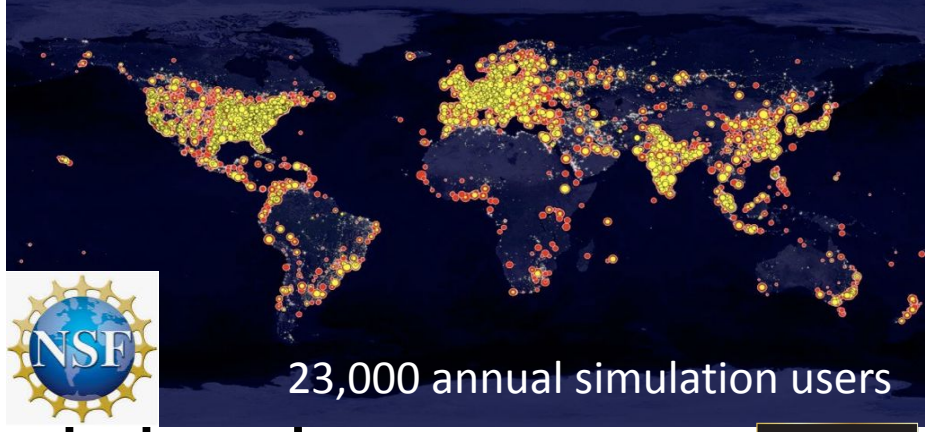

A guided tour of interactive Jupyter notebooks powered by nanoHUB

Tools for reproducible research and workflows in nanoHUB

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Purdue University
West Lafayette, Indiana USA

Agenda

1. Jupyter
   - IPython and other kernels
2. nanoHUB new features
   - Cell locking, variables inspection, themes, …
3. Atoms and Molecules
   - AtomMan, NGLView, py3DMol, ipyspeck
4. Matlab kernel
   - Matlab notebook, load python objects into matlab
5. Data Analysis
   - Pandas, ResultsDB, Floatview
6. GUI Development
   - ipywidgets, nanohub-uidl

Jupyter

IPython

[2001] UC Berkeley - Fernando Pérez

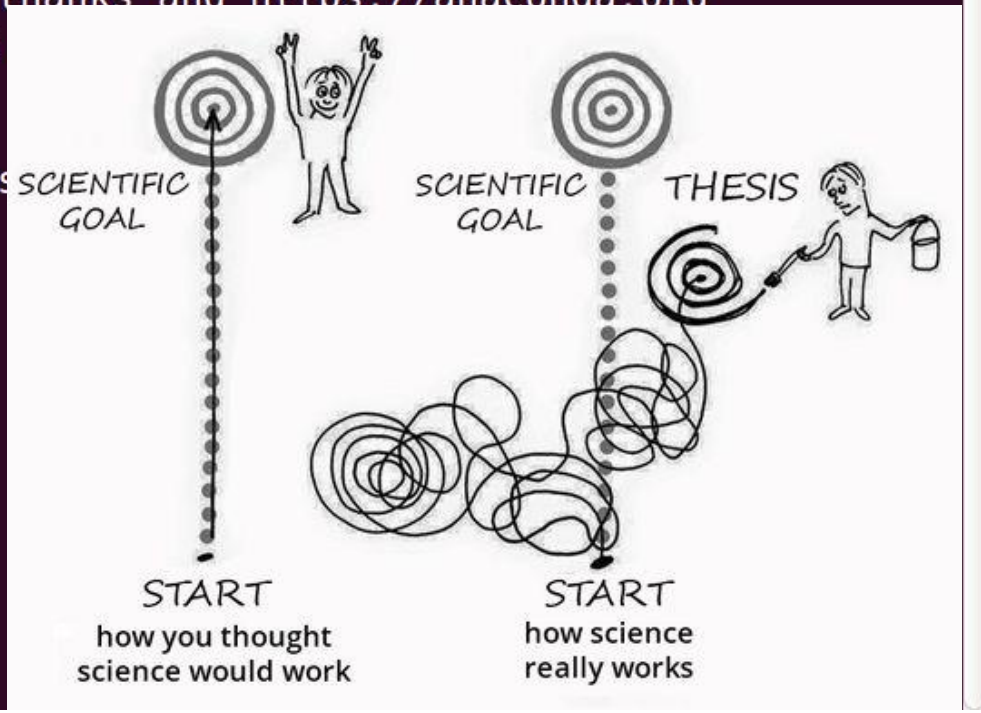
```
Python 3.4.3 |Anaconda 2.3.0 (64-bit)| (default, Jun  4 2015, 15:29:08)
Type "copyright", "credits" or "license" for more information.

IPython 3.2.0 -- An enhanced Interactive Python.
Anaconda is brought to you by Continuum Analytics.
Please check out: http://continuum.io/thanks and https://anaconda.org
?         -> Introduction and overview
%quickref -> Quick reference.
help      -> Python's own help system.
object?   -> Details about 'object', us

In [1]: print("Hello world!")
Hello world!

In [2]: 2 * 3
Out[2]: 6

In [3]:
```



