Slides, videos, links and more:
https://github.com/physicell-training/ws2021

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 is possible, with our help)

- Intracellular models are 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)

Assumptions

- You have installed the Anaconda Python distribution:
  - https://github.com/MathCancer/PhysiCell/blob/master/documentation/Quickstart.md#python
  - If you need more setup details: https://github.com/physicell-training/ws2021#pre-workshop-materials

- 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

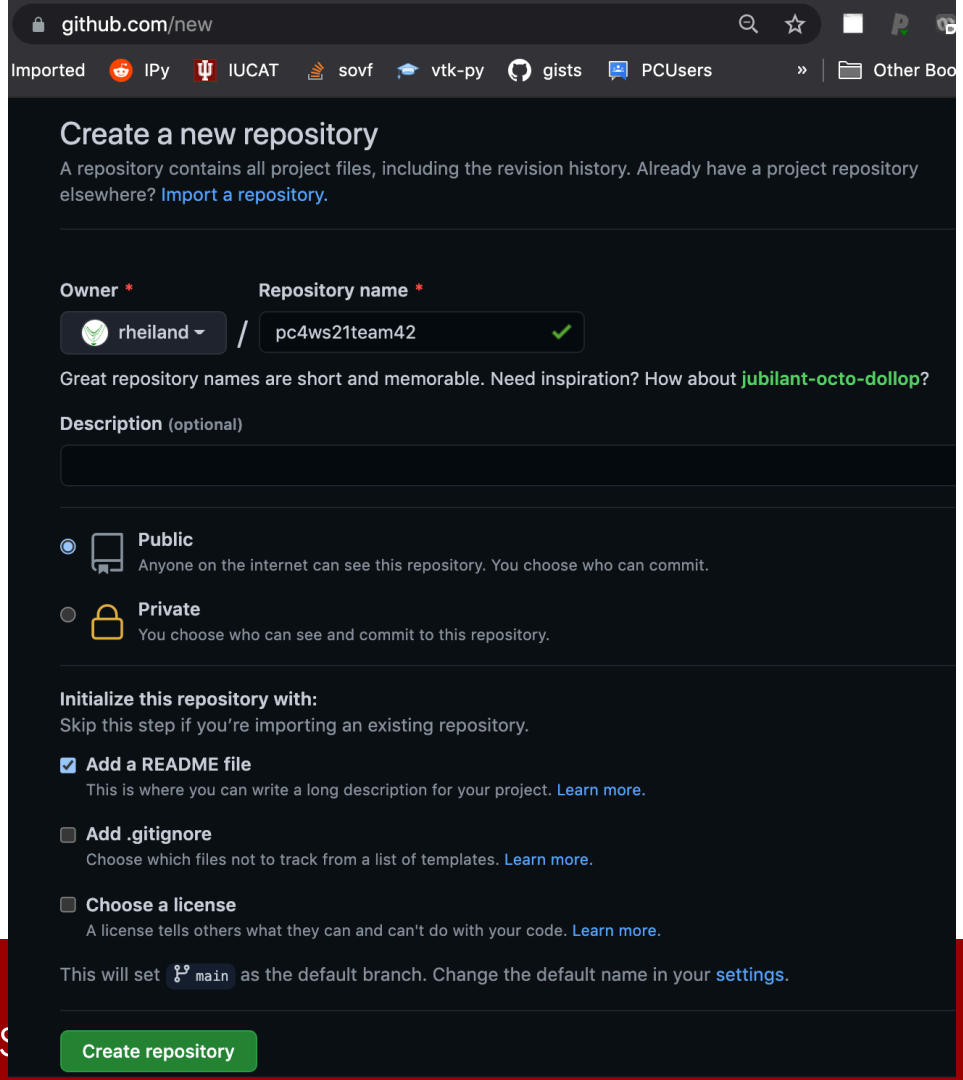
- Follow the steps here:
  - https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md
  - https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#steps-to-follow
    - ♦ Instead of using “ise_proj1”, you may want to use: “pc4ws21teamN” (PhysiCell for Workshop 2021, where N=1,2,etc (whatever your team # is)) – see next slide
  - 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.

The following slides try to illustrate these steps.

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_V.1.9.0.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-1.4$ **python setup_new_proj.py ~/pc4ws21team42 ~/PhysiCell pc4ws21team42**
...

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
```

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!

