CompuCell 3D

Computer Setup Guide

Version 0.5

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MacOS Account Setup Guide

Note: Everything on the Mac is case sensitive, so make sure you type the username and password exactly as they are given to you.

Because the class will be sharing common disk space, before you begin your adventure with CompuCell you need to set up some directories in the shared account. In particular, you will need to create your own directory to keep your materials separate from those of your classmates.

First, in the course home directory create a directory for yourself where you will store the results of your simulations.

First, open X-Terminal by clicking the X-icon at the bottom center of the screen and type:

```
mkdir <your_name> - create your personal directory.
cd <your_name> - change directories into the newly created one.
mkdir simulations - create a subdirectory where you will store the results of your simulations.
```

Next you will copy the run script and cellsort.xml into your simulation directory. Type:

```
cd simulations – change directories into the simulation subdirectory.
```

cp /usr/local/CompuCell/run* - copy the CompuCell execution file into your simulation directory.

cp /usr/local/CompuCell/cellsort.xml – copy the cell sorting sample file into your simulation subdirectory.

As you can see CompuCell is installed in the /usr/local/CompuCell directory on our Mac machines.

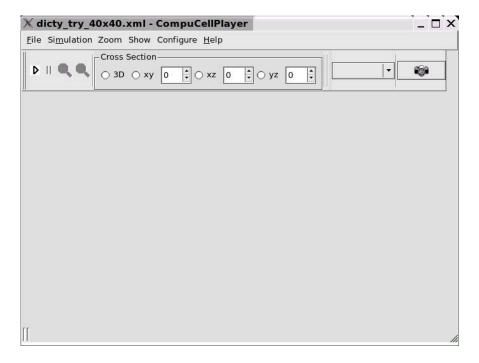
Now, to run CompuCell, while in simulations directory type:

```
./run_CompuCellNew.sh
```

This command will pop up the player window. Before you start running your simulation, spend some time configuring the player. You will need to configure cell colors (do so for at least 5 cell types, for future convenience) and screenshot frequency.

Note: Please do not switch to 3D mode as this mode currently runs extremely slowly under MacOS and may crash CompuCell. Apparently the Qt library on MacOS does not have good support for 3D graphics or some settings may be misconfigured. We will work to fix these problems in the coming weeks.

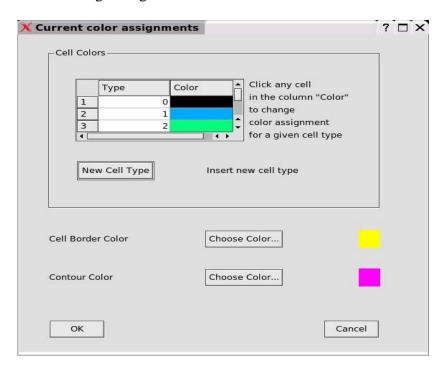
Your screen should now contain a window that looks like this:



This is CompuCell Player's main window.

Cell Color Configuration

Before we go further, let's configure cell colors so that when you start simulations cells will be visible on the screen. Click on Configure in the top menu bar and select Cell Type Colors You should see the following dialog window:

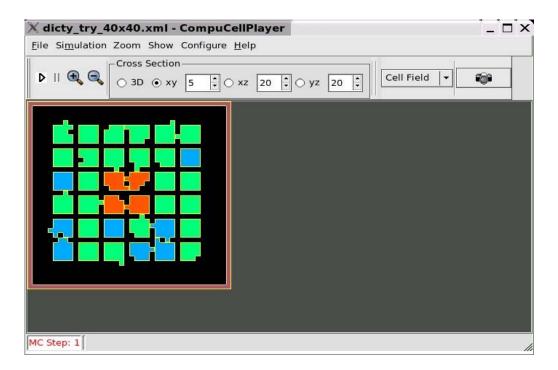


To add new cell types, click on the button New Cell Type. In the table below new row will be inserted (you may need to scroll down the table to see this new field). In the column labeled Type, type the new type id number for the new cell type (we recommend starting your cell-type numbering from zero and

using ascending integers). TypeId=0 is reserved for the cell type Medium. User-defined types will have TypeIds greater than 0. Now, click the field in the column labeled Color. The Familiar Color Dialog Box will pop up. Use it to choose a color. You may add as many cell types as you like following same procedure. Add as many cell types as you wish (you are unlikely, however, to use more that 10 types in this class). Adding colors now will save you work in the future. You may also choose the color for cell borders by clicking the Choose Color... button next to the label Cell Border Color. Once you are done with color configuration click OK and click Configure to pull down a file menu and select Save Default Settings to save your settings.

