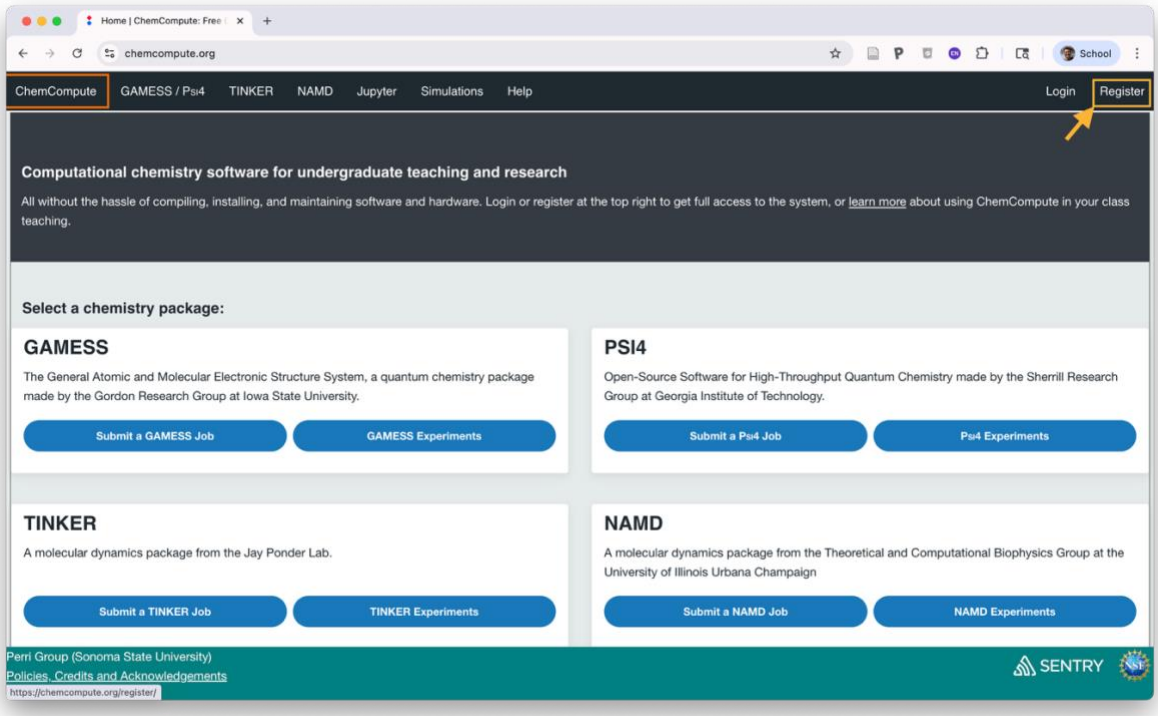
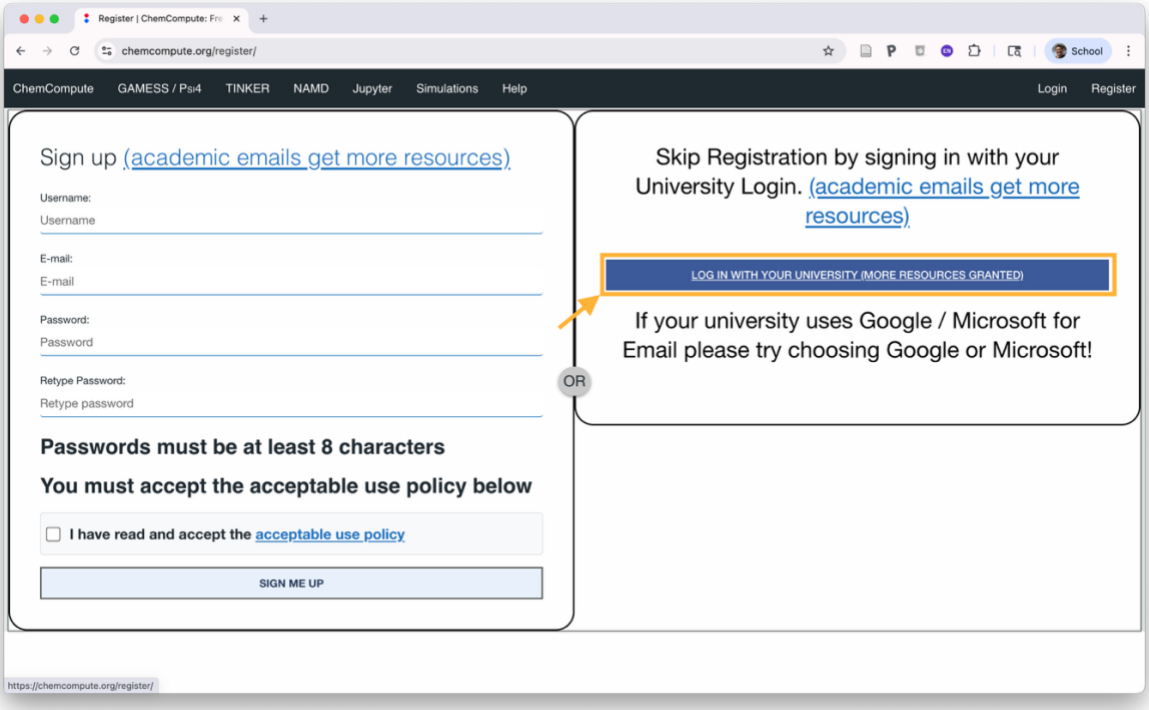
Document 1: Getting Started

