

## Document 1: Getting Started

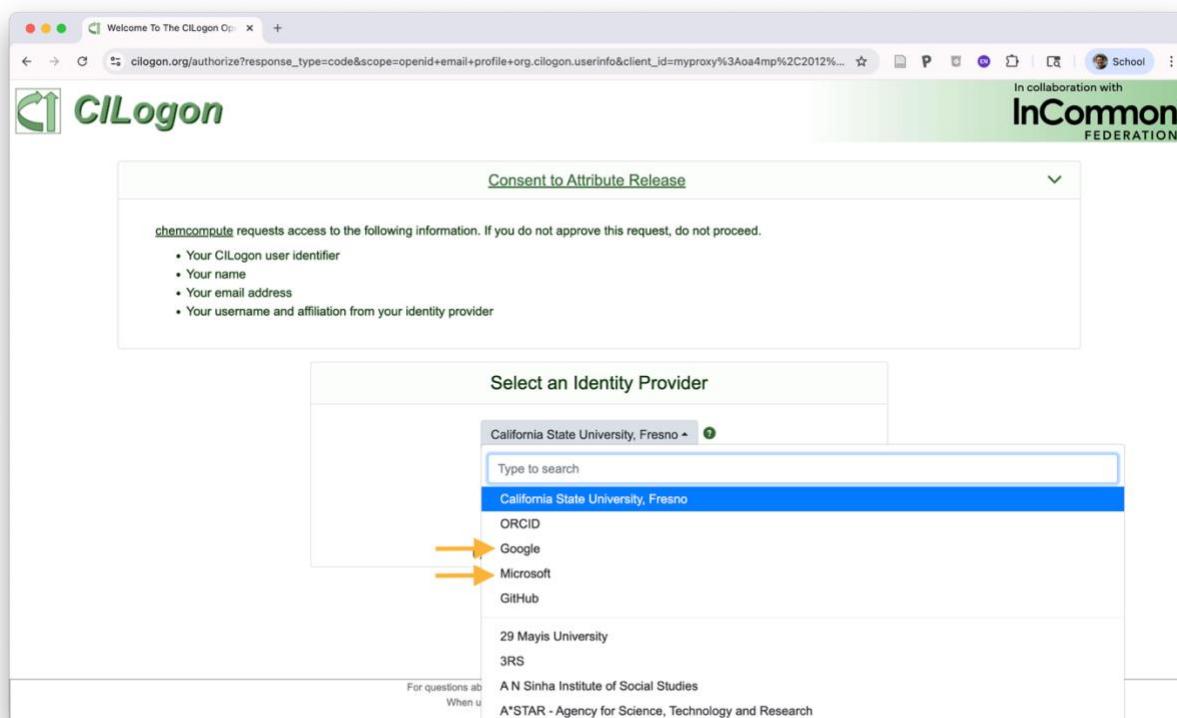
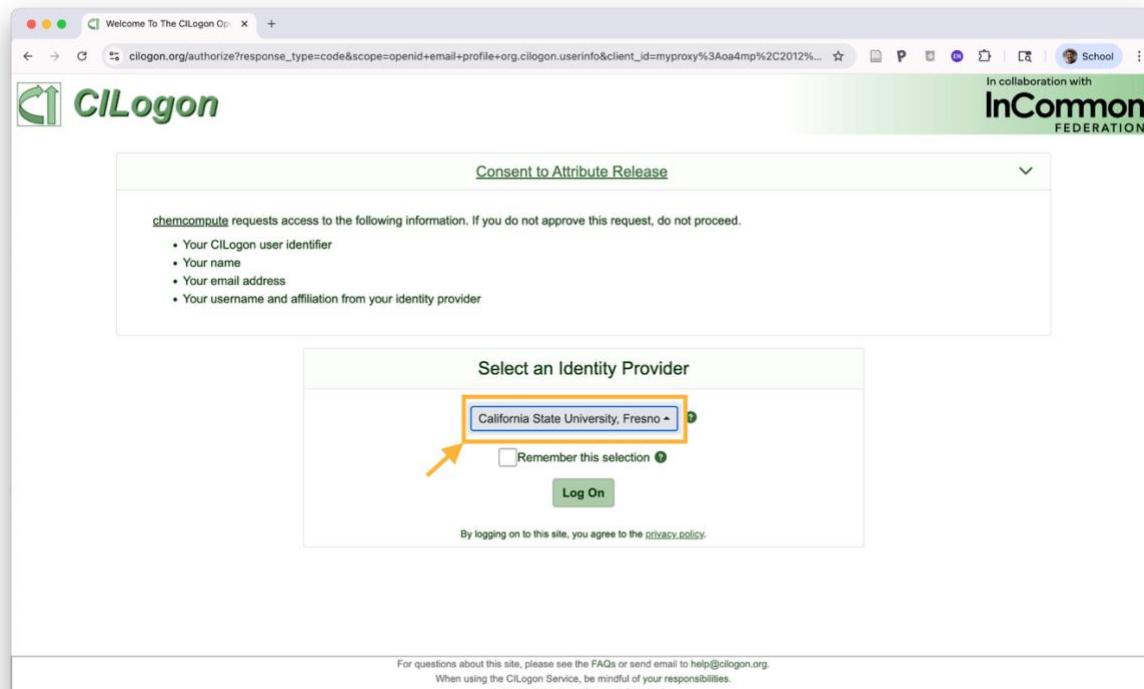
1. In your web browser, look up ChemCompute or enter this link into your address bar <https://chemcompute.org/>.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).

