The MAterials Simulation Toolkit for Machine Learning (MAST-ML): Automating Development and Evaluation of Machine Learning Models for Materials Property Prediction

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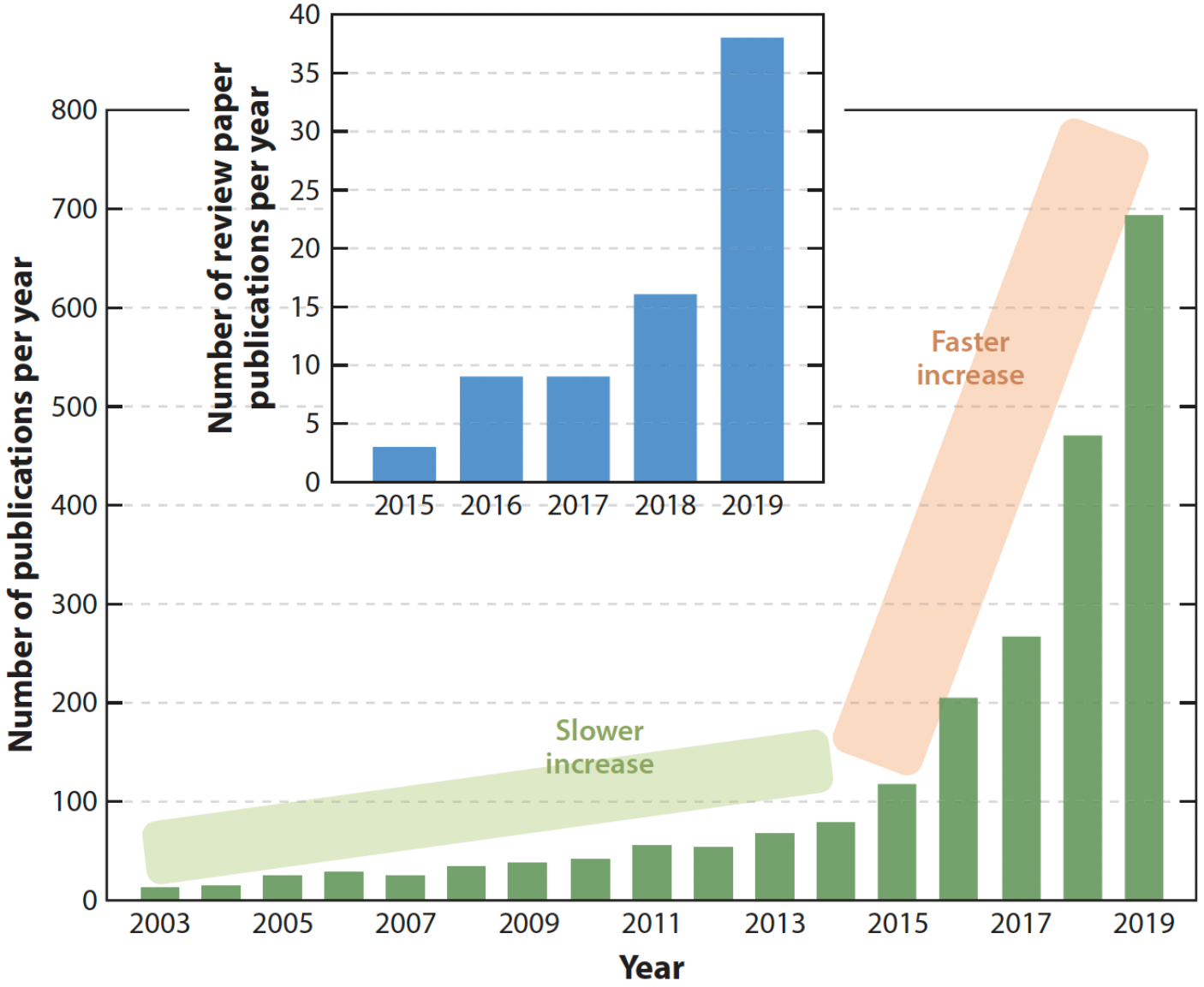
https://github.com/uw-cmg/MAST-ML

