

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)

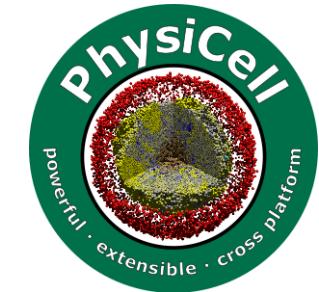


Randy Heiland

 [@rheiland](https://twitter.com/@rheiland)

PhysiCell Project

July 25-31, 2021



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)~~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 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.

github.com/new

Imported IPy IUCAT sovf vtk-py gists PCUsers Other Boo

Create a new repository

A repository contains all project files, including the revision history. Already have a project repository elsewhere? [Import a repository](#).

Owner * Repository name *

 rheiland / pc4ws21team42 

Great repository names are short and memorable. Need inspiration? How about [jubilant-octo-dollop](#)?

Description (optional)

 Public Anyone on the internet can see this repository. You choose who can commit.

 Private You choose who can see and commit to this repository.

Initialize this repository with:

Skip this step if you’re importing an existing repository.

Add a README file This is where you can write a long description for your project. [Learn more](#).

Add .gitignore Choose which files not to track from a list of templates. [Learn more](#).

Choose a license A license tells others what they can and can’t do with your code. [Learn more](#).

This will set  main as the default branch. Change the default name in your [settings](#).

[Create repository](#)

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_MultiCellIDS.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_MultiCellIDS.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.  
~$
```

```
~/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
```

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



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: `xml2jupyter`

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



The Journal of Open Source Software

xml2jupyter: Mapping parameters between XML and Jupyter widgets

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DOI: [10.21105/joss.01408](https://doi.org/10.21105/joss.01408)

Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Submitted: 08 April 2019
Published: 01 July 2019

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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).

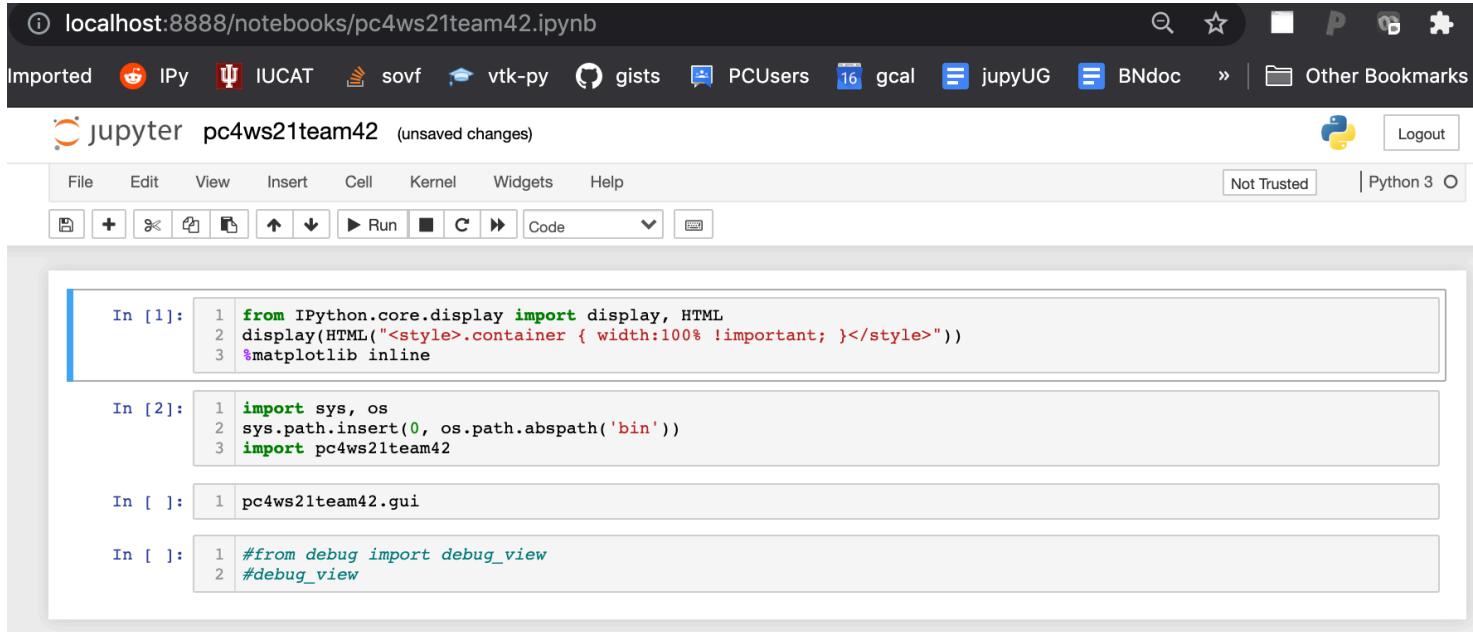
A PhysiCell configuration file defines model-specific `<user_parameters>` in XML. Each parameter element consists of its name with attributes, defining its data type, units (optional),

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
```

