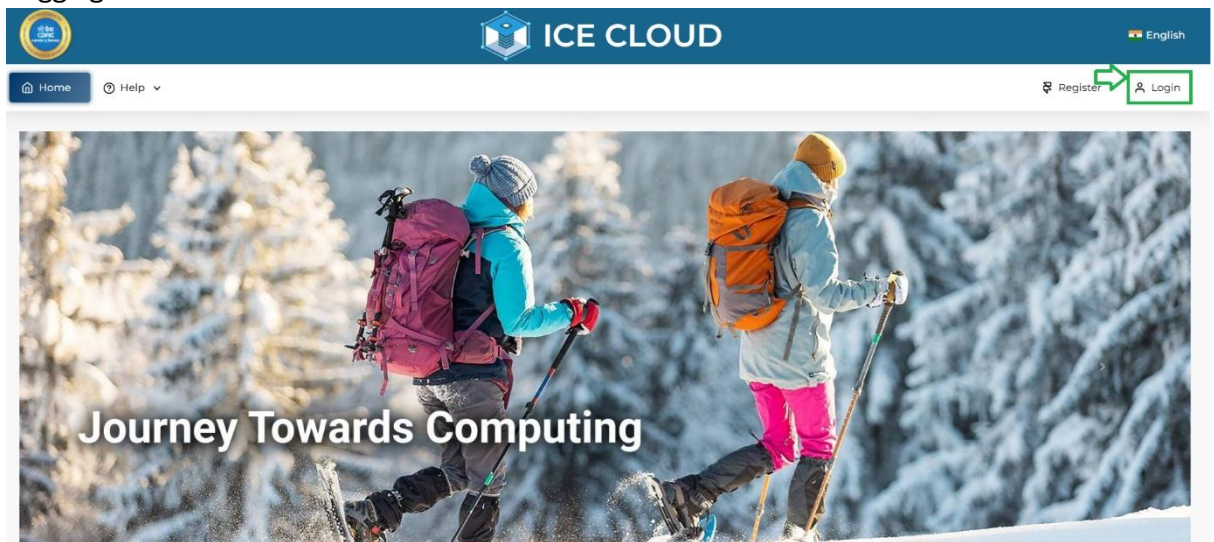


# Development of a framework for HPC-AI synergy using Integrated Computing Environment (ICE) on PARAM Rudra cluster

1. Accessing ICE  
<https://icecloud.in/home>

2. Logging into ICE Cloud



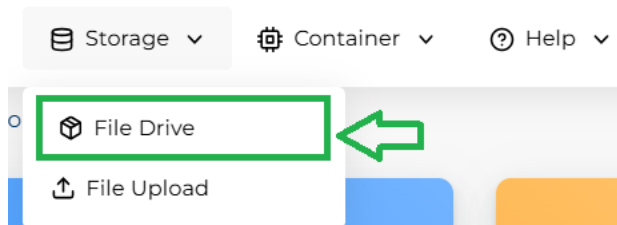
- Click on Login
- Enter username: testuser
- Password: testuser123
- Click the Login button

The screenshot shows the "Sign In" page of the ICE - Indigenous Cloud Environment. The page has a light blue background with a snowflake icon. The title "ICE - Indigenous Cloud Environment" is at the top, followed by "Sign In". There are two input fields: "Username or Email" with the value "testuser" and "Password" with the value "testuser123". A "Forgot Password?" link is located below the password field. A large orange "Login" button with a downward arrow is centered below the fields. At the bottom, there is a link "Create new account" for new users and contact information: "For any queries kindly contact at [braf-help@cdac.in](mailto:braf-help@cdac.in) , [ice@cdac.in](mailto:ice@cdac.in)".

