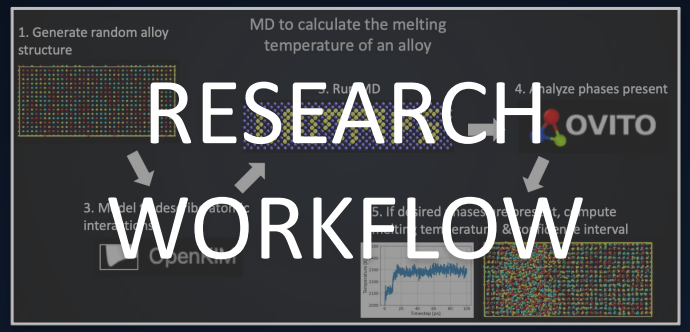
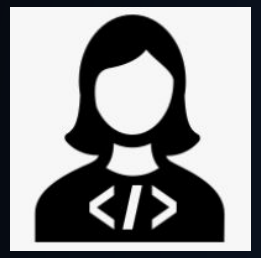
Introduction to nanoHUB notebooks

Inputs



Output(s)



Developer

nH

Users

SimTool:

- Declare inputs & outputs (including metadata)
- Implement every step connecting INs to OUTs

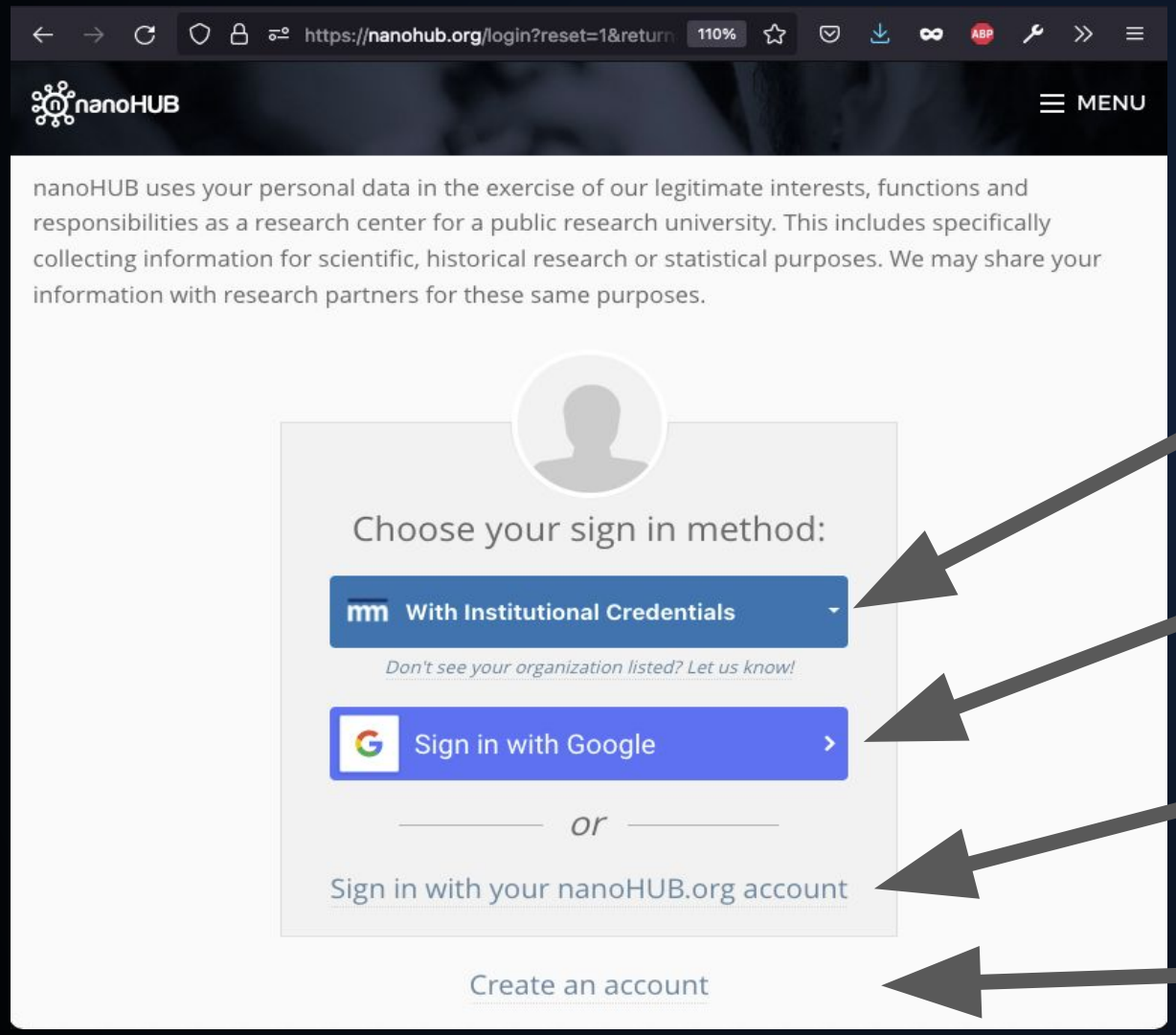
- USING JUPYTER NOTEBOOKS

SimTool library

- SimTools are registered & queryable
- Inputs and outputs (incl. metadata) are queryable
- Inputs are verified (incl. unit conversion) before run
- Outputs are checked after workflow execution
- Published SimTools have DOIs & are indexed by WoS and google scholar
- Results are automatically cached & queryable (data & metadata)