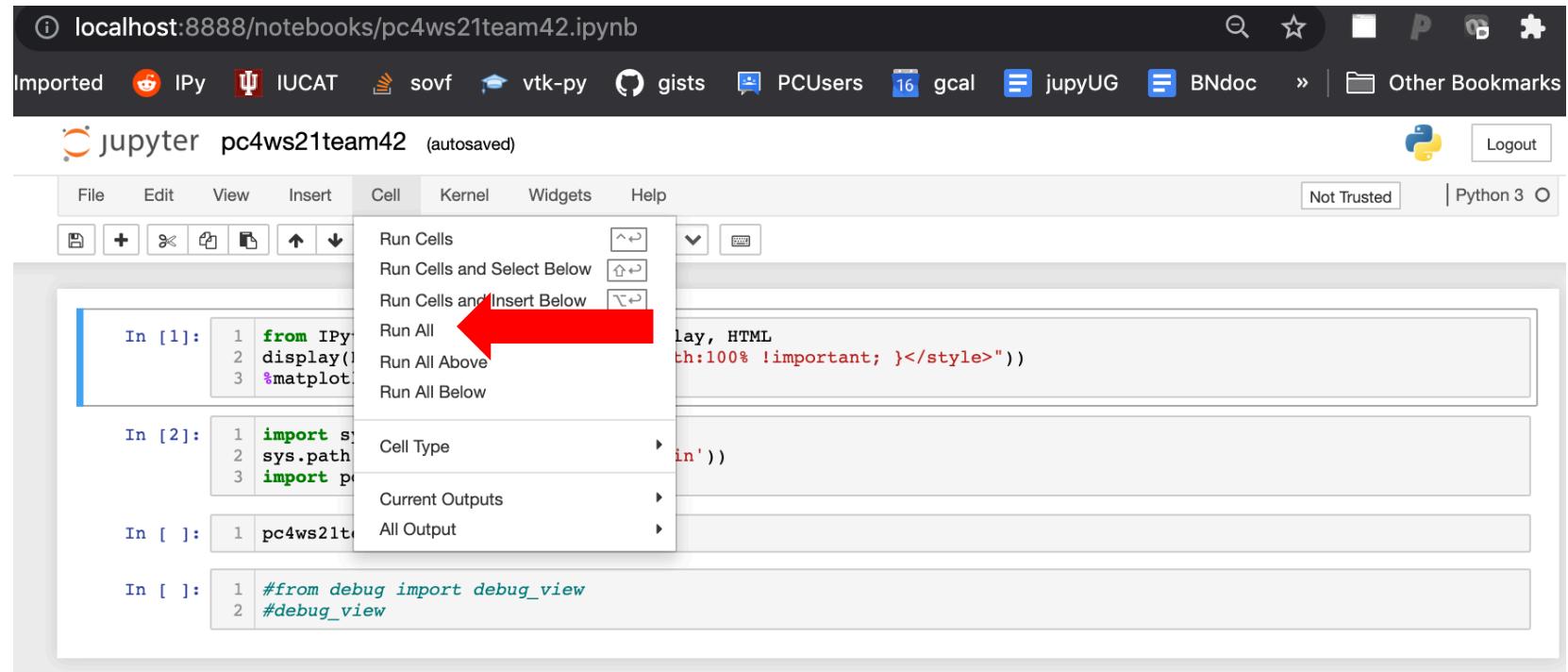
...