jupyter

2014

Jupyter

https://github.com/jupyter/jupyter/wiki/Jupyter-kernels

IPython

Ju(lia)Pyt(hon)R

* image from
https://www.simplilearn.com/best-programming-languages-start-learning-today-article

Jupyter

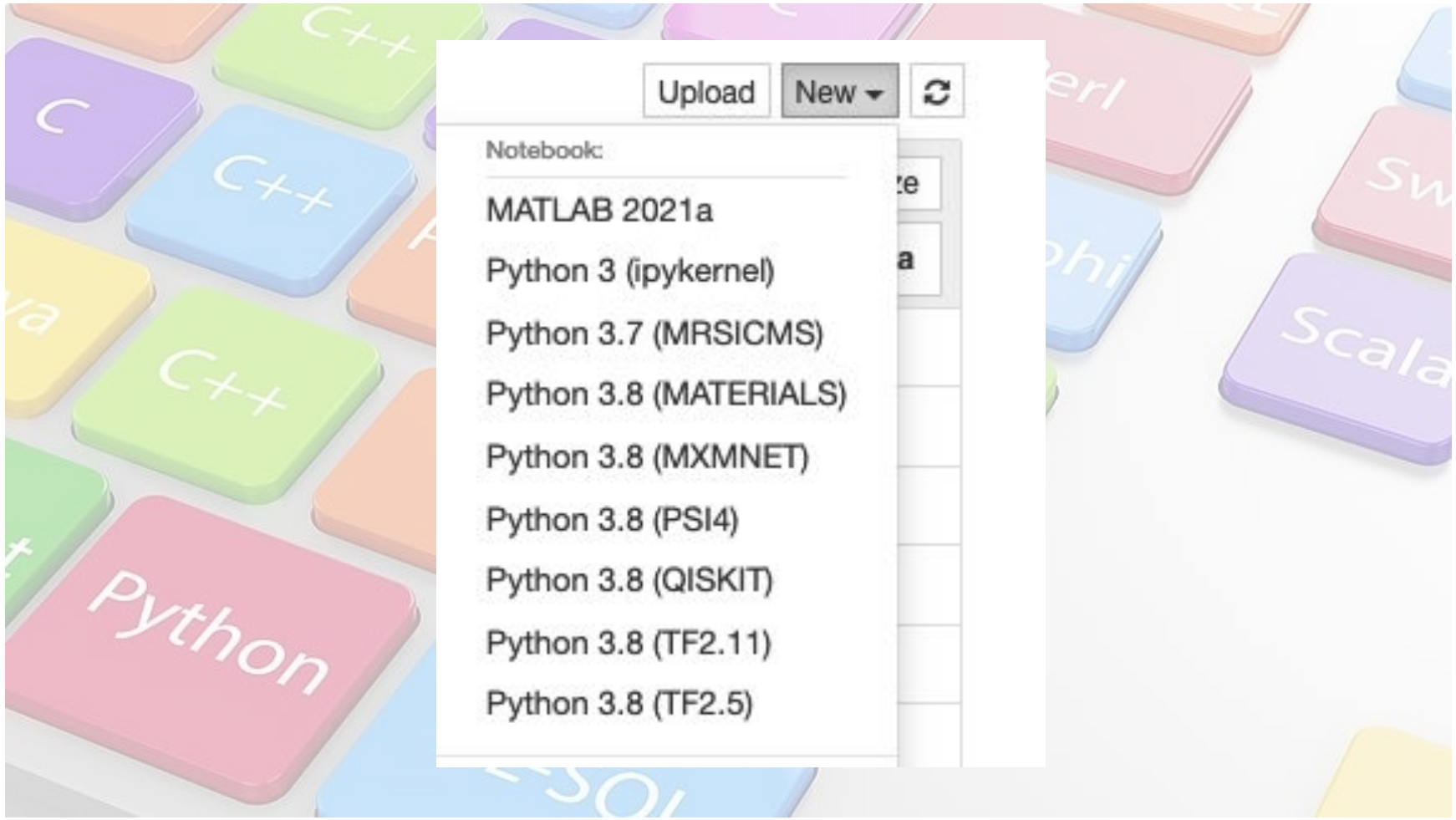
https://github.com/jupyter/jupyter/wiki/Jupyter-kernels

