



nanoHUB: getting started guide to tool developers



Develop and publish tools in nanoHUB

Make your research reproducible and your workflows and data FAIR

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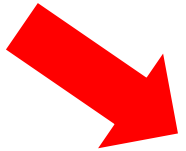
School of Materials Engineering &

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West Lafayette, Indiana USA

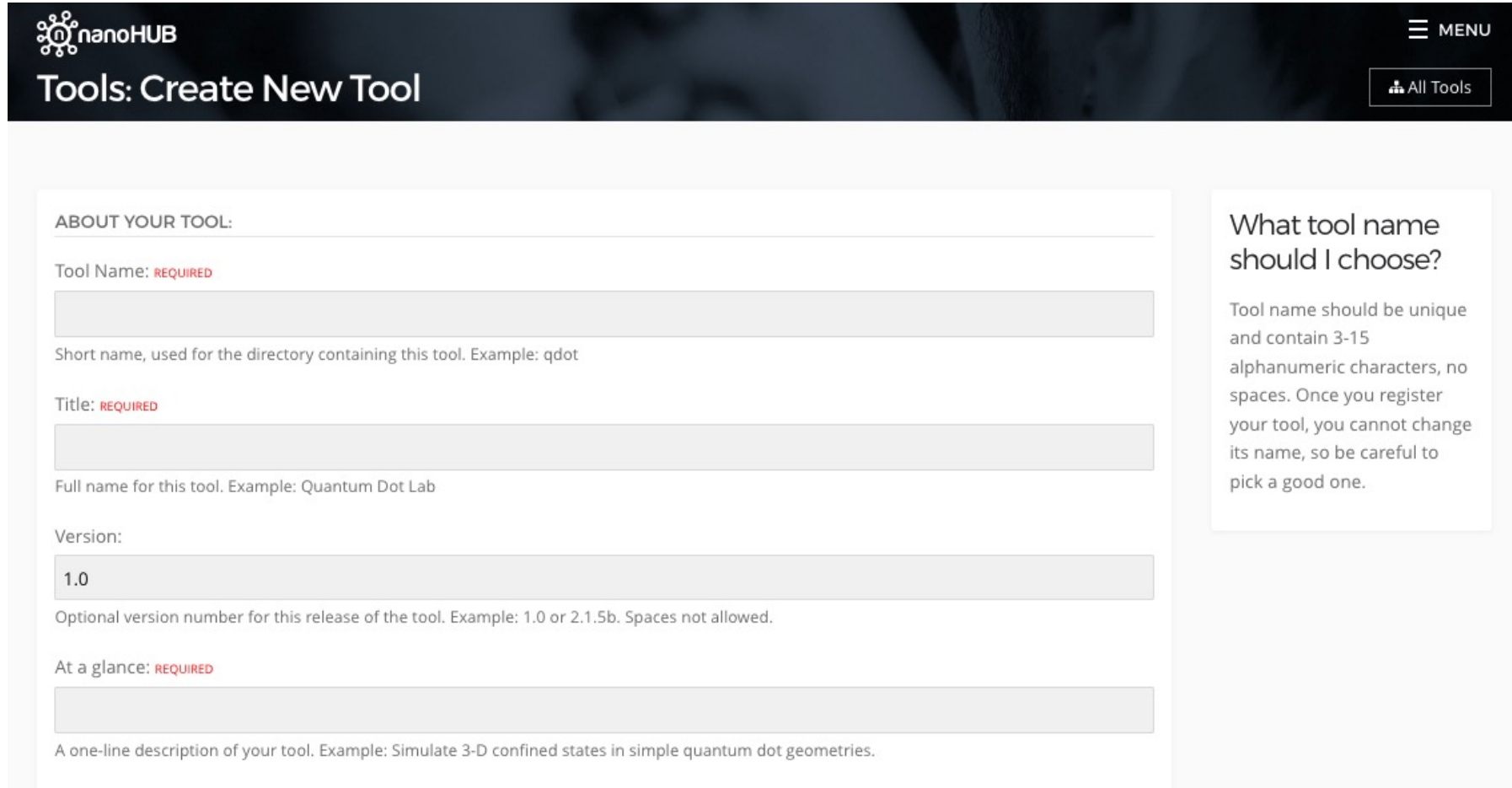
Overview

1. Why publish tools & apps in nanoHUB?
 - Tools are publications (DOIs and indexed by Web of Science)
 - Share your work with your community (22,000+ annual sim users)
2. Various tool and app types
 - Apps, workflows, Jupyter notebooks, commercial codes, X11 GUIs
3. Sim2Ls, FAIR workflows and data
 - Develop and publish Sim2Ls
4. Developing Apps
 - Connecting Sim2Ls to Jupyter and Web Apps
5. Tool Publication process
 - Register, deploy, test, and publish
6. Development environment
 - A Unix development environment (Jupyter or Linux desktop)
7. Simulation and data as a service
 - Launching tools and querying the ResultsDB



Step 1: Register your tool in nanoHUB

Go to <https://nanohub.org/tools/create> to register your tool in nanoHUB



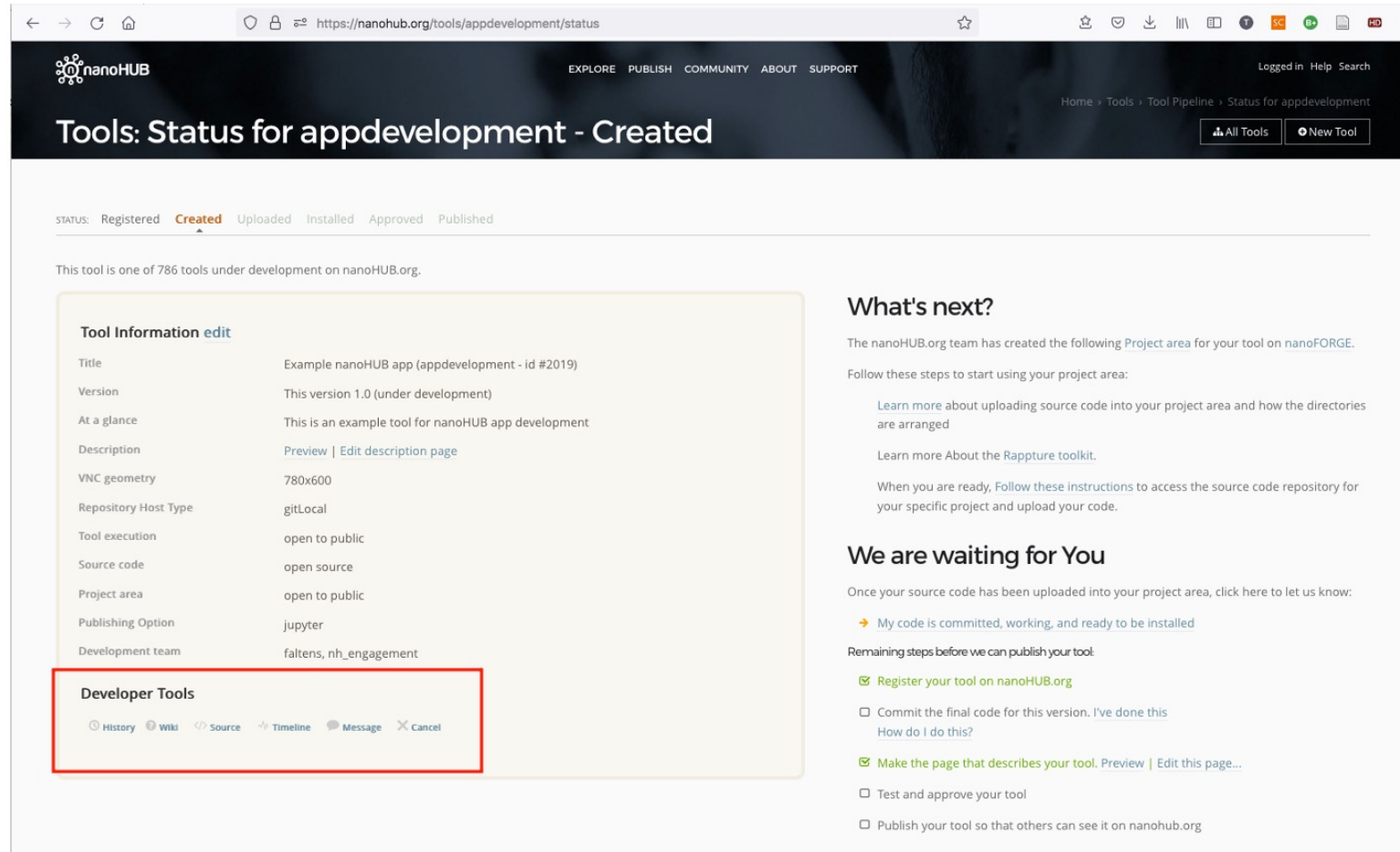
The screenshot shows the nanoHUB website's 'Tools: Create New Tool' page. The header includes the nanoHUB logo and a 'MENU' button. A 'All Tools' button is also visible. The main content area is titled 'ABOUT YOUR TOOL:' and contains several input fields with labels and requirements:

- Tool Name:** REQUIRED. A text input field with a placeholder.
- Short name:** used for the directory containing this tool. Example: qdot.
- Title:** REQUIRED. A text input field with a placeholder.
- Full name:** Full name for this tool. Example: Quantum Dot Lab.
- Version:** A text input field containing '1.0'.
- Optional version number:** Optional version number for this release of the tool. Example: 1.0 or 2.1.5b. Spaces not allowed.
- At a glance:** REQUIRED. A text input field with a placeholder.
- One-line description:** A one-line description of your tool. Example: Simulate 3-D confined states in simple quantum dot geometries.

On the right side, there is a box titled 'What tool name should I choose?' with the following text: 'Tool name should be unique and contain 3-15 alphanumeric characters, no spaces. Once you register your tool, you cannot change its name, so be careful to pick a good one.'

Step 2: Access the nanoHUB Developer Tools

Follow the link that Contribtool emails you to get to your tool's status page, which will be of the form: [https://nanohub.org/tools/*alias*/status](https://nanohub.org/tools/<i>alias</i>/status)



The screenshot shows the nanoHUB website interface for the 'appdevelopment' tool status page. The page title is 'Tools: Status for appdevelopment - Created'. The status is 'Created', and the tool is one of 786 tools under development. The 'Tool Information edit' section contains the following details:

Title	Example nanoHUB app (appdevelopment - id #2019)
Version	This version 1.0 (under development)
At a glance	This is an example tool for nanoHUB app development
Description	Preview Edit description page
VNC geometry	780x600
Repository Host Type	gitLocal
Tool execution	open to public
Source code	open source
Project area	open to public
Publishing Option	jupyter
Development team	faltens, nh_engagement

The 'Developer Tools' section is highlighted with a red box and includes links for History, Wiki, Source, Timeline, Message, and Cancel. The 'What's next?' section provides instructions on how to proceed, including links to learn more about uploading source code and accessing the source code repository. The 'We are waiting for You' section lists the remaining steps before the tool can be published, such as registering the tool on nanoHUB.org, committing the final code, and making the page that describes the tool.

Step 2: Access the nanoHUB Developer Tools

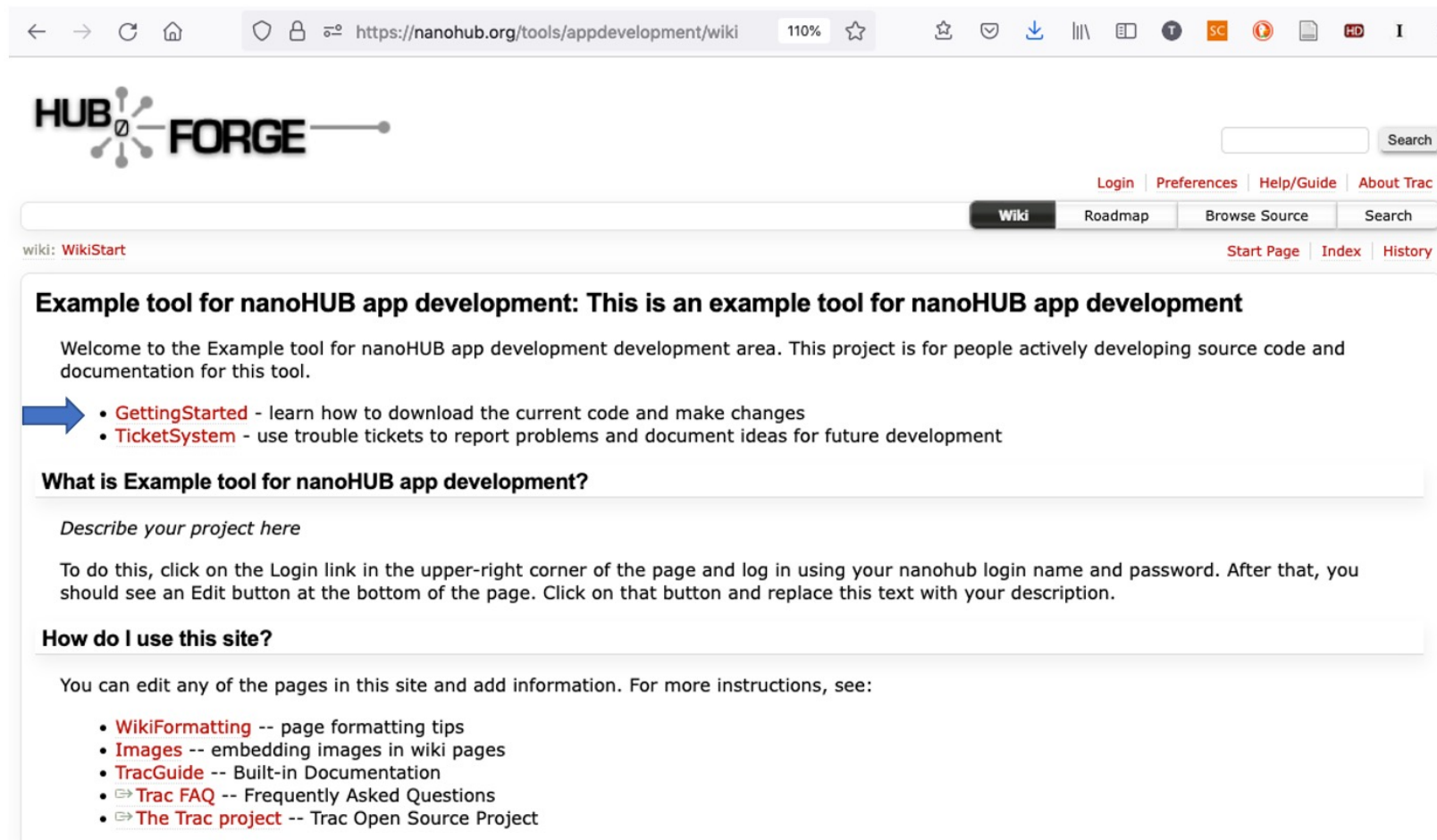
The Developer tools are located at the bottom left of the tool status page.

The screenshot shows the nanoHUB website interface. The main heading is "Tools: Status for appdevelopment - Created". Below this, there are tabs for "STATUS: Registered", "Created" (highlighted), "Uploaded", "Installed", "Approved", and "Published". A green callout box on the left contains the text: "The [wiki](#) link will take you to your tool development area in nanoFORGE." At the bottom of the page, a red box highlights the "Developer Tools" section, which includes links for "History", "Wiki", "Source", "Timeline", "Message", and "Cancel". The "Wiki" link is the one mentioned in the callout.

The [wiki](#) link will take you to your tool development area in nanoFORGE.

Step 3a: Get your code template from nanoFORGE

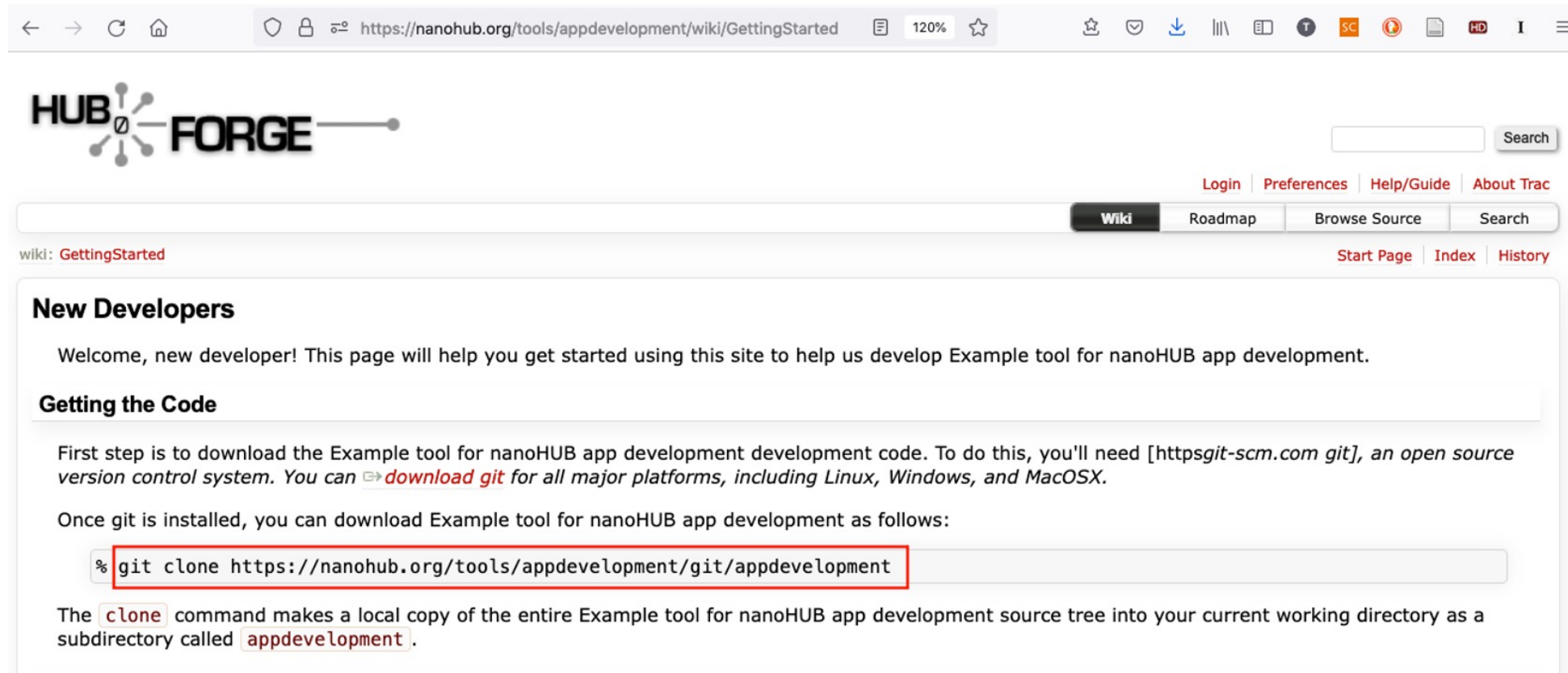
Click on the **GettingStarted** link on your tool development area in nanoFORGE.



The screenshot shows a web browser window displaying the nanoHUB wiki page for 'Example tool for nanoHUB app development'. The page features the nanoHUB logo at the top left, a search bar, and navigation links such as 'Login', 'Preferences', 'Help/Guide', and 'About Trac'. Below the navigation, there are tabs for 'Wiki', 'Roadmap', 'Browse Source', and 'Search'. The main content area includes a heading 'Example tool for nanoHUB app development: This is an example tool for nanoHUB app development', a welcome message, and a list of links: 'GettingStarted' (highlighted with a blue arrow) and 'TicketSystem'. Below this, there are sections for 'What is Example tool for nanoHUB app development?' and 'How do I use this site?'. The 'How do I use this site?' section lists various resources like 'WikiFormatting', 'Images', 'TracGuide', 'Trac FAQ', and 'The Trac project'.

Step 3a: Get your code template from nanoFORGE

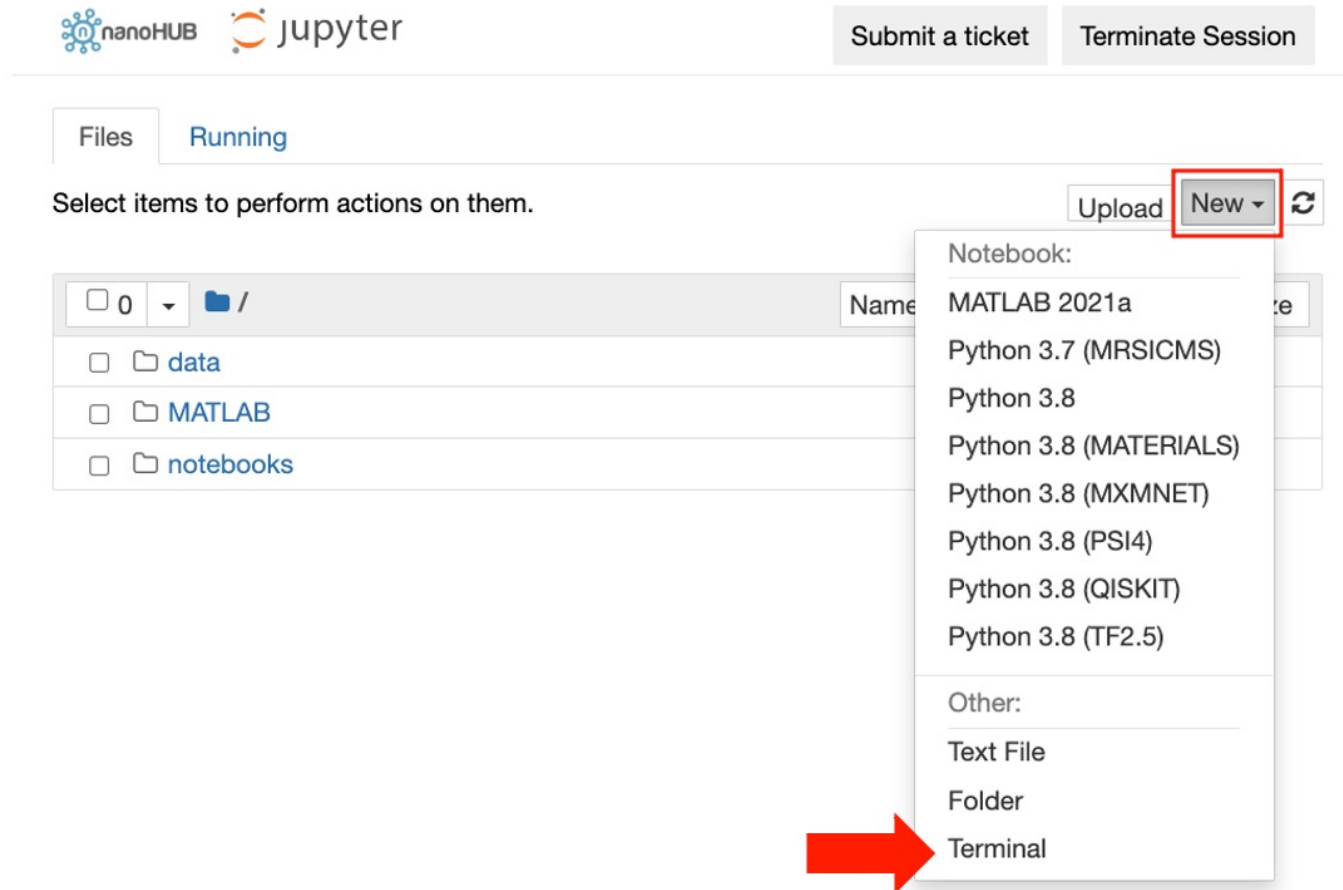
Git is already installed in nanoHUB. Copy the code snippet for cloning your repo into your personal nanoHUB filespace.



The screenshot shows a web browser window displaying the nanoHUB wiki page for 'GettingStarted'. The browser's address bar shows the URL: `https://nanohub.org/tools/appdevelopment/wiki/GettingStarted`. The page features the nanoHUB logo and a search bar. Navigation links include 'Login', 'Preferences', 'Help/Guide', and 'About Trac'. A secondary navigation bar contains 'Wiki', 'Roadmap', 'Browse Source', and 'Search'. The main content area is titled 'wiki: GettingStarted' and includes a 'Start Page', 'Index', and 'History' link. The page content is organized into sections: 'New Developers' with a welcome message, and 'Getting the Code' which provides instructions on downloading the code. A code snippet for cloning the repository is highlighted with a red box: `% git clone https://nanohub.org/tools/appdevelopment/git/appdevelopment`. Below the code, a paragraph explains that the 'clone' command creates a local copy of the source tree in the current directory as a subdirectory named 'appdevelopment'.

Step 3b: Open a nanoHUB Jupyter Terminal

Open a terminal in the latest version of Jupyter notebooks in nanoHUB (<https://nanohub.org/tools/jupyter70> in 2023).



The screenshot displays 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, there are tabs for 'Files' and 'Running'. The 'Files' tab is active, showing a file browser with a list of folders: 'data', 'MATLAB', and 'notebooks'. A red box highlights the 'New' button in the top right corner of the file browser. A dropdown menu is open from this button, listing various options under 'Notebook:' and 'Other:'. The 'Terminal' option is highlighted with a red arrow pointing to it.

nanoHUB jupyter

Submit a ticket Terminate Session

Files Running

Select items to perform actions on them.

Upload New ↕

	Name	
<input type="checkbox"/>	0	/
<input type="checkbox"/>	data	
<input type="checkbox"/>	MATLAB	
<input type="checkbox"/>	notebooks	

Notebook:

- MATLAB 2021a
- Python 3.7 (MRSICMS)
- Python 3.8
- Python 3.8 (MATERIALS)
- Python 3.8 (MXMNET)
- Python 3.8 (PSI4)
- Python 3.8 (QISKIT)
- Python 3.8 (TF2.5)

Other:

- Text File
- Folder
- Terminal

Step 3c: Clone your tool repo

Navigate to the folder you want and paste in and run the code snippet you copied from nanoFORGE to clone your tool repo to your nanoHUB account.





Submit a ticket

Terminate Session

```
nh_engagement@nanohub_2145700_8:~$ cd notebooks
nh_engagement@nanohub_2145700_8:~/notebooks$ git clone https://nanohub.org/tools/appdevelopment
/git/appdevelopment
Cloning into 'appdevelopment'...
remote: Counting objects: 9, done.
remote: Compressing objects: 100% (5/5), done.
remote: Total 9 (delta 0), reused 0 (delta 0)
Unpacking objects: 100% (9/9), done.
nh_engagement@nanohub_2145700_8:~/notebooks$
```

Step 3d: Add your code to nanoHUB and test

Add your code to the code template in your nanoHUB filespace, and test it there.

  jupyter Submit a ticket Terminate Session

Files Running

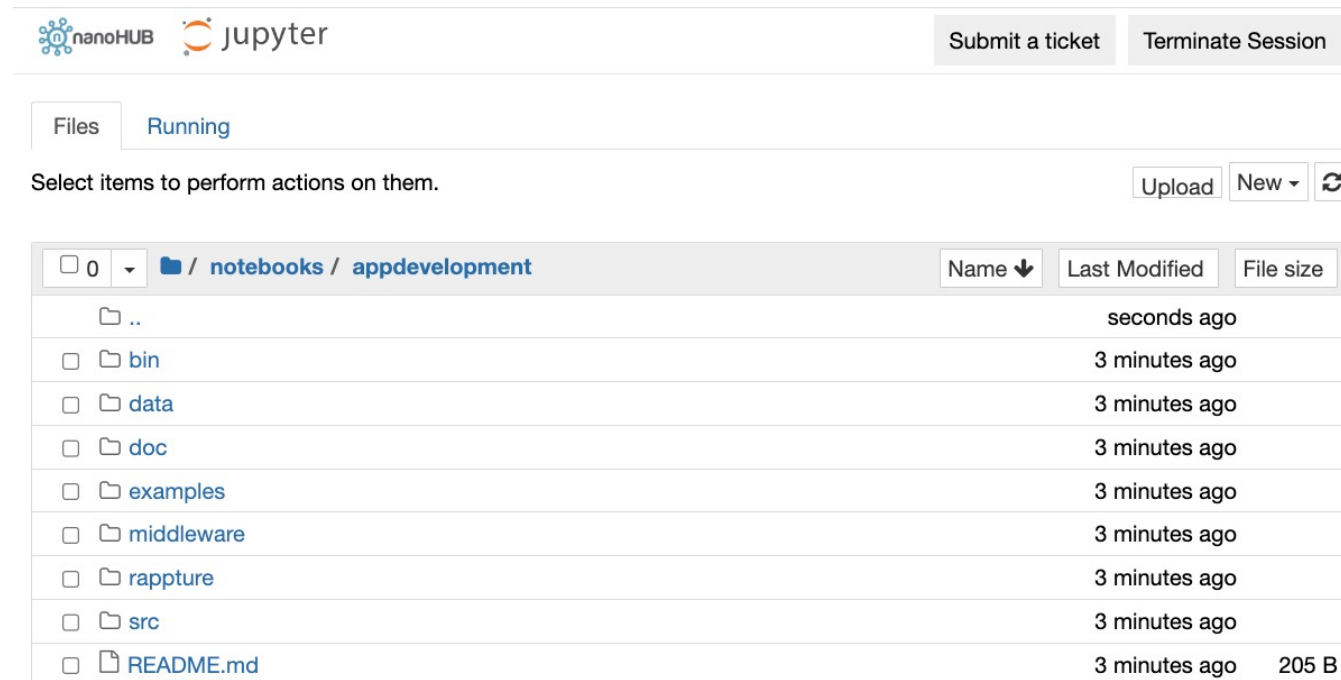
Select items to perform actions on them.

Upload New ▾ ↻

<input type="checkbox"/> 0 ▾	/ notebooks / appdevelopment	Name ↓	Last Modified	File size
<input type="checkbox"/>	..		seconds ago	
<input type="checkbox"/>	bin		3 minutes ago	
<input type="checkbox"/>	data		3 minutes ago	
<input type="checkbox"/>	doc		3 minutes ago	
<input type="checkbox"/>	examples		3 minutes ago	
<input type="checkbox"/>	middleware		3 minutes ago	
<input type="checkbox"/>	rappture		3 minutes ago	
<input type="checkbox"/>	src		3 minutes ago	
<input type="checkbox"/>	README.md		3 minutes ago	205 B

Notes about the nanoHUB tool file structure

- Keep the folder structure that nanoHUB expects for tools
- Jupyter Notebooks can go in bin or stay in the top-level directory. Note that the first notebook can only access files within the same folder or below.
- The middleware folder contains the invoke script
- Use the Messages Developer Tool to get help in creating the correct invoke script



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, there are tabs for "Files" and "Running". A message says "Select items to perform actions on them." with buttons for "Upload", "New", and a refresh icon. The main area displays a file browser for the path "/ notebooks / appdevelopment". The file browser has columns for "Name", "Last Modified", and "File size". The files listed are:

	Name	Last Modified	File size
<input type="checkbox"/>	..	seconds ago	
<input type="checkbox"/>	bin	3 minutes ago	
<input type="checkbox"/>	data	3 minutes ago	
<input type="checkbox"/>	doc	3 minutes ago	
<input type="checkbox"/>	examples	3 minutes ago	
<input type="checkbox"/>	middleware	3 minutes ago	
<input type="checkbox"/>	rappture	3 minutes ago	
<input type="checkbox"/>	src	3 minutes ago	
<input type="checkbox"/>	README.md	3 minutes ago	205 B

Request help in setting up your invoke script.

The Messages Developer tool is located at the bottom left of the tool status page.

Use **messages** to get help with building your tool.

The screenshot shows the nanoHUB interface for a tool status page. The browser address bar displays <https://nanohub.org/tools/appdevelopment/status>. The page title is "Tools: Status for appdevelopment - Created". The status is "Created". The tool details include: "Example nanoHUB app (appdevelopment - id #2019)", "This version 1.0 (under development)", "This is an example tool for nanoHUB app development", "Preview | Edit description page", "780x600", "gitLocal", "open to public", "Source code: open source", "Project area: open to public", "Publishing Option: jupyter", "Development team: faltens, nh_engagement". A red box highlights the "Developer Tools" section at the bottom left, which contains a "Message" button. The "What's next?" section provides instructions for starting the project area. The "We are waiting for You" section lists remaining steps for publishing the tool.

Step 4: Install your code in nanoHUB

Use git commands to add, commit and push your code to nanoFORGE. Click the link on the Tool Status page to install your code in nanoHUB.

The screenshot shows the nanoHUB interface for a tool in the 'Created' status. The page title is 'Tools: Status for appdevelopment - Created'. The status bar shows 'Registered', 'Created' (highlighted), 'Uploaded', 'Installed', 'Approved', and 'Published'. The tool information includes:

Tool Information edit	
Title	Example nanoHUB app (appdevelopment - id #2019)
Version	This version 1.0 (under development)
At a glance	This is an example tool for nanoHUB app development
Description	Preview Edit description page
VNC geometry	780x600
Repository Host Type	gitLocal
Tool execution	open to public
Source code	open source
Project area	open to public
Publishing Option	jupyter
Development team	faltens, nh_engagement

Below the tool information is a 'Developer Tools' section with links for History, Wiki, Source, Timeline, Message, and Cancel.

The 'What's next?' section provides instructions on how to proceed. A red arrow points to the step: 'My code is committed, working, and ready to be installed'.

What's next?
The nanoHUB.org team has created the following Project area for your tool on nanoFORGE. Follow these steps to start using your project area:

- Learn more about uploading source code into your project area and how the directories are arranged
- Learn more About the Rapture toolkit.
- When you are ready, Follow these instructions to access the source code repository for your specific project and upload your code.

We are waiting for You
Once your source code has been uploaded into your project area, click here to let us know:

- My code is committed, working, and ready to be installed

Remaining steps before we can publish your tool:

- Register your tool on nanoHUB.org
- Commit the final code for this version. I've done this
How do I do this?
- Make the page that describes your tool. Preview | Edit this page...
- Test and approve your tool
- Publish your tool so that others can see it on nanohub.org

Step 5: Update your tool info

Click the link to edit the Description Page to update your tool information.

The screenshot shows the nanoHUB interface for a tool named 'gitlocaltool'. The page title is 'Tools: update for gitlocaltool - Uploaded'. A green notification bar at the top states 'Tool status successfully changed'. Below this, a status filter shows 'Uploaded' as the active status. The main content area is divided into two sections: 'Tool Information edit' and 'What's next?'. The 'Tool Information edit' section contains a table with the following details:

Title	My nanoHUB app using git with nanoFORGE (gitlocaltool - id #1810)
Version	This version 1.0 [all versions]
At a glance	nanoHUB demonstration app using git with nanoFORGE
Description	Preview Edit description page
VNC geometry	780x600
Repository Host Type	gitLocal
Tool execution	open to public
Source code	open source [change license]
Project area	open to public
Publishing Option	jupyter
Development team	faltens, nh_engagement

Below the table, there is a 'Developer Tools' section with links for History, Wiki, Source, Timeline, and Message. The 'What's next?' section provides instructions on the next steps for publishing the tool, including a list of tasks with checkboxes. A red arrow points to the 'Edit description page' link in the 'Tool Information' section.

What's next?

The nanoHUB.org team needs to deploy your latest code on nanoHUB.org so you can test it out. It's been 1 second since the last change to your tool status. You should normally receive response within 3 days.

Remaining steps before we can publish your tool

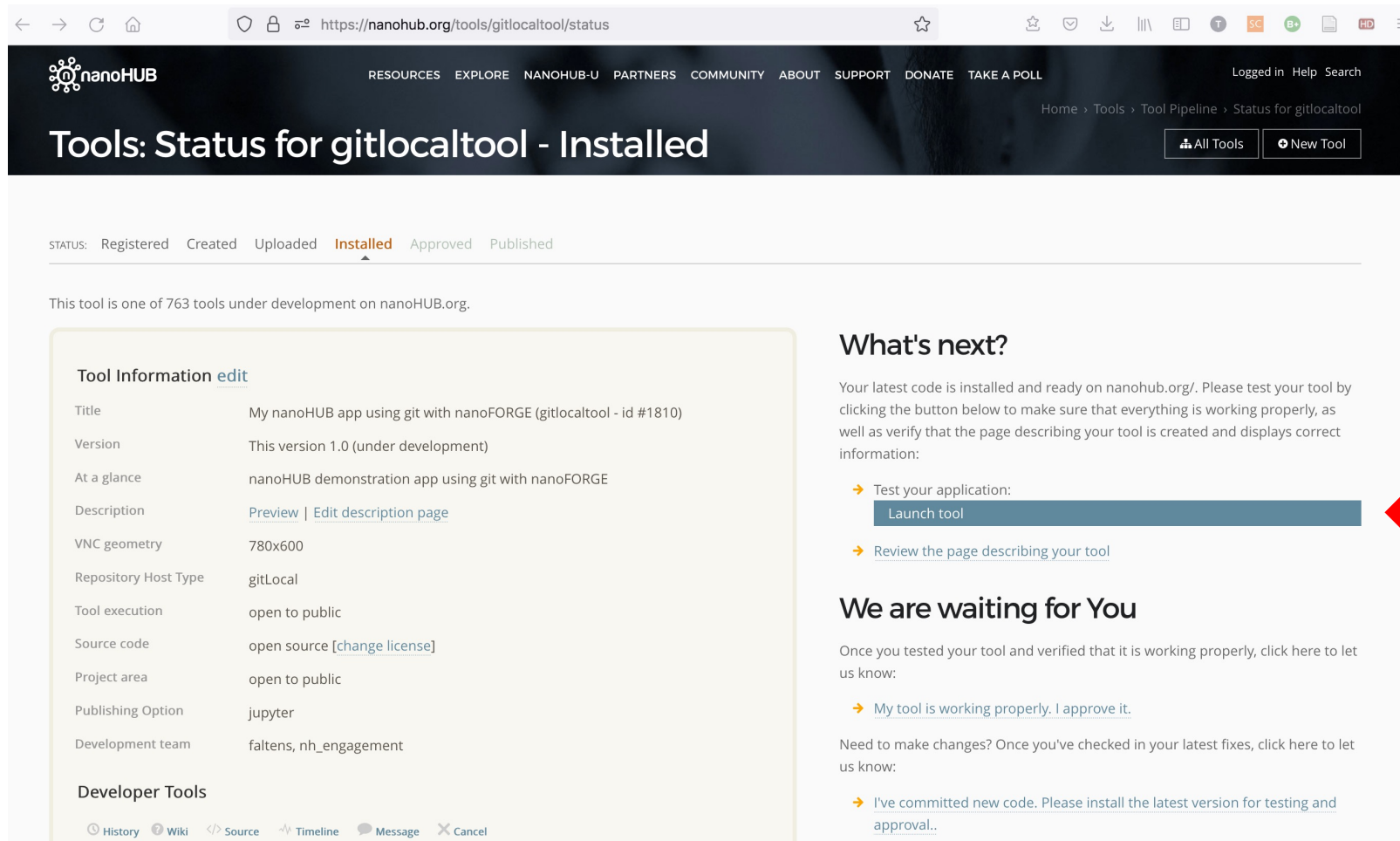
- Register your tool on nanoHUB.org
- Upload your source code into your project area on nanoFORGE
- Make the page that describes your tool. [Preview](#) | [Edit this page...](#)
- Test and approve your tool
- Publish your tool so that others can see it on nanohub.org

Step 5: Update your tool info

There are multiple pages and fields to fill in. You don't have to use all of the fields.

Step 6: Test your code in nanoHUB

Once you receive a message that your code has been installed, click the Launch Tool button to test it in nanoHUB apps.



The screenshot shows the nanoHUB website interface. At the top, the nanoHUB logo is on the left, and navigation links (RESOURCES, EXPLORE, etc.) and user status (Logged in) are on the right. The main heading is "Tools: Status for gitlocaltool - Installed". Below this, there are tabs for tool status: Registered, Created, Uploaded, Installed (highlighted), Approved, and Published. A message states: "This tool is one of 763 tools under development on nanoHUB.org." On the left, a "Tool Information" table lists details like Title, Version, Description, and Repository Host Type. On the right, a "What's next?" section contains a "Launch tool" button, which is highlighted by a red arrow. Below that, there are links for "Review the page describing your tool" and "We are waiting for You" with instructions on how to proceed.

Tool Information edit	
Title	My nanoHUB app using git with nanoFORGE (gitlocaltool - id #1810)
Version	This version 1.0 (under development)
At a glance	nanoHUB demonstration app using git with nanoFORGE
Description	Preview Edit description page
VNC geometry	780x600
Repository Host Type	gitLocal
Tool execution	open to public
Source code	open source [change license]
Project area	open to public
Publishing Option	jupyter
Development team	faltens, nh_engagement

What's next?

Your latest code is installed and ready on nanohub.org/. Please test your tool by clicking the button below to make sure that everything is working properly, as well as verify that the page describing your tool is created and displays correct information:

- Test your application:
[Launch tool](#)
- [Review the page describing your tool](#)

We are waiting for You

Once you tested your tool and verified that it is working properly, click here to let us know:

- [My tool is working properly. I approve it.](#)

Need to make changes? Once you've checked in your latest fixes, click here to let us know:

- [I've committed new code. Please install the latest version for testing and approval..](#)

Step 7: Approve your code for publication

If your code runs properly, click the link to approve your code for publication.

We are waiting for You

Once you tested your tool and verified that it is working properly, click here to let us know:

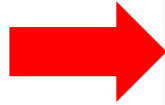
→ [My tool is working properly. I approve it.](#)

Need to make changes? Once you've checked in your latest fixes, click here to let us know:

→ [I've committed new code. Please install the latest version for testing and approval..](#)

Remaining steps before we can publish your tool:

- [Register your tool on nanoHUB.org](#)
- [Upload your source code into your project area on nanoFORGE](#)
- [Make the page that describes your tool.](#) [Preview](#) | [Edit this page...](#)
- [Test and approve your tool.](#) [I approve it](#) | [I've made changes](#)
- [Publish your tool so that others can see it on nanohub.org/](#)



Step 8: Your tool is ready to run in nanoHUB!

Your tool be be available at: <https://nanohub.org/tools/yourtoolname>

Machine Learning for Materials Science: Part 1

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Launch Tool

Version 1.4 - published on 19 Mar 2021
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2561 users, detailed usage
0 Citation(s)
1 question (Ask a question)
3 review(s) (Review this)
0 wish(es) (New Wish)
Share: [Facebook] [Twitter] [LinkedIn] [Email]

Materials Science

Category: Tools
Published on: 19 Mar 2021

Abstract
Data science and machine learning are playing increasingly important roles in science and engineering, and materials science and engineering is no exception. This online tool provides machine learning examples in the field of materials science using Jupyter notebooks, which contain step by step explanations of the activities along with live code that can be modified by users for hands-on learning.

The initial set of tutorials focus on:

- i) data query, organization and visualization
- ii) developing a simple model using linear regression to explore correlations between materials properties
- iii) neural network models trained to predict materials properties from basic element properties

Suggested exercises are included in each Jupyter notebook.

This tool was used in the Hands-on Machine Learning and Data Science Training Workshop conducted by nanoHUB in April 2020. Offerings for the tutorial can be found in nanoHUB resources [here](#) and [here](#).

Check out your usage numbers and measure your impact