How to register to nanoHUB

https://nanohub.org/kb/registration/how-to-create-a-free-nanohub-account



https://nanohub.org/login

INCOMMON

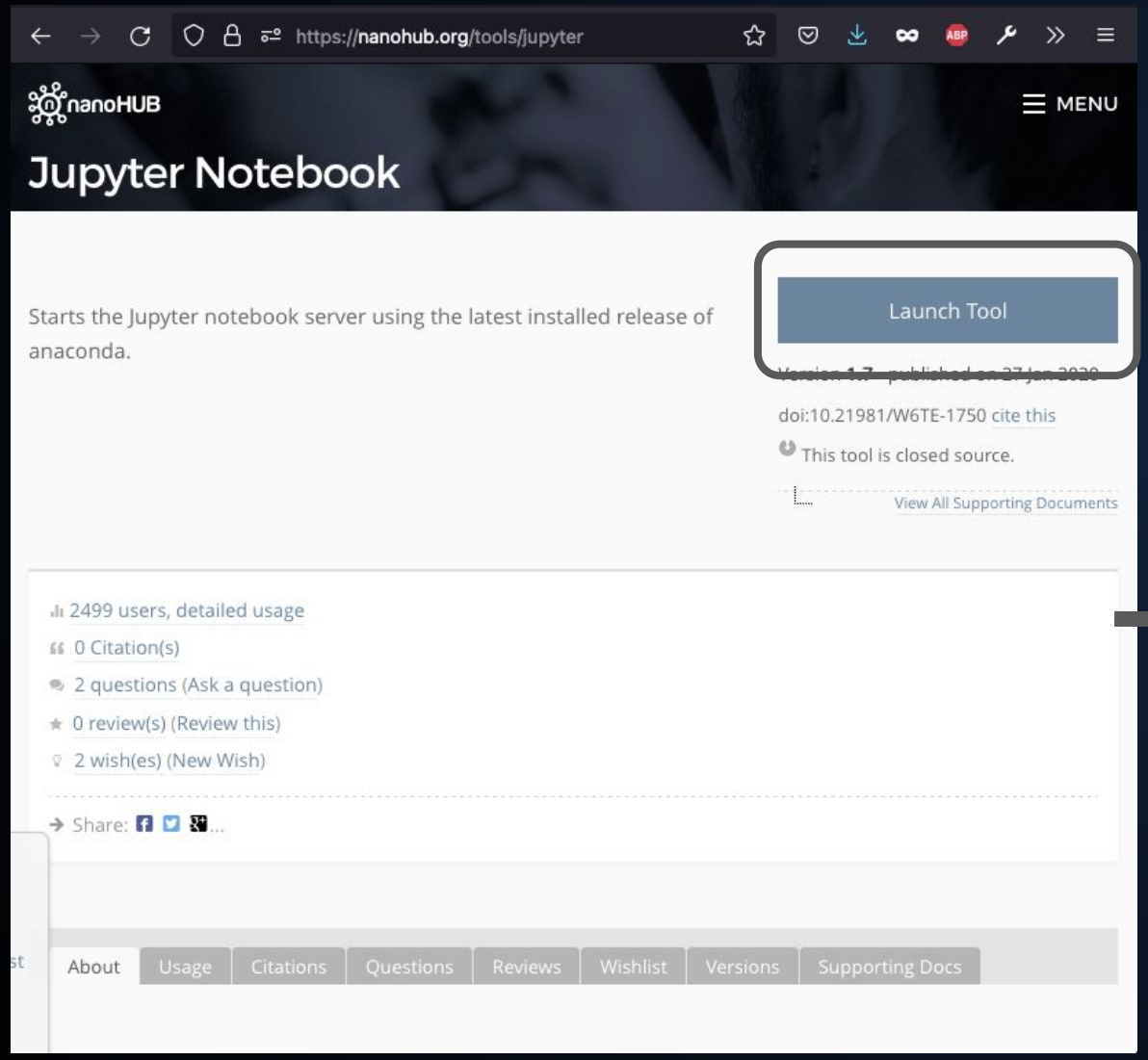
GOOGLE

LOGIN/PWD

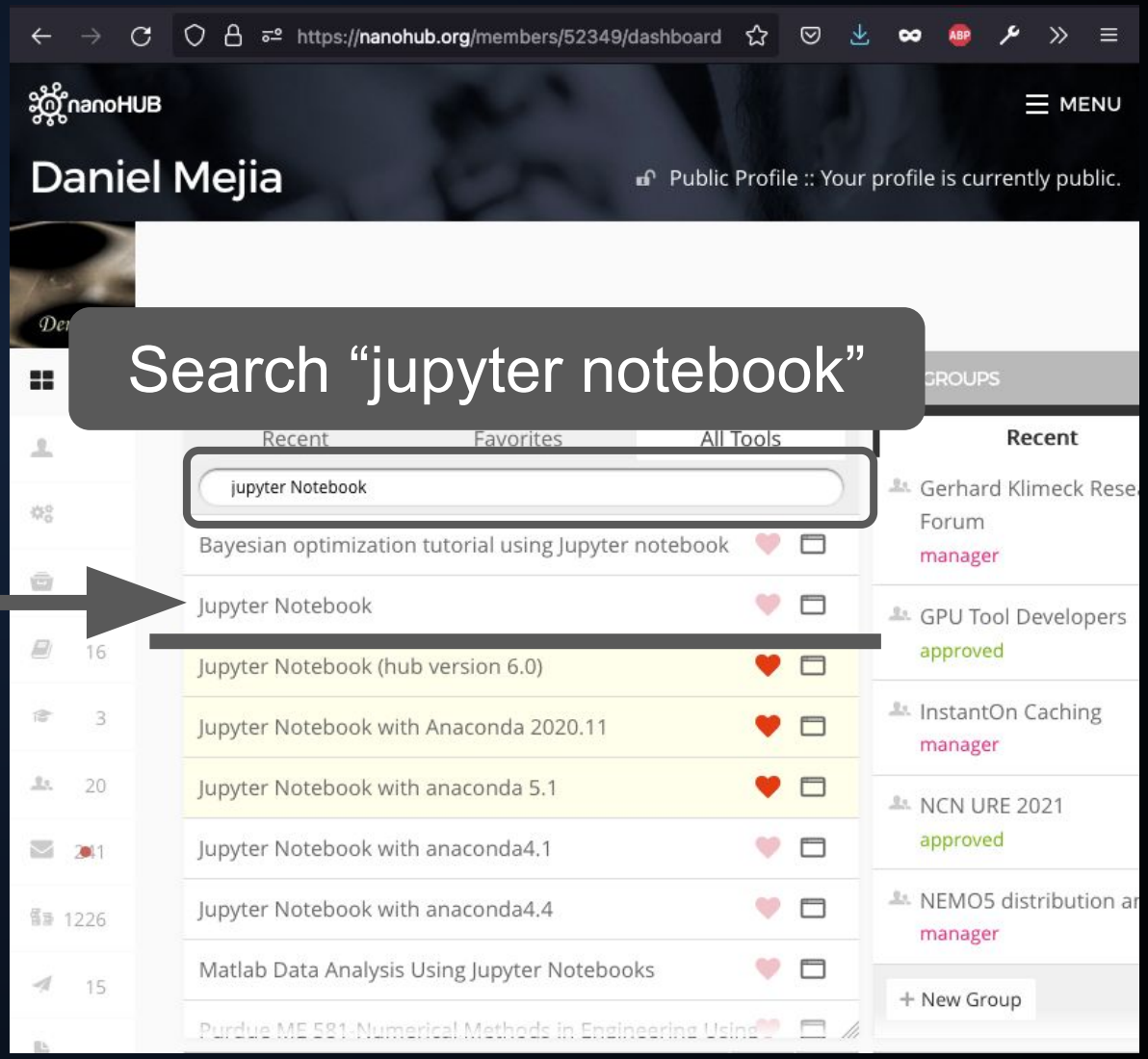