IPython

Ju(lia)Pyt(hon)R

* image from
https://www.simplilearn.com/best-programming-languages-start-learning-today-article

Jupyter



* image from https://www.simplilearn.com/best-programming-languages-start-learning-today-article

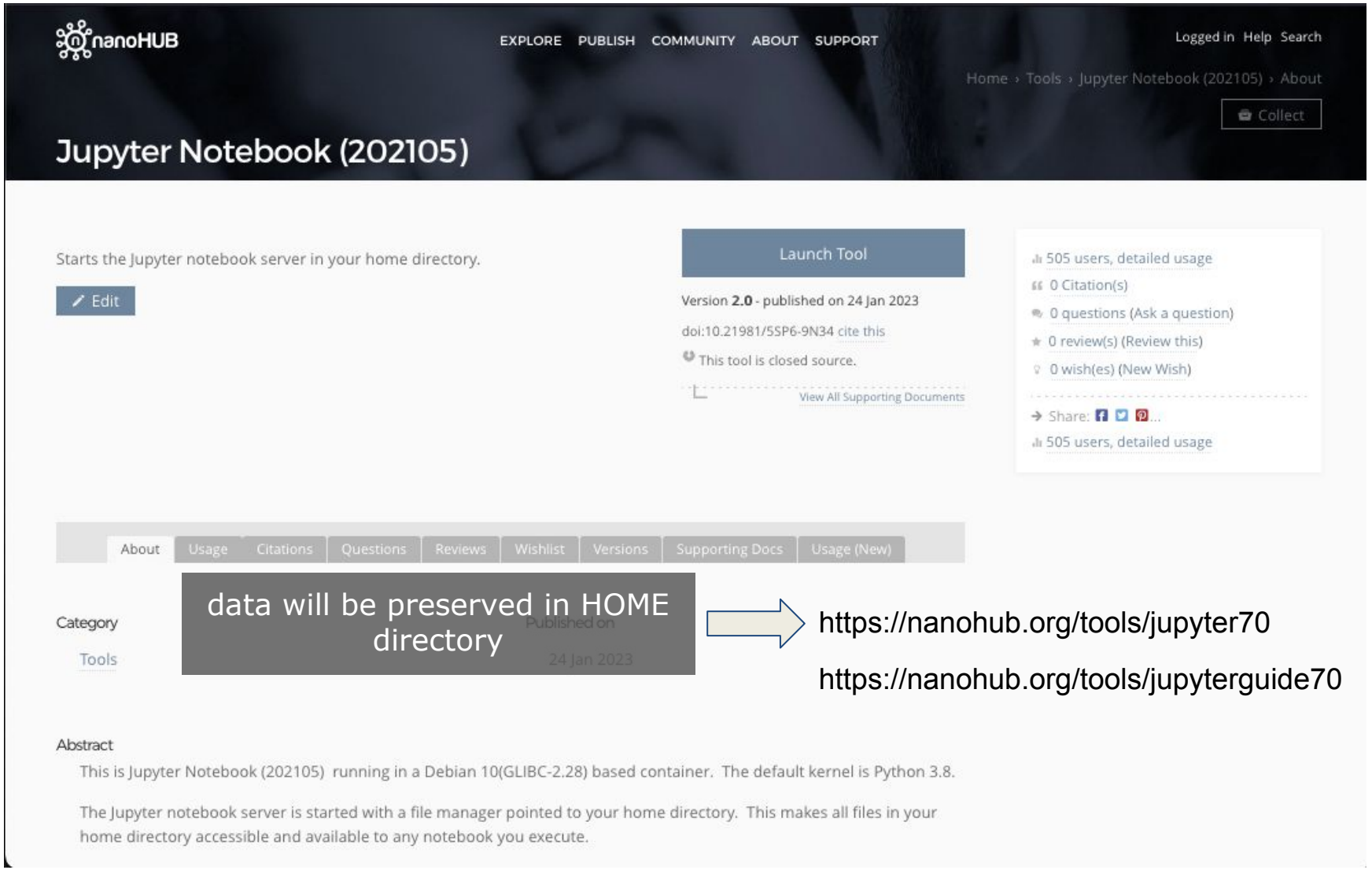
Jupyter

Python 3 (ipykernel)

