VCell Tutorial

FRAP: Fluorescence Redistribution After Photo bleaching

Create a simple biomodel and spatial (PDE) application to simulate a photobleaching experiment and view the results.
In this tutorial...

- Gain a basic introduction to the Virtual Cell interface
- Create a very simple biomodel with species but no reactions
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a simple geometry
- Define initial concentrations that are non-uniform using Boolean expressions
- View and analyze results of a spatial simulation
To re-open a model, click on the folder that the model was saved in and double-click on the model.
Choose the select tool and select the compartment. Type “EC” under Structure Name and “Extra Cellular” under Annotation.
Click on the compartment tool, and right-click the dotted black lines so that they turn green and click “Add Membrane”.
Next to Structure Name type “PM” (which stands for Plasma Membrane).

Click on the select tool.

Click on the label “m0”.

Click on the label “PM”.
Click on the compartment tool, and to the right of PM, right click on the dotted black lines so that they turn green and click “Add Compartment”.
Click on the select tool and click on the newest compartment. Next to Structure Name type “Cyt” and next to Annotation type “Cytosol”.
Select the species tool. Click on a point within the “Cyt” compartment and click to create a new species.
Next to Species Name type “Dex” and next to Annotation type “Dextran”.

Species Name: Dex
Annotation: Dextran
Click "Applications" > "Add New" > "Deterministic".
Double click on the name box and rename the application as “FRAP”. Press “Enter” on your keyboard to finalize.
Double click “FRAP” and click on “Geometry” > “Geometry Definition” > “Add Geometry” > “New”. 
Click “Analytic Equations (2D)” > “OK”.
Double click on “Subdomain0” and type in “EC”. Press “Enter” on your keyboard to finalize the name.
Click "Add Subdomain" > "Analytic".
Click the drop down menu next to “Select Subdomain Shape:” and click “Circle”.

Type in “10” for the radius.

Click “Add New Subdomain”.
Double click on the name box of the new subdomain and type in “Cyt”. Press “Enter” on your keyboard to finalize the name.
Click the black down arrow icon to adjust the Slice View window.
Click “Edit Domain”
In the "Size" row, type in "22" for X and Y. In the "Origin" row, type in ":-11" for X and Y.

Click "OK".
Your “Slice View” should be a circle inside of a square.

Click “Front” or “Back” to rearrange the geometry order. The order determines which subdomain a point in space belongs to; the front layer “hides” layers below.
Under Geometry > Structure mapping, select the line tool.

Drag a line from the structures to their corresponding subdomains.
Click “Specifications” > “Species”.

Double click on the “Initial Condition” box for Dex and type in “(10.0*((x<-5.0)||(x>5.0)||(y<-5.0)||(y>5.0)))”. Press “Enter” on your keyboard to finalize. This Boolean expression for the initial concentration evaluates to 10 um everywhere except from x = -5 to 5 and from y = -5 to 5, where the expression evaluates to 0.
Type in “20” under “Diffusion Constant”. Press “Enter” on your keyboard to finalize.
Click “Simulations” and the new simulation icon.
Double click on “Simulation0” and type in “FRAP”. Press “Enter” on your keyboard to finalize.
Click the edit simulation icon.
Click “Mesh”.

Leave “Lock aspect ratio” checked. Type in “51” for X “Mesh Size”.
Click “Solver”.

Type “3.0” for the Ending Time Bound.

Type in “.01” for the Maximum Time Step.

Type “0.05” for the Output Interval.

Click “OK”.

Press the green play button to run the simulation.
Type in a name for your FRAP model.

Click “Save”.

Please type a new name:
FRAPTutorial

Save
Cancel
Under “Running Status” you can view the status of the simulation. You can view the results as soon as there are time points saved to the database.
To change the time frame being viewed, type in a value under “Time” or hold down and drag the slider under “Time”.

The maximum and minimum values correspond to the colors shown.
Select the line tool, click on a point within the data and click on another point. A line will form and connect the two points.

Click “Plot” > “Spatial”.
Click the spreadsheet icon to open a spreadsheet of the graph.

Click “X” to close.
Select the dot tool and click on a point within the data and click on another point.

Click “Plot” > “Time”.
Click “X” to close.

Click the spreadsheet icon to open a spreadsheet of the graph.
Next VCell tutorial: FRAP with Binding