Slides, videos, links and more:
https://github.com/physicell-training/02-How-to-nanoHUB

Lesson 2: How to use a PhysiCell nanoHUB app

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last updated: November 13, 2019

nanoHUB Account

- These tutorials use cloud-hosted PhysiCell models on nanoHUB.org.
- nanoHUB is **free**, but it requires a one-time registration.
- **Steps**:
  1. Visit https://nanohub.org/register
  2. Choose "Sign in with Google"
  3. Choose a Google account
  4. Click "No" (so it doesn't try to associate with some other nanoHIB account)
  5. Finish filling in details, and you're done!
  6. Use your google account for future logins.

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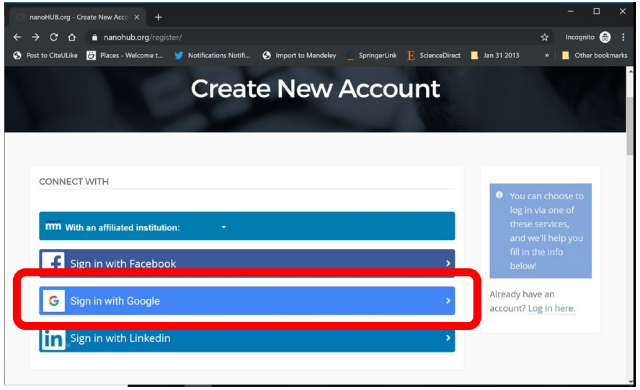

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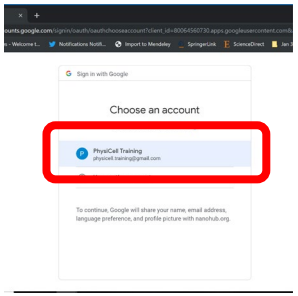

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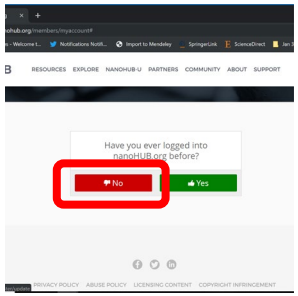


Goals

- Many of the PhysiCell lessons are paired with **educational microapps**:

  targeted cloud-hosted models designed to illustrate a core PhysiCell concept.

- All PhysiCell-powered nanoHUB apps share common features.

- This brief lesson will walk you through those features.

Tools versus Apps

- After considerable debate, the nanoHUB community arrived at these definitions:
  - A **tool** is an application with broader feature sets and less constrained use cases. A tool tends to require more extensive training to understand the full feature set.
    - Future PhysiCell-powered nanoHUB resources may be tools if they allow general-purpose modeling using PhysiCell as the engine.
  - An **app** is purpose-driven model or constrained tool with relatively constrained and focused use cases. Users can generally learn an app in one or two unguided sessions.
    - Most PhysiCell-powered nanoHUB resources are apps.
- There may be blurred distinctions between tools and apps in some cases, such as PhysiCell apps that can simulate a broad variety of nanotherapies.