* image from https://www.linkedin.com/pulse/top-10-python-libraries-pranshu-jaryal

Jupyter 70

Python 3 (ipykernel)



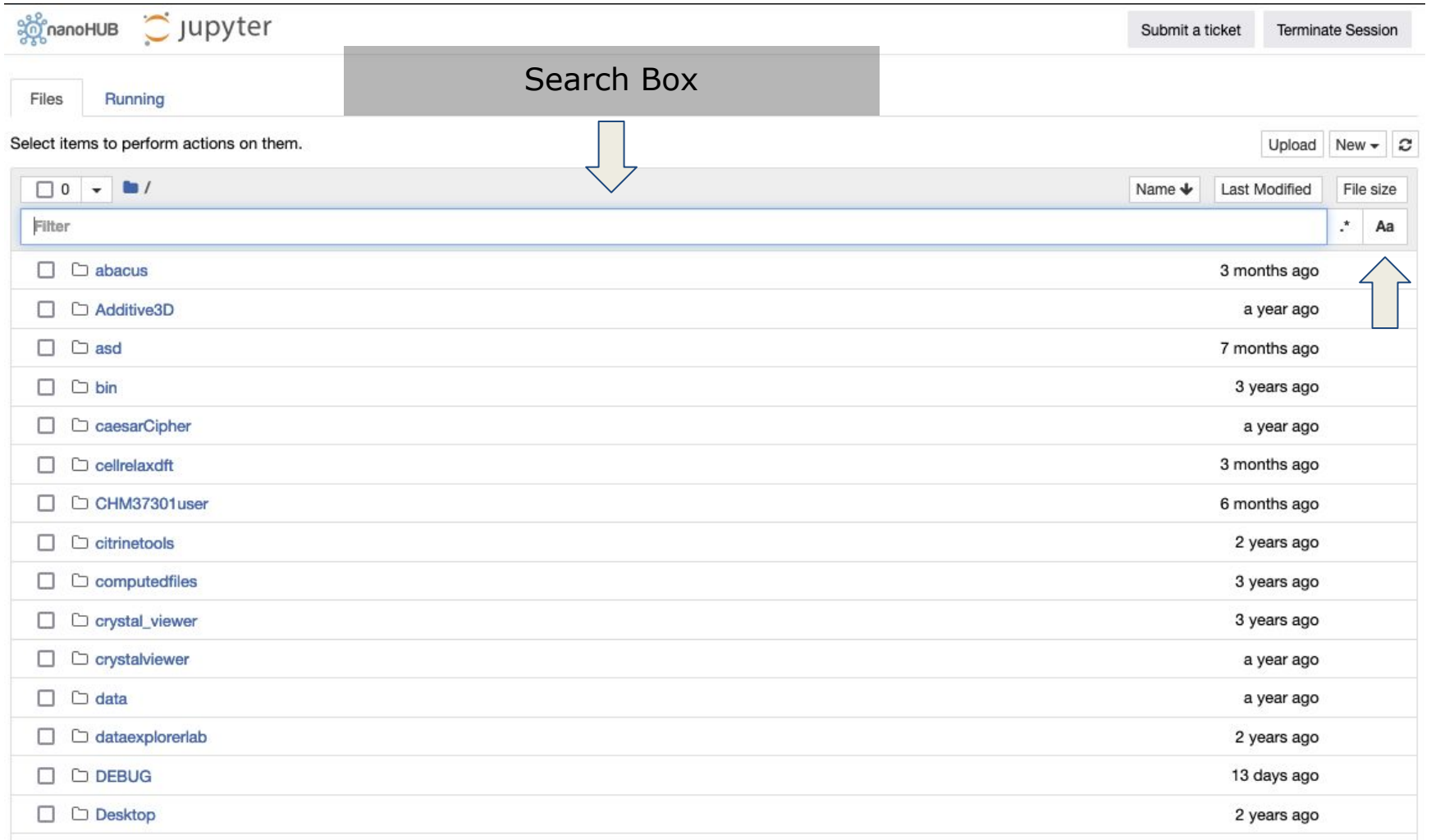
data will be preserved in HOME directory

