

**Slides, videos, links and more:**

<https://github.com/physicell-training/cecam23>

# Introducing: PhysiMESS

## Model Builder & Fibre Initialisation

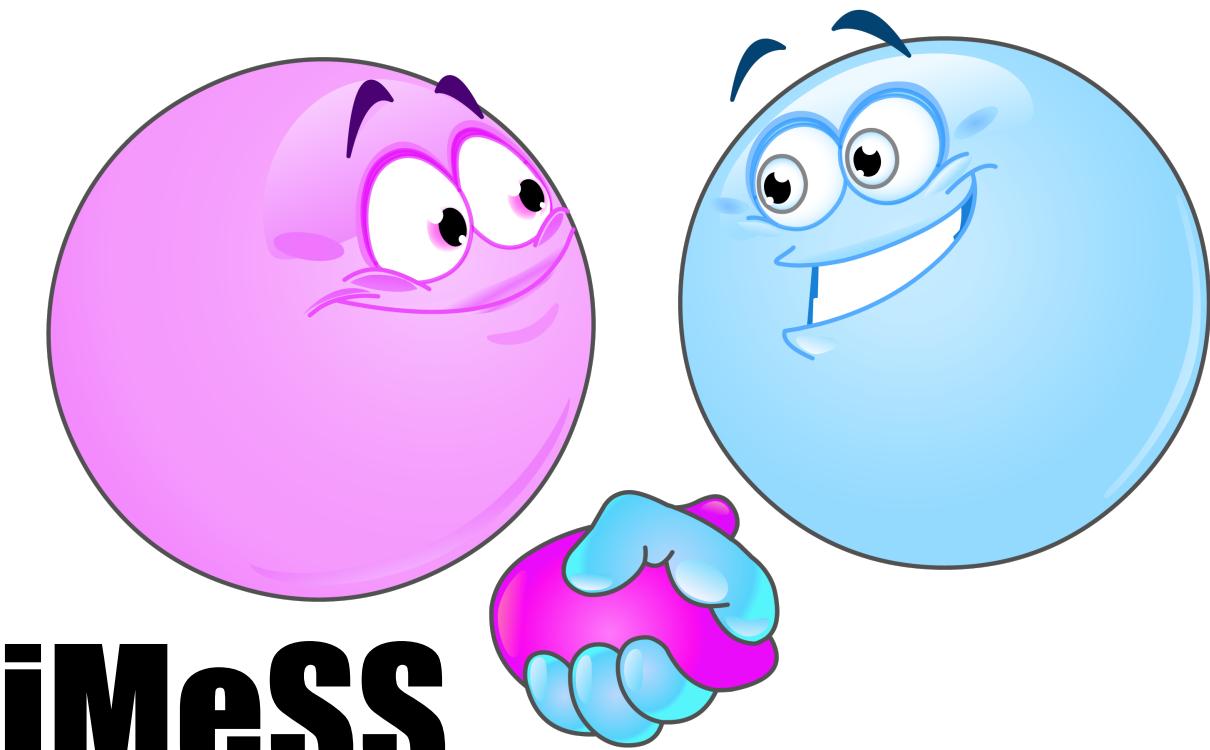


PhysiCell Hackathon  
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Cicely Macnamara