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

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JOSS
The Journal of Open Source Software

xml2jupyter: Mapping parameters between XML and Jupyter widgets

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Software

- Review
- Repository
- Archive

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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),

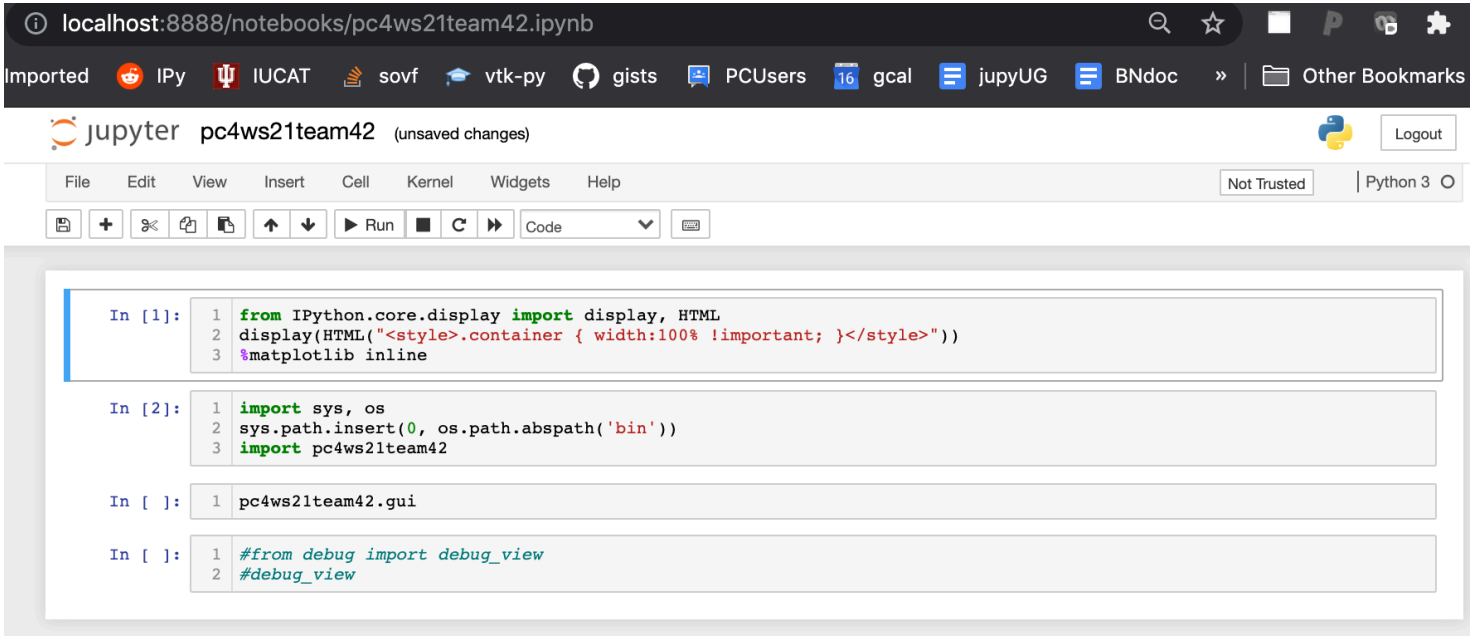
Test your notebook on your computer

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

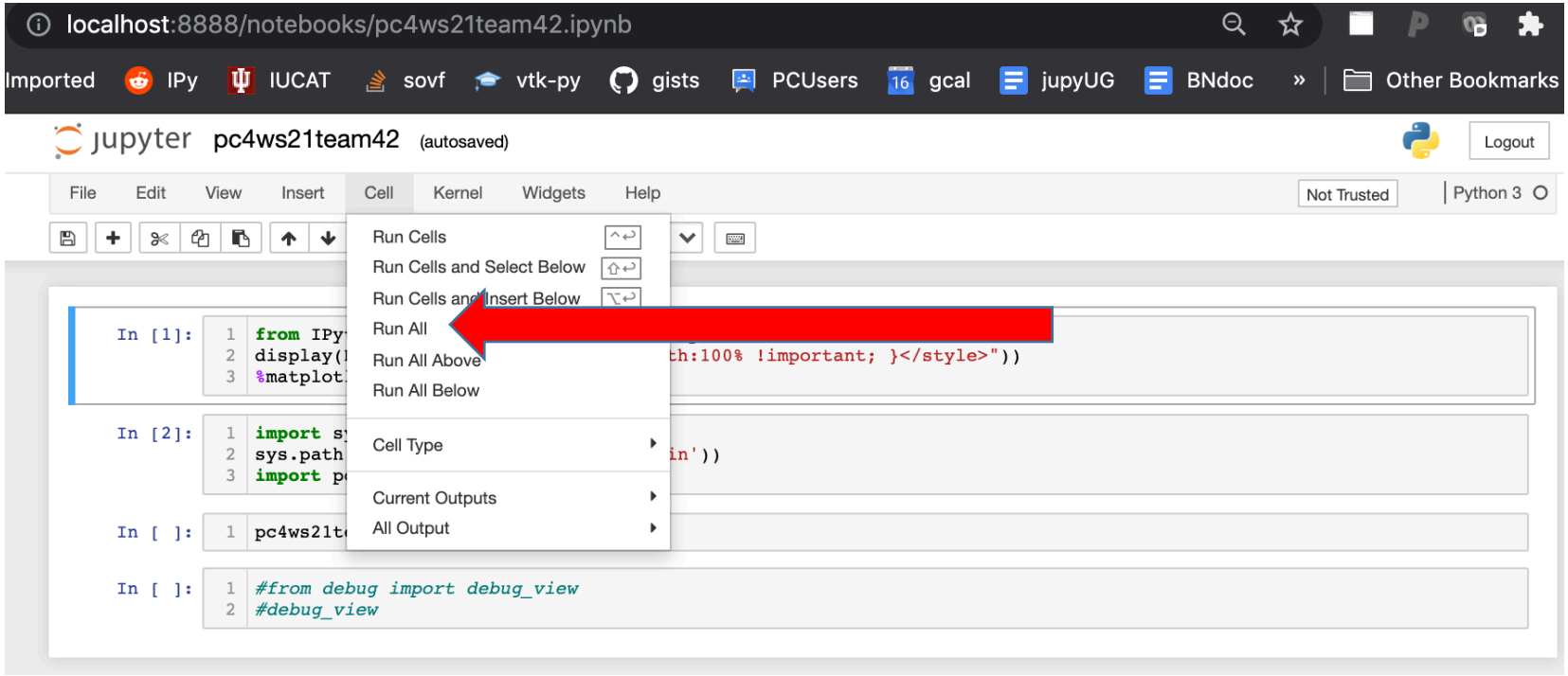
~/pc4ws21team42$ **jupyter notebook pc4ws21team42.ipynb**

...

