

# **Cybershuttle MD Local Agent**

## **Tutorial Instructions**

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V1.0

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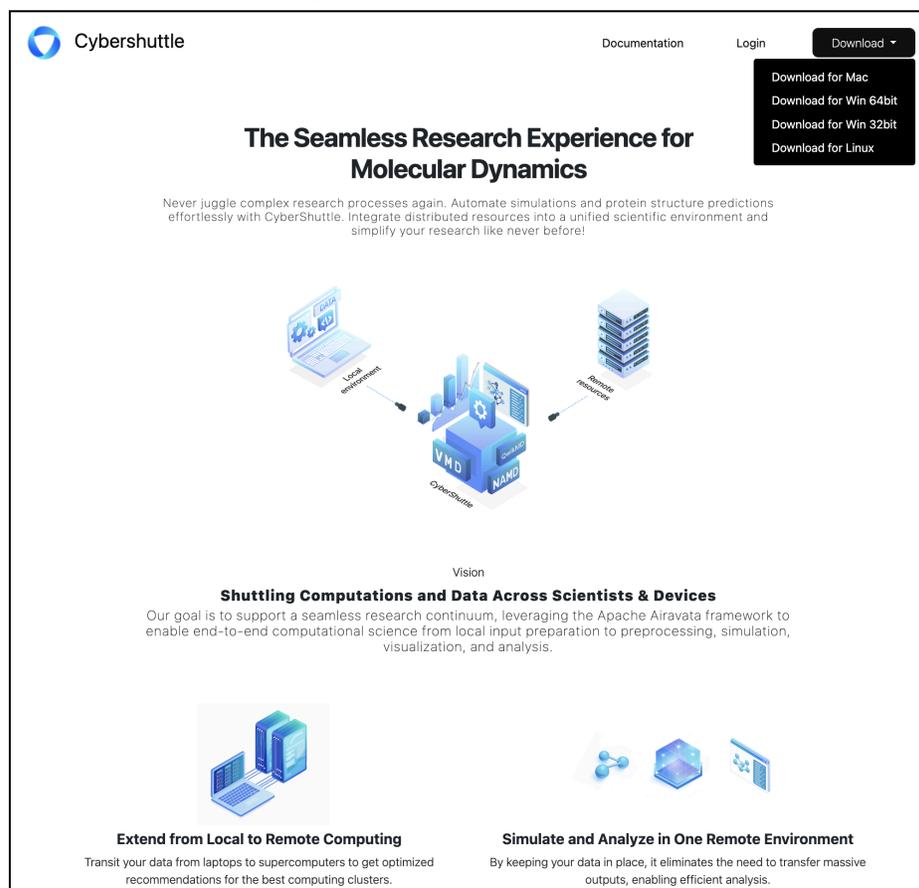
# Cybershuttle (CS) Local Agent for Molecular Dynamics (MD)

**Cybershuttle (CS) Local Agent** is a desktop client powered by Apache Airavata middleware. It enables domain scientists, researchers, and students to seamlessly execute their research workflows across a variety of resources, including local laptops, remote computing resources, and cloud environments. Additionally, it facilitates connections with multiple data locations of their choice, ensuring a smooth and efficient research experience.

In this documentation, we provide detailed instructions for using the CS Local Agent with Molecular Dynamics (MD) applications, specifically focusing on running NAMD simulations and performing post-analysis tasks. You will learn how to initiate VMD and Jupyter notebooks to run on remote data seamlessly.

## Download MD Local Agent

1. Visit <https://md.cybershuttle.org/>
2. Download Local Agent for you



The screenshot shows the Cybershuttle MD Web Portal homepage. At the top left is the Cybershuttle logo. Navigation links for 'Documentation', 'Login', and 'Download' are in the top right. A 'Download' dropdown menu is open, showing options for 'Download for Mac', 'Download for Win 64bit', 'Download for Win 32bit', and 'Download for Linux'. The main heading is 'The Seamless Research Experience for Molecular Dynamics'. Below this is a sub-heading: 'Never juggle complex research processes again. Automate simulations and protein structure predictions effortlessly with CyberShuttle. Integrate distributed resources into a unified scientific environment and simplify your research like never before!'. A central diagram illustrates the workflow: 'Local environment' (laptop) connects to 'CyberShuttle' (central hub with VMD and NAMD icons), which connects to 'Remote resource' (server rack). Below the diagram is the section 'Vision: Shuttling Computations and Data Across Scientists & Devices'. The text states: 'Our goal is to support a seamless research continuum, leveraging the Apache Airavata framework to enable end-to-end computational science from local input preparation to preprocessing, simulation, visualization, and analysis.' Two key features are highlighted: 'Extend from Local to Remote Computing' (Transit your data from laptops to supercomputers to get optimized recommendations for the best computing clusters.) and 'Simulate and Analyze in One Remote Environment' (By keeping your data in place, it eliminates the need to transfer massive outputs, enabling efficient analysis.)

