

Xml2jupyter: Mapping parameters between XML and Jupyter widgets

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DOI: [00.00000/joss.00000](https://doi.org/10.00000/joss.00000)

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Software

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Submitted: 31 January 2019

Published: 01 March 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 (hopefully in some standard format) to provide parameter values. Xml2jupyter is a Python package that bridges this gap. 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. Users modify parameter values via the widgets and the values are written to the XML configuration file. Xml2jupyter has been tested using the PhysiCell (Ghaffarizadeh et al. 2018) simulation software and 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), *description* (optional), and the parameter's default value. The attributes will determine the appearance and behavior of the Jupyter widget. For numeric widgets (the most common type for PhysiCell), xml2jupyter will calculate a delta step size as a function of the default value and this step size will be used by the widget's graphical increment/decrement feature.

To illustrate, we show the following contrived XML example, containing each of the four allowed data types (currently):

```
<PhysiCell_settings>
  <user_parameters>
    <radius type="double" units="micron">250.0</radius>
    <threads type="int">8</threads>
    <color type="string">red</color>
    <fix_persistence type="bool">True</fix_persistence>
  </user_parameters>
</PhysiCell_settings>
```

When we map this into Jupyter widgets, we obtain the following rendered result. The name of the widget and the units (if present) are rendered as (disabled) button widgets. This choice, plus the alternating colors on rows of widgets, provide a more visually appealing layout. For numeric widgets (type “int” or “double”), we compute a delta step value based on the magnitude (log) of the initial value. For example, the `radius` widget will have a step value of 10, whereas `threads` will have a step value of 1.

radius	250	micron
threads	8	
color	red	
fix_persistence	<input checked="" type="checkbox"/>	

For a more realistic example, consider the `config_biorobots.xml` configuration file (found in the `config_samples` directory). The XML elements in the `<user_parameters>` block include the (optional) *description* attribute which briefly describes the parameter and is displayed in another widget. To demonstrate `xml2jupyter` on this XML file, one would: 1) clone or download the repository, 2) copy the XML configuration file to the root directory, and 3) run the `xml2jupyter.py` script, providing the XML file as a argument.

```
$ cp config_samples/config_biorobots.xml .
$ python xml2jupyter.py config_biorobots.xml
```

The `xml2jupyter.py` script parses the XML and generates a Python module, `user_params.py`, containing the Jupyter widgets, together with methods to populate their values from the XML and write their values back to the XML. To “validate” the widgets were generated correctly, one could, minimally, open `user_params.py` in an editor and inspect it.

But to actually see the widgets rendered in a notebook, we provide a simple test:

```
$ python xml2jupyter.py config_biorobots.xml test_user_params.py
$ jupyter notebook test_gui.ipynb
```

This should produce the following notebook in your browser after selecting `Run all` in the `Cell` menu:

jupyter test_gui Last Checkpoint: 02/03/2019 (autosaved) Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 C

In [1]: 1 `import test_user_params`
`full_xml_filename= /Users/heiland/git/xml2jupyter/config_biorobots.xml`