You should see this Jupyter notebook displayed in your browser:

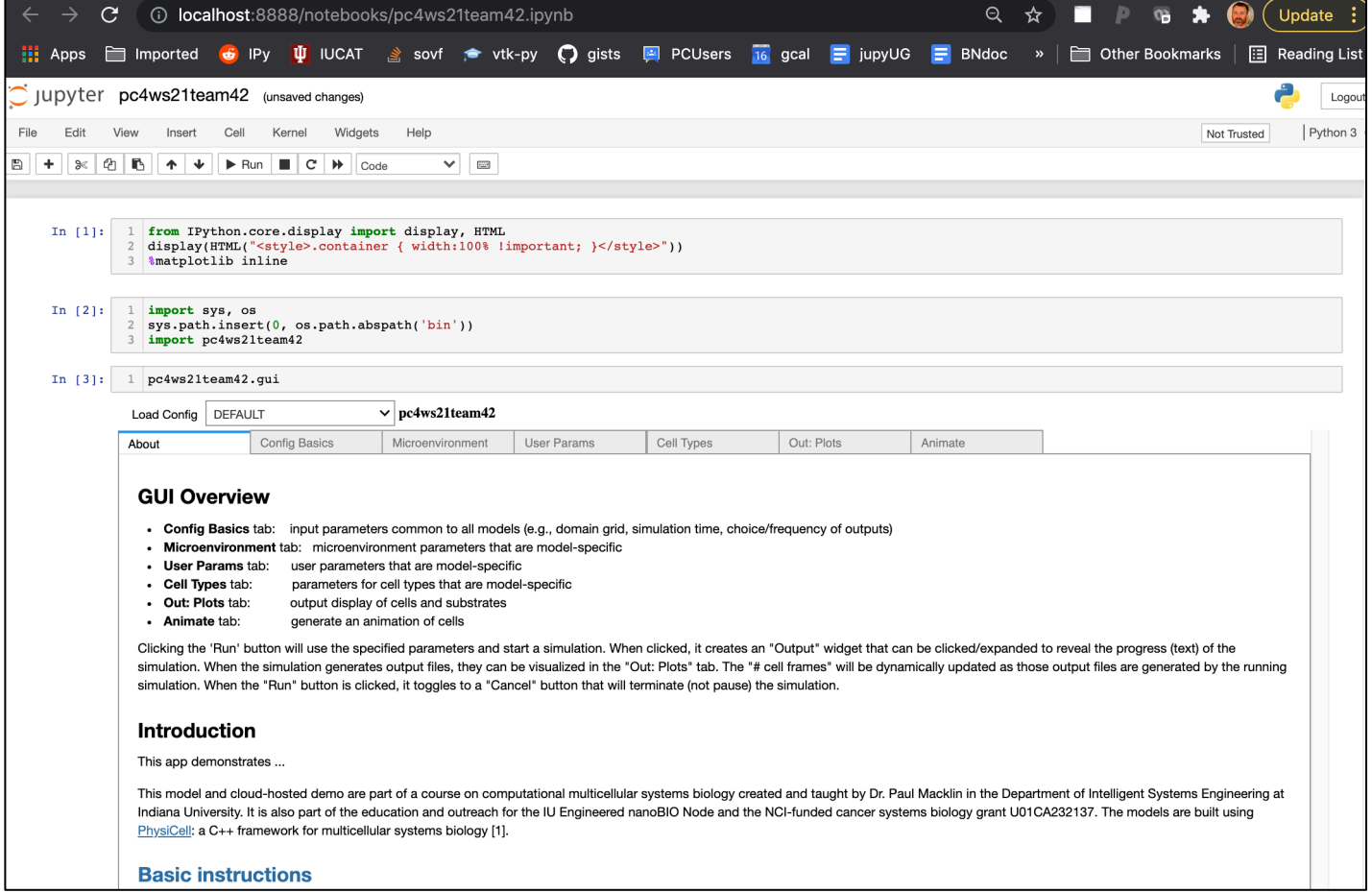


Click the ‘Cell’ menu, ‘Run All’, wait for each notebook “cell” to execute...