The screenshot shows the ChemCompute homepage. At the top right, there are 'Login' and 'Register' buttons. A yellow arrow points to the 'Register' button. Below the header, there's a section titled 'Computational chemistry software for undergraduate teaching and research'. It lists four chemistry packages: GAMESS, Psi4, TINKER, and NAMD. Each package has a 'Submit a Job' button and an 'Experiments' button. At the bottom left, there's a footer with links to 'Perri Group (Sonoma State University)', 'Policies', 'Credits and Acknowledgements', and the URL 'https://chemcompute.org/register/'. On the right side, there are logos for 'SENTRY' and 'NSF'.

3. Login with your University Login.

The screenshot shows the 'Register' page of the ChemCompute website. It has two main sections. The left section is for 'Sign up' and includes fields for Username, E-mail, Password, and Retype Password. It also contains a checkbox for accepting the acceptable use policy and a 'SIGN ME UP' button. The right section is for 'Skip Registration by signing in with your University Login' and includes a 'LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)' button. A yellow arrow points to this button. Below it, text says 'If your university uses Google / Microsoft for Email please try choosing Google or Microsoft!' and an 'OR' button is shown. At the bottom left, there's a footer with the URL 'https://chemcompute.org/register/'.

4. Select your Identity Provider from the dropdown menu. If your school is not listed, select a third-party identity provider based on your school account. If your student email uses Google, select “Google”. If your student email uses Outlook, select “Microsoft”.