 @CicelyKrystyna

CECAM 2023



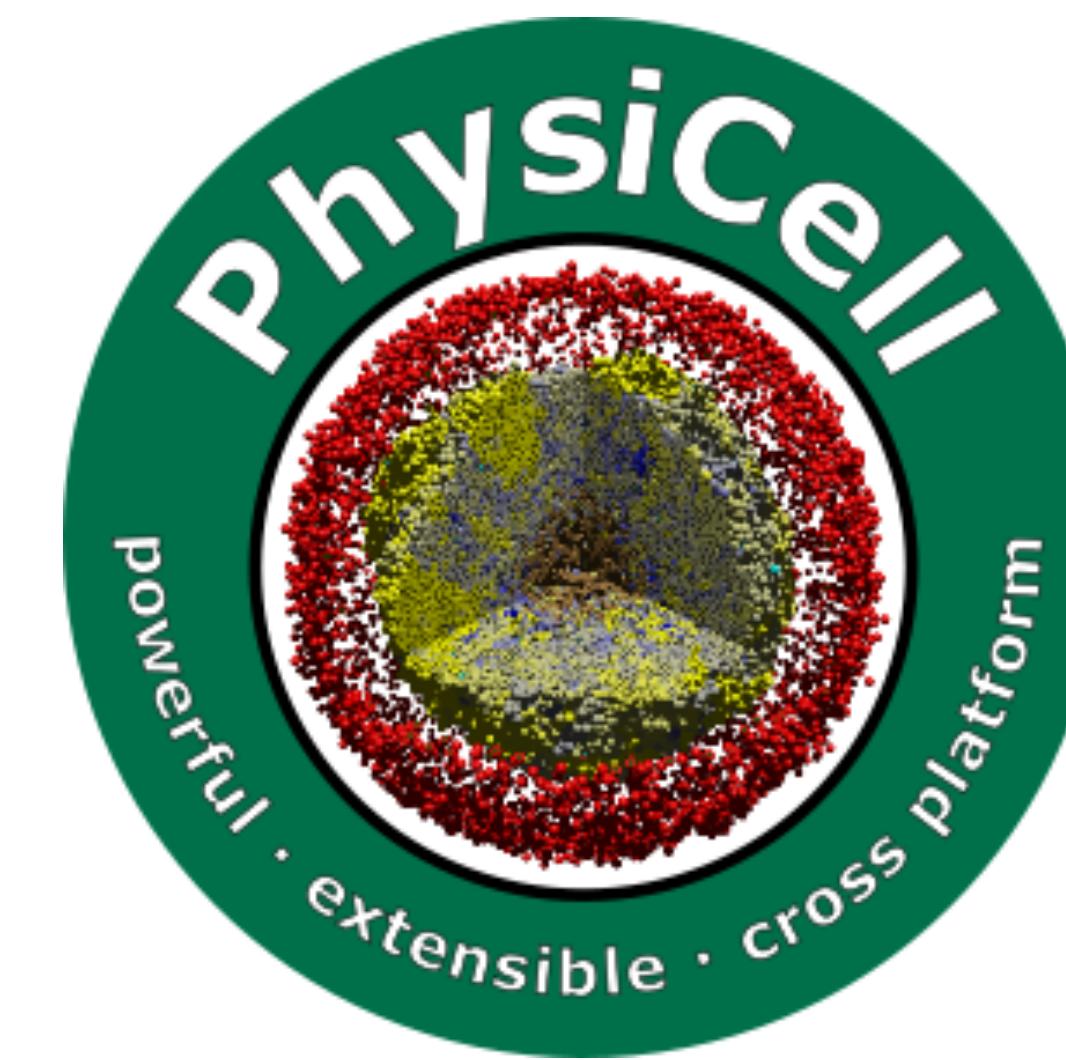
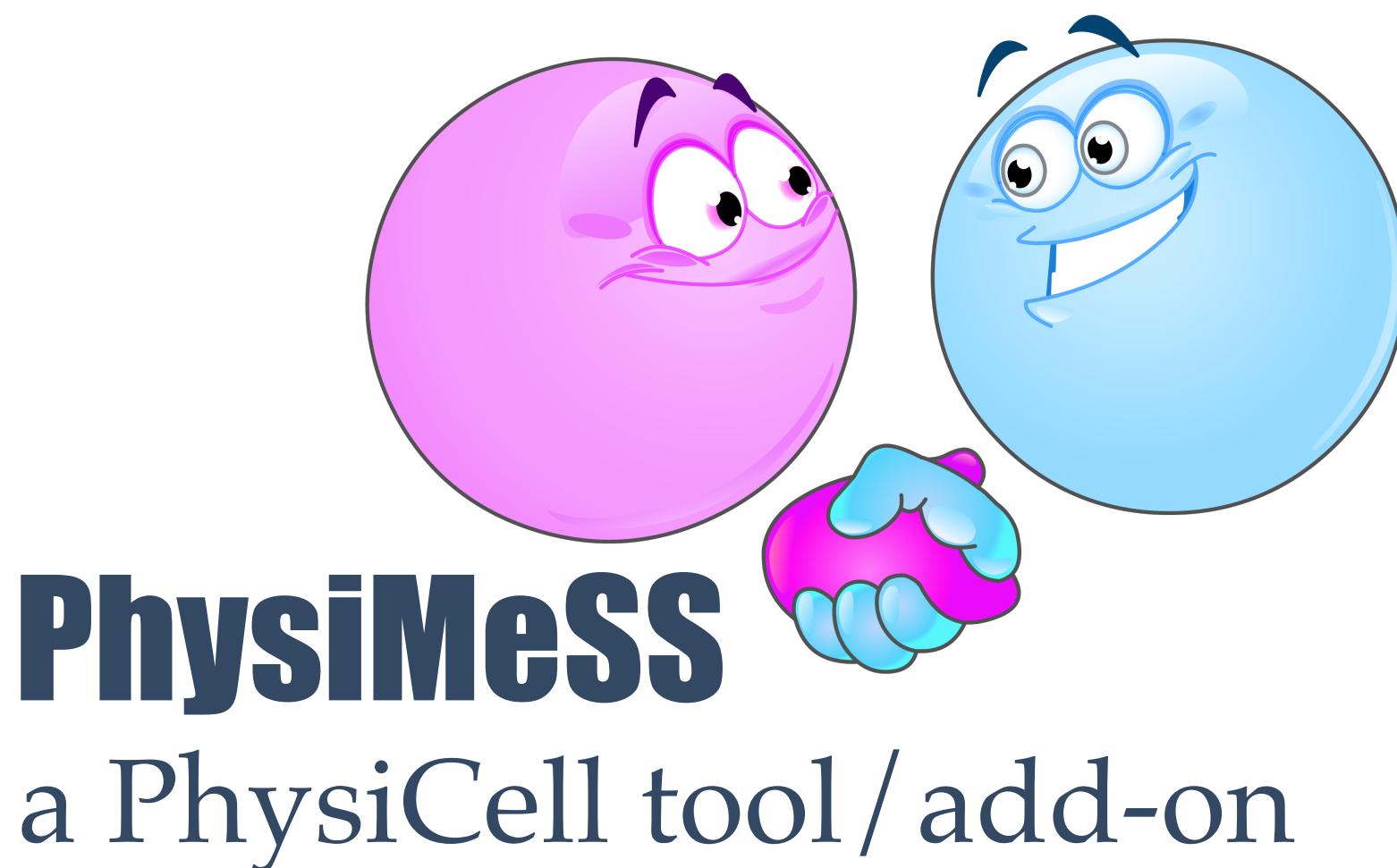
**PhysiMESS**  
a PhysiCell tool / add-on

