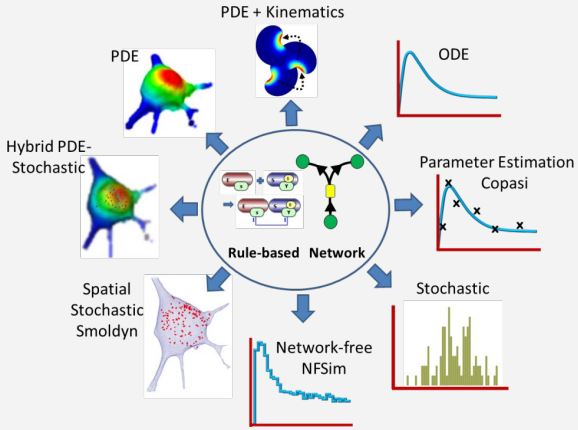
VCell

The Virtual Cell

A modeling environment for the simulation of cellular events. Download at vcell.org
Version 7.7 July 2025



Constructive Solid Geometry: Dendritic Spine

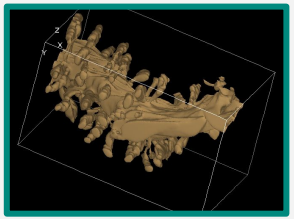
Virtual Cell is developed by the Center for Cell Analysis and Modeling at the University of Connecticut Health Center. It is funded by the National Institute of General Medical Sciences (NIGMS)

NIH National Institute of General Medical Sciences
VCell is funded by the NIGMS

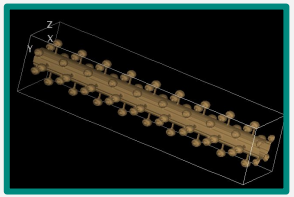
CCAM VCell is developed at CCAM
Center for Cell Analysis & Modeling

Dendritic Spine CSG Introduction

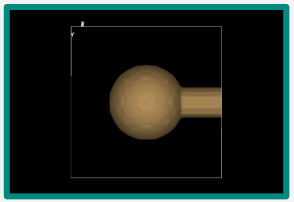
Dendritic spines are small membrane protrusions from a neuron's dendrite that aid in the transduction of electrical signals between nerve cells. To the top right is a VCell representation of a dendrite based on z-stack of microscopy images (see Tutorial for Image Based Geometry) The model is described in Brown wt al., 2008 https://vcell.org/brown-et-al-2008



To develop faster and more understandable simulations, it is better to start with an artificial geometry where all effects are clearly seen. In the middle right is a **Constructive Solid Geometry** (CSG) model of a dendrite.



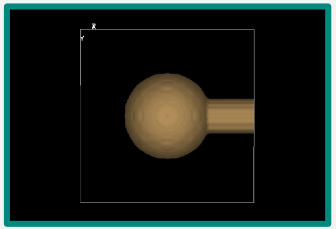
In this tutorial, we will focus on creating a model of one dendritic spine (see bottom right), which consists of a bouton (a sphere with a radius 0.5 um) on a dendritic stem (a cylinder with a length of 0.5 um and a diameter of 0.4 um). We will simulate it in a 3D space that is 2 x 2 x 2 um.



Constructive Solid Geometry: Dendritic Spine

Objective:

Create a single Biomodel of a dendritic spine using Constructive Solid Geometry (CSG) in Virtual Cell modeling and analysis software.



Goals:

- ➔ Learn basic CSG concepts, such as defining solid bodies, scaling, translation and union.
- ➔ Run a simulation to verify accuracy of your model.

General familiarity with VCell software is recommended. Although this tutorial can be followed by a VCell novice, it is recommended that novice users first look through the VCell tutorials available at https://vcell.org/support

Model building can be matched to the BioModel **Tutorial_CSG_DendriticSpine** in the Tutorial folder in the **VCell Database.**

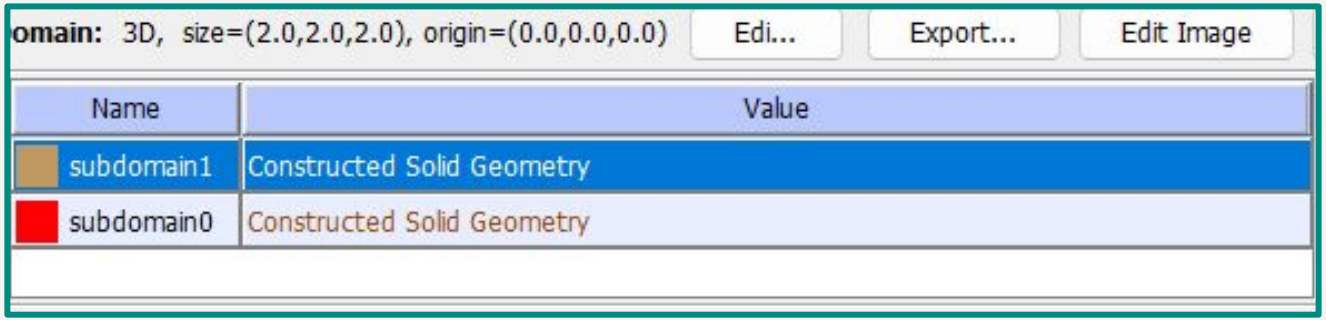
Table of Contents

1. Starting Constructive Solid Geometry
    - 1.1 Create Application and Geometry
    - 1.2 Select Appropriate Framework
2. Creating the Bouton (Sphere)
    - 2.1 Define the Bouton of the Spine
    - 2.2 Scale Sphere to the Proper Size
    - 2.3 Move Sphere to the Desired Position
3. Creating the Neck (Cylinder)
    - 3.1 Define the Neck of the Spine
    - 3.2 Scale Cylinder to the Proper Size
    - 3.3 Move Cylinder to the Desired Position
    - 3.4 Viewing the Model in Slice View
    - 3.5 Verifying the Model's Dimensions

Table of Contents

4. Testing the Model via Diffusion Simulation
    - 4.1 Set up Model Physiology
    - 4.2 Link Model Physiology to Geometry
    - 4.3 Specify Species Concentrations and Diffusions
    - 4.4 Start the Simulation
    - 4.5 Navigating the Simulation
    - 4.6 Viewing Volume Simulation
    - 4.7 Viewing Membrane Simulation

1



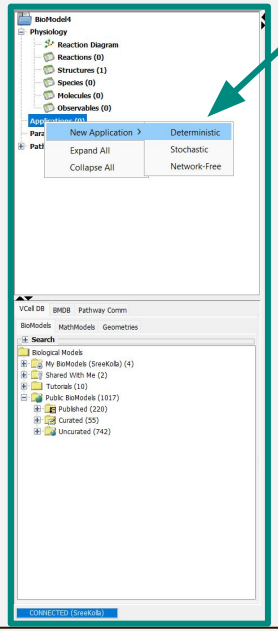
Starting Constructive Solid Geometry

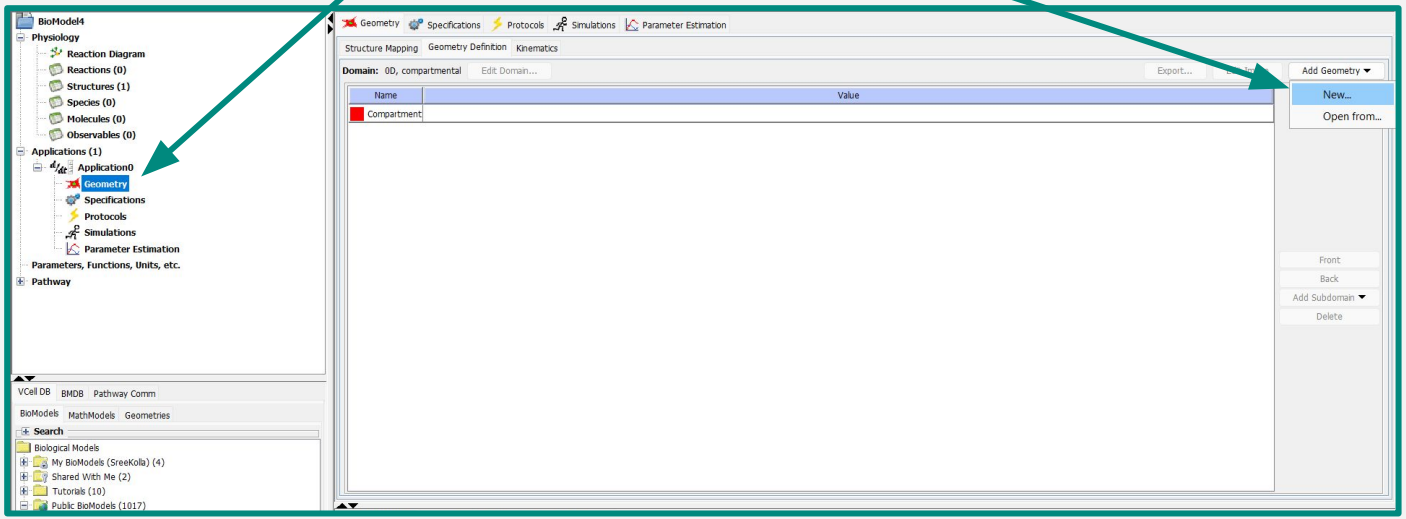
1.1 Create Application and Geometry

Select **Application**. Right click, then select **New Application → Deterministic**.