https://nanohub.org/tools/jupyter70

https://nanohub.org/tools/jupyterguide70

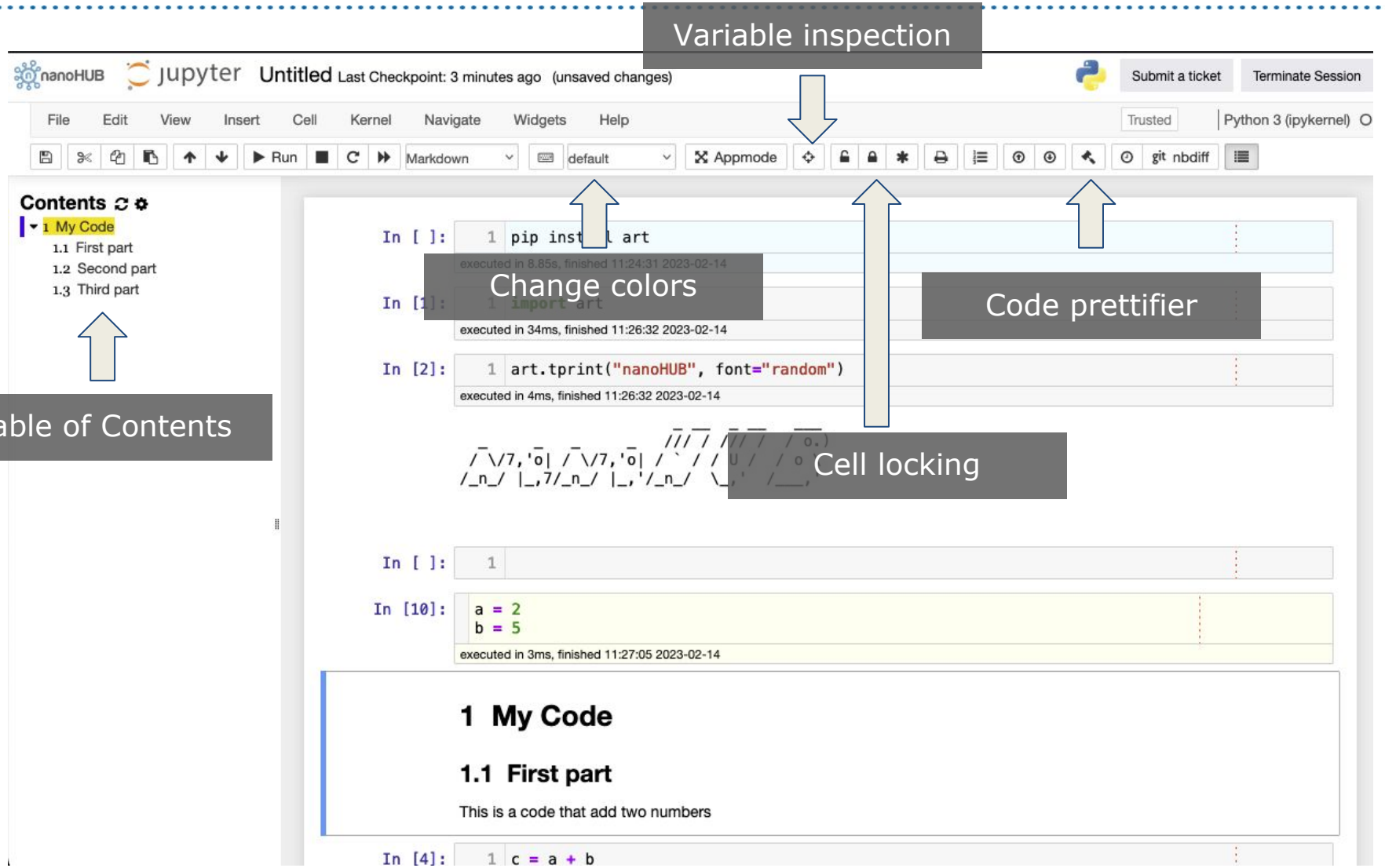
Jupyter 70 - new features

Python 3 (ipykernel)