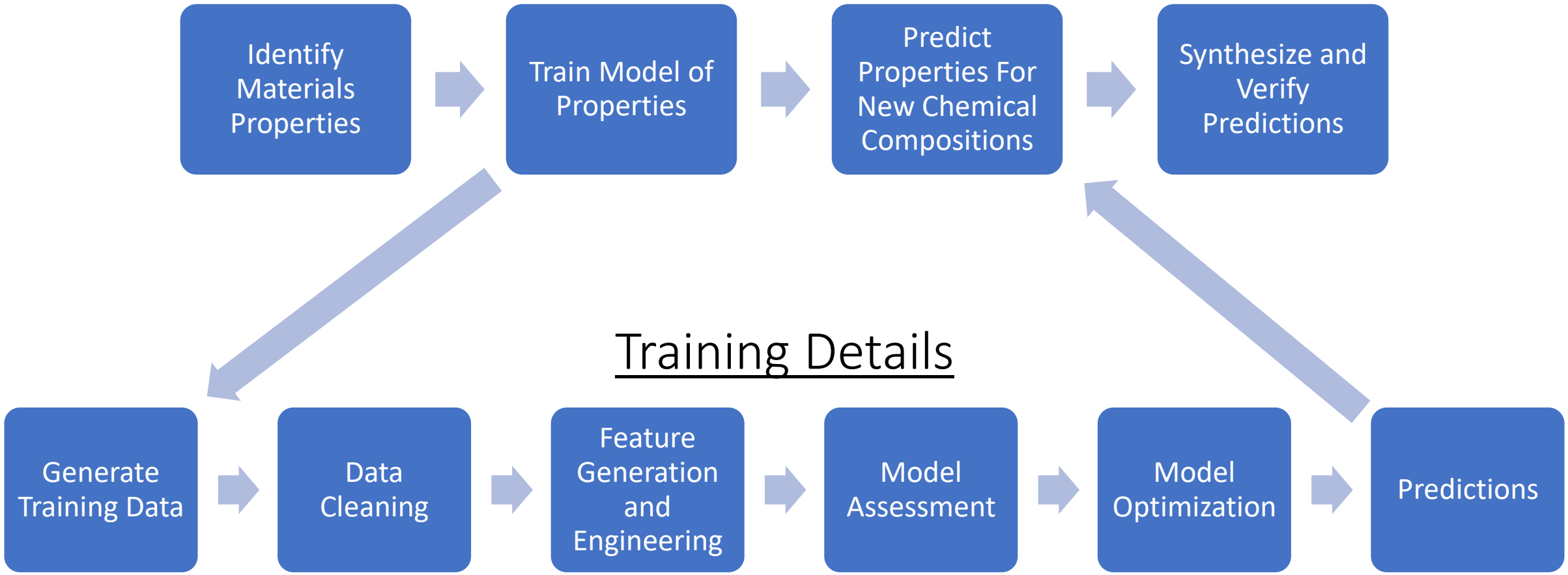
NanoHub ML Workshop
5/19/2021

Machine learning in Materials Science is Exploding



Jacobs and Morgan, Ann. Rev. Mat. Res. (2020), https://doi.org/10.1146/annurev-matsci-070218-010015

A Basic Materials Design Workflow



What is MAST-ML?

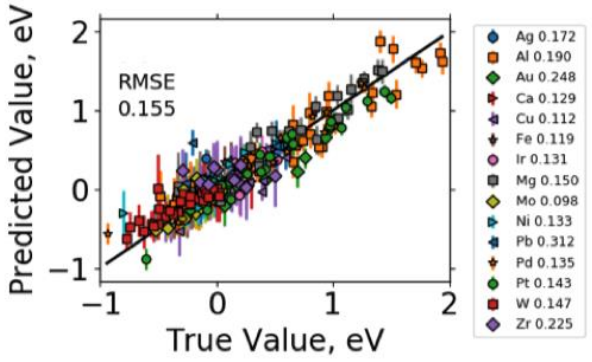
MAST-ML is an open-source Python package designed to broaden and accelerate the use of machine learning in materials science research, particularly for non-experts.

