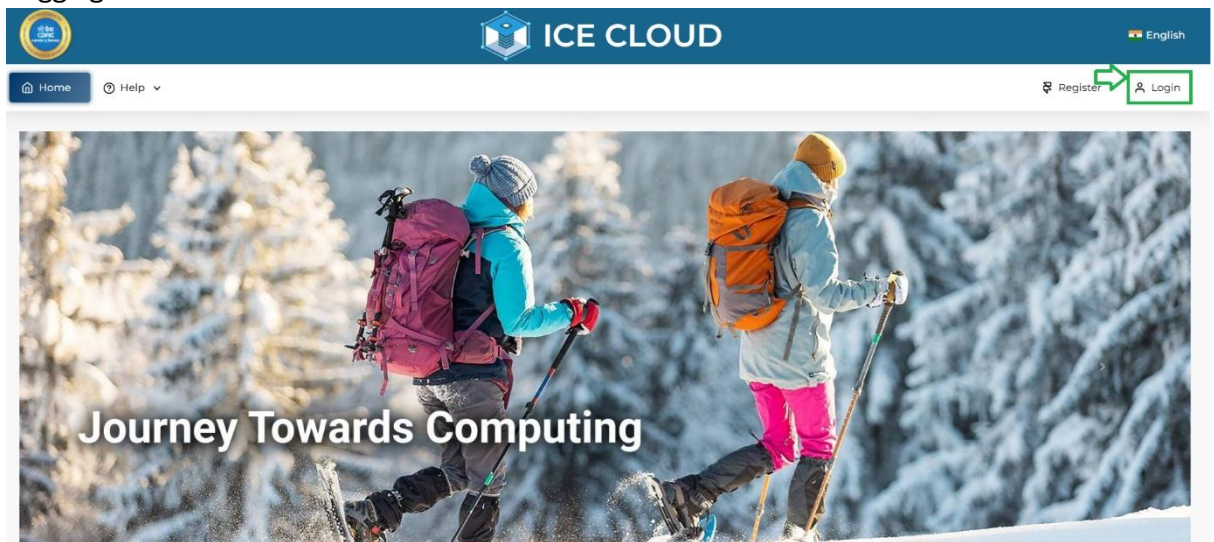# Development of a framework for HPC-AI synergy using Integrated Computing Environment (ICE) on PARAM Rudra cluster

1. Accessing ICE
   https://icecloud.in/home
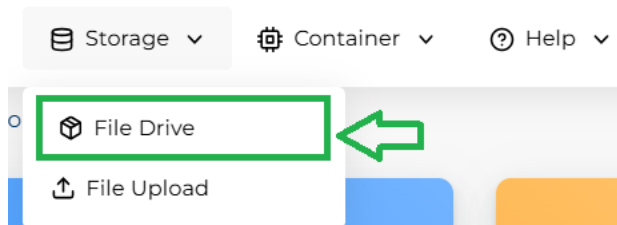
2. Logging into ICE Cloud

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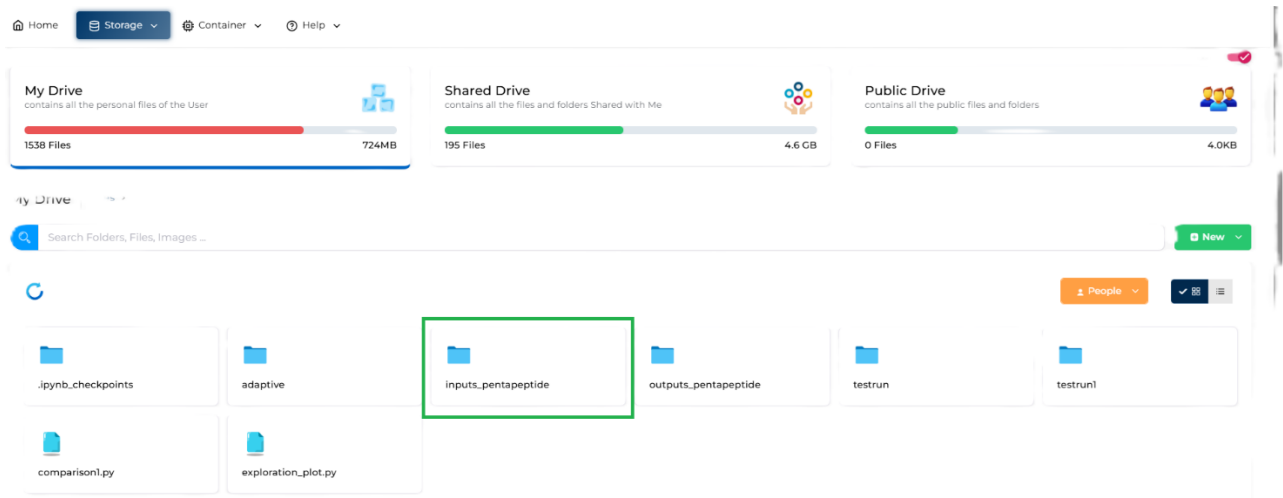   - Click the Login button

