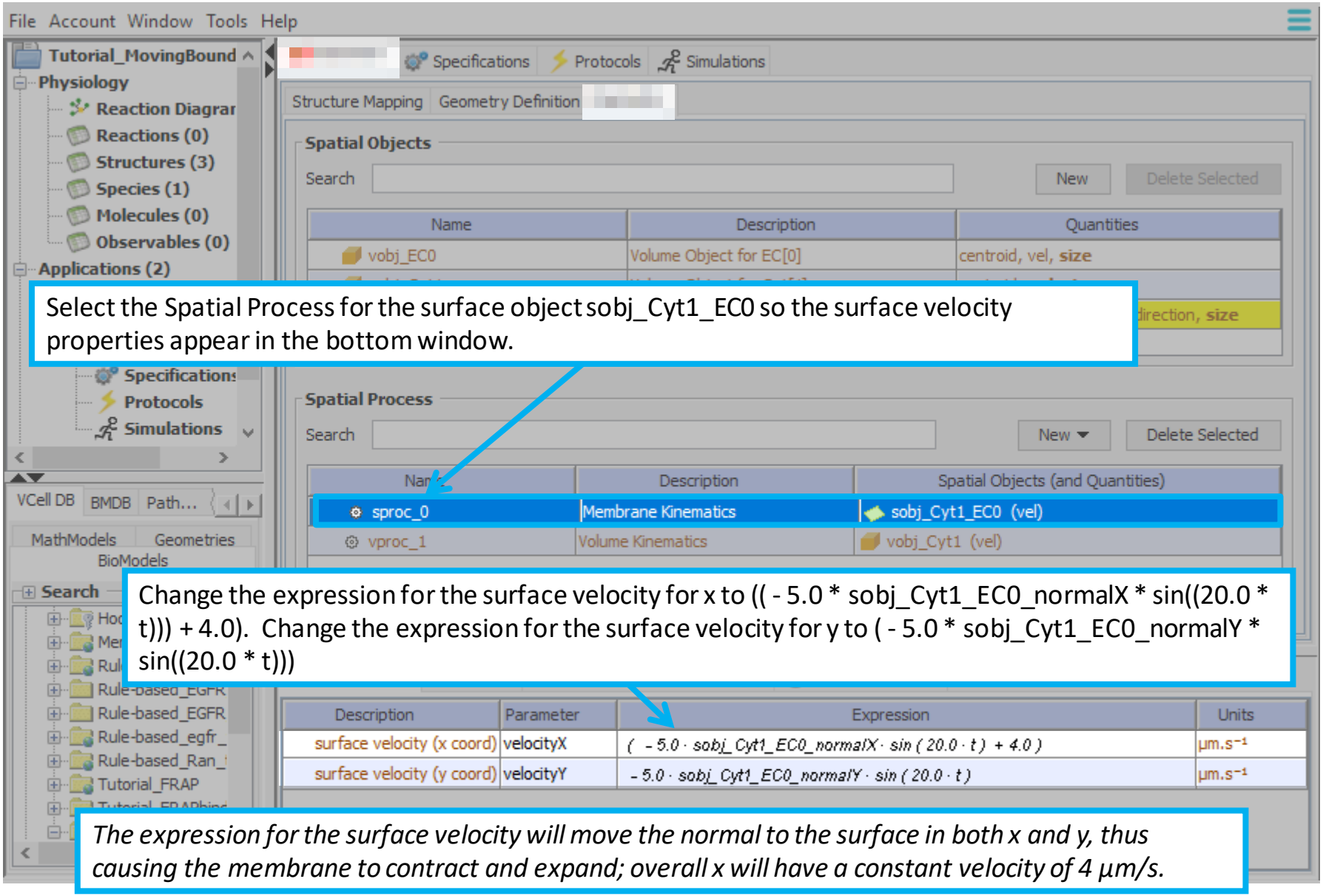

File Account Window Tools Help
Tutorial_MovingBoundary
Physiology
Molecules (0)
Observables (0)
Applications (2)
FRAP
Parameters, Functions, Uni
Pathway
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
We can call the new Application "Modified FRAP". You need to use the enter key to accept the new name.
Solver
Running Status
Results
FRAP_1
1.0
every 0.02 s
Moving
not saved
no
VCell DB
BMDB
Path...
MathModels
Geometries
BioModels
Search
Hodgkin_Huxley
Membrane Frap
Rule-based_egfr_
Rule-based_EGFR
Rule-based_EGFR
Rule-based_egfr_
Rule-based_Ran_
Tutorial_FRAP
Tutorial_FRAPbinc
Tutorial_MovingBc
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

