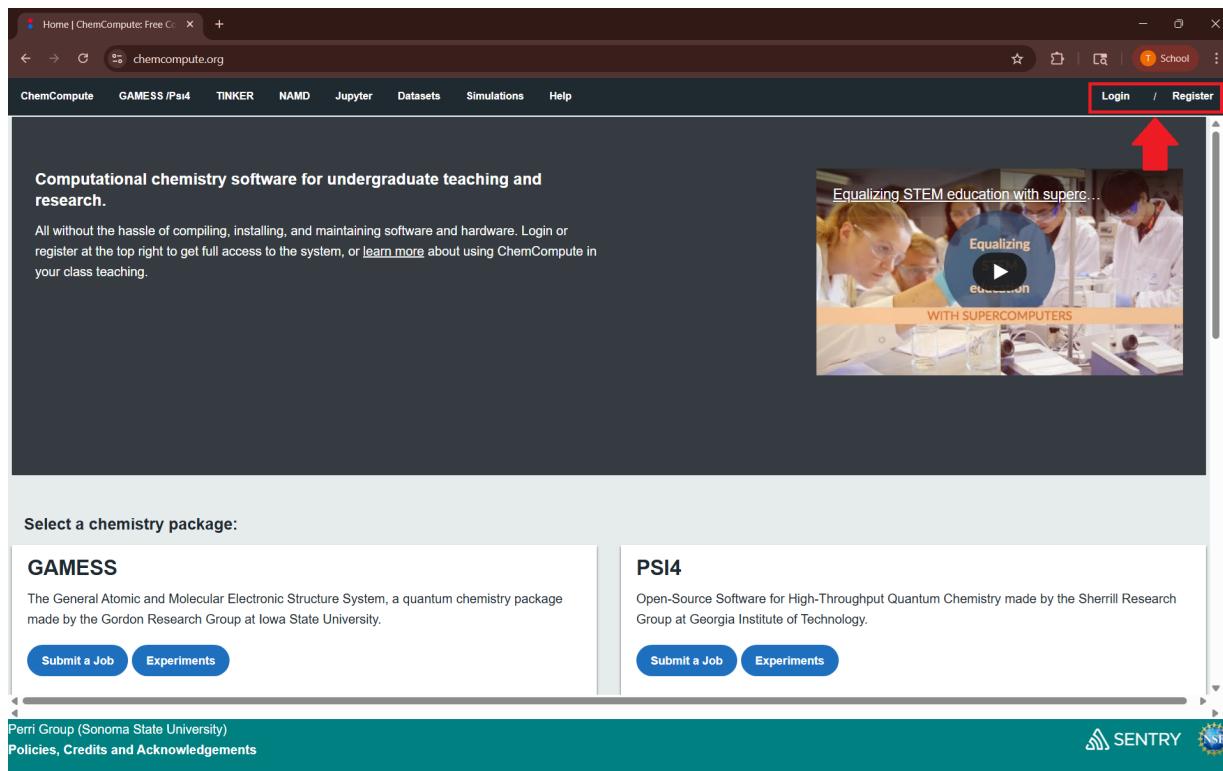


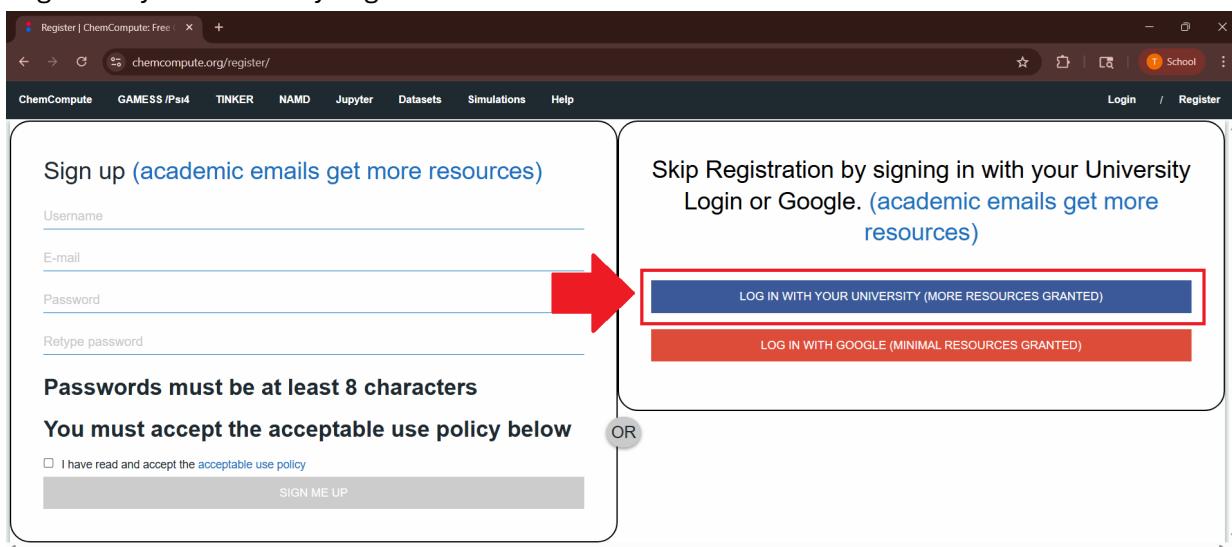
Document 1: Getting Started

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).



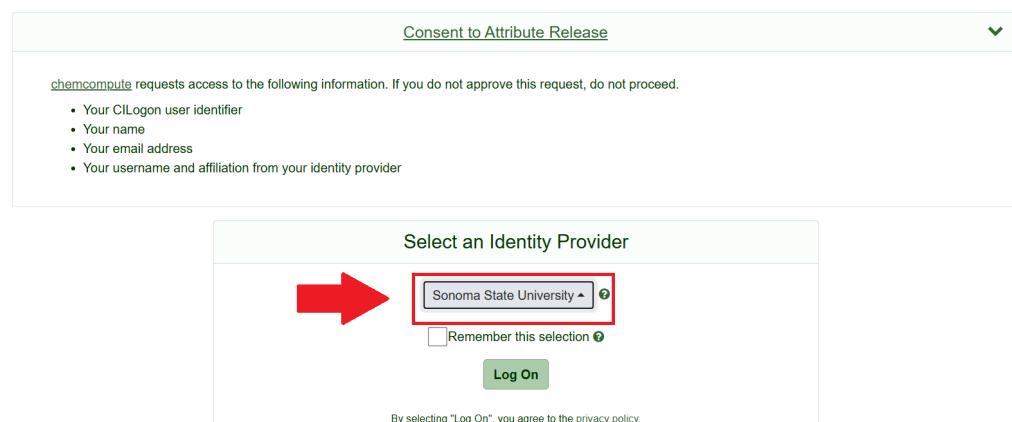
The screenshot shows the ChemCompute homepage. At the top right, there is a 'Login / Register' button. A red arrow points to this button. The page features a banner with the text 'Equalizing STEM education with super...' and 'WITH SUPERCOMPUTERS'. Below the banner, there are sections for 'Select a chemistry package:' with options for 'GAMESS' and 'PSI4', each with 'Submit a Job' and 'Experiments' buttons. The bottom of the page includes links for 'Perri Group (Sonoma State University)', 'Policies, Credits and Acknowledgements', and logos for 'SENTRY' and 'NSF'.

3. Login with your University Login.



The screenshot shows the ChemCompute registration page. On the left, there is a form for 'Sign up (academic emails get more resources)' with fields for 'Username', 'E-mail', 'Password', and 'Relype password'. Below these fields, there are two required terms: 'Passwords must be at least 8 characters' and 'You must accept the acceptable use policy below'. A red arrow points from the 'Sign up' section to the 'LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)' button. On the right, there is a box for 'Skip Registration by signing in with your University Login or Google. (academic emails get more resources)' with two buttons: 'LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)' (highlighted with a red box) and 'LOG IN WITH GOOGLE (MINIMAL RESOURCES GRANTED)'. A 'OR' button is located between the two sections.