Make sure to select **Geometry** under the Application subsection.

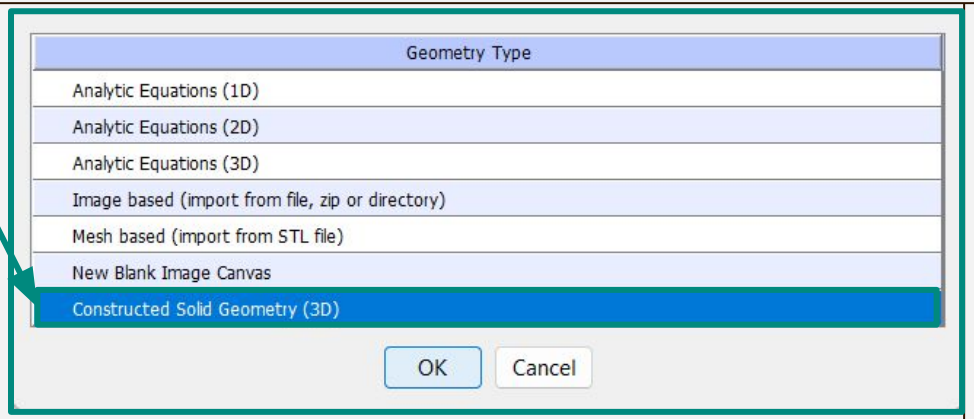
Click **Add Geometry** and select **New**.

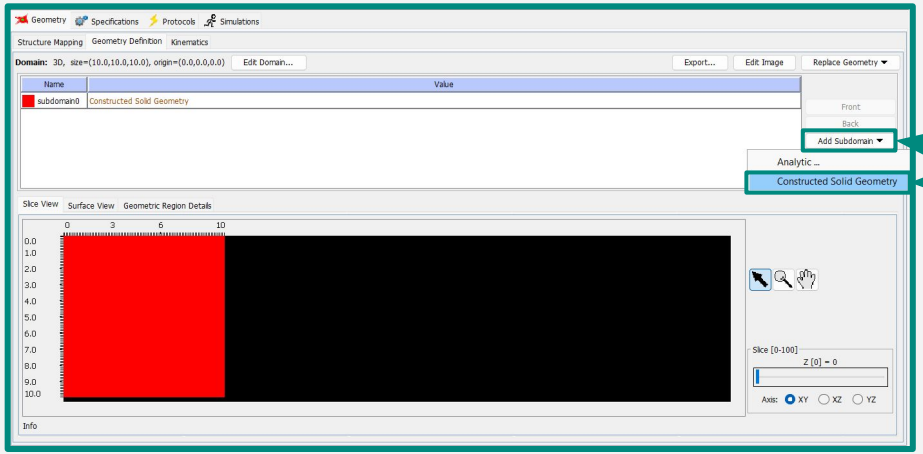




Select **Constructed Solid Geometry (3D)** and click OK.

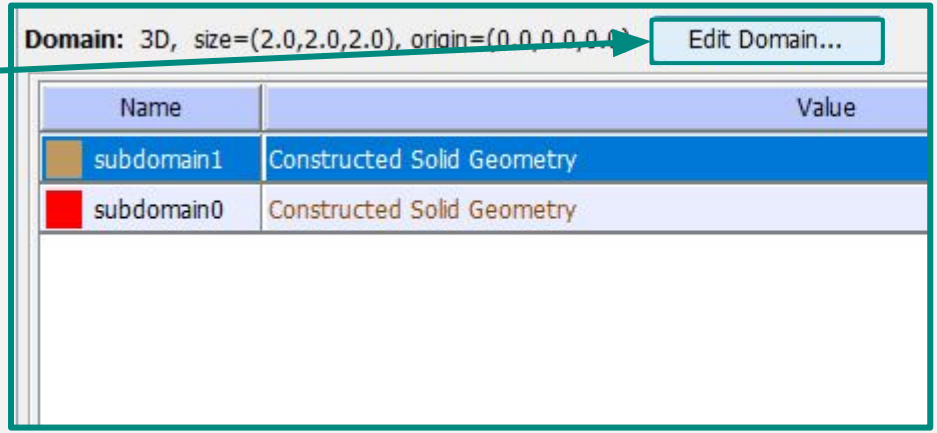
Select **Surface View** to better view the model

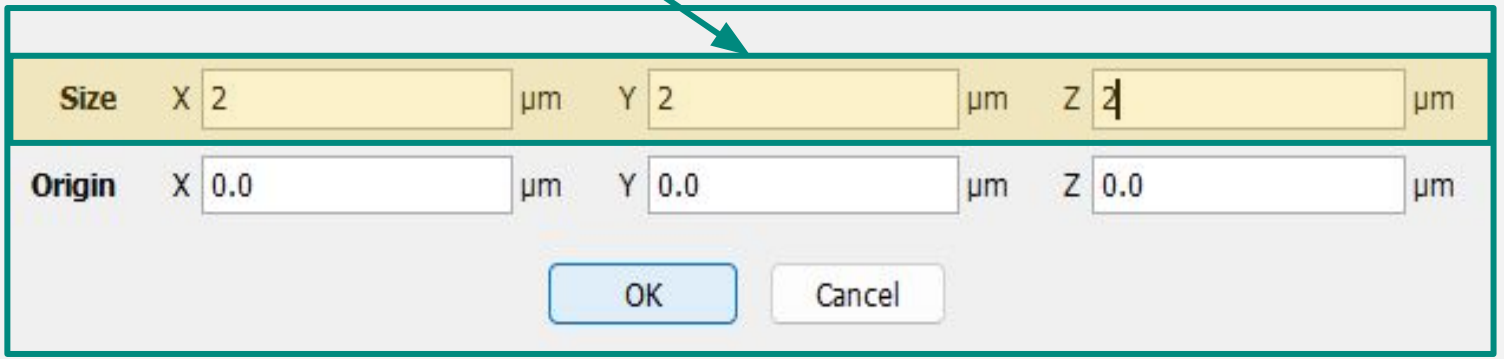




Then, click **Add Subdomain**, and select **Constructed Solid Geometry.**

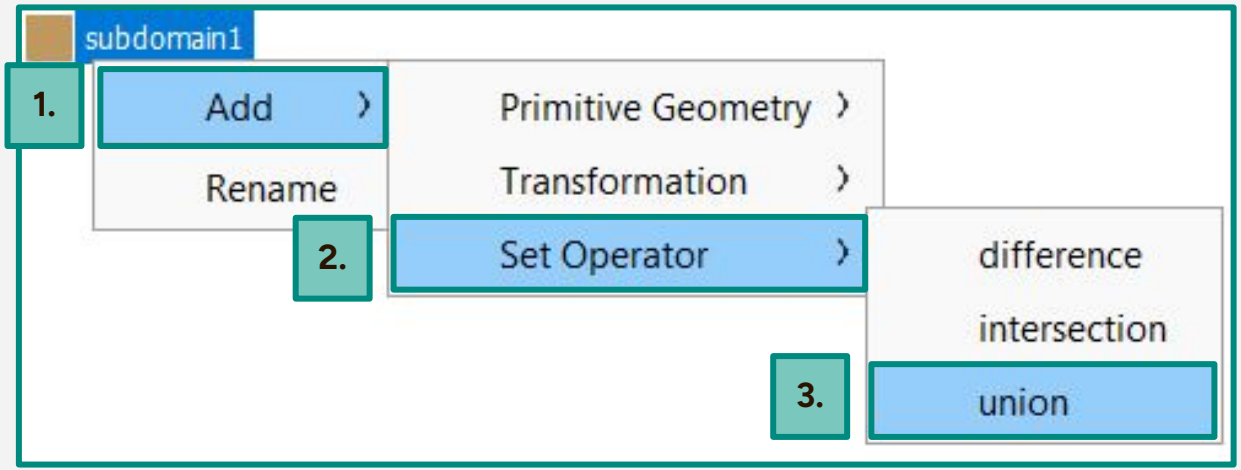
To set the dimensions of the simulation space, click **Edit Domain.** When prompted to set X, Y, and Z parameters, set all of them to **2 um.**





