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

Preparing your PhysiCell model to share on nanoHUB

(or, just run the Jupyter notebook GUI locally)

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PhysiCell Project

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Overview

- nanoHUB (https://nanohub.org/) is an open and free platform for computational research, education, and collaboration in nanotechnology, materials science, and related fields.

- nanoHUB lets users run interactive apps from a browser.

- This tutorial will explain how you port an existing PhysiCell (2-D) model to run on nanoHUB.

Some Limitations (currently)

- Only 2-D models, not 3-D (but customization may be possible, with our help)

- Intracellular models are (probably) not supported on nanoHUB
  - We need to work with nanoHUB to pre-install the necessary libraries

- ~~The “Cell Types” tab will represent the actual cell type hierarchy found in your `PhysiCell_settings.xml`, e.g.,~~

~~<cell_definition name="A" ID="1" parent_type="default">~~

~~(this could be considered a limitation because it doesn’t expose every cell_definition parameter for every cell type)~~

Starting with v1.5 of PhysiCell-Jupyter-GUI, the Cell Types are “flattened” to expose all parameters in each type.

Assumptions

- You have installed the latest Anaconda Python 3.x distribution:
- You have a working PhysiCell 2-D model that adheres to the default directory structure, file naming scheme (`Makefile`, `main.cpp`, `config/PhysiCell_settings.xml`), and contains the `output/initial.xml` file from a simulation.
- You have downloaded and installed (unzipped) the latest release from https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/releases

Detailed instructions

- Follow the steps here:
  - https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md
  - https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#steps-to-follow
    - Instead of using “ise_proj1”, you may want to use: “pc4wsXXteamN” (where XX=workshop year, e.g. “22”, and N=1,2,etc (whatever your team # is)) – see next slide

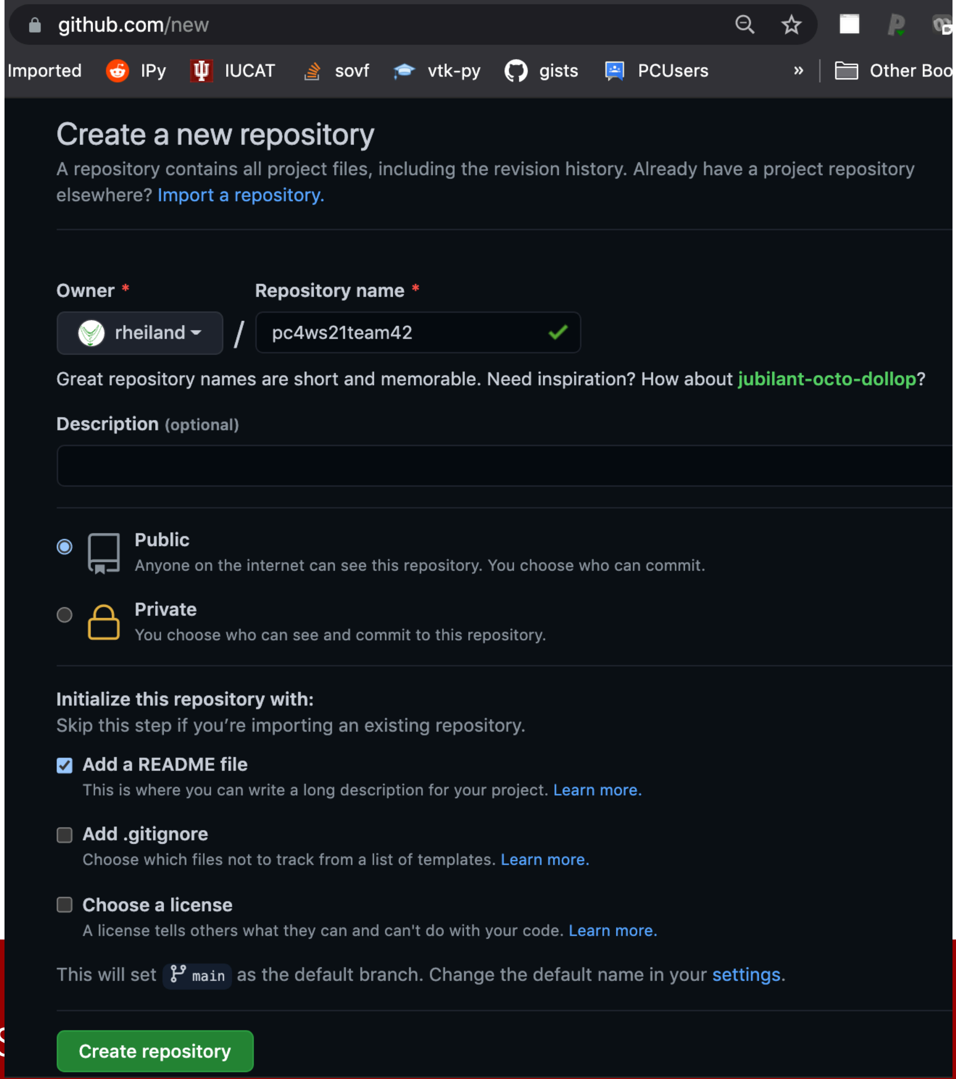
The following slides try to illustrate these steps.

  - These instructions should let you create a Jupyter notebook that you can run locally (on your computer) before installing it on nanoHUB.
  - Creating a nanoHUB app is considered optional (https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#create-a-nanohub-tool-optional), but we are assuming you will do it in this tutorial. Let us know if you need help.

Create a new GitHub repo for your nanoHUB project. E.g., I created "pc4ws21team42"

The repo needs to be "public" for nanoHUB.

For a team project, one person can create it on their personal account and add others as collaborators.



Using celltypes3 as an example (1)

~$ **unzip PhysiCell.zip**
...
~$ **cd PhysiCell**

~/PhysiCell$ **make celltypes3-sample**
... (copies over this sample's files) ...

~/PhysiCell$ **make**
...
g++-11 -march=native -O3 -fomit-frame-pointer -mfpmath=both -fopenmp -m64 -std=c++11 -o celltypes3 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 custom.o main.cpp

~/PhysiCell$ **./celltypes3**
... Let it run just for a very brief time (to generate the `/output/initial.xml`) and then ctl-c to kill it

Note: we use MacOS/Linux commands in these slides. In a Windows shell, your syntax will likely vary, e.g., "\" instead of "/", using ".exe" suffix on a model's executable, "dir" instead of "ls", etc.

Using celltypes3 as an example (2)

- Verify you have these 4 critical files:

~/PhysiCell$ **ls Makefile main.cpp config/PhysiCell_settings.xml output/initial.xml**
Makefile   main.cpp
config/PhysiCell_settings.xml   output/initial.xml

Clone your GitHub repo

~$ **git clone git@github.com:rheiland/pc4ws21team42.git**
Cloning into 'pc4ws21team42'...
remote: Enumerating objects: 3, done.
remote: Counting objects: 100% (3/3), done.
remote: Total 3 (delta 0), reused 0 (delta 0), pack-reused 0
Receiving objects: 100% (3/3), done.
~$

Rf. https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#steps-to-follow for options and for Windows command syntax.