CREATE ACCOUNT

How to register to nanoHUB

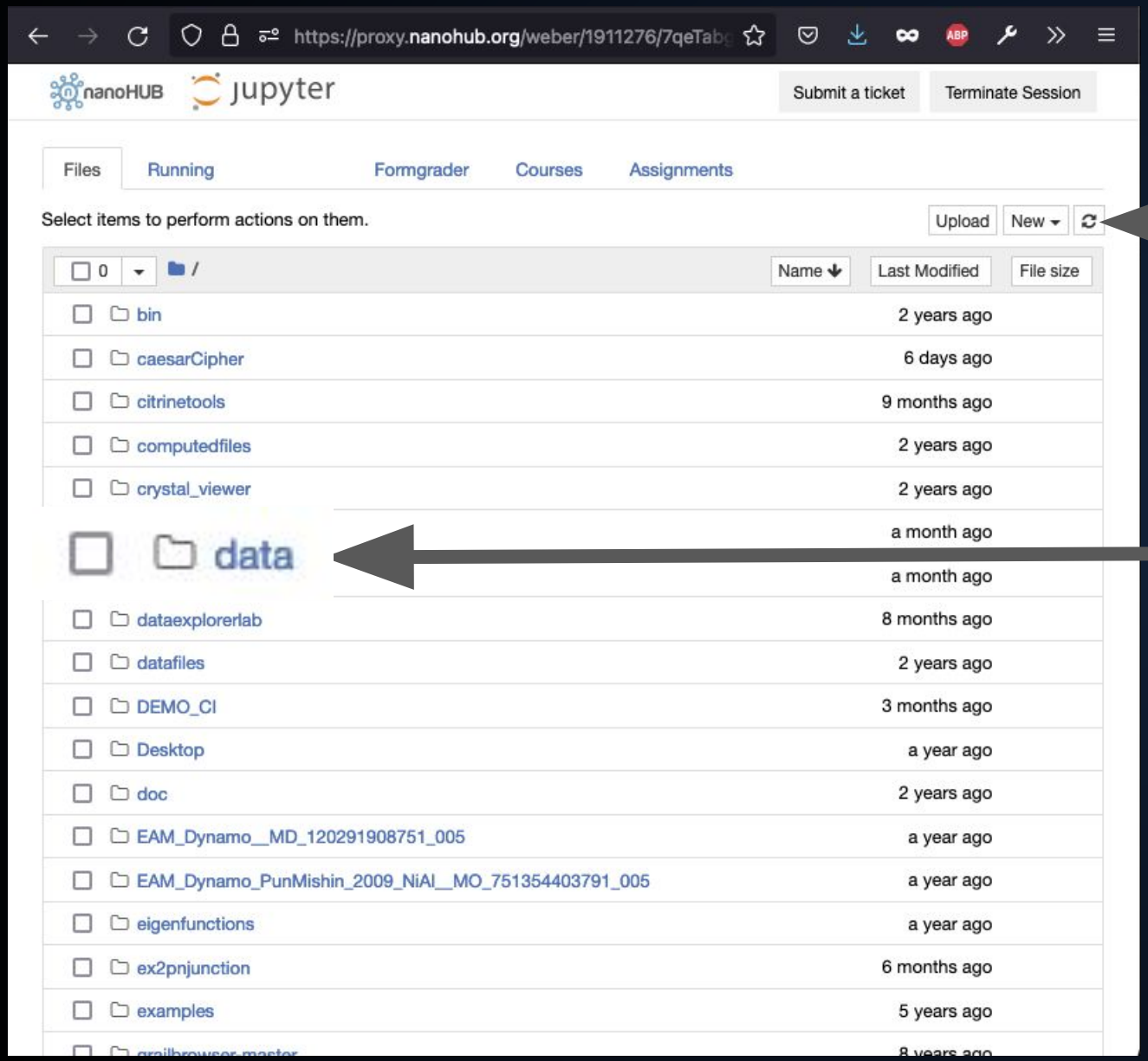
https://nanohub.org/tools/jupyter



Dashboard



Jupyter File explorer

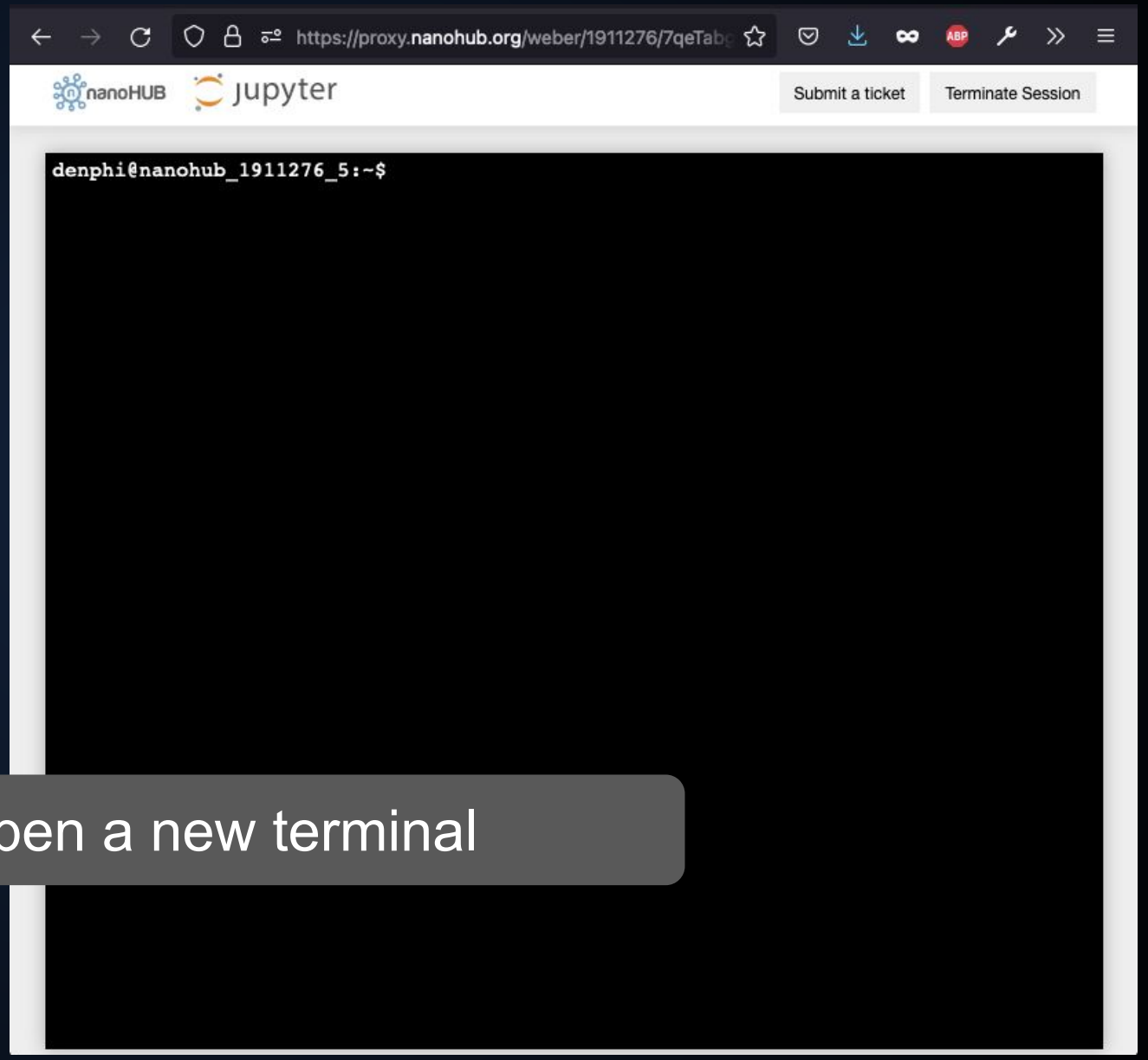


New
Folder, Notebook,
Terminal, Desktop