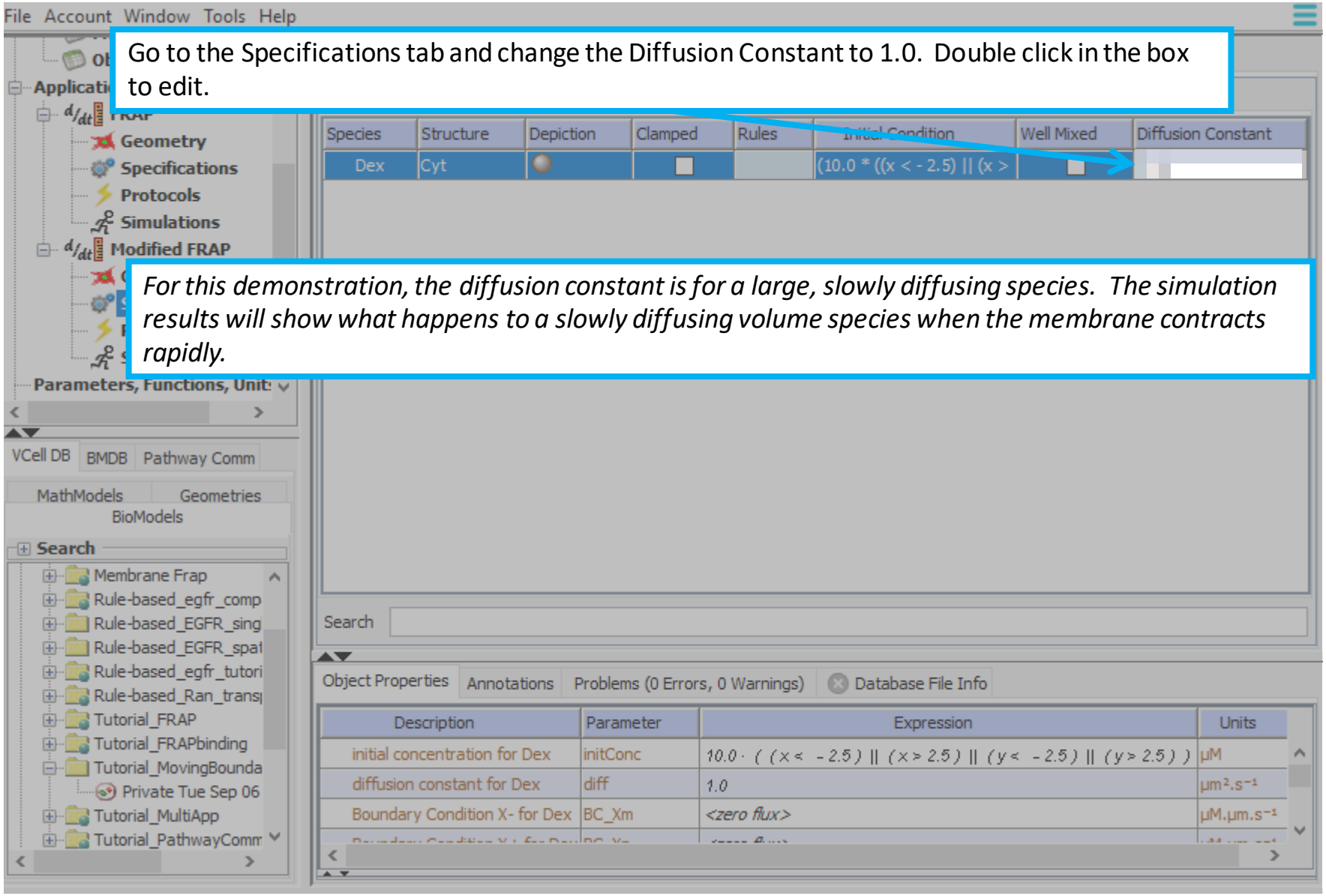
Return to the Geometry > Kinematics tab

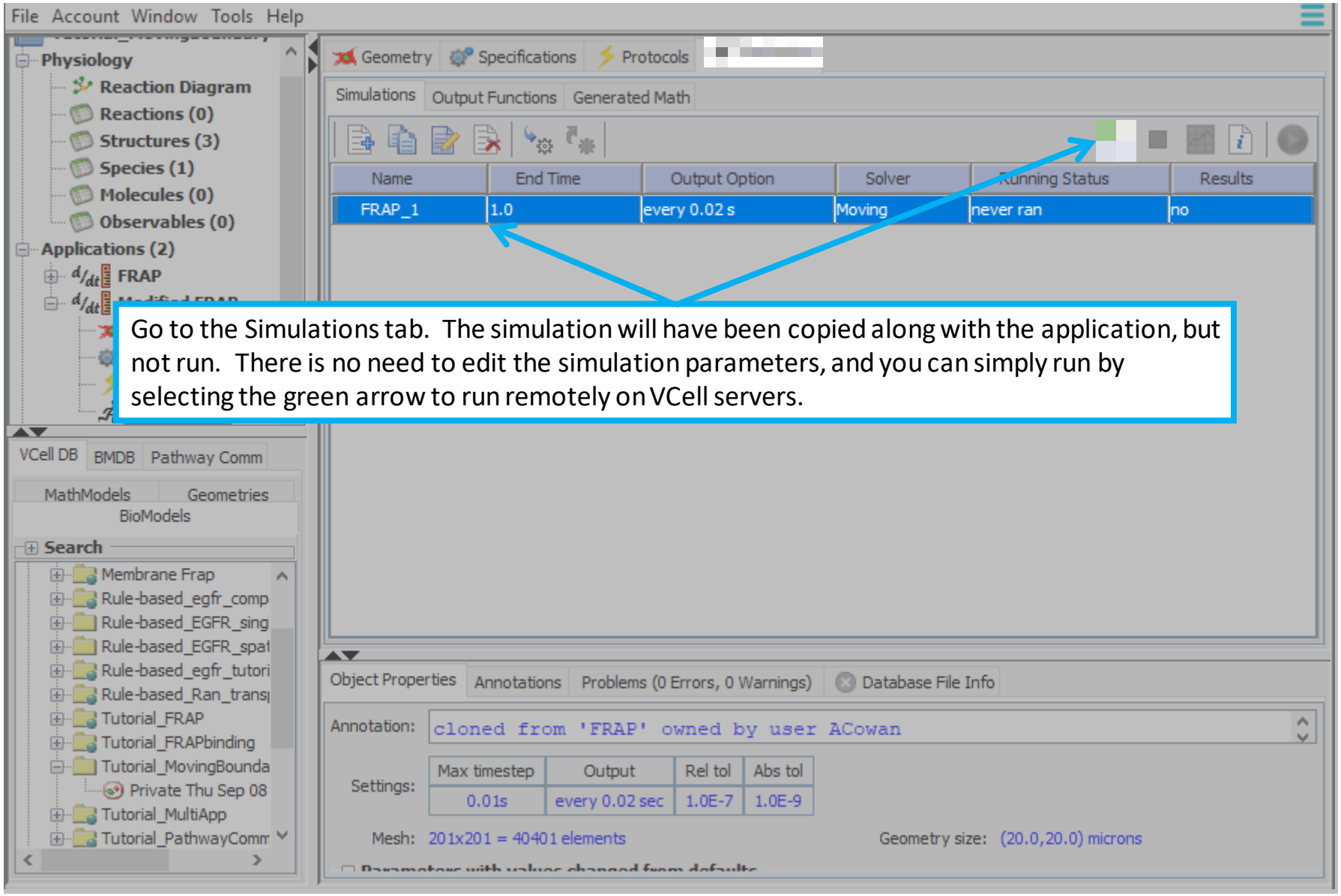


