Slides, videos, links and more:
https://github.com/physicell-training/ws2022

Setting up MacOS for PhysiCell

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PhysiCell Project

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Presentation overview

- OpenMP-enabled g++ (using Homebrew)
- Test building the default model (“heterogeneity”)

Minimum setup

- Python 3 (using Anaconda distribution)
- Test building an intracellular model
- ImageMagick
- PhysiCell Model Builder

Modeler setup

- COPASI
- C++ code editor
- Git and Github

Hackathon setup + additional options

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) 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).

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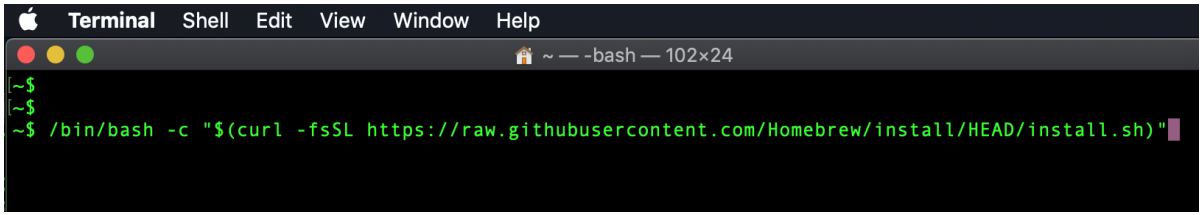
OpenMP-enabled g++

- 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.
- https://brew.sh/

Click to copy the bash command

- 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. It should include or end with something like this (perhaps with the name of your macOS version instead of "monterey")

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: https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#macos

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 *new* Terminal shell, you can verify that this is defined:

```
echo $PHYSICELL_CPP
```

You should see this printed out:

```
g++-11
```

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Test build/run: PhysiCell model (1)

- Get PhysiCell
  - Open browser and navigate to https://raw.githubusercontent.com/physicell-training/ws2022/main/setup/get_physicell.py
  - Using Menus → File → Save Page As → **get_physicell.py** (the default name) in **Downloads**
    - Can view other releases and release notes at: https://github.com/MathCancer/PhysiCell/releases
- Unzip PhyisCell

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++-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_cell_container.o PhysiCell_standard_models.o PhysiCell_cell.o
PhysiCell_custom.o PhysiCell_utilities.o PhysiCell_constants.o PhysiCell_basic_signaling.o  PhysiCell_SVG.o PhysiCell_pathology.o
PhysiCell_MultiCellDS.o PhysiCell_various_outputs.o PhysiCell_pugixml.o PhysiCell_settings.o PhysiCell_geometry.o heterogeneity.o main.cpp

Executable name is heterogeneity

~/PhysiCell$
```

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 1.10.3
                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
```

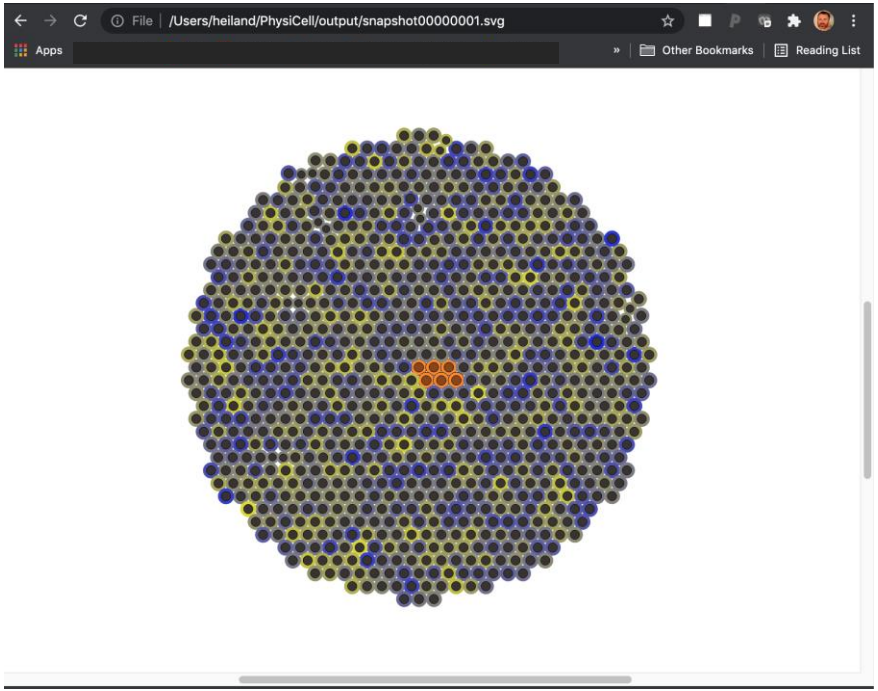
Test build/run: PhysiCell model (4)

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: **ls output** # list files created in the /output directory

```
^C
~/PhysiCell$ ls output/
PhysiCell_settings.xml              initial_microenvironment0.mat       output00000001_cells.mat
empty.txt                           legend.svg                          output00000001_cells_physicell.mat
initial.svg                         output00000000.xml                  output00000001_microenvironment0.mat
initial.xml                         output00000000_cells.mat            snapshot00000000.svg
initial_cells.mat                   output00000000_cells_physicell.mat  snapshot00000001.svg
initial_cells_physicell.mat         output00000000_microenvironment0.mat
initial_mesh0.mat                   output00000001.xml
~/PhysiCell$
```

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 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).

