

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 red box around the "Login / Register" button. A red arrow points upwards from the bottom of the page towards this button. The main content area features a banner about equalizing STEM education with supercomputers. Below the banner, there are two sections: "Select a chemistry package:" with options for GAMESS and PSI4, each with "Submit a Job" and "Experiments" buttons. At the bottom, there is a teal footer bar with 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 Retype password. It also includes a note about password length ("Passwords must be at least 8 characters") and a checkbox for accepting the acceptable use policy ("You must accept the acceptable use policy below"). A large red arrow points from the "Sign up" section to the "Skip Registration" section on the right. On the right, there is a box for "Skip Registration by signing in with your University Login or Google. (academic emails get more resources)". It contains two buttons: "LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)" (highlighted with a red border) and "LOG IN WITH GOOGLE (MINIMAL RESOURCES GRANTED)". Below these buttons is the text "OR".

4. Select your University from the dropdown menu.

The screenshot shows a web browser window titled "Welcome To The CILogon Open". The URL in the address bar is "cilogon.org/authorize?response_type=code&scope=openid+email+profile+org.cilogon.userInfo&client_id=myproxy%3Aoa4mp%2C2012%3A%2Fclient_id%2F251c447c13457...". The main content is a "Consent to Attribute Release" form. It asks for permission to access information from "chemcompute", specifically the user's CILogon user identifier, name, email address, and affiliation. Below this is a "Select an Identity Provider" section. A red arrow points to a dropdown menu where "Sonoma State University" is selected. There is also a checkbox for "Remember this selection" and a "Log On" button. At the bottom, there is a note about agreeing to the privacy policy.

5. Select Jupyter.

The screenshot shows a web browser window titled "Home | ChemCompute: Free Cloud Computing for Chemistry". The URL in the address bar is "chemcompute.org". The top navigation bar includes links for "ChemCompute", "GAMESS /Psi4", "TINKER", "NAMD", "Jupyter" (which is highlighted with a red box and a red arrow pointing to it), "Datasets", "Simulations", and "Help". The main content area features a banner with the text "Equalizing STEM education with supercomputers" and "WITH SUPERCOMPUTERS". Below the banner, there is a section titled "Computational chemistry software for undergraduate teaching and research." It explains that users can log in or register to get full access. There is also a "learn more" link. To the right of this text is a video thumbnail showing students in a lab. Below this, there are two sections: "Select a chemistry package:" with options for "GAMESS" and "PSI4", each with "Submit a Job" and "Experiments" buttons, and "Peri Group (Sonoma State University)" with links for "Policies, Credits and Acknowledgements". At the bottom right, there are logos for "SENTRY" and "NSF".

6. Select “clone a repo from github”.

Jupyterhub / Jupyter Notebooks

How does Psi4 / JUPYTERHUB work?

- From the top menu select Jupyter -- Use Jupyter Notebook
- Clone a repo from github**
- 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: perrim@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:

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

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

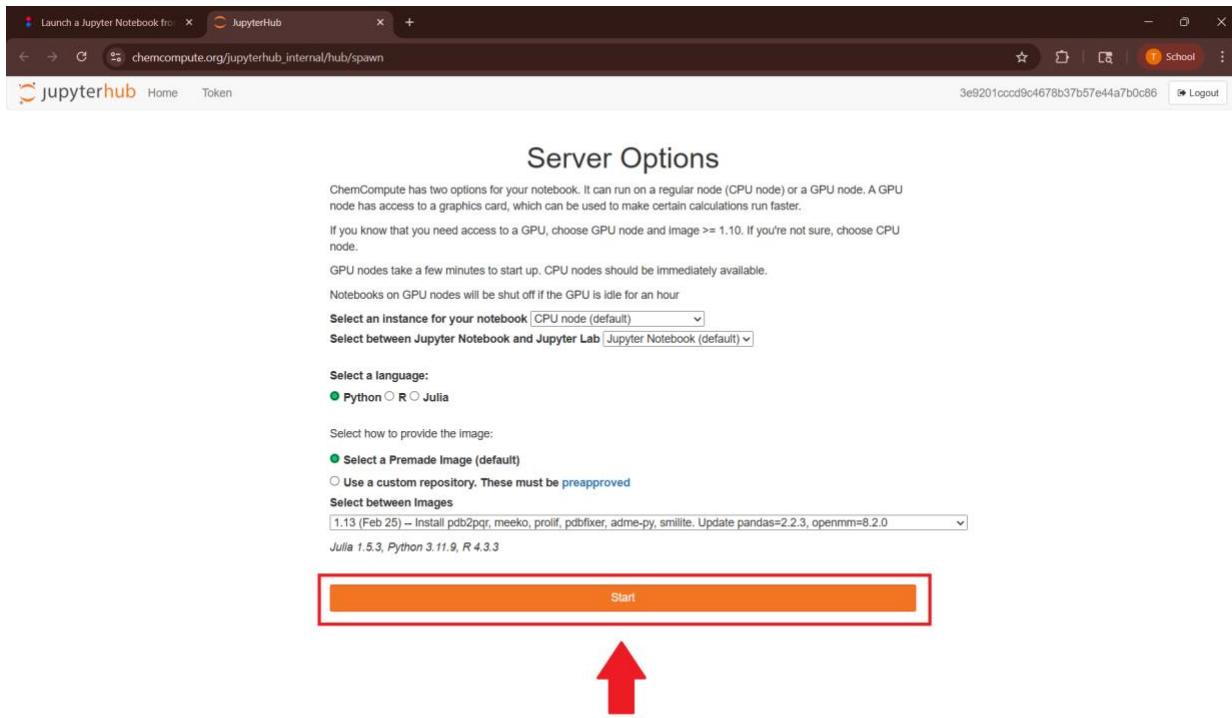
Optional: enter branch (if not master or main)