Default Folder / Sessions / Results

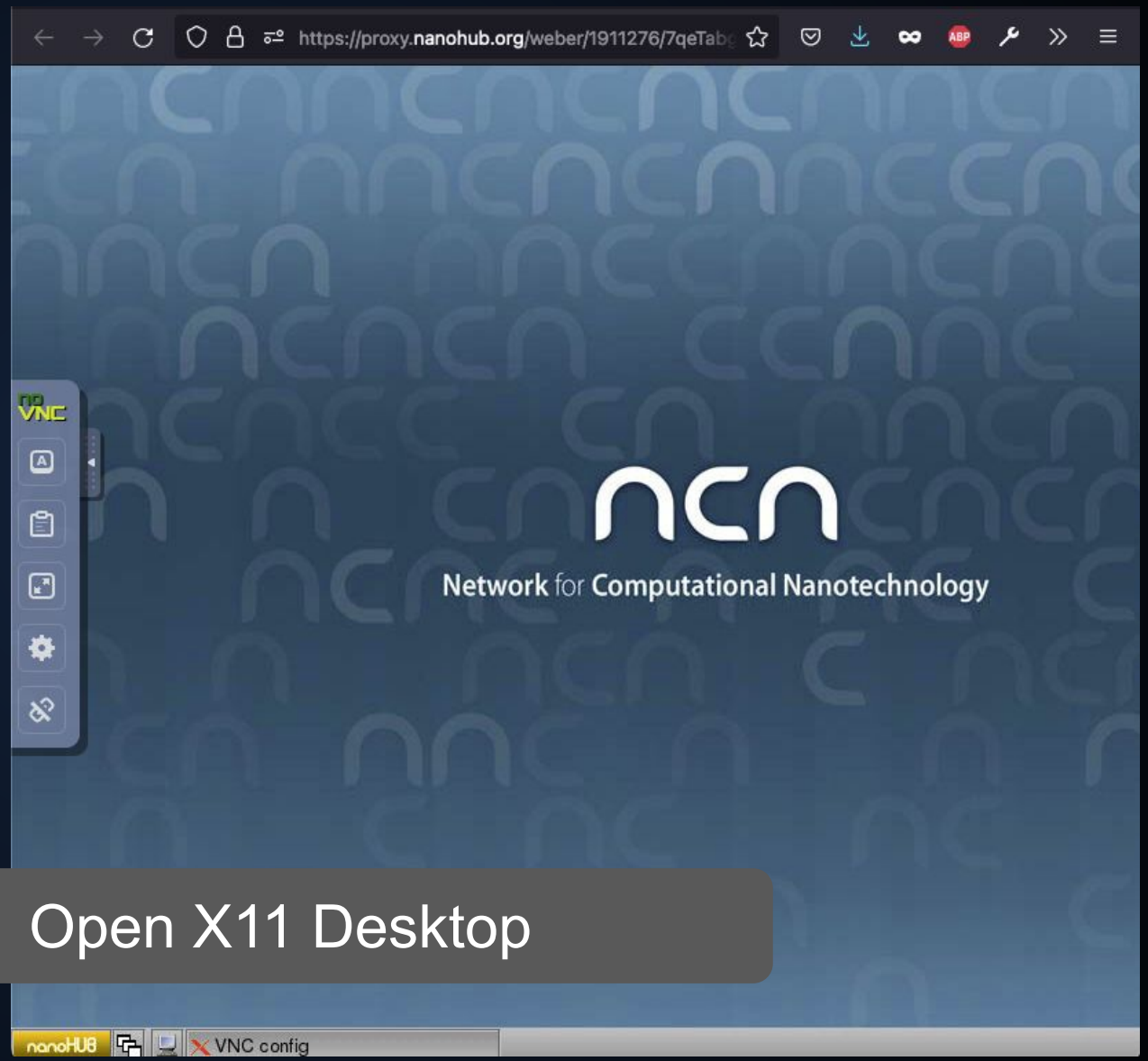
Create Terminal

Open a new terminal



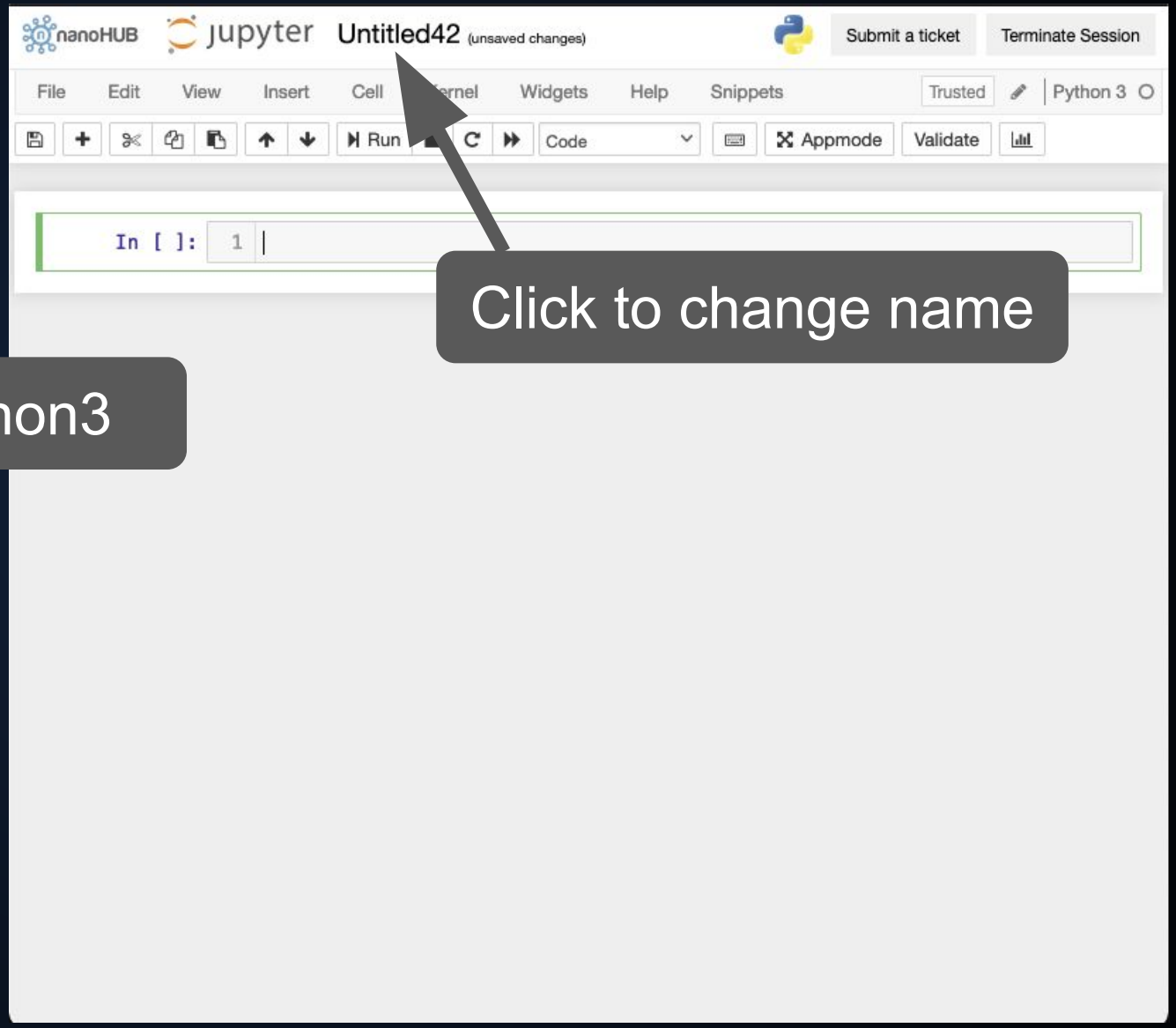
Create Terminal / Desktop

Open X11 Desktop



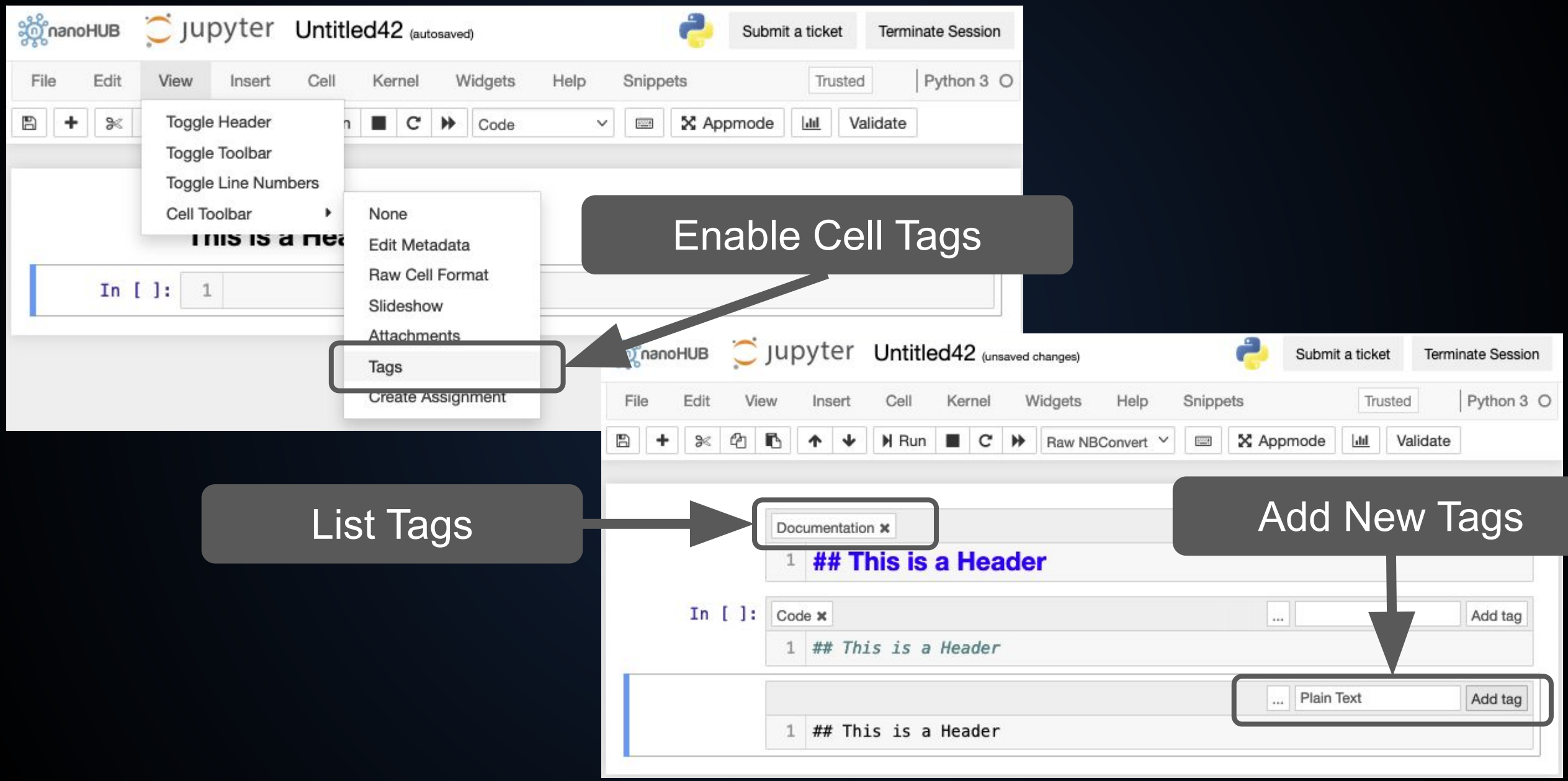
Create New Notebook