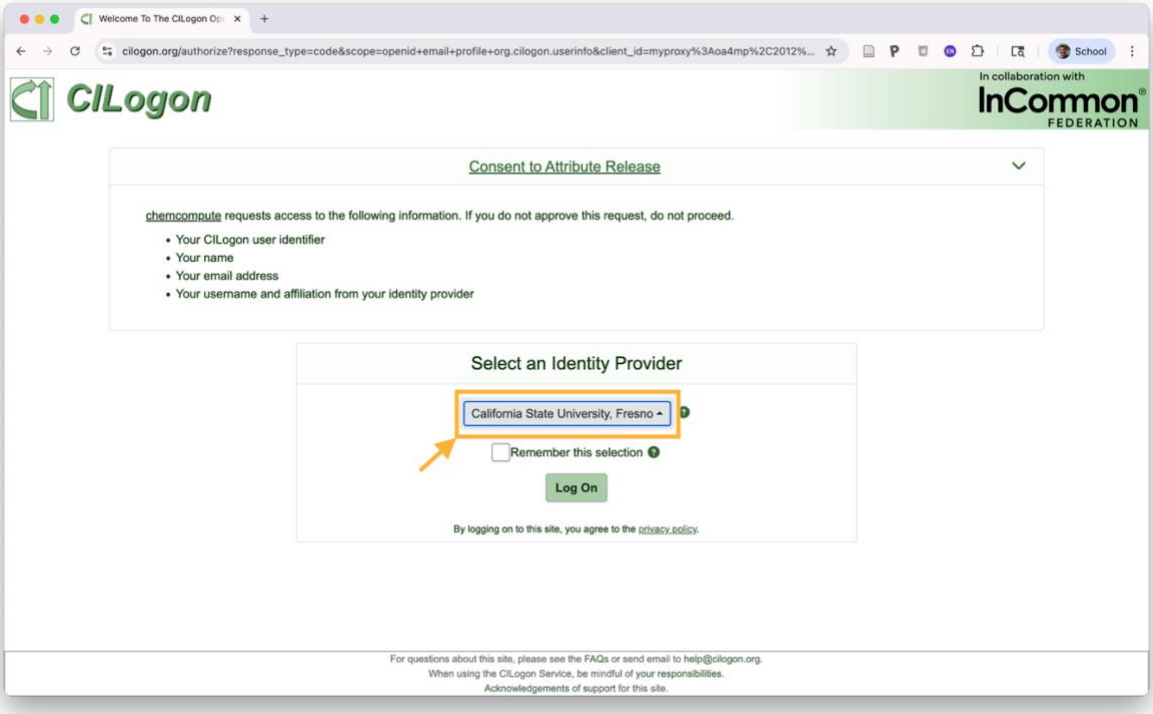
1. In your web browser, look up ChemCompute or enter this link into your address bar https://chemcompute.org/.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).