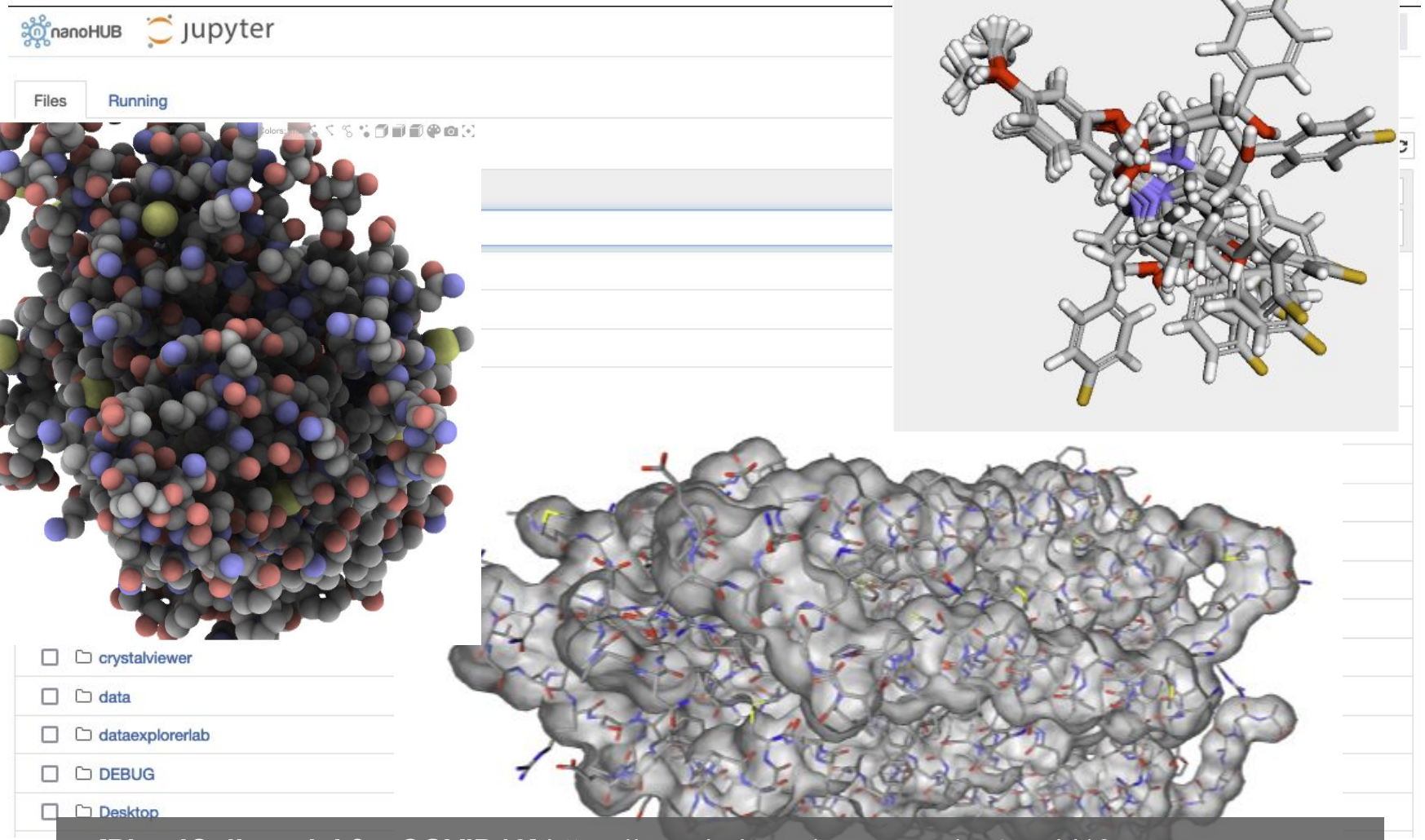
Jupyter 70 - new features

Python 3 (ipykernel)