~/PhysiCell-Jupyter-GUI-1.5.1$ **python setup_new_proj.py ~/pc4ws21team42 ~/PhysiCell pc4ws21team42**
...

Note: if you need to re-run the `setup_new_proj.py` script for any reason, it is probably best to first delete all the files & directories that were previously created. HOWEVER, if you made edits to your `doc/about.html`, make a backup copy!

This will generate these files in your cloned nanoHUB project:

~/pc4ws21team42$ **ls**

LICENSE	examples/	rappture/
README.md	make_my_tool.py	src/
bin/	middleware/	tmpdir/
data/	mod_makefile.py	
doc/	pc4ws21team42.ipynb	

← This will be your project's name

FYI: `setup_new_proj.py` is an extension of an earlier project: xml2jpyter

https://doi.org/10.21105/joss.01408

The Journal of Open Source Software

xml2jupyter: Mapping parameters between XML and Jupyter widgets

Randy Heiland[1], Daniel Mishler[1], Tyler Zhang[1], Eric Bower[1], and Paul Macklin[1]

1 Intelligent Systems Engineering, Indiana University

DOI: 10.21105/joss.01408

Software

- Review
- Repository
- Archive

Submitted: 08 April 2019
Published: 01 July 2019

Summary

Jupyter Notebooks (Kluyver et al., 2016, Perkel (2018)) provide executable documents (in a variety of programming languages) that can be run in a web browser. When a notebook contains graphical widgets, it becomes an easy-to-use graphical user interface (GUI). Many scientific simulation packages use text-based configuration files to provide parameter values and run at the command line without a graphical interface. Manually editing these files to explore how different values affect a simulation can be burdensome for technical users, and impossible to use for those with other scientific backgrounds. xml2jupyter is a Python package that addresses these scientific bottlenecks. It provides a mapping between configuration files, formatted in the Extensible Markup Language (XML), and Jupyter widgets. Widgets are automatically generated from the XML file and these can, optionally, be incorporated into a larger GUI for a simulation package, and optionally hosted on cloud resources. Users modify parameter values via the widgets, and the values are written to the XML configuration file which is input to the simulation's command-line interface. xml2jupyter has been tested using PhysiCell (Ghaffarizadeh, Heiland, Friedman, Mumenthaler, & Macklin, 2018), an open source, agent-based simulator for biology, and it is being used by students for classroom and research projects. In addition, we use xml2jupyter to help create Jupyter GUIs for PhysiCell-related applications running on nanoHUB (Madhavan et al., 2013).

A PhysiCell configuration file defines model-specific `<user_parameters>` in XML. Each parameter element consists of its name with attributes, defining its data *type*, *units* (optional),

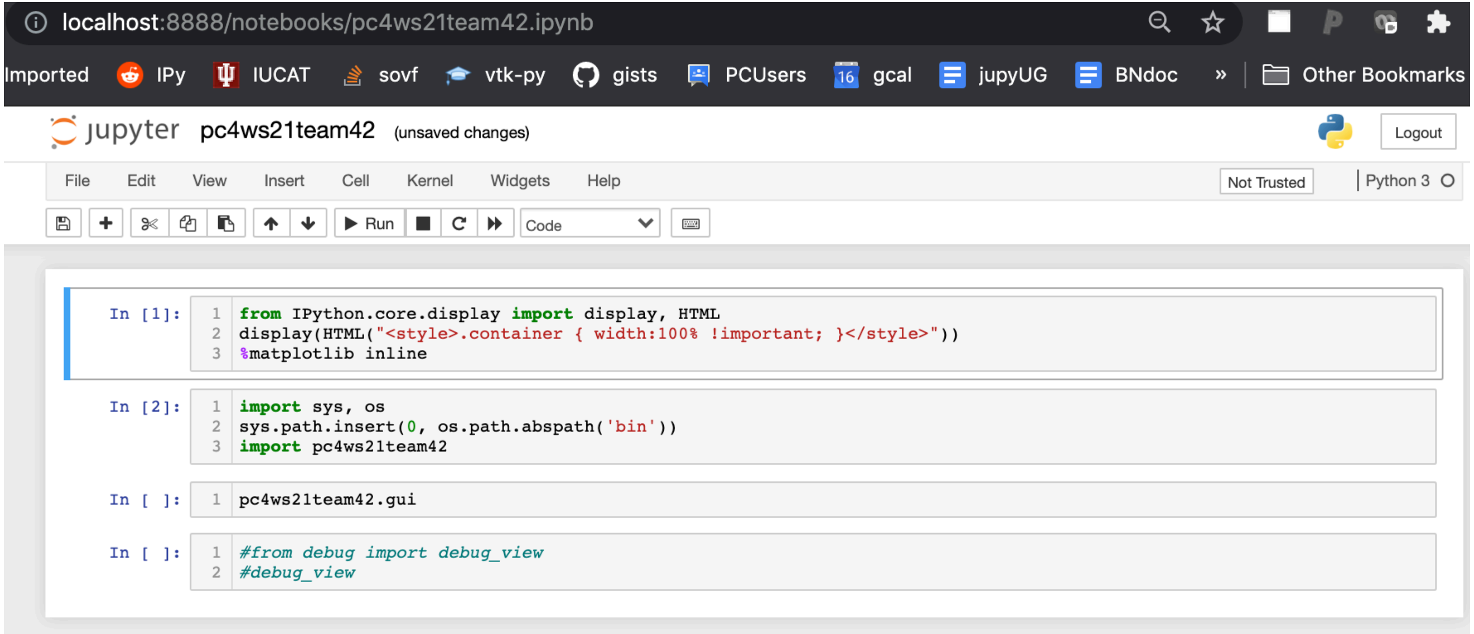
Test your notebook on your computer

Have a Web browser running, then run the following command from a shell window:

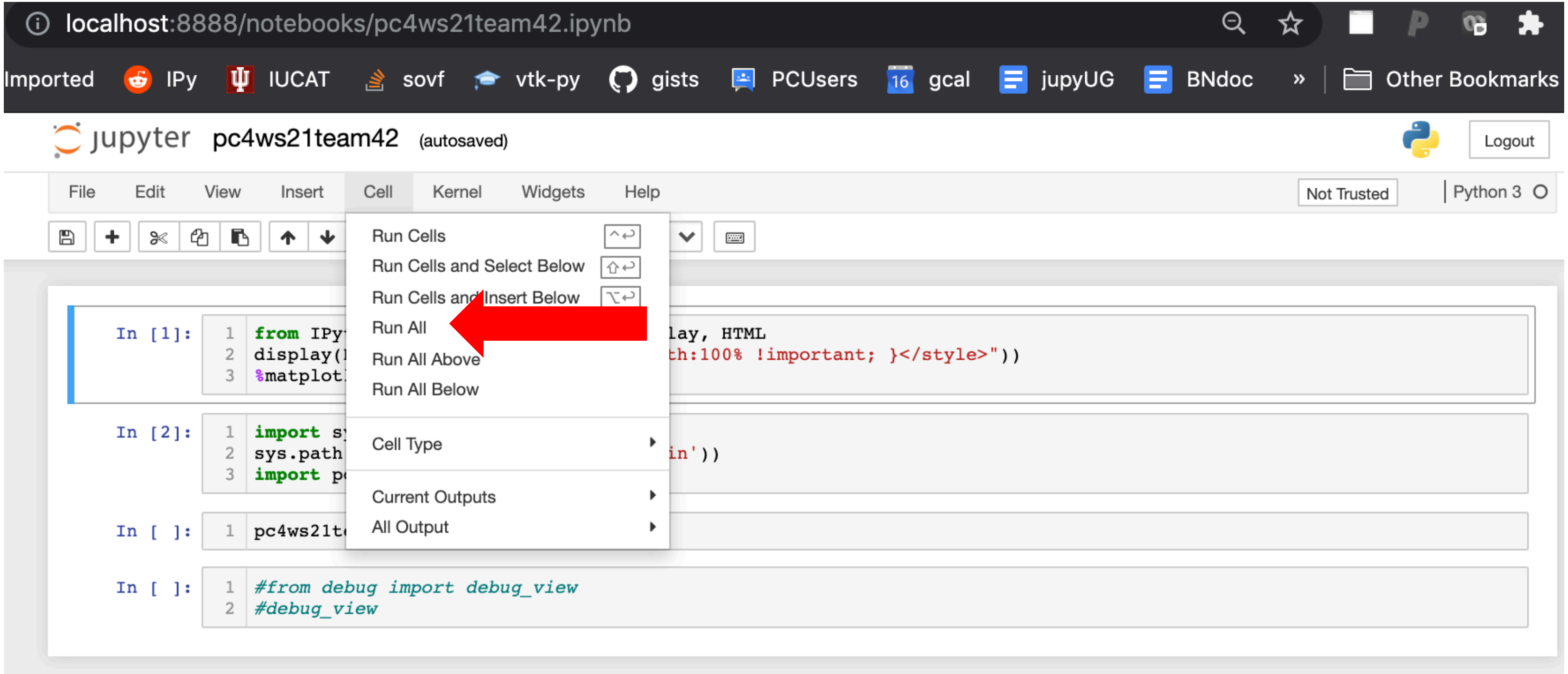
~/pc4ws21team42$ **jupyter notebook pc4ws21team42.ipynb**

...

You should see this Jupyter notebook displayed in your browser:

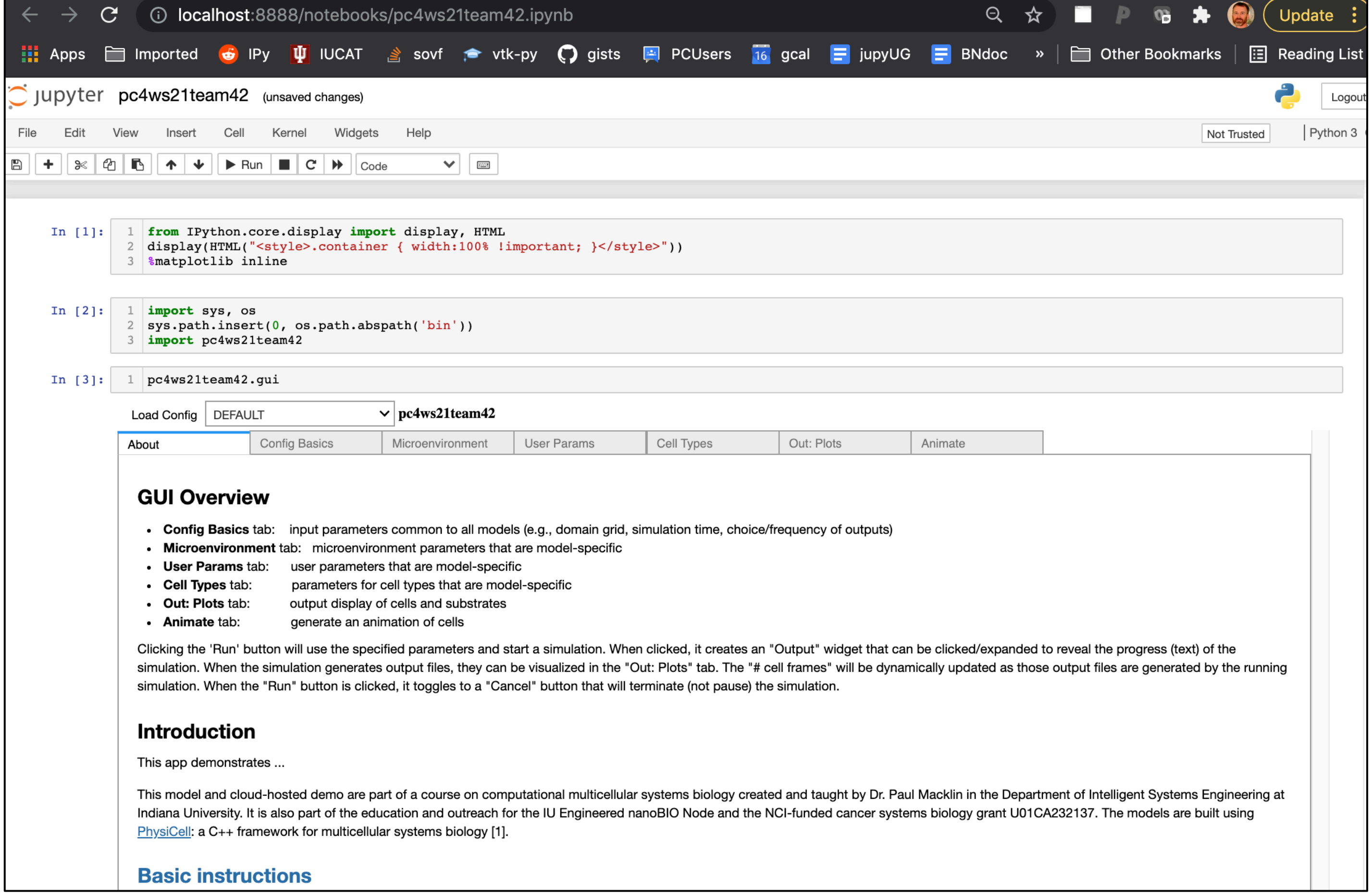


Click the ‘Cell’ menu, ‘Run All’, wait for each notebook “cell” to execute...