4. Select your University from the dropdown menu.



Consent to Attribute Release

chemcompute requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

Select an Identity Provider

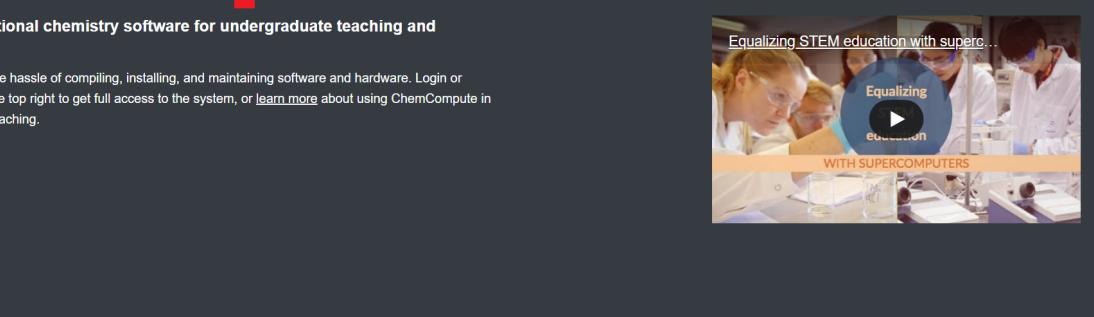
Sonoma State University

Remember this selection

By selecting "Log On", you agree to the [privacy policy](#).

For questions about this site, please see the FAQs or send email to help@cilogon.org.
Know your responsibilities for using the CILogon Service.
See acknowledgements of support for this site.

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



Home | ChemCompute: Free Cloud Computing for Chemistry

ChemCompute GAMESS /Psi4 TINKER NAMD **Jupyter** Datasets Simulations Help

Tanner's Dashboard

Computational chemistry software for undergraduate teaching and research.

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.

Equalizing STEM education with supercomputers

Equalizing education WITH SUPERCOMPUTERS

Select a chemistry package:

GAMESS

The General Atomic and Molecular Electronic Structure System, a quantum chemistry package made by the Gordon Research Group at Iowa State University.

[Submit a Job](#) [Experiments](#)

PSI4

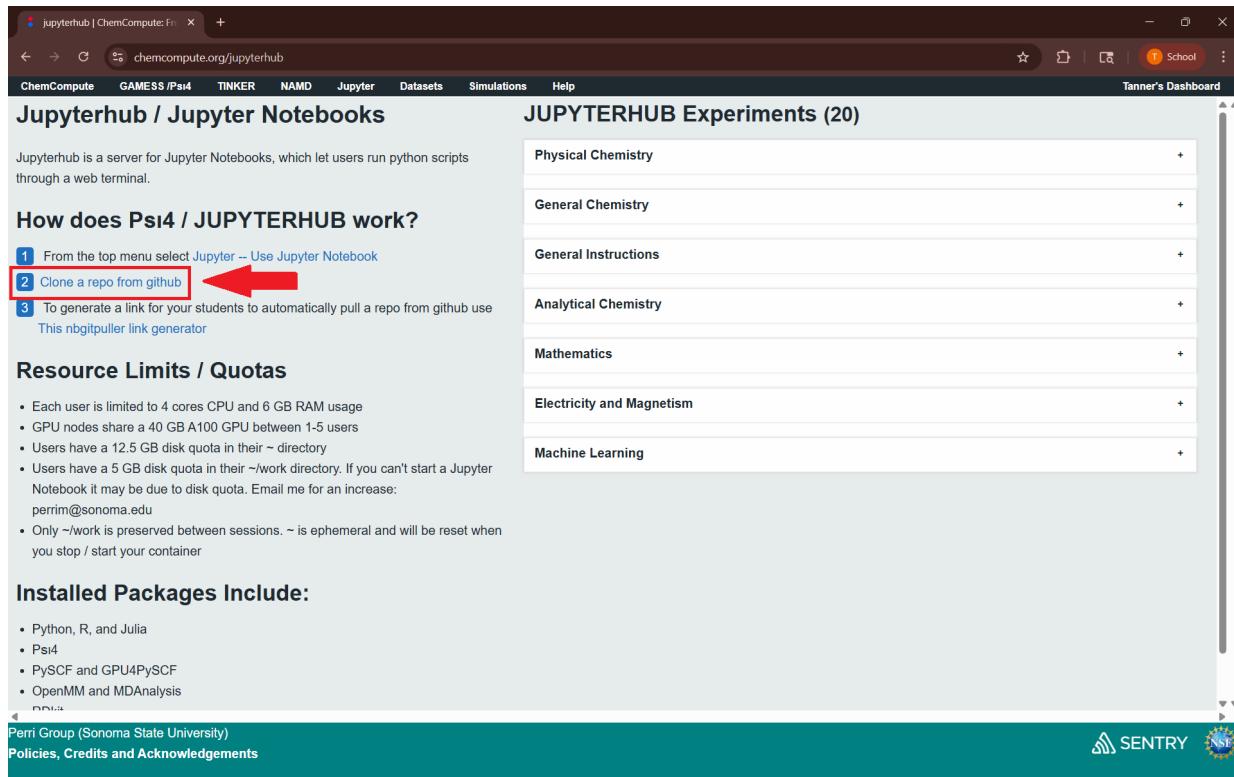
Open-Source Software for High-Throughput Quantum Chemistry made by the Sherrill Research Group at Georgia Institute of Technology.