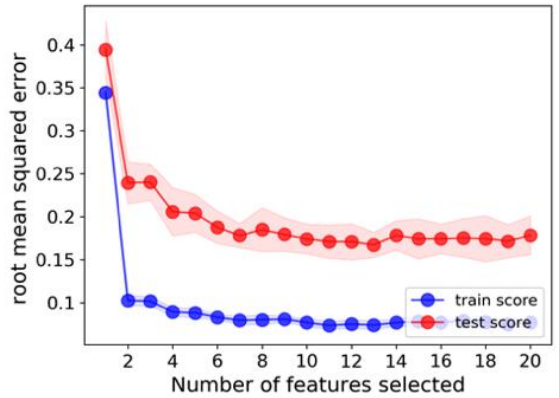
MAST-ML

MAterials Simulation Toolkit

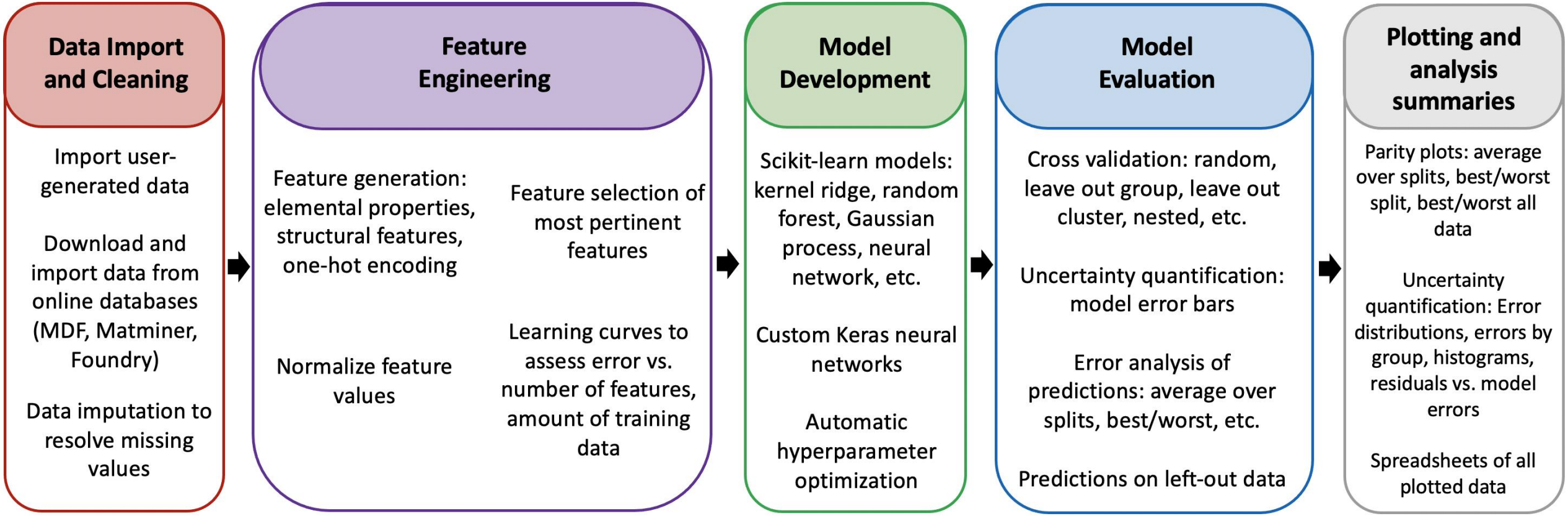
Automated machine learning tools for materials informatics research (MAST-ML)

https://github.com/uw-cmg/MAST-ML





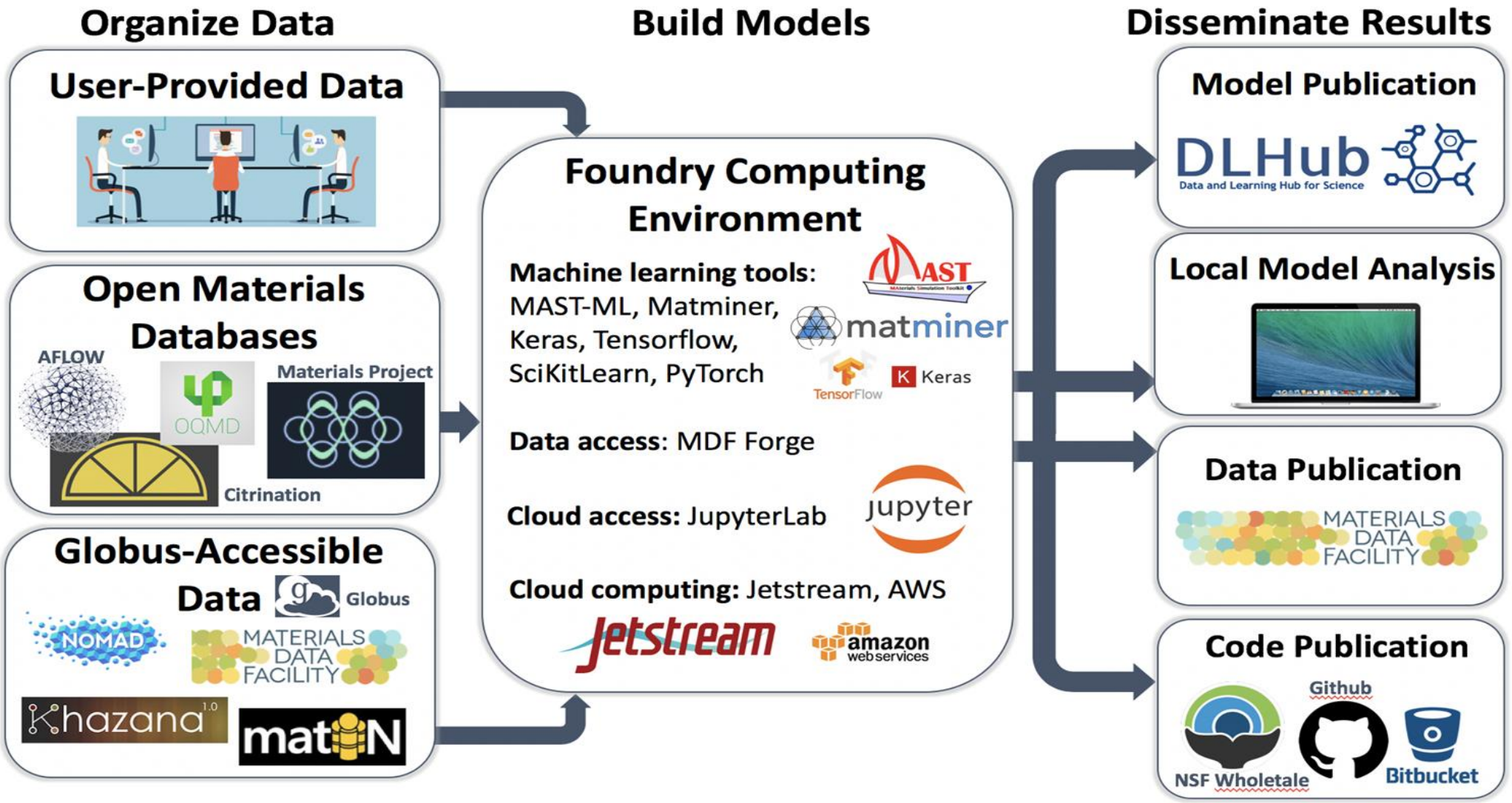
MAST-ML automates the supervised learning workflow