Python3

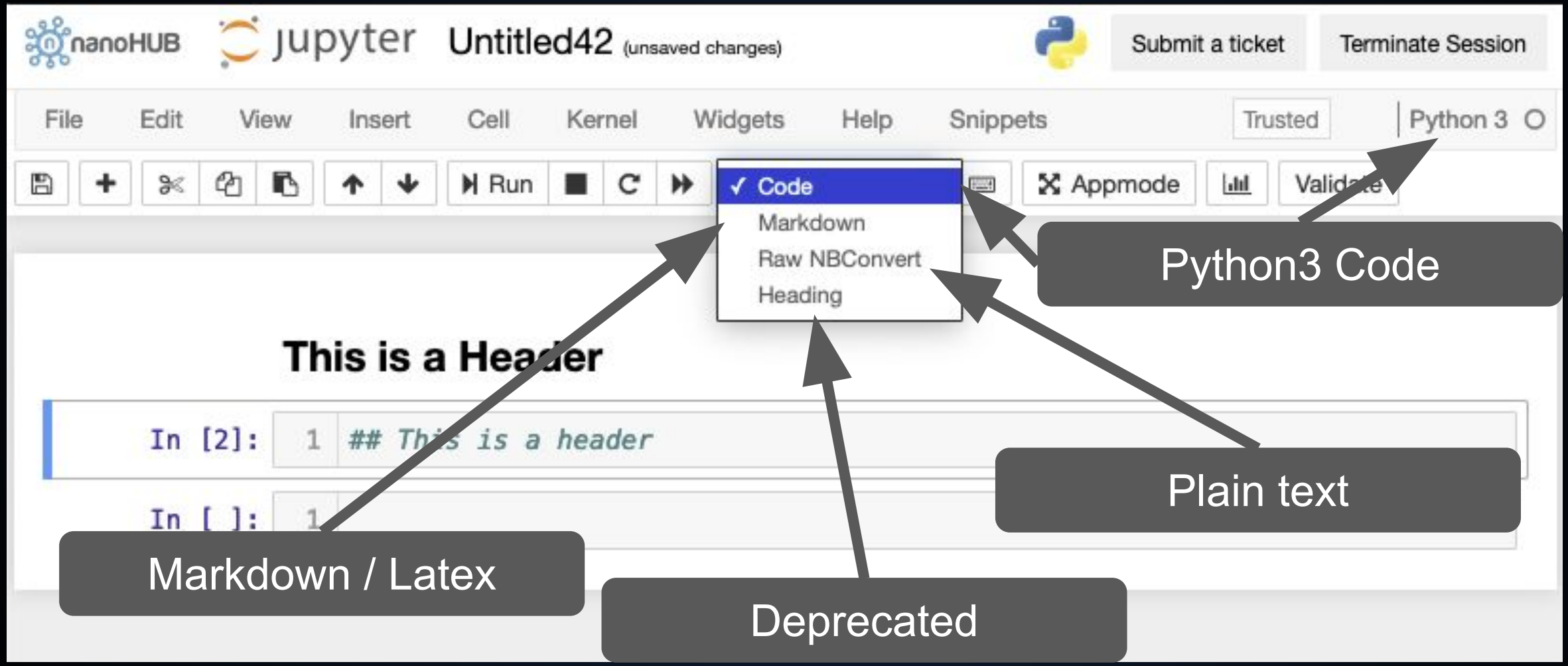


Click to change name

Enable Tags


nanoHUB
jupyter
Untitled42 (autosaved)
Submit a ticket
Terminate Session
File Edit View Insert Cell Kernel Widgets Help Snippets
Trusted
Python 3
Code
Appmode
Validate
Toggle Header
Toggle Toolbar
Toggle Line Numbers
Cell Toolbar
None
Edit Metadata
Raw Cell Format
Slideshow
Attachments
Tags
Create Assignment
In [ ]:
1
Enable Cell Tags
nanoHUB
jupyter
Untitled42 (unsaved changes)
Submit a ticket
Terminate Session
File Edit View Insert Cell Kernel Widgets Help Snippets
Trusted
Python 3
Run
Raw NBConvert
Appmode
Validate
List Tags
Documentation
This is a Header
In [ ]:
Code
Add tag
This is a Header
Add New Tags
Plain Text
Add tag
This is a Header