[Submit a Job](#) [Experiments](#)

Peri Group (Sonoma State University)
Policies, Credits and Acknowledgements

SENTRY 

6. Select “clone a repo from github”.



Jupyterhub is a server for Jupyter Notebooks, which let users run python scripts through a web terminal.

How does Psi4 / JUPYTERHUB work?

- 1 From the top menu select Jupyter -- Use Jupyter Notebook
- 2 **Clone a repo from github**
- 3 To generate a link for your students to automatically pull a repo from github use [This nbgitpuller link generator](#)

Resource Limits / Quotas

- Each user is limited to 4 cores CPU and 6 GB RAM usage
- GPU nodes share a 40 GB A100 GPU between 1-5 users
- Users have a 12.5 GB disk quota in their ~ directory
- Users have a 5 GB disk quota in their ~/work directory. If you can't start a Jupyter Notebook it may be due to disk quota. Email me for an increase: perm@sonoma.edu
- Only ~/work is preserved between sessions. ~ is ephemeral and will be reset when you stop / start your container

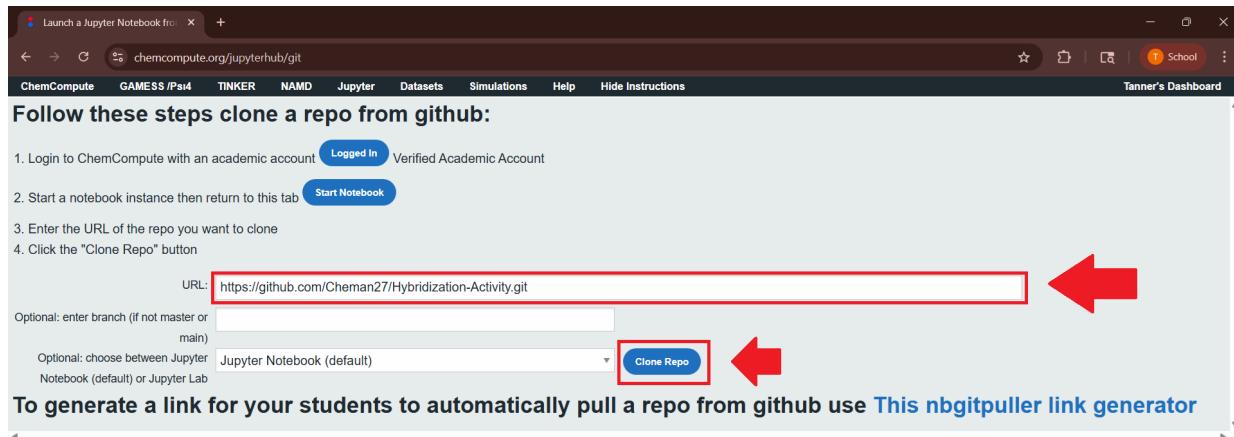
Installed Packages Include:

- Python, R, and Julia
- Psi4
- PySCF and GPU4PySCF
- OpenMM and MDAnalysis

Perri Group (Sonoma State University)
Policies, Credits and Acknowledgements

SENTRY NSF

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



Follow these steps clone a repo from github:

1. Login to ChemCompute with an academic account [Logged In](#) Verified Academic Account
2. Start a notebook instance then return to this tab [Start Notebook](#)
3. Enter the URL of the repo you want to clone
4. Click the “Clone Repo” button