- MAST-ML supports the full library of scikit-learn modules, and can be used to construct neural networks with Keras (based on tensorflow)

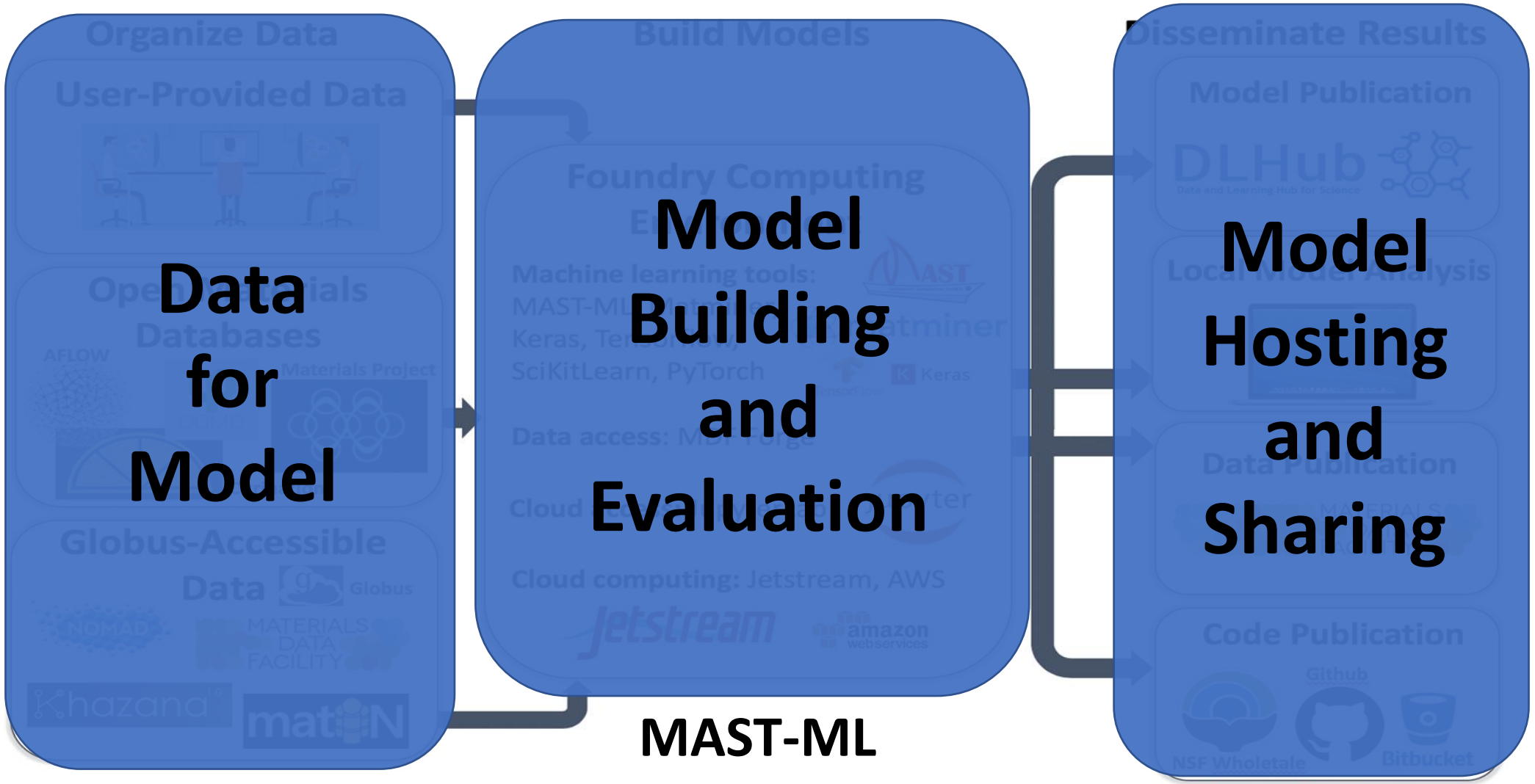
- MAST-ML allows for the simultaneous execution of an arbitrary combination of data preprocessing, feature generation/selection, model types and model evaluation metrics

