https://github.com/physicell-training/ws2022

# **Setting up MacOS** for PhysiCell

Randy Heiland and John Metzcar



@PhysiCell

## PhysiCell Project

July 17, 2022



### **Overview**

- Apple Intel CPU vs. Silicon (M1) 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 page at end).

Minimal

setup

- OpenMP-enabled g++ (using Homebrew)
- Test building the default model ("heterogeneity")
- Python 3 (using Anaconda distribution)
- Test building an intracellular model
- ImageMagick
- PhysiCell Model Builder

\*At the end of the slides, we includes notes on other useful software including COPASI. **COPASI is required** for the 2022 PhysiCell workshop – *so make it through to the end!* 



Traditional\*

setup

## Brief note on this presentation

- 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.

## 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/HEAD/install.sh)"

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

```
Terminal Shell Edit View Window Help

| Comparison of the comparis
```

Continue to next slide →

https://docs.brew.sh/Installation - more 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. It should include or end with something like this (perhaps with the name of your macOS version instead of "monterey")

```
=> Installing gcc

=> Pouring gcc--11.3.0_2.monterey.bottle.tar.gz
```

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

#### which g++-11

Again, this may be:

/usr/local/bin/g++-11

or,

/opt/homebrew/bin/g++-11

or whatever path homebrew used as its default directory.

Continue to next slide →



### PHYSICELL CPP

 As described in the Quickstart guide: <a href="https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#macos">https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#macos</a>

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++-11

(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++-11 >> ~/.bash_profile
or,
echo export PHYSICELL_CPP=g++-11 >> ~/.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: g++-11

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- PhysiCell Model Builder

## Test build/run: PhysiCell model (1)

- At this point, you should be able to compile and run the default PhysiCell model.
- Download the latest release of PhysiCell from: <a href="https://github.com/MathCancer/PhysiCell/releases">https://github.com/MathCancer/PhysiCell/releases</a> e.g.,

https://github.com/MathCancer/PhysiCell/releases/download/1.10.3/PhysiCell V.1.10.3.zip

Assuming the file is downloaded to your ~/Downloads directory, move it to your home directory:

```
~/Downloads$ mv PhysiCell_V.1.10.3.zip ~ # move this .zip file to your home directory ~/Downloads$ cd ~ # change to home directory ~$ unzip -q PhysiCell_V.1.10.3.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++-11 -march=native -O3 -fomit-frame-pointer -mfpmath=both -fopenmp -m64 -std=c++11 -c ./BioFVM/BioFVM_vector.cpp
... (continues to compile files)...
g++-11 -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_container.o PhysiCell_standard_models.o PhysiCell_cell.o
PhysiCell_custom.o PhysiCell_utilities.o PhysiCell_constants.o PhysiCell_basic_signaling.o PhysiCell_geometry.o heterogeneity.o main.cpp
```

Executable name is heterogeneity

~/PhysiCell\$



## Test build/run: PhysiCell model (3)

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

...  $\rightarrow$  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 1.10.3

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)

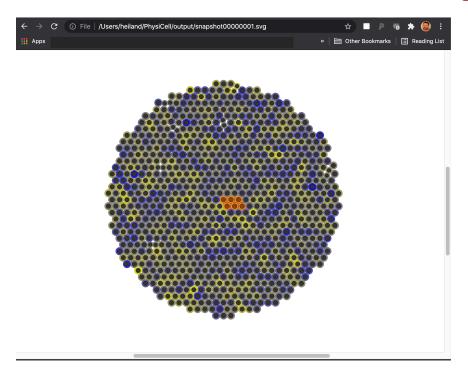
total agents: 896

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

```
~/PhysiCell$ ls output/
                                        initial microenvironment0.mat
PhysiCell settings.xml
                                                                                 output00000001 cells.mat
                                                                                 output00000001 cells physicell.mat
emptv.txt
                                        legend.svg
                                        output00000000.xml
                                                                                 output0000001 microenvironment0.mat
initial.svg
                                        output00000000 cells.mat
                                                                                 snapshot00000000.svg
initial.xml
initial cells.mat
                                        output00000000 cells physicell.mat
                                                                                 snapshot00000001.svg
initial_cells_physicell.mat
                                        output0000000 microenvironment0.mat
initial mesh0.mat
                                        output00000001.xml
/PhvsiCell$
```

## 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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- PhysiCell Model Builder
- Git (optional)

## **Python**

Python is a requirement for certain aspects of PhysiCell:

- It is needed to install certain libraries for the intracellular models.
- It can be used for visualization and data analysis scripts.
- It is used for Jupyter notebook apps of PhysiCell models.
- 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).

- 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/

First, we illustrate using the "64-Bit Command Line Installer" (later, the Graphical installer)

~/Downloads\$ /bin/bash Anaconda3-2022.05-MacOSX-x86\_64.sh

Welcome to Anaconda3 2022.05

In order to continue the installation process, please review the license agreement.

Please, press ENTER to continue

>>>

Note: even if you are using a newer M1/M2 Mac with the arm64 chip, we recommend installing the "x86\_64" version of Anaconda.



Please, press ENTER to continue >>>

... (keep pressing 'enter')...

Do you accept the license terms? [yes|no]
[no] >>> yes

Anaconda3 will now be installed into this location:

/Users/heiland/anaconda3 (Note this is for the user "heiland"; your username will appear here)

- Press ENTER to confirm the location
- Press CTRL-C to abort the installation
- Or specify a different location below

[/Users/heiland/anaconda3] >>> (just press Enter to confirm the default location, then wait a few mins for installation...) PREFIX=/Users/heiland/anaconda3 Unpacking payload ...

• •

Preparing transaction: done Executing transaction: / done

It's OK if you see this warning. You can disregard it for now.

#### WARNING:

installation finished.

You currently have a PYTHONPATH environment variable set. This may cause unexpected behavior when running the Python interpreter in Anaconda3. For best results, please verify that your PYTHONPATH only points to directories of packages that are compatible with the Python interpreter in Anaconda3: /Users/heiland/anaconda3

Do you wish the installer to initialize Anaconda3
by running conda init? [yes|no]
[yes] >>> (just press 'enter' to continue)

...

Do you wish the installer to initialize Anaconda3 by running conda init? [yes|no] [yes] >>> (just press 'enter' to continue)

...

==> For changes to take effect, close and re-open your current shell. <==

If you'd prefer that conda's base environment not be activated on startup, set the auto activate base parameter to false:

conda config --set auto\_activate\_base false

Thank you for installing Anaconda3!

-----

Working with Python and Jupyter notebooks is a breeze with PyCharm Pro, designed to be used with Anaconda. Download now and have the best data tools at your fingertips.

PyCharm Pro for Anaconda is available at: https://www.anaconda.com/pycharm

This means you!!! The base python environment you just installed won't load until you RESTART your shell.

A simple way to do this is close your current Terminal session and restart it. Or to open a new Terminal window.

• After installation is complete, verify that "python" points to the Anaconda version:

#### ~\$ which python

/Users/heiland/anaconda3/bin/python

(your path may differ, but if you run "python", it should say "Anaconda" in the 2<sup>nd</sup> line of the startup prompt)

#### \$ python

```
Python 3.9.12 (main, Apr 5 2022, 01:53:17)
```

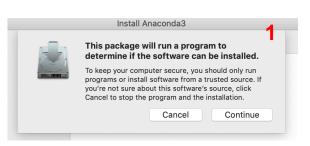
[Clang 12.0.0]:: Anaconda, Inc. on darwin

Type "help", "copyright", "credits" or "license" for more information.

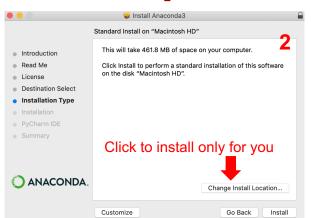
>>>

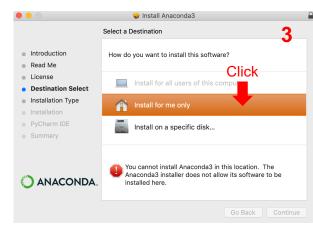
### **Anaconda Graphical Installer**

~\$ open Anaconda3-2022.05-MacOSX-x86\_64.pkg

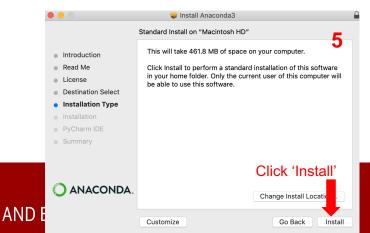


Keep clicking 'Continue' and agree to their license.



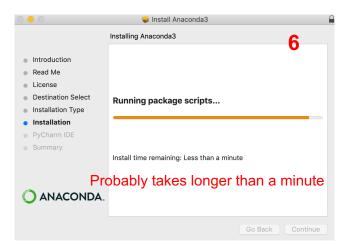


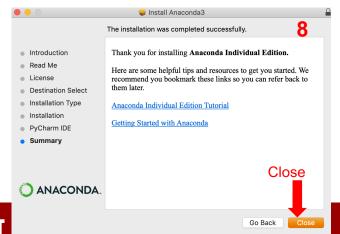


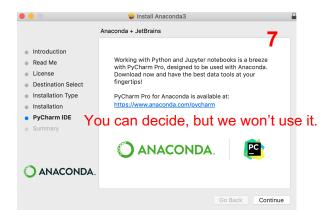


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Open a New Terminal shell to verify you are using the Anaconda Python as your default:

#### ~\$ which python

/Users/heiland/opt/anaconda3/bin/python

(your path may differ, but if you run "python", it should say "Anaconda" in the 2<sup>nd</sup> line of the startup prompt)



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### Intracellular sample project (uses Python 3 to install a lib)

#### ~/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

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...

Done.

The ODE solver library is downloaded

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

(from previous 'make')

```
g++-11 -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++-11 -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

g++-11 -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++-11 -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\_pugixml.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

When we try to run the model, we get an error, but it was expected and serves as a reminder if/when you ever see it again. See next slide.

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You will see this output (but not

highlighted ... ) if the executable

was successfully made

## **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

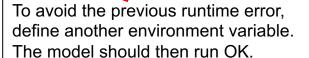
current simulated time: 60 min (max: 1440 min)

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
Of,

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, including Makefile targets: <a href="https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#imagemagick">https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#imagemagick</a>

For 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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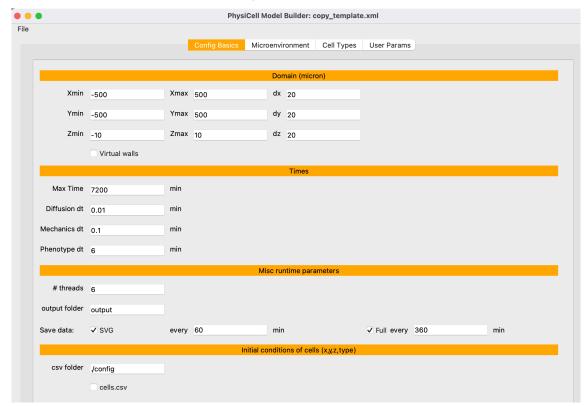
## PhysiCell Model Builder (1)

- The Model Builder is a GUI to let you create/edit a .xml configuration file that defines (nearly all of) a PhysiCell model.
- Download the latest release at:
   https://github.com/PhysiCell-Tools/PhysiCell-model-builder/releases
- Uncompress the .zip, change directory into it, and run it, e.g.:

```
$ unzip PhysiCell-model-builder-2.5.0.zip
$ cd PhysiCell-model-builder-2.5.0
$ python bin/pmb.py
```

This should display the GUI (next page):

## PhysiCell Model Builder (2)



A User Guide for the Model Builder is still be written.

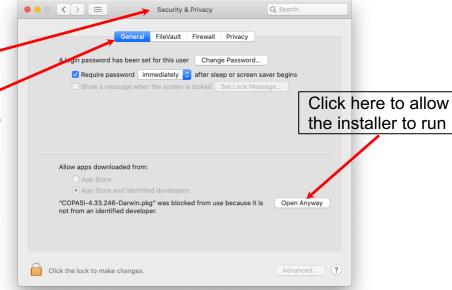
This tool is still being actively developed, so your feedback will be very valuable.

### 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
  - To note it, there are other SBML editors (search "SBML editors" for other options)
- For the 2022 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...



### 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>.

### Funding Acknowledgements







### **PhysiCell Development:**

- Breast Cancer Research Foundation
- Jayne Koskinas Ted Giovanis Foundation for Health and Policy
- National Cancer Institute (U01CA232137)
- National Science Foundation (1720625)

### **Training Materials:**

Administrative supplement to NCI U01CA232137 (Year 2)