# Cybershuttle MD Local Agent Tutorial Instructions

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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



Image - Cybershuttle MD Web Portal

3. Install the Local Agent.

# Local Agent Login

1. After the installation open the Local Agent.

	Contacts		
	Cybershuttle MD	Open	
Aa	Dictionary	Show Package Contents	
	Docker	Move to Trash	
	draw.io	Get Info Rename	

Image - Open the Local Agent

• • •	cybershuttle-md-local-agent
Cybershuttle MD Local Agen	t v1.0.1
	Cybershuttle MD Local Agent
	Cybershuttle MD Local Agent, developed by the Cybershuttle project, empowers researchers by providing seamless access to a comprehensive range of computational resources. The agent bridges the gap between local, institutional, and national-scale computing resources, enhancing productivity and collaboration in scientific research. By integrating diverse computing environments into a unified interface, Apache Airavata eliminates traditional barriers, enabling researchers to focus on innovation and discovery.
	Features
	<ul> <li>Connects local machines, lab servers, and workstations with remote HPC resources and cloud services.</li> <li>Automates the installation and execution of scientific software.</li> <li>Facilitates collaboration among researchers across different locations.</li> <li>Supports graphical interfaces, Jupyter Notebooks, and low-code Python annotations.</li> <li>Manages data transfer and synchronization between local and remote environments.</li> </ul>

Image - Local Agent Home Page

2. Login with your institutional login through CILogon

• • •	cybershuttle-md-local-agent
Cybershuttle MD Local Agent v1.0.1	
	Cybershuttle MD Local Agent
	Log in with your existing organizational login
	Login with ClLogon
	Back to home

Image - Login Page

•••	Welcome To The CILogon OpenID Connect Authorization Service	
Cî ClLogon		
	Consent to Attribute Release	
<u>Molecular Dynamic</u> proceed. • Your CILogon • Your name • Your email ac • Your usernam	<u>es Gateway</u> requests access to the following information. If you do not approve this request, do not in user identifier ddress ne and affiliation from your identity provider	
	Select an Identity Provider Georgia Institute of Technology A & Remember this selection & Log On By selecting "Log On", you agree to the <u>privacy policy</u> .	
	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.	

Image - CILogon for Institutional Login

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

• • •			cybershuttle-n	nd-local-agent			
Cybershuttle MD Local A	Agent v1.0.1				Eroma	Abey (eroma.abe	y@gmail.com), Log Out
							Create NAMD Experiment
A List Experiments							
NAMD		<ul> <li>Application</li> </ul>	~	Experiment Status	~	Reset	Search
NAME	USER	APPLICATION	RESOURCE	CREATED	STATU	JS	ACTIONS
			Previous No ex	periments Next			

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.

• • •			cybersh	uttle-n	nd-local-ager	t					
Cybershuttle MD Local Ag	ent v1.0.1						Eror	ma Ab	ey (eroma.ab 🤇	ey@gmail.com	n), Log Out Experiment
A List Experiments											
NAMD	~	Application		~	Experiment	t Status		~	Reset	Sea	arch
NAME	USER		APPLICATION		RESOURCE	CRI	EATED	:	STATUS	ACTIONS	
NAMD-Expanse- GPU-Shared-1	EROMA.ABE	Y@GMAIL.COM	NAMD		expanse	35	minutes ago		EXECUTING	Jupyter	VMD
			Previous	Show	ving 1 to 1	Next					

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.

ocation			
Default			~
ompute Resource	)		
expanse			~
	10 10	30 minutes	MB
1			
Node Count	Core Count	Time Limit	Physical Memory
<b>1</b> Node Count mail Settings	Core Count	Time Limit	Physical Memory
Node Count mail Settings	Core Count	Time Limit	Physical Memory

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.

• • •		cybershuttle-	md-local-agent			
Cybershuttle MD Local Ag	gent v1.0.1			Erc	oma Abey (eroma.abe	y@gmail.com), Log Out Create NAMD Experiment
倄 List Experiments						
NAMD	✓ Application	~	Experiment S	tatus	∽ Reset	Search
NAME	USER	APPLICATION	RESOURCE	CREATED	STATUS	ACTIONS
NAMD-Expanse- GPU-Shared-1	EROMA.ABEY@GMAIL.COM	NAMD	expanse	35 minutes ago	EXECUTING	Jupyter
		Previous Show	wing 1 to 1	Next		

