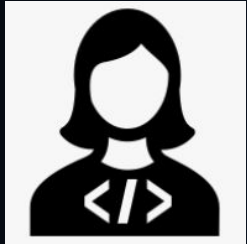
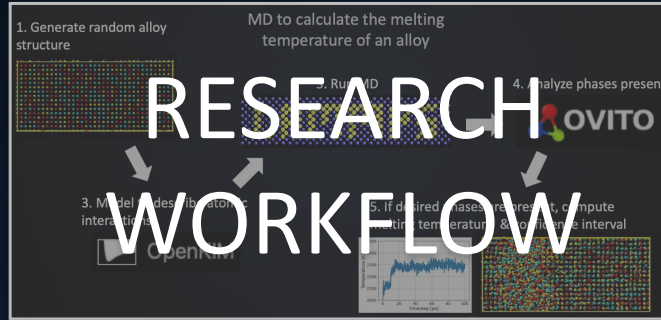


# Introduction to nanoHUB notebooks

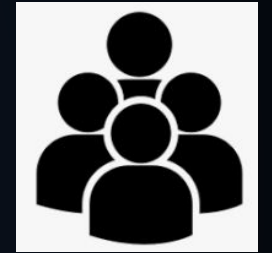
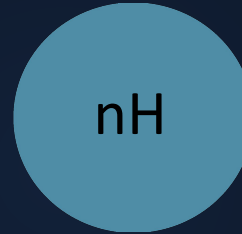
Inputs



Developer



Output(s)