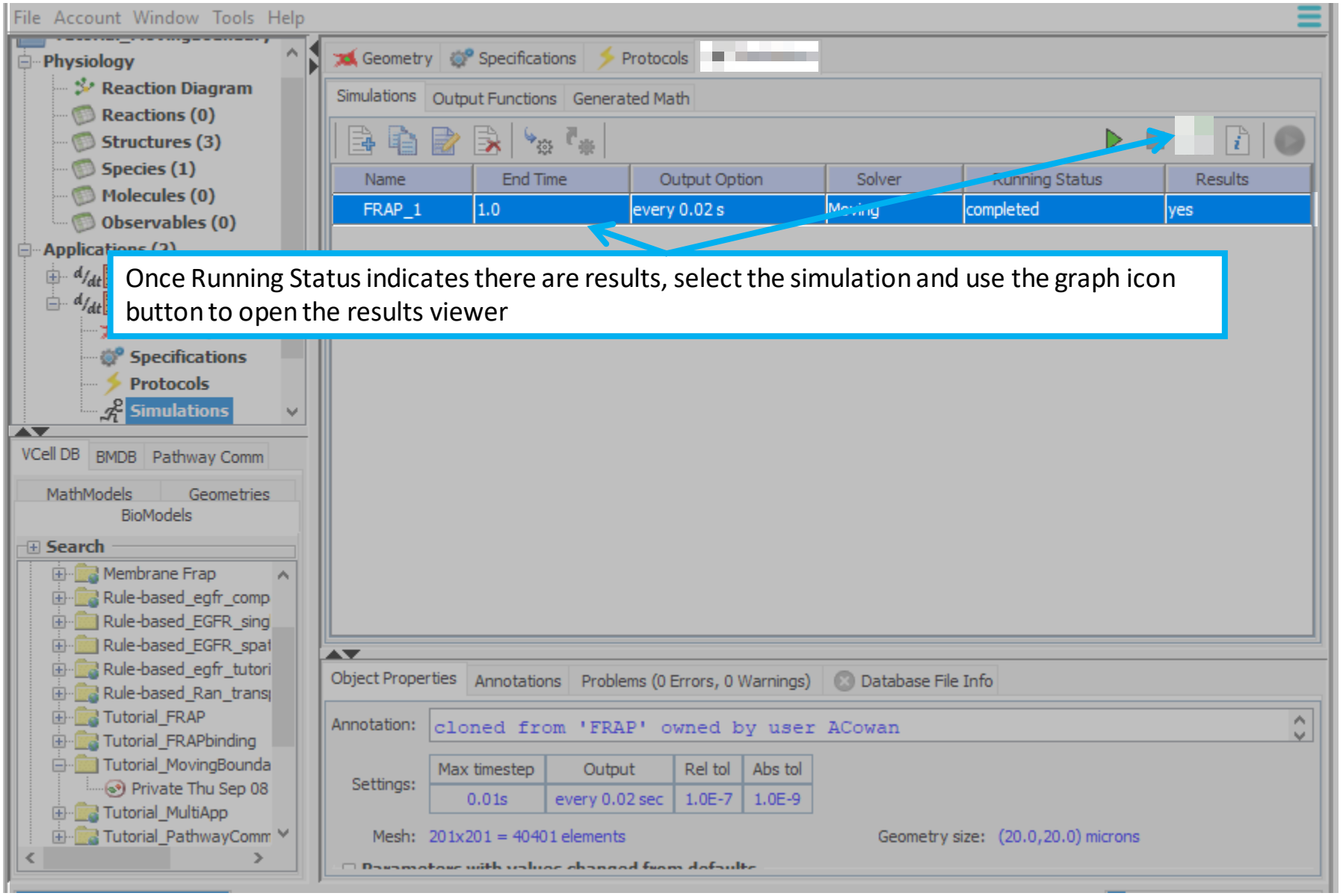
Select the surface object sobj_Cyt1_EC0

Select the “Surface Normal” check box to enable a kinematic process to apply to the normal to the surface.