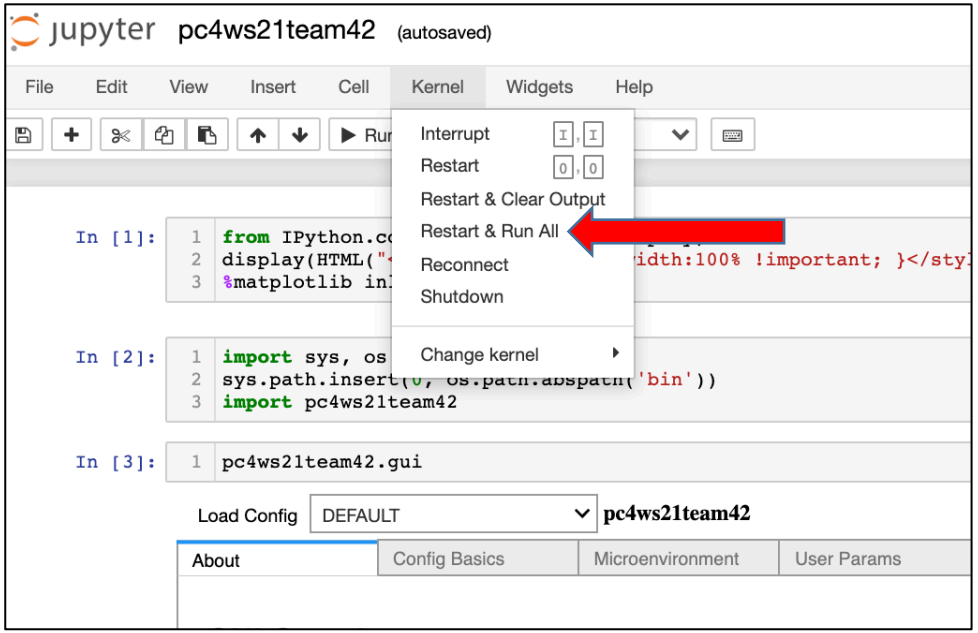


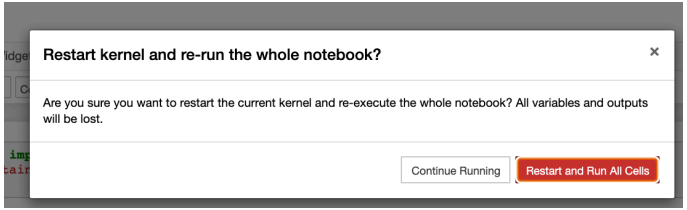
You should see a similar looking notebook GUI for your project.

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).

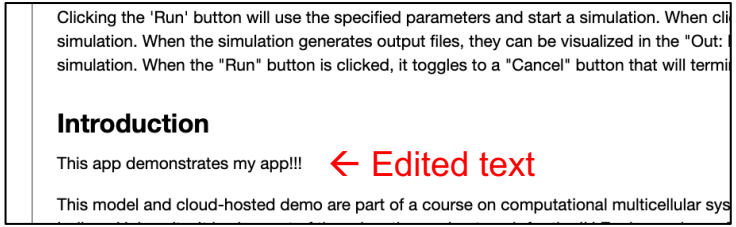


After editing the “doc/about.html”, Click the ‘Kernel’ menu, ‘Restart & Run All’, then click the pop-up button to confirm:

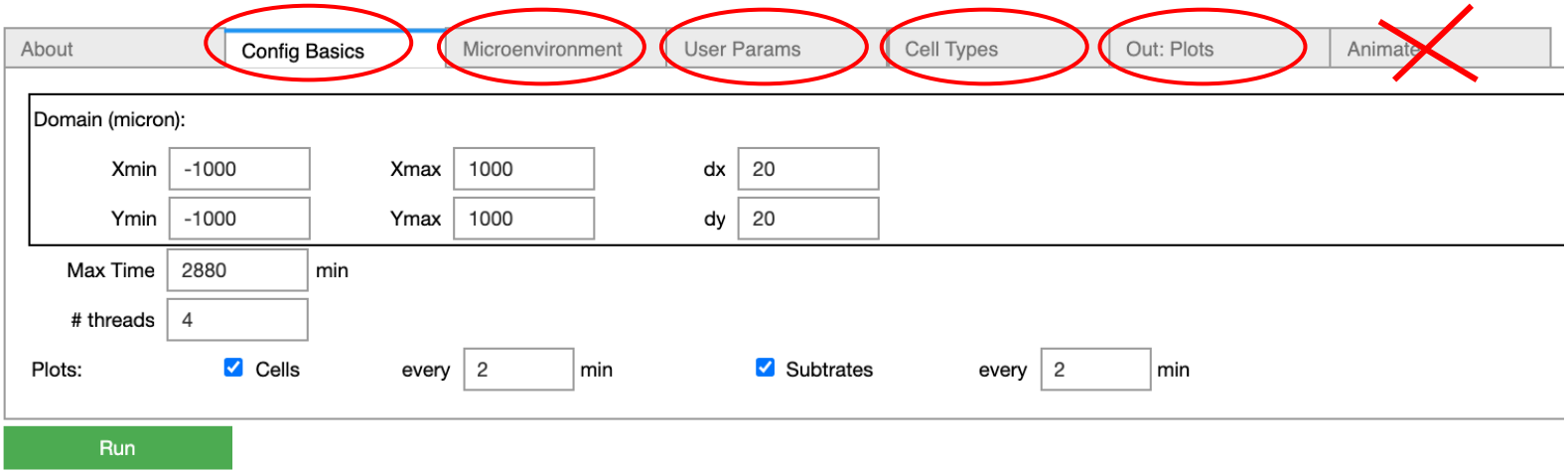




The notebook will refresh, showing your edited text:



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

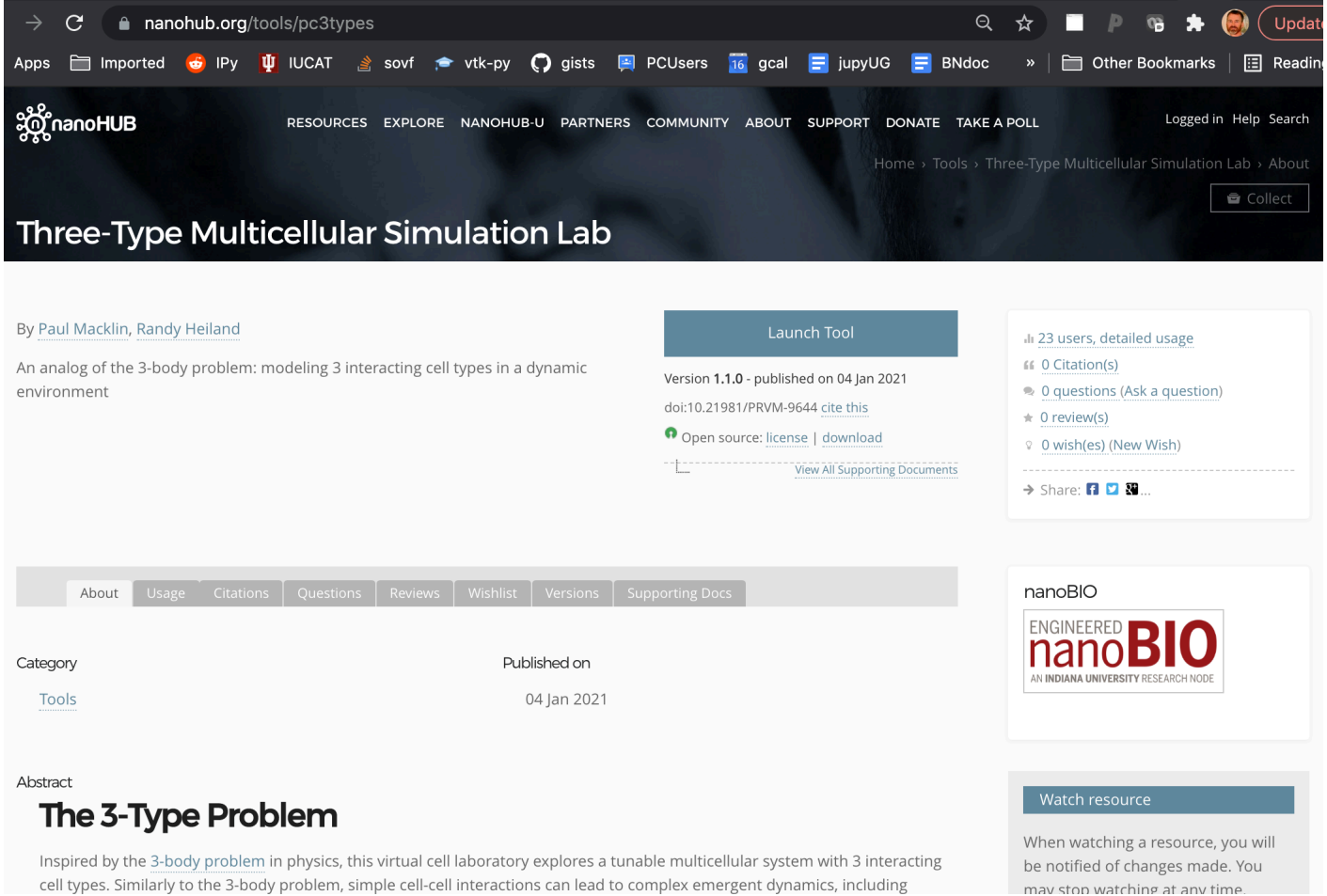


Final steps for nanoHUB app

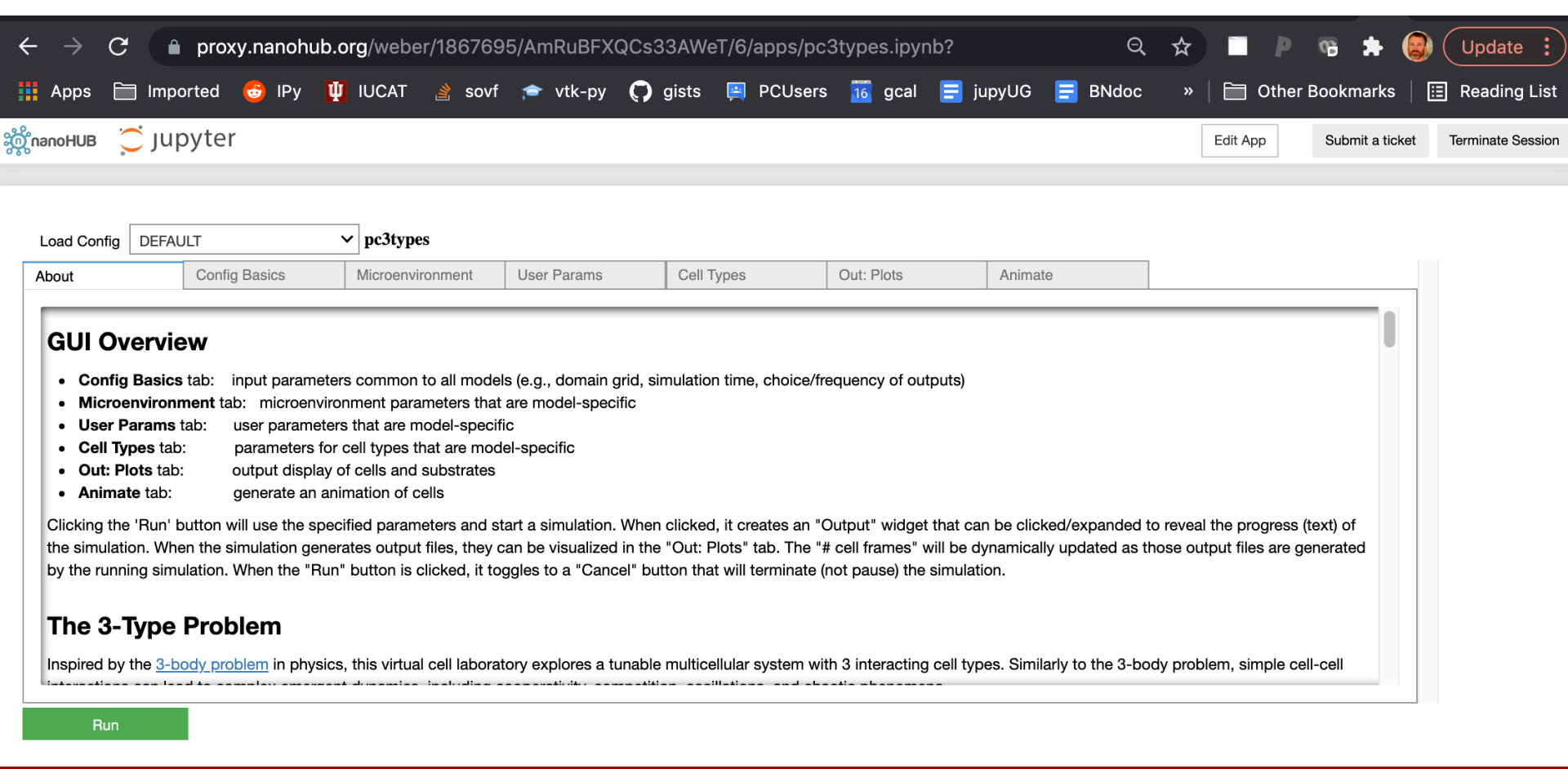