Users

## SimTool:

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

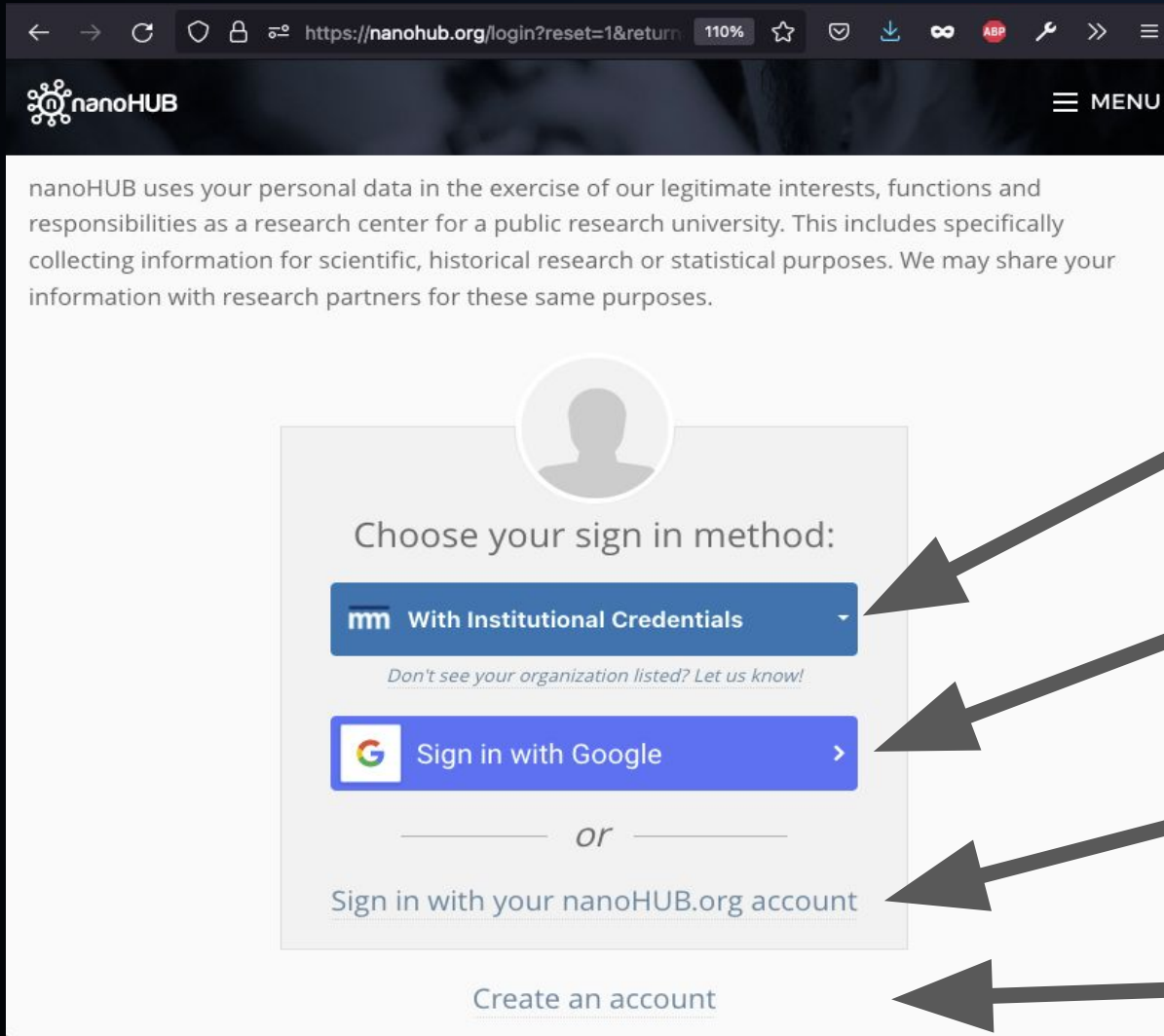
## • USING JUPYTER NOTEBOOKS

## 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>



The screenshot shows the nanoHUB login page. At the top, there is a navigation bar with the nanoHUB logo and a 'MENU' button. Below the navigation bar, a privacy notice states: 'nanoHUB uses your personal data in the exercise of our legitimate interests, functions and responsibilities as a research center for a public research university. This includes specifically collecting information for scientific, historical research or statistical purposes. We may share your information with research partners for these same purposes.' The main content area features a sign-in section with a placeholder for a profile picture. The text 'Choose your sign in method:' is followed by two buttons: 'With Institutional Credentials' (with a dropdown arrow) and 'Sign in with Google' (with a right arrow). Below these buttons is the word 'or' and the text 'Sign in with your nanoHUB.org account'. At the bottom of the sign-in section is a link that says 'Create an account'.

<https://nanohub.org/login>

INCOMMON

GOOGLE

LOGIN/PWD

CREATE ACCOUNT

# How to register to nanoHUB

<https://nanohub.org/tools/jupyter>

The screenshot shows the nanoHUB website's tool page for Jupyter Notebook. The URL in the browser is <https://nanohub.org/tools/jupyter>. The page features a 'Launch Tool' button, which is highlighted with a red rectangle. Below the button, it states 'Version 1.7 published on 27 Jan 2020' and 'doi:10.21981/W6TE-1750 cite this'. It also mentions 'This tool is closed source.' and a link to 'View All Supporting Documents'. On the left, there are statistics: '2499 users, detailed usage', '0 Citation(s)', '2 questions (Ask a question)', '0 review(s) (Review this)', and '2 wish(es) (New Wish)'. At the bottom, there is a share button and a navigation bar with tabs: About, Usage, Citations, Questions, Reviews, Wishlist, Versions, and Supporting Docs.

Dashboard

The screenshot shows the nanoHUB dashboard for a user named Daniel Mejia. The URL in the browser is <https://nanohub.org/members/52349/dashboard>. The dashboard displays a list of tools under the 'Recent' tab. A search bar is highlighted with a red rectangle, containing the text 'jupyter Notebook'. Below the search bar, a list of tools is shown, including 'Jupyter Notebook', 'Jupyter Notebook (hub version 6.0)', 'Jupyter Notebook with Anaconda 2020.11', 'Jupyter Notebook with anaconda 5.1', 'Jupyter Notebook with anaconda4.1', 'Jupyter Notebook with anaconda4.4', 'Matlab Data Analysis Using Jupyter Notebooks', and 'Purdue ME 581 Numerical Methods in Engineering Using'. A red arrow points from the 'Launch Tool' button in the previous screenshot to the 'Jupyter Notebook' entry in this list. On the right side of the dashboard, there is a 'Recent' section with a list of groups, including 'Gerhard Klimeck Research Forum', 'GPU Tool Developers', 'InstantOn Caching', 'NCN URE 2021', and 'NEMO5 distribution and management'. A '+ New Group' button is at the bottom right.