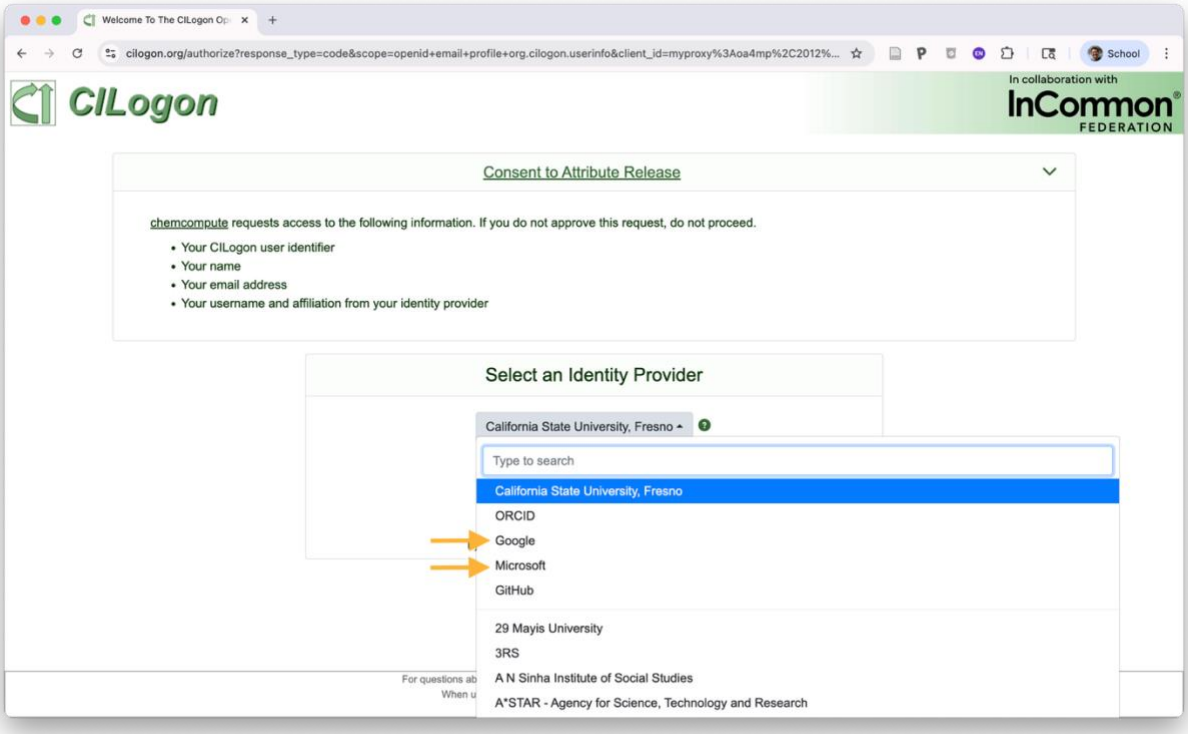


3. Login with your University Login.

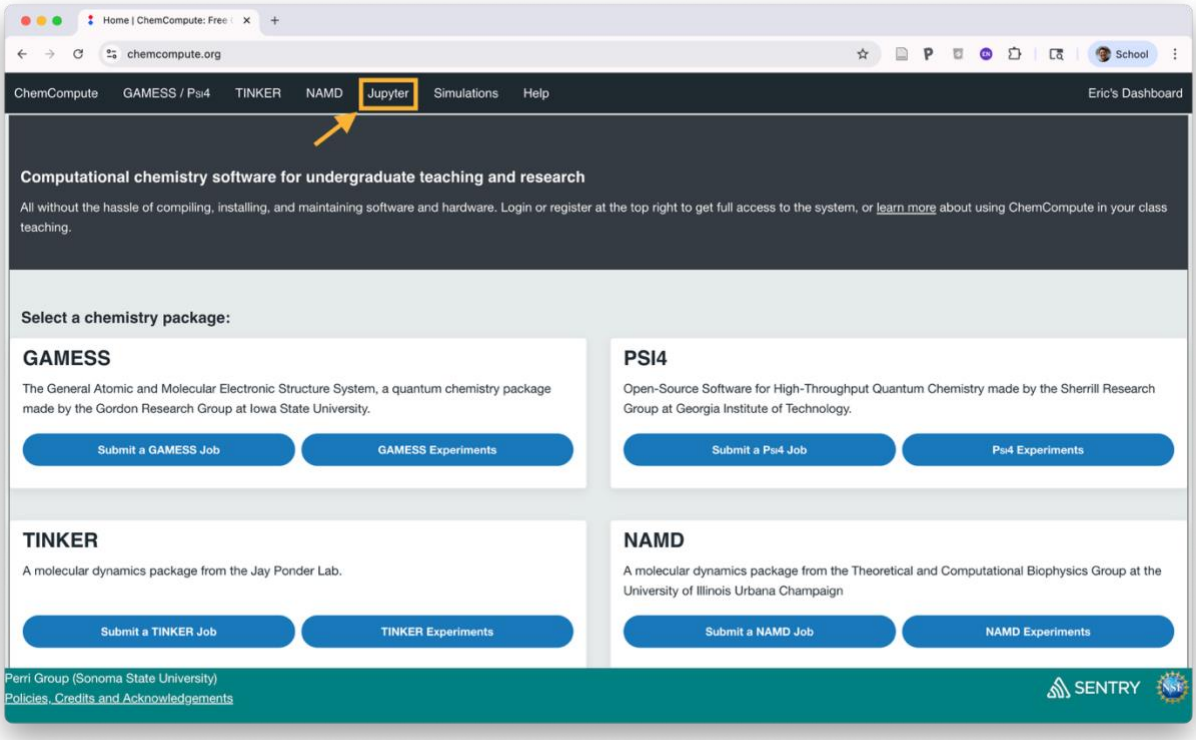


4. Select your Identity Provider from the dropdown menu. If your school is not listed, select a third-party identity provider based on your school account. If your student email uses Google, select “Google”. If your student email uses Outlook, select “Microsoft”.