(NSF CSSI) Machine Learning Materials Innovation Infrastructure



(PIs Dane Morgan, Paul Voyles, Michael Ferris, Ryan Jacobs, Ben Blaiszik)

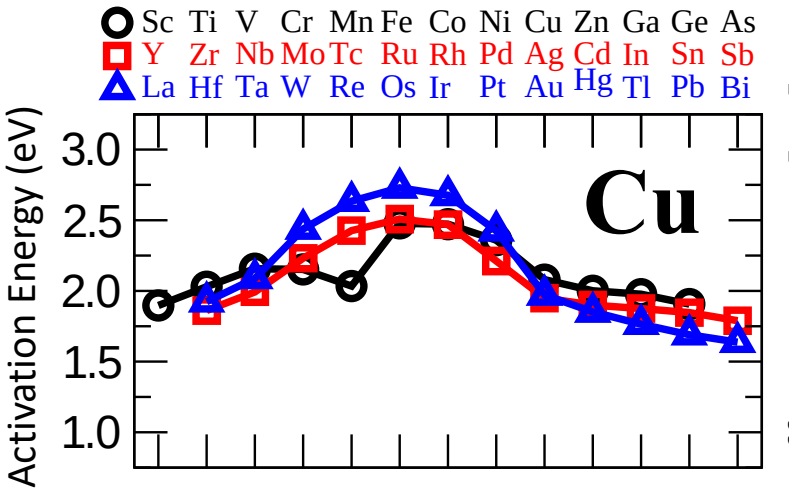
(NSF CSSI) Machine Learning Materials Innovation Infrastructure



Model building, evaluation, and key connections between data and model dissemination

Test Problem: Impurity Diffusion Database

- Diffusion of dilute impurity X in host H. We have DFT calculations of 440 values, but want ~4,000. [1, 2]
- Assume Y= Activation energies measured relative to host, X= Host descriptors, Impurity descriptors. Find Y=F(X).
- Descriptors = elemental properties like melting temperature, bulk modulus, electronegativity, … and their ratios, differences, etc. (MAGPIE set)[3]
- F is determined using standard machine learning regression methods (e.g., Gaussian Process Regression (Gaussian Kernel) (GPR), Random Forest (RF), neural network).
- Fit F with calculated data (15 hosts, 440 M-X pairs)