A screenshot of a Jupyter Notebook interface running in a web browser. The title bar shows the URL as "localhost:8888/notebooks/pc4ws21team42.ipynb". The browser's address bar also displays "Imported" and other bookmarks. The main window shows a Jupyter logo and the title "jupyter pc4ws21team42 (unsaved changes)". The toolbar includes File, Edit, View, Insert, Cell, Kernel, Widgets, Help, and various icons for file operations like Open, Save, and Run. Below the toolbar, there are four code cells labeled In [1] through In [4].

```
In [1]: 1 from IPython.core.display import display, HTML  
2 display(HTML("<style>.container { width:100% !important; }</style>"))  
3 %matplotlib inline  
  
In [2]: 1 import sys, os  
2 sys.path.insert(0, os.path.abspath('bin'))  
3 import pc4ws21team42  
  
In [ ]: 1 pc4ws21team42.gui  
  
In [ ]: 1 #from debug import debug_view  
2 #debug_view
```

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).

The screenshot shows a Jupyter Notebook interface with three code cells and a generated GUI overview page.

In [1]:

```
1 from IPython.core.display import display, HTML
2 display(HTML("<style>.container { width:100% !important; }</style>"))
3 %matplotlib inline
```

In [2]:

```
1 import sys, os
2 sys.path.insert(0, os.path.abspath('bin'))
3 import pc4ws21team42
```

In [3]:

```
1 pc4ws21team42.gui
```

Below the code cells, there is a configuration dropdown set to "pc4ws21team42".

The main content area displays a "GUI Overview" page with the following tabs:

- 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.

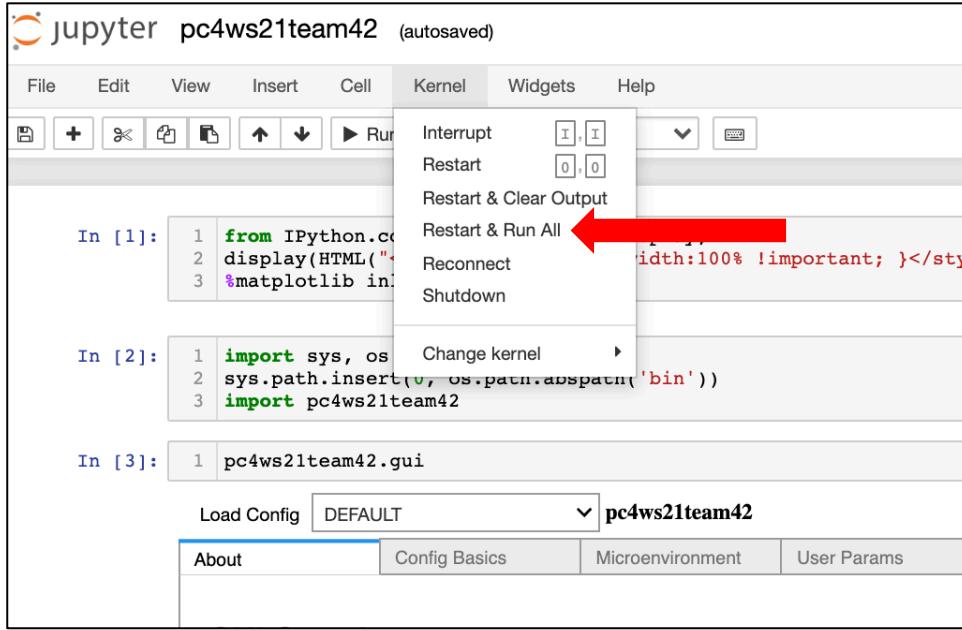
Introduction

This app demonstrates ...

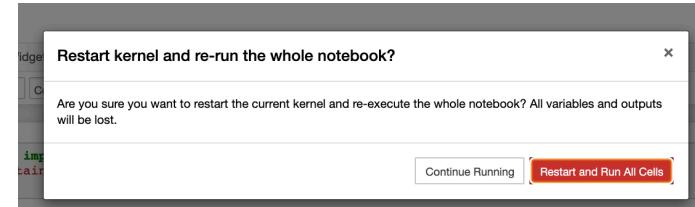
This model and cloud-hosted demo are part of a course on computational multicellular systems biology created and taught by Dr. Paul Macklin in the Department of Intelligent Systems Engineering at Indiana University. It is also part of the education and outreach for the IU Engineered nanoBIO Node and the NCI-funded cancer systems biology grant U01CA232137. The models are built using PhysiCell: a C++ framework for multicellular systems biology [1].

