

23,000 annual simulation users

A guided tour of interactive Jupyter notebooks powered by nanoHUB

2020
**R&D
100**
WINNER

Tools for reproducible research and workflows in nanoHUB

Daniel Mejia

dmejiapa@purdue.edu

Network for Computational Nanotechnology / nanoHUB

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

[2001] UC Berkeley - Fernando Pérez

IP[y]:

IPython

```
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.
```

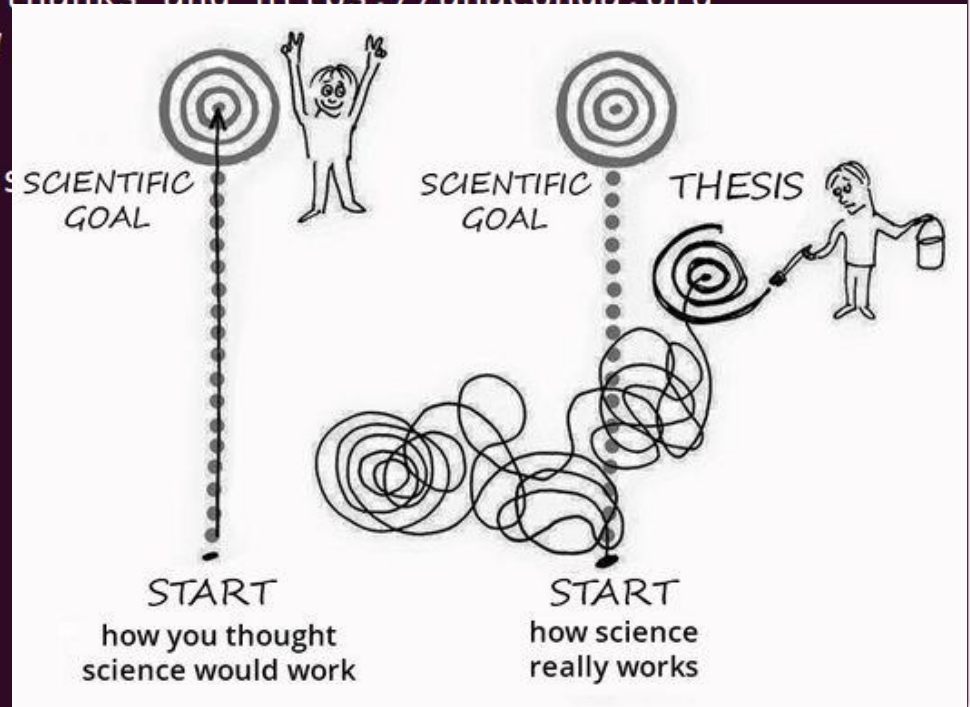
```
IPython 3.2.0 -- An enhanced Interactive Python.
Anaconda is brought to you by Continuum Analytics.
Please check out: http://continuum.io/thanks and https://anaconda.org
```

```
? -> 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]: █
```

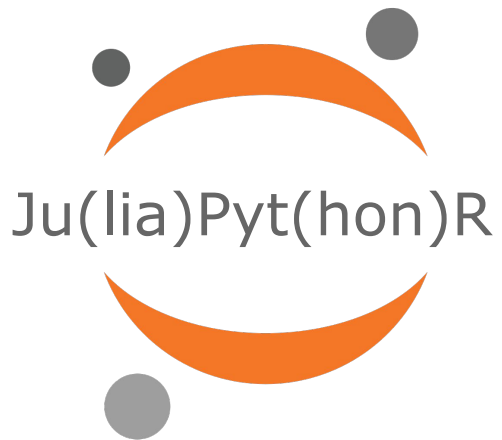


2014

Jupyter

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

IP[y]:
IPython



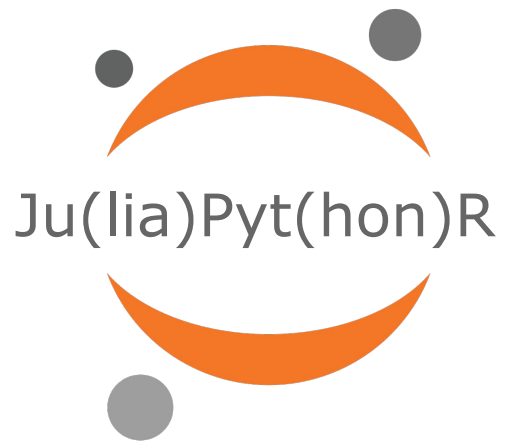
* image from

<https://www.simplilearn.com/best-programming-languages-start-learning-today-article>