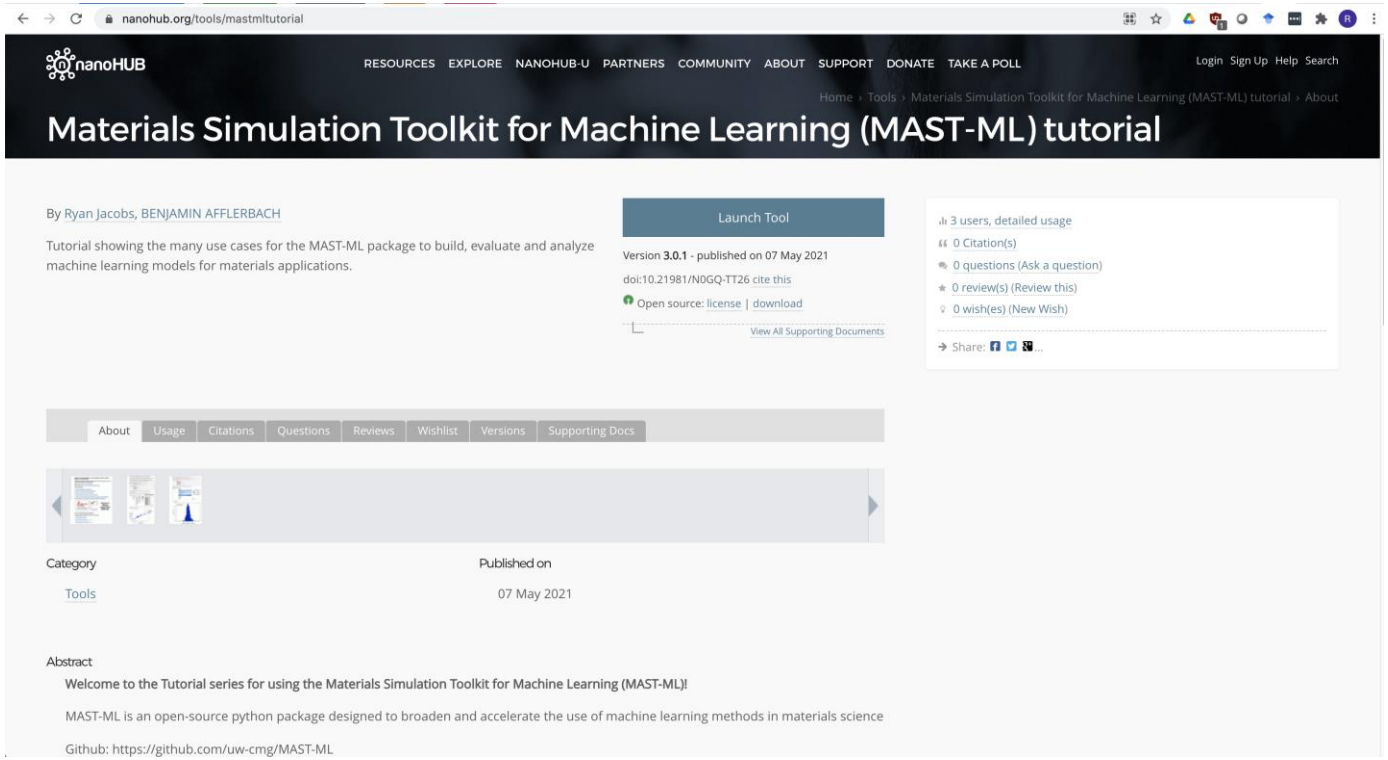


http://diffusiondata.materialshub.org/

[1] H. Wu, et al., *Comp. Mat. Sci* '17; [2] H. Lu, et al., *Comp Mat Sci* '19; [3] L. Ward, et al. *npj Comp. Mat.* '16

Getting Started with the MAST-ML tutorial on NanoHub

- Link to Tool: https://nanohub.org/tools/mastmltutorial
- Select “Launch Tool”
- A Jupyter notebook environment will open (may take a minute)
- Click on cell and run with Shift+return
- Data will be saved to local directory, see next slides for how to download results



Downloading results from MAST-ML tutorial

Each numbered step has a screenshot on the next few slides

Step 1.) Can visualize and zip saved files by clicking File-> Open in Jupyter notebook. A new window will open displaying your folders

Step 2.) To download a saved folder, need to zip it first. On right-hand side of window displaying folders, go to New->Terminal. A new window will open displaying a Unix-style Terminal.

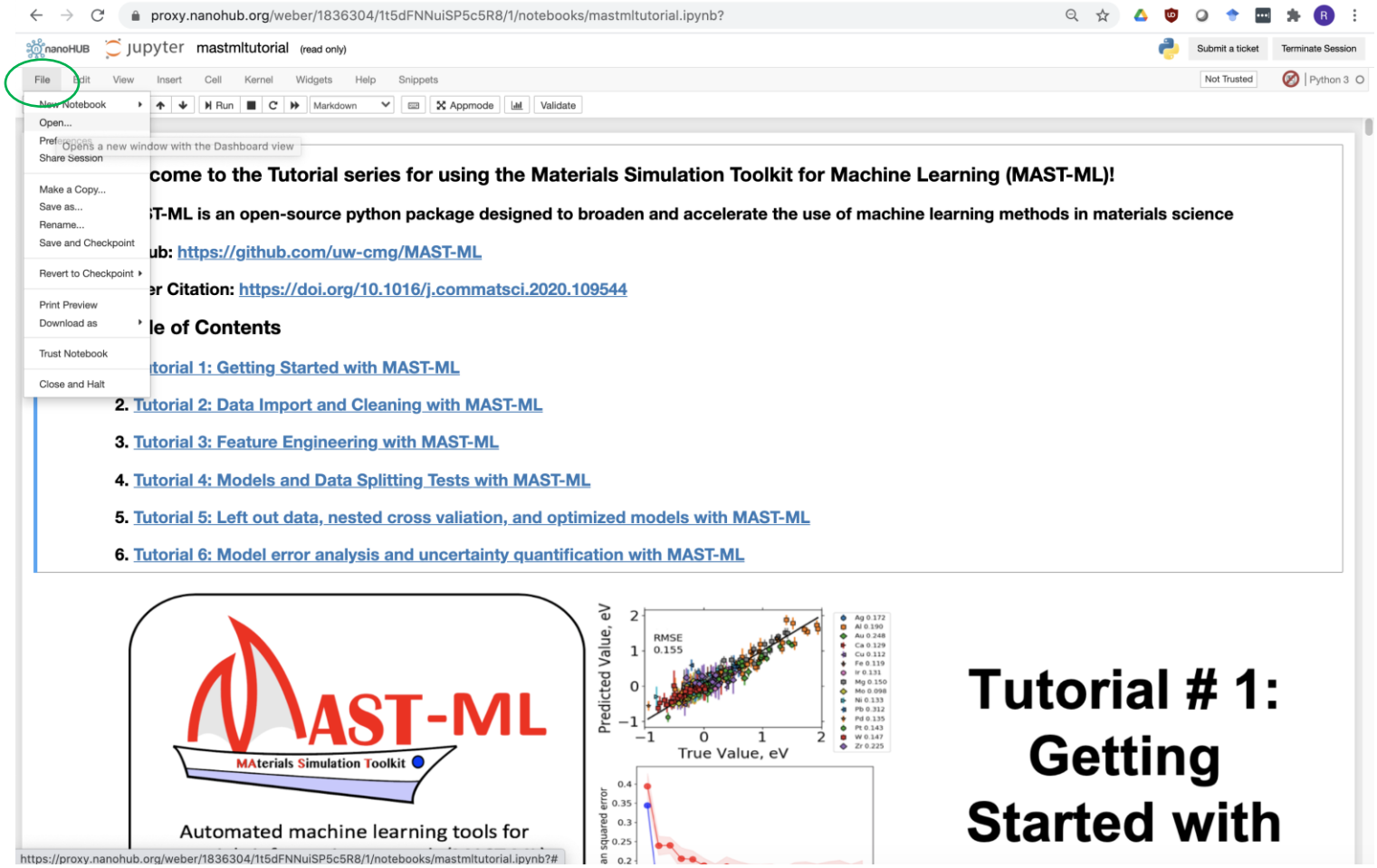
Step 3.) Zip the folder you want to download with the command:

- tar –zcvf folder_name.tar.gz folder_name

Step 4.) Look back at your displayed folders: there is now a new .tar.gz folder. You can click the box next to this folder and click the “Download” button.

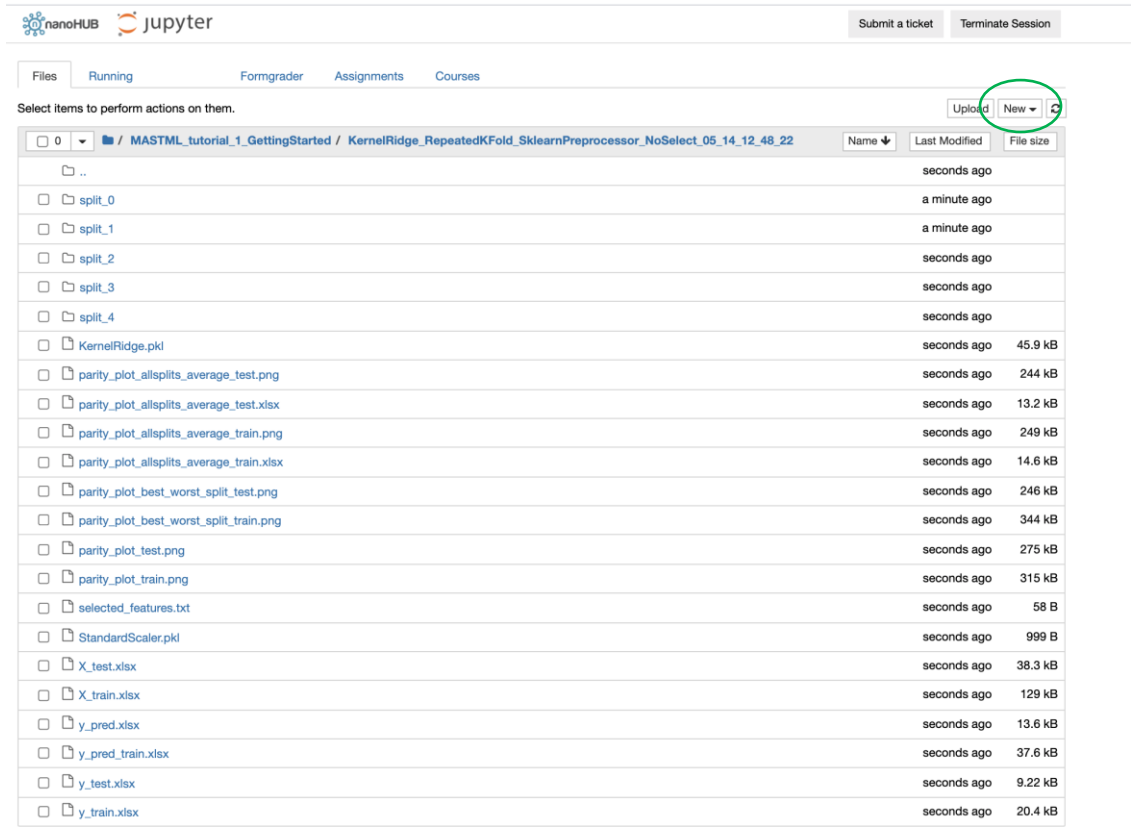
Downloading results from MAST-ML tutorial: Step 1