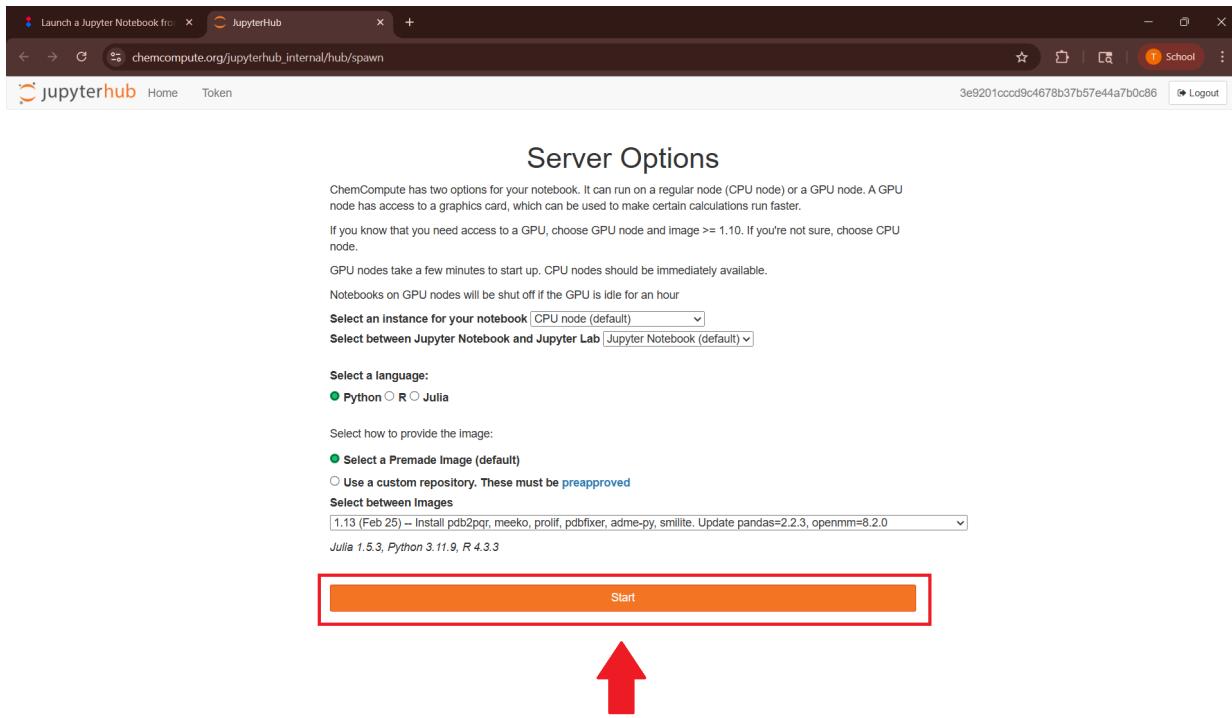
URL: <https://github.com/Cheman27/Hybridization-Activity.git>

Optional: enter branch (if not master or main)
Optional: choose between Jupyter Notebook (default) Notebook (default) or Jupyter Lab

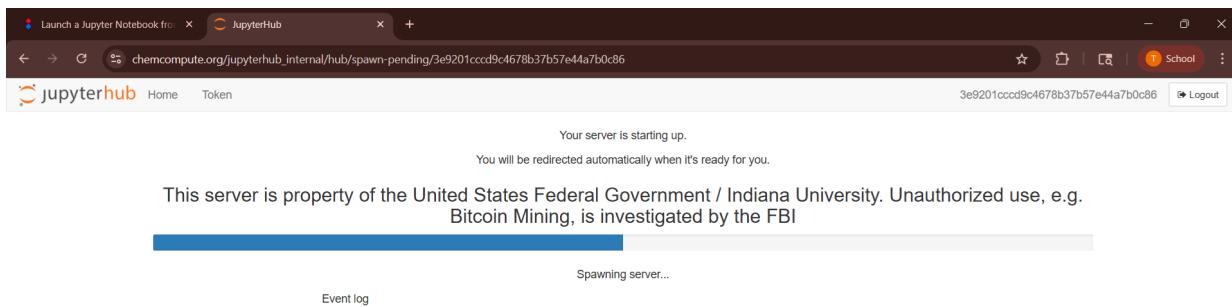
Clone Repo

To generate a link for your students to automatically pull a repo from github use [This nbgitpuller link generator](#)