Optional: choose between Jupyter Notebook (default) or Jupyter Lab

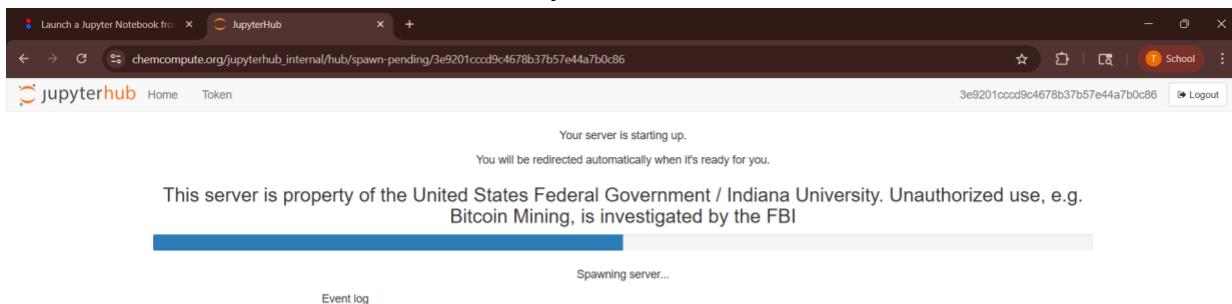
Clone Repo

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 while 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.

Jupyter Notebooks | ChemCom

chemcompute.org/jupyterhub/submit

ChemCompute GAMESS /Psi4 TINKER NAMD Jupyter Datasets Simulations Help Hide Instructions

Instructions Download

(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 ngitpuller link generator](#)

All notebooks will open in another tab. Leave this tab as is so that you can come back to it.

Logout Control Panel

Files Running Clusters Nbextensions

Select items to perform actions on them.

Upload New

Name	Last Modified	File size
Hybridization-Activity.git	2 days ago	
datasets	2 days ago	
experiments	2 hours ago	
psieducation	2 days ago	
SciComforChemists	2 days ago	

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

Launch a Jupyter Notebook fro Hybridization-Activity.git

chemcompute.org/jupyterhub_internal/user/3e9201cccd9c4678b37b57e44a7b0c86/tree/Hybridization-Activity.git

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. Don't show anymore

jupyterhub

Logout Control Panel

Files Running Clusters Nbextensions

Select items to perform actions on them.

Upload New

Name	Last Modified	File size
Hybridization-Activity.git	seconds ago	
Hybridization_Intervention_1.2.ipynb	seconds ago	2.18 MB
3D_static_acetonitrile.png	seconds ago	134 kB
3D_static_formaldehyde.png	seconds ago	148 kB
3D_static_methylamine.png	seconds ago	127 kB
3D_static_pyrrrole.png	seconds ago	146 kB
acetonitrile.xyz	seconds ago	320 B
formaldehyde.xyz	seconds ago	210 B
Hybridization_worksheet.docx	seconds ago	35.7 kB
methylamine.xyz	seconds ago	366 B
pyrrrole.xyz	seconds ago	373 B
SMILES.txt	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 tabs for "Launch a Jupyter Notebook from..." and "Hybridization_Activity.git/ Hybridization_Intervention_1.2". A message at the top says "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." The toolbar below has options like File, Edit, View, Insert, Cell, Kernel, Widgets, Help, and a Python 3 (ipykernel) kernel indicator. The main area contains a section titled "3. Jupyter Notebooks and Color Scheme Explained". Below it, several colored boxes illustrate the color scheme: a grey box for "Information that is meant to be read will be in this grey color.", a green box for "Sections that will require you to type a response will be in this green color.", a yellow box for "Sections that will require you to answer on the worksheet will be in this yellow color", and a blue box for "And sections that will require you to code or execute a cell will be in this blue color.". A note at the bottom states: "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."