File Account Window Tools Help
Tutorial_MovingBound
Physiology
Reaction Diagrar
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (2)
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Spatial Objects
Search
New
Delete Selected
Name
Description
Quantities
vobj_EC0
Volume Object for EC[0]
centroid, vel, size
Select the Spatial Process for the surface object sobj_Cyt1_EC0 so the surface velocity properties appear in the bottom window.
Spatial Process
Search
New
Delete Selected
Description
Spatial Objects (and Quantities)
sproc_0
Membrane Kinematics
sobj_Cyt1_EC0 (vel)
vproc_1
Volume Kinematics
vobj_Cyt1 (vel)
VCell DB
BMDB
MathModels
Geometries
BioModels
Search
Change the expression for the surface velocity for x to ((- 5.0 * sobj_Cyt1_EC0_normalX * sin((20.0 * t))) + 4.0). Change the expression for the surface velocity for y to (- 5.0 * sobj_Cyt1_EC0_normalY * sin((20.0 * t)))
Description
Parameter
Expression
Units
surface velocity (x coord)
velocityX
(- 5.0 · sobj_Cyt1_EC0_normalX · sin (20.0 · t) + 4.0)
μm.s⁻¹
surface velocity (y coord)
velocityY
- 5.0 · sobj_Cyt1_EC0_normalY · sin (20.0 · t)
μm.s⁻¹
The expression for the surface velocity will move the normal to the surface in both x and y, thus causing the membrane to contract and expand; overall x will have a constant velocity of 4 μm/s.


File Account Window Tools Help
Go to the Specifications tab and change the Diffusion Constant to 1.0. Double click in the box to edit.
Species
Structure
Depiction
Clamped
Rules
Well Mixed
Diffusion Constant
Dex
Cyt
(10.0 * ((x < - 2.5) || (x >
Geometry
Specifications
Protocols
Simulations
Modified FRAP
Parameters, Functions, Unit
For this demonstration, the diffusion constant is for a large, slowly diffusing species. The simulation results will show what happens to a slowly diffusing volume species when the membrane contracts rapidly.
VCell DB
BMDB
Pathway Comm
MathModels
Geometries
BioModels
Search
Membrane Frap
Rule-based_egfr_comp
Rule-based_EGFR_sing
Rule-based_EGFR_spat
Rule-based_egfr_tutori
Rule-based_Ran_trans
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MovingBounda
Private Tue Sep 06
Tutorial_MultiApp
Tutorial_PathwayComm
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for Dex
initConc
10.0 · ((x < - 2.5) || (x > 2.5) || (y < - 2.5) || (y > 2.5))
µM
diffusion constant for Dex
diff
1.0
µm².s⁻¹
Boundary Condition X- for Dex
BC_Xm
<zero flux>
µM.µm.s⁻¹


File Account Window Tools Help
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Applications (2)
FRAP
Geometry
Specifications
Protocols
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
FRAP_1
1.0
every 0.02 s
Moving
never ran
no
Go to the Simulations tab. The simulation will have been copied along with the application, but not run. There is no need to edit the simulation parameters, and you can simply run by selecting the green arrow to run remotely on VCell servers.
VCell DB
BMDB
Pathway Comm
MathModels
Geometries
BioModels
Search
Membrane Frap
Rule-based_egfr_comp
Rule-based_EGFR_sing
Rule-based_EGFR_spat
Rule-based_egfr_tutori
Rule-based_Ran_transp
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MovingBounda
Private Thu Sep 08
Tutorial_MultiApp
Tutorial_PathwayComm
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
cloned from 'FRAP' owned by user ACowan
Settings:
Max timestep
Output
Rel tol
Abs tol
0.01s
every 0.02 sec
1.0E-7
1.0E-9
Mesh: 201x201 = 40401 elements
Geometry size: (20.0,20.0) microns