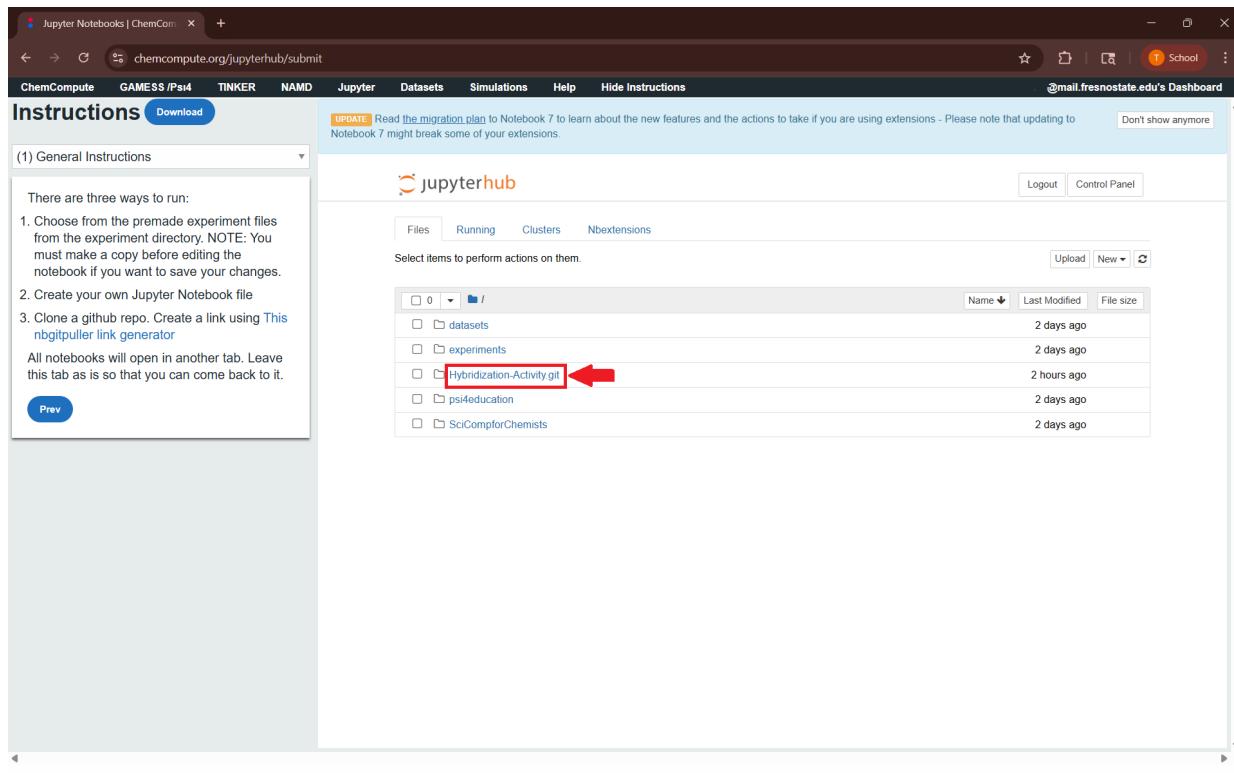
8. Once redirected, ensure “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, then press start.



9. You will be redirected to a new tab. This may take a minute or two to load.



10. Once loading is complete, press Hybridization-Activity.git. If this folder does not show up, click on the tab from step 7 and repeat steps 7 – 9.