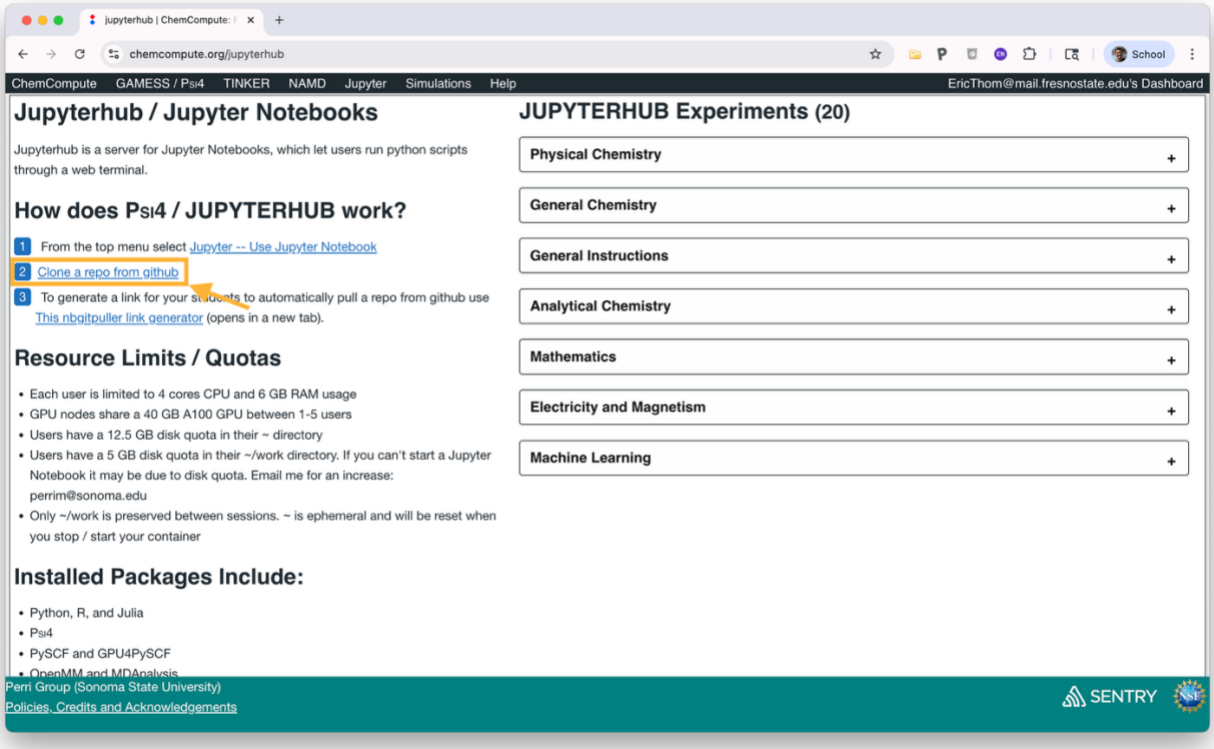




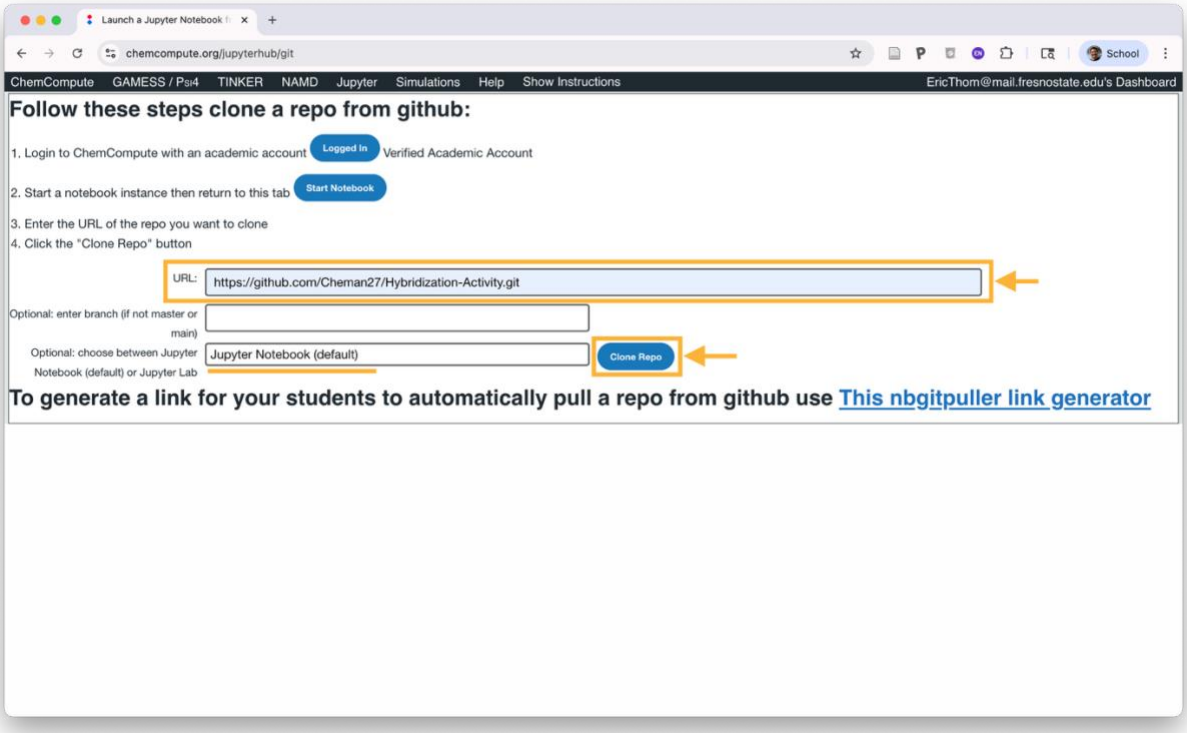
5. Select Jupyter (Dropdown menu when hovering is not relevant).