# Download PhysiMESS

- Download/Clone the cecam23 training repo on Git which contains the PhysiMESS source code

```
git clone https://github.com/physicell-training/cecam23.git
```

Please note: PhysiMESS was originally built on PhysiCell v1.10.1  
the cecam23 training repo version of was built on v1.10.4.  
PhysiMESS is as yet unpublished please use responsibly.



## PhysiMESS Directory

PhysiMESS (PhysiCell MicroEnvironment Structure Simulation) is a PhysiCell add-on which allows users to simulate ECM components as agents.

This source code is for the CECAM-Lorentz workshop "The Extracellular Matrix: How to model structure complexity"

### Directory files

- Source code built on PhysiCell v1.10.4 with PhysiMESS modifications (see DOCUMENTATION.txt)
- Makefile
- config directory with pre-loaded examples
- setup guide

### Pre-loaded examples

#### Fibre\_Initialisation

- mymodel\_initialisation.xml and initialfibres.csv files for initialising fibres in the domain

#### Fibre\_Degradation

- mymodel\_fibre\_degradation.xml and cells\_and\_fibres\_attractant.csv to model one cell degrading fibres to reach attractant
- mymodel\_matrix\_degradation.xml and cells\_and\_fibres.csv to model growth of cell mass degrading matrix