Image - Cybershuttle MD Web Portal

3. Install the Local Agent.

# Local Agent Login

1. After the installation open the Local Agent.

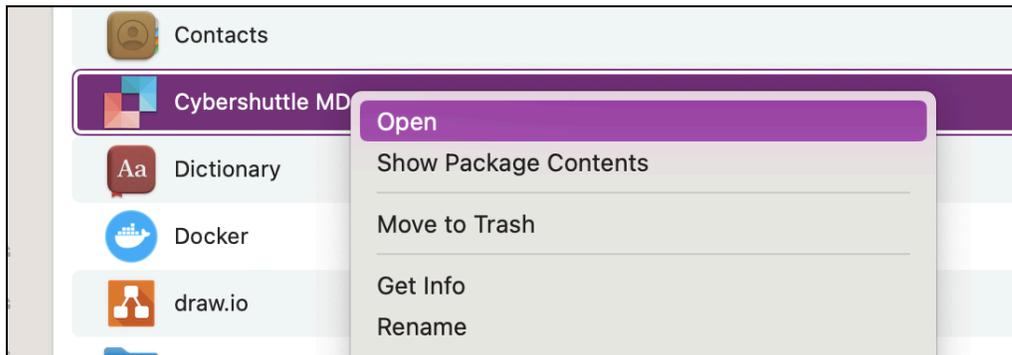


Image - Open the Local Agent

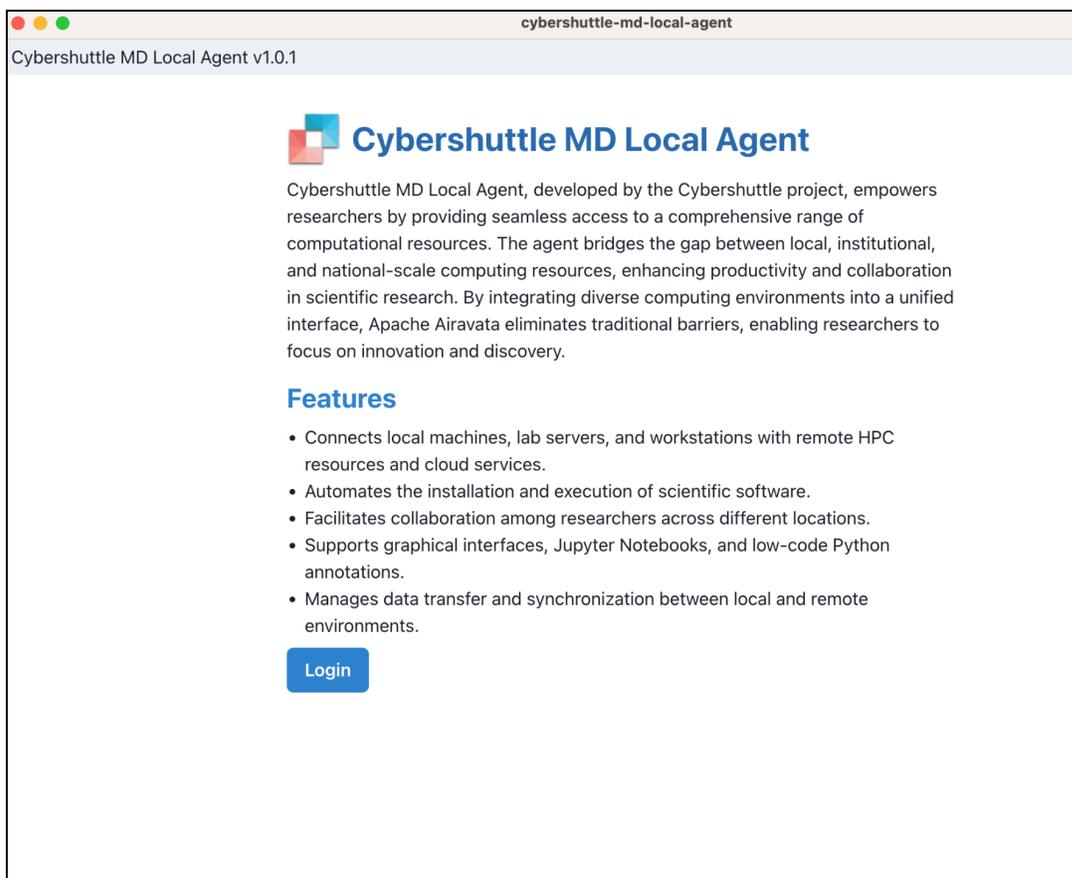


Image - Local Agent Home Page

2. Login with your institutional login through CILogon

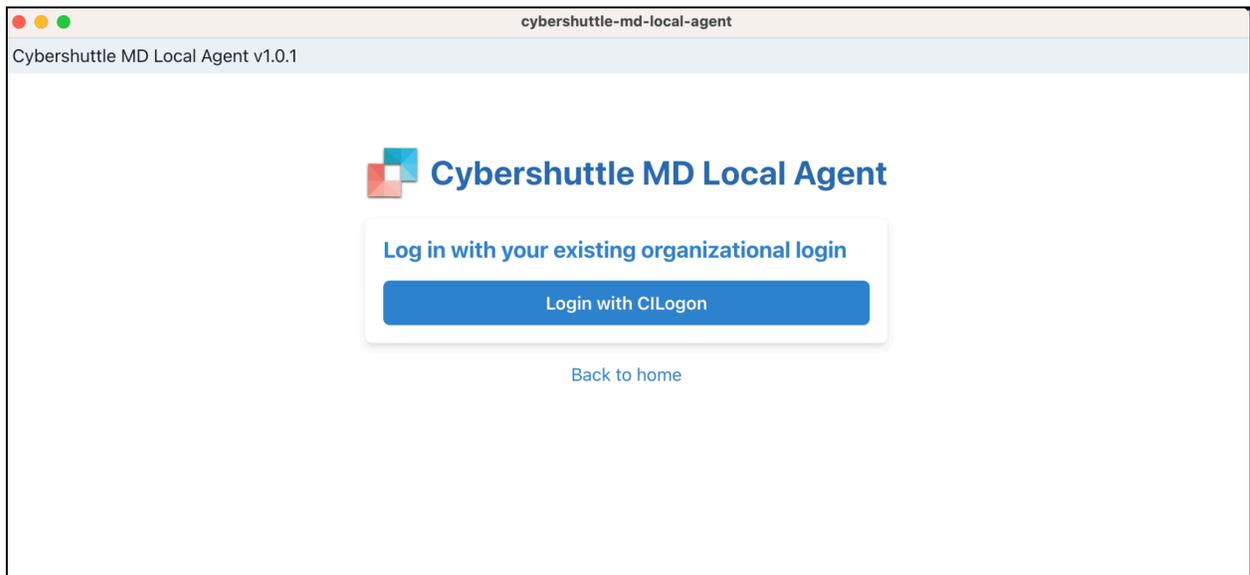


Image - Login Page

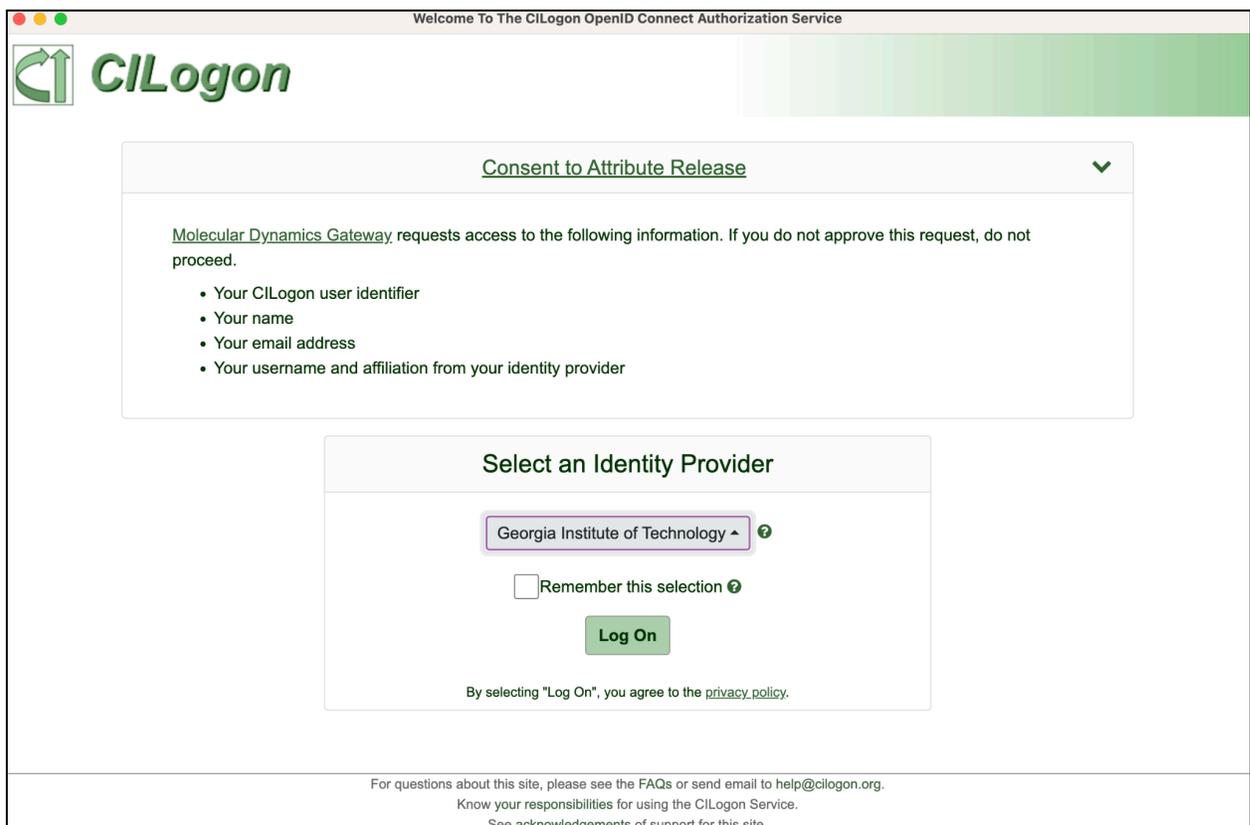


Image - CILogon for Institutional Login

3. You are in the main workspace. For new users this space would be empty.

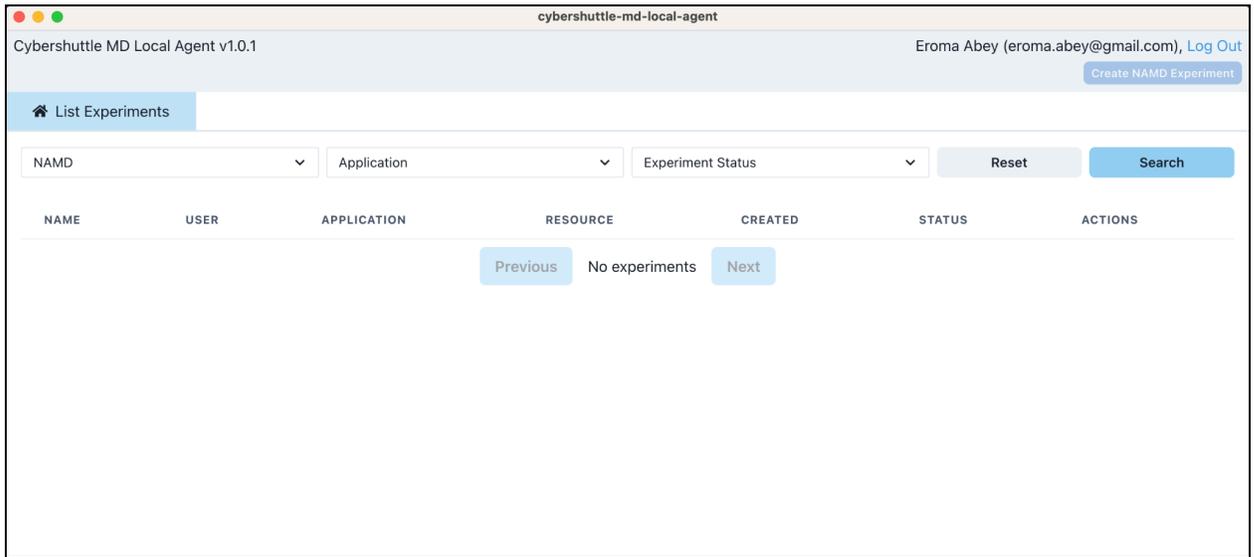


Image - Main View Before User Activation

4. Your account will be activated in order to launch NAMD jobs in recomputing resources.
5. You will see the 'Create NAMD Experiment' button enabled when activated.