Jupyter 70 - Atoms and Molecules

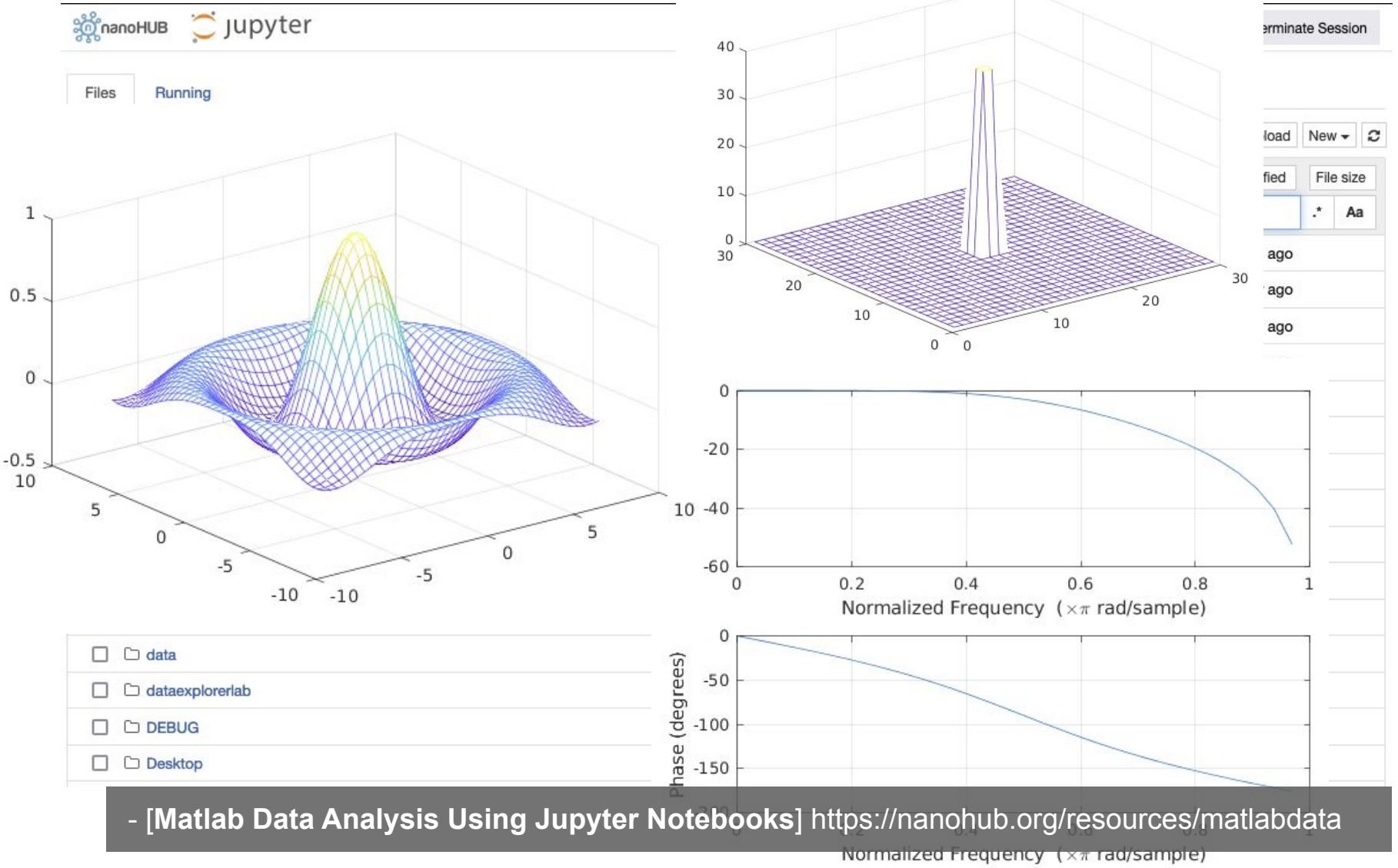
Python 3 (ipykernel)



- [**PhysiCell model for COVID19**] https://nanohub.org/resources/pc4covid19
- [T**wo-dimensional Lattice Protein Simulator**] https://nanohub.org/tools/latticeprotein

Jupyter 70 - Matlab

Python 3 (ipykernel)



- [**Matlab Data Analysis Using Jupyter Notebooks**] https://nanohub.org/resources/matlabdata