#### Cell\_Fibre\_Mechanics

- mymodel\_fibremaze.xml and fibre\_maze.csv to model cell moving around a maze made of fibres
- mymodel\_potentials.xml and snowplough.csv to model both fibre pushing and rotation by cells
- mymodel\_hinge.xml and hinge.csv to model fibres being rotated at their hinge crosslink point by a cell

# Model Building

Save model as mymodel.xml

- Open a terminal/shell and navigate to ./code/PhysiMESS/config directory
- Launch the GUI using the command:

```
python ../../PhysiCell-Model-Builder/bin/pmb.py --studio
```

```
<PhysiCell settings version="devel-version">
  <domain>
    <x_min>-400</x_min>
    <x_max>400</x_max>
    <y_min>-400</y_min>
    <y_max>400</y_max>
    <z_min>-10</z_min>
    <z_max>10</z_max>
    <dx>20</dx>
    <dy>20</dy>
    <dz>20</dz>
    <use_2D>true</use_2D>
  </domain>

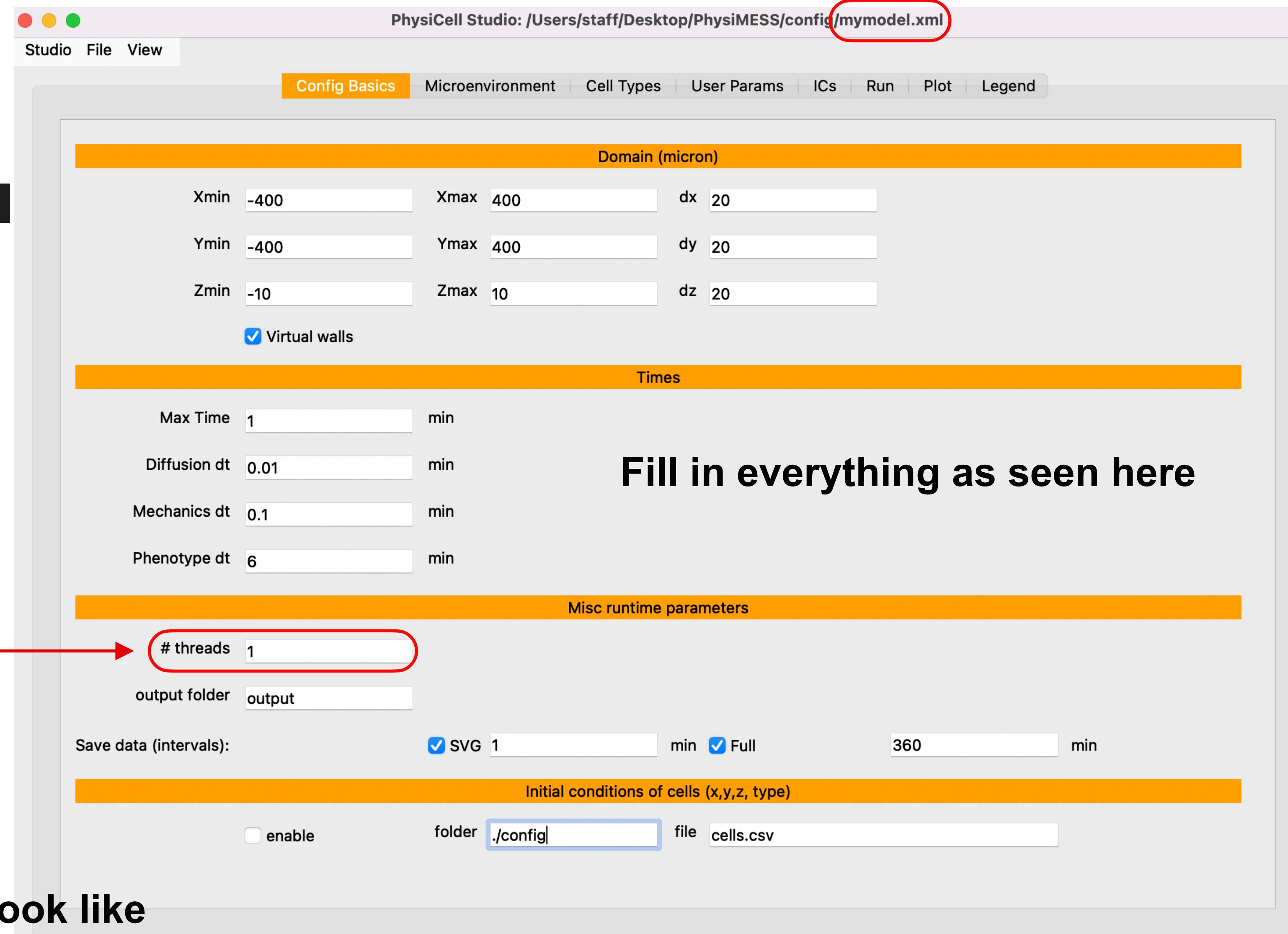
  <overall>
    <max_time units="min">1</max_time>
    <time_units>min</time_units>
    <space_units>micron</space_units>

    <dt_diffusion units="min">0.01</dt_diffusion>
    <dt_mechanics units="min">0.1</dt_mechanics>
    <dt_phenotype units="min">6</dt_phenotype>
  </overall>

  <parallel>
    <omp_num_threads>1</omp_num_threads>
  </parallel>
</PhysiCell>
```