In [2]: 1 `test_user_params.gui`

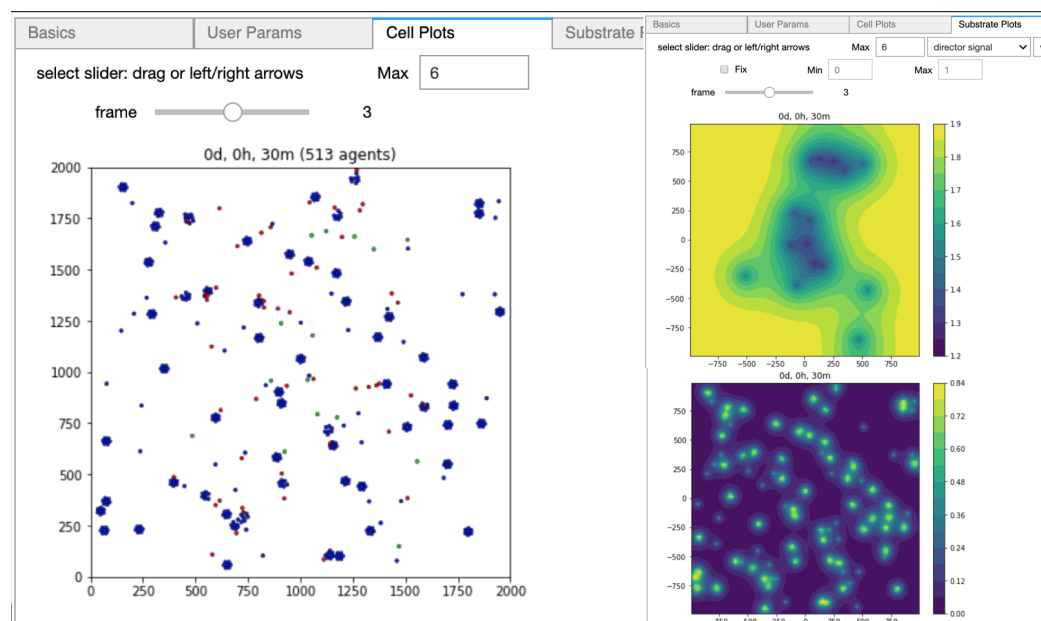
User Params

cargo_signal_D	1000	micron/min^2	cargo signal diffusion coefficient
cargo_signal_decay	0.4	1/min	cargo signal decay rate
director_signal_D	1000	micron/min^2	director signal diffusion coefficient
director_signal_decay	0.1	1/min	director signal decay rate
elastic_coefficient	0.05	1/min	elastic coefficient of cells
worker_motility_persiste...	5	min	persistence time for worker motility
worker_migration_speed	5	micron/min	speed of worker cells
attached_worker_migrati...	1		migration bias of attached workers
unattached_worker_migr...	0.5		migration bias of unattached workers
number_of_directors	15		# of director cells
number_of_cargo_clusters	100		# of cargo clusters
number_of_workers	50		# of worker cells
drop_threshold	0.4		threshold to drop cargo
worker_color	red		color of worker cells

Write

PhysiCell Jupyter GUI

Our ultimate goal is to generate a fully functional GUI for PhysiCell users. Xml2jupyter provides one important piece of this - dynamically generating widgets for custom user parameters for a model. With other Python modules that provide additional components (tabs) of the GUI, common to all PhysiCell models, a user can configure, run, and visualize output from a simulation. Two tabs that provide visualization of output files are shown below with results from the *biorobots* simulation. Note that some of the required modules are not available in the Python standard library, e.g., Matplotlib (Hunter 2007) and SciPy. We provide instructions for installing these additional dependencies in the repository README.