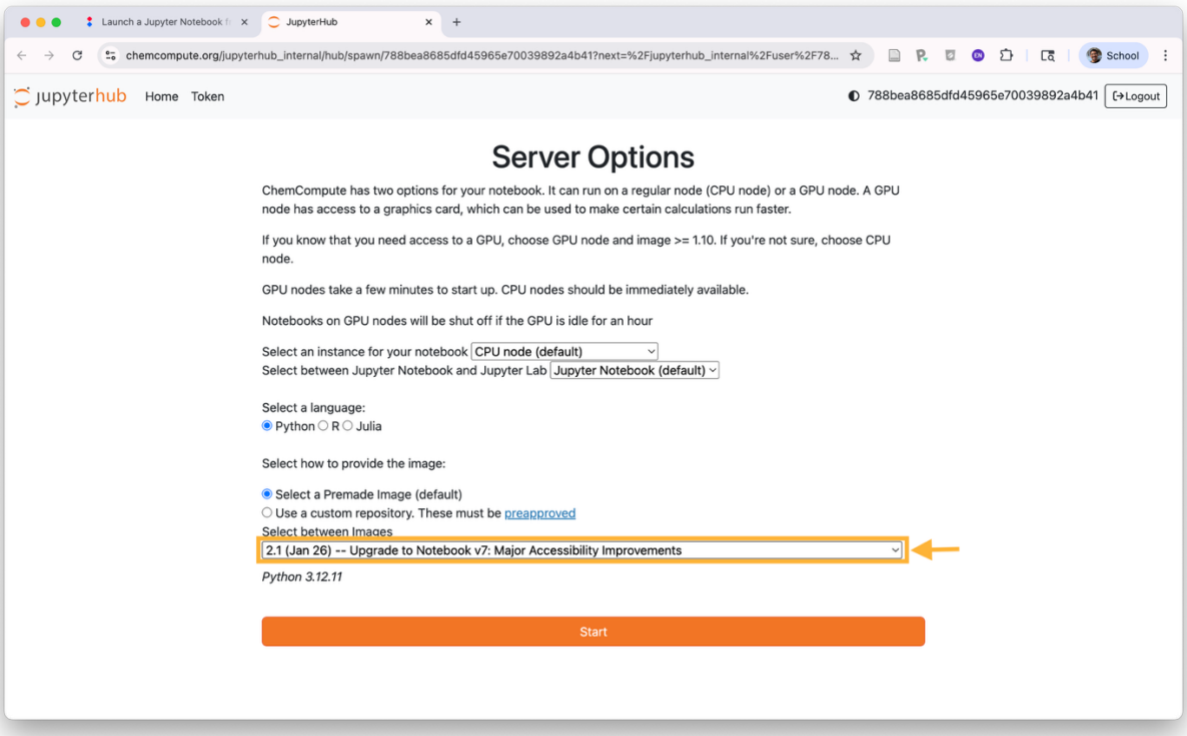
6. Select “clone a repo from github”.