Jupyter

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

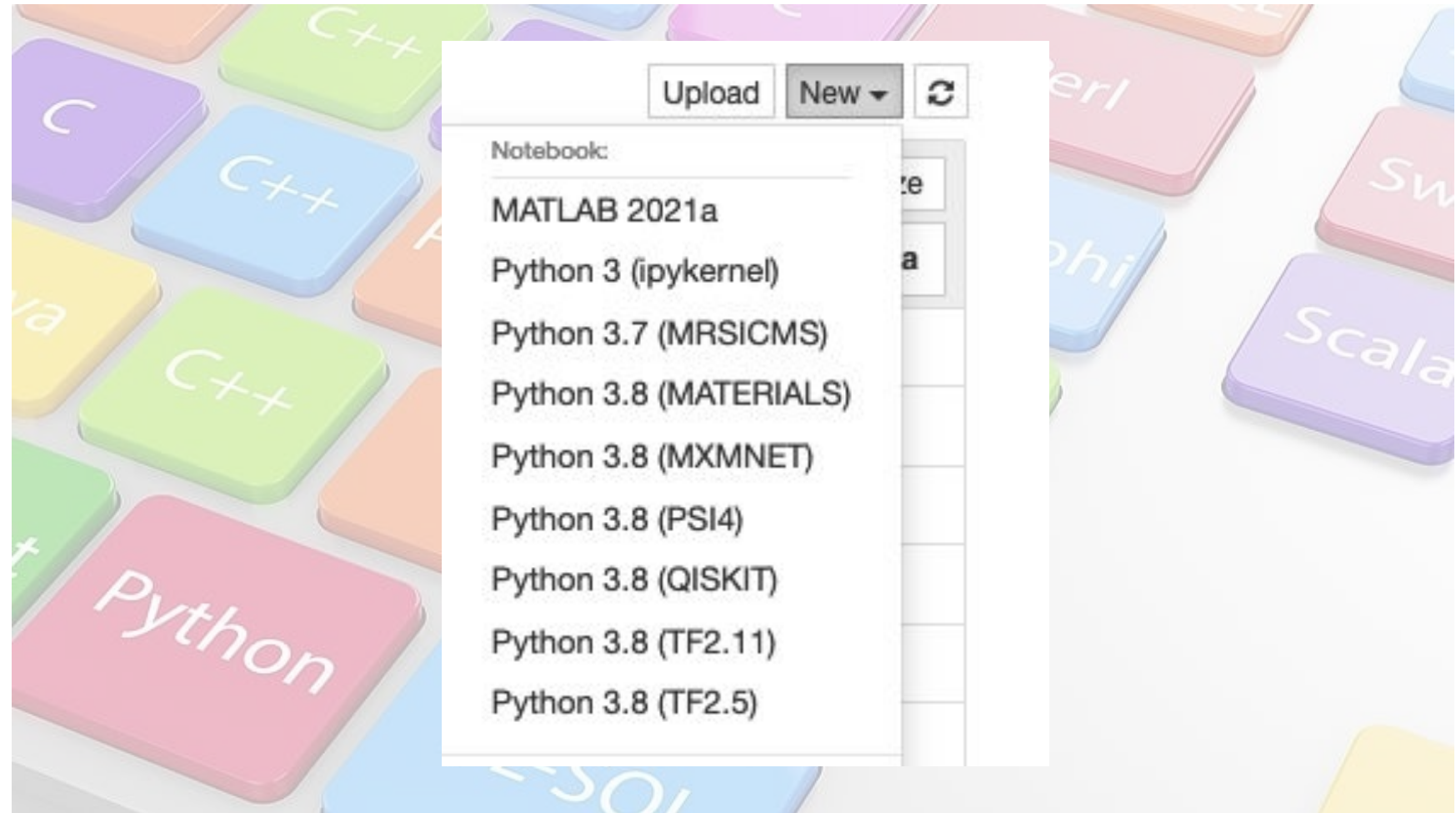
IP[y]:
IPython



* 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)



Jupyter 70



**Python 3
(ipykernel)**



Jupyter Notebook (202105)

Starts the Jupyter notebook server in your home directory.