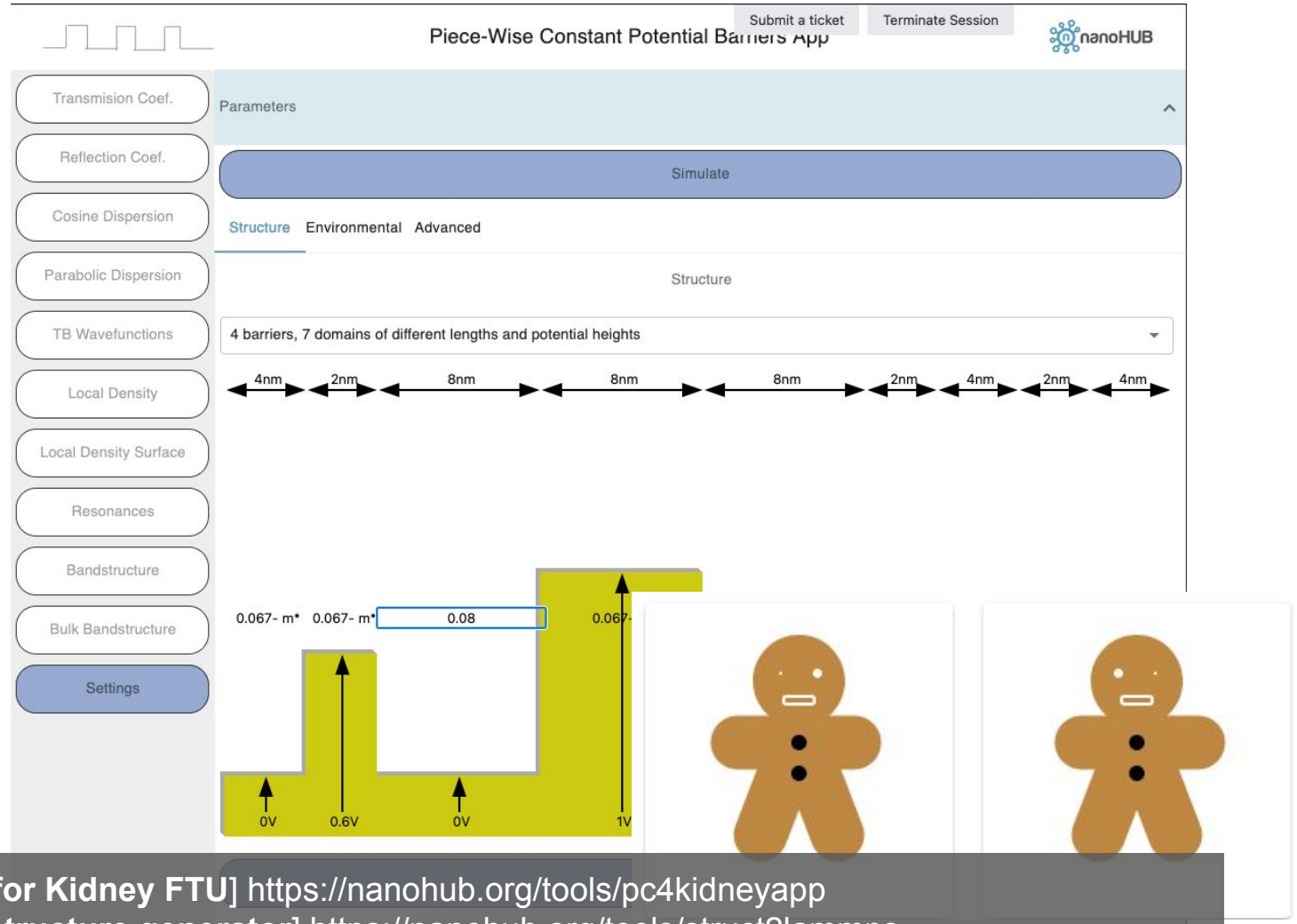
Jupyter 70 - Data Analysis

Python 3 (ipykernel)

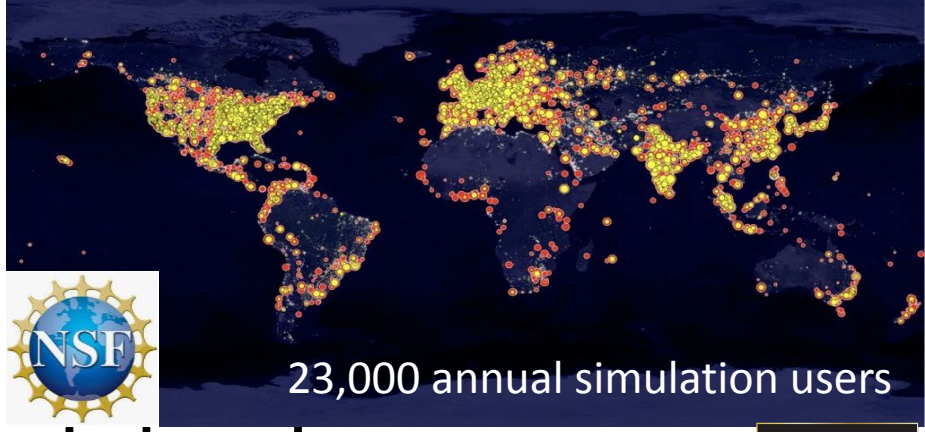
- [**Machine Learning for Materials Science**] https://nanohub.org/resources/mseml
- [**Citrine Tools for Materials Informatics**] https://nanohub.org/resources/citrinetools

Jupyter 70 - GUI / ipywidgets / nanohubUIDL

Python 3 (ipykernel)



- [**PhysiCell for Kidney FTU**] https://nanohub.org/tools/pc4kidneyapp
- [**LAMMPS structure generator**] https://nanohub.org/tools/struct2lammps
- [**Visual representation of a MOSFET**] https://nanohub.org/tools/mosfet2sat



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2020 R&D 100 WINNER

QUESTIONS?

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