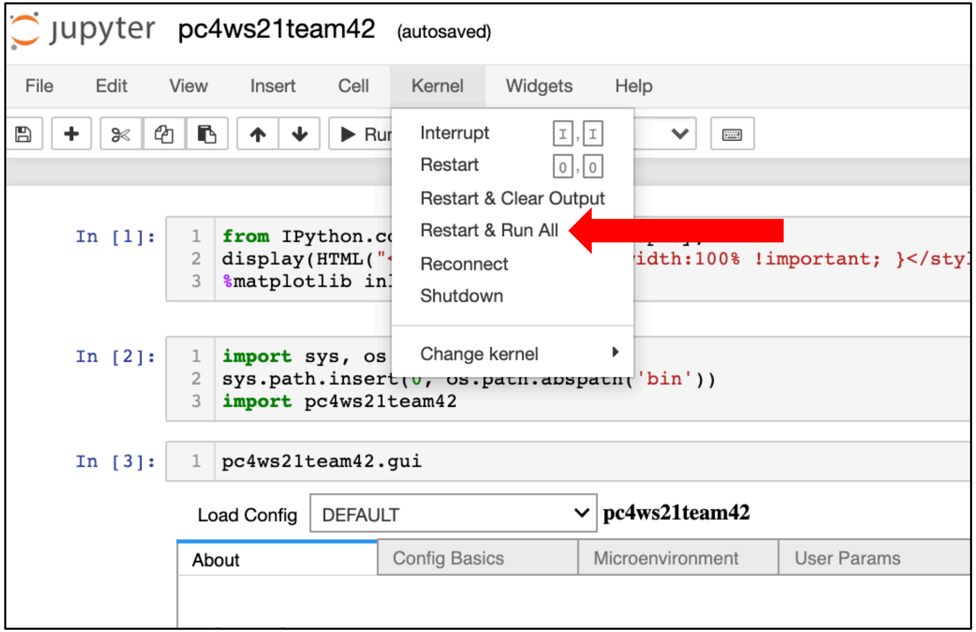


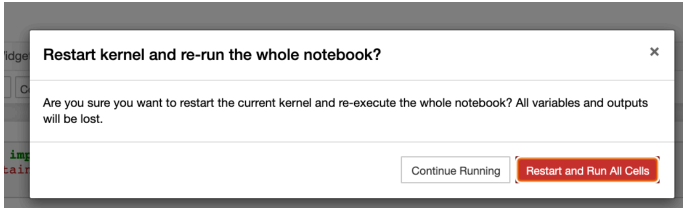
You should see a similar looking notebook GUI for your project.

Now or later:
You can leave this running, then edit the `doc/about.html` file to update this page's contents and (see next page).

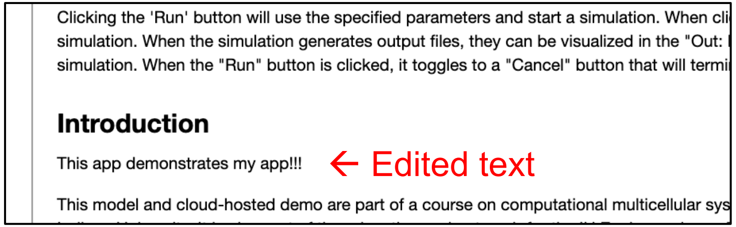


After editing the “doc/about.html”, Click the ‘Kernel’ menu, ‘Restart & Run All’, then click the pop-up button to confirm:

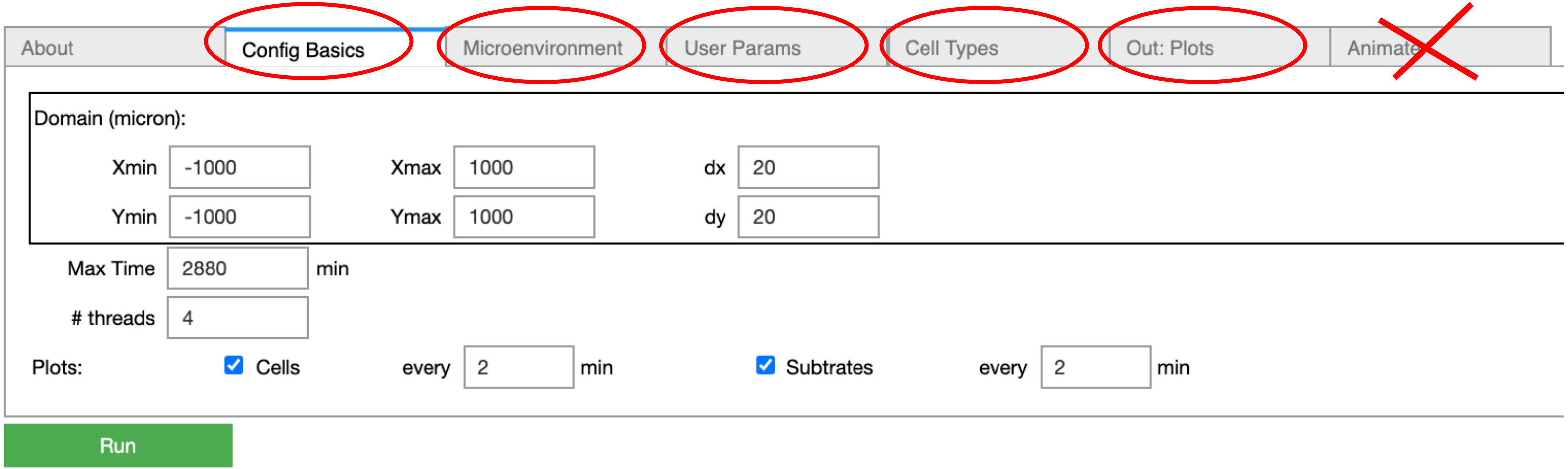




The notebook will refresh, showing your edited text:



Explore the other tabs of the GUI (but disregard the Animate tab for now)