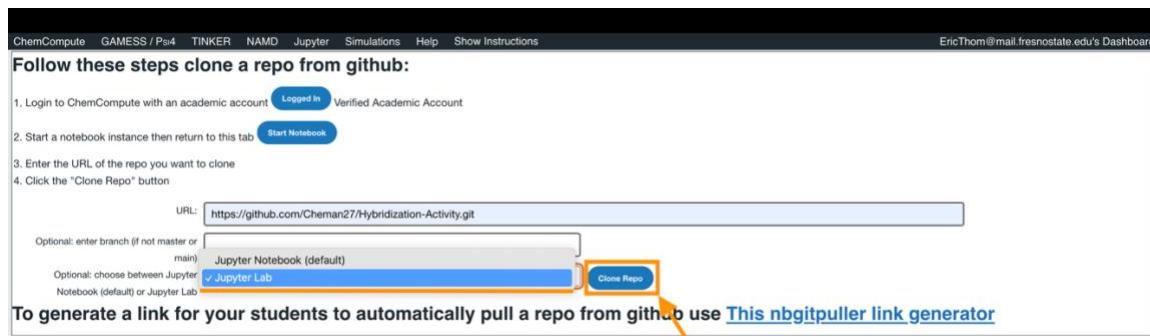
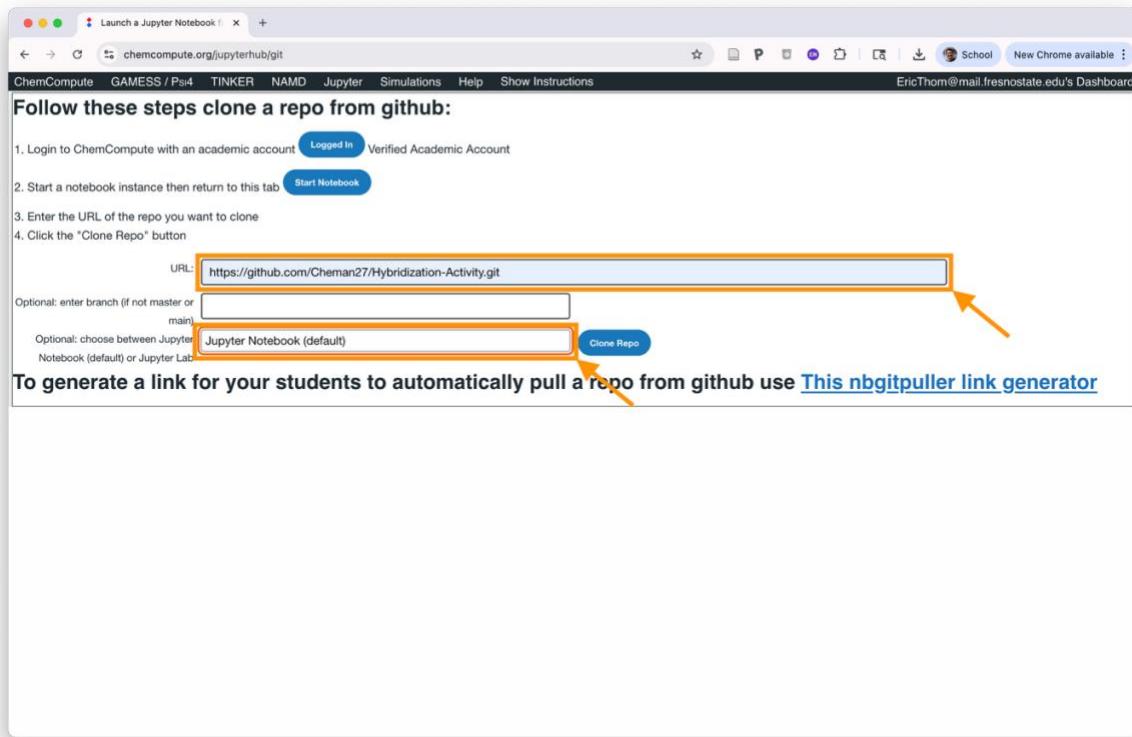
5. Select Jupyter (Dropdown menu when hovering is not relevant).

The screenshot shows the ChemCompute homepage. At the top, there is a navigation bar with links for ChemCompute, GAMESS / Psi4, TINKER, NAMD, Jupyter (which is highlighted with a yellow box and has an orange arrow pointing to it), Simulations, and Help. To the right of the navigation bar is a "Eric's Dashboard" link. Below the navigation bar, the page title is "Computational chemistry software for undergraduate teaching and research". A sub-header says "All without the hassle of compiling, installing, and maintaining software and hardware. Login or register at the top right to get full access to the system, or [learn more](#) about using ChemCompute in your class teaching." There are four main sections: GAMESS, PSI4, TINKER, and NAMD. Each section has a brief description, a "Submit a Job" button, and an "Experiments" button. At the bottom of the page, there is a green footer bar with the Perri Group logo, a "Policies, Credits and Acknowledgements" link, and SENTRY and NSF logos.

