# Setting up MacOS for PhysiCell



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@PhysiCell

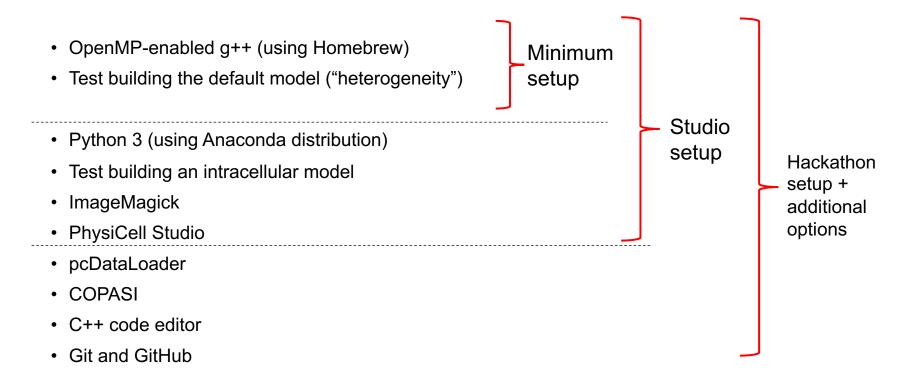
# **PhysiCell Project**

July 2023





### **Presentation overview**



# Brief notes on this install guide

- We tried to make all the Terminal commands bold face and able to be directly copied (command + c) and pasted (command + v) directly into the Terminal
- Note that this is a static document it is possible that the commands could vary slightly as version numbers change.
- Apple Intel CPU vs. Silicon (M1/M2) CPU
  - ◆ You may experience some problems with our setup instructions if you have the newer Apple Silicon CPU. If so, please contact us (see Support links at end).

- OpenMP-enabled g++ (using Homebrew)
- Test building the default model ("heterogeneity")
- Python 3 (using Anaconda distribution)
- Test building an intracellular model
- ImageMagick
- PhysiCell Studio
- pcDataLoader
- COPASI
- C++ code editor
- · Git and GitHub

# OpenMP-enabled g++

- The default /usr/bin/g++ (clang) that comes with macOS is not OpenMP-enabled. You need to install one that is.
- Homebrew (a package-manager for macOS) will let you do this.
- <a href="https://brew.sh/">https://brew.sh/</a>
  Install Homebrew
  Click to copy the bash command
  \$ /bin/bash -c "\$(curl -fs\$L https://raw.githubusercontent.com/Homebrew/install.sh)"

Open a new 'Terminal' window and paste the copied command there:

Continue to next slide →

https://docs.brew.sh/Installation - additional useful information if needed

Press 'return' to execute the command you copied into the Terminal window. Then 'return' again to continue the installation of Homebrew.

This will take a few minutes, depending on your network speed.

When installation is finished, you can see where it got installed using the "which" command:

#### which brew

This may result in:

/usr/local/bin/brew

or, possibly here, on the Mac M1/M2:

/opt/homebrew/bin/brew

or possibly a different path, but it's not that important, except for some of the following instructions.

Continue to next slide →

Once you've completed installing the basic Homebrew package manager, proceed to install an OpenMP-enabled g++ using the Terminal command:

#### brew install gcc

Again, this will take a few minutes. This page <a href="https://formulae.brew.sh/formula/gcc">https://formulae.brew.sh/formula/gcc</a> will tell you the current stable gcc/g++ version, e.g., 13.1.0

When it completes, you can again use "which" to see where it is installed:

#### which g++-13

Again, this may be:
/usr/local/bin/g++-13
or,
/opt/homebrew/bin/g++-13

or whatever path homebrew used as its default directory.

Continue to next slide →

Once you've completed installing the basic Homebrew package manager, proceed to install an OpenMP-enabled g++ using the Terminal command:

#### brew install gcc

Again, this will take a few minutes. This page <a href="https://formulae.brew.sh/formula/gcc">https://formulae.brew.sh/formula/gcc</a> will tell you the current stable gco/g. r version, e.g., 13.1.0

When it completes, you can again use "which" to see where it is installed:

#### which g++-13

Again, this may be: /usr/local/bin/g++-13

or,

/opt/homebrew/bin/g++-13

or whatever path homebrew used as its default directory.