Not everything  
has been  
checked  
thread-safe

what the xml will look like



# Model Building

## Microenvironment settings:

- set up to allow diffusion of nutrient from attractant to cell

The screenshot shows the 'Microenvironment' tab selected in the top navigation bar. On the left, there is a sidebar titled '--- Substrate ---' with a single entry 'nutrient'. The main panel contains four parameter settings: 'diffusion coefficient' set to 100.0 (micron^2/min), 'decay rate' set to 0.1 (1/min), 'initial condition' set to 1.0 (mmHg), and 'Dirichlet BC' set to 0 (mmHg). A checkbox labeled 'on' is located to the right of the Dirichlet BC input field.

Parameter	Value	Unit
diffusion coefficient	100.0	micron <sup>2</sup> /min
decay rate	0.1	1/min
initial condition	1.0	mmHg
Dirichlet BC	0	mmHg

# Model Building

**Cell settings:**  
- no birth;  
no death;  
chemotaxis  
(towards nutrient)

The image displays three vertically stacked screenshots of the PhysiCell software interface, specifically the 'Cell Types' tab.

- Top Screenshot (Cycle):** Shows the 'Cycle' tab selected. A dropdown menu indicates 'live cells'. A parameter 'phase 0->0 transition rate' is set to '0.0' with a unit of '1/min'. A 'Fixed' checkbox is checked.
- Middle Screenshot (Death):** Shows the 'Death' tab selected. An 'Apoptosis' section is visible. The 'death rate' is set to '0' with a unit of '1/min'.
- Bottom Screenshot (Motility):** Shows the 'Motility' tab selected. Parameters include 'speed' (1 micron/min), 'persistence time' (10 min), and 'migration bias' (.5). Checkboxes for 'enable motility' and '2D' are checked. A 'Chemotaxis' section is present, with 'nutrient' selected and 'towards' chosen as the direction.

# Model Building

## Fibre settings:

- copy cell but not motile
- Recognised names: “ecm” “matrix” “fibre” “fiber” “rod”

Any of these agent names  
will signal a cylindrical/  
rod-like agent

The screenshot shows the PhysiCell Studio interface with the title "PhysiCell Studio: /Users/staff/Desktop/PhysiMESS/config/mymodel.xml". The menu bar includes "Studio", "File", "View", "Config Basics", "Microenvironment", "Cell Types" (which is selected), "User Params", "ICs", "Run", "Plot", and "Legend". The "Cell Types" tab is active, displaying a list of cell types: "cell" and "ecm". The "ecm" entry is highlighted with a gray background. On the right, the "Motility" tab is selected under the "Cell Types" section. It shows parameters: speed (0 micron/min), persistence time (0 min), migration bias (0), and a checkbox for "enable motility" which is unchecked. Below these, the "Chemotaxis" section is highlighted in yellow, showing "nutrient" as the chemoattractant with a dropdown set to "towards" and a radio button for "against". Other tabs like "Cycle", "Death", "Volume", "Mechanics", "Secretion", "Interactions", "Intracellular", and "Custom Data" are also visible.