6. Select “clone a repo from github”.

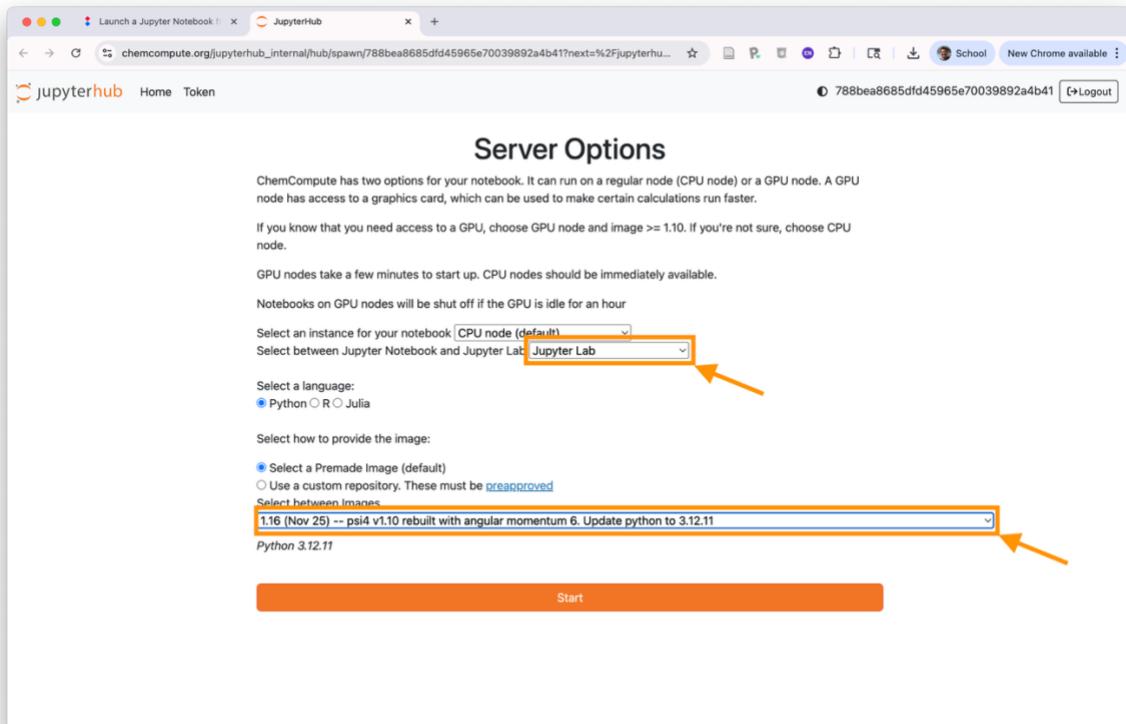
The screenshot shows the Jupyterhub page. At the top, there is a navigation bar with links for ChemCompute, GAMESS / Psi4, TINKER, NAMD, Jupyter (which is highlighted with a yellow box and has an orange arrow pointing to it), Simulations, and Help. To the right of the navigation bar is a "EricThom@mail.fresnostate.edu's Dashboard" link. The main content area is titled "Jupyterhub / Jupyter Notebooks". It contains a section "How does Psi4 / JUPYTERHUB work?" with three numbered steps: 1. From the top menu select [Jupyter -- Use Jupyter Notebook](#), 2. **Clone a repo from github** (which is highlighted with a yellow box and has an orange arrow pointing to it), and 3. To generate a link for your students to automatically pull a repo from github use [This nbgritpuller link generator](#) (opens in a new tab). There is also a section "Resource Limits / Quotas" with a bulleted list of usage details and a contact email (perrim@sonoma.edu). On the right side, there is a sidebar titled "JUPYTERHUB Experiments (20)" with categories like Physical Chemistry, General Chemistry, General Instructions, Analytical Chemistry, Mathematics, Electricity and Magnetism, and Machine Learning, each with a "+" sign to expand. At the bottom of the page, there is a green footer bar with the Perri Group logo, a "Policies, Credits and Acknowledgements" link, and SENTRY and NSF logos.