Image - Experiment View

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

•••		cybershuttle-r	nd-local-agent				
Cybershuttle M	D Local Agent v1.0.1			Eroma Abey (eroma.abey@gma	iil.com), Log Out		
				Create	NAMD Experiment		
🔏 List Exp	Experiment Details (NAM	D-Expanse-GPU-Sha	ared1)	×			
NAMD	Experiment Actions				Search		
NAME	Cancel Experiment				พร		
NAMD-Exp	Name: NAMD-Expanse-GPU-Sh	nared1					
GPU-Share	Status: EXECUTING				er VMD		
NAMD on	~ Outputs						
Expanse G Shared	✓ Inputs				er VMD		
NAMD-Exp	Description:						
GPU-Share	ExperimentID: NAMD-Expanse-GPU-Shared1_27ed3380-3422-4ec2-952f-29aa89a61dc6						
	Creation Time: 6/28/2024, 8:16	::24 AM					
	Owner: eroma.abey@gmail.com	1					
	Compute Resource: expanse						
	Queue: gpu-shared						
	Node Count: 1						
	<b>CPU Count:</b> 10						
	Total Physical Memory: 0 MB						
	Wall Time Limit: 120 minutes						
	Jobs						
	NAME	ID	STATUS	CREATION TIME			
	A392122964	31725828	ACTIVE	a few seconds ago			
	Errors						

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.

• • •		cybershuttle-r	nd-local-agent			
Cybershuttle MD Local Age	ent v1.0.1				Eroma Abey (ero	oma.abey@gmail.com), Log Out
						Create NAMD Experiment
🖀 List Experiments	VMD NAMD-Expanse-GP ×					
NAMD	✓ Application	~	Experiment Status		✓ Reset	Search
NAME	USER	APPLICATION	RESOURCE	CREATED	STATUS	ACTIONS
NAMD-Expanse-GPU-Sh	eroma.aBey@GMAIL.COM	NAMD	expanse	an hour ago	EXECUTING	Jupyter VMD
NAMD on Expanse GPU-	Shared EROMA.ABEY@GMAIL.COM	NAMD	expanse	an hour ago	FAILED	Jupyter VMD
NAMD-Expanse-GPU-Sh	eroma.aBey@GMAIL.COM	NAMD	expanse	2 hours ago	COMPLETED	Jupyter VMD
		Previous Show	ving 1 to 3 Next			



2. The VMD opens a separate tab.

			cybershuttle-md-local-ag	gent	
List Experiments	VMD NAMD-Expanse-GP	. ×			
				VMD 1.9.4a55 OpenGL Display	
	VMD Main	×			
File Molecule 0	raphics Display Mouse Extens	ions Help			
ID TADFMo O TADFst	lecule Atoms ructure.psf 97196	Frames Vol 3939 0			
3938		] #			
<b>▲ ▲</b> zoom <b>□</b>	Loop 🔽 step 🚺 1 🕨 speed				
			y		
			- z		
	The VMD	session will become in	active if it detects it is be	ing unused for an extended period of	
		time. Please click th	ne refresh connection but	ton below if it is inactive.	
			Refresh Connection		
Dev Settings					
ocket URL: wss://ap	i.cybershuttle.org/proxy/914	6			
cation ID: VMD-ed8	1d73e-d93f-4317-bfa9-9ed	183ff2619			

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.

				cybershuttle-md-local-agent	
ershuttle MD	D Local Agent v1.0.1			Eroma Abey (eroma.abey@gmail.	com), Lo
				Create NA	мо Ехре
List Experi	iments JN NAMD	-Expanse-GP	×U		
upyterLab is	s ready to use in a new	window			
e: If you clo	se this tab, your jupyte	ar session will	no longer sa	le any changes	
or in you olo			no longer eu		
			<b>A</b> 111	CyderSnuttle JupyterLab	
~	File Edit View Run	i Kernel lat	os Settings	Help	-
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0	Filter files by name	Ч.			¥
	• /			61th Workshop on Computational Biophysics	
≣	Name 🔺	Modified		o the workshop on compatational biophysics	
	A1595356250	1m ago		CyberShuttle - Example analysis using Junytor Lab	
*	A1650517862	1h ago		Cyber Shuttle - Example analysis using Jupyter Lab	
	🕒 b4pull.pdb	1h ago	[57]:	# Import python modules	
	b4pull.restart.co	in ago		import pandas as pd	
	b4pull.restart.ver	In ago		from matplotlib import pyplot as plt	
	CyberShuttle A	1h ago	[89]:	# If you need another module use pip install	
	P iob 2141433517	1h ago		!pip install numpy	
	□ job_741328516	1m ago		Requirement already satisfied: numpy in /home/dgomes/miniconda3/envs/analysis/lib/python3.12/site	
	JupyterLab.stderr	1s ago		-packages (1.26.0)	
	JupyterLab.stdout	1m ago		Read RMSD	
	NAMD.stderr	37m ago			
	NAMD.stdout	37m ago	[58]:	!head trajrmsd.dat	
	number_of_cont	1h ago		frame mol0	
	par_all36_water	1h ago		0 NA	
	par_all36m_prot	1h ago		2 0.493	
	Plot_contacts.ip	1h ago		3 0.535	
	pull.conf	1h ago		4 0.547 5 0.524	
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	system.1.4.dcd	37m ago	[29]:	delim_whitespace=True)	
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		- D. II T	[60] ·	rmed	

Image - Jupyter Notebook for Outputs

8. 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@groups.gatech.edu**