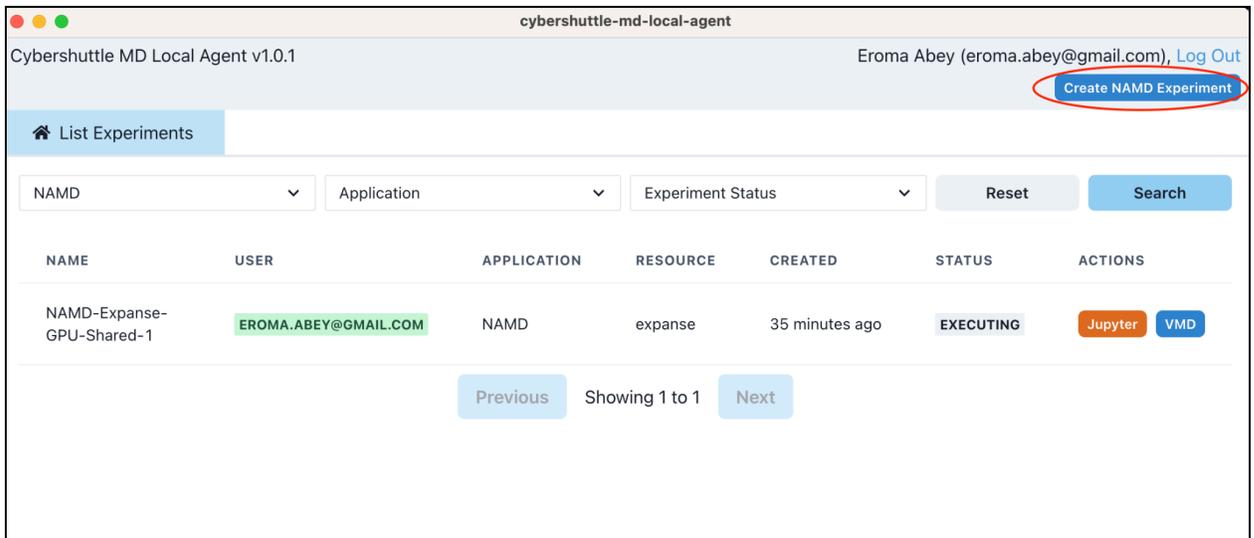


Image - Main View After User Activation

# Create NAMD Experiment

1. To launch a job on the remote resource, use the “Create NAMD Experiment” button in the top right corner.

Image - Create NAMD Experiment

2. In the interface provide the required inputs and computing resources and ‘Save and Launch’ the experiment.

Allocation

Default

Compute Resource

expanse

**Settings for queue gpu-shared**

<b>1</b>	<b>10</b>	<b>30 minutes</b>	<b>MB</b>
Node Count	Core Count	Time Limit	Physical Memory

Email Settings

Receive email notification of experiment status

[Back to Experiments](#) 
Save
Save and Launch

Image - Computing Resource Section

3. For the workshop purposes, you will launch under 'Default' allocation and Expanse resource.
4. These are by default made available for you.
5. Once launched, you will be directed to the main view.

## Local Agent Experiment View

1. After the experiment launch, the main view will have the experiment listed with status.

The screenshot shows the 'List Experiments' view in the Cybershuttle MD Local Agent v1.0.1. The interface includes a search bar with filters for 'NAMD', 'Application', and 'Experiment Status', along with 'Reset' and 'Search' buttons. A table displays the following experiment:

NAME	USER	APPLICATION	RESOURCE	CREATED	STATUS	ACTIONS
NAMD-Expanse-GPU-Shared-1	EROMA.ABEY@GMAIL.COM	NAMD	expanse	35 minutes ago	EXECUTING	Jupyter VMD

Navigation controls at the bottom show 'Previous', 'Showing 1 to 1', and 'Next' buttons.

Image - Experiment View

2. This 'Experiment Status' auto-refreshes. For further information, click on the name and navigate to view more details.