[Edit](#)

[Launch Tool](#)

Version **2.0** - published on 24 Jan 2023
doi:10.21981/55P6-9N34 cite this
This tool is closed source.

[View All Supporting Documents](#)

[505 users, detailed usage](#)
[0 Citation\(s\)](#)
[0 questions \(Ask a question\)](#)
[0 review\(s\) \(Review this\)](#)
[0 wish\(es\) \(New Wish\)](#)
Share: [f](#) [t](#) [p](#)...
[505 users, detailed usage](#)

[About](#) [Usage](#) [Citations](#) [Questions](#) [Reviews](#) [Wishlist](#) [Versions](#) [Supporting Docs](#) [Usage \(New\)](#)

Category: [Tools](#)

data will be preserved in HOME directory → <https://nanohub.org/tools/jupyter70>
<https://nanohub.org/tools/jupyterguide70>

Published on 24 Jan 2023

Abstract
This is Jupyter Notebook (202105) running in a Debian 10(GLIBC-2.28) based container. The default kernel is Python 3.8.
The Jupyter notebook server is started with a file manager pointed to your home directory. This makes all files in your home directory accessible and available to any notebook you execute.

Jupyter 70 - new features



**Python 3
(ipykernel)**



The screenshot shows the nanoHUB Jupyter interface. At the top, there are logos for nanoHUB and Jupyter, along with buttons for "Submit a ticket" and "Terminate Session". Below the logos is a "Search Box" with a downward arrow pointing to a file list. The file list has a "Filter" input field and columns for "Name", "Last Modified", and "File size". The file list contains the following items:

Name	Last Modified	File size
<input type="checkbox"/> abacus	3 months ago	
<input type="checkbox"/> Additive3D	a year ago	
<input type="checkbox"/> asd	7 months ago	
<input type="checkbox"/> bin	3 years ago	
<input type="checkbox"/> caesarCipher	a year ago	
<input type="checkbox"/> cellrelaxdft	3 months ago	
<input type="checkbox"/> CHM37301user	6 months ago	
<input type="checkbox"/> citrinetools	2 years ago	
<input type="checkbox"/> computedfiles	3 years ago	
<input type="checkbox"/> crystal_viewer	3 years ago	
<input type="checkbox"/> crystalviewer	a year ago	
<input type="checkbox"/> data	a year ago	
<input type="checkbox"/> dataexplorerlab	2 years ago	
<input type="checkbox"/> DEBUG	13 days ago	
<input type="checkbox"/> Desktop	2 years ago	

Jupyter 70 - new features



Python 3
(ipykernel)



The screenshot shows the JupyterLab interface with several new features highlighted by callouts:

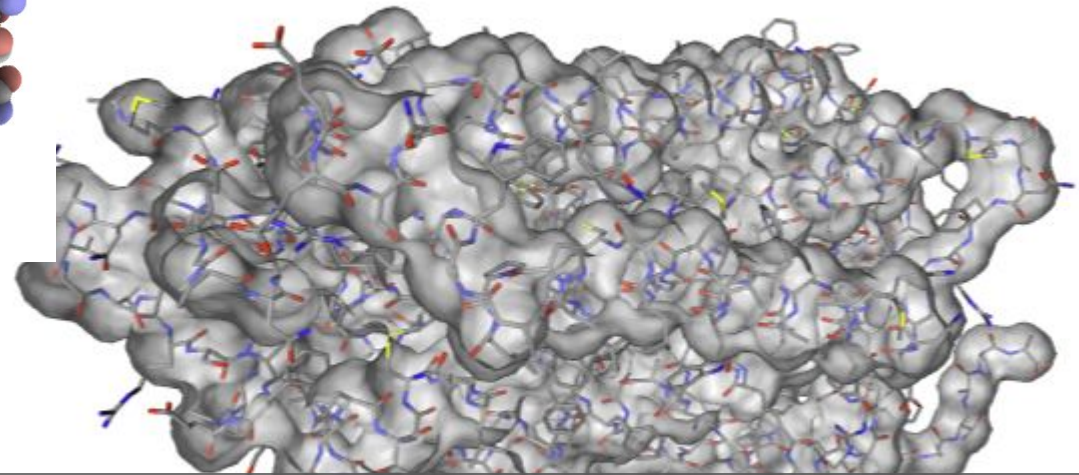
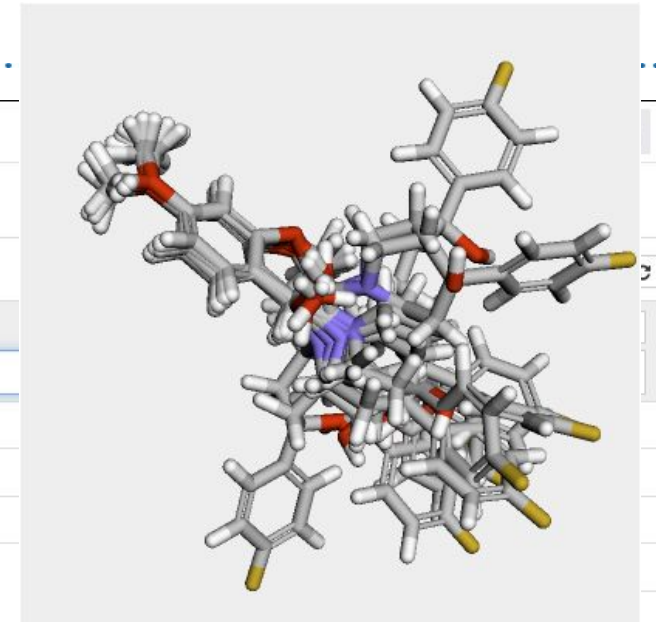
- Variable inspection:** A callout points to the top right toolbar, specifically to the icon that allows inspecting variables in the current environment.
- Change colors:** A callout points to the code editor, highlighting the ability to change the background color of code cells.
- Code prettifier:** A callout points to the code editor, highlighting the ability to automatically format code.
- Cell locking:** A callout points to the code editor, highlighting the ability to lock a cell to prevent further editing.
- Table of Contents:** A callout points to the left sidebar, highlighting the new Table of Contents view.

The interface also shows a file browser on the left with a 'Contents' panel, a top menu bar (File, Edit, View, Insert, Cell, Kernel, Navigate, Widgets, Help), and a toolbar with various icons for file operations and execution. The main workspace contains several code cells with Python code and their execution results.

Jupyter 70 - Atoms and Molecules



Python 3
(ipykernel)



- [PhysiCell model for COVID19] <https://nanohub.org/resources/pc4covid19>
- [Two-dimensional Lattice Protein Simulator] <https://nanohub.org/tools/latticeprotein>

Jupyter 70 - Matlab

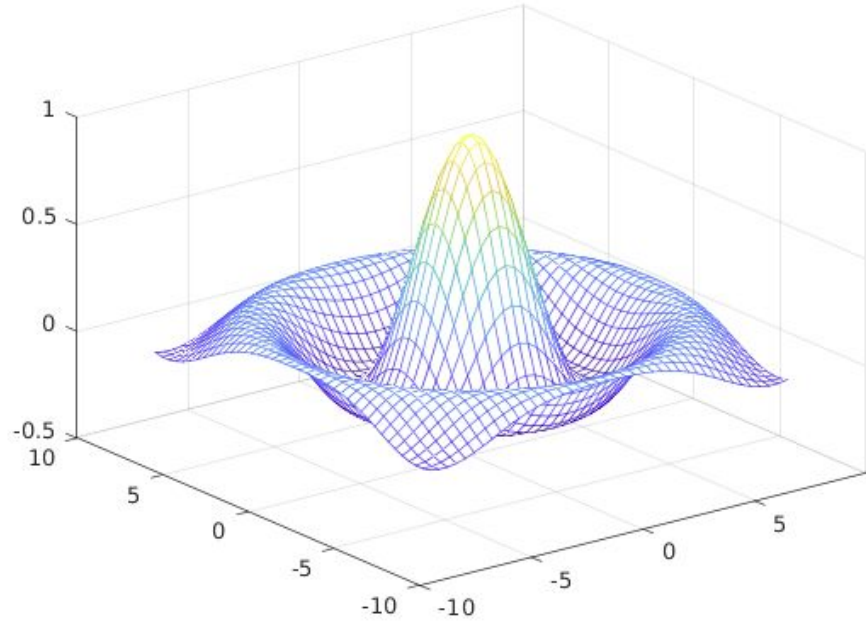


Python 3
(ipykernel)