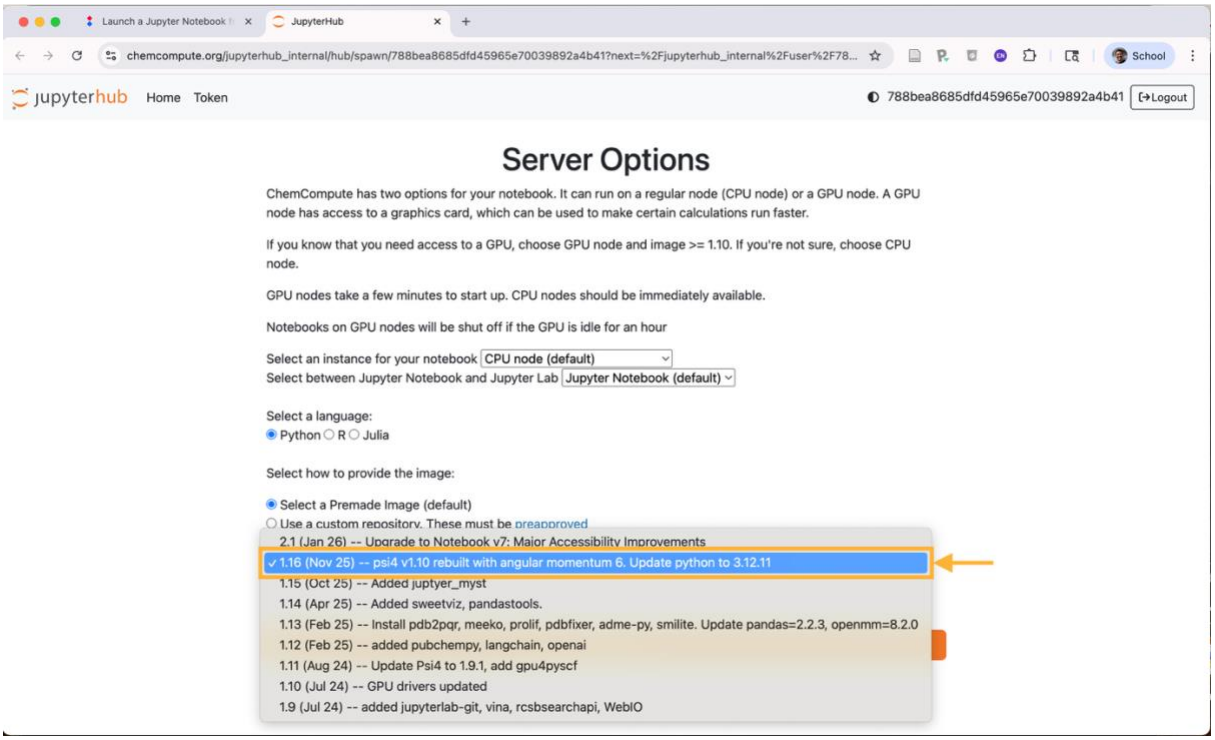
7. Paste the URL https://github.com/Cheman27/Hybridization-Activity.git into the designated portion, then select “Clone Repo” button.



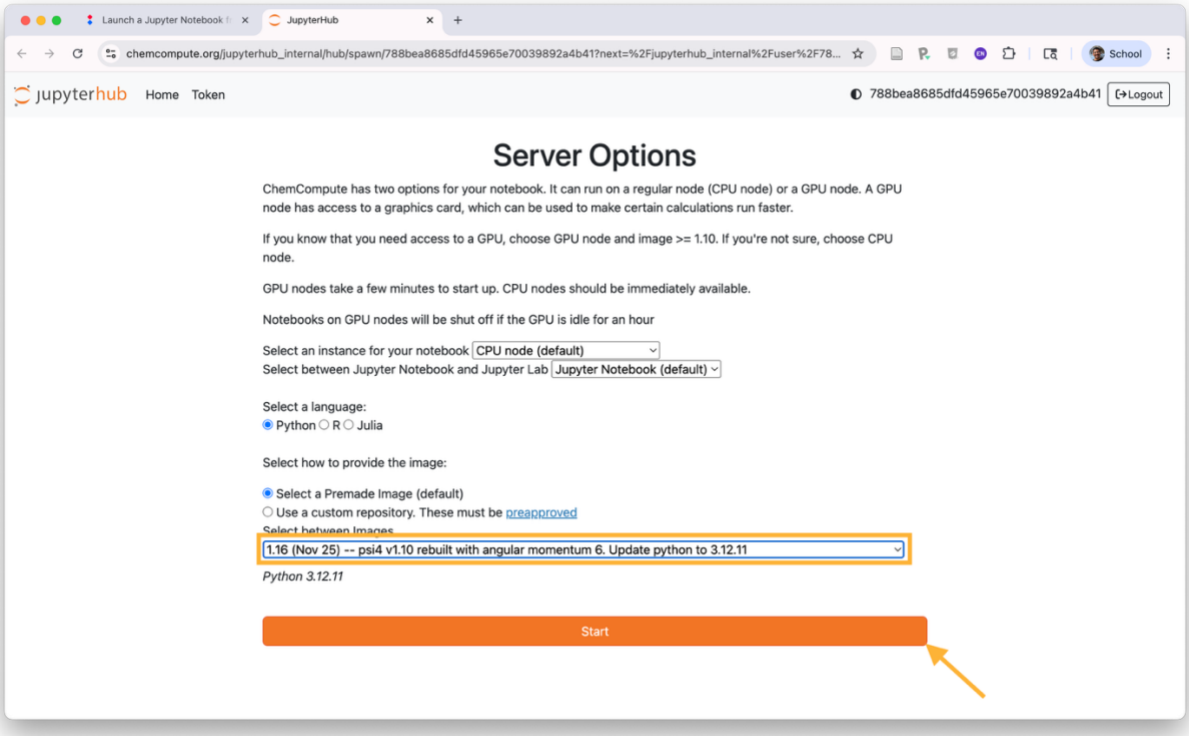
8. Once redirected, ensure “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, and lastly, you will need to change “Select between Images” by clicking on the dropdown menu.