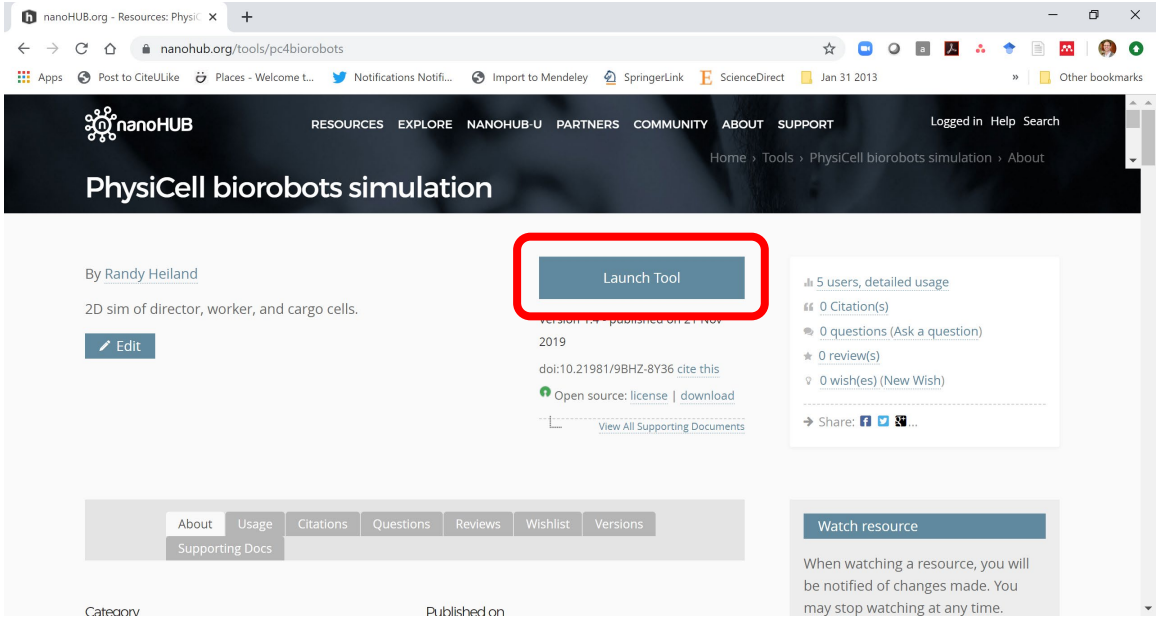
Sample nanoHUB app: biorobots

- This sample model explores how engineered cells could be used as a **multicellular cargo delivery system.**
- **Director cells:** Release a chemoattractant to guide delivery of cargo
- **Cargo cells:** Release a chemoattractant to guide worker cells until they are attached.
- **Worker cells:** When unattached to cargo, use chemotaxis to seek cargo cells and adhere to them.

  When attached to cargo, use chemotaxis to drag cargo towards directors for delivery.

Splash screen and launching the tool

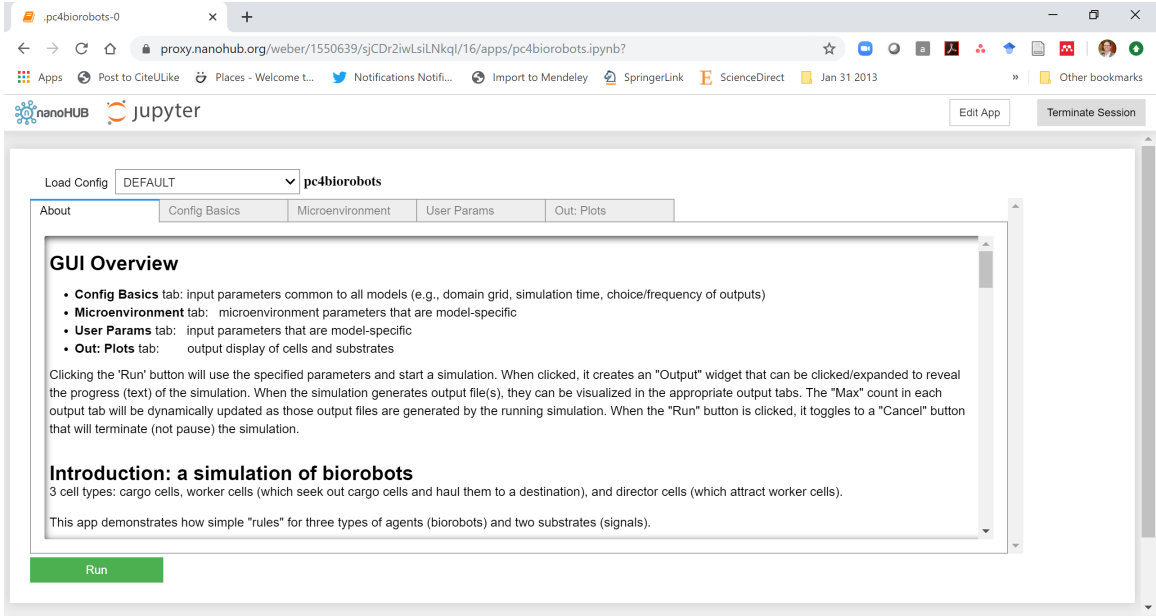
- Each PhysiCell-powered nanoHUB app has a splash page:
  - Background information on the tool and model
  - Use metrics
  - Citation information
  - A **LAUNCH TOOL** button. Click this!