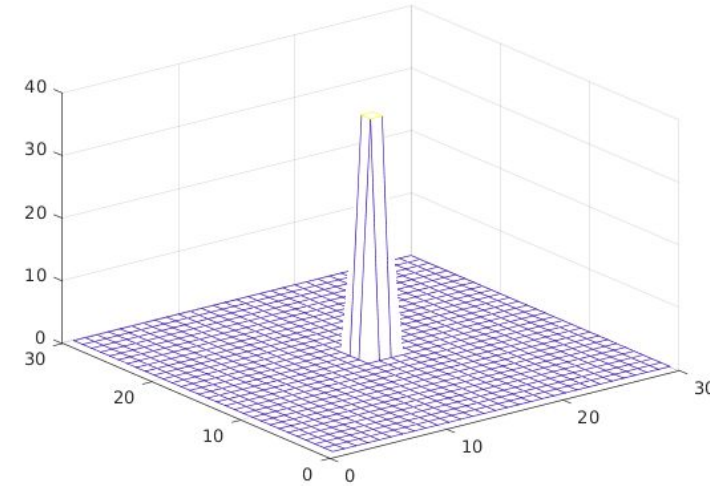


nanoHUB jupyter

Files Running



- data
- dataexplorerlab
- DEBUG
- Desktop



Terminate Session

load New ↕ ↻

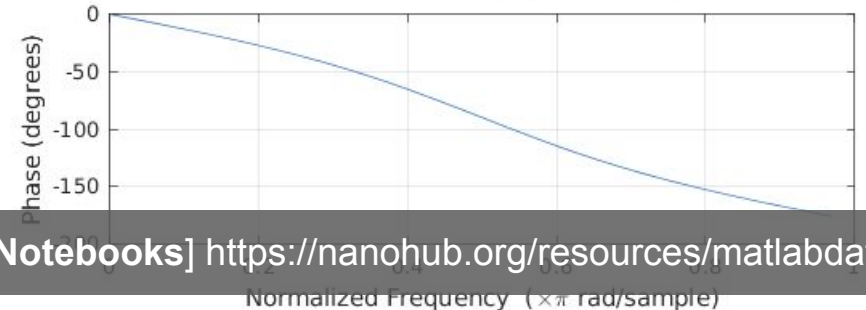
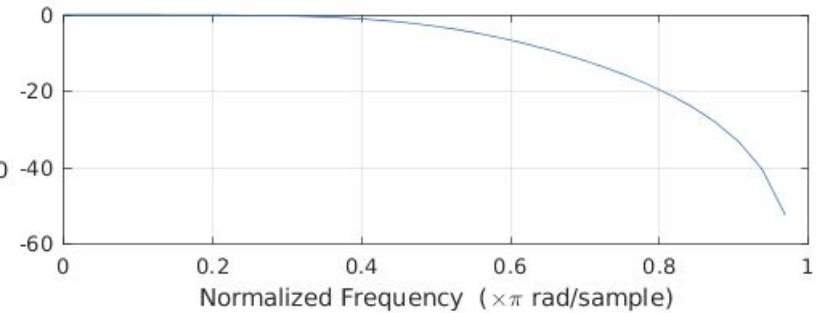
File size