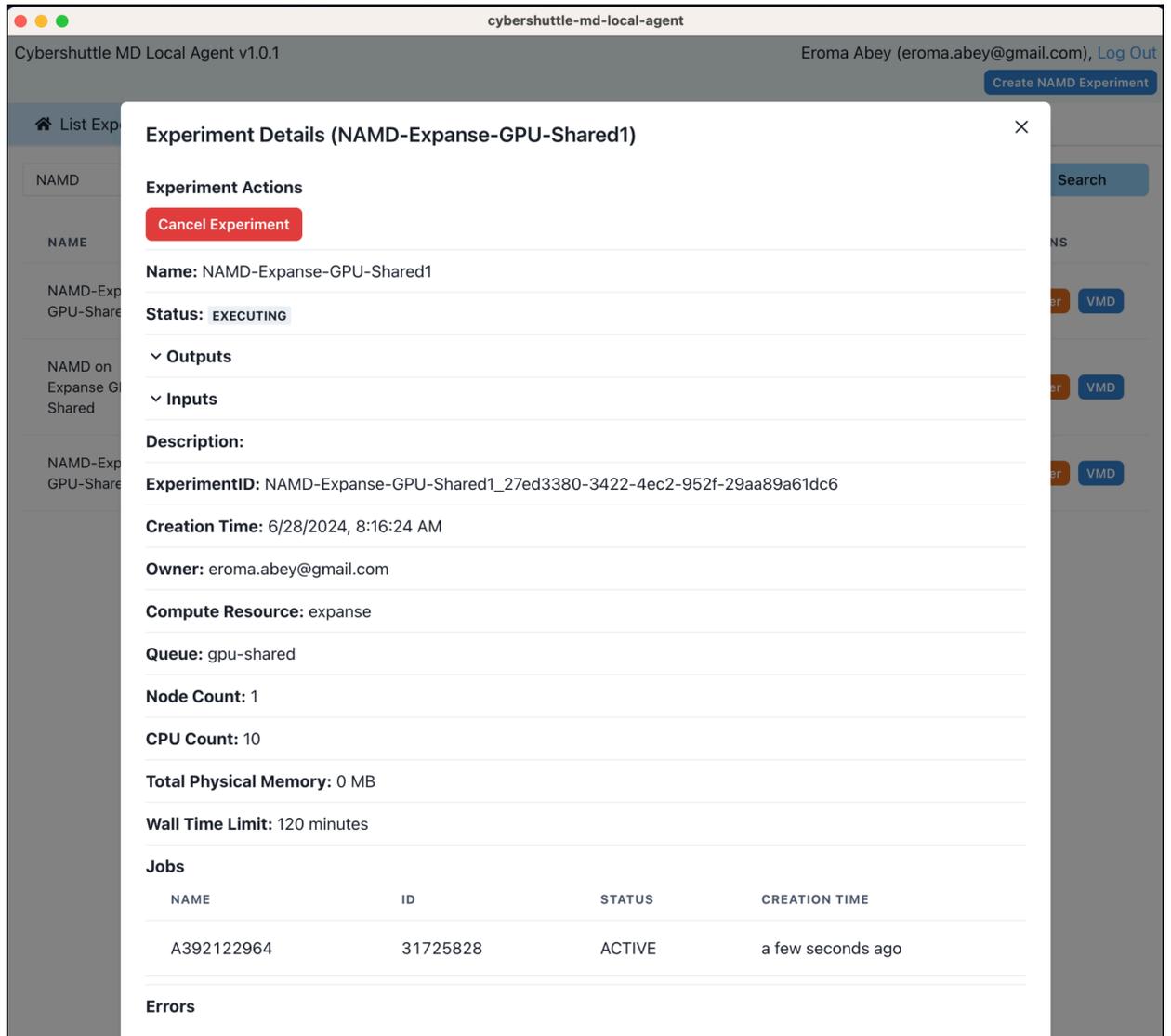


Image - Detail Experiment View

3. The 'Experiment Details' view displays the status and details of a remote resource job. It shows the inputs provided and outputs generated by the job.