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/

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.

Anaconda Python 3.x

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 ...

Anaconda Python 3.x

...

Preparing transaction: done
Executing transaction: /
done
installation finished.
WARNING:
    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**)

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

Anaconda Python 3.x

...
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.

Anaconda Python 3.x

- After installation is complete, verify that “python” points to the Anaconda version:

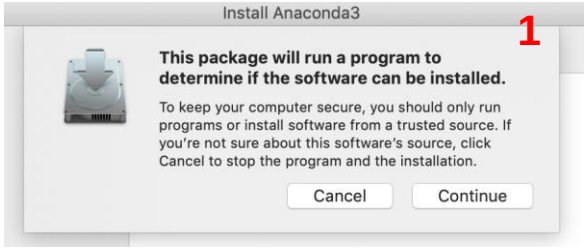
~$ **which python**
/Users/heiland/anaconda3/bin/python

(your path may differ, but if you run ”python”, it should say “Anaconda” in the 2nd line of the startup prompt)

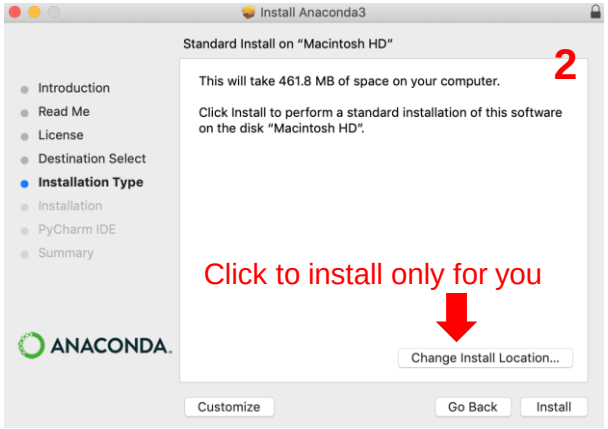
$ **python**
Python 3.9.12 (main, Apr 5 2022, 01:53:17)
[Clang 12.0.0] :: Anaconda, Inc. on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>

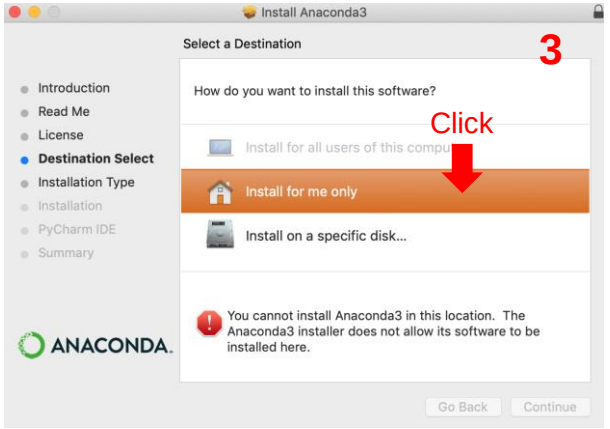
Anaconda Graphical Installer

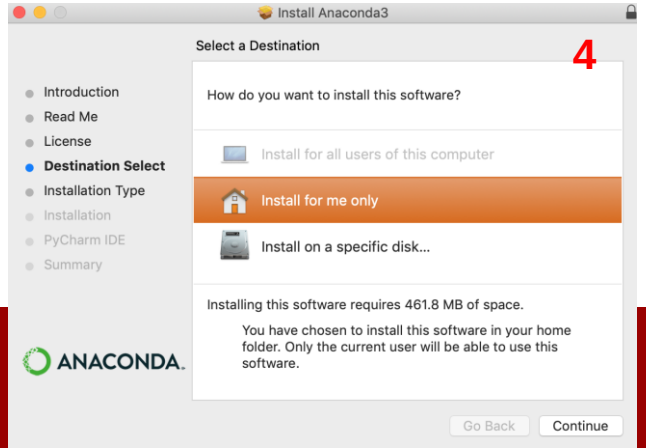
~$ open Anaconda3-2022.05-MacOSX-x86_64.pkg

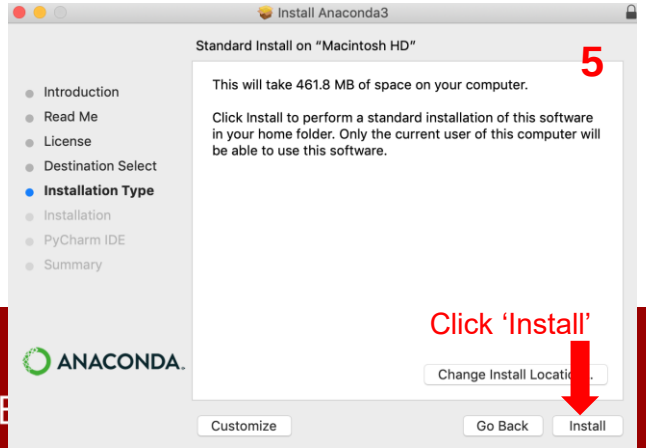


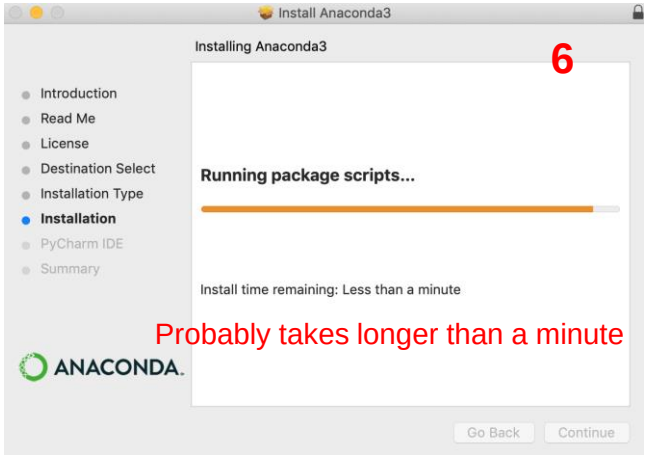
Keep clicking 'Continue' and agree to their license.

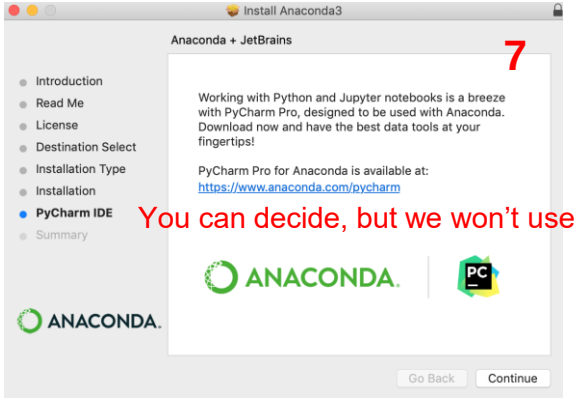


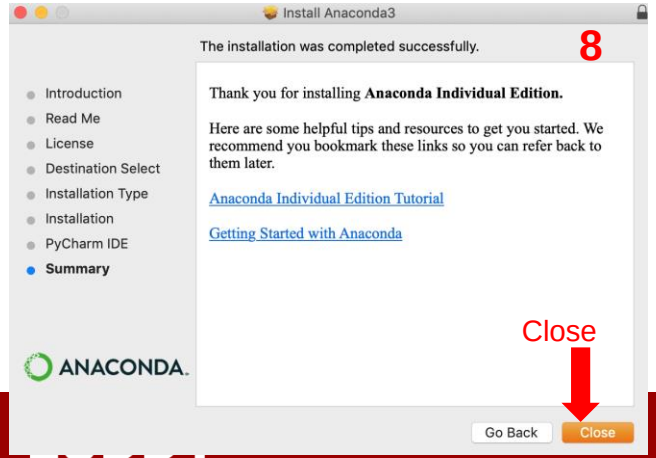












Open a New Terminal shell to verify you are using the Anaconda Python as your default:

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

(your path may differ, but if you run "python", it should say "Anaconda" in the 2nd 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_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
```

You will see this output (but not highlighted …) if the executable was successfully made

```
~/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 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)...
```

To avoid the previous runtime error, define another environment variable. The model should then run OK.

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
```

or,

```
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)

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

```
$ brew install imagemagick
```

(probably will install lots of dependencies)

```
...
==> Installing imagemagick dependency: openexr
...
```

You should then have access to various ImageMagick commands, for example:

```
$ which convert
/usr/local/bin/convert
```

ImageMagick (2)

Refer to the Quickstart guide for helpful ImageMagick commands, including Makefile targets:
https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#imagemagick

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
```

Overview

- 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
- COPASI
- C++ code editor
- Git and Github

PhysiCell Model Builder (1)