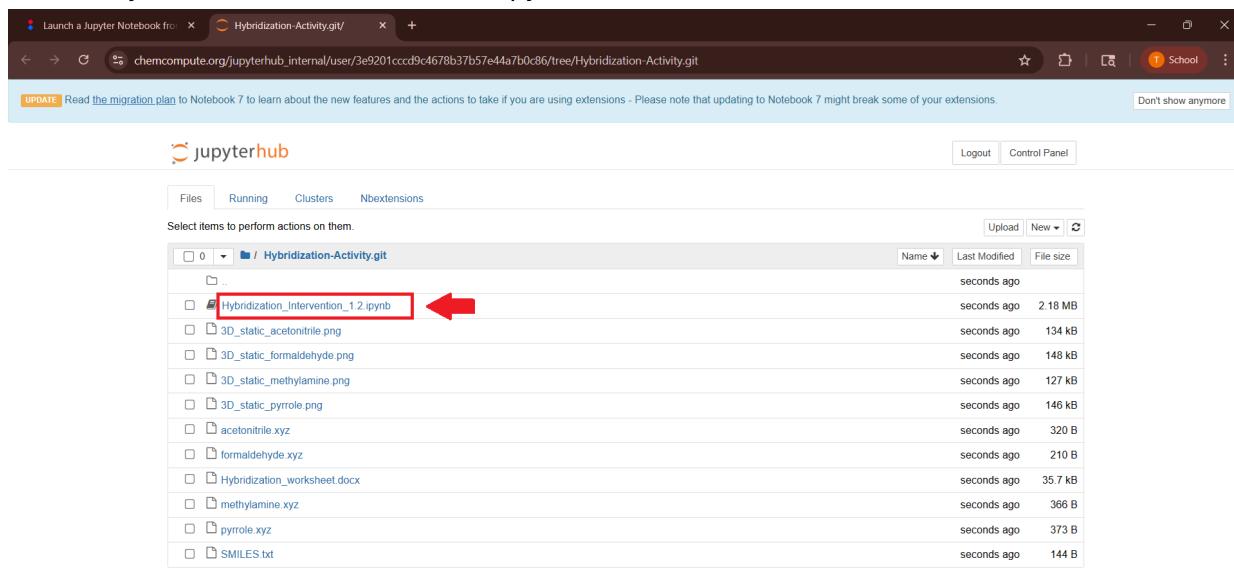


The screenshot shows a web browser window with the following details:

- Address Bar:** chemcompute.org/jupyterhub/submit
- Header:** ChemCompute, GAMESS/PS4, TINKER, NAMD, Jupyter, Datasets, Simulations, Help, Hide Instructions, @mail.fresnostate.edu's Dashboard
- Left Sidebar (Instructions):**
 - (1) General Instructions
 - There are three ways to run:
 1. Choose from the premade experiment files from the experiment directory. NOTE: You must make a copy before editing the notebook if you want to save your changes.
 2. Create your own Jupyter Notebook file
 3. Clone a github repo. Create a link using [This nbgitpuller link generator](#)
 - All notebooks will open in another tab. Leave this tab as is so that you can come back to it.
- Main Content (jupyterhub):**
 - Files tab selected.
 - File list:
 - 0 /
 - datasets
 - experiments
 - Hybridization-Activity.git (highlighted with a red box and arrow)
 - psi4education
 - SciComforChemists
 - File list table:

Name	Last Modified	File size
2 days ago	2 days ago	
2 hours ago	2 hours ago	
2 days ago	2 days ago	
2 days ago	2 days ago	