Step 1.) Can visualize and zip saved files by clicking File-> Open in Jupyter notebook. A new window will open displaying your folders



Downloading results from MAST-ML tutorial: Step 2

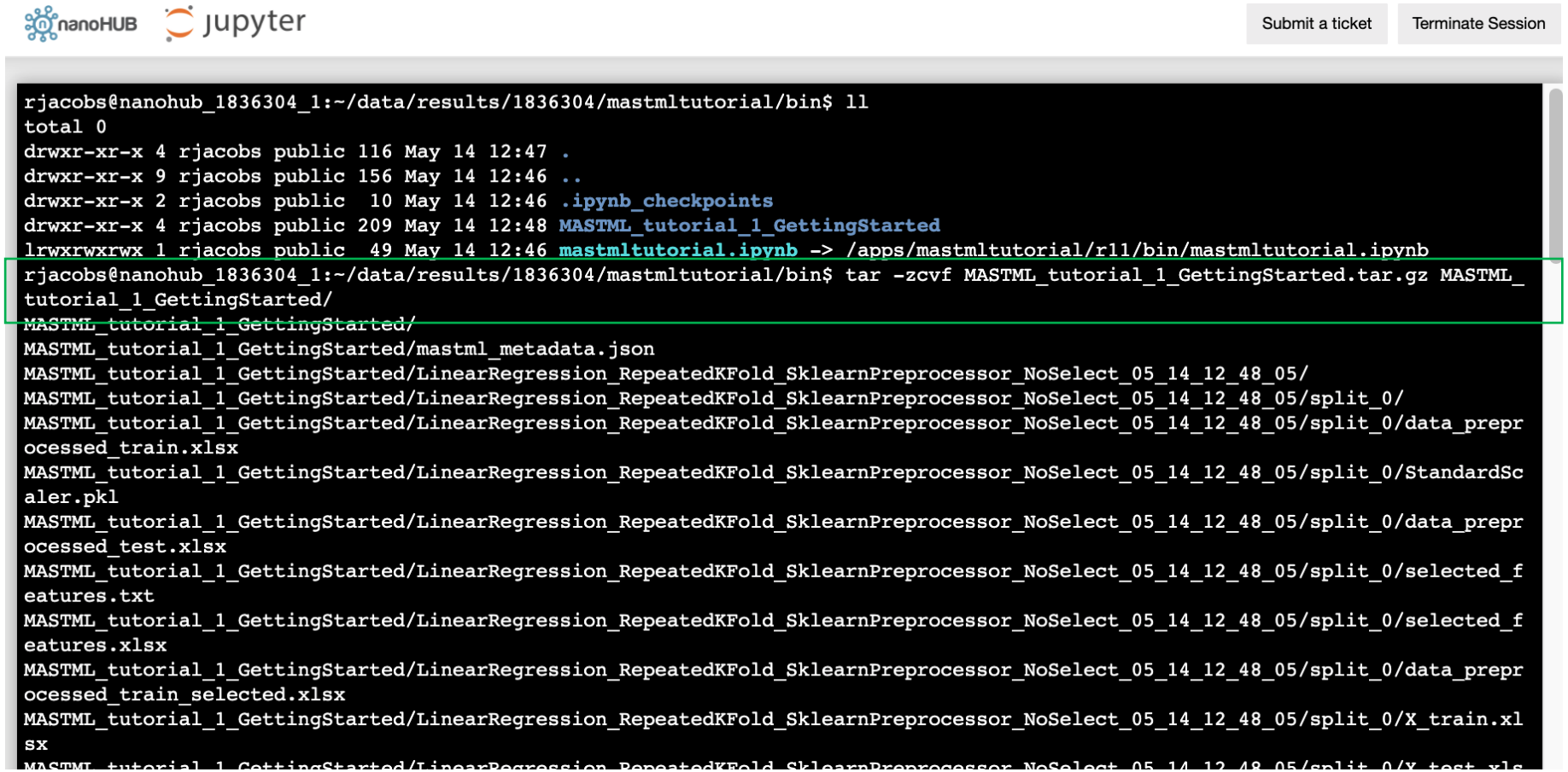
Step 2.) To download a saved folder, need to zip it first. On right-hand side of window displaying folders, go to New->Terminal. A new window will open displaying a Unix-style Terminal.



Downloading results from MAST-ML tutorial: Step 3

Step 3.) Zip the folder you want to download with the command:

- tar –zcvf folder_name.tar.gz folder_name
- In this case, I ran Tutorial 1, and the folder name was “MASTML_tutorial_1_GettingStarted”



Downloading results from MAST-ML tutorial: Step 4

Step 4.) Look back at your displayed folders: there is now a new .tar.gz folder. You can click the box next to this folder and click the "Download" button.