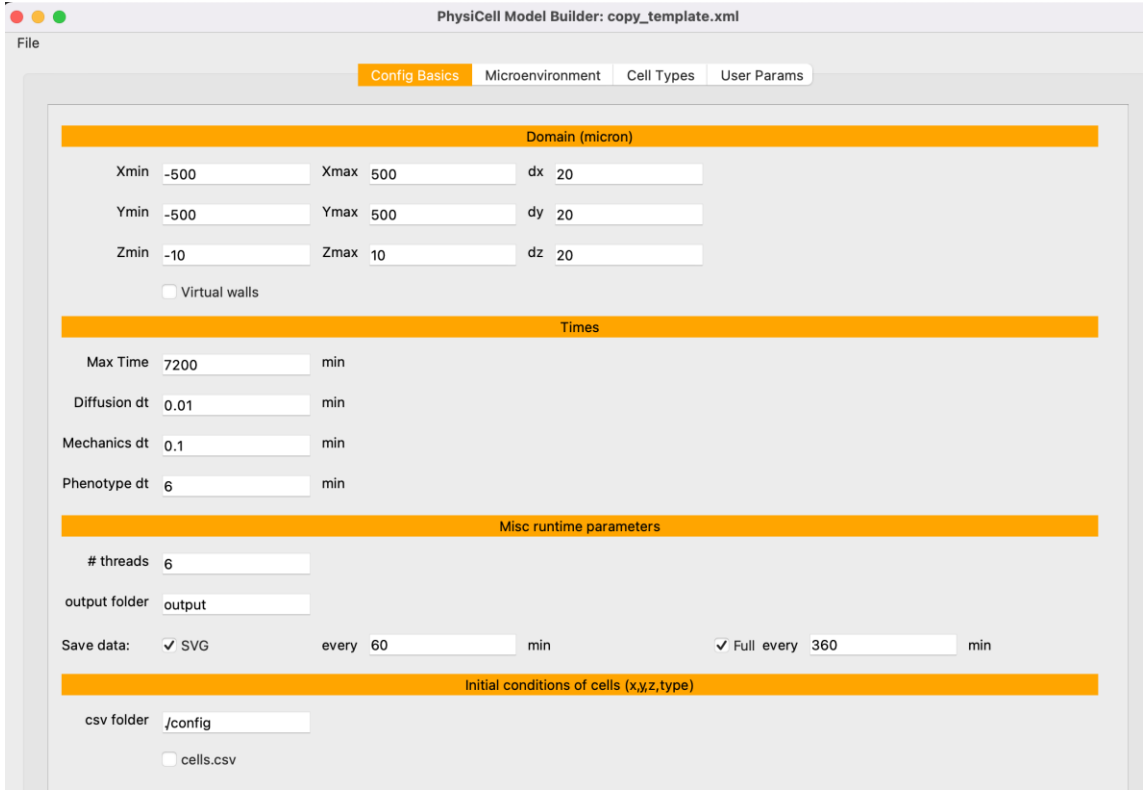
- The Model Builder is a GUI to let you create/edit a .xml configuration file that defines (nearly all of) a PhysiCell model.
- Download the latest release at:

  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.

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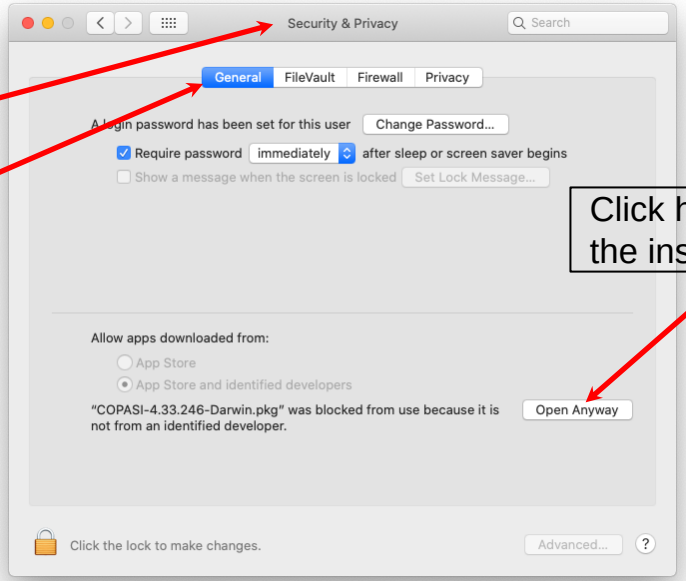
SBML editors: COPASI (1)

- 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
  - 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 http://copasi.org/Download/ and download COPASI for Mac OS X
- Follow instructions here: http://copasi.org/Support/Installation/Mac_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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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 (https://code.visualstudio.com/).

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, github.com 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 PhysiCell community Slack channel. There, you can post questions (#troubleshooting), answer questions, and (hopefully) share successful modeling stories.
- Alternatively, you can submit problem tickets at https://sourceforge.net/p/physicell/tickets/
- Finally, please follow us on Twitter @PhysiCell and @MathCancer.

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