If you use this install guide later (much after July 2023), this is an example of a command that may need updated.

Homebrew will, at some point, switch to g++-14. There are other similar points later in the presentation – pretty much any time there is a version number – that version number might have changed by the time you use the guide!!!

Continue to next slide →

### PHYSICELL CPP

• As described in the Quickstart guide: Quickstart (note – this is deprecated), but may be helpful if you have trouble – hopefully the video will get you where you need to be!

You need to define an environment variable that will point to this g++ so that a PhysiCell Makefile will know to use it. export PHYSICELL\_CPP=g++-13

(Your PATH env var should have the full path to homebrew's /bin in it and therefore be able to find it)

• Furthermore, we recommend that you make this a permanent feature of any new Terminal Shell window that you open. To do this, you want to copy/paste the above export command into a special, existing configuration file. This file will be in your HOME directory (type: echo \$HOME) and the name of the config file will depend on the type of shell that you are using — most likely either "bash" or "zsh". To find out which, run:

echo \$SHELL

It should print out either: /bin/bash or /bin/zsh
If you are using "bash", you should have a .bash\_profile file (has a preceding "."); if "zsh" then a .zshenv file in your home directory. If this file does not exist, you will need to create it. From a Terminal shell do:

```
cd ~ # go to your home directory
touch .bash profile # or for zsh, touch .zshenv
```

https://support.apple.com/guide/terminal/use-environment-variables-apd382cc5fa-4f58-4449-b20a-41c53c006f8f/mac for more about env vars



### PHYSICELL CPP (cont'd)

• To permanently put the previous export command into your shell's configuration file, so that it is executed each time a new shell is opened, run one of the following in your Terminal (again, depending on which shell you are using):

```
echo export PHYSICELL_CPP=g++-13 >> ~/.bash_profile
or,
echo export PHYSICELL_CPP=g++-13 >> ~/.zshenv
```

When you open a <u>new</u> Terminal shell, you can verify that this is defined:
 echo \$PHYSICELL CPP

You should see this printed out: q++-13

### PHYSICELL CPP (cont'd)

• To permanently put the previous export command into your shell's configuration file, so that it is executed each time a new shell is opened, run one of the following in your Terminal (again, depending on which shell you are using):

```
echo export PHYSICELL_CPP=g++-13 >> ~/.bash_profile
or,
echo export PHYSICELL_CPP=g++-13 >> ~/.zshenv
```

When you open a new Terminal shell, you can verify that this is defined:

```
echo $PHYSICELL_CPP
```

You should see this printed out:

This instruction appears several times. We really mean it. When you start a new terminal, that causes multiple programs to relaunch. In this case, you will "source" your bash profile/zshenv.

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# Test build/run: PhysiCell model (1)

- Get PhysiCell
  - Open browser and navigate to <a href="https://raw.githubusercontent.com/physicell-training/ws2023/main/setup/get">https://raw.githubusercontent.com/physicell-training/ws2023/main/setup/get</a> physicell.py
  - Using the menu, go to File → Save Page As → get\_physicell.py in Downloads
    - ◆ Can view other releases and release notes at: <a href="https://github.com/MathCancer/PhysiCell/releases">https://github.com/MathCancer/PhysiCell/releases</a>
- Unzip PhysiCell

```
Assuming the get physicell.py is downloaded to your ~/Downloads directory:
```

- ~/Downloads\$ python get\_physicell.py
- ~/Downloads\$ mv PhysiCell.zip ~ # move this .zip file to your home directory
- ~/Downloads\$ cd ~ # change to home directory
- ~\$ unzip -q PhysiCell.zip
- ~\$ cd PhysiCell
- ~/PhysiCell\$



# Test build/run: PhysiCell model (2)

~/PhysiCell\$ make # from this directory, just run 'make' (or make -j 2 to use 2 cores and speed up compilation)

→ You will see the following output:

make heterogeneity-sample

```
cp ./sample_projects/heterogeneity/custom_modules/* ./custom_modules/
touch main.cpp && cp main.cpp main-backup.cpp
cp ./sample_projects/heterogeneity/main-heterogeneity.cpp ./main.cpp
cp Makefile Makefile-backup
cp ./sample_projects/heterogeneity/Makefile .
cp ./config/PhysiCell_settings.xml ./config/PhysiCell_settings-backup.xml
cp ./sample_projects/heterogeneity/config/* ./config/
make
g++-13 -march=native -O3 -fomit-frame-pointer -mfpmath=both -fopenmp -m64 -std=c++11 -c ./BioFVM/BioFVM_vector.cpp
... (continues to compile files)...
g++-13 -march=native -O3 -fomit-frame-pointer -mfpmath=both -fopenmp -m64 -std=c++11 -o heterogeneity BioFVM_vector.o BioFVM_mesh.o
BioFVM_microenvironment.o BioFVM_solvers.o BioFVM_matlab.o BioFVM_utilities.o BioFVM_basic_agent.o BioFVM_MultiCellDS.o
BioFVM_agent_container.o pugixml.o PhysiCell_phenotype.o PhysiCell_cell_container.o PhysiCell_standard_models.o PhysiCell_cell.o
PhysiCell_custom.o PhysiCell_utilities.o PhysiCell_constants.o PhysiCell_settings.o PhysiCell_geometry.o heterogeneity.o main.cpp
```



~/PhysiCell\$

Executable name is heterogeneity

# Test build/run: PhysiCell model (3)

~/PhysiCell\$ ./heterogeneity # run the model

... > lots of model configuration info will be printed out, and then info at each specified output interval:

Oncoprotein summary:

\_\_\_\_\_

mean: 1.00687

standard deviation: 0.250737 [min max]: [0.205535 1.71906]

Using PhysiCell version 1.12.0

Please cite DOI: 10.1371/journal.pcbi.1005991 Project website: http://PhysiCell.MathCancer.org

See ALL CITATIONS.txt for this list.

current simulated time: 0 min (max: 64800 min)

total agents: 890

interval wall time: 0 days, 0 hours, 0 minutes, and 2.1e-05 seconds total wall time: 0 days, 0 hours, 0 minutes, and 2.4e-05 seconds

Using method diffusion decay solver constant coefficients LOD 2D (2D LOD with Thomas Algorithm) ...

current simulated time: 60 min (max: 64800 min)

total agents: 896

interval wall time: 0 days, 0 hours, 0 minutes, and 1.89867 seconds total wall time: 0 days, 0 hours, 0 minutes, and 1.8987 seconds



# Test build/run: PhysiCell model (4)

current simulated time: 60 min (max: 64800 min)

total agents: 896

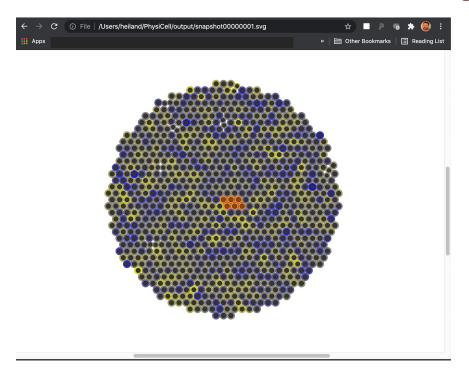
interval wall time: 0 days, 0 hours, 0 minutes, and 1.89867 seconds total wall time: 0 days, 0 hours, 0 minutes, and 1.8987 seconds

You can press "control-c" to cancel the simulation and then type: **Is output** # list files created in the /output directory

```
(base) M1P~/PhysiCell$ ls output/
PhysiCell settings.xml
                                                output00000000.xml
                                                                                                 output00000002.xml
empty.txt
                                                output00000000 attached cells graph.txt
                                                                                                 output00000002 attached cells graph.txt
                                                output00000000 cell_neighbor_graph.txt
                                                                                                 output00000002 cell_neighbor_graph.txt
initial.svg
initial.xml
                                                output00000000 cells.mat
                                                                                                 output00000002 cells.mat
initial attached cells graph.txt
                                                output00000000 microenvironment0.mat
                                                                                                 output00000002 microenvironment0.mat
initial_cell_neighbor_graph.txt
                                                output00000001.xml
                                                                                                 snapshot00000000.svg
initial_cells.mat
                                                output00000001_attached_cells_graph.txt
                                                                                                 snapshot0000001.svg
initial mesh0.mat
                                                output00000001 cell neighbor graph.txt
                                                                                                 snapshot00000002.svg
initial microenvironment0.mat
                                                output00000001 cells.mat
                                                output00000001 microenvironment0.mat
legend.svg
```



# Test build/run: PhysiCell model (5)



To easily visualize the cells at a particular output interval, you can simply open one of the .svg files in your Web browser. Beware that it will be rather large, but you can use the scrollbars to find the heterogeneous tumor of cells at the center of the domain.

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# **Python**

Python is a requirement for certain aspects of PhysiCell:

- It is used for PhysiCell Studio.
- It is needed to install certain libraries for the intracellular models.
- It can be used for visualization and data analysis scripts.
- It can be used for parameter explorations of models.

# Python 3 (not Python 2)

Note that your Mac may have Python 2 installed, by default:

### ~\$ which python /usr/bin/python

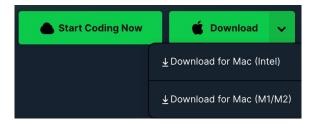
```
~$ python
```

Python 2.7.16 (default, Jan 27 2020, 04:46:15)
[GCC 4.2.1 Compatible Apple LLVM 10.0.1 (clang-1001.0.37.14)] on darwin Type "help", "copyright", "credits" or "license" for more information.

 We want Python 3. (And even if the newer Macs come bundled with Python 3, it will not contain all the modules that we want).

## **Anaconda Python 3.x**

- Download a (free) Python distribution that comes bundled with lots of useful modules that are not in the standard Python library.
- https://www.anaconda.com/products/individual#Downloads
- https://docs.anaconda.com/anaconda/install/mac-os/



Download the appropriate one - Intel or M1/M2(Silicon) for your Mac. If you're unsure, clicking on the Apple logo in your menu bar and "About This Mac" will tell you which "Chip" it has.

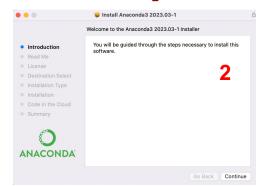
### **Anaconda Graphical Installer**

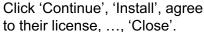
#### ~\$ open Anaconda3-2023.03-1-MacOSX-arm64.pkg

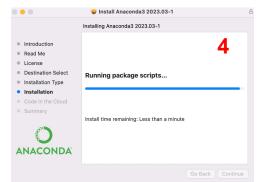
Your installation should resemble these screenshots:

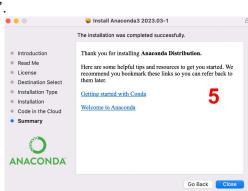


Click 'Allow'









Customize

■ Install Anaconda3 2023.03-1
Standard Install on "Macintosh HD"

will be able to use this software.

IntroductionRead Me

Destination Select

Installation Type

ANACONDA

License

This will take 3.55 GB of space on your computer.

Click Install to perform a standard installation of this software in your home folder. Only the current user of this computer

Change Install Location..

Go Back

### **Confirm Installation**

Open a New Terminal shell to verify you are using the Anaconda Python as your default:

```
~$ which python
/Users/heiland/anaconda3/bin/python

~$ python
Python 3.10.9 (main, Mar 1 2023, 12:20:14) [Clang 14.0.6 ] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

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### Advanced topic: Intracellular sample project

#### ~/PhysiCell\$ make reset

```
rm -f *.cpp
cp ./sample_projects/Makefile-default Makefile
rm -f ./custom_modules/*
touch ./custom_modules/empty.txt
touch ALL_CITATIONS.txt
touch ./core/PhysiCell_cell.cpp
rm ALL_CITATIONS.txt
cp ./config/PhysiCell_settings-backup.xml ./config/PhysiCell_settings.xml
touch ./config/empty.csv
rm -f ./config/*.csv
```

#### ~/PhysiCell\$ make list-projects

Sample projects: template biorobots-sample cancer-biorobots-sample cancer-immune-sample celltypes3-sample heterogeneity-sample pred-prey-farmer virus-macrophage-sample worm-sample interaction-sample mechano-sample rules-sample

Sample intracellular projects: ode-energy-sample physiboss-cell-lines-sample cancer-metabolism-sample

~/PhysiCell\$



### **ODE** intracellular model (1)

#### ~/PhysiCell\$ make ode-energy-sample

```
cp ./sample_projects_intracellular/ode/ode_energy/custom_modules/* ./custom_modules/ touch main.cpp && cp main.cpp main-backup.cpp cp ./sample_projects_intracellular/ode/ode_energy/main.cpp ./main.cpp cp Makefile Makefile-backup cp ./sample_projects_intracellular/ode/ode_energy/Makefile . cp ./config/PhysiCell_settings.xml ./config/PhysiCell_settings-backup.xml cp ./sample projects intracellular/ode/ode energy/config/* ./config/
```

#### ~/PhysiCell\$ **make** python3 beta/setup libroadrunner.py

This model requires the libRoadrunner libraries which will now be downloaded. (for your Darwin operating system) libRoadRunner will now be installed into this location: addons/libRoadrunner

Beginning download of libroadrunner into addons/libRoadrunner ...

https://sourceforge.net/projects/libroadrunner/files/libroadrunner-1.4.18/roadrunner-osx-10.9-cp36m.tar.gz/download
my\_file = addons/libRoadrunner/roadrunner-osx-10.9-cp36m.tar.gz
rrlib\_dir = addons/libRoadrunner/roadrunner-osx-10.9-cp36m
100.0% 96092160 / 96087190
installing (uncompressing) the file...

The ODE solver library is downloaded

Or, for M1/M2: https://github.com/PhysiCell-Tools/intracellular\_libs/raw/main/ode/roadrunner\_macos\_ar m64.tar.gz



Done.

### **ODE** intracellular model (2)

(from previous 'make')

g++-13 -march=native -O3 -fomit-frame-pointer -fopenmp -m64 -std=c++11 -D ADDON ROADRUNNER -I./addons/libRoadrunner/roadrunner/include/rr/C -c ./core/PhysiCell\_cell.cpp

g++-13 -march=native -O3 -fomit-frame-pointer -fopenmp -m64 -std=c++11 -D ADDON ROADRUNNER -I./addons/libRoadrunner/roadrunner/include/rr/C -c ./custom\_modules/custom.cpp

q++-13 -march=native -O3 -fomit-frame-pointer -fopenmp -m64 -std=c++11 -D ADDON ROADRUNNER -I./addons/libRoadrunner/roadrunner/include/rr/C -c ./addons/libRoadrunner/src/librr intracellular.cpp

Your OS= -D OSX

LIBRR CFLAGS= -I./addons/libRoadrunner/roadrunner/include/rr/C

LIBRR LIBS= ./addons/libRoadrunner/roadrunner/lib

g++-13 -march=native -O3 -fomit-frame-pointer -fopenmp -m64 -std=c++11 -D ADDON ROADRUNNER -I./addons/libRoadrunner/roadrunner/include/rr/C -o ode energy BioFVM vector.o BioFVM mesh.o BioFVM microenvironment.o BioFVM solvers.o BioFVM matlab.o BioFVM utilities.o BioFVM basic agent.o BioFVM MultiCellDS.o BioFVM agent container.o pugixml.o PhysiCell phenotype.o PhysiCell cell container.o PhysiCell standard models.o PhysiCell cell.o PhysiCell custom.o PhysiCell utilities.o PhysiCell constants.o PhysiCell SVG.o PhysiCell pathology.o PhysiCell MultiCellDS.o PhysiCell various outputs.o PhysiCell pugixml.o PhysiCell settings.o custom.o librr intracellular.o main.cpp -L./addons/libRoadrunner/roadrunner/lib -lroadrunner c api

created ode energy

~/PhysiCell\$ ./ode energy

dyld: Library not loaded: @rpath/libroadrunner c api.dylib Referenced from: /Users/heiland/PhysiCell/./ode energy Reason: image not found

Abort trap: 6 ~/PhysiCell\$ When we try to run the model, we get an error, but it was expected and serves as a reminder

You will see this output (but not

highlighted ... ) if the executable

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@PhysiCell

was successfully made

if/when you ever see it again. See next slide.



# **ODE** intracellular model (3)

~/PhysiCell\$ export DYLD\_LIBRARY\_PATH=\$DYLD\_LIBRARY\_PATH:./addons/libRoadrunner/roadrunner/lib

~/PhysiCell\$ ./ode\_energy

... model info output...

current simulated time: 30 min (max: 1440 min)

total agents: 144

interval wall time: 0 days, 0 hours, 0 minutes, and 4.27858 seconds total wall time: 0 days, 0 hours, 0 minutes, and 4.27861 seconds

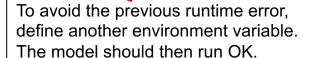
current simulated time: 60 min (max: 1440 min)

total agents: 144

interval wall time: 0 days, 0 hours, 0 minutes, and 4.33063 seconds total wall time: 0 days, 0 hours, 0 minutes, and 8.60924 seconds

----- start: librr\_intracellular.cpp: start() called

... (lots more output)...



And once again, you could use your browser to open one of the .svg files that are created in /output

## **ODE** intracellular model (4)

As before, permanently put this environment variable in your (bash or zsh) shell's config startup file:

export DYLD\_LIBRARY\_PATH=\$DYLD\_LIBRARY\_PATH:./addons/libRoadrunner/roadrunner/lib >> ~/.bash\_profile
OI,

export DYLD\_LIBRARY\_PATH=\$DYLD\_LIBRARY\_PATH:./addons/libRoadrunner/roadrunner/lib >> ~/.zshenv

Then when you start a *new* Terminal Shell window, this environment variable will be defined.

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### ImageMagick (1)

<u>https://imagemagick.org/</u> - free, powerful image conversion, composition, editing software.

# ImageMagick (2)

Refer to the Quickstart guide for helpful ImageMagick commands, (note – this is deprecated but may be helpful) including Makefile targets:

As an example, if you have generated some .svg files (in /output), you should be able to generate an animation, using something like the following set of commands in your shell:

```
convert snapshot000034*.svg foo.gif
magick animate foo.gif  # may be huge, if original SVGs were; downsize in following steps
convert foo.gif -coalesce tmp.gif
identify snapshot00003471.svg  # get size of a single image (e.g. 1500x1605)
convert -size 1500x1605 tmp.gif -resize 20% small.gif
magick animate small.gif
```

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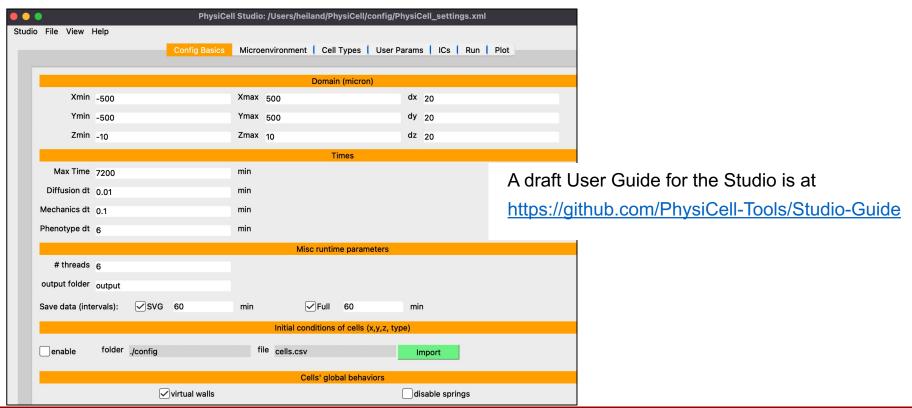
# PhysiCell Studio (1)

- PhysiCell Studio is a desktop graphical tool to let you create/edit a .xml configuration file that defines a PhysiCell model. The Studio also lets you run a simulation, plot results, and more.
- Download the latest release at: <a href="https://github.com/PhysiCell-Tools/PhysiCell-Studio/releases">https://github.com/PhysiCell-Tools/PhysiCell-Studio/releases</a>
- Copy or move the .zip to the same level as your PhysiCell directory, unzip it, and run the Studio, e.g.:

```
~$ unzip PhysiCell-Studio-2.26.7.zip
~$ python ~/PhysiCell-Studio-2.26.7/bin/studio.py
```

This should display the Studio (next page):

# PhysiCell Studio (2)



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### pcDataLoader

- Used to load PhysiCell data
  - Python based data loader
  - Facilitates post-simulation analysis
- Additional information (tutorials, reference guide etc) and latest releases at: <a href="https://github.com/PhysiCell-Tools/python-loader">https://github.com/PhysiCell-Tools/python-loader</a>

- From any running terminal:
   ~/PhysiCell\$ pip3 install pcdl
- pcDataloader should now be available for import at any python prompt

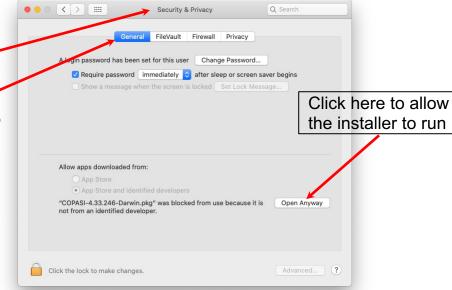
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## SBML editors: COPASI (1)

- COPASI, SBML, and SBML editors:
  - COPASI can simulate some categories of mathematical models (ordinary and stochastic differential equations) among other features
  - COPASI Provides a graphical interface for editing Systems Biology Markup Language (SBML)
    - ♦ SBML is a language used to encode biological models, often intracellular models
      - » The ode-sample-model is written in SBML as is the FBA example
  - Note: there are other SBML editors (search "SBML editors" for other options)
- For the PhysiCell workshop, SBML model creation and editing will be demonstrated with COPASI

# SBML editors: COPASI (2)

- Navigate to <a href="http://copasi.org/Download/">http://copasi.org/Download/</a> and download COPASI for Mac OS X
- Follow instructions here: <a href="http://copasi.org/Support/Installation/Mac">http://copasi.org/Support/Installation/Mac</a> OS X/
- Once downloaded and activated, you may be challenged by Apple security as this app isn't from the App Store
  - To get around this:
    - ◆ Go to Settings → Security & Privacy, then the General tab in Security & Privacy
    - ◆ If you recently ran the package file, there will be something like "COPASI" was blocked from use because it is not from an identified developer." and an option "Open Anyway" → Click "Open Anyway"
- Complete installation via the COPASI Installer
  - It should be fine to accept the defaults...



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- Git and GitHub

### C++ Code editor

When you get to the point of editing the custom C++ code for your model, you will want a decent code editor. If you're already using one (for C or C++), great! - keep using it. But if you are new to programming, we recommend keeping it pretty simple. If you just search "C++ code editor macOS", you'll find some good suggestions.

One popular, free integrated development environment (IDE) that can be used in a minimal fashion for editing is VSCode (<a href="https://code.visualstudio.com/">https://code.visualstudio.com/</a>).

### **Version control**

When you get to the point of editing the custom C++ code, python scripts for analysis, etc, it is common to use version control for your code and to share with collaborators. If you are already using version control great! - keep using it. If you are new to programming, we recommend using git. A search for "git mac install" will yield helpful results. (You may even already have it – it is included in XCode command line tools).

Once you have git, <u>github.com</u> is a common place to share code. There are also many graphical interfaces for git (GitHub has one for example.)

## **Support**

- We encourage you to join and actively use the <u>PhysiCell community</u>
   <u>Slack channel</u>. There, you can post questions (<u>#troubleshooting</u>), answer questions, and (hopefully) share successful modeling stories.
- Alternatively, you can submit problem tickets at <a href="https://sourceforge.net/p/physicell/tickets/">https://sourceforge.net/p/physicell/tickets/</a>
- Finally, please follow us on Twitter <u>@PhysiCell</u> and <u>@MathCancer</u>.

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