7. Paste the URL <https://github.com/Cheman27/Hybridization-Activity.git> into the designated portion. Click on the menu option for “Optional: choose between Jupyter Notebook (default) or Jupyter Lab” and select “Jupyter Lab”, then select “Clone Repo” button.

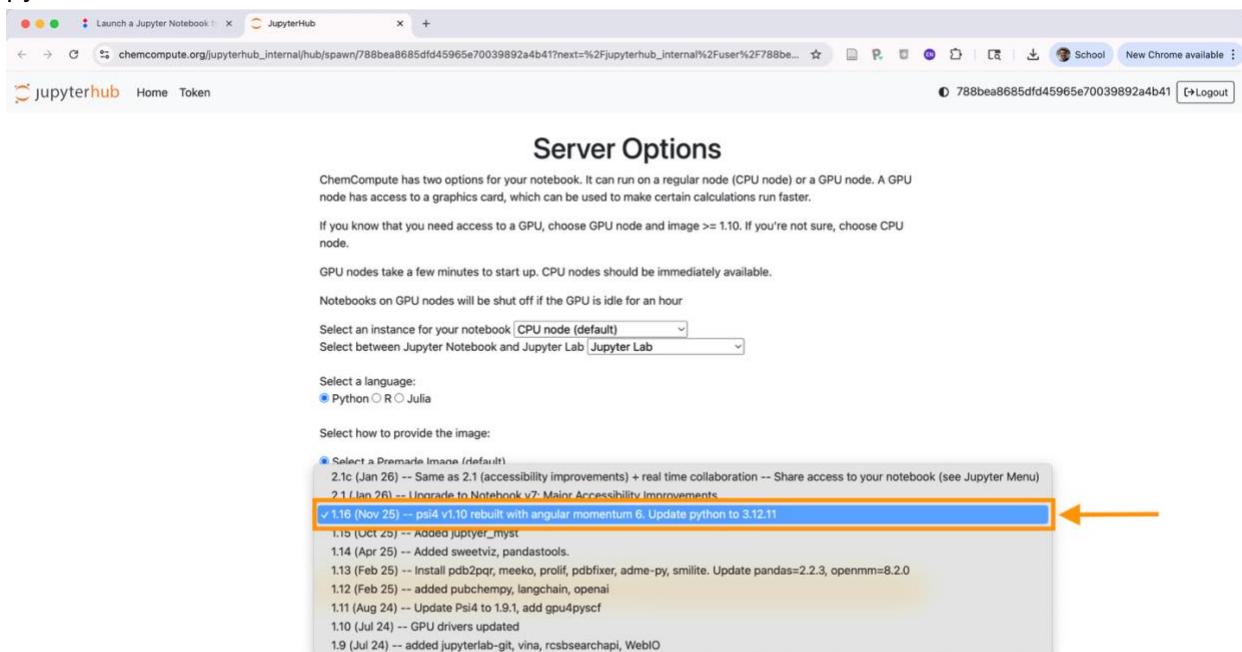


8. Once redirected, ensure “Select between Jupyter Notebook and Jupyter Lab” option is set to “Jupyter Lab”, and the “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, and lastly, you will need to change “Select between Images” by