About

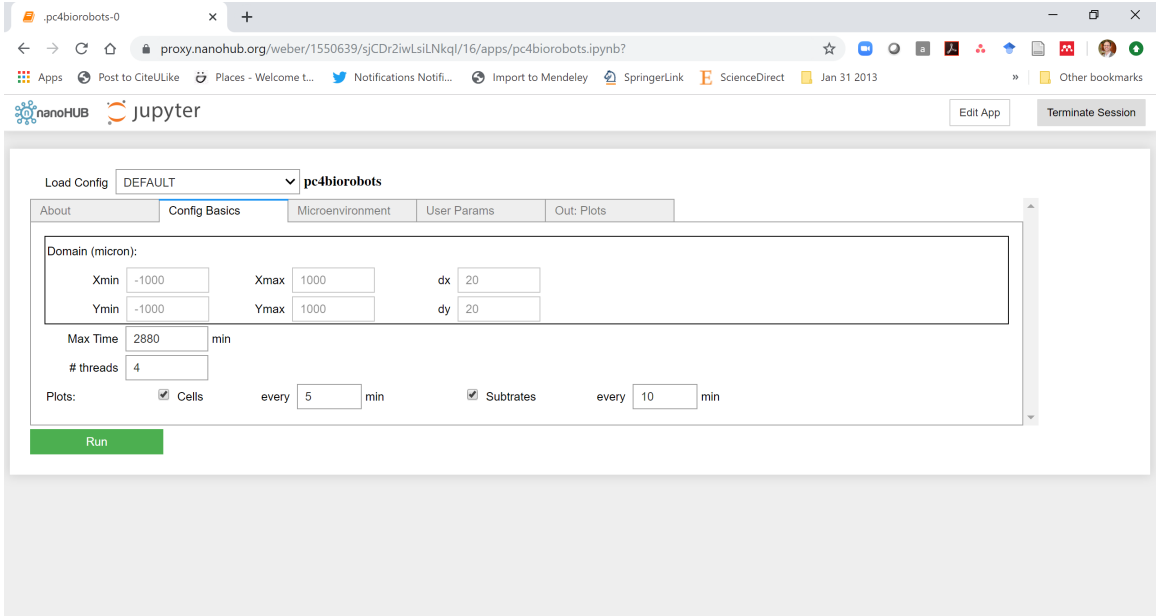
- The **about** tab gives *in-app* documentation about the mathematics of the model:
  - background
  - diffusing substrates
  - key cell types and behaviors

- This tab also describes the main user parameters of the model.