.* Aa

ago

ago

ago



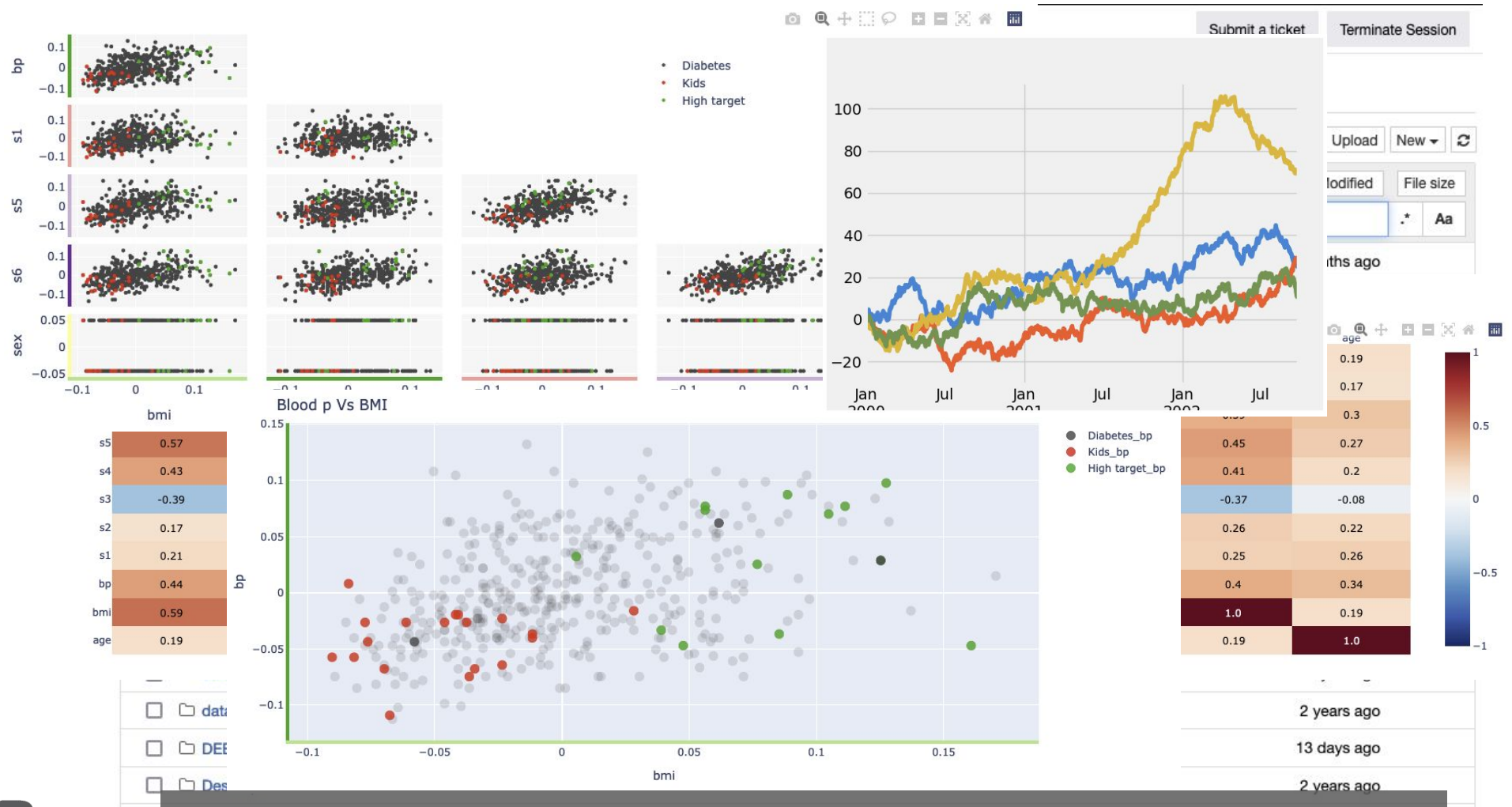
- [Matlab Data Analysis Using Jupyter Notebooks] <https://nanohub.org/resources/matlabdata>

Normalized Frequency ($\times \pi$ rad/sample)

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/citriuptools>

Jupyter 70 - GUI / ipywidgets / nanohubUIDL



Python 3
(ipykernel)



Piece-Wise Constant Potential Barriers App

Submit a ticket Terminate Session nanoHUB

Parameters

Simulation

Structure Environmental Advanced

Structure

4 barriers, 7 domains of different lengths and potential heights

4nm 2nm 8nm 8nm 8nm 2nm 4nm 2nm 4nm

0.067- m* 0.067- m* 0.08 0.067-

0V 0.6V 0V 1V

- [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>



A guided tour of interactive Jupyter notebooks powered by nanoHUB



QUESTIONS?

Daniel Mejia

dmejiapa@purdue.edu

Network for Computational Nanotechnology / nanoHUB

Purdue University

West Lafayette, Indiana USA