## VMD and Jupyter Notebook

1. Click the VMD button in line with the experiment to initiate a VMD and view and visualize the outputs.

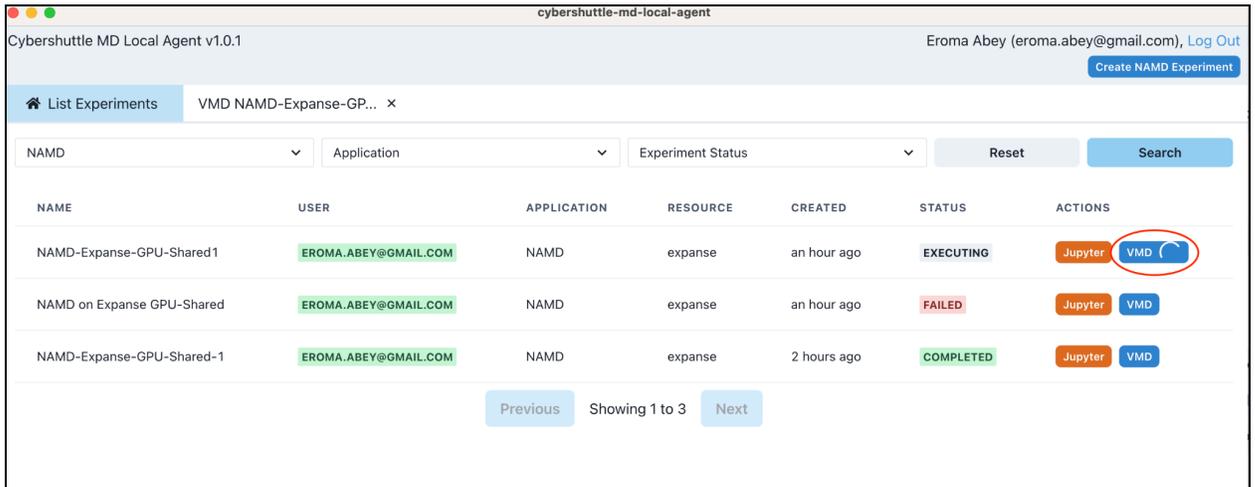


Image - Initiate the VMD for an Experiment

2. The VMD opens a separate tab.

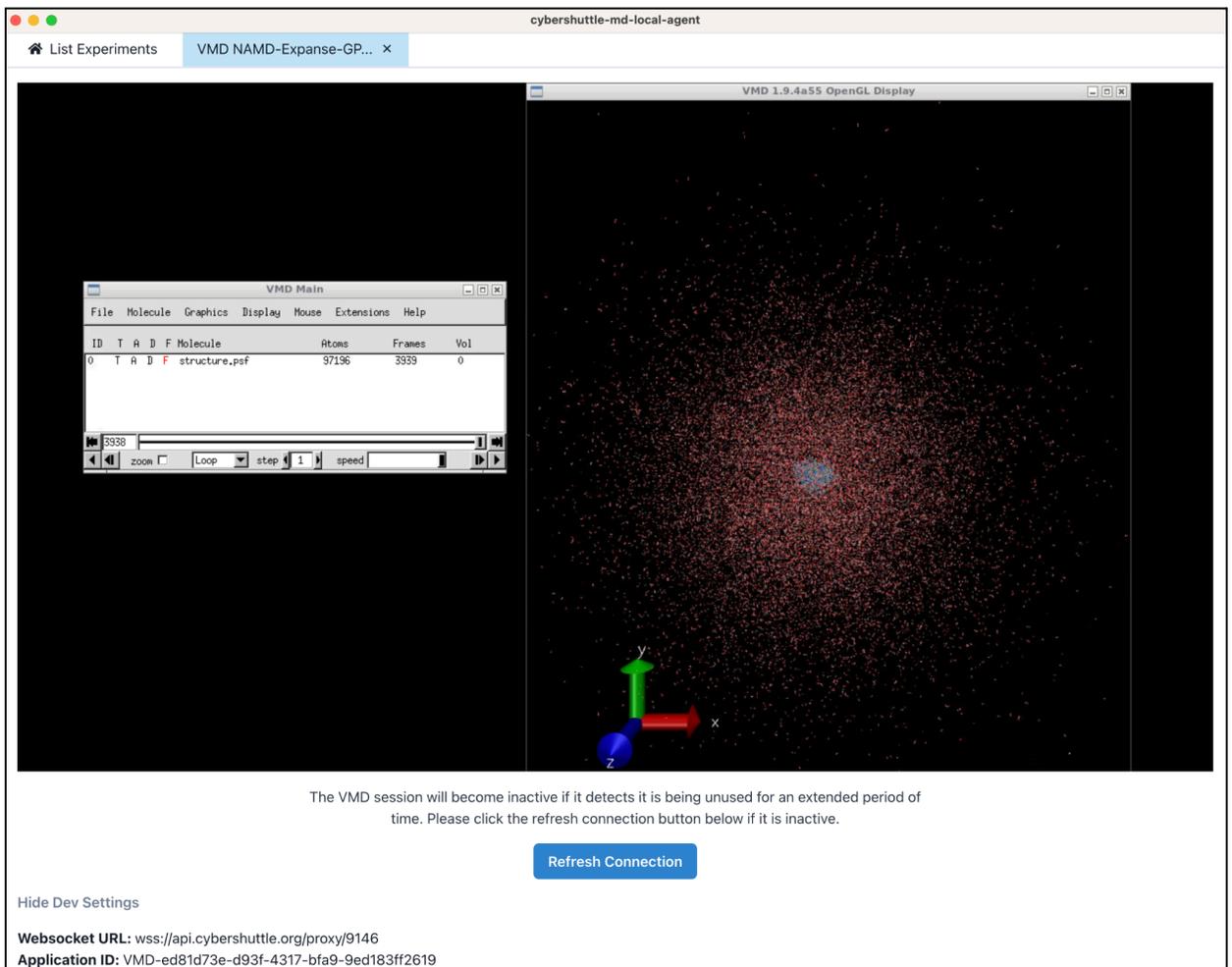


Image - VMD within Local Agent

3. Please note that closing the VMD tab will terminate the session. Depending on computing resource availability, another session may take time to initiate.

