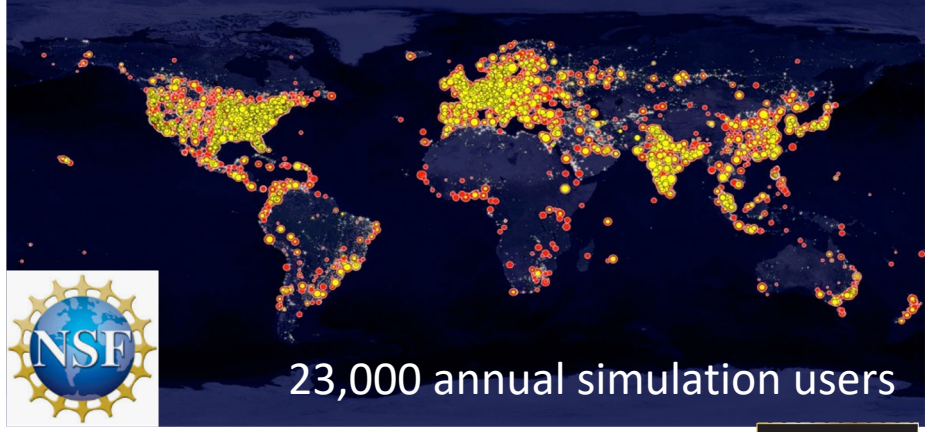

nanoHUB:
getting started guide to tool developers

Develop and publish tools in nanoHUB
Make your research reproducible and your workflows and data FAIR

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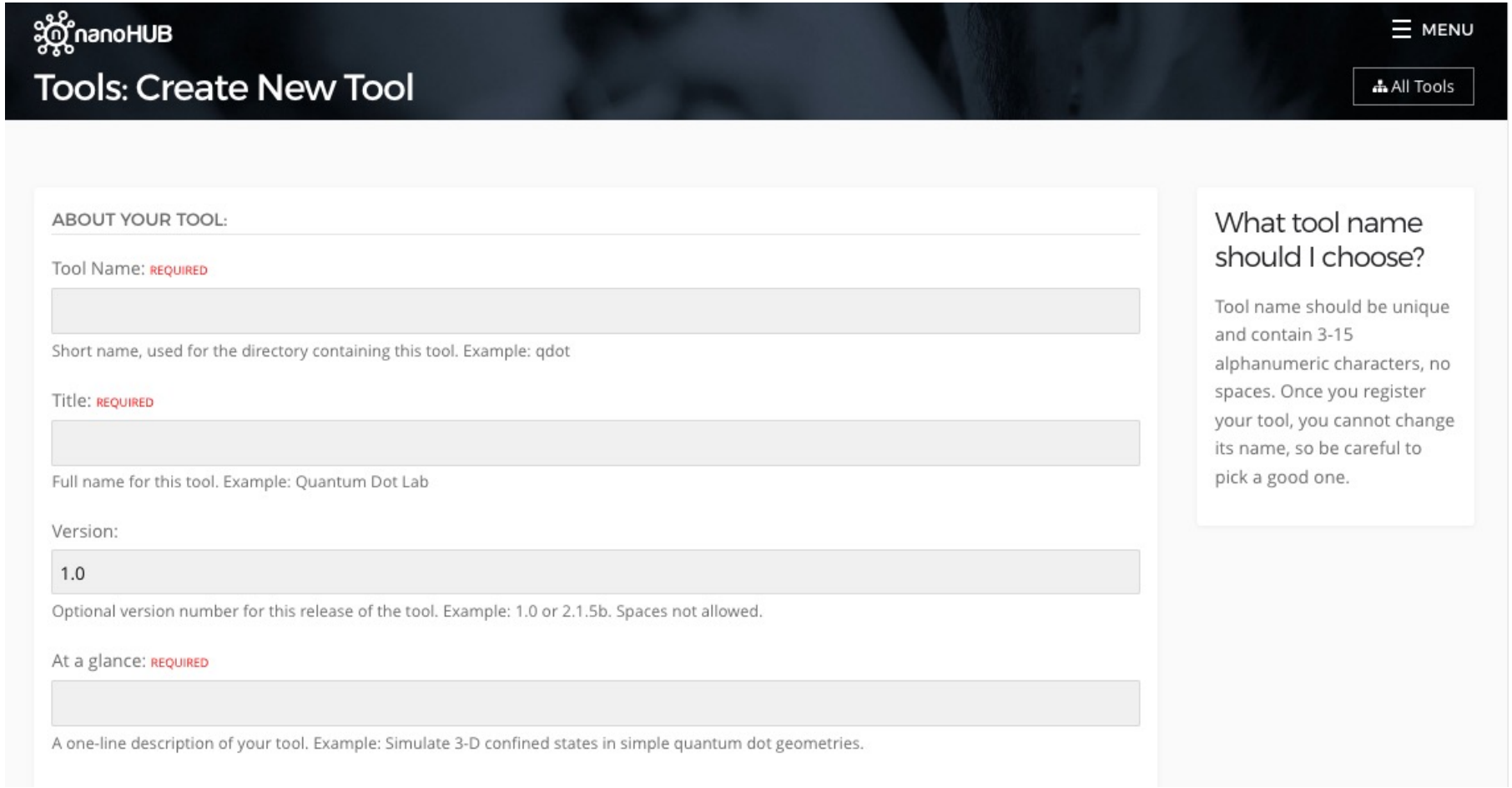
Overview

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

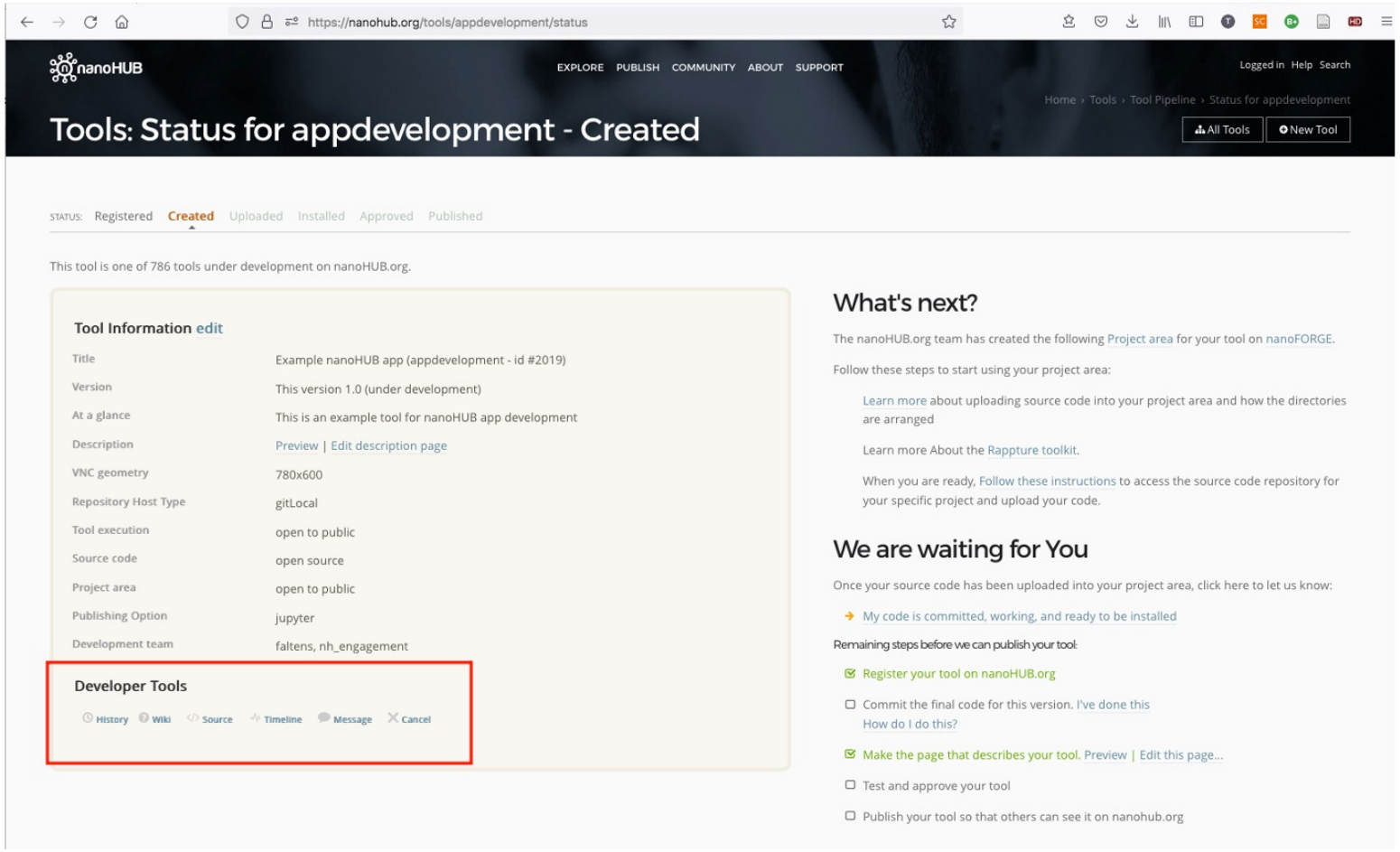
Step 1: Register your tool in nanoHUB

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



Step 2: Access the nanoHUB Developer Tools

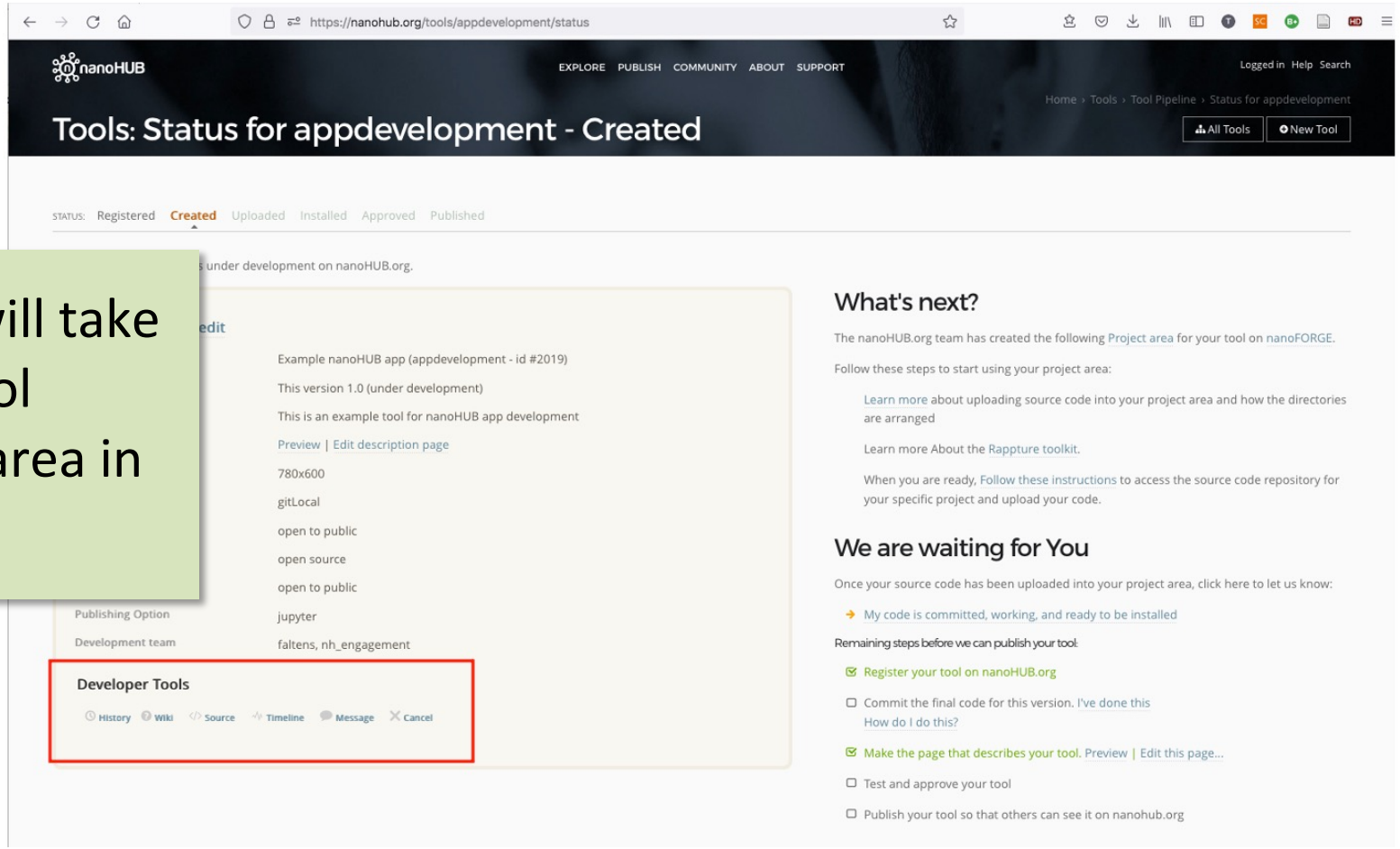
Follow the link that Contribtool emails you to get to your tool's status page, which will be of the form: https://nanohub.org/tools/*alias*/status



Step 2: Access the nanoHUB Developer Tools

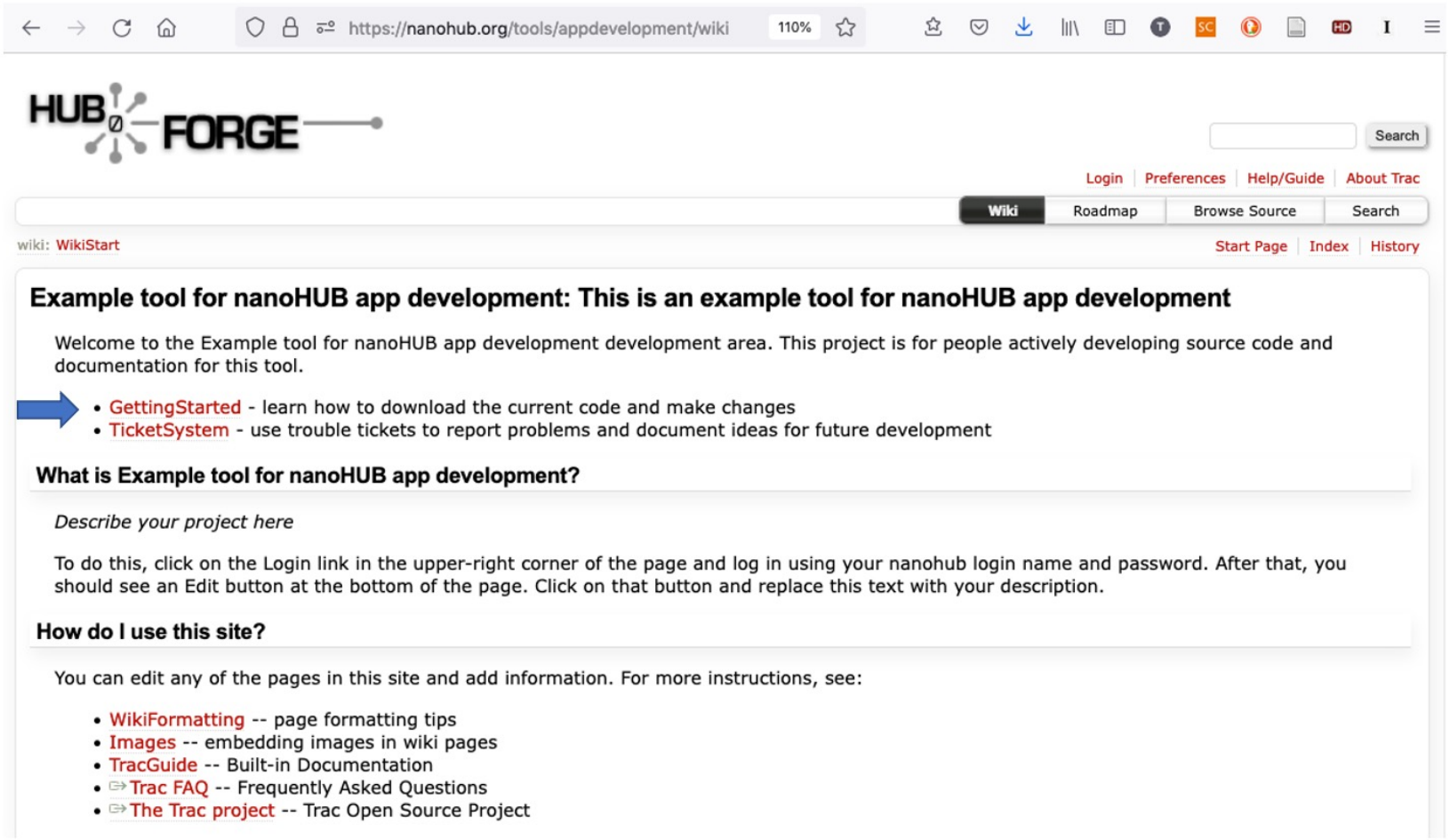
The Developer tools are located at the bottom left of the tool status page.

The **wiki** link will take you to your tool development area in nanoFORGE.



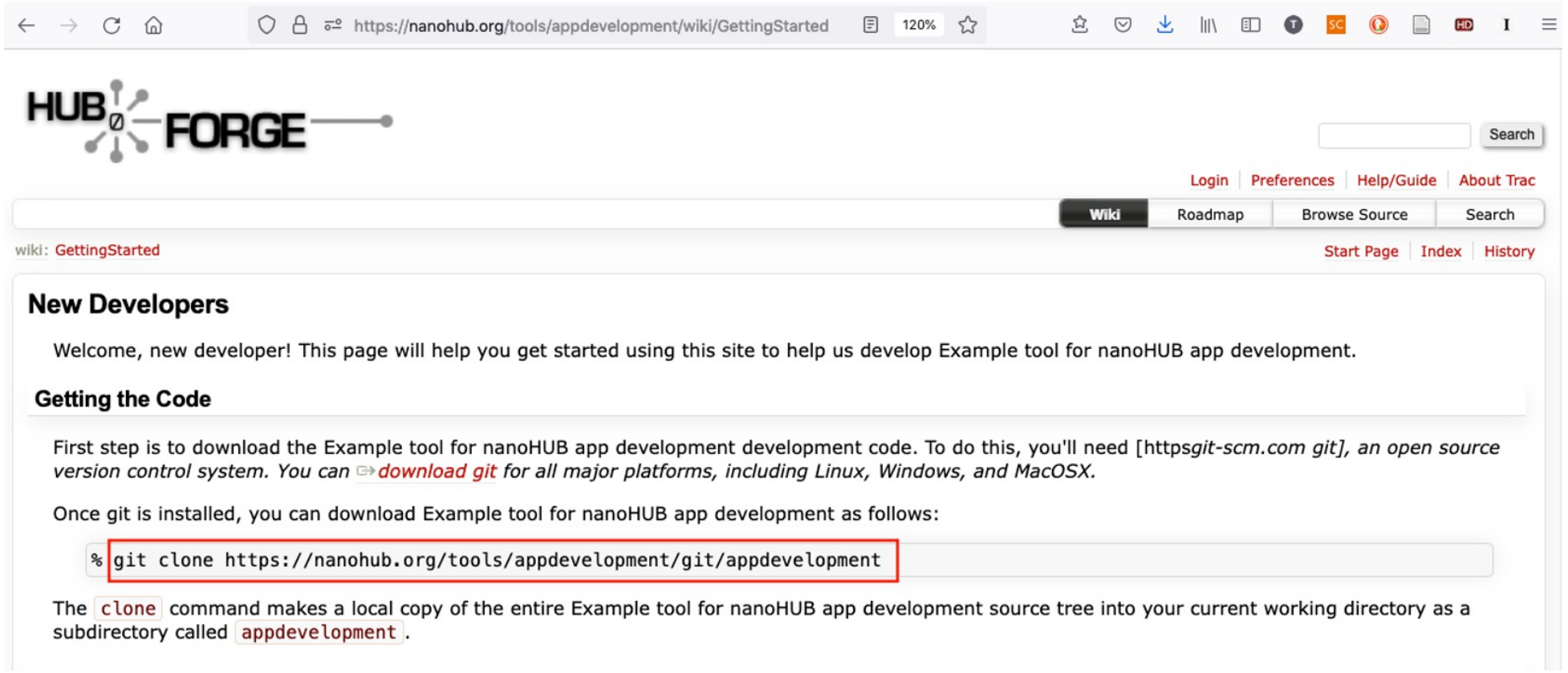
Step 3a: Get your code template from nanoFORGE

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



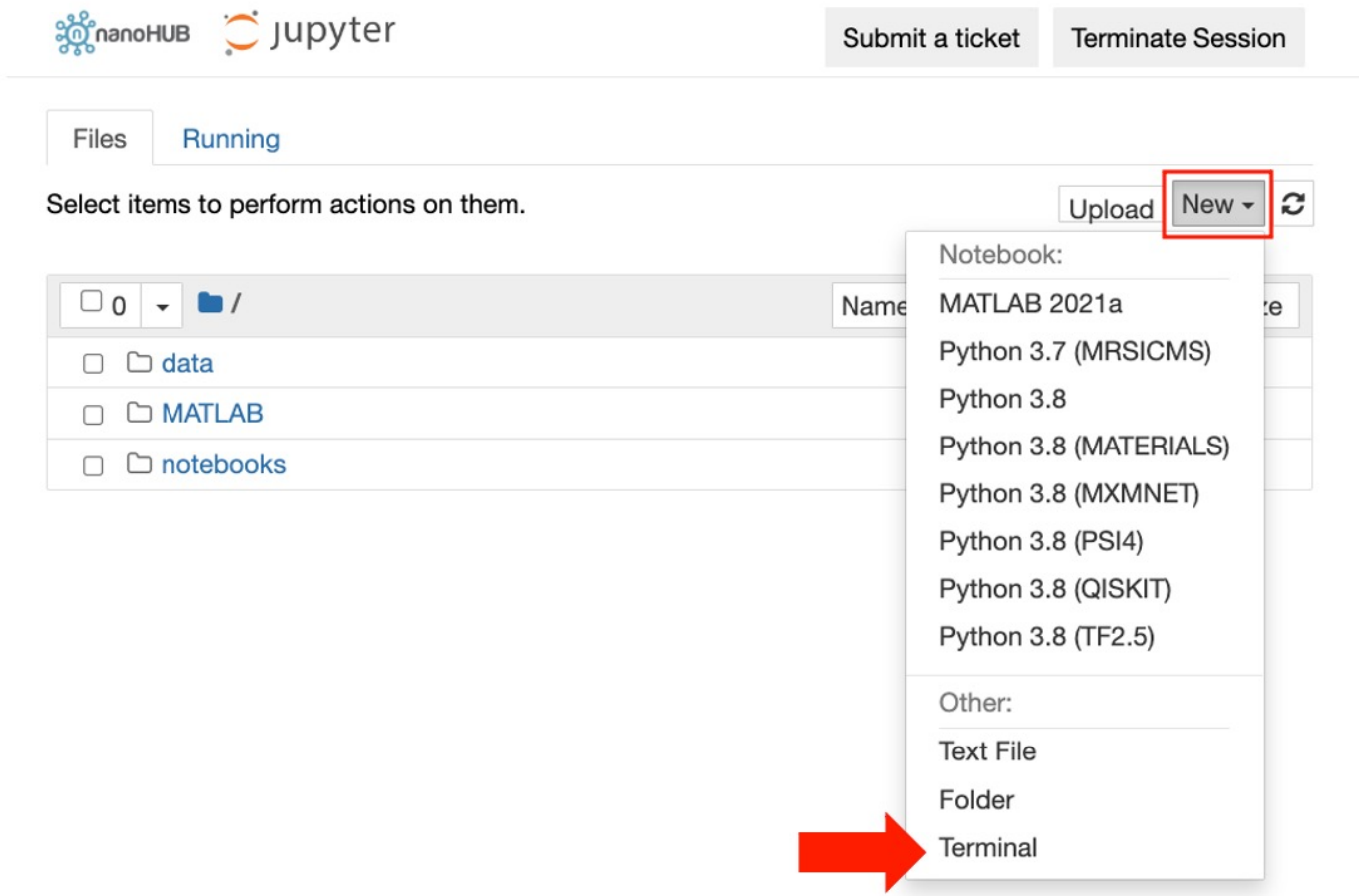
Step 3a: Get your code template from nanoFORGE

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



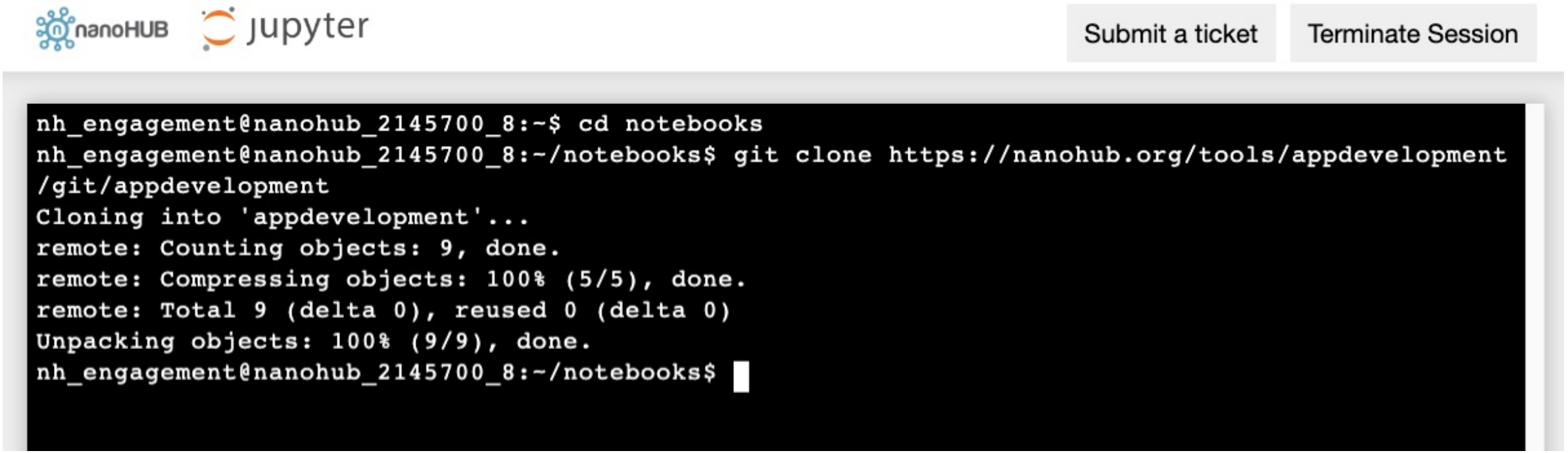
Step 3b: Open a nanoHUB Jupyter Terminal

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



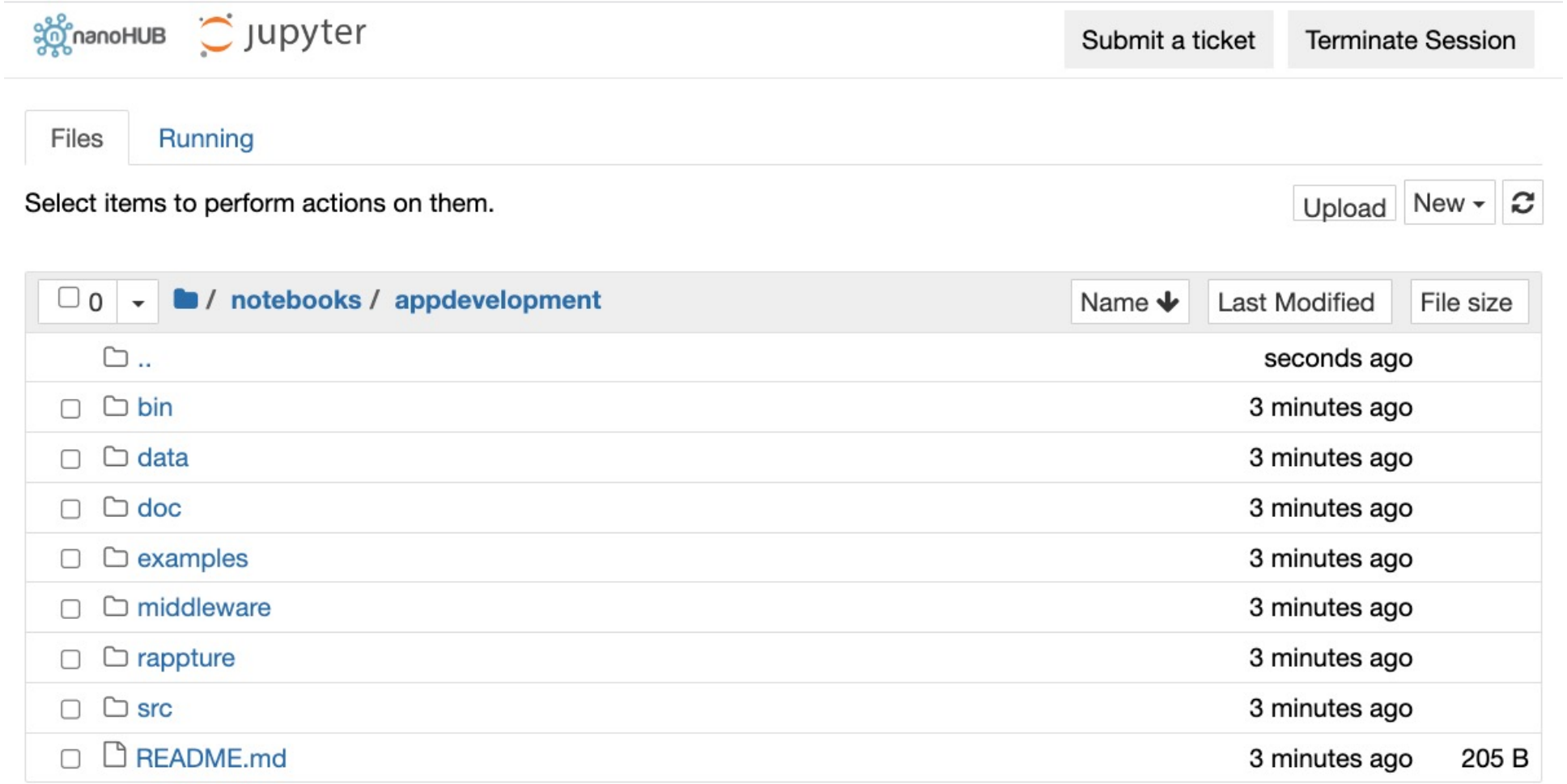
Step 3c: Clone your tool repo

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.



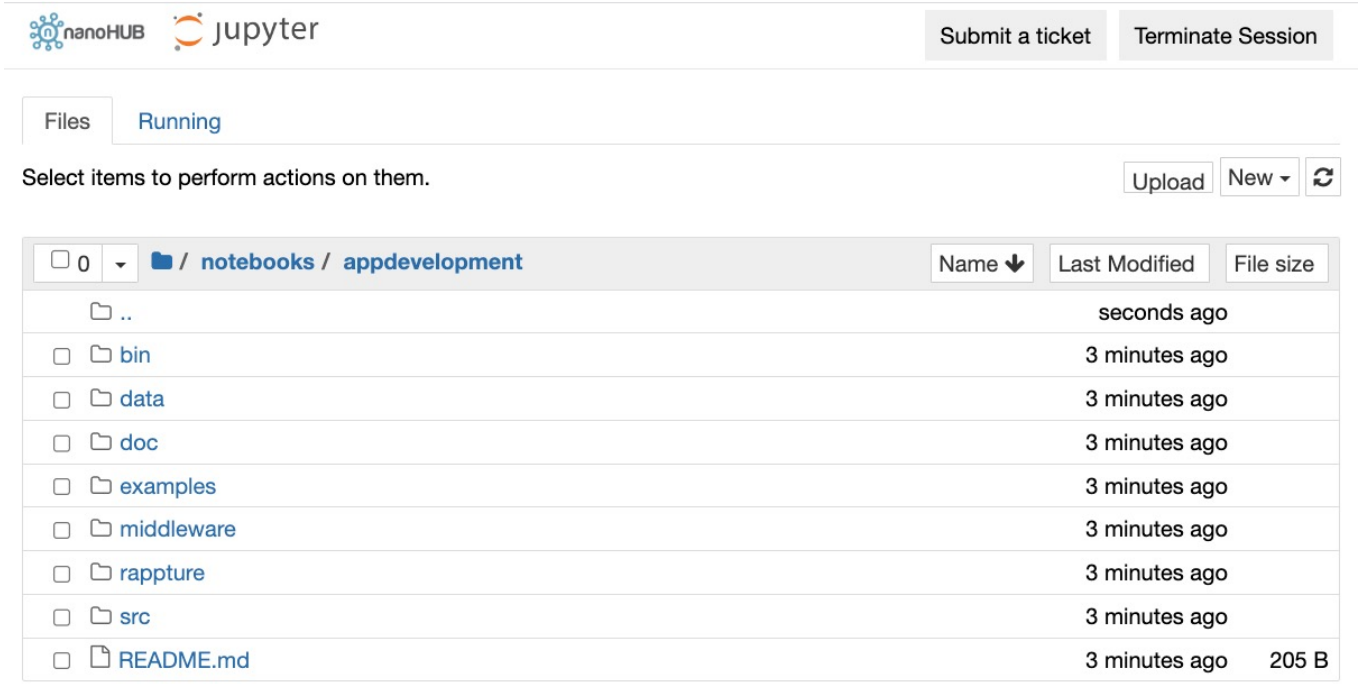
Step 3d: Add your code to nanoHUB and test

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



Notes about the nanoHUB tool file structure

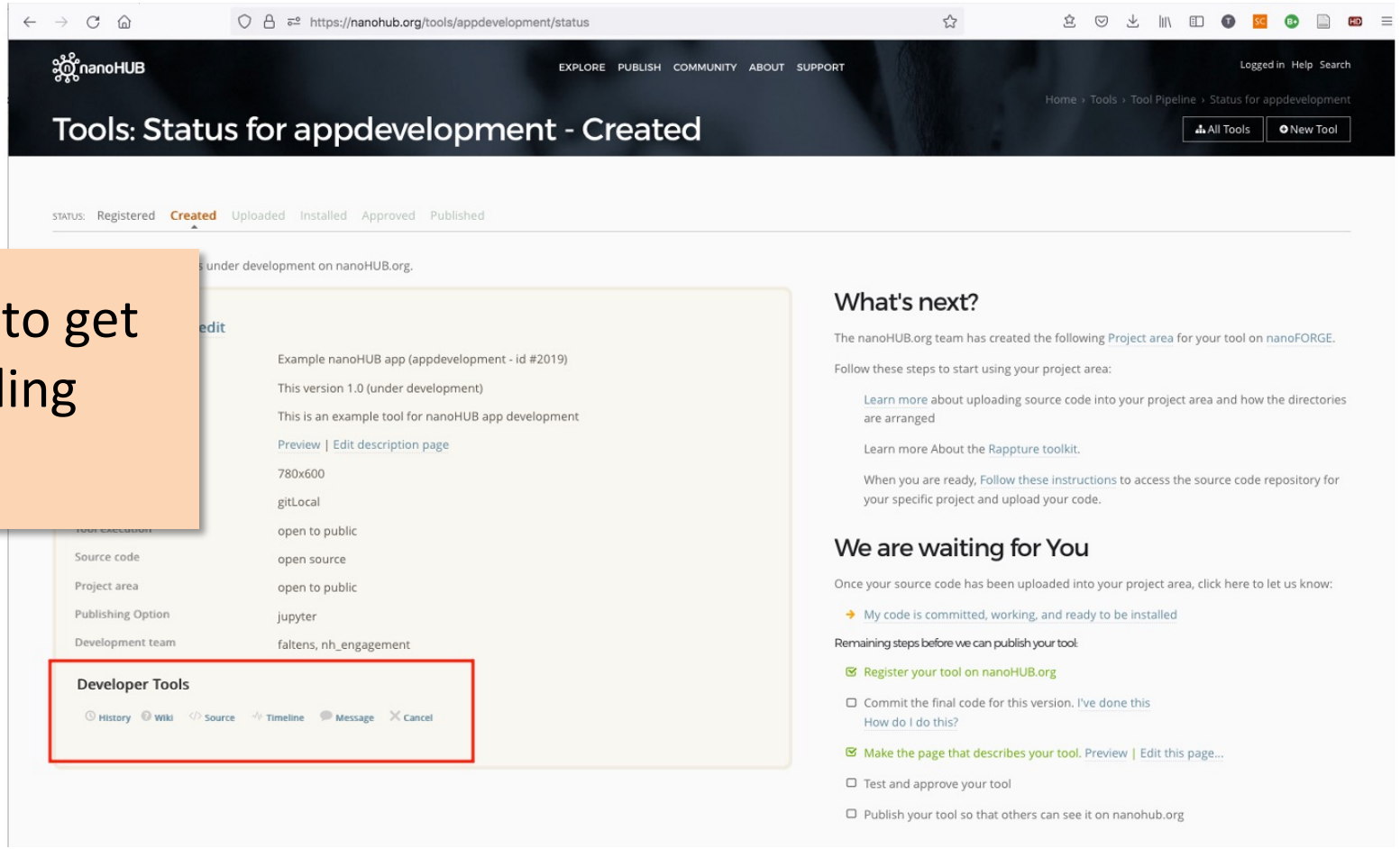
- Keep the folder structure that nanoHUB expects for tools
- Jupyter Notebooks can go in bin or stay in the top-level directory. Note that the first notebook can only access files within the same folder or below.
- The middleware folder contains the invoke script
- Use the Messages Developer Tool to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



Request help in setting up your invoke script.

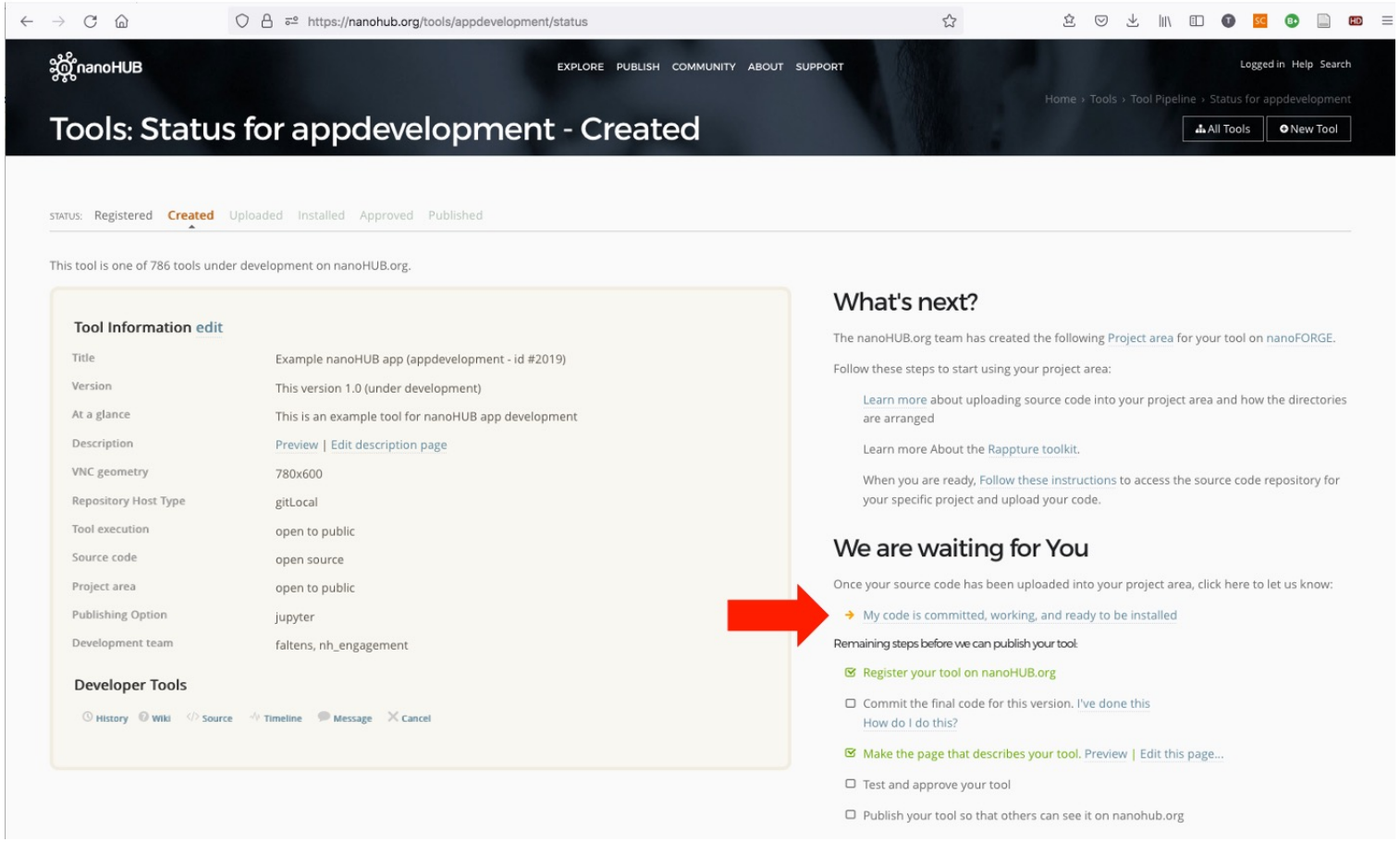
The Messages Developer tool is located at the bottom left of the tool status page.

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



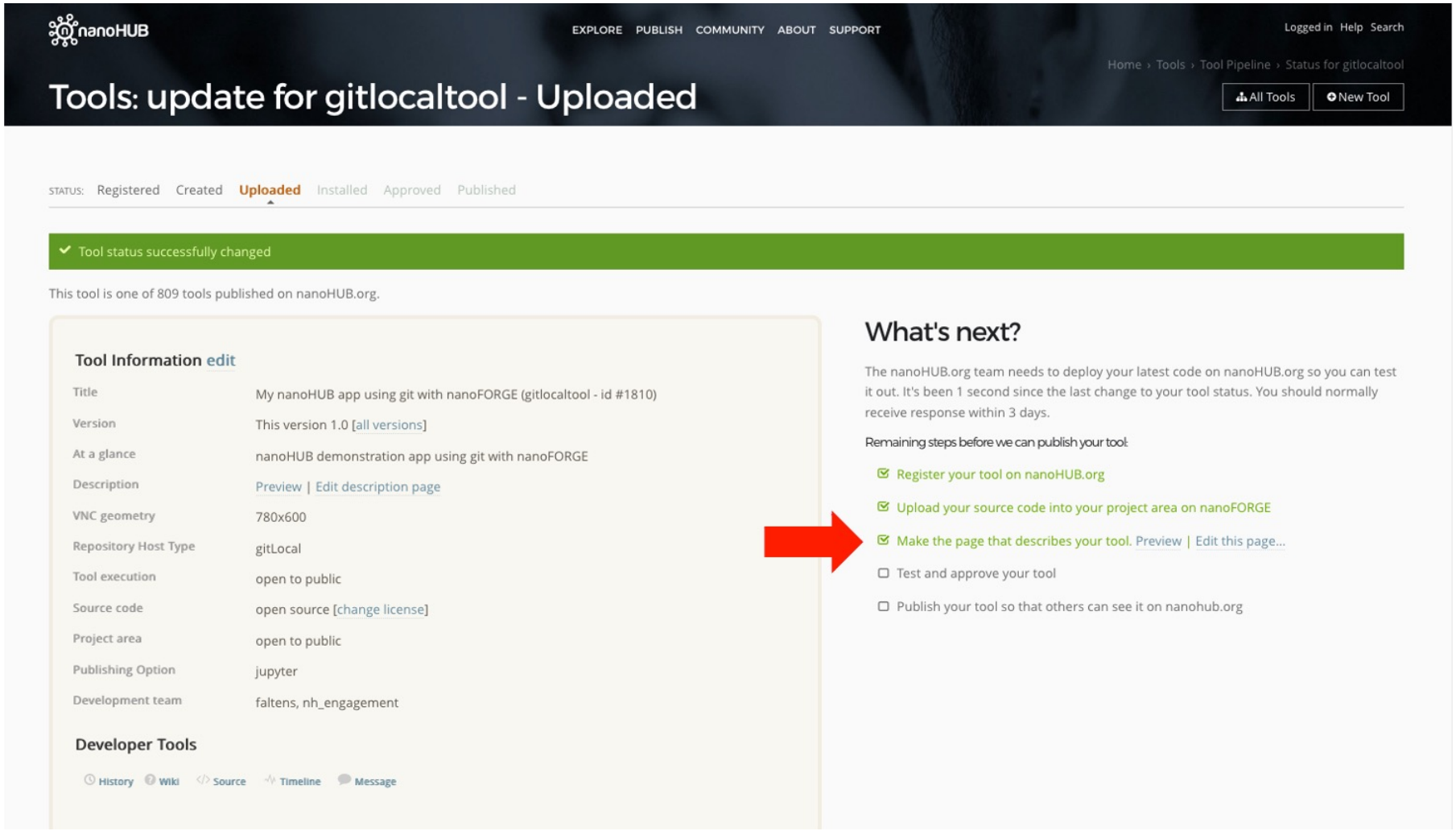
Step 4: Install your code in nanoHUB

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.



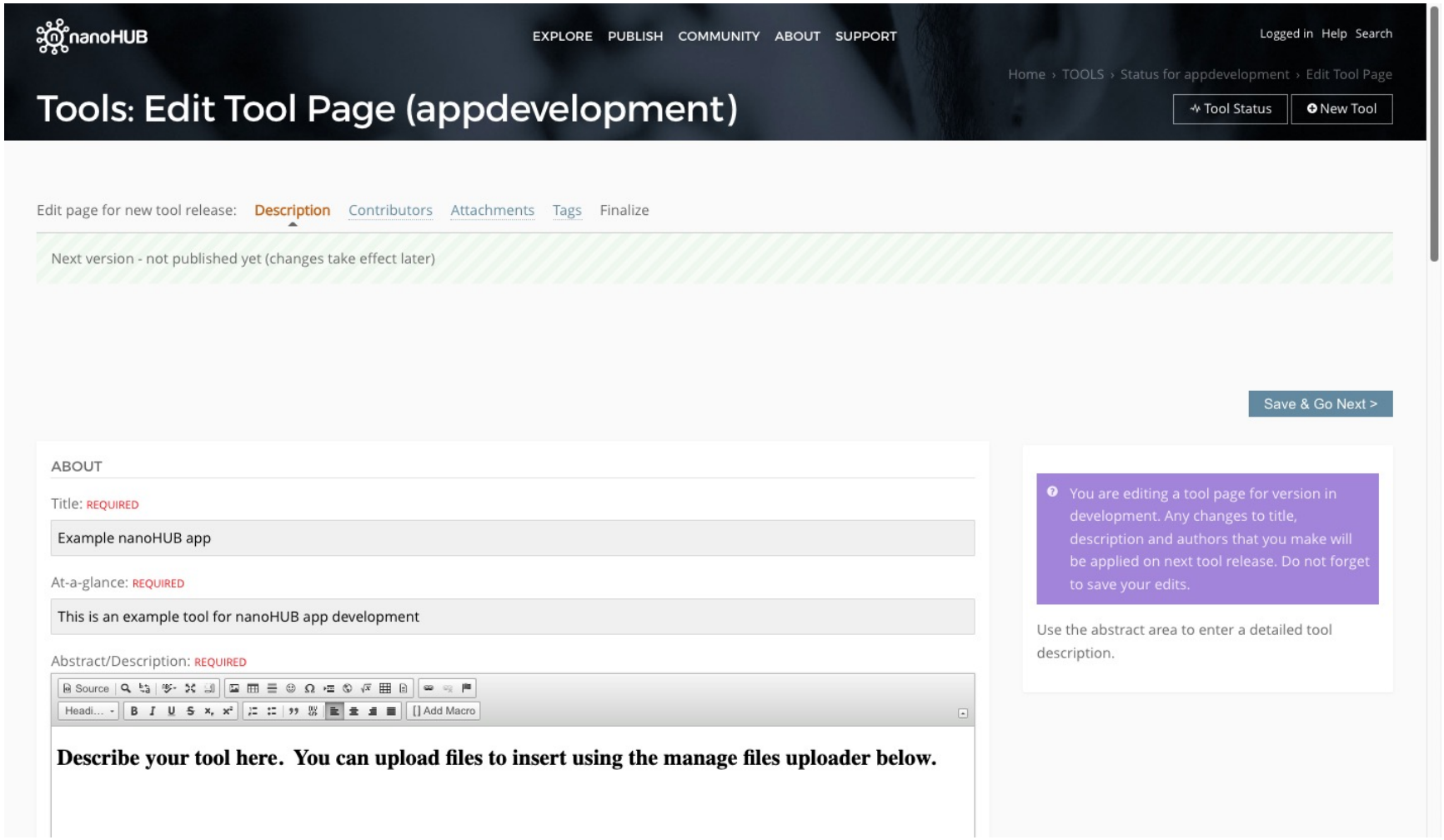
Step 5: Update your tool info

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



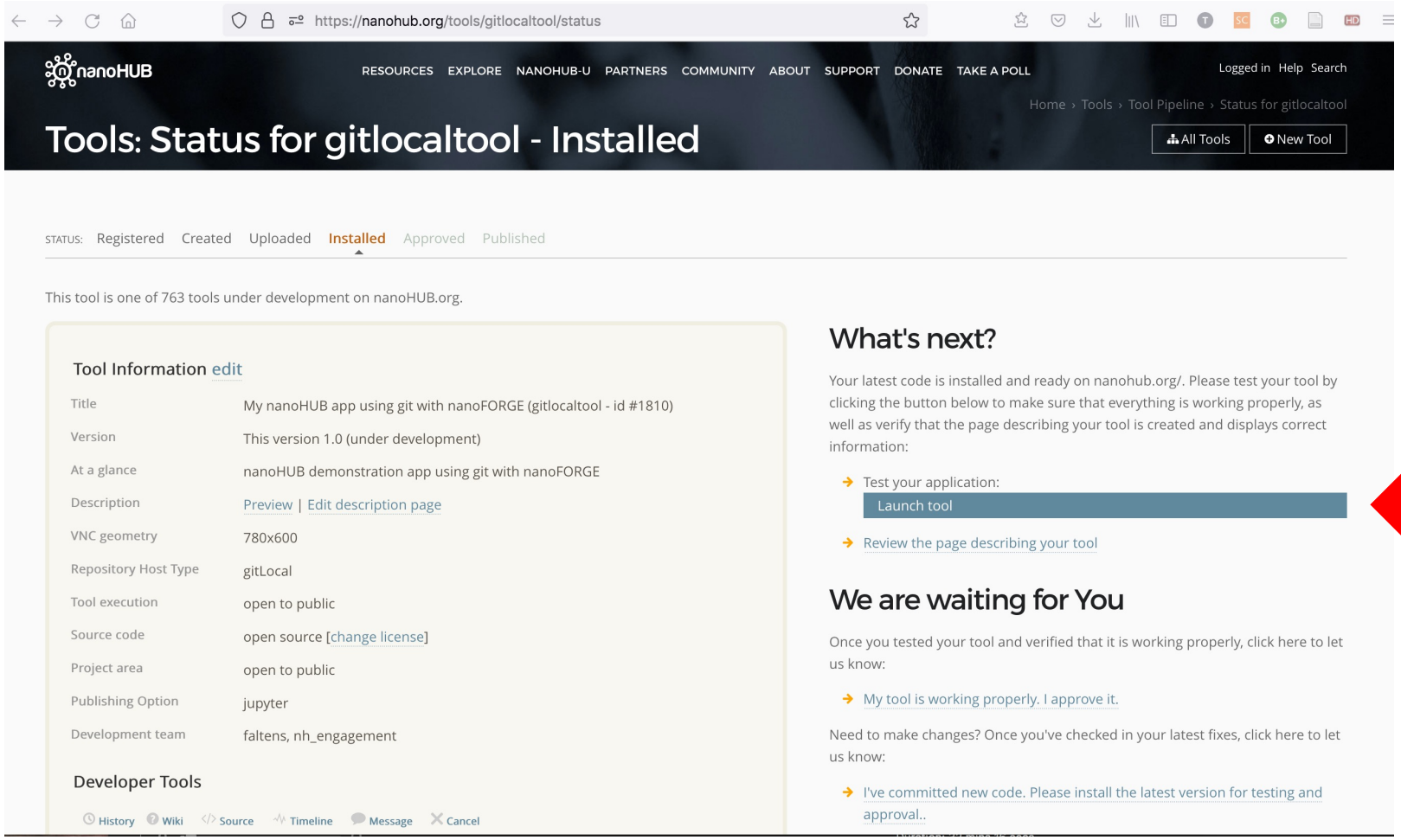
Step 5: Update your tool info

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



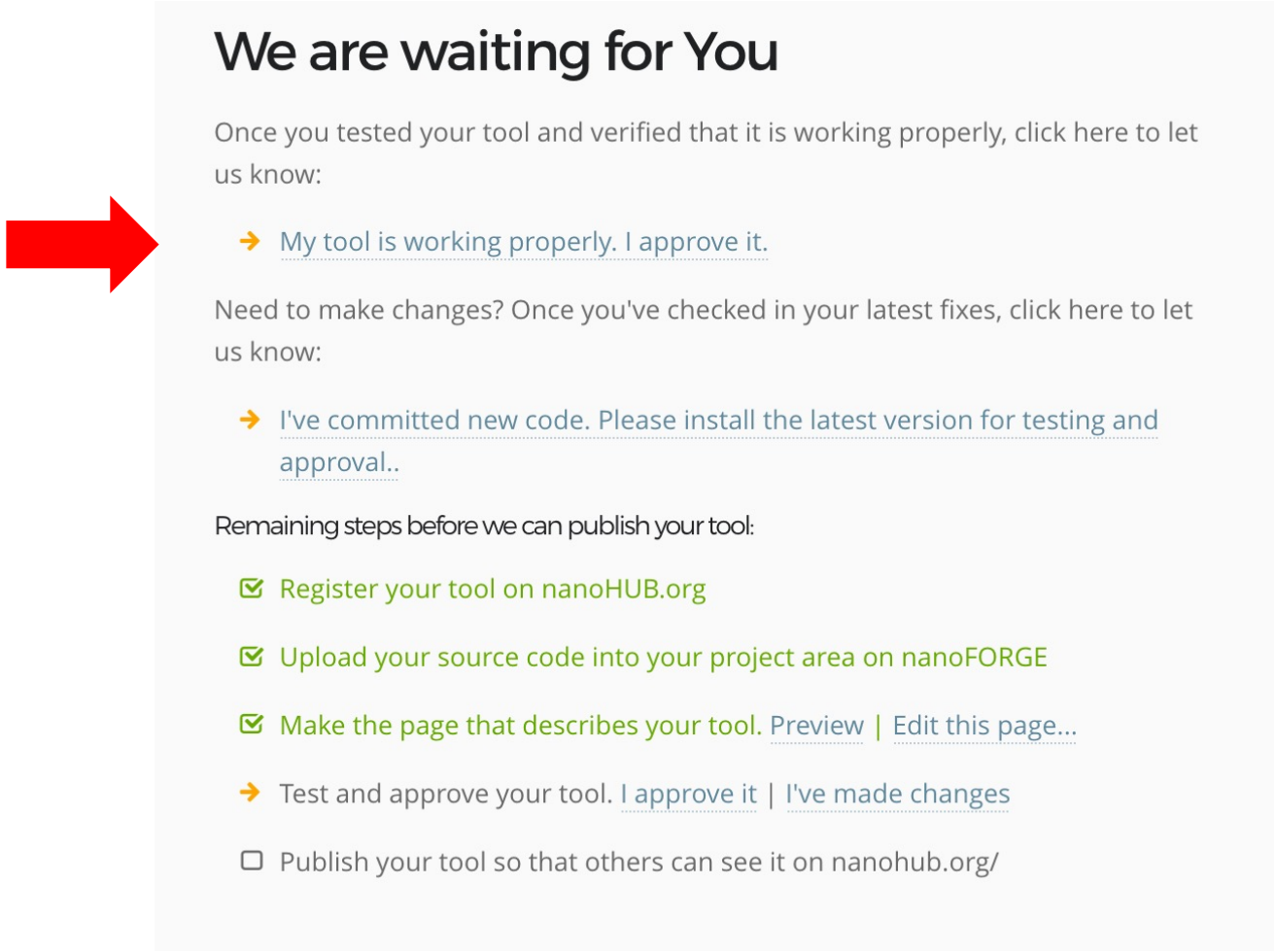
Step 6: Test your code in nanoHUB

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



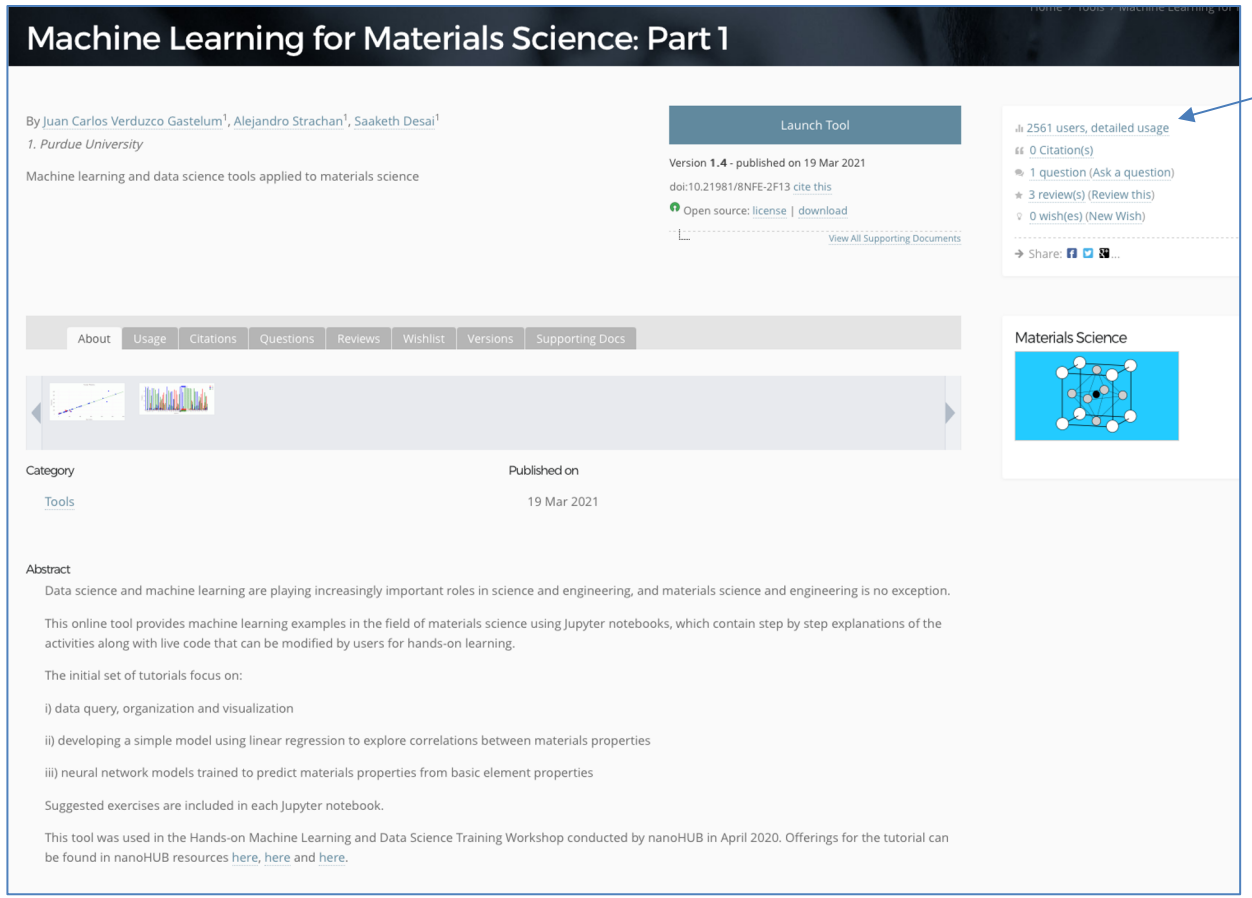
Step 7: Approve your code for publication

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



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

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



Check out your usage numbers and measure your impact