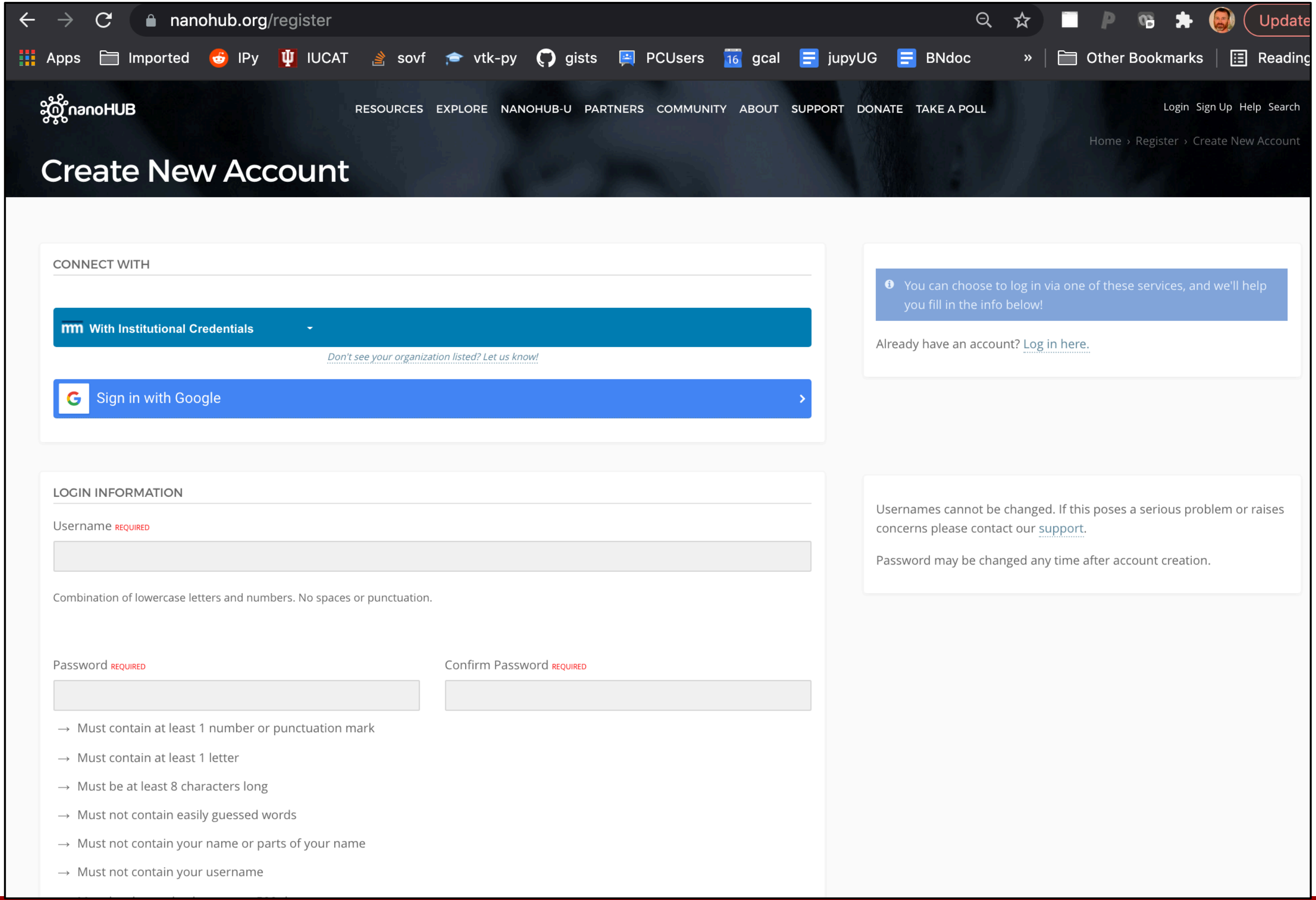


Final steps for nanoHUB app

- If your local Jupyter notebook looks correct, you have the option of compiling your project and making sure you can Run it from the notebook - rf. Steps 4 and 5 in:
- https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#steps-to-follow
- However, you can probably skip straight to getting it ready to test on nanoHUB:
- https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#create-a-nanohub-tool-optional (not "optional" if you plan to do it ☺)

  - ♦ https://nanohub.org/register/ – register for a nanoHUB account if you haven't
  - ♦ https://nanohub.org/tools/create – create your app's basic info
  - ♦ Make sure your middleware/invoke script is "executable" (rf. github link above)

nanohub.org/register/



Tools: Create New Tool

nanohub.org/tools/create

ABOUT YOUR TOOL:

Tool Name: REQUIRED

pc4ws21team42

Short name, used for the directory containing this tool. Example: qdot

Title: REQUIRED

PhysiCell 3-types model

Full name for this tool. Example: Quantum Dot Lab

Version:

1.0

Optional version number for this release of the tool. Example: 1.0 or 2.1.5b. Spaces not allowed.

At a glance: REQUIRED

Simulate 3-body-like dynamics between 3 cell types

A one-line description of your tool. Example: Simulate 3-D confined states in simple quantum dot geometries.

SUGGESTED SCREEN SIZE:

W 780 x H 600

Specify a screen size for your application in pixels.

REPOSITORY HOST:

- ○ Host subversion repository on HUB
- ○ Host GIT repository on HUB
- ◉ Host GIT repository on GitHUB

REPOSITORY HOST:

- ○ Host subversion repository on HUB
- ○ Host GIT repository on HUB
- ◉ Host GIT repository on GitHUB

GIT REPOSITORY URL:

Git Repository for Source Code:

https://github.com/rheiland/pc4ws21team42

Public URL: https://github.com/yourgithubrepo
Private URL: ssh://github.com/yourgithubrepo

PUBLISHING OPTION:

- ○ Rappture or Linux-GUI
- ◉ Jupyter notebook
- ○ SimTool

ACCESS:

Tool Access: REQUIRED — What should I choose?

Anyone can run tool

Source Code Access: REQUIRED — What should I choose?

Open source (anyone can access code)

Project Area Access: REQUIRED — What should I choose?