- If your local Jupyter notebook looks correct, you have the option of compiling your project and making sure you can Run it from the notebook - rf. Steps 4 and 5 in:
- https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#steps-to-follow
- However, you can probably skip straight 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 ☺)

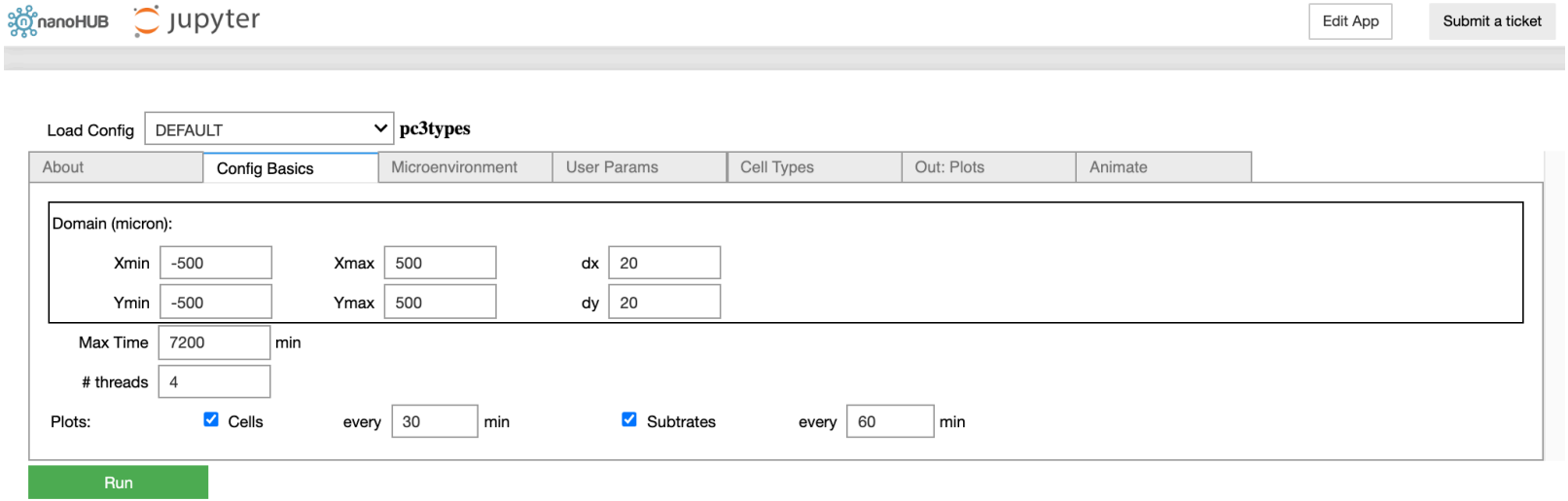