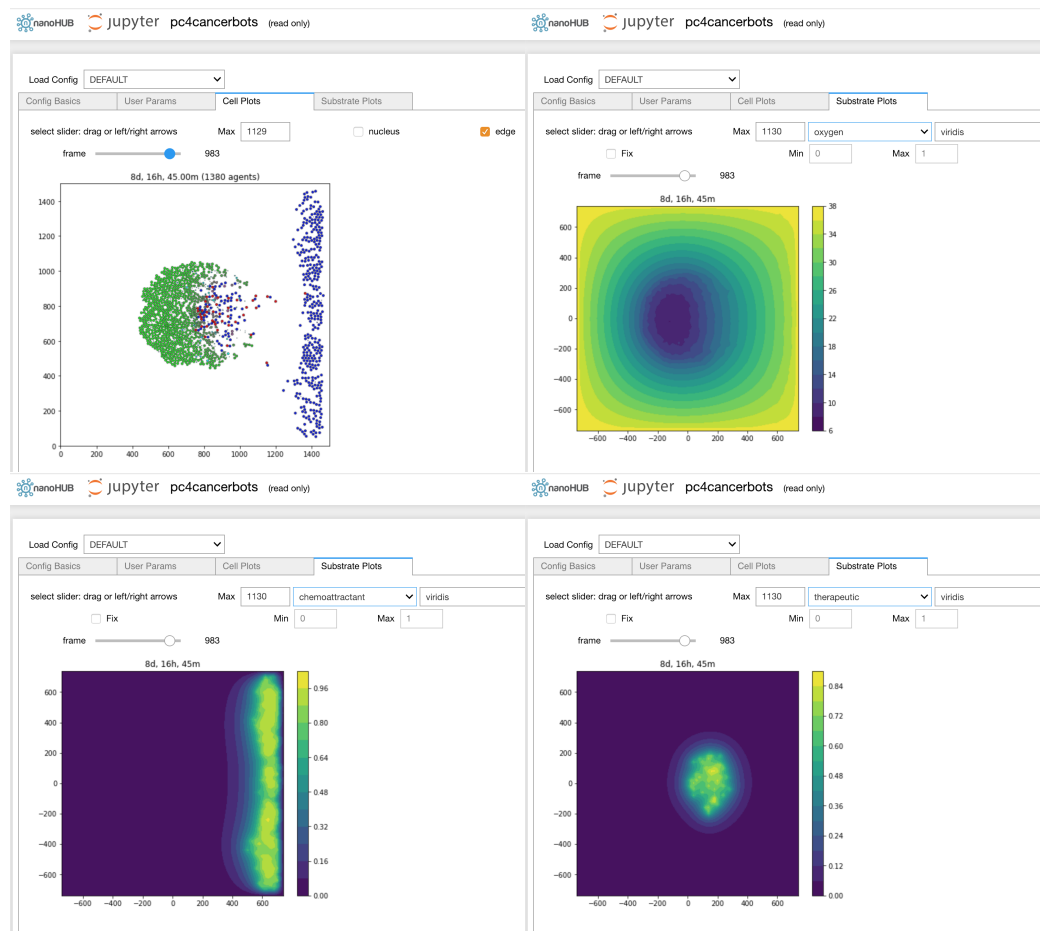
Extensions and Discussion

We hope others will be inspired to extend the core idea of this project to other text-based configuration files. XML is only one of several data-interchange formats. It just happens to be the one of interest to us for PhysiCell. And while the additional Python modules that provide visualization are also tailored to PhysiCell output, they can serve as templates for other file formats and provide similar functionality.

Xml2jupyter has helped us port PhysiCell-related Jupyter tools to nanoHUB, a scientific cloud for nanoscience education and research that includes running interactive simulations in a browser. For example, we show screen shots from our [pc4cancerbots](#) tool running on nanoHUB, where the *User Params* tab has been generated using the `xml2jupyter.py` script. Other PhysiCell-related nanoHUB tools that have been created using xml2jupyter include [pc4heterogen](#) and [pcISA](#). Readers can create an account on nanoHUB and run these simulations for themselves. We encourage students to use xml2jupyter to create their own nanoHUB tools of PhysiCell models that can 1) be run and evaluated by the instructor, 2) be shared with others, and 3) become part of a student's living portfolio. (Another repository, <https://github.com/rheiland/tool4nanobio>, provides instruction and scripts to help)

Load Config DEFAULT			
Config Basics	User Params	Cell Plots	Substrate Plots
therapy_activation_time	10080	min	time at which worker and cargo cells are injected
number_of_injected_cells	500		number of injected cells for therapy
worker_fraction	0.1		fraction of injected cells that are workers
save_interval_after_therapy_start	3	min	save (output) interval after therapy begins
cargo_o2_relative_uptake	0.1		cargo cell oxygen uptake rate (relative to cancer cells)
cargo_apoptosis_rate	0.00004065	1/min	apoptosis rate for cargo cells
cargo_relative_adhesion	0		cargo cell adhesion (relative to cancer cells)
cargo_relative_repulsion	5		cargo cell repulsion (relative to cancer cells)
worker_o2_relative_uptake	0.1		worker cell oxygen uptake rate (relative to cancer cells)
worker_apoptosis_rate	0	1/min	apoptosis rate for workers
worker_relative_adhesion	0		worker cell adhesion (relative to cancer cells)
worker_relative_repulsion	5		worker cell repulsion (relative to cancer cells)
worker_motility_persistence_time	5	min	motility persistence time for workers
worker_migration_speed	2	micron/min	migration speed for workers
attached_worker_migration_bias	0.5		migration bias for attached workers
unattached_worker_migration_bias	0.5		migration bias for unattached workers

In the four screenshots below, we show the cell plot tab (upper-left) and three different substrate plots. This particular model and simulation is described in this [video](#).



We welcome suggestions and contributions to xml2jupyter. For example, currently, we

arrange the generated parameter widgets vertically, one row per parameter. This is an appropriate layout for an educational setting. But if a GUI will be used by researchers who are already familiar with the parameters, it may be preferable to generate a more compact layout of widgets, e.g., in a matrix with only the parameter names and values.

Also, we currently provide just 2-D visualizations of (spatial) data. Obviously, we want to provide 3-D visualizations for 3-D models in the near future.

Acknowledgements

We thank the National Science Foundation (1720625) and the National Cancer Institute (U01-CA232137-01) for generous support. We also thank our collaborators at Purdue University, especially Martin Hunt and Steve Clark, who provided technical support with nanoHUB and Jupyter.

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