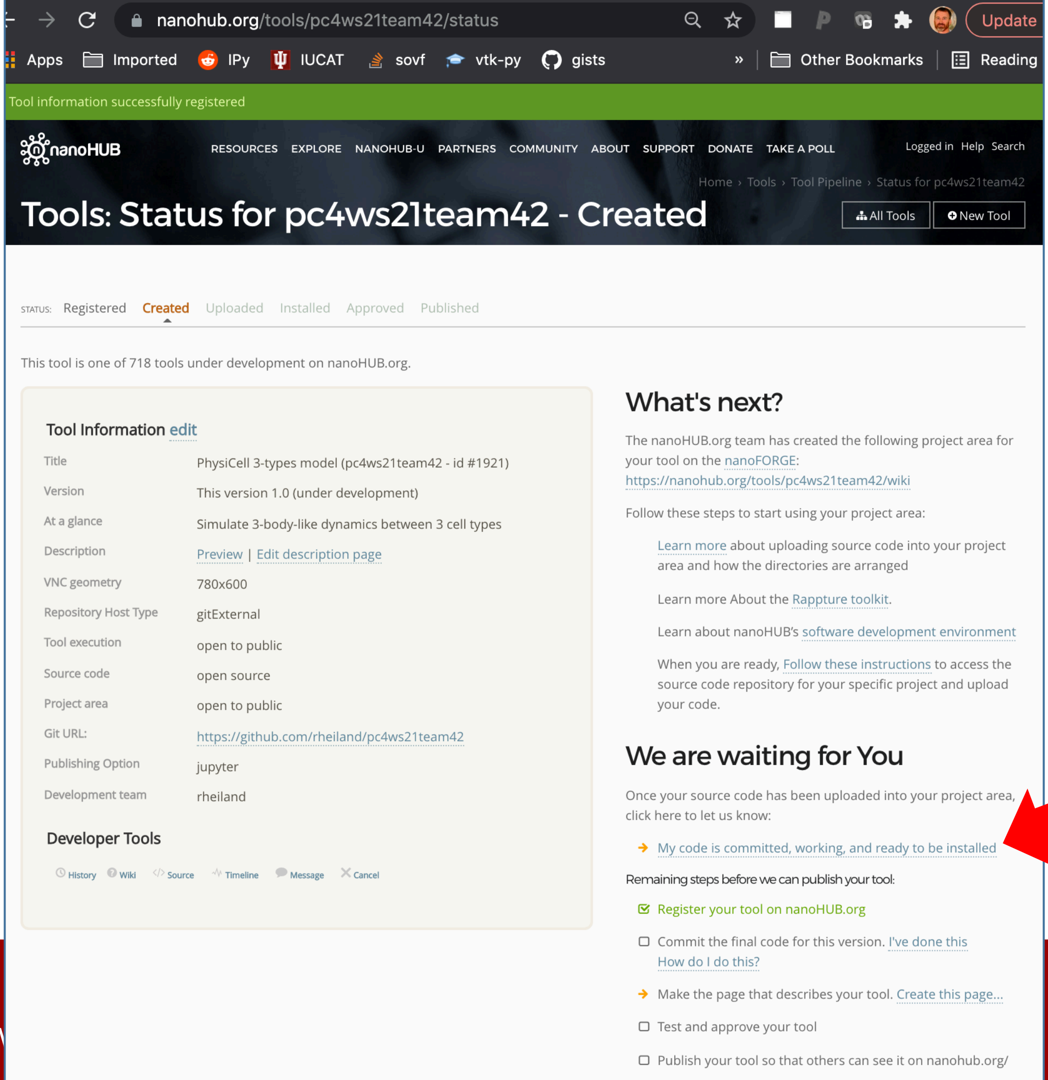
Open to public

Development team: REQUIRED

rheiland, mathcancer

nanoHUB.org logins for people allowed to modify your code. Example: mylogin, fred, barney, wilma

Register Tool



After committing your files to your team project's GitHub repo:

Tools: update for pc4ws21team42 - Uploaded

All Tools | New Tool

STATUS: Registered Created **Uploaded** Installed Approved Published

✔ Tool status successfully changed

This tool is one of 718 tools under development on nanoHUB.org.

Tool Information edit

Title	PhysiCell 3-types model (pc4ws21team42 - id #1921)
Version	This version 1.0 (under development)
At a glance	Simulate 3-body-like dynamics between 3 cell types
Description	Preview | Edit description page
VNC geometry	780x600
Repository Host Type	gitExternal
Tool execution	open to public
Source code	open source [change license]
Project area	open to public
Git URL:	https://github.com/rheiland/pc4ws21team42
Publishing Option	jupyter
Development team	rheiland

Developer Tools

History Wiki Source Timeline Message Cancel

What's next?

The nanoHUB.org team needs to deploy your latest code on nanoHUB.org so you can test it out. It's been 0 seconds since the last change to your tool status. You should normally receive response within 3 days.

Remaining steps before we can publish your tool:

- ☑ Register your tool on nanoHUB.org
- ☑ Upload your source code into your project area on nanoFORGE
- → Make the page that describes your tool. Create this page...
- ☐ Test and approve your tool
- ☐ Publish your tool so that others can see it on nanohub.org/

This page should appear next and you should receive an email:

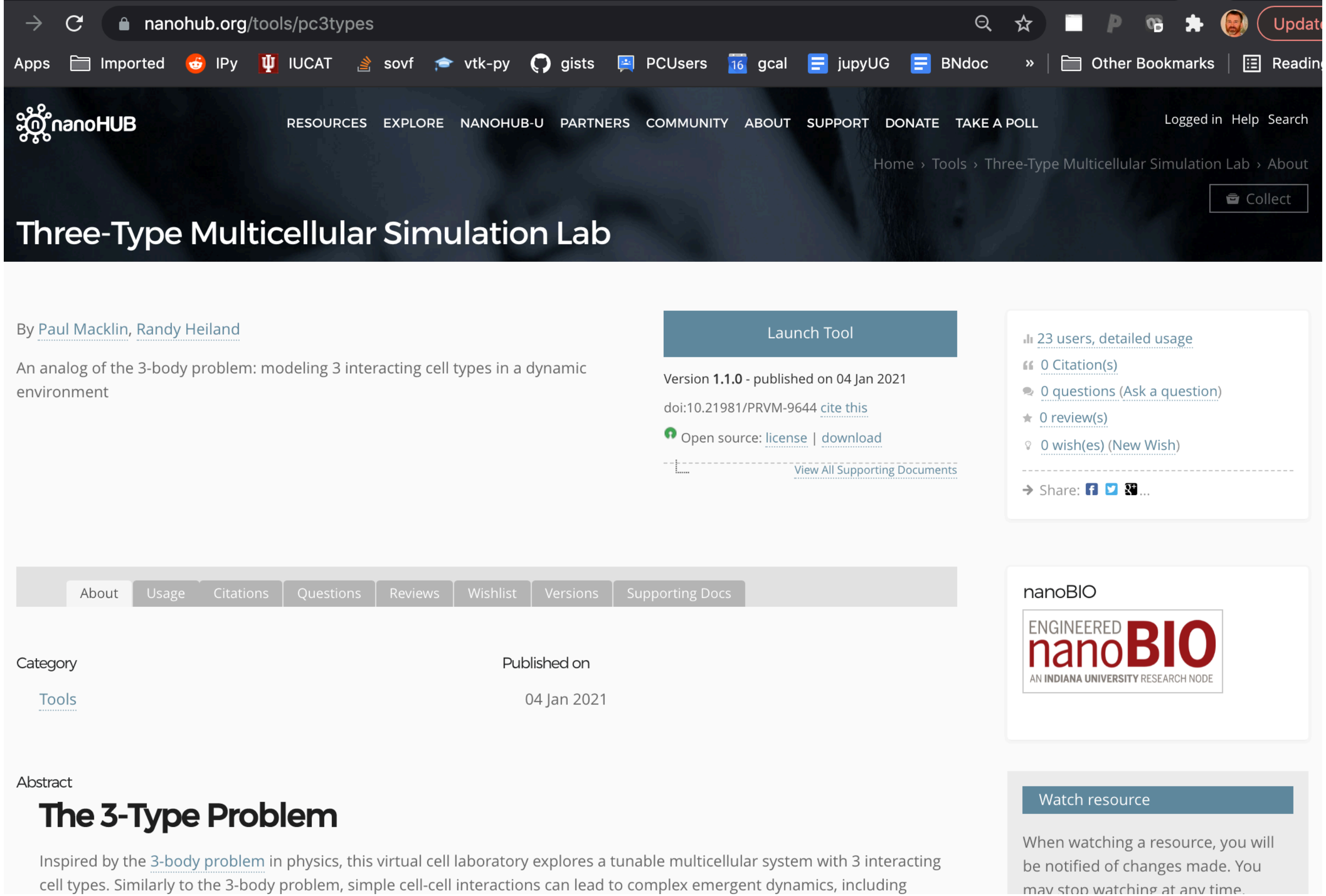
nanoHUB.org Contribtool
to me

TOOL: PhysiCell 3-types model (pc4ws21team42)
SUMMARY: Status changed from Created to Uploaded
WHEN 27 Jul 2021
BY: rheiland

To check the latest tool status and take required actions, go to:
https://nanohub.org/tools/pc4ws21team42/status

nanoHUB staff then attempt to install your code and you will receive another email – indicating success or failure. If successful, you'll be directed to a "status" page where you can launch/test your app. (If it fails to install, you'll be told why and will likely need to communicate with nanoHUB staff to figure out why).