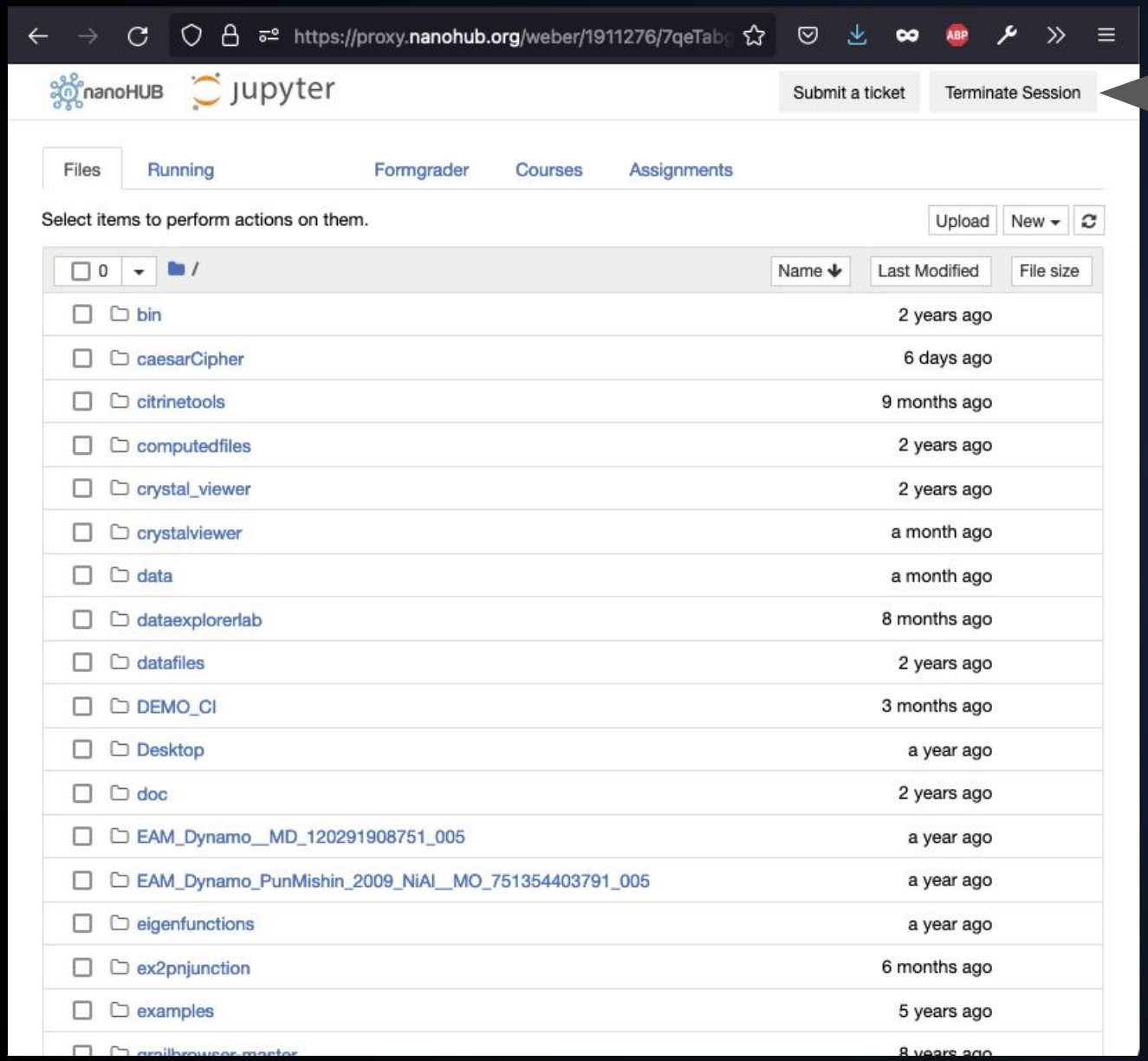
Cell Types


nanoHUB
jupyter
Untitled42 (unsaved changes)
Submit a ticket
Terminate Session
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Snippets
Trusted
Python 3
Run
Code
Markdown
Raw NBConvert
Heading
Appmode
This is a Header
In [2]:
1 ## This is a header
In [ ]:
1
Python3 Code
Plain text
Markdown / Latex
Deprecated

Run Cells


nanoHUB
jupyter
Untitled42 (unsaved changes)
Submit a ticket
Terminate Session
File
Edit
View
Insert
Cell
Kernel
Python 3
Run
Run Cell + Move to Next
Documentation
Add tag
This is a Header
CTRL + RETURN/ENTER
Run Cell + Stay in the cell
In [4]:
Code
...
Add tag
1 ## This is a Header
SHIFT + RETURN/ENTER
Run Cell + Move to Next
Add tag
1 ## This is a Header

End Sessions



Terminate the session

Files are preserved, All python kernels are ended

If a session is not Terminated, can be accessed from dashboard

Idle sessions are terminated, unsaved data maybe lost