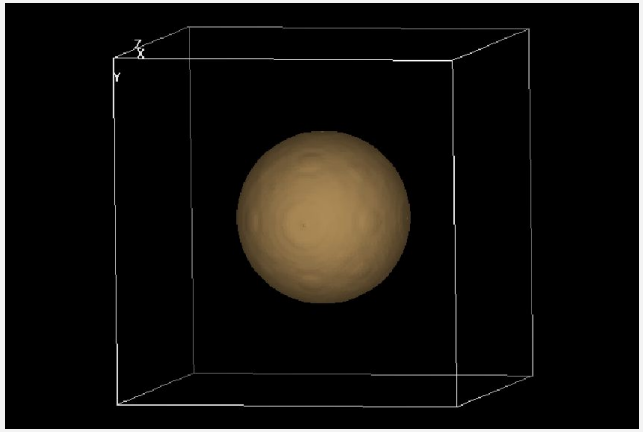
1.2 Select Appropriate Framework

Right click the subdomain, select **Add**, navigate to **Set Operator**, then select **Union**.



Note: It is important to select the operator BEFORE constructing the geometry. Selecting union ensures that whatever structures are made will join together when they touch.

2

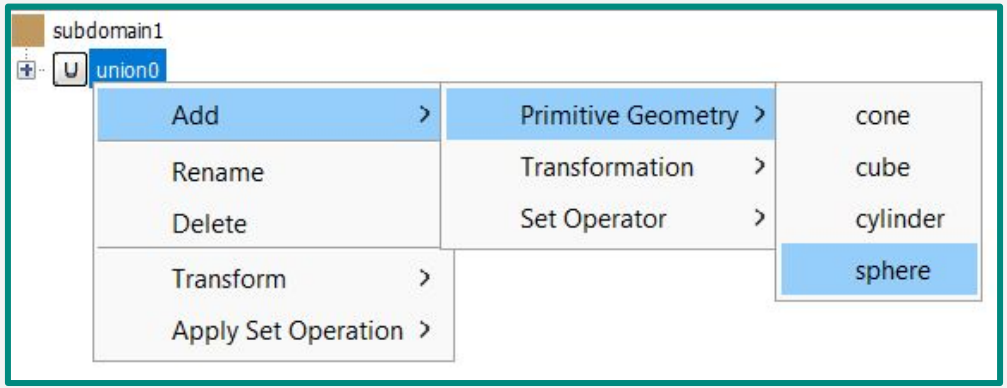


Creating the Bouton (Sphere)

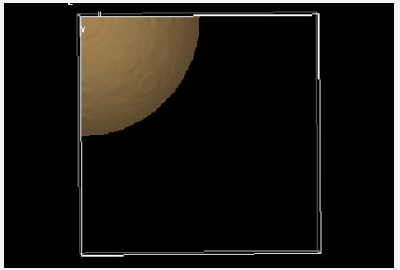
The construction of the dendritic spine will start by first creating a sphere that will represent the bouton (bulbous part of the spine).

2.1 Define the Bouton of the Spine

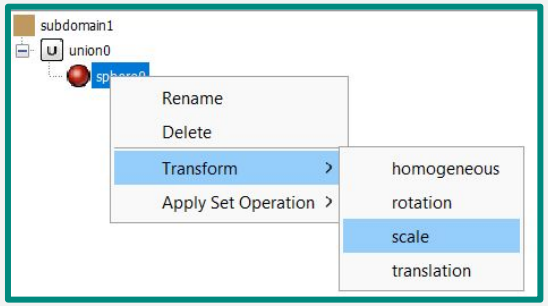
Right click **Union**, select **Add**, navigate to **Primitive Geometry**, then select **Sphere**.



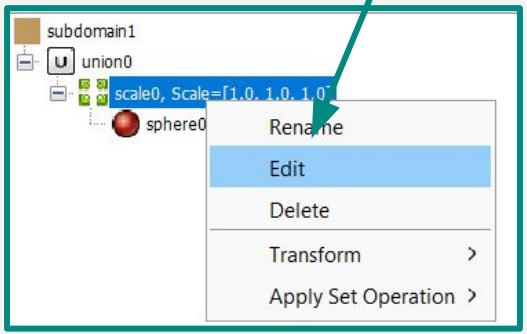
By default, the sphere will be created in the top left corner (the point with coordinates [0,0.0] and will have the radius 1. It needs go be translated to the desired position and scaled to the proper size.

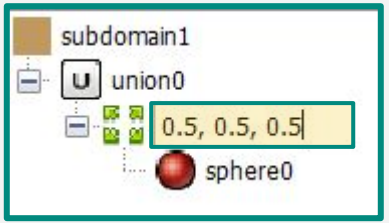


2.2 Scale Sphere to the Proper Size



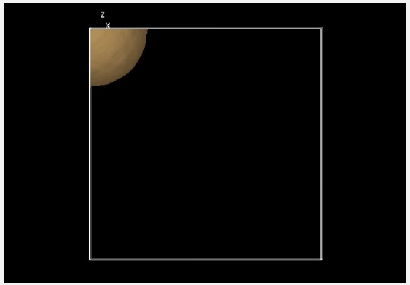
To edit the scale, right click the dimensions, select **Edit**, and set the scale. For this tutorial, decrease the sphere by half in all directions by scaling to 0.5. → **[0.5, 0.5, 0.5].**





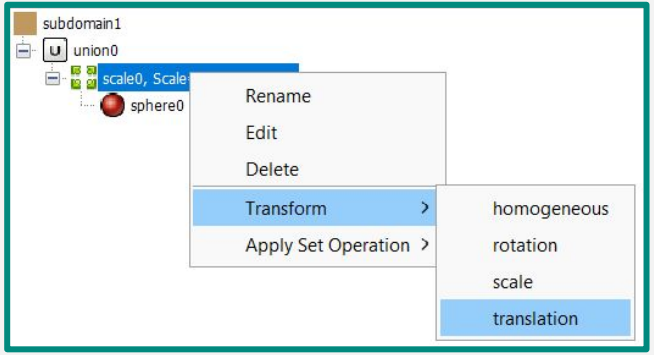
Now, scale the bouton. Right click on **sphere0**, and select **Transform**, then **scale**.

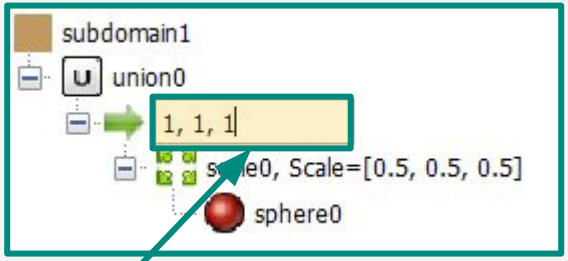
This is how the model will appear in **Surface View** after scaling.



2.3 Move Sphere to the Desired Position

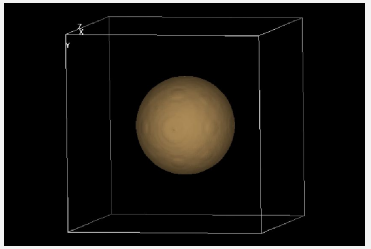
Next, translate the sphere so that it fits in the center of the simulation space. Right click on **scale0**, select **Transform**, then **translation**.