  - https://nanohub.org/register/ – register for a nanoHUB account if you haven’t
  - https://nanohub.org/tools/create – create your app’s basic info
  - Make sure your middleware/invoke script is “executable” (rf. github link above)

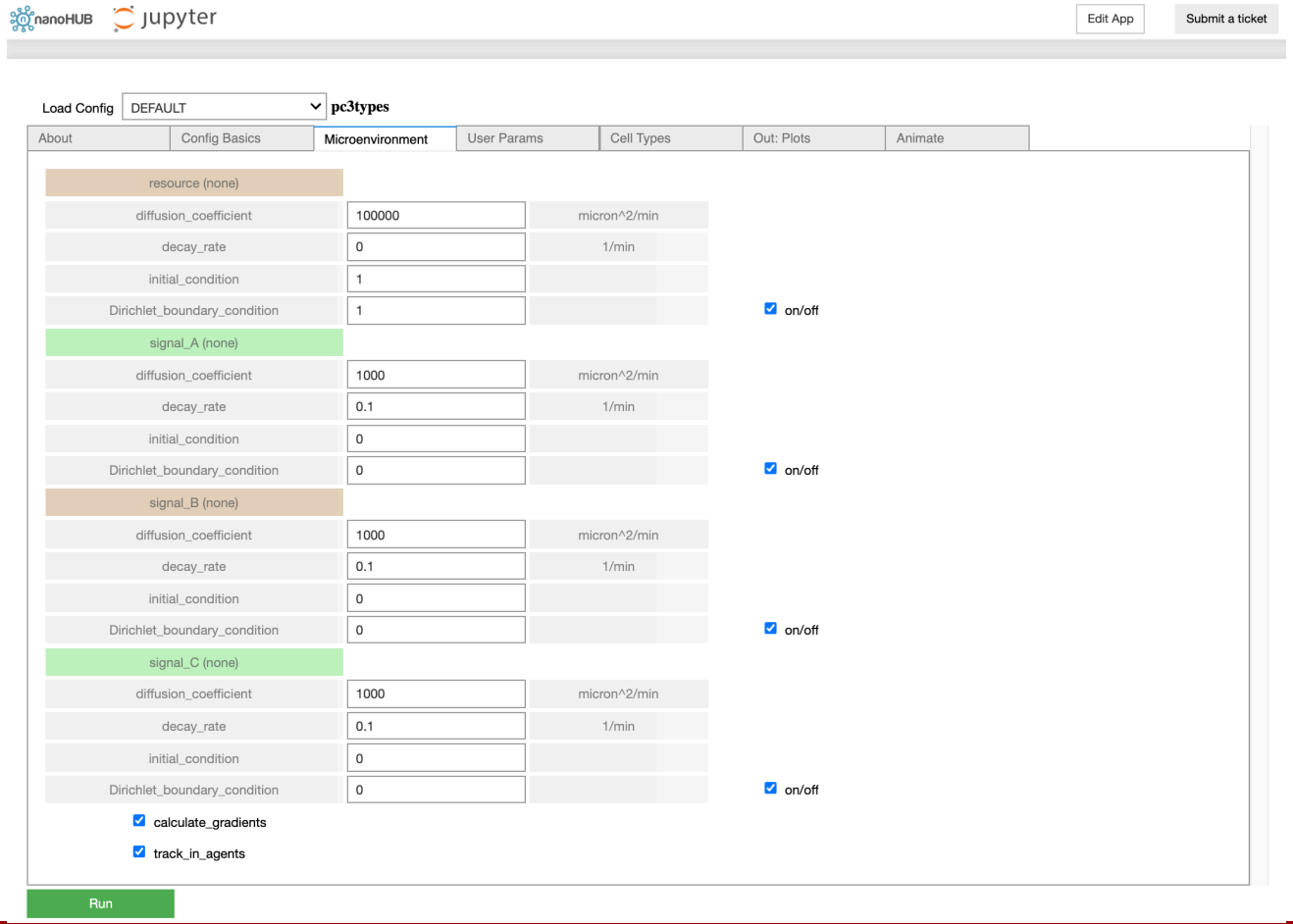
This is our previously published **pc3types** app on nanoHUB.