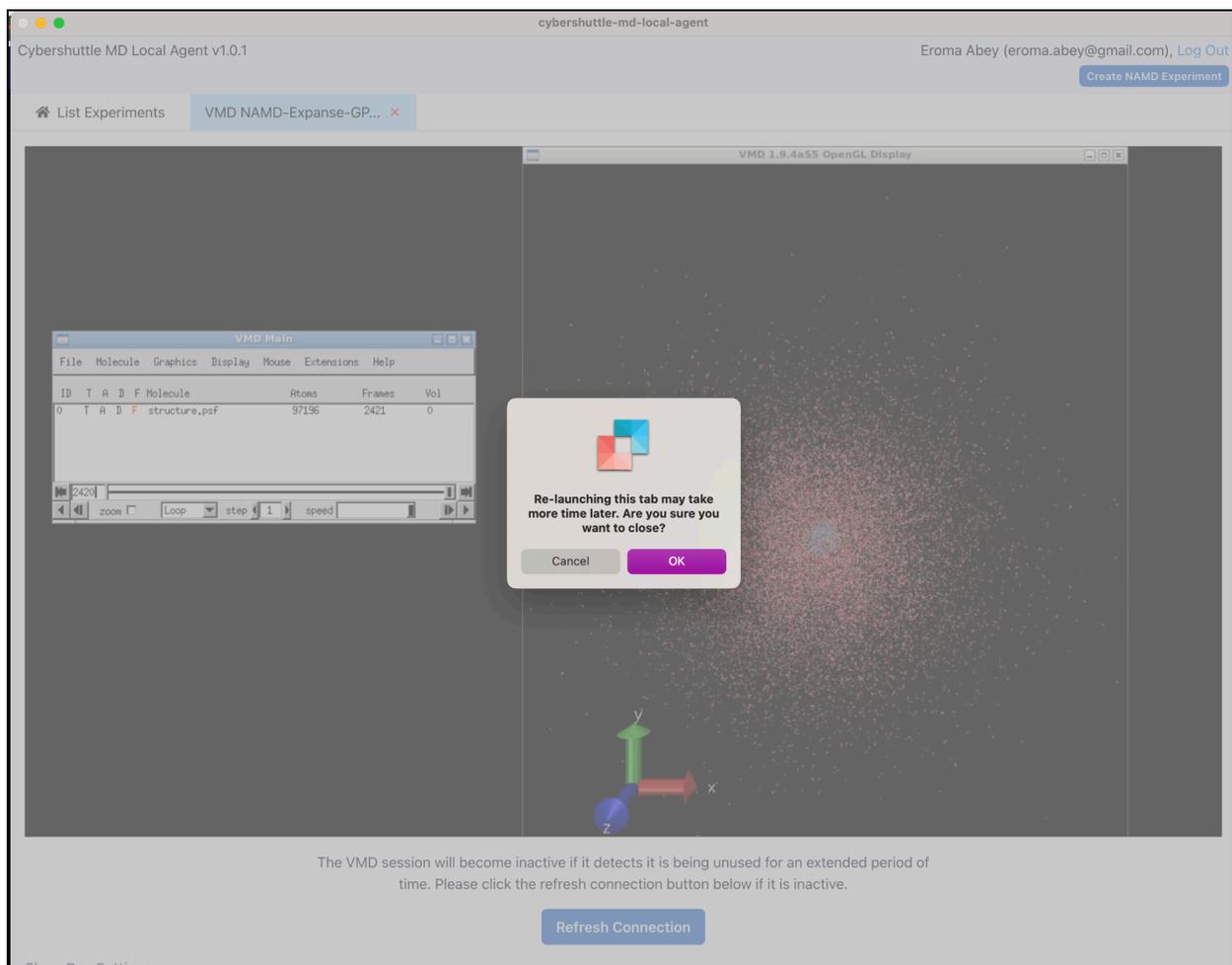
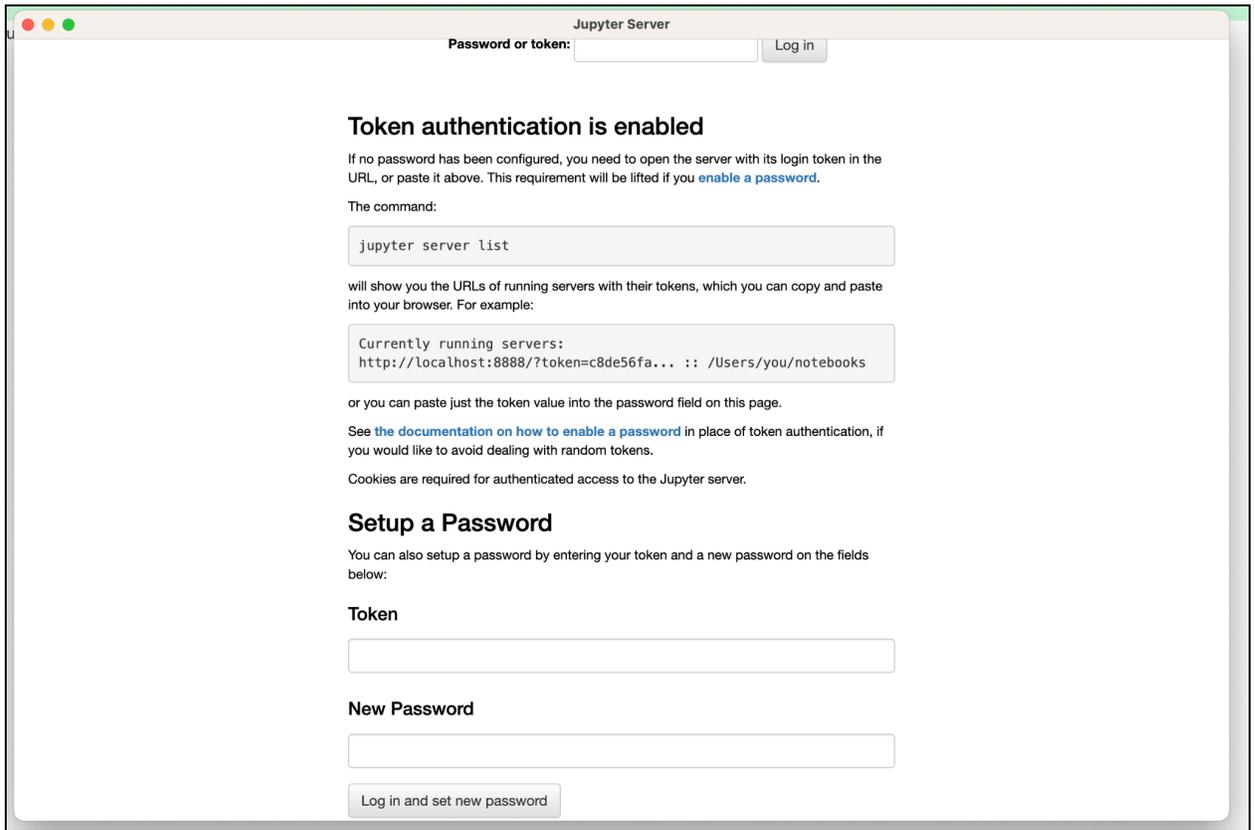