Running the Simulation

Now, let's come back to the main CompuCell Player window. We hope that when you look at this window you will be able to figure out for yourself what you need to do in order to start running a simulation. You need to go to pull down the File menu and choose Open (or type Ctrl-o). Once you are in the Open File dialog, choose any file which contains an .xml description of your simulation (we recommend that you give such files the extension .xml because this is the extension that Player looks for by default). Once you select the file, the title bar will display the simulation source file name and the window should look like this:



Once you have selected your .xml file, you start running your simulation by clicking the Play button, which is labeled button on the toolbar. If the .xml file contains a valid model, the simulation will start and the screen will display a two dimensional projection of a slice through the simulation lattice. In the picture above we have just started a simulation using the .xml file dicty_try_40x40.xml

Next to the button you can see the Pause button, labeled II, which allows you to pause (temporarily halt) the simulation to examine the simulation lattice. To restart the simulation click the Play button again—just as on a CD player.

Running and pausing a simulation was simple. Now let's familiarize ourselves with the rest of the toolbar:

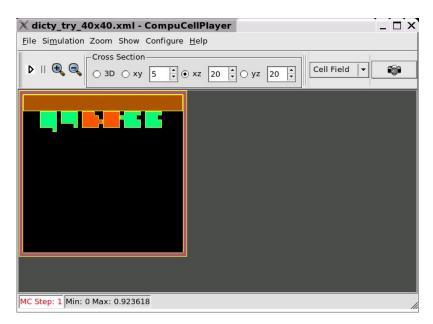


Next to the Play and Pause buttons are Zoom In and Zoom Out buttons, labeled. These magnify or shrink image that the Player displays.

Next to the Zoom In and Zoom Out buttons are a group of buttons you can use to view different projections through the lattice or to switch to 3D visualization.

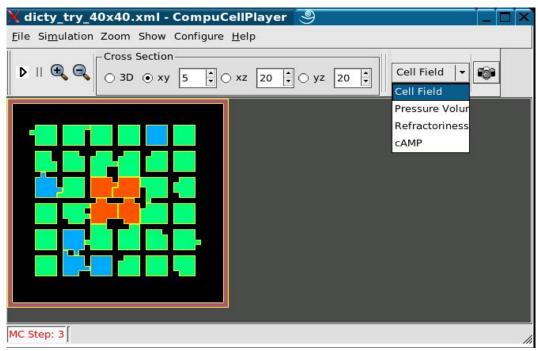
Viewing Lattice Projections

You can select the direction of the displayed slice through the simulation lattice using the radio buttons labeled xy, xz, yz. For example if you click on the xy button to select it, the screen will display a slice along the xy plane of the simulation lattice. The z coordinate of the slice is shown by the value in the scroll box next to the xy button. In the picture above, this value is 5. Below, we show another projection, a view of the simulation lattice sliced by the xz plane for y=20:

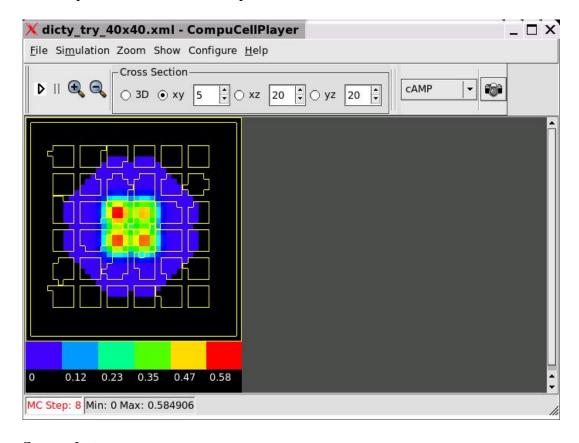


Switching plot types

CompuCell Player can display not only cells but also other quantities associated with the simulation. For example whenever you are using chemical field in your simulation, you can visualize concentration by selecting appropriate item from the pull down list next to Cross Section group:

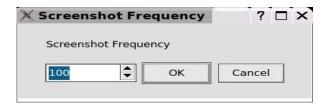


Here you can see that in addition to displaying colored cells themselves you can see concentration profile of cAMP or of the inhibitor (we call it here refractoriness). You can also visualize pressure inside the cell (which we define to be the difference between target volume and volume of the cell). As an example we will show cAMP profile:



Screenshots

When the simulation is running whatever you see on the screen is recorded on your hard drive as .png image. You can configure frequency (expressed in MCS) with which screenshots are saved by going to Configure->Screenshot Frequency dialog. The following window will pop-up:



Additional Screenshots

Quite often when you run a simulation you want to be able to record not just one lattice view, but several. For example you want to see what cells are doing but also want to follow changes in chemical concentration. CompuCell Player allows to store lattice views that are not visible on the screen. The way you do it is the following; you start simulation. Once started you may pause it, although it is not a requirement. Now you may switch to a different lattice view, say cAMP profile, and press the camera

button located on a toolbar. From now on, the view for which you have pressed the camera button will be saved even if you switch to a different view.