# Jupyter File explorer

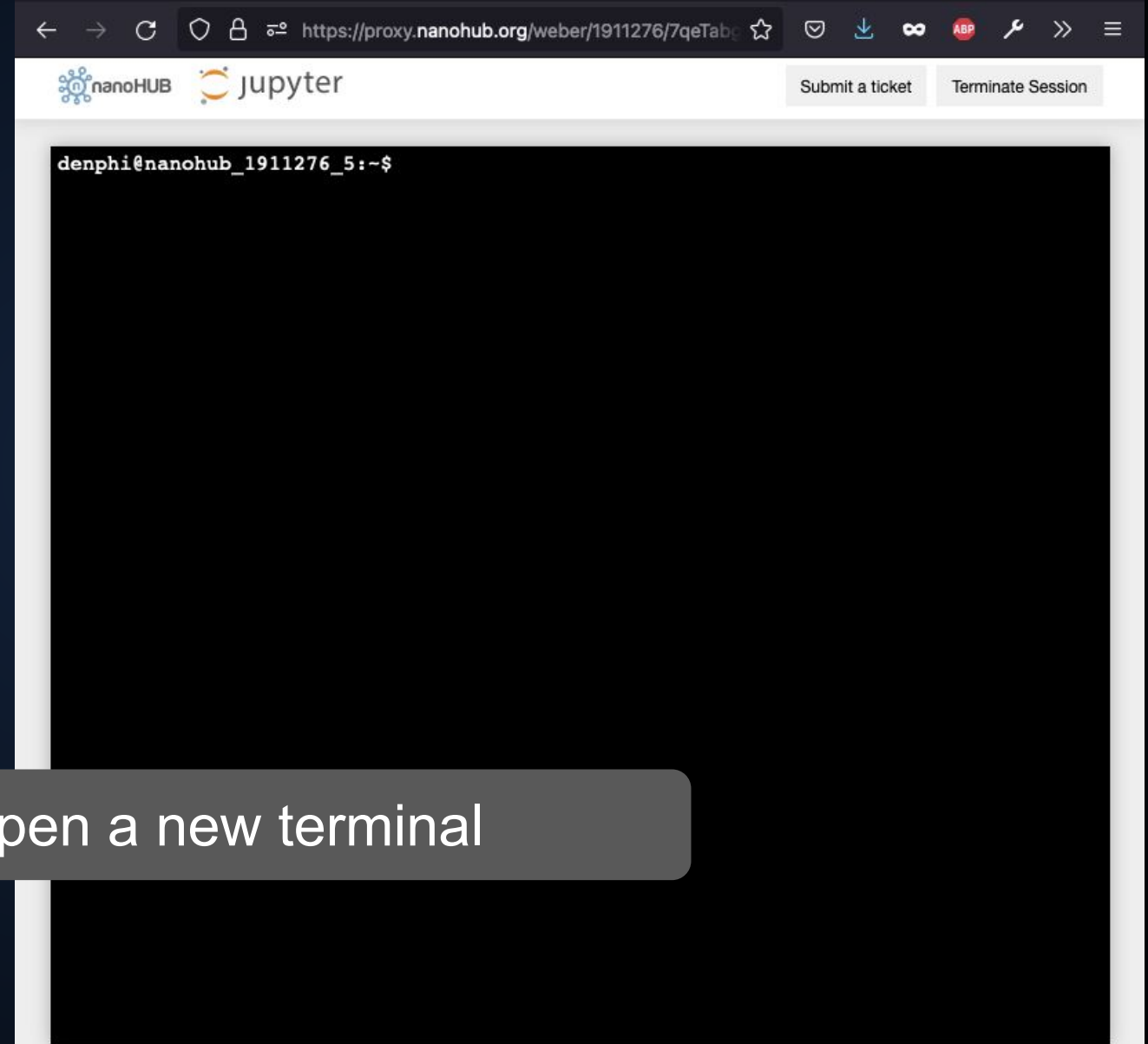
The screenshot shows the Jupyter File Explorer interface. At the top, there's a navigation bar with 'Files', 'Running', 'Formgrader', 'Courses', and 'Assignments'. Below this, there's a section for 'Select items to perform actions on them.' with buttons for 'Upload', 'New', and a refresh icon. The main area displays a list of folders and files with columns for 'Name', 'Last Modified', and 'File size'. The 'data' folder is highlighted with a yellow background. A large arrow points from the 'data' folder to a callout box on the right. Another arrow points from the 'New' button to a callout box above it.

Name	Last Modified	File size
bin	2 years ago	
caesarCipher	6 days ago	
citrinetools	9 months ago	
computedfiles	2 years ago	
crystal_viewer	2 years ago	
data	a month ago	
dataexplorerlab	8 months ago	
datafiles	2 years ago	
DEMO_CI	3 months ago	
Desktop	a year ago	
doc	2 years ago	
EAM_Dynamo__MD_120291908751_005	a year ago	
EAM_Dynamo_PunMishin_2009_NiAl__MO_751354403791_005	a year ago	
eigenfunctions	a year ago	
ex2pnjunction	6 months ago	
examples	5 years ago	
grailbrowser-master	8 years ago	

New  
Folder, Notebook,  
Terminal, Desktop

Default Folder / Sessions / Results

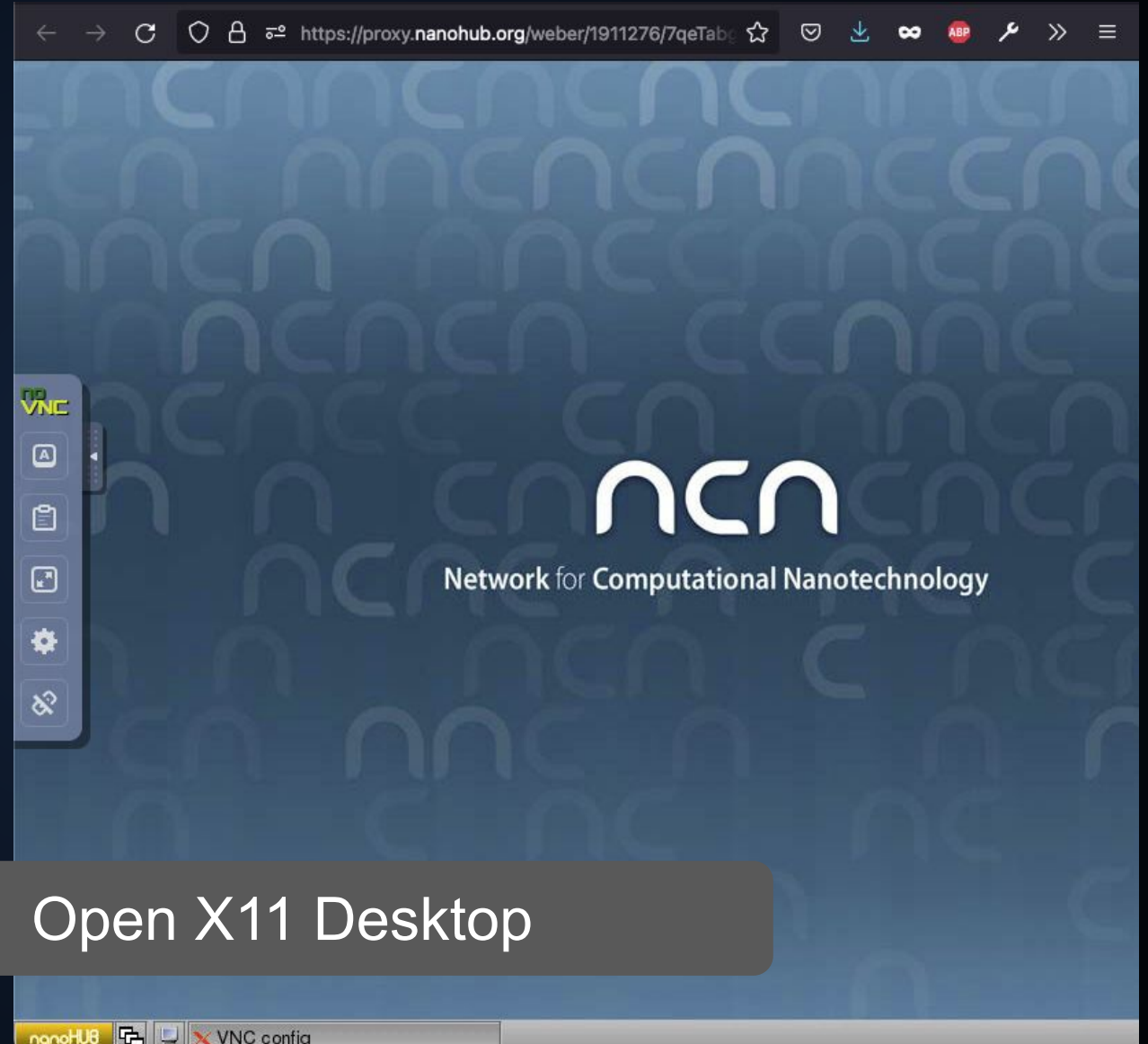
# Create Terminal



Open a new terminal



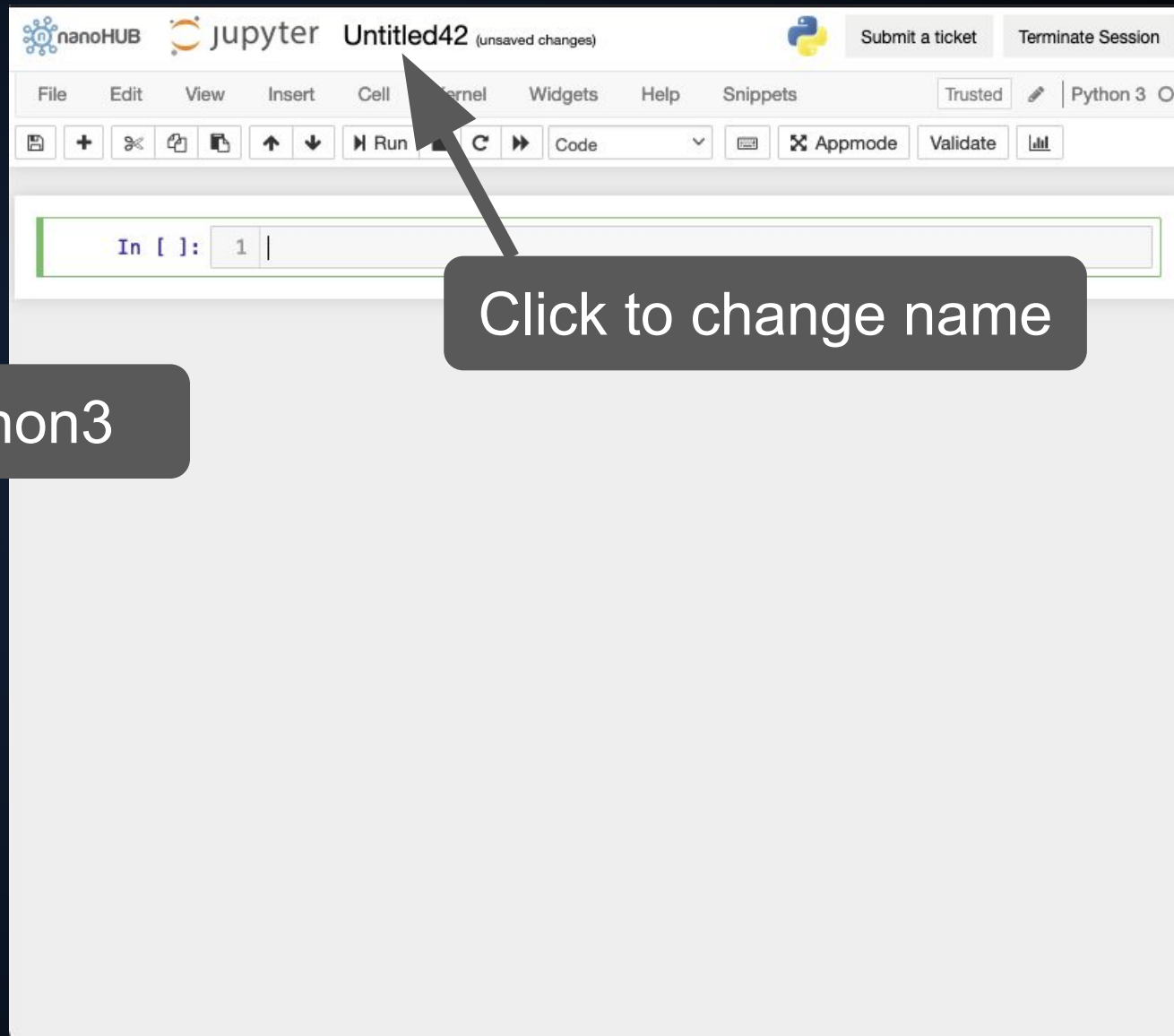
# Create Terminal / Desktop



# Create New Notebook



Python3



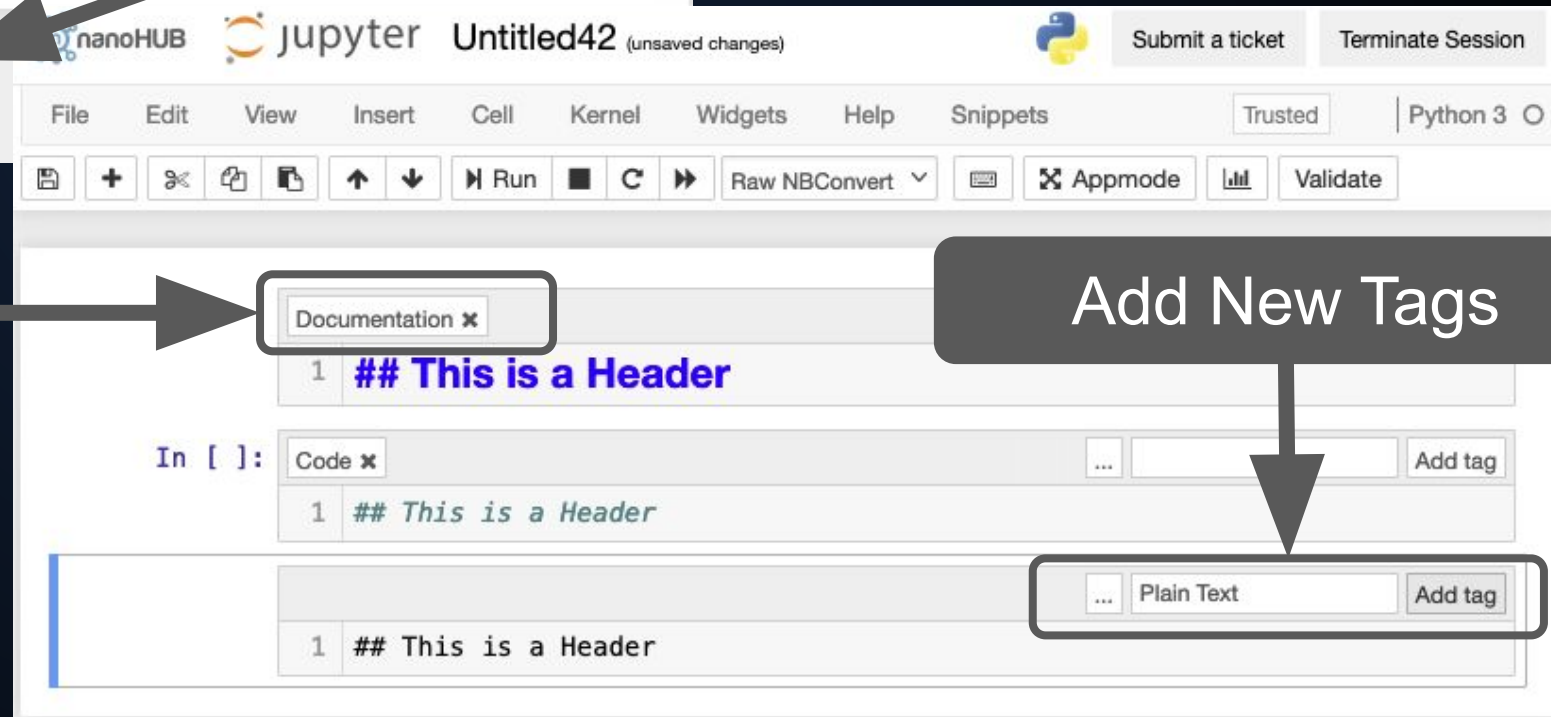
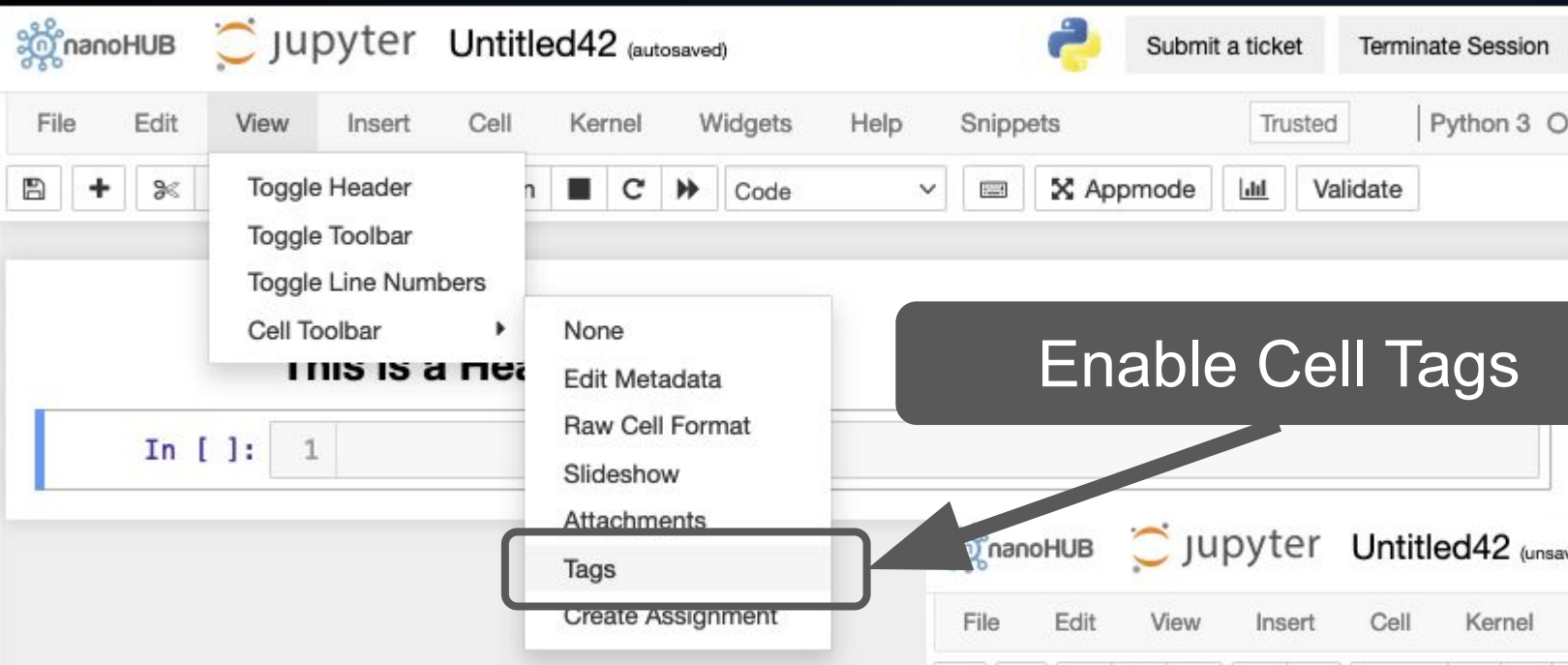
Click to change name

# Enable Tags

Enable Cell Tags

List Tags

Add New Tags





# Cell Types

The image shows a Jupyter Notebook interface with the following elements:

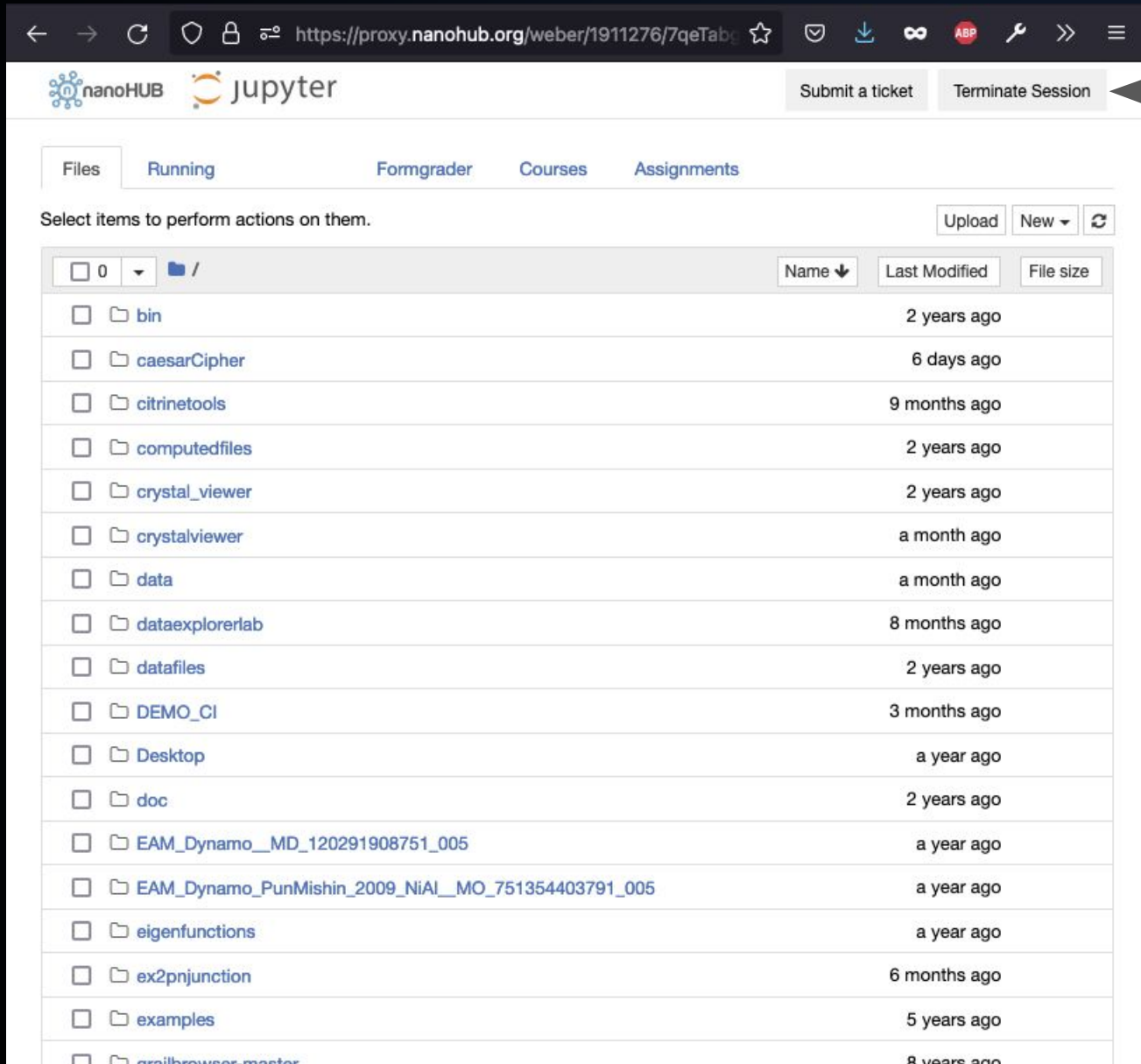
- Top Bar:** nanoHUB logo, Jupyter logo, "Untitled42 (unsaved changes)", Python logo, "Submit a ticket", and "Terminate Session".
- Menu Bar:** File, Edit, View, Insert, Cell, Kernel, Widgets, Help, Snippets.
- Toolbar:** Icons for saving, adding cells, undo, redo, and running cells. A dropdown menu is open under the "Cell" menu, showing options:
  - ✓ Code
  - Markdown
  - Raw NBConvert
  - Heading
- Cell Content:** A code cell containing the text `## This is a header`. Above the cell, the text "This is a Header" is displayed.
- Labels and Arrows:** Four dark gray boxes with white text and arrows pointing to the Cell menu options:
  - "Python3 Code" points to the "Code" option.
  - "Plain text" points to the "Markdown" option.
  - "Deprecated" points to the "Raw NBConvert" option.
  - "Markdown / Latex" points to the "Heading" option.

# Run Cells

The screenshot shows the JupyterLab interface with the following elements:

- Top Bar:** nanoHUB logo, Jupyter logo, "Untitled42 (unsaved changes)", Python 3 logo, "Submit a ticket", and "Terminate Session".
- Menu Bar:** File, Edit, View, Insert, Cell, Kernel, Windows.
- Toolbar:** Contains icons for Save, New, Copy, Paste, Undo, Redo, and a "Run" button (a play icon). A callout box points to the "Run" button with the text "Run Cell + Move to Next".
- Code Cells:** Two code cells are visible. The first cell is titled "Documentation x" and contains the text "This is a Header". A callout box points to it with the text "CTRL + RETURN/ENTER Run Cell + Stay in the cell". The second cell is titled "Code x" and contains the text "1 ## This is a Header". A callout box points to it with the text "SHIFT + RETURN/ENTER Run Cell + Move to Next".

# End Sessions



The screenshot shows the nanoHUB Jupyter interface. At the top, there's a browser address bar with the URL `https://proxy.nanohub.org/weber/1911276/7qeTabg`. Below the browser bar, the nanoHUB and Jupyter logos are visible. To the right of the logos are two buttons: "Submit a ticket" and "Terminate Session". An arrow points from the "Terminate Session" button to a text box on the right. Below the logos, there are tabs for "Files", "Running", "Formgrader", "Courses", and "Assignments". The "Files" tab is selected. Below the tabs, there's a message "Select items to perform actions on them." and buttons for "Upload", "New", and a refresh icon. A table lists files and folders with columns for "Name", "Last Modified", and "File size". The table contains the following entries:

	Name	Last Modified	File size
<input type="checkbox"/>	0		
<input type="checkbox"/>	bin	2 years ago	
<input type="checkbox"/>	caesarCipher	6 days ago	
<input type="checkbox"/>	citrinetools	9 months ago	
<input type="checkbox"/>	computedfiles	2 years ago	
<input type="checkbox"/>	crystal_viewer	2 years ago	
<input type="checkbox"/>	crystalviewer	a month ago	
<input type="checkbox"/>	data	a month ago	
<input type="checkbox"/>	dataexplorerlab	8 months ago	
<input type="checkbox"/>	datafiles	2 years ago	
<input type="checkbox"/>	DEMO_CI	3 months ago	
<input type="checkbox"/>	Desktop	a year ago	
<input type="checkbox"/>	doc	2 years ago	
<input type="checkbox"/>	EAM_Dynamo_MD_120291908751_005	a year ago	
<input type="checkbox"/>	EAM_Dynamo_PunMishin_2009_NiAl_MO_751354403791_005	a year ago	
<input type="checkbox"/>	eigenfunctions	a year ago	
<input type="checkbox"/>	ex2pnjunction	6 months ago	
<input type="checkbox"/>	examples	5 years ago	
<input type="checkbox"/>	grailbrowser-master	8 years ago	

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