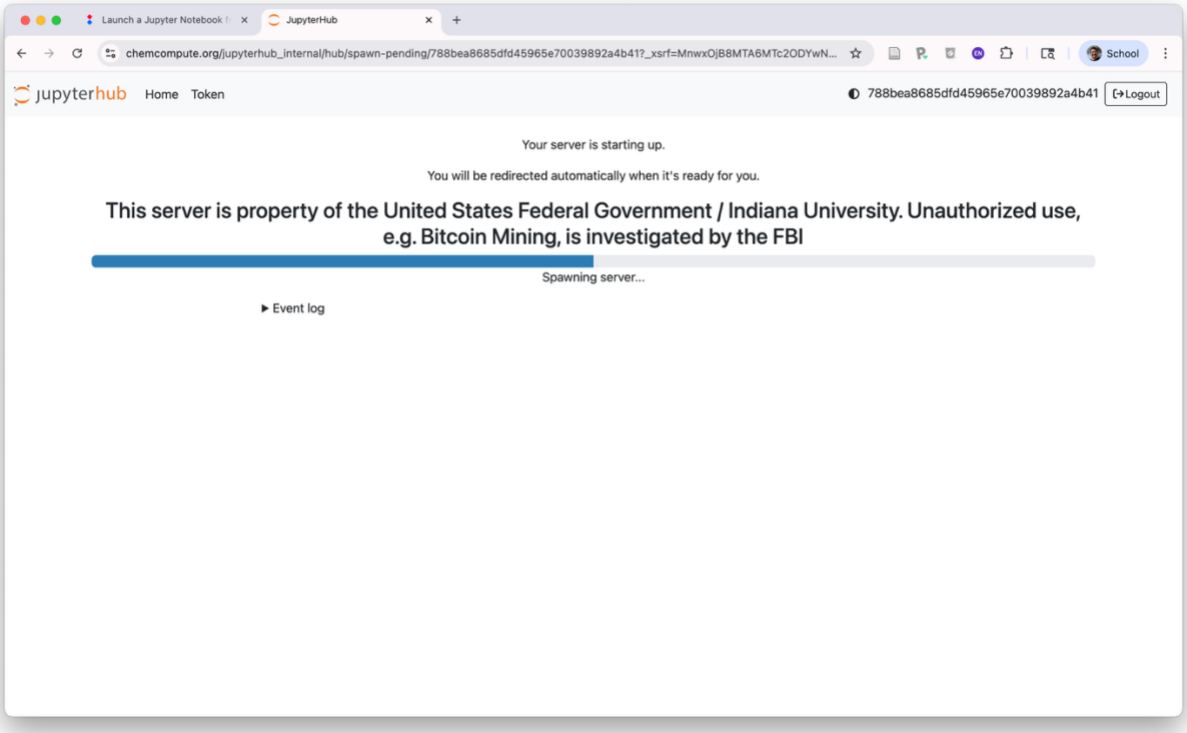
9. From the dropdown menu select “1.16 (Nov25) – psi4 v1.10rebuilt with angular momentum 6. Update python to 3.12.11”.