Image - End of VMD Session

4. Similar to VMD, the user can initiate a Jupyter Notebook session to run on job outputs.
5. For this use the 'Jupyter' button and the Jupyter Notebook session will open in a pop-up window.



.Image - Jupyter Server Authentication

6. In the above, provide '1234' as the 'Password or token'
7. This will open the notebook session with your remote job files on the left.

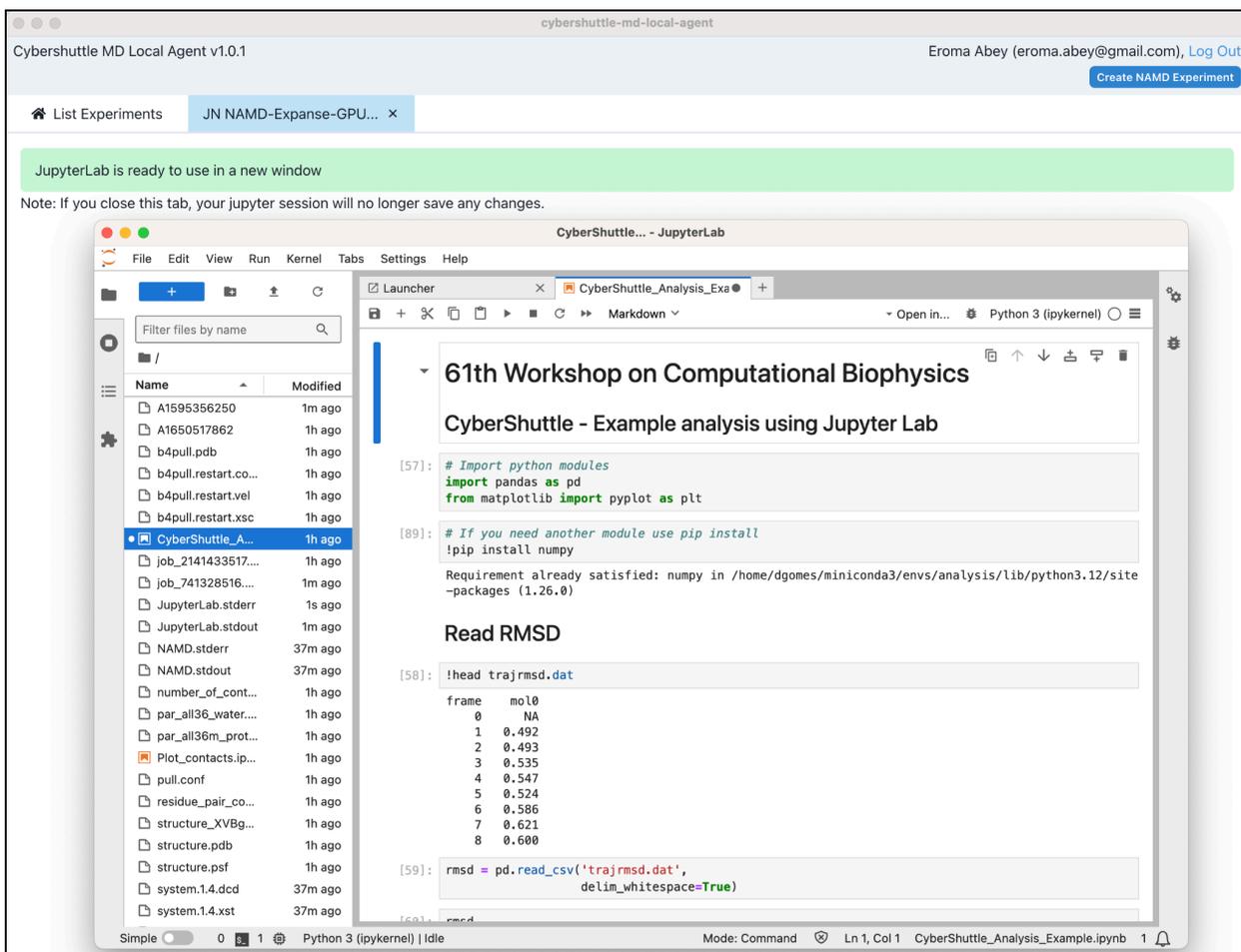


Image - Jupyter Notebook for Outputs

- When you close the notebook window, make sure to close the tab linked, to terminate the session on remote resource.

## Contact

For further communications and collaborations on Cybershuttle, use [ARTISAN@gatech.edu](mailto:ARTISAN@gatech.edu)