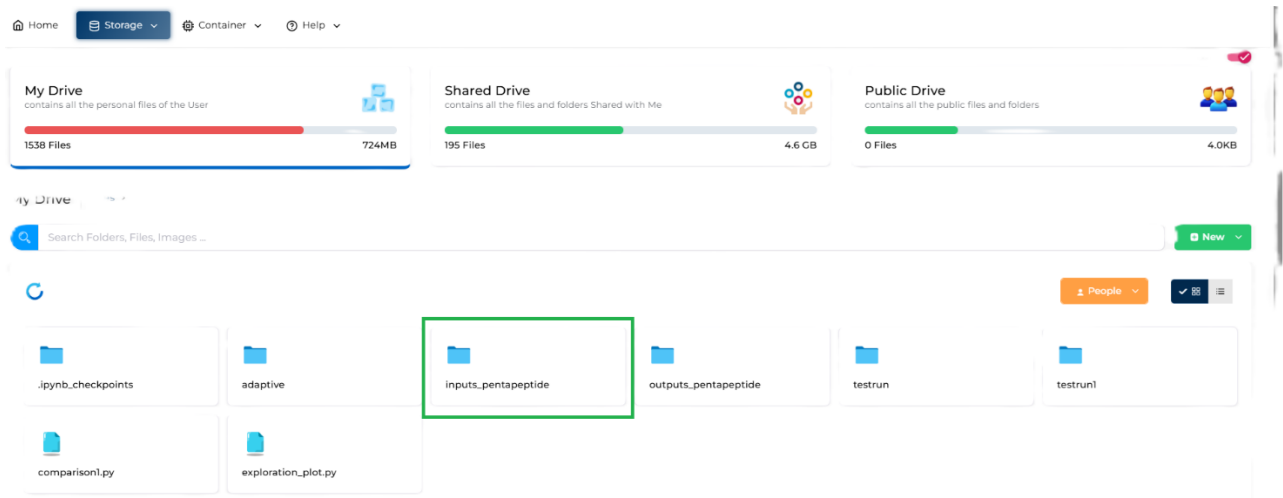
3. Preparing inputs for adaptive sampling



- After logging in successfully, click on the “Storage”, as shown in the figure above.
- Further, click on the “File Drive” as shown below,