Basic instructions

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



The screenshot shows a Jupyter Notebook window titled "jupyter pc4ws21team42 (autosaved)". The "Kernel" menu is open, displaying options: Interrupt, Restart, Restart & Clear Output, **Restart & Run All** (highlighted with a red arrow), Reconnect, Shutdown, and Change kernel. Below the menu, there are three code cells labeled In [1], In [2], and In [3]. Cell In [1] contains code to import IPython and display HTML. Cell In [2] imports sys, os, and pc4ws21team42. Cell In [3] imports pc4ws21team42.gui. At the bottom, there is a "Load Config" dropdown set to "DEFAULT" and a "pc4ws21team42" tab selected. A navigation bar at the bottom includes "About", "Config Basics", "Microenvironment", and "User Params".



The notebook will refresh,
showing your edited text:

Clicking the 'Run' button will use the specified parameters and start a simulation. When clicking 'Run', the simulation will begin. When the simulation generates output files, they can be visualized in the "Output" tab. When the "Run" button is clicked, it toggles to a "Cancel" button that will terminate the simulation.

Introduction

This app demonstrates my app!!! **← Edited text**

This model and cloud-hosted demo are part of a course on computational multicellular systems.

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

The screenshot shows the PhysiCell software interface. At the top, there is a navigation bar with several tabs: About, Config Basics, Microenvironment, User Params, Cell Types, Out: Plots, and Animate. The 'Config Basics' tab is currently active, indicated by a blue background. Red circles highlight the 'Microenvironment', 'User Params', 'Cell Types', and 'Out: Plots' tabs. A large red 'X' is drawn over the 'Animate' tab. Below the tabs, there are various configuration settings:

- Domain (micron):**
 - Xmin: -1000
 - Xmax: 1000
 - dx: 20
 - Ymin: -1000
 - Ymax: 1000
 - dy: 20
- Max Time:** 2880 min
- # threads:** 4
- Plots:** Cells every 2 min Substrates every 2 min

A green 'Run' button is located at the bottom left.

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:
 - [\(not “optional” if you plan to do it ☺\)](https://github.com/PhysiCell-Tools/PhysiCell-Jupyter-GUI/blob/master/README.md#create-a-nanohub-tool-optional)
 - ◆ <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)

The screenshot shows the 'Create New Account' page on the nanohub.org website. At the top, there's a navigation bar with links like 'RESOURCES', 'EXPLORE', 'NANOHUB-U', 'PARTNERS', 'COMMUNITY', 'ABOUT', 'SUPPORT', 'DONATE', and 'TAKE A POLL'. Below the navigation is a 'CONNECT WITH' section with two main options: 'With Institutional Credentials' (selected) and 'Sign in with Google'. A note below the first option says 'Don't see your organization listed? Let us know!'. To the right of this section is a blue box containing the text: 'You can choose to log in via one of these services, and we'll help you fill in the info below!' Below the connection options is a 'LOGIN INFORMATION' section. It includes fields for 'Username' (marked as REQUIRED), 'Password' (marked as REQUIRED), and 'Confirm Password' (marked as REQUIRED). Below the password fields is a list of seven validation rules: 'Must contain at least 1 number or punctuation mark', 'Must contain at least 1 letter', 'Must be at least 8 characters long', 'Must not contain easily guessed words', 'Must not contain your name or parts of your name', and 'Must not contain your username'. To the right of the login form, there are two informational boxes: one about usernames and another about passwords.

nanoHUB

RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

Login Sign Up Help Search

Home > Register > Create New Account

CONNECT WITH

With Institutional Credentials

Don't see your organization listed? Let us know!

Sign in with Google

LOGIN INFORMATION

Username REQUIRED

Combination of lowercase letters and numbers. No spaces or punctuation.

Password REQUIRED

Confirm Password REQUIRED

- Must contain at least 1 number or punctuation mark
- Must contain at least 1 letter
- Must be at least 8 characters long
- Must not contain easily guessed words
- Must not contain your name or parts of your name
- Must not contain your username

You can choose to log in via one of these services, and we'll help you fill in the info below!

Already have an account? [Log in here.](#)

Usernames cannot be changed. If this poses a serious problem or raises concerns please contact our support.

Password may be changed any time after account creation.

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-G

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

nanohub.org/tools/pc4ws21team42/status

Apps Imported IPy IUCAT sofv vtk-py gists Other Bookmarks Reading

Tool information successfully registered

nanoHUB

RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

Logged in Help Search

Home > Tools > Tool Pipeline > Status for pc4ws21team42

Tools: Status for pc4ws21team42 - Created

All Tools New Tool

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

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 |
| 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 has created the following project area for your tool on the [nanoFORGE](#):
<https://nanohub.org/tools/pc4ws21team42/wiki>

Follow these steps to start using your project area:

[Learn more about uploading source code into your project area and how the directories are arranged](#)

[Learn more About the Rappture toolkit.](#)

[Learn about nanoHUB's software development environment](#)

When you are ready, [Follow these instructions](#) to access the source code repository for your specific project and upload your code.

We are waiting for You

Once your source code has been uploaded into your project area, click here to let us know:

→ [My code is committed, working, and ready to be installed](#)

Remaining steps before we can publish your tool:

[Register your tool on nanoHUB.org](#)

[Commit the final code for this version. I've done this. How do I do this?](#)

→ [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/](#)

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

PhysiCell Project
PhysiCell.org
@PhysiCell

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) |
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| 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](#)



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>

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
- Create this page...
- Test and approve your tool
- Publish your tool so that others can see it on nanohub.org/

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).

PhysiCell Project
PhysiCell.org
@PhysiCell

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

nanohub.org/tools/pc3types

RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

Home > Tools > Three-Type Multicellular Simulation Lab > About

Collect

Three-Type Multicellular Simulation Lab

By Paul Macklin, Randy Heiland

An analog of the 3-body problem: modeling 3 interacting cell types in a dynamic environment

Launch Tool

Version 1.1.0 - published on 04 Jan 2021

doi:10.21981/PRVM-9644 cite this

Open source: license | download

View All Supporting Documents

Category: Tools

Published on: 04 Jan 2021

Abstract: **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 interactions can lead to complex emergent dynamics, including

23 users, detailed usage

0 Citation(s)

0 questions (Ask a question)

0 review(s)

0 wish(es) (New Wish)

Share: [f](#) [t](#) [s](#) ...

nanoBIO
ENGINEERED nanoBIO
AN INDIANA UNIVERSITY RESEARCH NODE

<https://nanohub.org/tools/pc3types>

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

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Domain (micron):

Xmin Xmax dx Ymin Ymax dy Max Time min# threads

Plots:

 Cellsevery min Substratesevery min[Run](#)

Load Config

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|--|-------------------------------------|--------------------------|-------------|------------|------------|--|
| resource (none) | | | | | | |
| diffusion_coefficient | <input type="text" value="100000"/> | micron ² /min | | | | |
| decay_rate | <input type="text" value="0"/> | 1/min | | | | |
| initial_condition | <input type="text" value="1"/> | | | | | |
| Dirichlet_boundary_condition | <input type="text" value="1"/> | | | | | <input checked="" type="checkbox"/> on/off |
| signal_A (none) | | | | | | |
| diffusion_coefficient | <input type="text" value="1000"/> | micron ² /min | | | | |
| decay_rate | <input type="text" value="0.1"/> | 1/min | | | | |
| initial_condition | <input type="text" value="0"/> | | | | | |
| Dirichlet_boundary_condition | <input type="text" value="0"/> | | | | | <input checked="" type="checkbox"/> on/off |
| signal_B (none) | | | | | | |
| diffusion_coefficient | <input type="text" value="1000"/> | micron ² /min | | | | |
| decay_rate | <input type="text" value="0.1"/> | 1/min | | | | |
| initial_condition | <input type="text" value="0"/> | | | | | |
| Dirichlet_boundary_condition | <input type="text" value="0"/> | | | | | <input checked="" type="checkbox"/> on/off |
| signal_C (none) | | | | | | |
| diffusion_coefficient | <input type="text" value="1000"/> | micron ² /min | | | | |
| decay_rate | <input type="text" value="0.1"/> | 1/min | | | | |
| initial_condition | <input type="text" value="0"/> | | | | | |
| Dirichlet_boundary_condition | <input type="text" value="0"/> | | | | | <input checked="" type="checkbox"/> on/off |
| <input checked="" type="checkbox"/> calculate_gradients <input checked="" type="checkbox"/> track_in_agents | | | | | | |
| <input type="button" value="Run"/> | | | | | | |

Load Config **DEFAULT** **pc3types**

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|----------------------------------|--------------------------|------------------|-------------|------------|--|---------|
| 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 | <input type="checkbox"/> | | | | 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) | |

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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 |

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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)

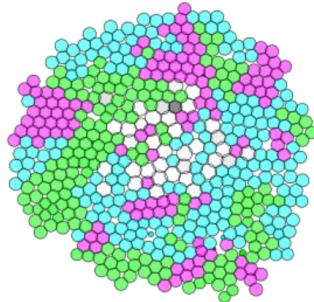
400

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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