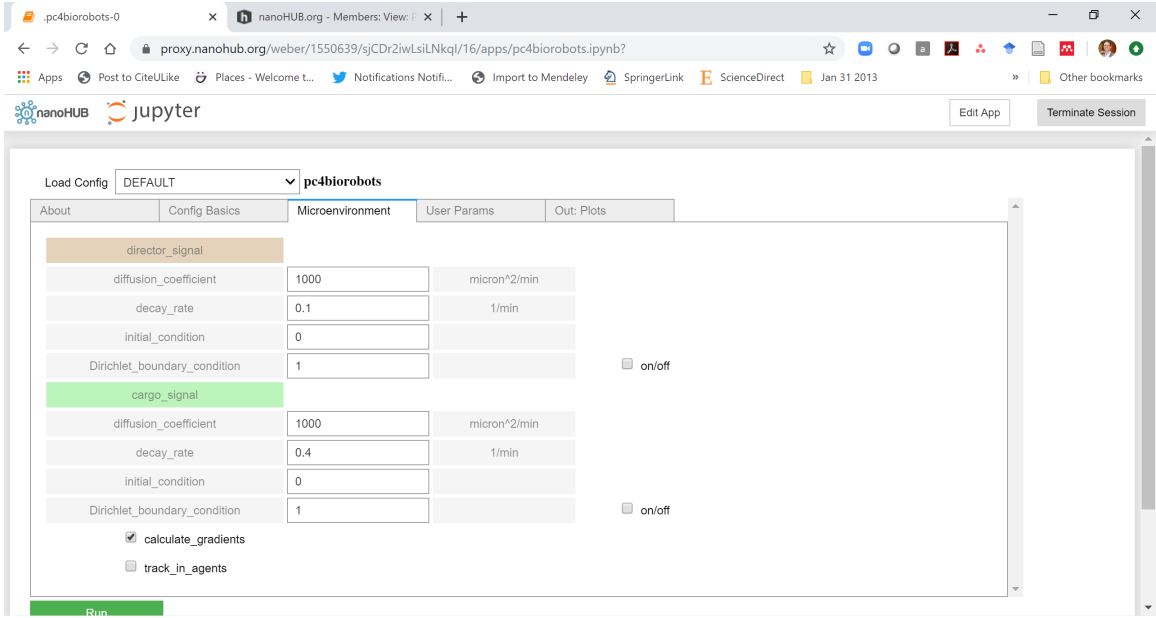
Configuration basics

- The **config basics** tab lets you set up the simulation:
  - Set the domain size and spatial resolution
    - ♦ Might be disabled in some apps.
  - Set the final simulation time
  - Set the number of threads (capped at 4 on nanoHUB)
  - Specify how often to save cell plots
  - Specify how often to save diffusing substrate data



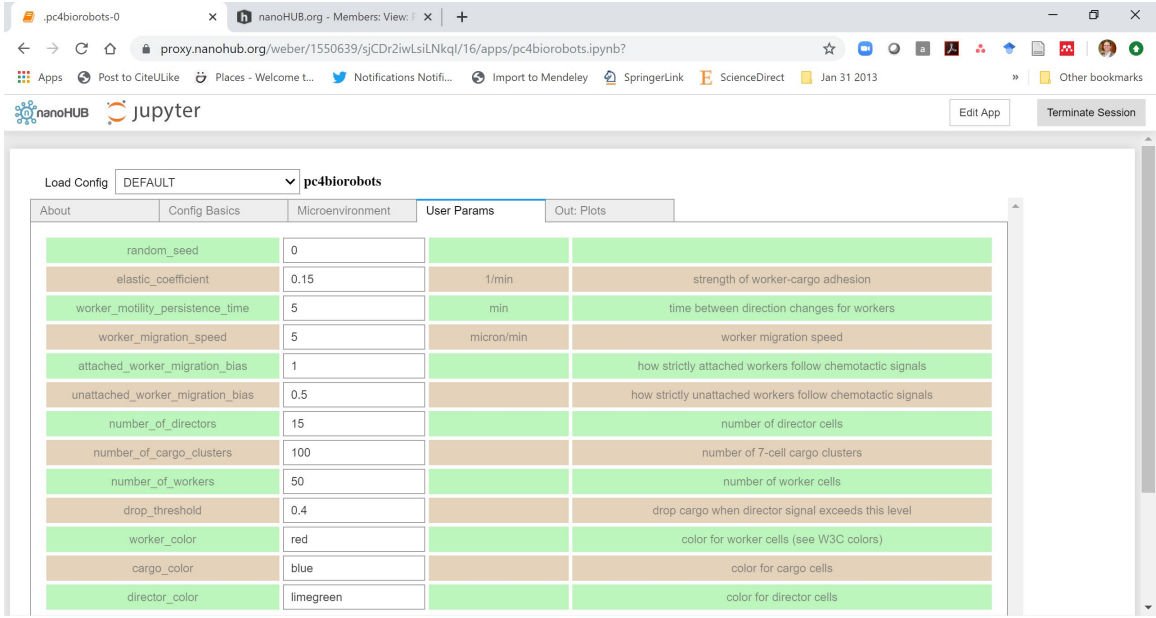
Microenvironment

- The **microenvironment** tab lets you set diffusion options:
  - For each substrate, set:
    - ♦ diffusion coefficient
    - ♦ decay rate
    - ♦ initial condition
      - » applied uniformly throughout the domain
    - ♦ Dirichlet boundary condition
      - » applied uniformly to the boundary
      - » "uncheck" to disable this and revert to Neumann (zero flux) conditions
  - Enable or disable calculation of substrate gradients
    - ♦ needed for cell chemotaxis
  - Enable or disable full tracking of internalized substrates in each cell
    - ♦ needed for some models



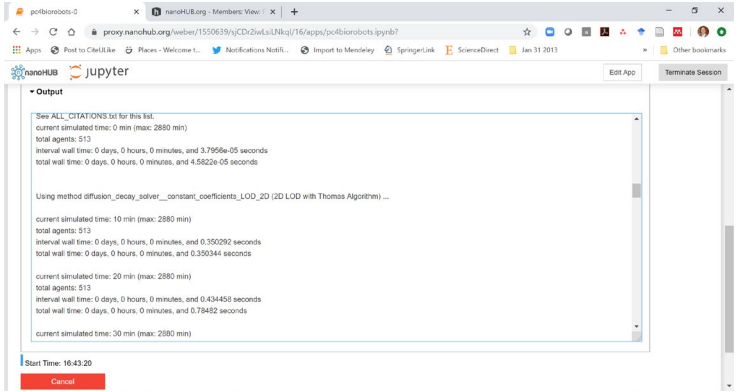
User parameters

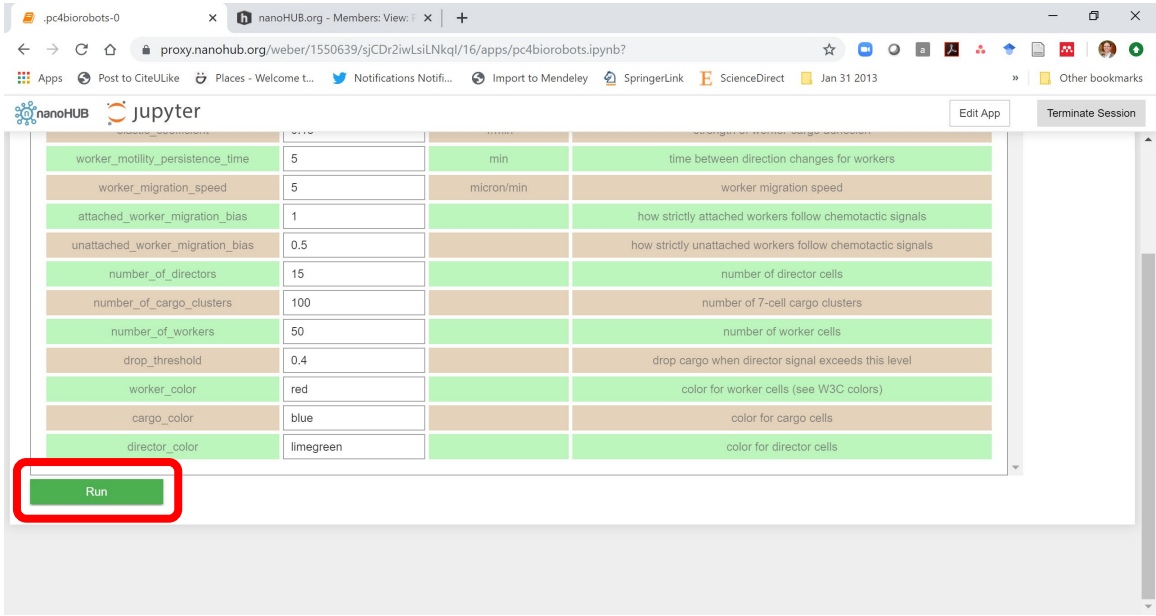
- The **user parameters** tab is where you set parameters that are specific to the app.
- Each row is a parameter:
  - parameter name
  - parameter value
  - units
  - short parameter description
- Consult the **about** tab for more mathematical information on the parameters