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

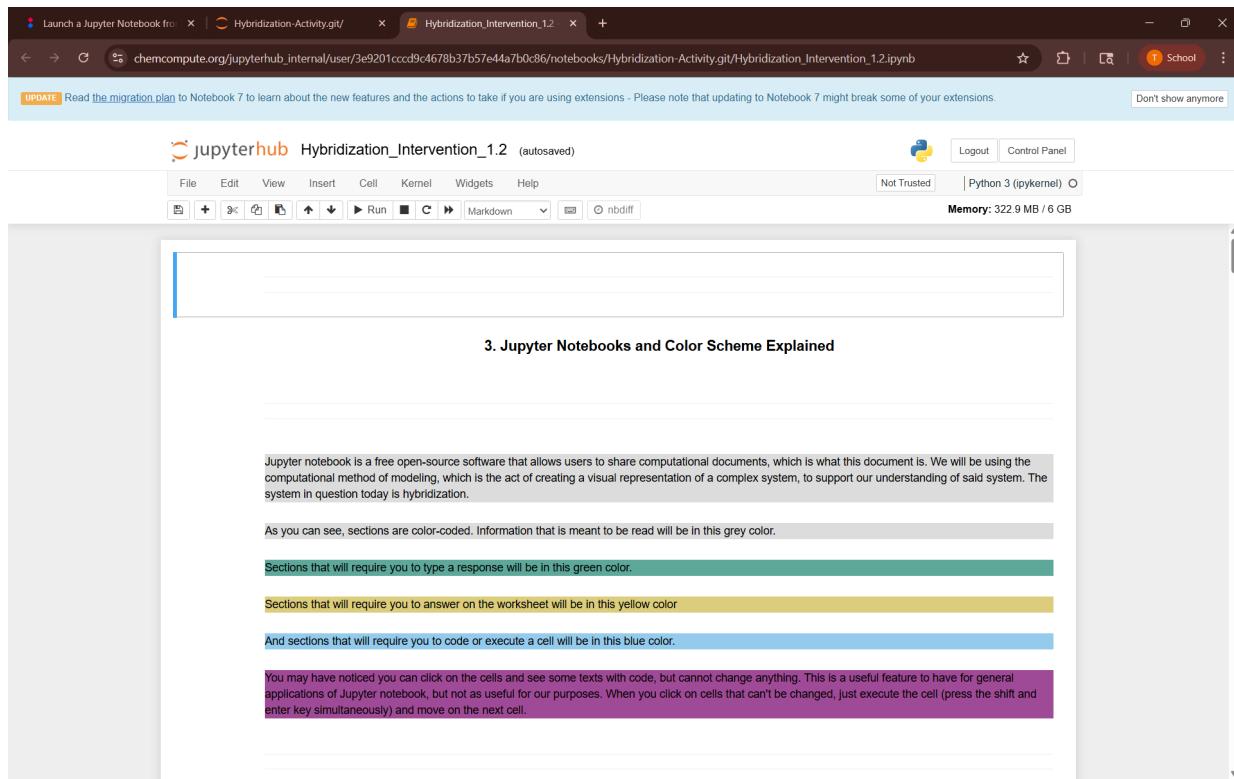


The screenshot shows a web browser window with the following details:

- Address Bar:** chemcompute.org/jupyterhub/internal/user/3e9201cccd9c4678b37b57e44a7b0c86/tree/Hybridization-Activity.git
- Header:** ChemCompute, GAMESS/PS4, TINKER, NAMD, Jupyter, Datasets, Simulations, Help, Hide Instructions, @mail.fresnostate.edu's Dashboard
- Left Sidebar (Instructions):**
 - (1) General Instructions
 - There are three ways to run:
 1. Choose from the premade experiment files from the experiment directory. NOTE: You must make a copy before editing the notebook if you want to save your changes.
 2. Create your own Jupyter Notebook file
 3. Clone a github repo. Create a link using [This nbgitpuller link generator](#)
 - All notebooks will open in another tab. Leave this tab as is so that you can come back to it.
- Main Content (jupyterhub):**
 - Files tab selected.
 - File list:
 - 0 / Hybridization-Activity.git
 - Hybridization_Intervention_1.2.ipynb (highlighted with a red box and arrow)
 - 3D_static_acetonitrile.png
 - 3D_static_formaldehyde.png
 - 3D_static_methylamine.png
 - 3D_static_pyrrrole.png
 - acetonitrile.xyz
 - formaldehyde.xyz
 - Hybridization_worksheet.docx
 - methylamine.xyz
 - pyrrrole.xyz
 - SMILES.txt
 - File list table:

Name	Last Modified	File size
seconds ago	2.18 MB	
seconds ago	134 kB	
seconds ago	148 kB	
seconds ago	127 kB	
seconds ago	146 kB	
seconds ago	320 B	
seconds ago	210 B	
seconds ago	35.7 kB	
seconds ago	366 B	
seconds ago	373 B	
seconds ago	144 B	

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



The screenshot shows a Jupyter Notebook interface with the title "jupyterhub Hybridization_Intervention_1.2 (autosaved)". The top bar includes a "Logout" button and a "Control Panel" button. A message at the top of the notebook says: "UPDATE Read the migration plan to Notebook 7 to learn about the new features and the actions to take if you are using extensions - Please note that updating to Notebook 7 might break some of your extensions." Below this, the notebook content is displayed in a large text area. The content is a color-coded legend for sections:

- Grey background: "3. Jupyter Notebooks and Color Scheme Explained"
- Grey background: "As you can see, sections are color-coded. Information that is meant to be read will be in this grey color."
- Green background: "Sections that will require you to type a response will be in this green color."
- Yellow background: "Sections that will require you to answer on the worksheet will be in this yellow color"
- Blue background: "And sections that will require you to code or execute a cell will be in this blue color."
- Purple background: "You may have noticed you can click on the cells and see some texts with code, but cannot change anything. This is a useful feature to have for general applications of Jupyter notebook, but not as useful for our purposes. When you click on cells that can't be changed, just execute the cell (press the shift and enter key simultaneously) and move on the next cell."