# Model Building

## Attractant settings:

- copy fibre but secretes nutrient

The screenshot shows the 'Cell Types' tab selected in the top navigation bar. On the left, a sidebar lists 'Cell Type' options: 'cell', 'ecm', and 'attractant', with 'attractant' currently selected. The main panel displays settings for the selected 'nutrient' type under the 'Secretion' tab. The settings are as follows:

Parameter	Value	Unit
secretion rate	10	1/min
target	1	sub. density
uptake rate	0	1/min
net export rate	0	total/min

# Model Building

## Parameters

Config Basics | Microenvironment | Cell Types | User Params | ICs | Run | Plot

Append 10 more rows | Clear selected rows

Name	Type	Value
<input type="checkbox"/> random_seed	int	0
Description:		
<input type="checkbox"/> number_of_cells	int	0
Description: initial number of cells (for each cell type)		
<input type="checkbox"/> number_of_fibres	int	2000
Description: initial number of fibres (for each fibre type)		
<input type="checkbox"/> anisotropic_fibres	bool	false
Description: flag for whether we want anisotropic fibres		
<input type="checkbox"/> fibre_length	double	75.0
Description: length of fibres		
<input type="checkbox"/> length_normdist_sd	double	0.0
Description: standard deviation of fibre length		
<input type="checkbox"/> fibre_radius	double	2.0
Description: radius of fibres		
<input type="checkbox"/> fibre_angle	double	0.0
Description: angle of fibre orientation		

```

<user_parameters>
<random_seed type="int" units="dimensionless" description="">0</random_seed>
<number_of_cells type="int" units="none" description="initial number of cells (for each cell type)">0</number_of_cells>
<number_of_fibres type="int" units="none" description="initial number of fibres (for each fibre type)">2000</number_of_fibres>
<anisotropic_fibres type="bool" units="none" description="flag for whether we want anisotropic fibres">false</anisotropic_fibres>
<fibre_length type="double" units="microns" description="length of fibres">75.0</fibre_length>
<length_normdist_sd type="double" units="microns" description="standard deviation of fibre length">0.0</length_normdist_sd>
<fibre_radius type="double" units="microns" description="radius of fibres">2.0</fibre_radius>
<fibre_angle type="double" units="radians" description="angle of fibre orientation">0.0</fibre_angle>
<angle_normdist_sd type="double" units="radians" description="standard deviation of fibre orientation angle">0.0</angle_normdist_sd>

```

Config Basics | Microenvironment | Cell Types | User Params | ICs | Run | Plot | Legend

Append 10 more rows | Clear selected rows

<input type="checkbox"/> angle_normdist_sd	double	0.0
Description: standard deviation of fibre orientation angle		
<input type="checkbox"/> fibre_degradation	bool	false
Description: flag for fibre degradation		
<input type="checkbox"/> fibre_deg_rate	double	0.01
Description: fibre degradation rate		
<input type="checkbox"/> fibre_stuck	double	10.0
Description: time before stuck cell can degrade fibre		
<input type="checkbox"/> vel_adhesion	double	0.6
Description: cell velocity parallel to fibre		
<input type="checkbox"/> fibre_pushing	bool	false
Description: flag for fibre pushing		
<input type="checkbox"/> vel_contact	double	0.1
Description: cell velocity orthogonal to fibre		
<input type="checkbox"/> fibre_sticky	double	1.0
Description: measure of how easy it is to move a fibre		
<input type="checkbox"/> cell_velocity_max	double	1.0
Description: max cell velocity		
<input type="checkbox"/> fibre_rotation	bool	false
Description: flag for fibre rotation		