This is our previously published **pc3types** app on nanoHUB.



https://nanohub.org/tools/pc3types

proxy.nanohub.org/weber/1867695/AmRuBFXQCs33AWeT/6/apps/pc3types.ipynb?

Apps | Imported | IPy | IUCAT | sovf | vtk-py | gists | PCUsers | gcal | jupyUG | BNdoc | Other Bookmarks | Reading List

nanoHUB jupyter

Edit App | Submit a ticket | Terminate Session

Load Config DEFAULT **pc3types**

About | Config Basics | Microenvironment | User Params | Cell Types | Out: Plots | Animate

GUI Overview

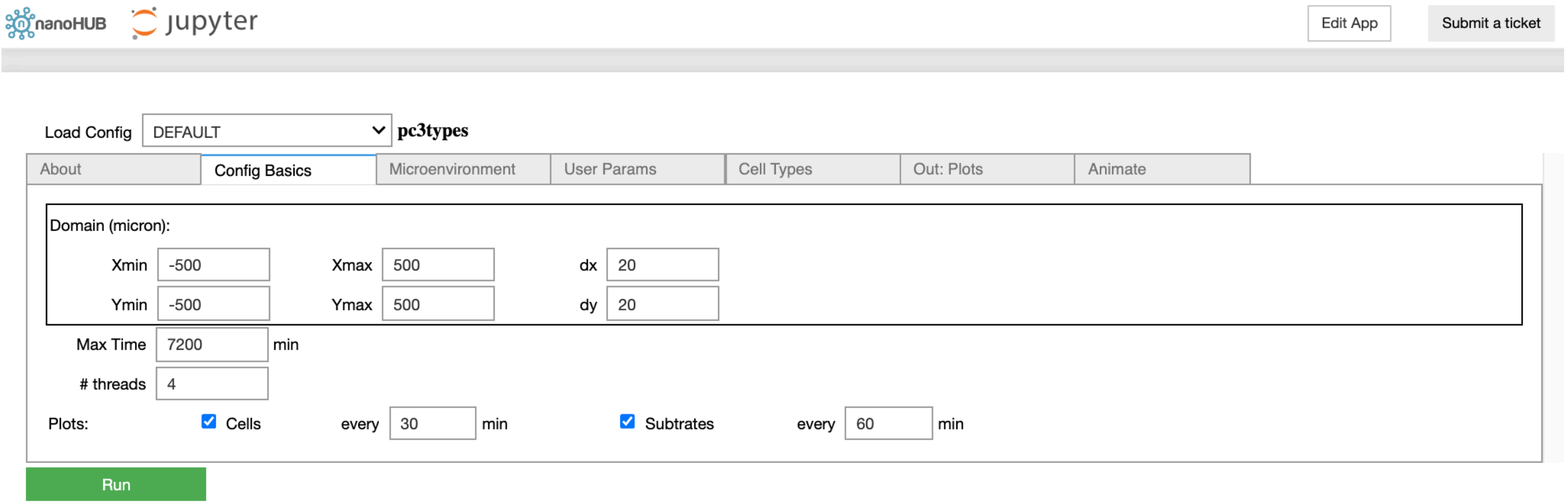
- **Config Basics** tab: input parameters common to all models (e.g., domain grid, simulation time, choice/frequency of outputs)
- **Microenvironment** tab: microenvironment parameters that are model-specific
- **User Params** tab: user parameters that are model-specific
- **Cell Types** tab: parameters for cell types that are model-specific
- **Out: Plots** tab: output display of cells and substrates
- **Animate** tab: generate an animation of cells

Clicking the 'Run' button will use the specified parameters and start a simulation. When clicked, it creates an "Output" widget that can be clicked/expanded to reveal the progress (text) of the simulation. When the simulation generates output files, they can be visualized in the "Out: Plots" tab. The "# cell frames" will be dynamically updated as those output files are generated by the running simulation. When the "Run" button is clicked, it toggles to a "Cancel" button that will terminate (not pause) the simulation.

The 3-Type Problem

Inspired by the 3-body problem in physics, this virtual cell laboratory explores a tunable multicellular system with 3 interacting cell types. Similarly to the 3-body problem, simple cell-cell

Run


nanoHUB
jupyter
Edit App
Submit a ticket
Load Config
DEFAULT
pc3types
About
Config Basics
Microenvironment
User Params
Cell Types
Out: Plots
Animate
Domain (micron):
Xmin -500
Xmax 500
dx 20
Ymin -500
Ymax 500
dy 20
Max Time 7200 min
threads 4
Plots: Cells every 30 min
Subtrates every 60 min
Run

nanoHUB jupyter

Edit App | Submit a ticket

Load Config DEFAULT pc3types

About | Config Basics | Microenvironment | User Params | Cell Types | Out: Plots | Animate

resource (none)			
diffusion_coefficient	100000	micron^2/min	
decay_rate	0	1/min	
initial_condition	1		
Dirichlet_boundary_condition	1		on/off
signal_A (none)			
diffusion_coefficient	1000	micron^2/min	
decay_rate	0.1	1/min	
initial_condition	0		
Dirichlet_boundary_condition	0		on/off
signal_B (none)			
diffusion_coefficient	1000	micron^2/min	
decay_rate	0.1	1/min	
initial_condition	0		
Dirichlet_boundary_condition	0		on/off
signal_C (none)			
diffusion_coefficient	1000	micron^2/min	
decay_rate	0.1	1/min	
initial_condition	0		
Dirichlet_boundary_condition	0		on/off

calculate_gradients

track_in_agents

Run

nanoHUB jupyter

Edit App

Submit a ticket

Load Config DEFAULT **pc3types**

About | Config Basics | Microenvironment | User Params | Cell Types | Out: Plots | Animate