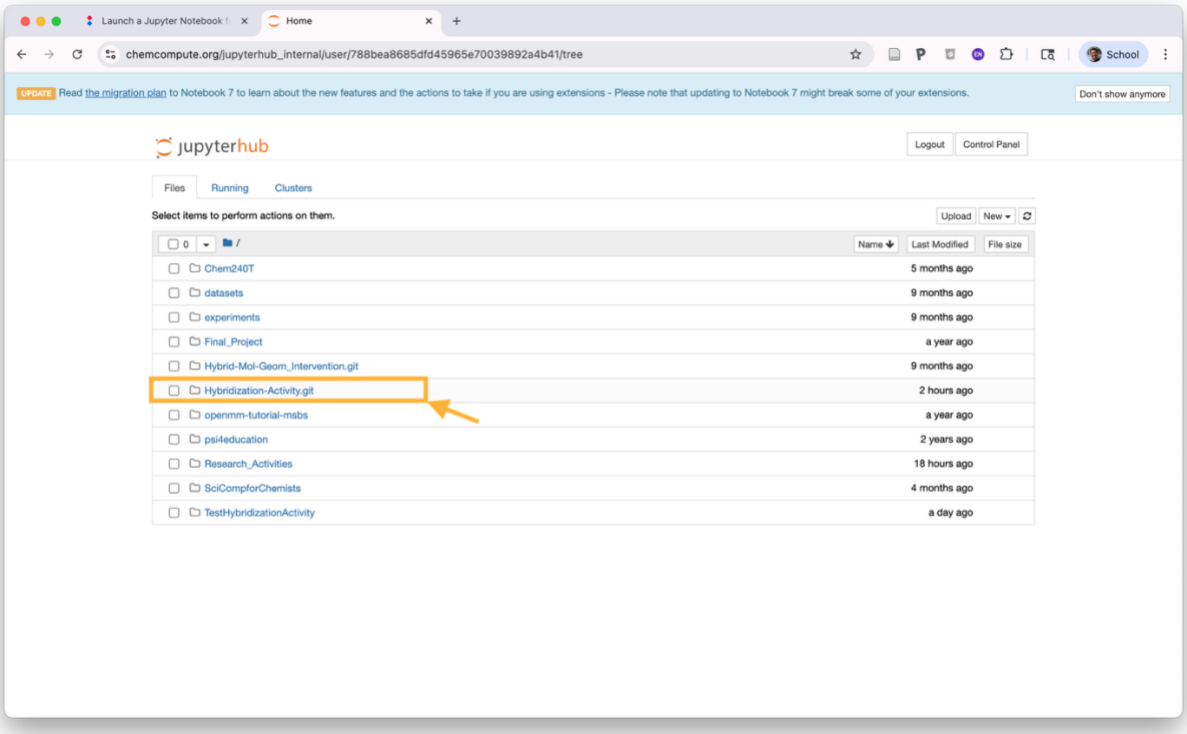
10. Now click Start.



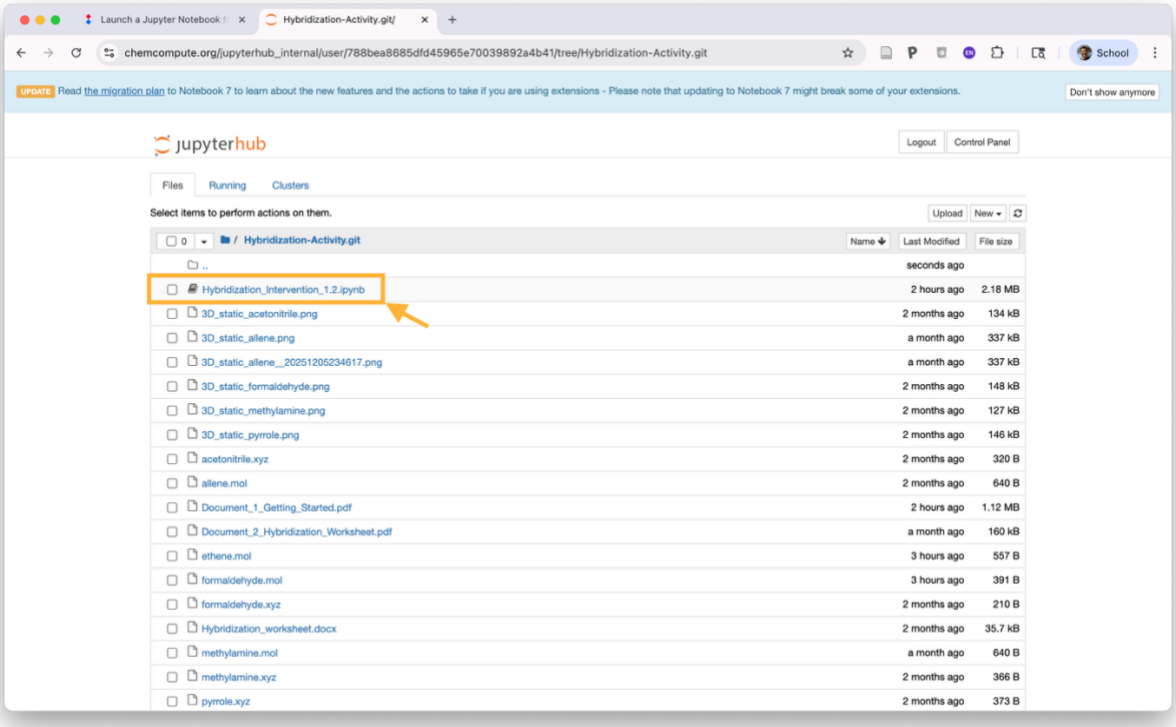
11. You will be redirected to a new tab. This may take a while if multiple students are setting up at the same time on the same server.



12. Once loading is complete, press Hybridization-Activity.git. Do not worry if your screen does not show as many folders as the image below. It is only important that you have the Hybridization-Activity.git folder.



13. Select “Hybridization_Intervention_1.2.ipynb”. You will be redirected to one more tab.



14. Now that you can access your Jupyter notebook, **proceed to Document 2: Hybridization Worksheet**.