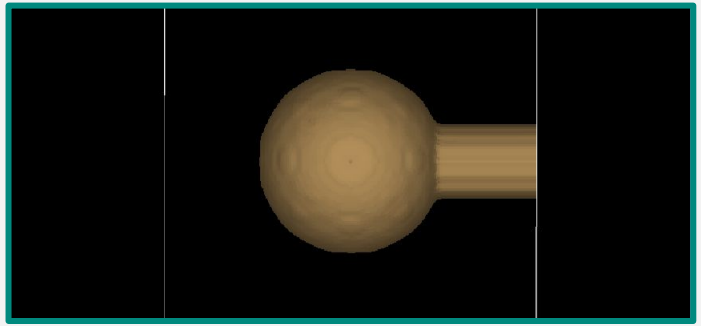


To move the center of the sphere from the point [0,0,0] to the point [1,1,1], right click the **Translation** (green arrow), click **Edit**, and set all parameters to 1. → **[1, 1, 1].**

This is what the model should look in **Surface View.**



3

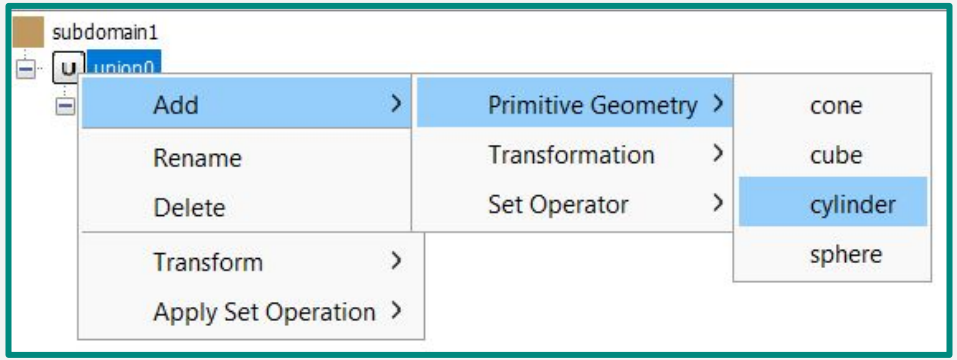


Creating the Neck (Cylinder)

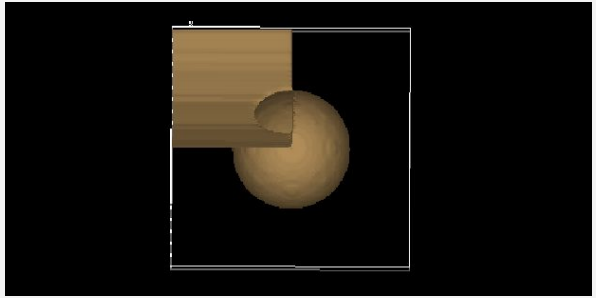
Following the creation of the bouton, the cylindrical portion of the spine (the neck) that connects to the bouton will be created.

3.1 Define the Neck of the Spine

Right click on the **Union** operation and click **Add.** Select **Primitive Geometry** and click on **Cylinder.**

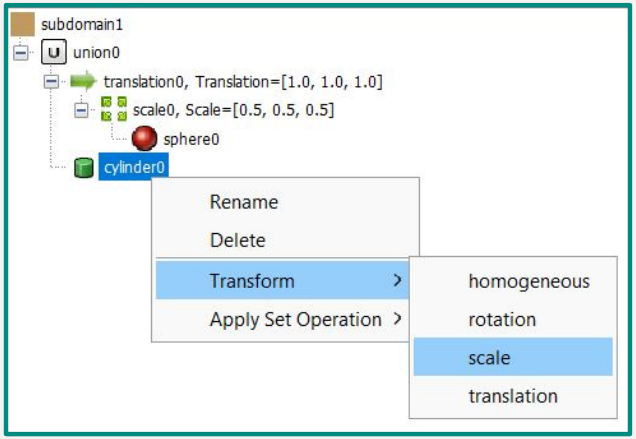


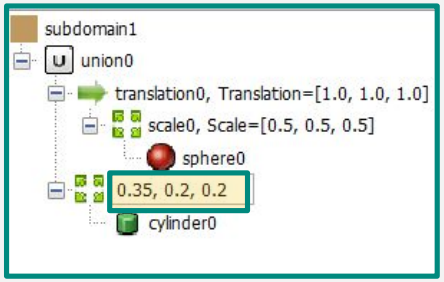
By default, the cylinder will be located in the top left corner (with coordinates [0,0,0]) and will have a radius of 1. The image shows half of the cylinder, so it needs to be scaled to the proper size and translated to the desired position.



3.2 Scale Cylinder to the Proper Size

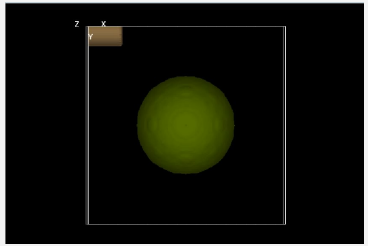
Like the bouton, the stem also needs to be scaled. Right click on **cylinder0**, and select **Transform**, then **Scale**.





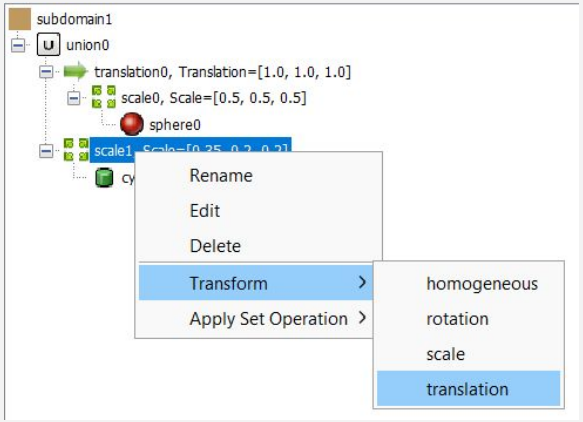
To create a cylinder of the length 0.5 and radius 0.2, it needs to be scaled to 0.25 in the length (x-direction) and 0.2 (in y and z directions). The cylinder is made longer than 0.5 to protrude inside a sphere with no holes. Note that with unions of solid bodies, protrusions do not matter. Right click on **scale1**, select **Edit**, and set the parameters to **[0.35, 0.2, 0.2].**

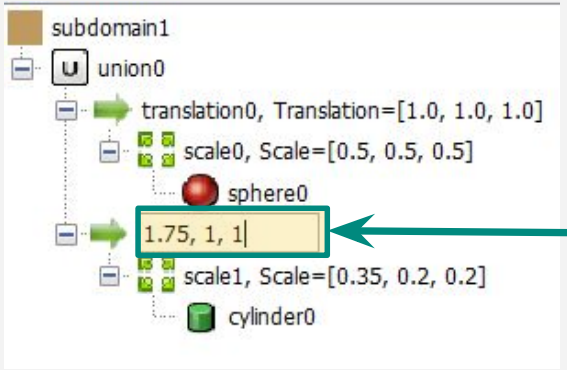
After scaling, the cylinder will remain at the coordinates [0,0,0]. To have it be correctly aligned with the sphere, it will be translated in the next slide.



3.3 Move Cylinder to the Desired Position

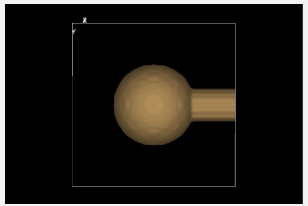
To translate the cylinder so that it is directly aligned with the sphere, right click on **scale1**, select **Transform**, and then **translation**.





Set the translation specifications to **[1.75, 1, 1]** so that the cylinder is placed adjacent to the sphere and to the right of the simulation space.

The cylinder (neck) should now be in direct alignment with the sphere (bouton).

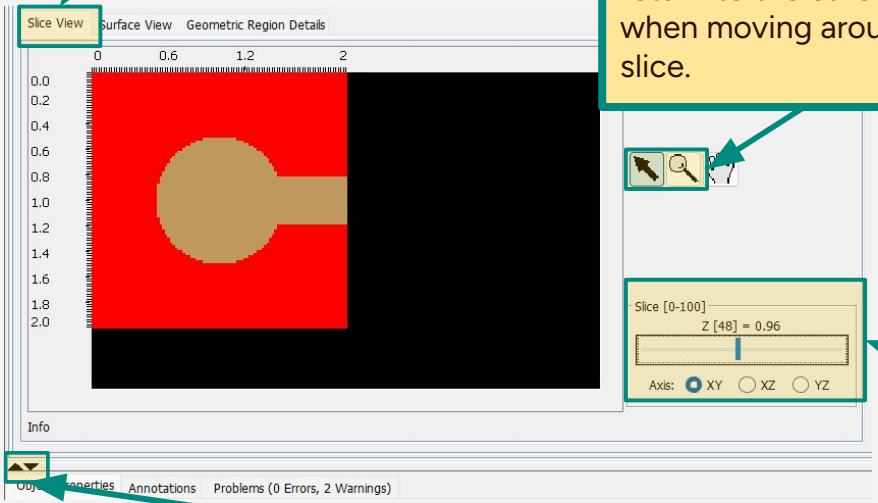


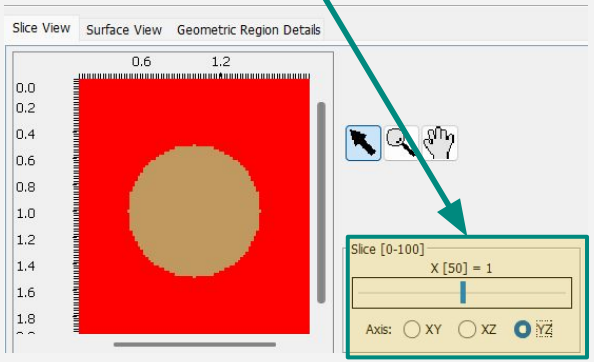
3.4 Viewing the Model in Slice View

To view the model in 2D, click **Slice View.**

Use the **magnifying glass** to zoom in. Make sure to return to the **cursor tool** when moving around the slice.

Select an option to switch between different projections (XY-plane vs YZ-plane). This is z=50 in the **YZ-Plane**





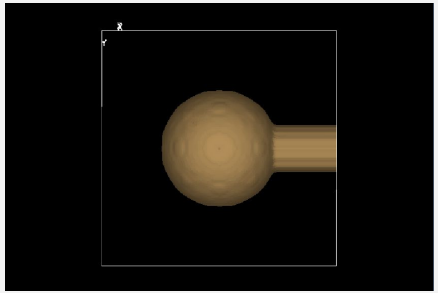
Use arrows at the bottom of the screen to get a better view of the model.

The geometry may not be visible if when at the border of simulation space. To fix this, use the **Z-Slider** to go to the slice that intersects the shape, e.g. **z=50.**

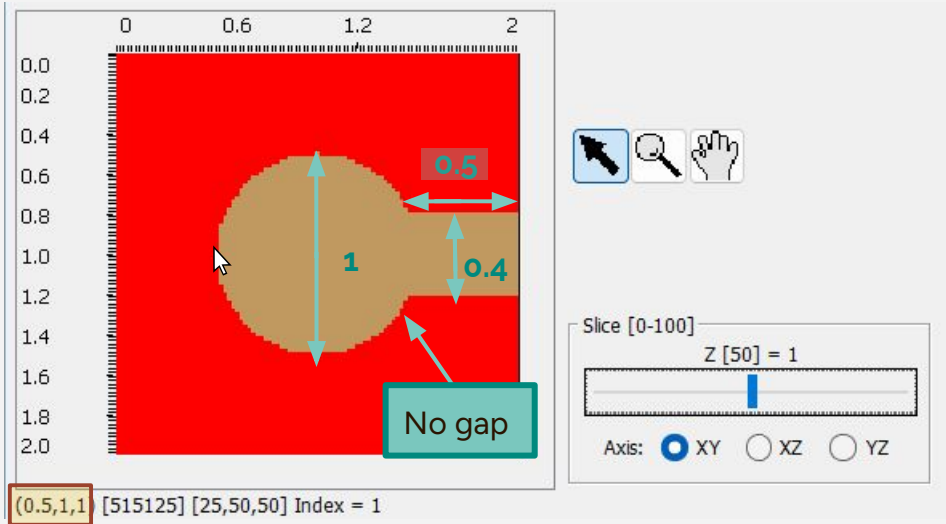
3.5 Verifying the Model's Dimensions

If done properly, the dendritic spine will have the following dimensions:

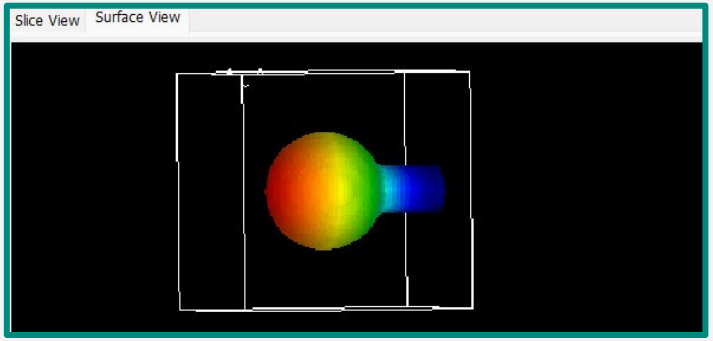
- Bouton (Sphere) Diameter = 1
- Neck (Cylinder) Diameter =0.4
- Neck (Cylinder) Height - 0.5



Note: Here, ensure that there are no gaps between the bouton and neck (sphere and cylinder) of the model, as this will disrupt reaction processes in during simulations.



4

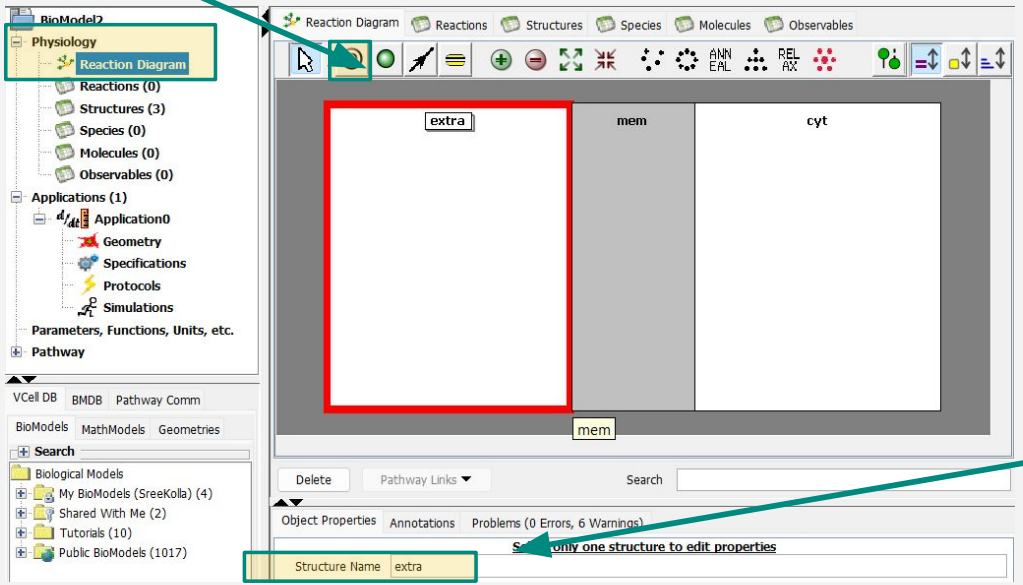


Testing the Model via Diffusion Simulation

To test if the model is functioning properly (i.e it doesn't have any holes that may leak species, touch the border, etc.), run a simulation of species diffusions in the volume and on the membrane.

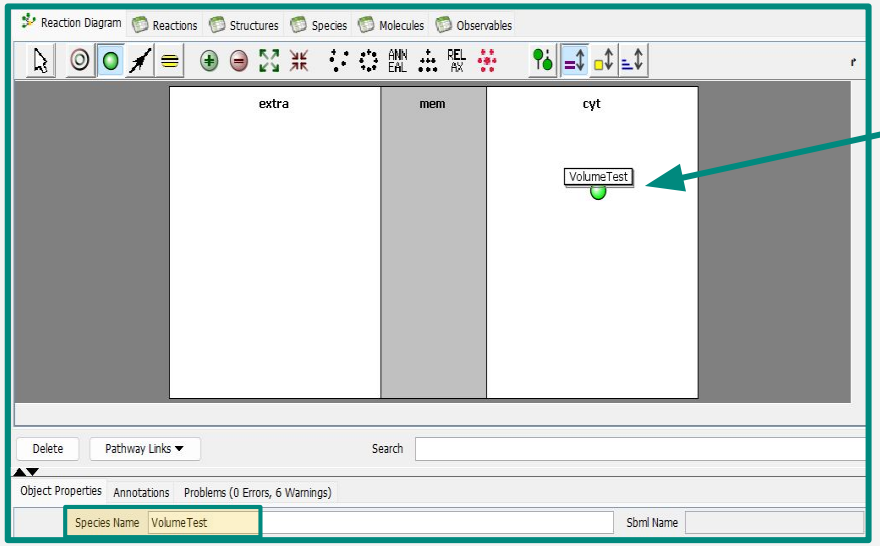
4.1 Set up Model Physiology

First, create a reaction diagram. Navigate to **Physiology** and under **Reaction Diagram**, create two compartments separated by one membrane.

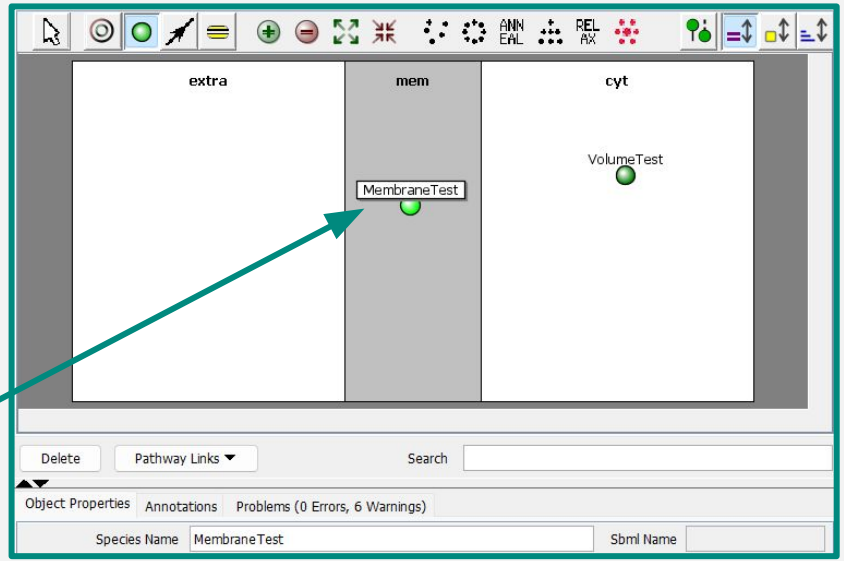


Note: More information about constructing model physiology, can be found in [Tutorial I.]

Click on each compartment or the membrane to rename it in the **Object Properties** tab. Name them according to the image (extra, mem, cyt)



To monitor the diffusion of the species in the volume, create a synthetic species **VolumeTest** that should be able to diffuse freely within the compartment.

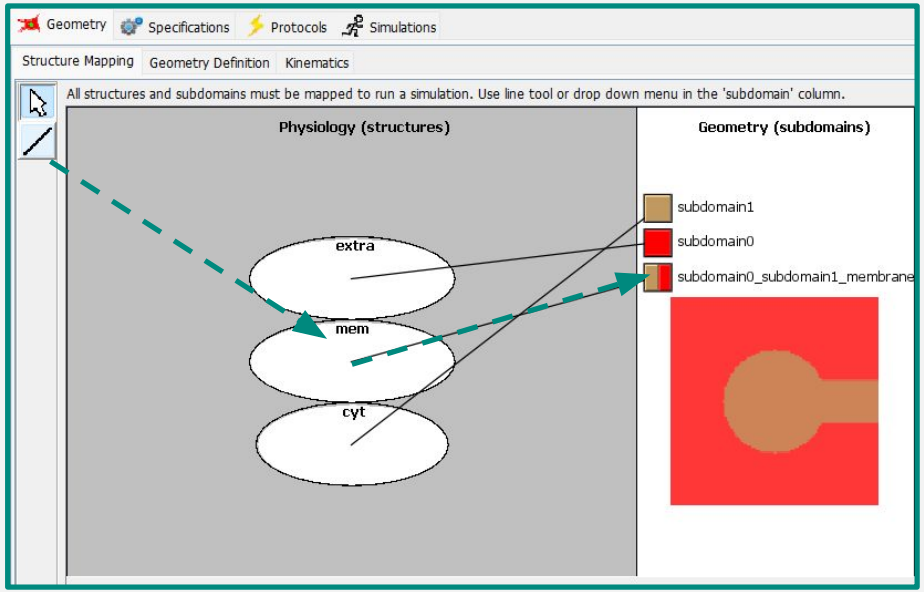


To observe the diffusion of the species in the membrane, create a synthetic species **MembraneTest** that should be able to diffuse freely in the membrane.

4.2 Link Model Physiology to Geometry

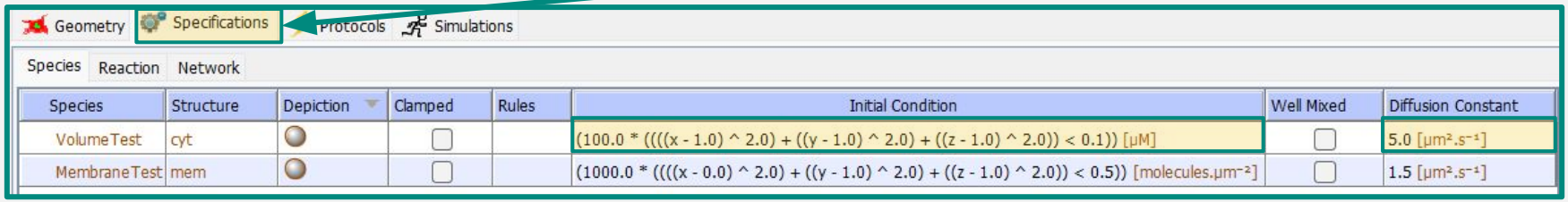
Link the compartments and membrane from the reaction diagram to subdomains to ensure that the physiology matches up with the model's geometry.

Open the **Geometry** section, and then click the **Structure Mapping** tab. Use the **Mapping Tool** to draw lines from the physiology to the appropriate geometry subdomain.



4.3 Specify Species Concentrations and Diffusions

Now, set specifications for the simulation. Navigate to the **Specifications** tab, choose **Species**.

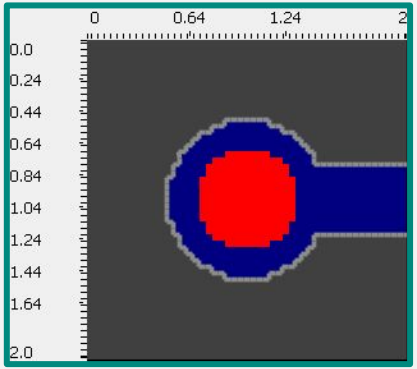


Species	Structure	Depiction	Clamped	Rules	Initial Condition	Well Mixed	Diffusion Constant
VolumeTest	cyt				(100.0 * ((((x - 1.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.1)) [µM]		5.0 [µm².s⁻¹]
MembraneTest	mem				(1000.0 * ((((x - 0.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.5)) [molecules.µm⁻²]		1.5 [µm².s⁻¹]

Initial Condition for Volume:

It is necessary to create a high concentration of a species inside the volume to monitor how the species diffuses within it. To do this, place all species, VolumeTest, within a sphere of a radius ≈ 0.3162 (square root of 0.1) and center at [1, 1, 1], so it is located completely within the bouton.

(100.0 * ((((x - 1.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.1))



Diffusion Constant for Volume = 5.0

The diffusion rate is set high so that the simulation only has to run for a short period of time.

Geometry | Specifications | Protocols | Simulations

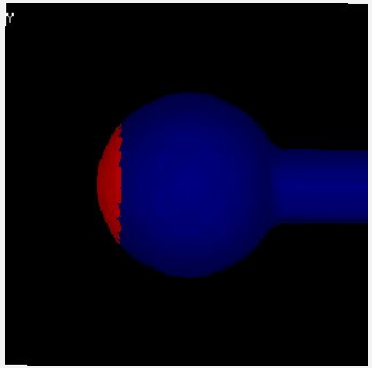
Species | Reaction | Network

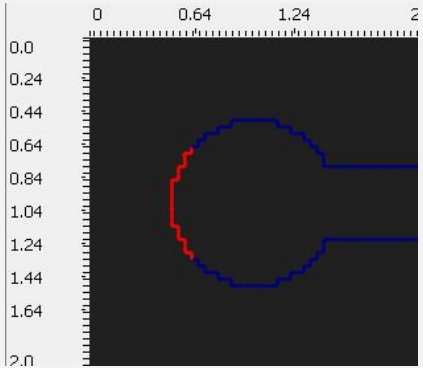
Species	Structure	Depiction	Clamped	Rules	Initial Condition	Well Mixed	Diffusion Constant
VolumeTest	cyt				(100.0 * ((((x - 1.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.1)) [µM]		5.0 [µm².s⁻¹]
MembraneTest	mem				(1000.0 * ((((x - 0.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.5)) [molecules.µm⁻²]		1.5 [µm².s⁻¹]

Initial Condition for Membrane:

It is necessary to place a high concentration of a species on the membrane. To do this, create a sphere of a species, MembraneTest for this example, with a center of [0,1,1] and a radius ≈ 0.7071 (square root of 0.5) so it intersects the membrane at the tip of the bouton, which is located at an x-coordinate of 0.5 in the 2x2x2 space.

(1000.0 * ((((x - 0.0) ^ 2.0) + ((y - 1.0) ^ 2.0) + ((z - 1.0) ^ 2.0)) < 0.5))



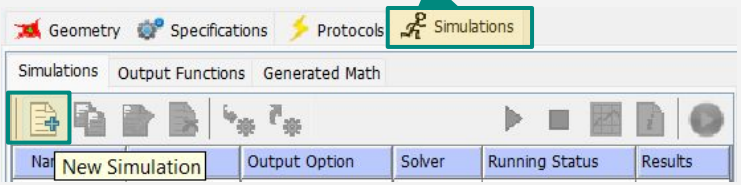


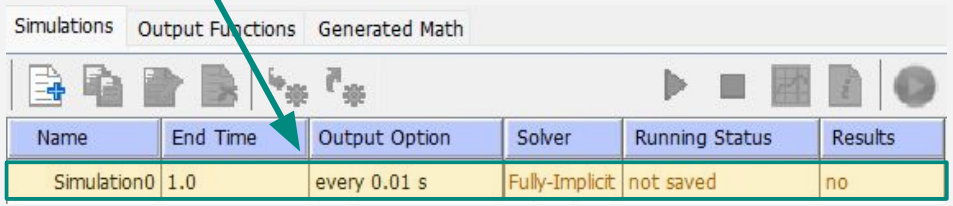
Diffusion Constant for MembraneTest = 1.5

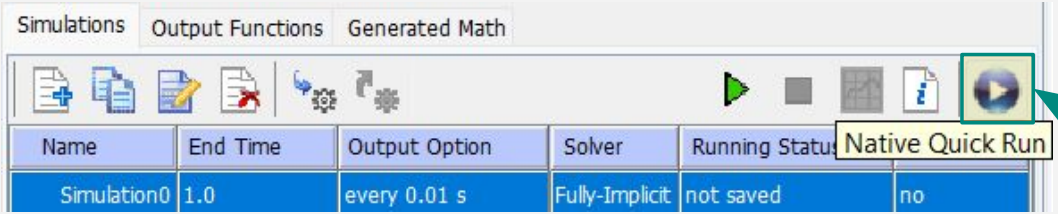
4.4 Start the Simulation

Navigate to the **Simulations** tab and click **New Simulation**. Input a small **End Time**, for example, 1.0 seconds. Set your **Output Option** to every 0.01 seconds to get 100 timepoints of the simulation's progress.

Tip: Start the simulation with a short end time to ensure the running device can load the simulation.

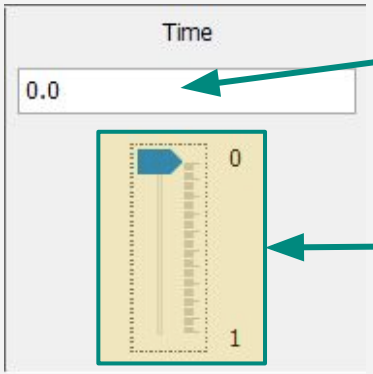






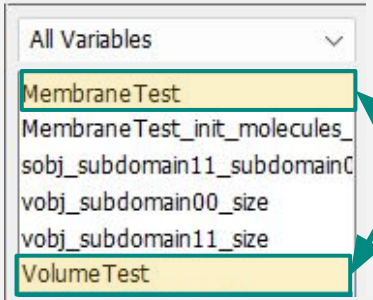
VCell can enable reactions in two ways. For this tutorial, click the blue button, **Native Quick Run**. This is preferred for quick simulations. For longer simulations, select the green button, which will run it in the VCell server.

4.5 Navigating the Simulation

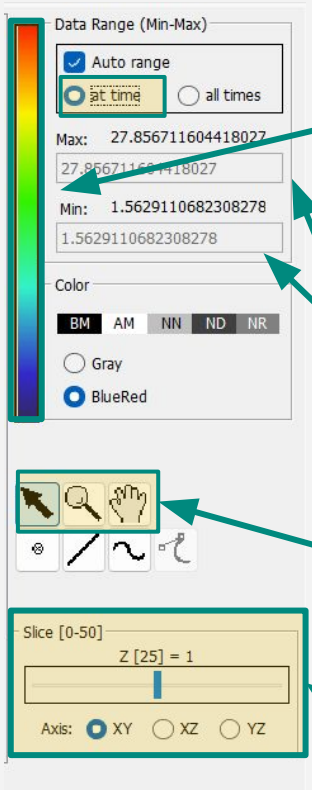


Enter the time to see the results.

This slider allows the user to view how the simulation progresses through the allotted time period.



Choose **MembraneTest** or **VolumeTest** to see the concentrations of the respective species..



To the right, there are tools that help to interpret and navigate the simulation.

The color scale shows the concentration of a selected species (blue is the minimum value, red is the maximal). The minimum and maximum values can be seen at a given time (selected), or at all times.

These are the maximal and minimal values of concentrations at a given time point.

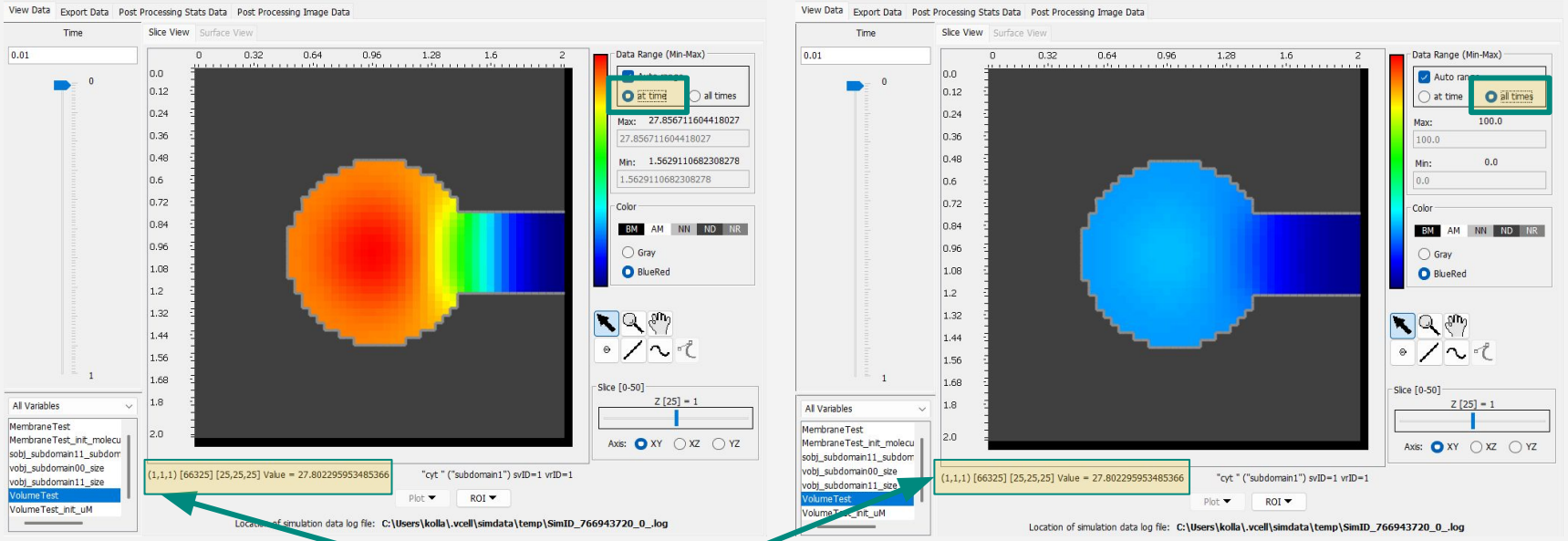
Use the mouse, zoom, and hand features to help you move around the simulation space.

Use the Z-Slider to choose the proper plane (e.g. XY) and shift through geometry slices (z=25 here).

At Time:

v.s.

All Times:



The concentration value at the cursor position [1,1,1] is 27

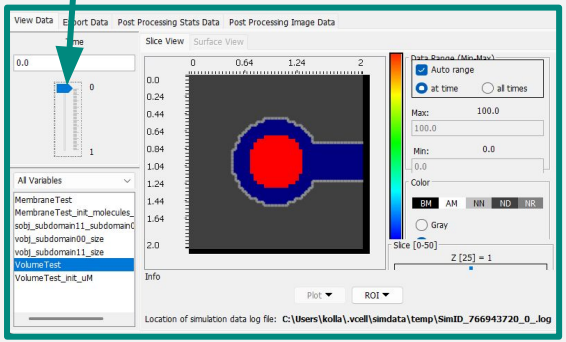
At Time shows the color scale relative to a specific time point, meaning that the red corresponds to the maximum concentration at that time and the blue represents the minimum.

All Times shows the species concentration relative to the entire duration of the simulation. In the color scale, the red would correspond to the highest concentration of a selected species over the entire simulation, whereas the blue corresponds to the lowest. One can see that at this time point, all concentrations are relatively low compared to the maximum value 100.

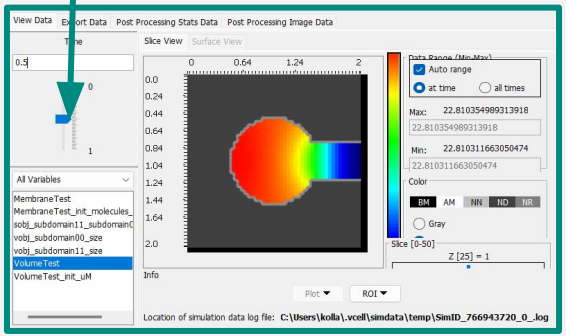
4.6 Viewing Volume Simulation

To view the simulation of the volume, click **Volume Test** under the left tab.

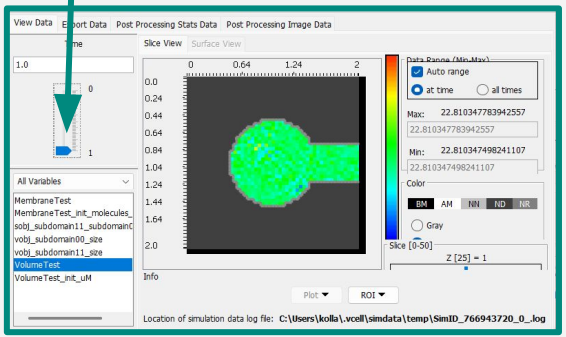
0 sec



0.5 sec



1 sec

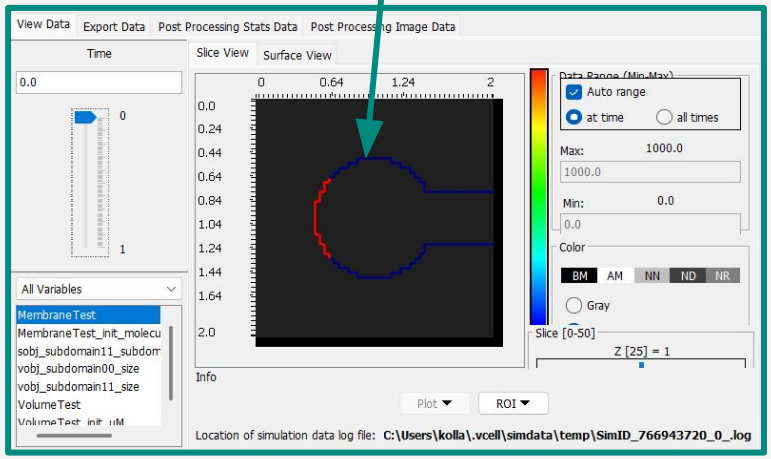


The simulation is correct if there are no leaks and the diffusion is everywhere where it is intended. At the end, the dendritic spine should be almost uniform in color.

4.7 Viewing Membrane Simulation

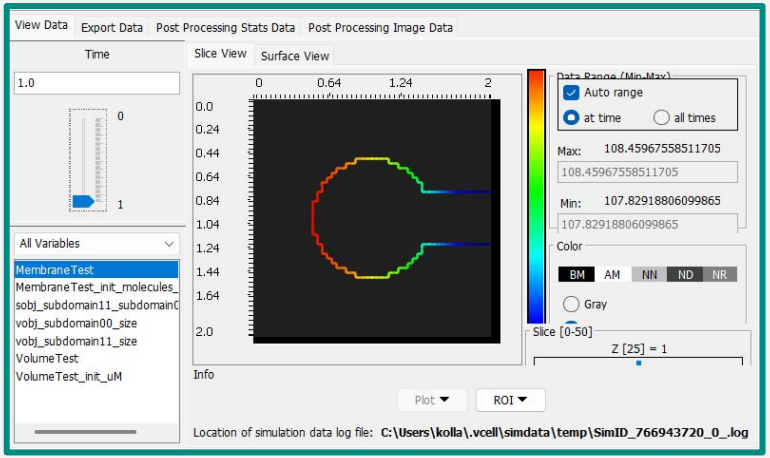
0 sec

Dark blue



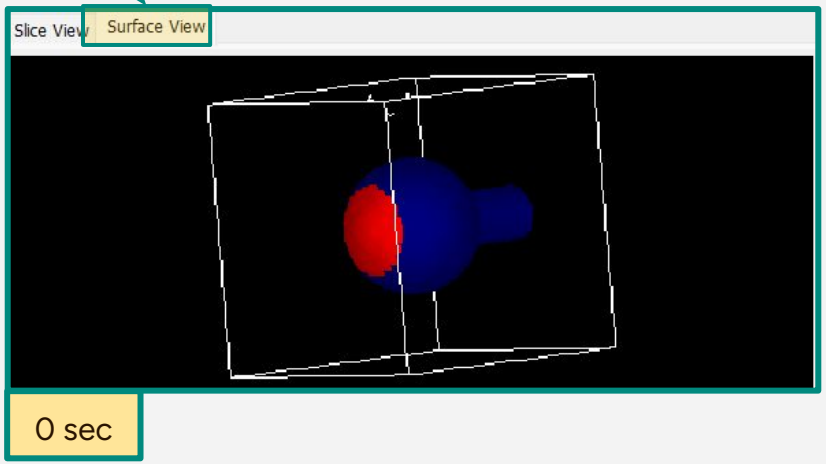
MembraneTest species is initially concentrated at the top of the bouton (the red value is 1,000), whereas the rest of the membrane has zero concentration (dark blue).

1 sec

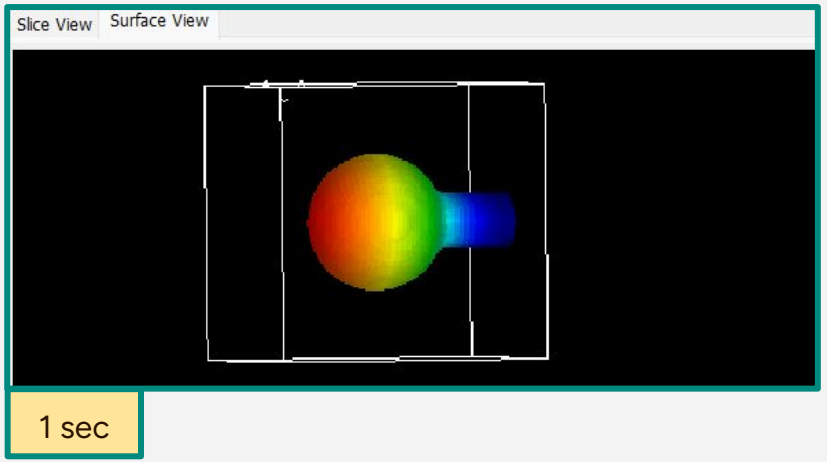


At 1 second, the species diffuses towards the neck. For the fast diffusion, the red value at the top is 108, while the blue value at the bottom of the neck is 107, which signifies that it is almost uniform.

To view the same simulation of membrane diffusion but in 3D, click on **Surface View.**



0 sec



1 sec

Don’t forget to save your model!

Acknowledgments

This tutorial was prepared by Sreekirthana Kolla (East Granby High School) and Justine Laureano (East Hartford High School) under the guidance of Dr. Michael L. Blinov, Associate Professor, Center for Cell Analysis and Modeling. The students were funded by the Department of Health Career Opportunity Programs; the Aetna Foundation; Connecticut State Legislative Fund; John and Valerie Rowe Health Professions Scholars Program; The Hartford; the University of Connecticut Foundation; the Friends of the Department of Health Career Opportunity Programs; and UConn Health.