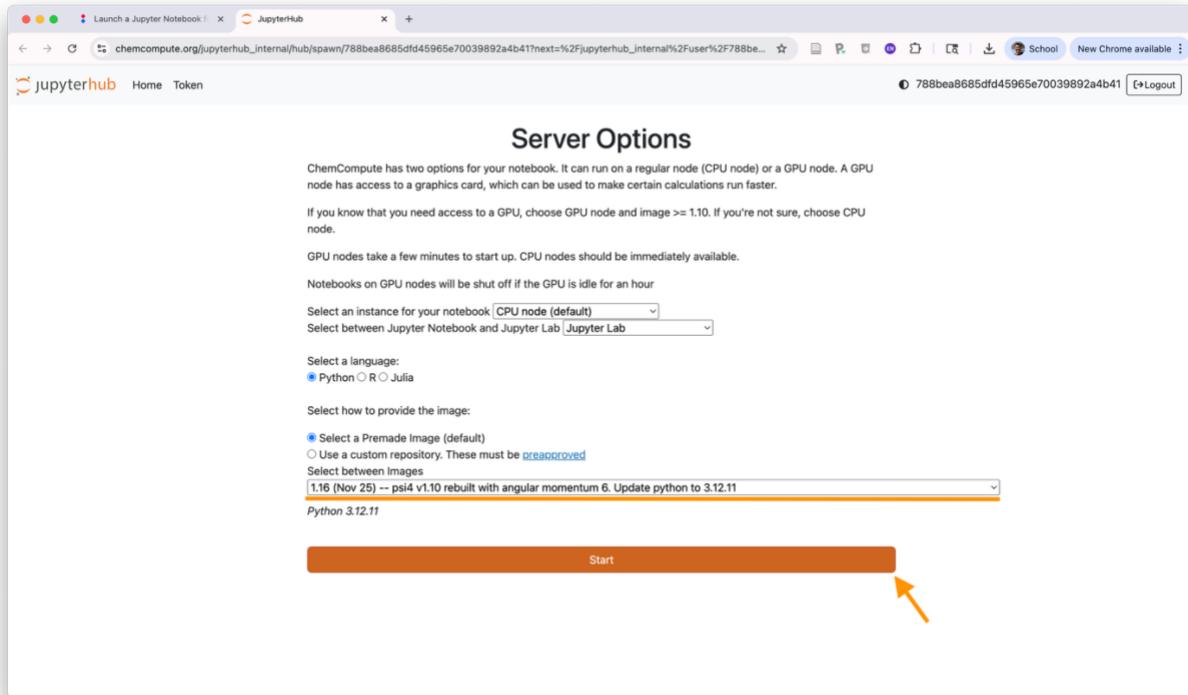
clicking on the dropdown menu.



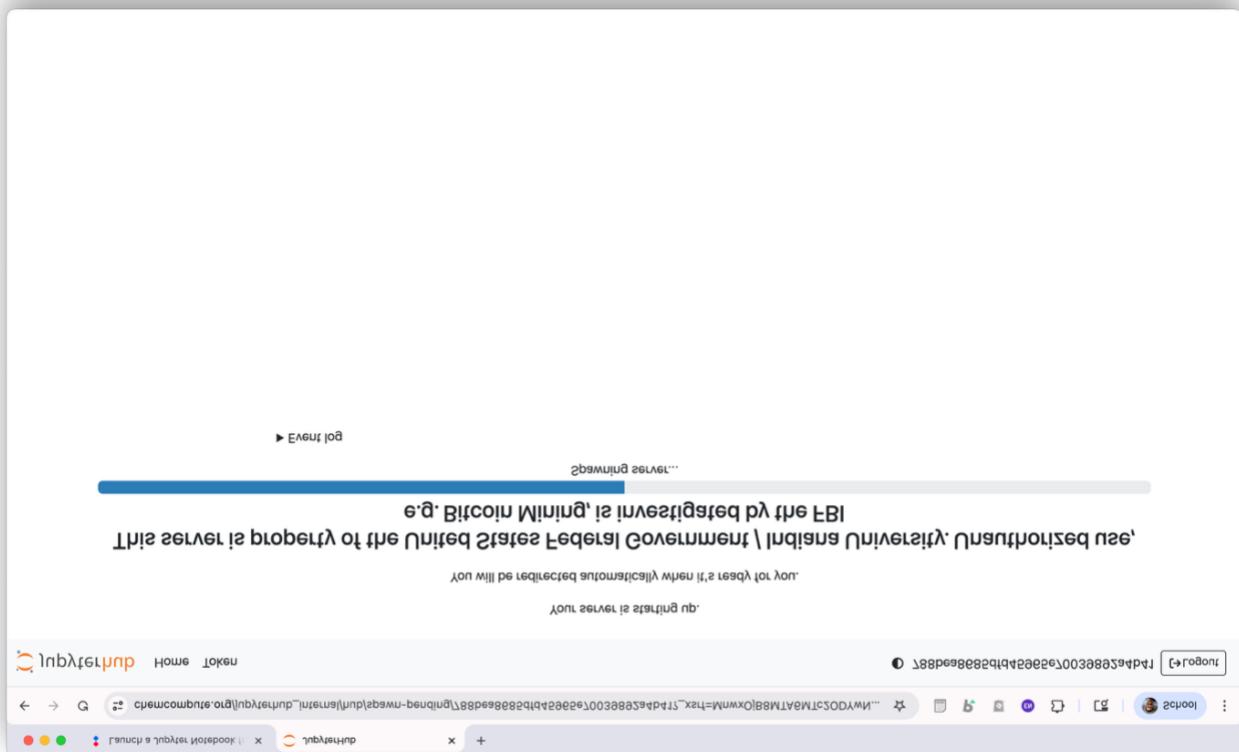
- From the dropdown menu select “1.16 (Nov25) – psi4 v1.10rebuilt with angular momentum 6. Update python to 3.12.11”.



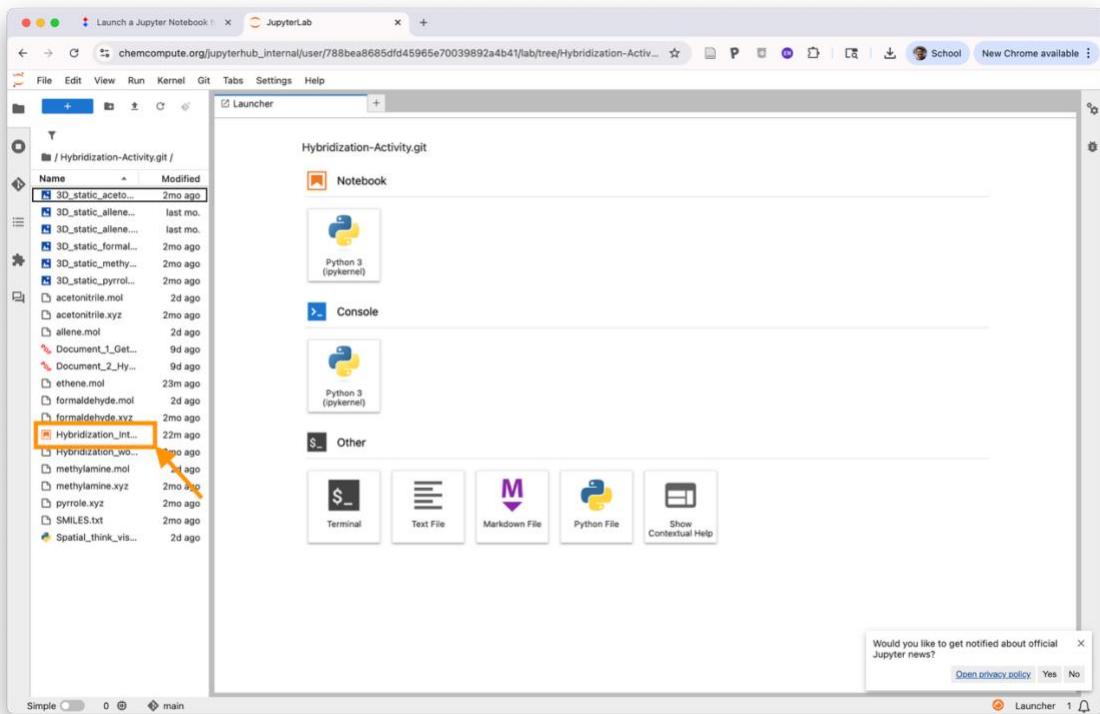
10. Now click Start.



11. You will be redirected to a new tab. This may take a while if multiple students are setting up at the same time on the same server.



12. Once loading is complete, click on Hybridization-Activity.git. Do not worry about clicking into any of the other files. It is only important that you interact with the Hybridization-Activity.git file.



13. The viewer window will open another tab. Now that you can access your jupyter notebook, **proceed to Document 2: Hybridization Worksheet**.