what the xml will look like

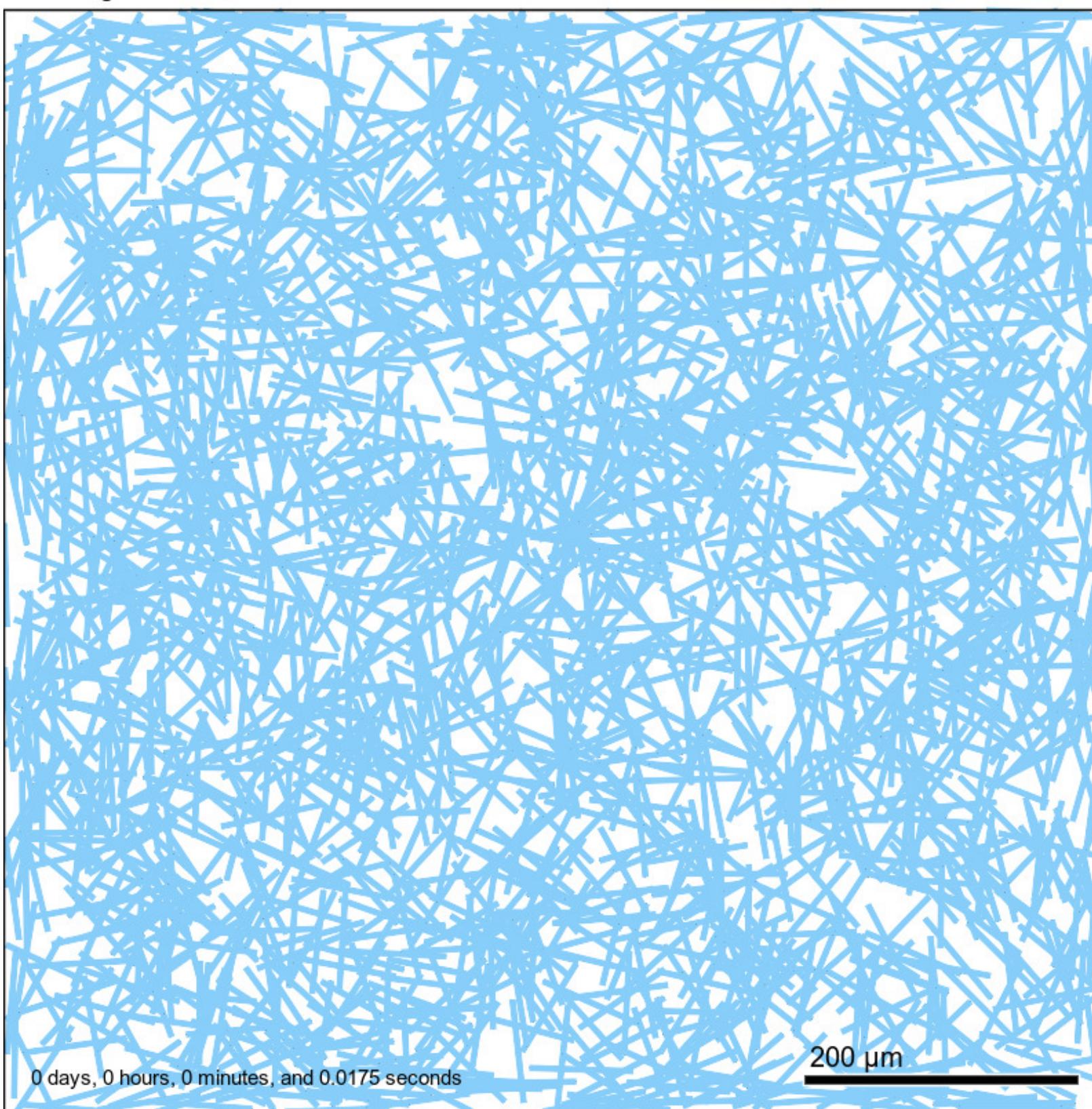
# Run Model inside PhysiMESS Directory

```
make clean; make
```