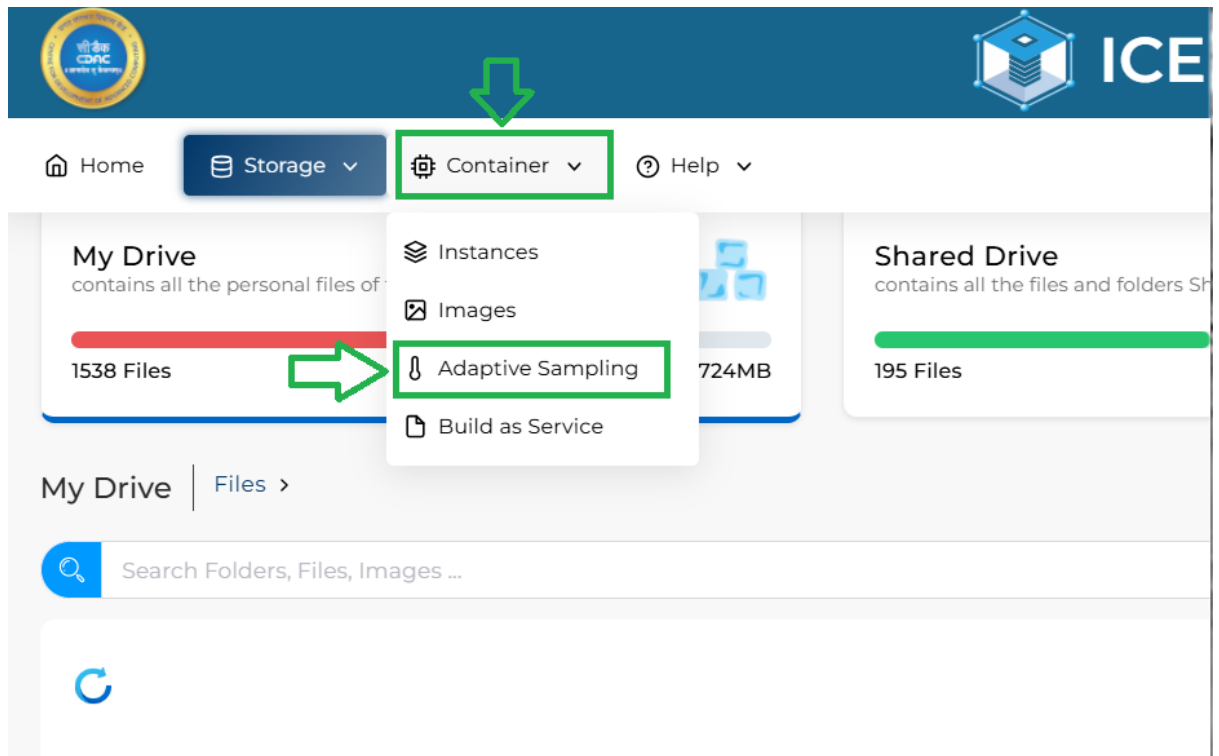


- The inputs are present in the folder “inputs\_pentapeptide”



#### 4. Running adaptive sampling

- Click on “Container” followed by “Adaptive Sampling” (as given in the figure below)



- The page shown in the figure below would appear. Kindly enter the following details:

### Adaptive Sampling

Job Name \*

CPU Utilization \*

Memory Allocation For Image \*

Number of cycles \*

Number of runs per cycle \*

Algorithm \*

Input path \*

[Create Adaptive Sampling](#)

- Job Name: outputs\_pentapeptide (an output folder with the identical name would be created in the home folder)
- CPU Utilization: number of cpus to be given (Currently given: 10)

- Memory Allocation for Image: memory to be given would be considered in GBs (Currently given: 40 GB)
- Adaptive Sampling specifications:
  - Number of cycles: Number of adaptive sampling cycles to be given here (Currently given, 5)
  - Number of runs per cycle: Number of frames to be selected at every cycle for continuing the adaptive sampling (Currently give, 5)
  - Algorithm: Selection of algorithm for finalizing the frames in every cycle. (Current selection: isolation forest)

Algorithm \*

isolation

Create Adaptive Sampling

- Inputs path: path to the folder where the inputs are present (Currently it is directed towards “inputs\_pentapeptide” which is present in the home folder)
- Finally, click on “Create Adaptive Sampling”

## 5. Output of the adaptive sampling

- Initially, the job status may be “Waiting”, followed by “Running” and “Completed”.

Show 10 Create Container Images Refresh job status Search Delete (0)