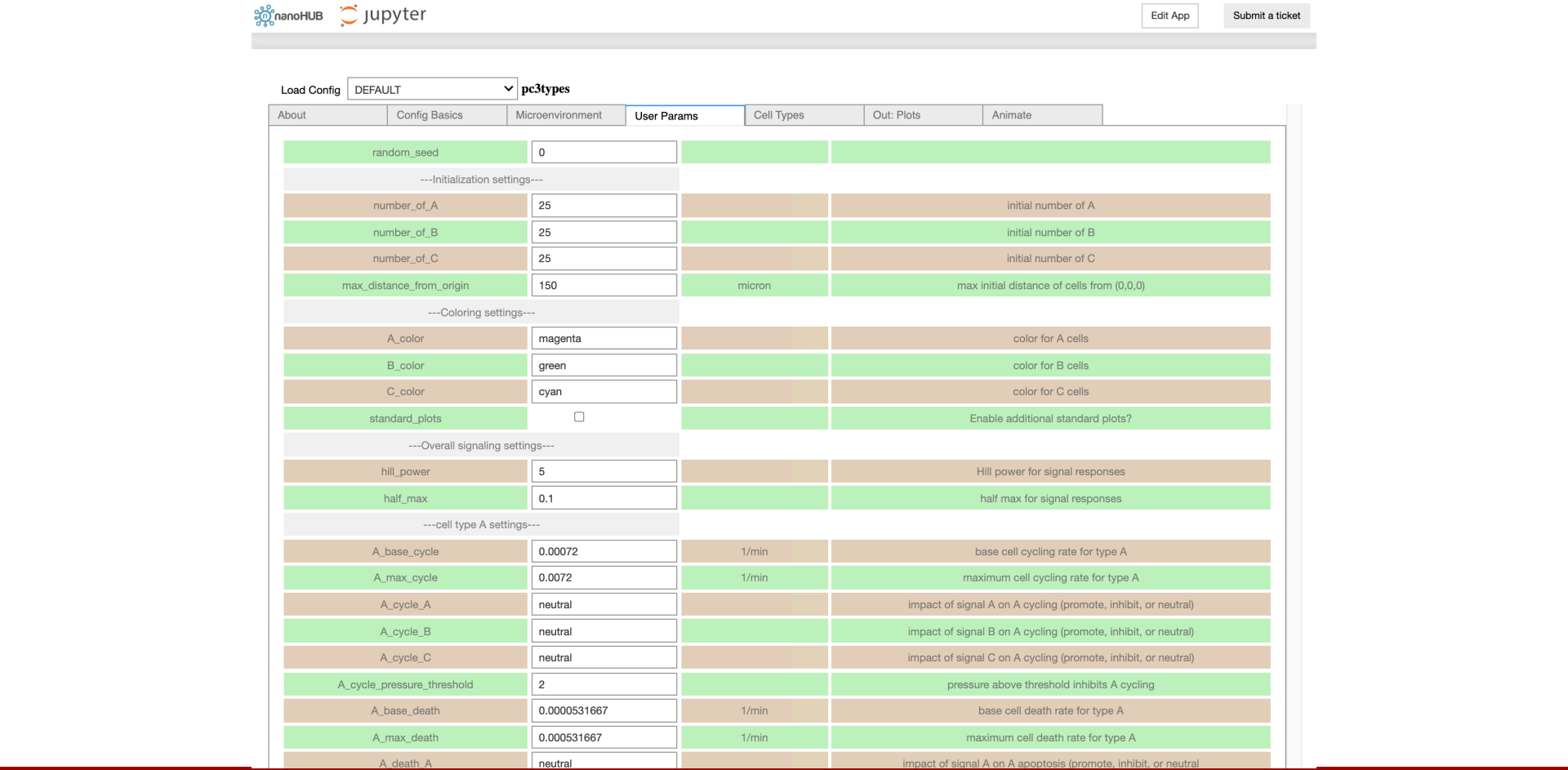


https://nanohub.org/tools/pc3types


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

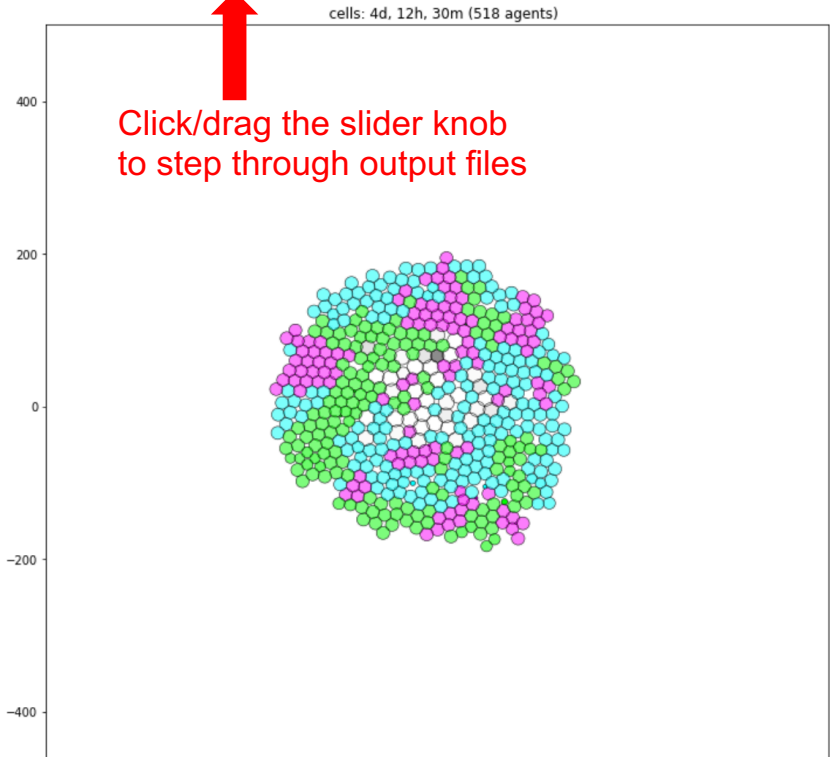
Load Config 2021-06-24 13:58:12.193933 **pc3types**

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



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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