File Account Window Tools Help
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (1)
Molecules (0)
Observables (0)
Specifications
Protocols
Simulations
VCell DB
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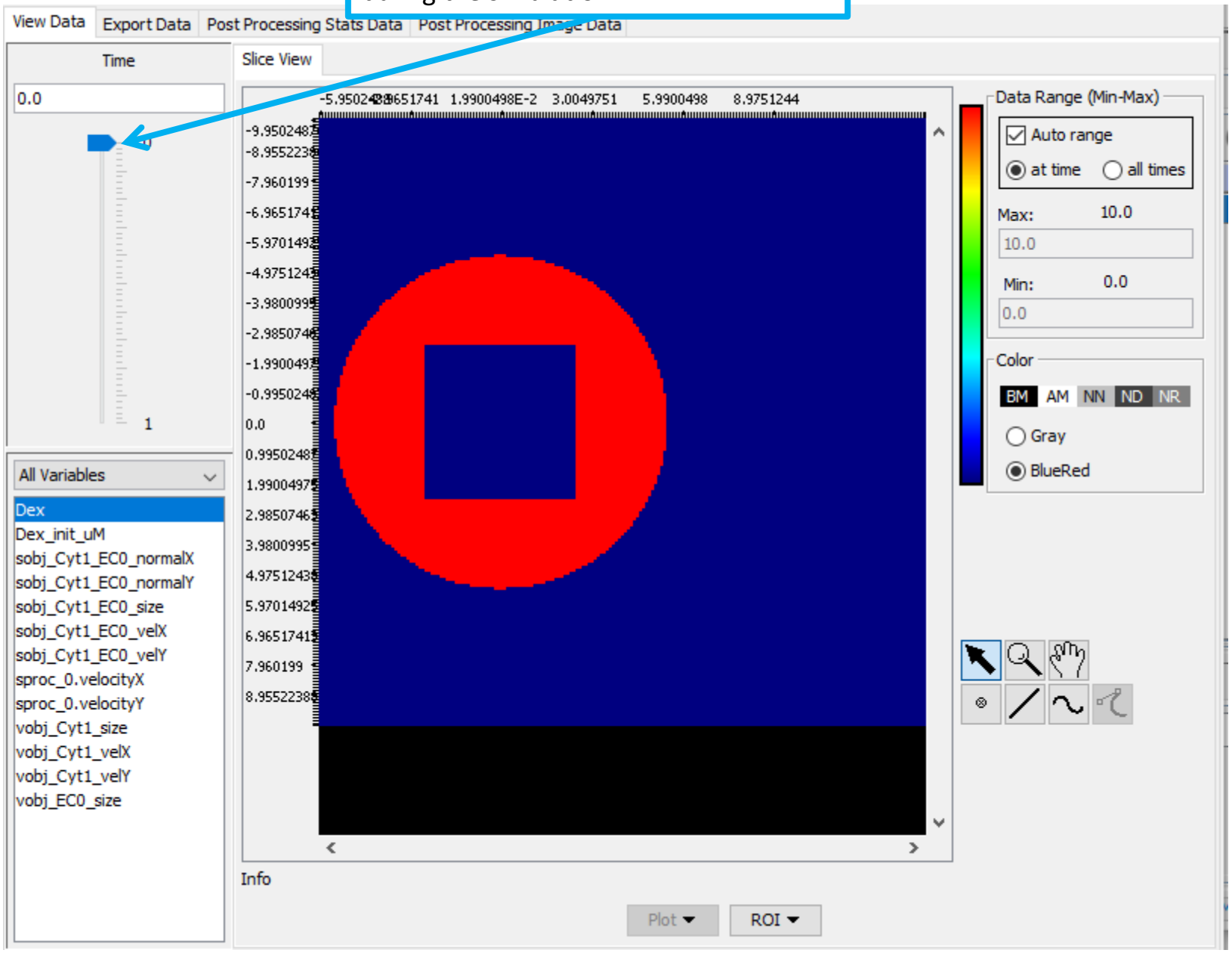
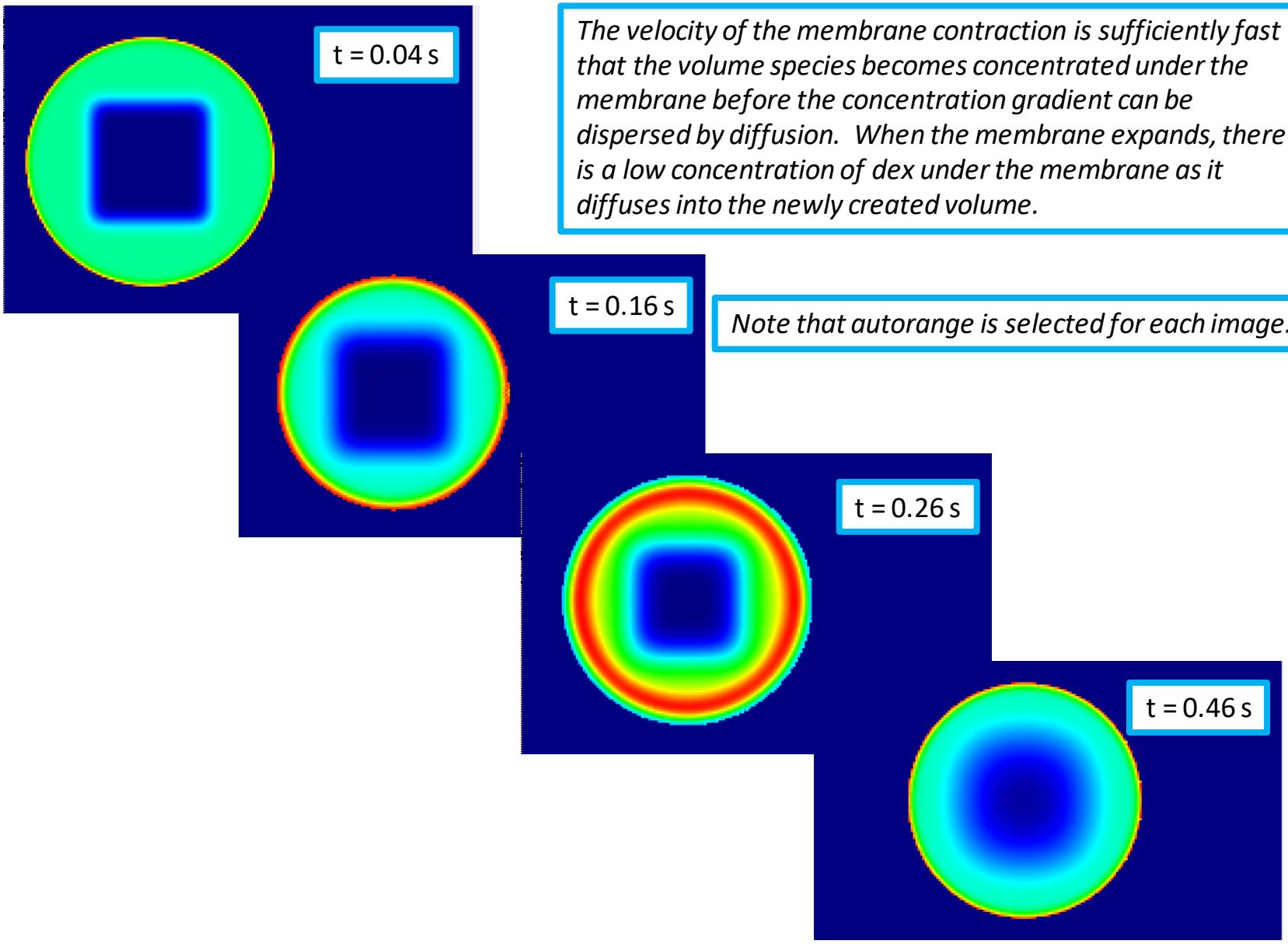
MathModels
Geometries
BioModels
Search
Membrane Frap
Rule-based_egfr_comp
Rule-based_EGFR_sing
Rule-based_EGFR_spat
Rule-based_egfr_tutori
Rule-based_Ran_trans
Tutorial_FRAP
Tutorial_FRAPbinding
Tutorial_MovingBounda
Private Thu Sep 08
Tutorial_MultiApp
Tutorial_PathwayComm
Geometry
Specifications
Protocols
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
FRAP_1
1.0
every 0.02 s
completed
yes
Once Running Status indicates there are results, select the simulation and use the graph icon button to open the results viewer
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
cloned from 'FRAP' owned by user ACowan
Settings:
Max timestep
Output
Rel tol
Abs tol
0.01s
every 0.02 sec
1.0E-7
1.0E-9
Mesh: 201x201 = 40401 elements
Geometry size: (20.0,20.0) microns

Use the Time slider to see what happens during the simulation.



Contents



The velocity of the membrane contraction is sufficiently fast that the volume species becomes concentrated under the membrane before the concentration gradient can be dispersed by diffusion. When the membrane expands, there is a low concentration of dex under the membrane as it diffuses into the newly created volume.

Note that autorange is selected for each image.