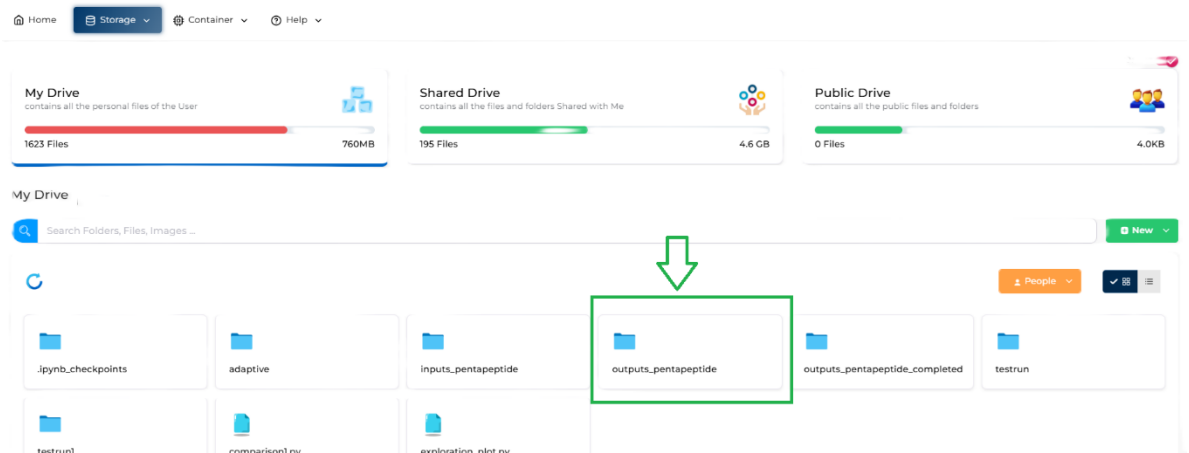
JOB NAME	IMAGE NAME	AGE	CPU USED	MEMORY USED	STATUS	PASSWORD	DELETE	CONNECT
<input type="checkbox"/> testuser-pod-gro-2jfd	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Waiting			
<input type="checkbox"/> testuser-pod-gro-2vst9	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Waiting			
<input type="checkbox"/> testuser-pod-gro-qtxgm	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Waiting			
<input checked="" type="checkbox"/> testuser-pod-gro-twbrn	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Waiting			
<input type="checkbox"/> testuser-pod-pyemma-qw6ml	pyemma	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/> testuser-pod-amber-br6bt	ambertools	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/> testuser-pod-gro-28kdj	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/> testuser-pod-gro-brbp7	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/> testuser-pod-gro-gfkw7	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/> testuser-pod-gro-mfx46	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			

**Current job status**

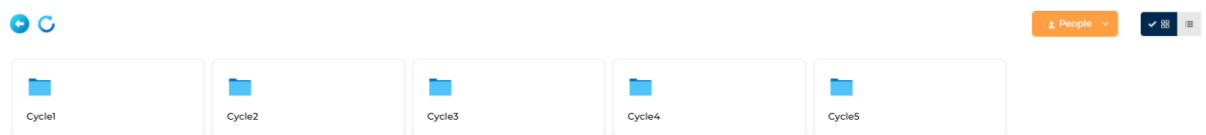
Show 10 Create Container Images ↻ Search Delete (0)

<input type="checkbox"/>	JOB NAME	IMAGE NAME	AGE	CPU USED	MEMORY USED	STATUS	PASSWORD	DELETE	CONNECT
<input type="checkbox"/>	testuser-pod-gro-2lfd	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Running			
<input type="checkbox"/>	testuser-pod-gro-2vst9	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Running			
<input type="checkbox"/>	testuser-pod-gro-BqBpw	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Running			
<input type="checkbox"/>	testuser-pod-gro-qtvgm	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Running			
<input type="checkbox"/>	testuser-pod-gro-twbrn	adaptive-gromacs	3 minutes ago	10 vCPU	40 GB	Running			
<input type="checkbox"/>	testuser-pod-pyemma-qw6ml	pyemma	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/>	testuser-pod-amber-br6bt	ambertools	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/>	testuser-pod-gro-28kdj	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/>	testuser-pod-gro-brbp7	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			
<input type="checkbox"/>	testuser-pod-gro-g9xw7	adaptive-gromacs	a day ago	10 vCPU	40 GB	Completed			

- On the main menu bar, Click on “Storage” >> “File Drive”
- The output folder by the name “output\_pentapeptide” (same as the given job name)



- Inside the main output folder, would be sub-folders with information of every cycle of adaptive sampling

















- Inside every sub-folder would be the information on the frames selected for every run in that particular cycle. The simulation data for each of the runs would be written in the individual “Run1/2/3/4/5” folders.



People



 Run1	 Run2	 Run3	 Run4	 Run5	 .all_traj.xtc.offsets.lock
 .all_traj.xtc.offsets.npz	 Sunexplored_KDE.csv	 Sunexplored_KDE_seperated.csv	 aligned_merged1.xtc	 all_traj.xtc	 combine.in
 cpp.log	 input_for_cycle2.txt				