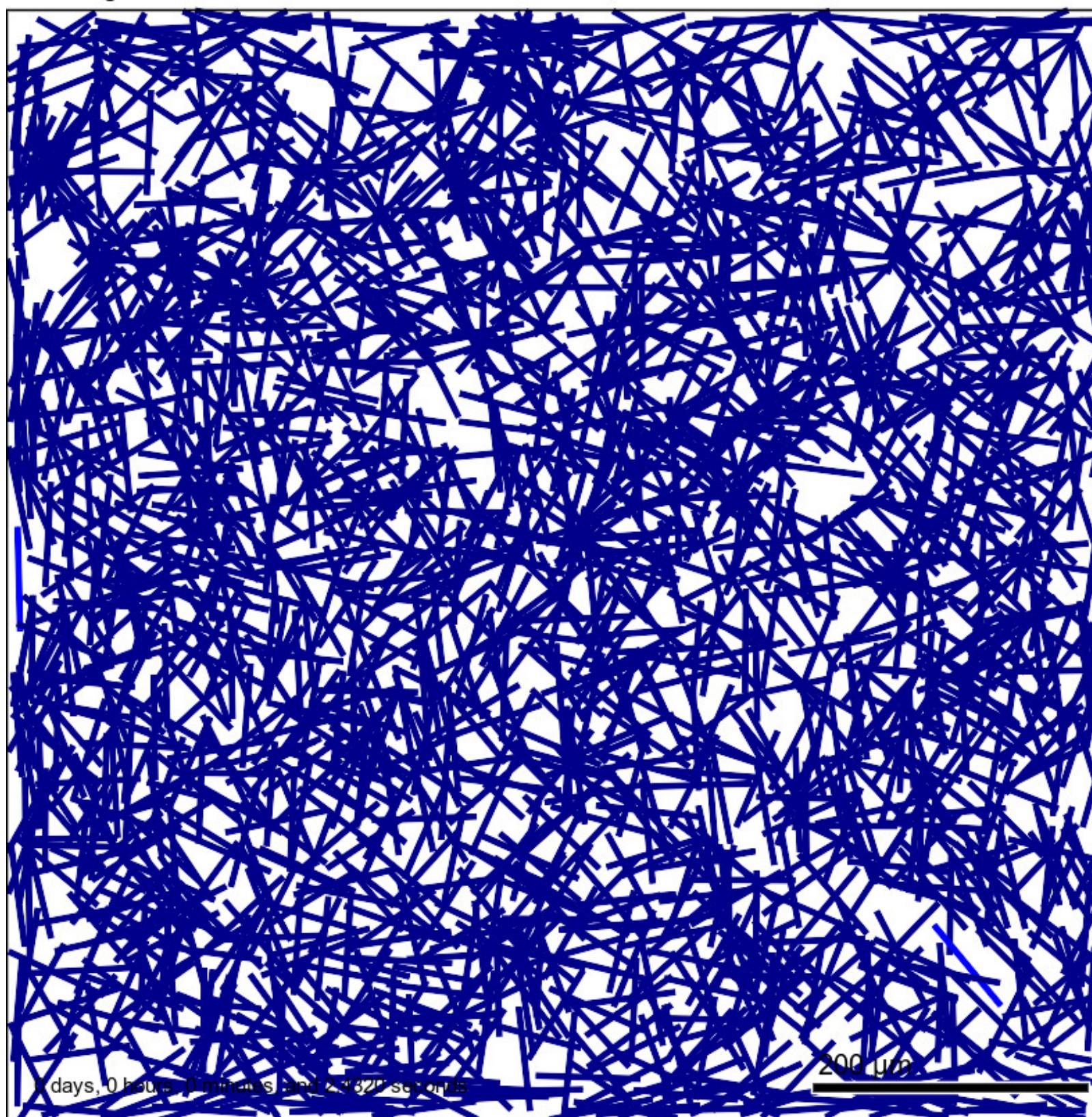
```
./project ./config/mymodel.xml
```

```
make jpeg
```

Current time: 0 days, 0 hours, and 0.00 minutes, z = 0.00 µm  
1931 agents



Current time: 0 days, 0 hours, and 1.00 minutes, z = 0.00 µm  
1931 agents



- This should create two files  
snapshot00000000.jpg & snapshot00000001.jpg

Note: if you can't use the model builder GUI you can use the pre-loaded mymodel.xml file in the ./PhysiMESS/config directory.

- You're now ready to play with PhysiMESS!!!

# Funding Acknowledgements



## PhysiCell Development:

- Breast Cancer Research Foundation
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## ECM Workshop:

