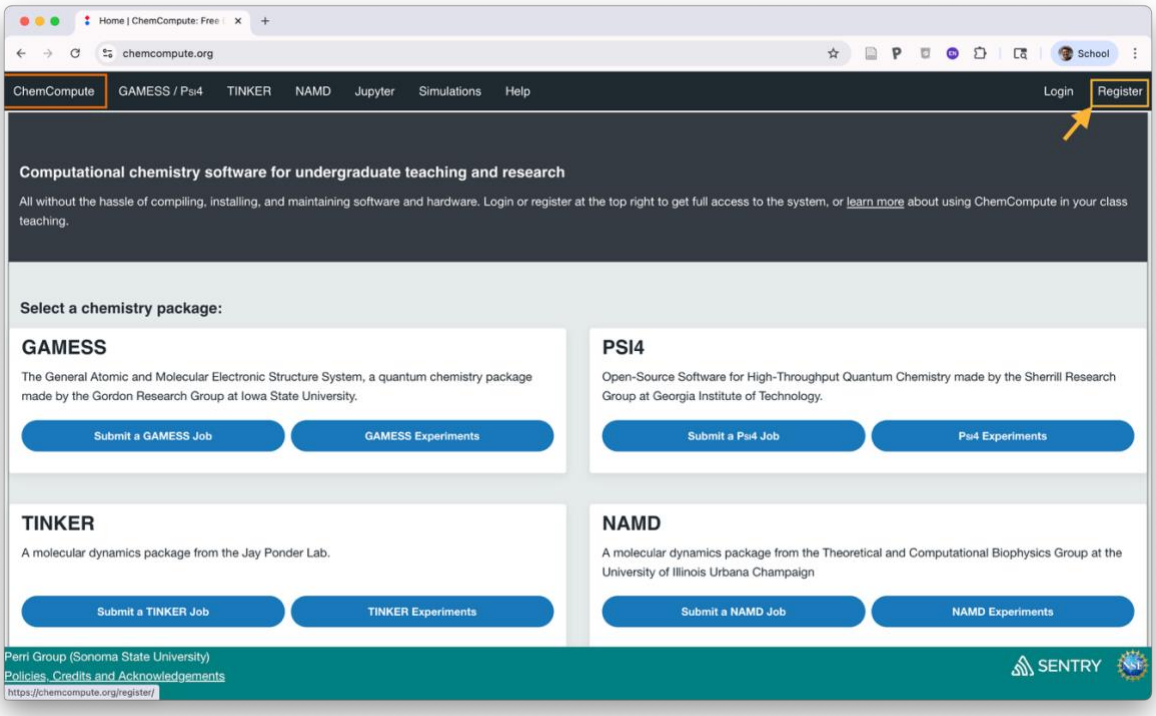
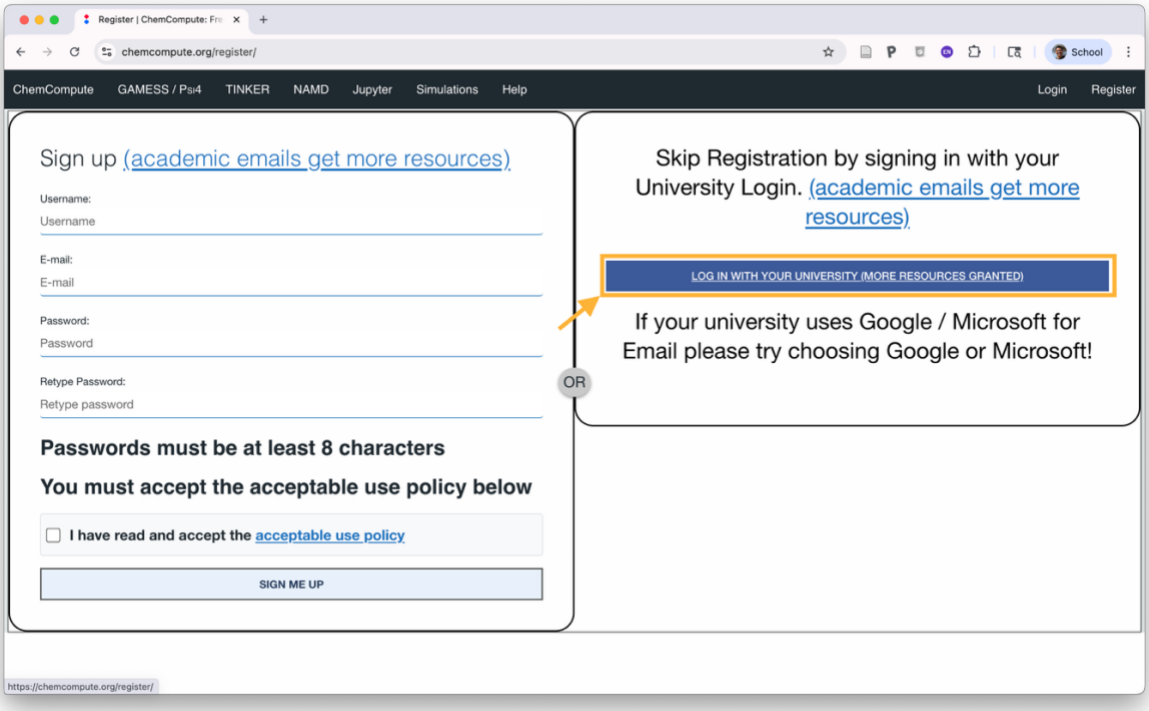
Document 1: Getting Started

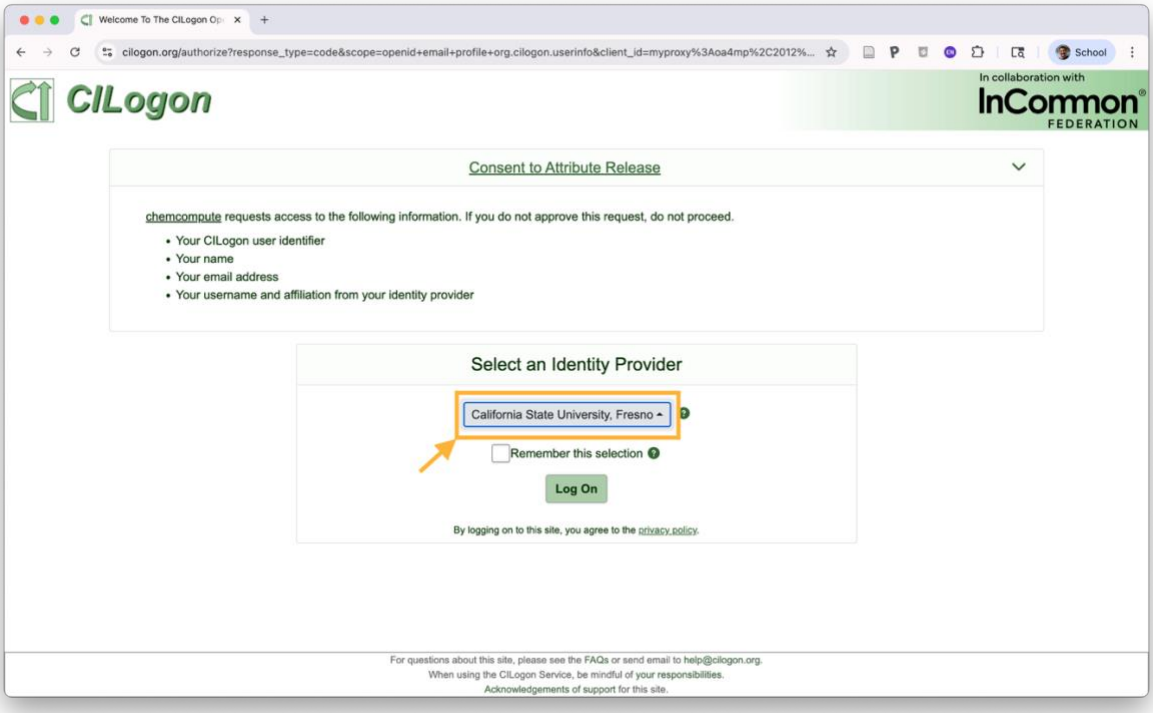
1. In your web browser, look up ChemCompute or enter this link into your address bar https://chemcompute.org/.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).

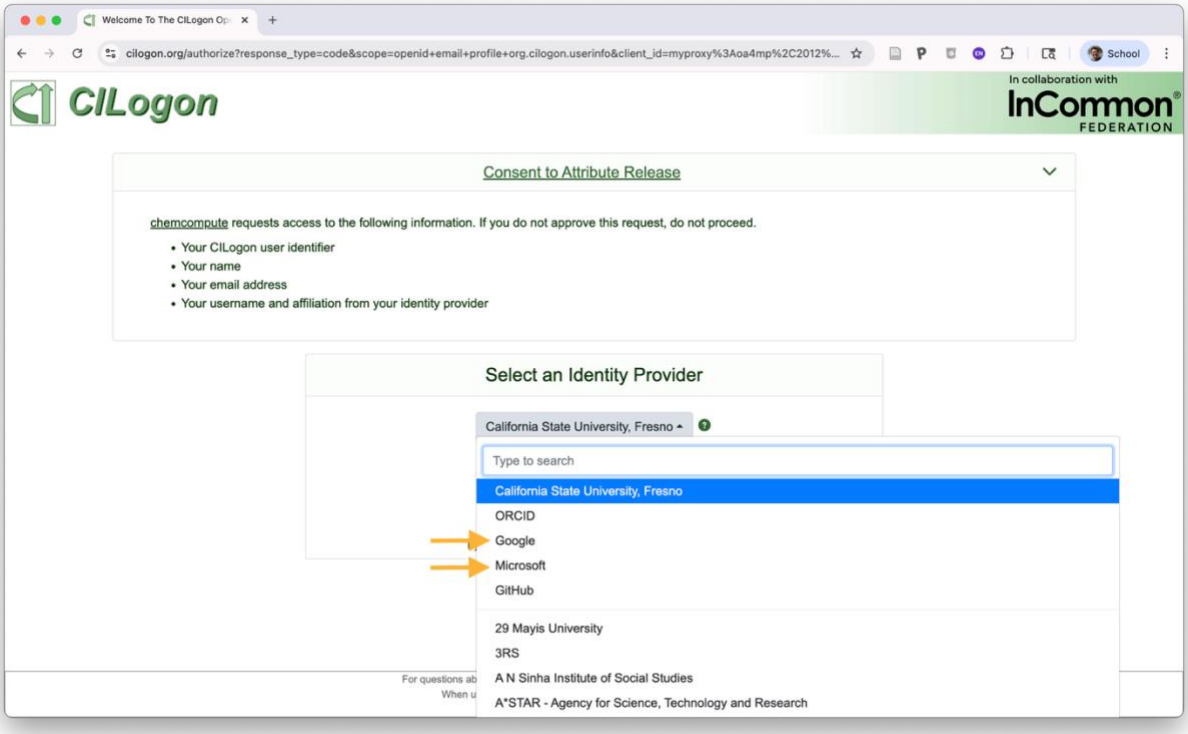


3. Login with your University Login.

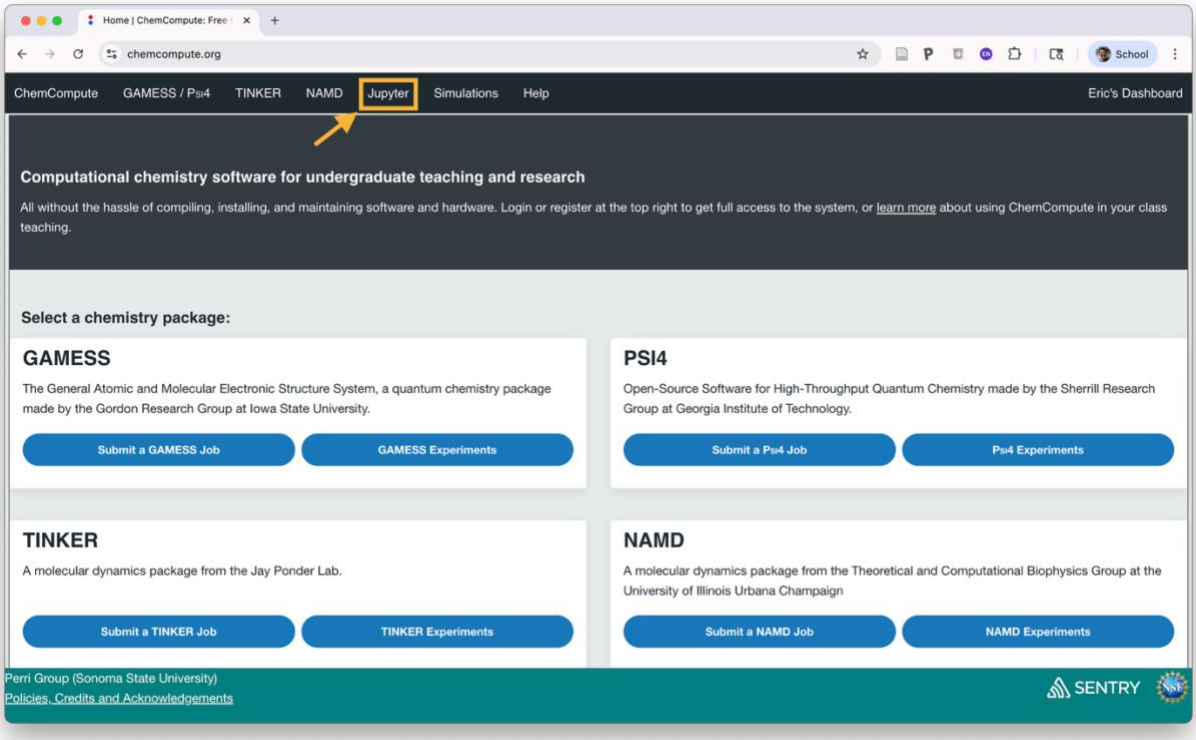


4. Select your Identity Provider from the dropdown menu. If your school is not listed, select a third-party identity provider based on your school account. If your student email uses Google, select “Google”. If your student email uses Outlook, select “Microsoft”.

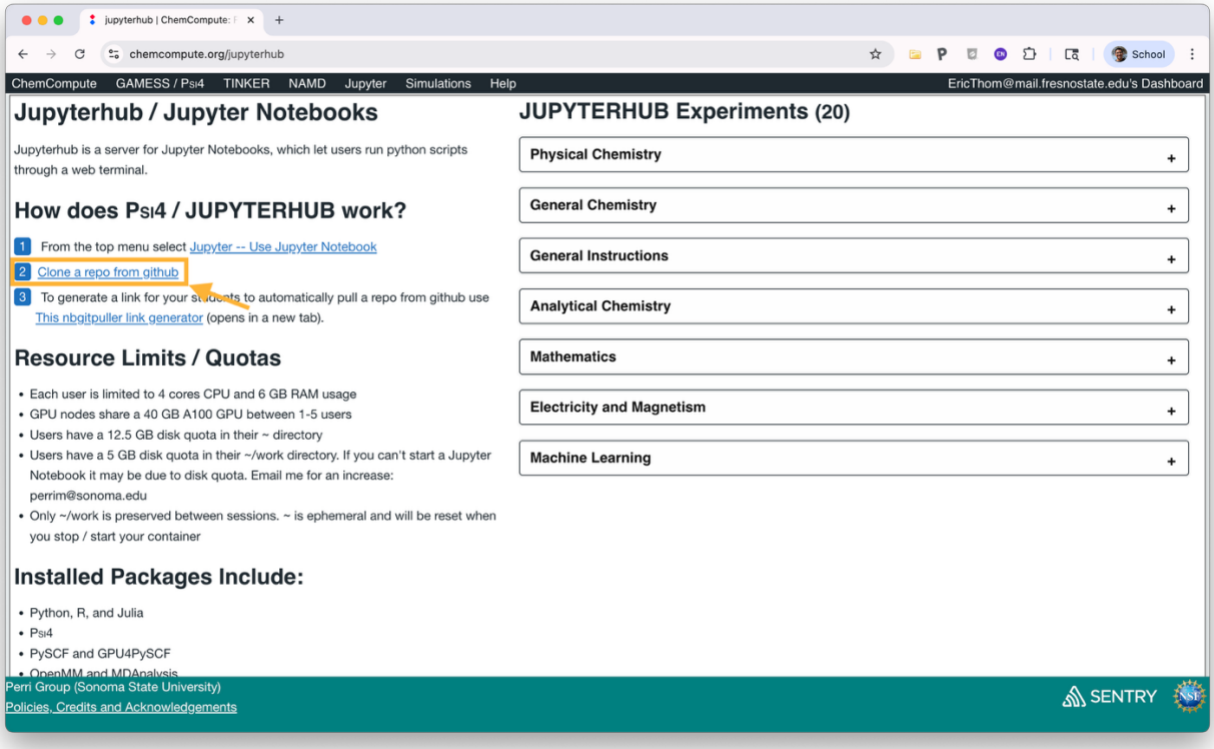




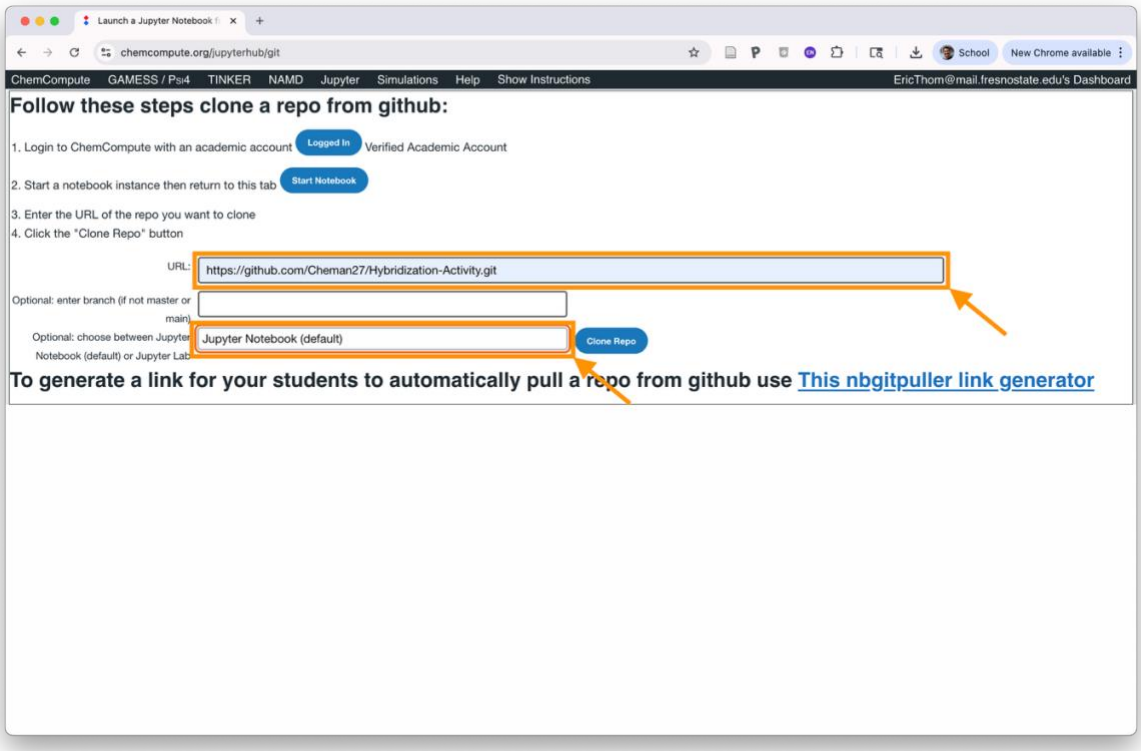
5. Select Jupyter (Dropdown menu when hovering is not relevant).

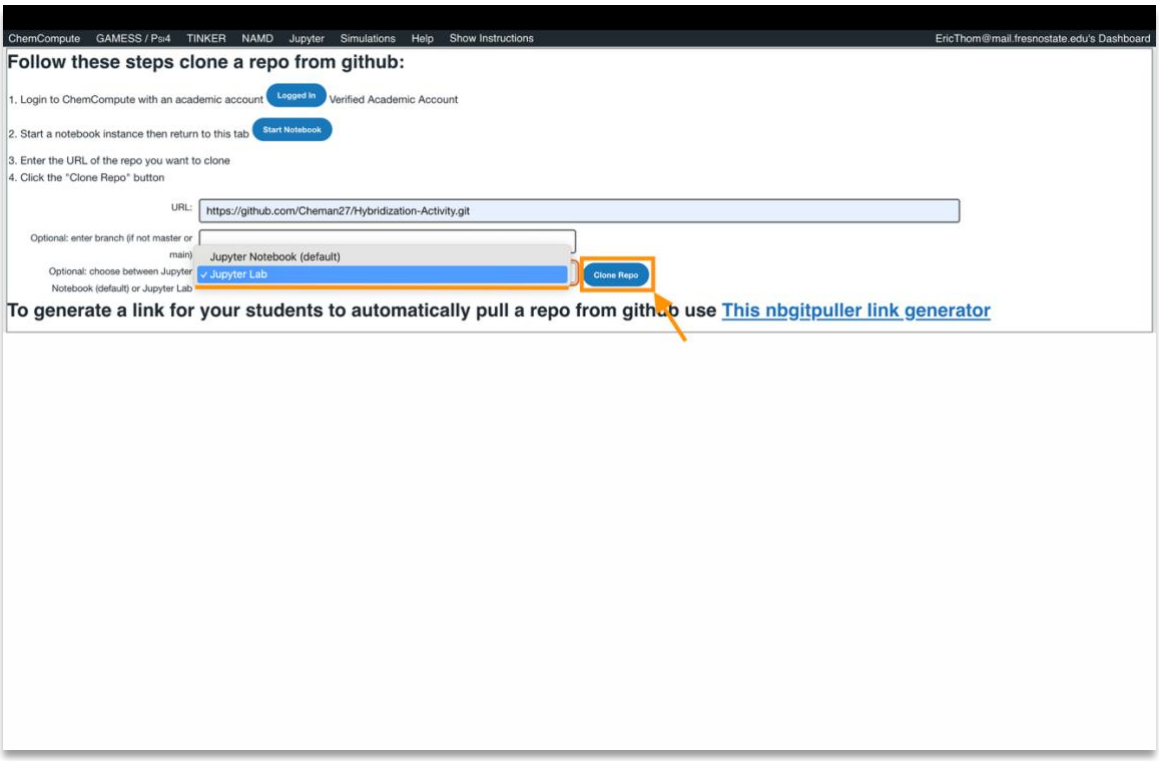


6. Select “clone a repo from github”.

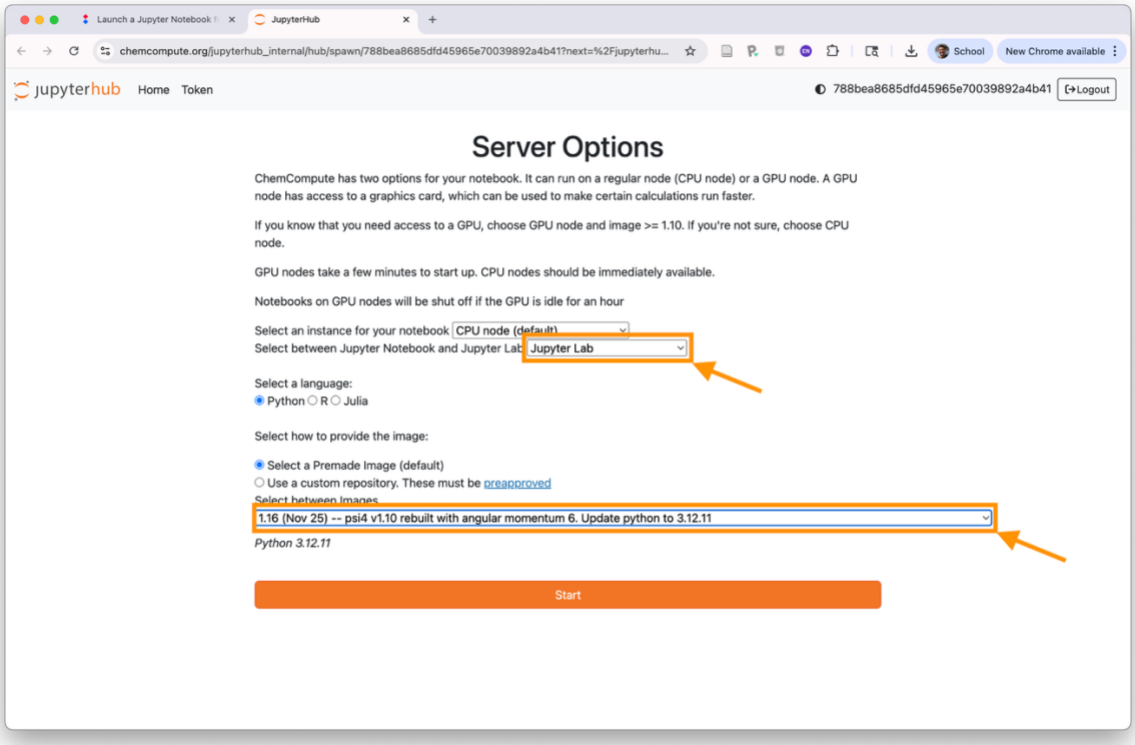


7. Paste the URL https://github.com/Cheman27/Hybridization-Activity.git into the designated portion. Click on the menu option for “Optional: choo between Jupyter Notebook (default) pr Jupyter Lab” and select “ Jupyter Lab”, then select “Clone Repo” button.