Running

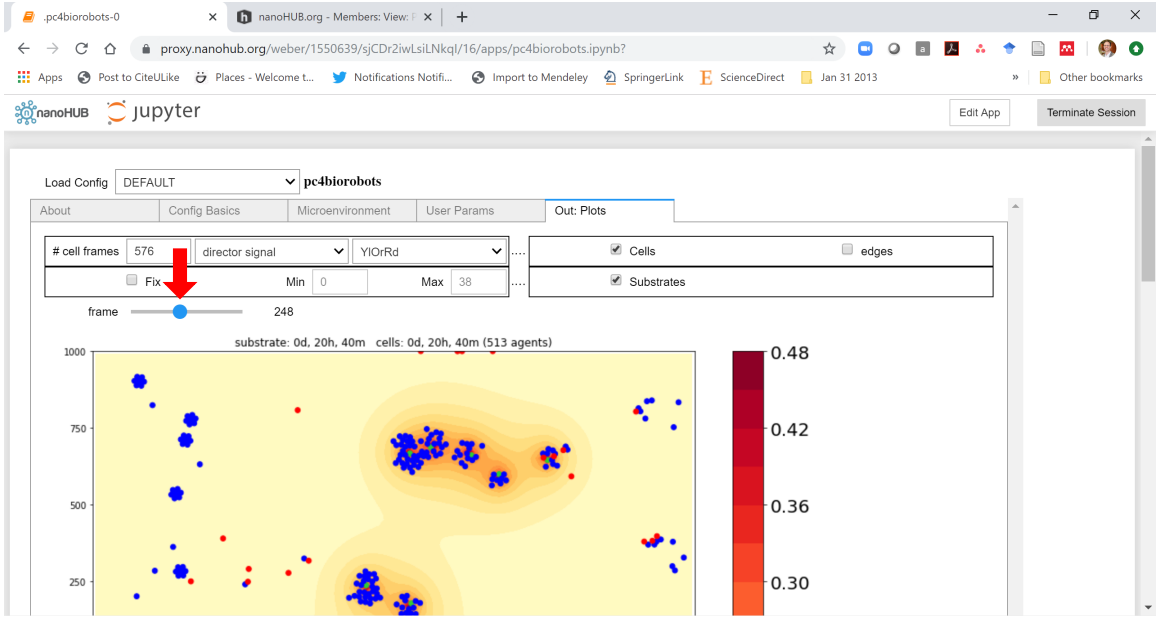
- Once ready, click **Run**
- The standard model outputs will start appearing below
- Click **Cancel** to end early and choose new parameters