random_seed	0		
---Initialization settings---			
number_of_A	25		initial number of A
number_of_B	25		initial number of B
number_of_C	25		initial number of C
max_distance_from_origin	150	micron	max initial distance of cells from (0,0,0)
---Coloring settings---			
A_color	magenta		color for A cells
B_color	green		color for B cells
C_color	cyan		color for C cells
standard_plots	☐		Enable additional standard plots?
---Overall signaling settings---			
hill_power	5		Hill power for signal responses
half_max	0.1		half max for signal responses
---cell type A settings---			
A_base_cycle	0.00072	1/min	base cell cycling rate for type A
A_max_cycle	0.0072	1/min	maximum cell cycling rate for type A
A_cycle_A	neutral		impact of signal A on A cycling (promote, inhibit, or neutral)
A_cycle_B	neutral		impact of signal B on A cycling (promote, inhibit, or neutral)
A_cycle_C	neutral		impact of signal C on A cycling (promote, inhibit, or neutral)
A_cycle_pressure_threshold	2		pressure above threshold inhibits A cycling
A_base_death	0.0000531667	1/min	base cell death rate for type A
A_max_death	0.000531667	1/min	maximum cell death rate for type A
A_death_A	neutral		impact of signal A on A apoptosis (promote, inhibit, or neutral

nanoHUB jupyter

Edit App | Submit a ticket

Load Config: DEFAULT **pc3types**

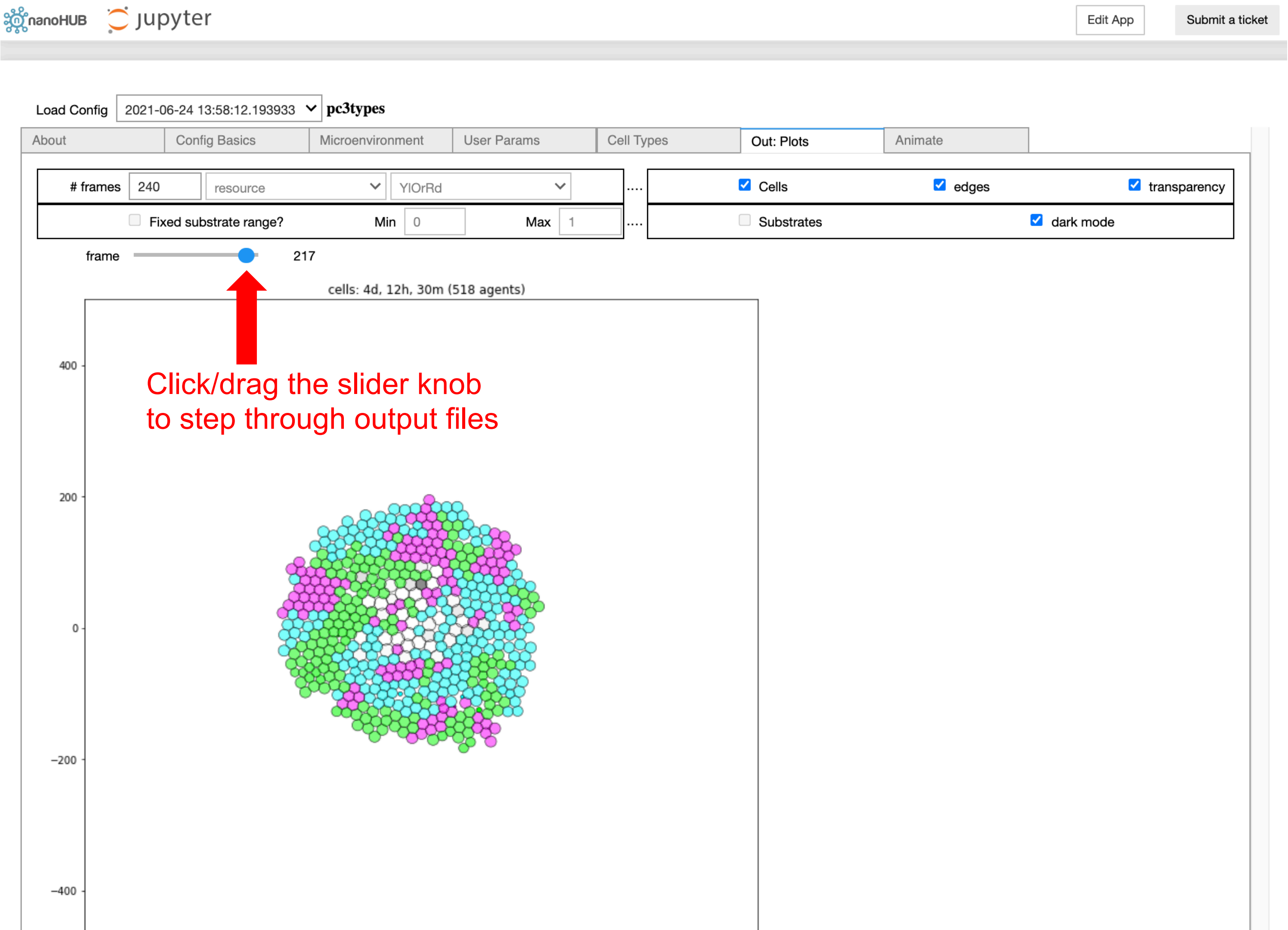
About | Config Basics | Microenvironment | User Params | Cell Types | Out: Plots | Animate

Cell type: default inherits properties from parent type: None

This cell line inherits its properties from its parent type. Any settings below override those inherited properties.

phenotype:cycle (model: live; code=5)		
Phase 0 -> Phase 0 transition rate	0.00072	1/min
phenotype:death		
model: apoptosis		
death rate	0.0000531667	1/min
unlysed_fluid_change_rate	0.05	1/min
lysed_fluid_change_rate	0	1/min
cytoplasmic_biomass_change_rate	0.0166667	1/min
nuclear_biomass_change_rate	0.00583333	1/min
calcification_rate	0	1/min
relative_rupture_volume	2	1/min
model: necrosis		
death rate	0	1/min
unlysed_fluid_change_rate	0.05	1/min
lysed_fluid_change_rate	0	1/min
cytoplasmic_biomass_change_rate	0.0166667	1/min
nuclear_biomass_change_rate	0.00583333	1/min
calcification_rate	0	1/min
relative_rupture_volume	2	1/min
phenotype:volume		
total	2494	1/min
fluid_fraction	0.75	1/min

NOTE: this version of the PhysiCell-Jupyter-GUI may not yet provide some of the newer phenotype parameters (in PhysiCell 1.10.x), e.g. <cell_adhesion_affinities> in <mechanics>, etc..


nanoHUB
jupyter
Edit App
Submit a ticket
Load Config
2021-06-24 13:58:12.193933
pc3types
About
Config Basics
Microenvironment
User Params
Cell Types
Out: Plots
Animate
frames
240
resource
YlOrRd
Cells
edges
transparency
Fixed substrate range?
Min
0
Max
1
Substrates
dark mode
frame
217
cells: 4d, 12h, 30m (518 agents)
400
200
0
−200
−400
Click/drag the slider knob
to step through output files

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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PhysiCell Development:

- Breast Cancer Research Foundation
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- National Cancer Institute (U01CA232137)
- National Science Foundation (1720625, 1818187)

Training Materials:

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Other Funding:

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- NIH Common Fund (3OT2OD026671-01S4)