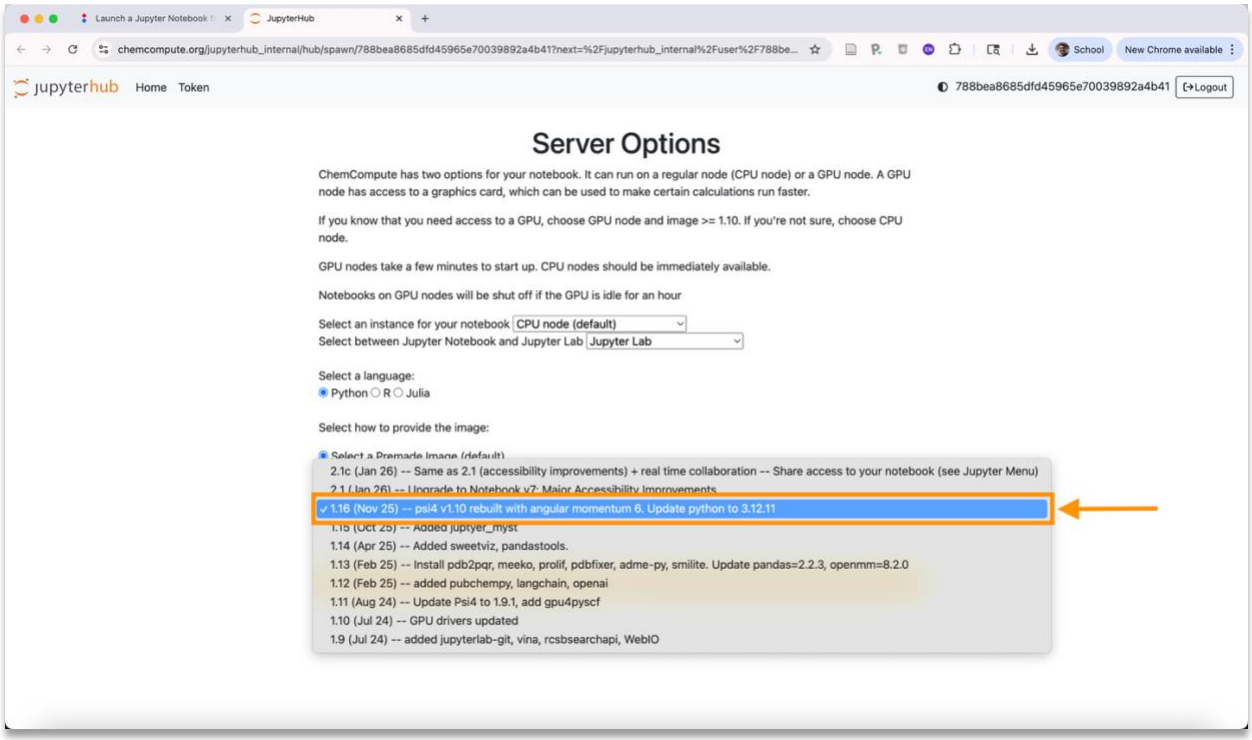




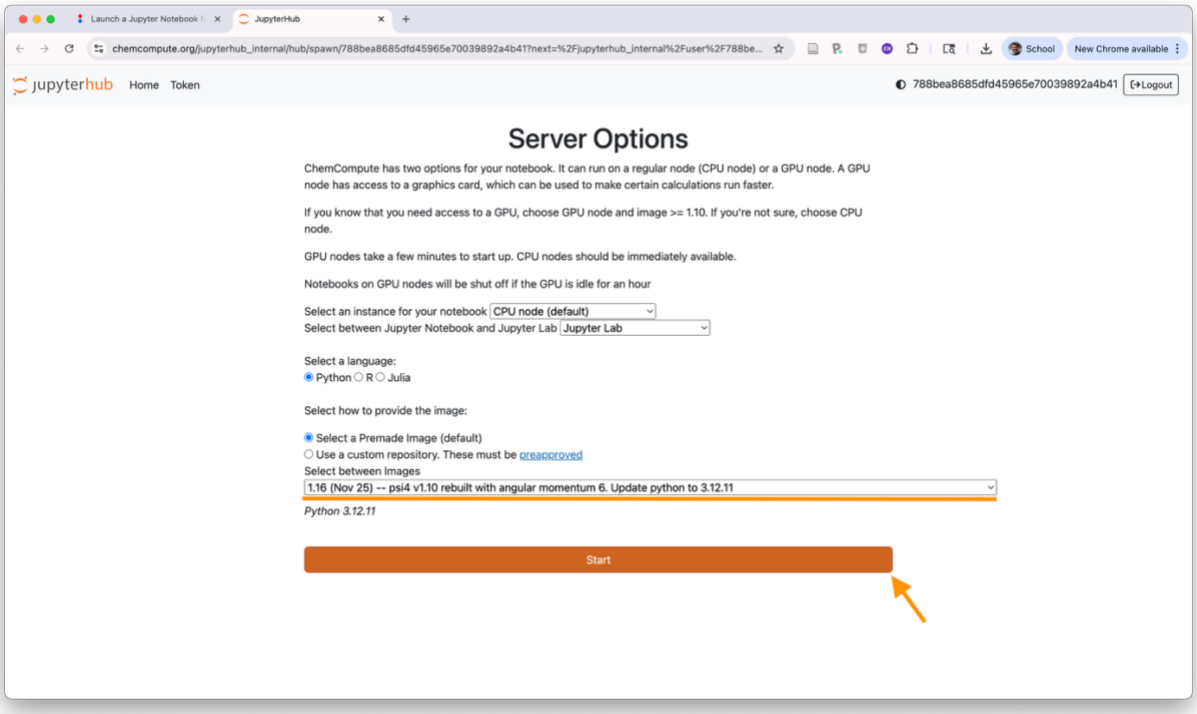
8. Once redirected, ensure “Select between Jupyter Notebook and Jupyter Lab” option is set to “Jupyter Lab”, and the “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, and lastly, you will need to change “Select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



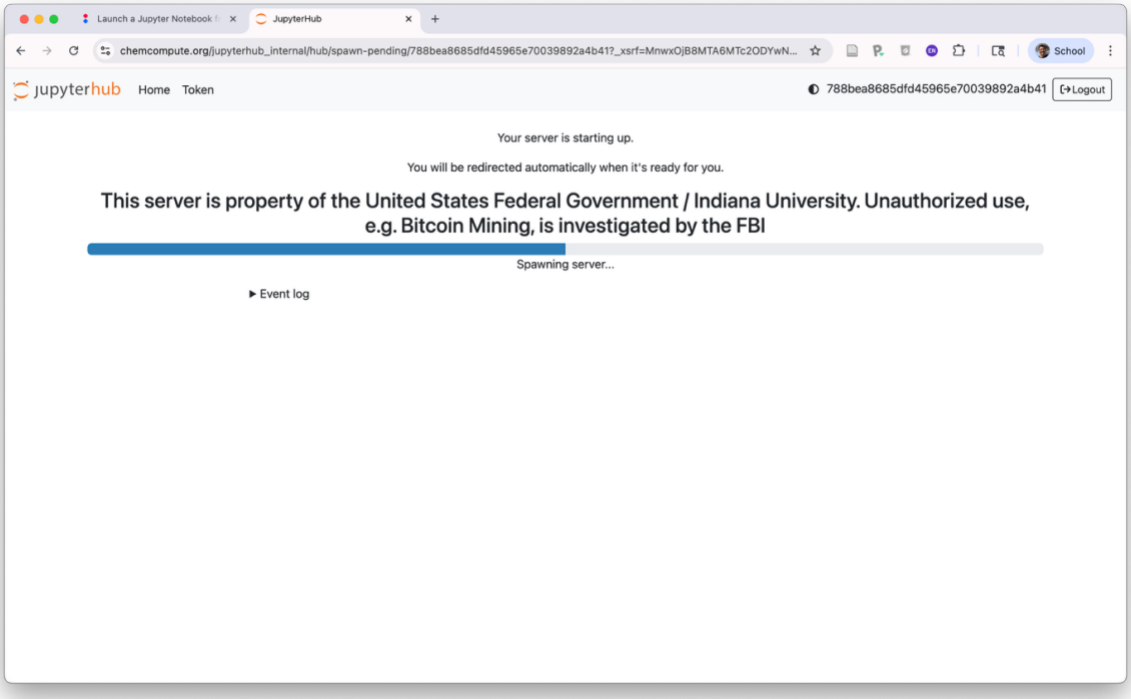
9. From the dropdown menu select “1.16 (Nov25) – psi4 v1.10rebuilt with angular momentum 6. Update python to 3.12.11”.



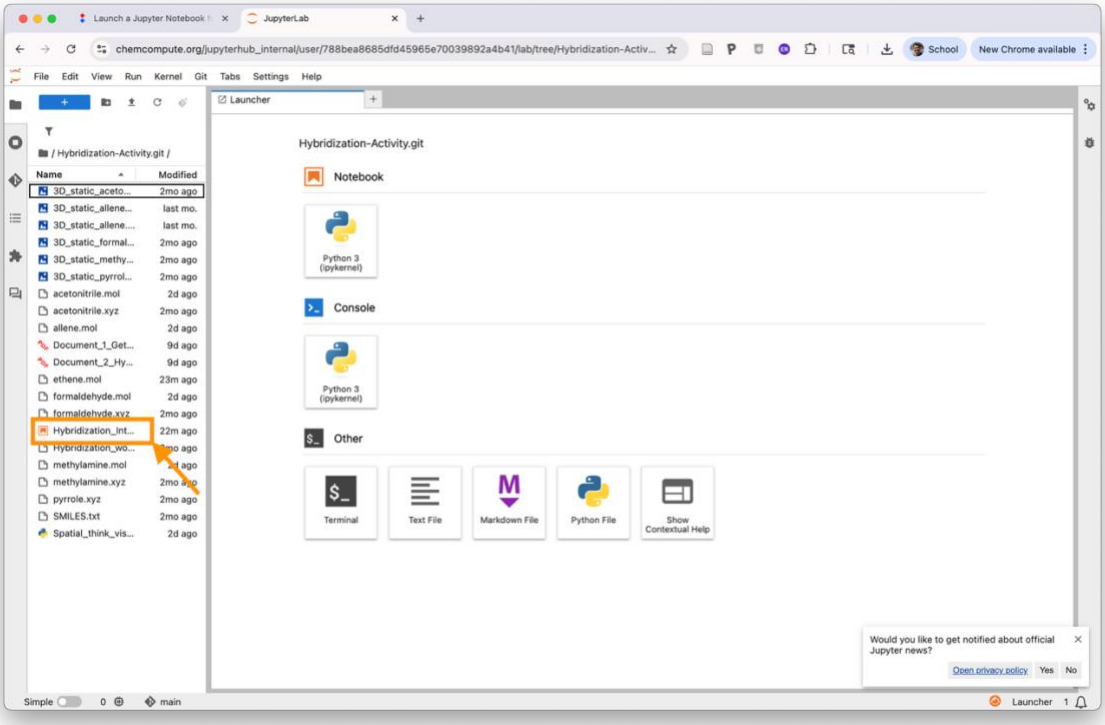
10. Now click Start.



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.**