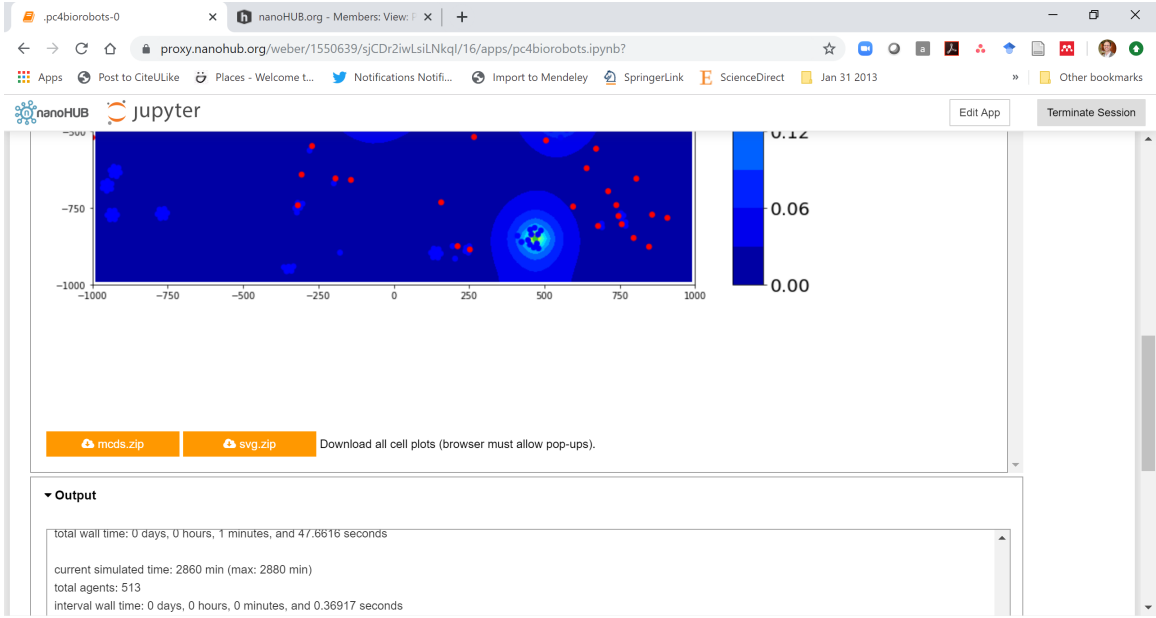
Simulation output

- The **Out: Plots** tab shows the simulation outputs as it runs.
- Slide the "frame" bar to advance time in the simulation.
- Use the dropdown box to choose a different substrate for visualization.
  - Use "fix" to manually set the plot range
  - Click the righthand dropdown box to change coloring (YlOrRd, viridis, jet, …)
- The checkboxes on the right let you choose plotting options for the cells.
- **Note:** Some older apps may split the output into separate "substrate" and "cell" tabs, rather than overlay them.



Downloading simulation plots and data

- At the bottom of the output tab, you can find options to download your simulation data.
- Click **svg.zip** to download all the SVG cell plots as a single ZIP file.
- Click **mcds.zip** to download all the simulation data (in MultiCellDS format) as a single ZIP file.
- **Note:** These download buttons only work after a simulation has finished running.
- See the PhysiCell-Tools ecosystem for tips on loading simulation data in Matlab, Python, and other environments.



Live demo

Next steps

Super fast: Please proceed to 4 (Introduction to PhysiCell)
link: https://github.com/physicell-training/04-PhysiCell-intro

Intermediate: Please proceed to 4 (Introduction to PhysiCell)
link: https://github.com/physicell-training/04-PhysiCell-intro

Full training: Please proceed to 3 (What is an agent-based model?)
link: https://github.com/physicell-training/03-What-is-ABM

More lessons: https://github.com/physicell-training/master-list

Credits

Lesson Planning: Paul Macklin, Drew Willis*, Randy Heiland

Slides: Paul Macklin, Drew Willis, Randy Heiland

Recording: Paul Macklin, Drew Willis*

Post-production: Paul Macklin, Drew Willis*, Kali Konstantinopoulos*

Microapps: https://www.nanohub.org/tools/pc4biorobots

* denotes undergraduate researcher

Funding:

PhysiCell Development:

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

Training materials:

* Administrative supplement to NCI U01CA232137 (Year 2)