3. Preparing inputs for adaptive sampling

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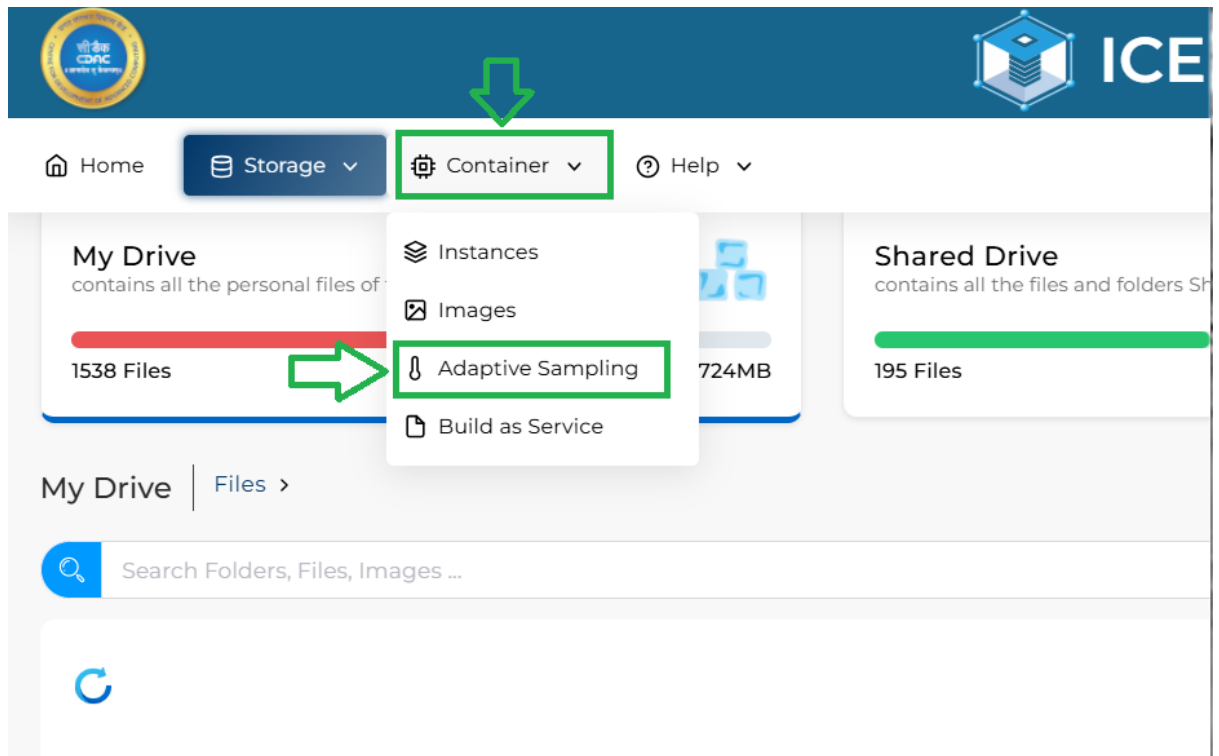- Further, click on the "File Drive" as shown below,

- 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:

- 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)

- o Memory Allocation for Image: memory to be given would be considered in GBs (Currently given: 40 GB)
- o 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)

- o 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)
- o Finally, click on "Create Adaptive Sampling"

5. Output of the adaptive sampling
   - Initially, the job status may be "Waiting", followed by "Running "and "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)
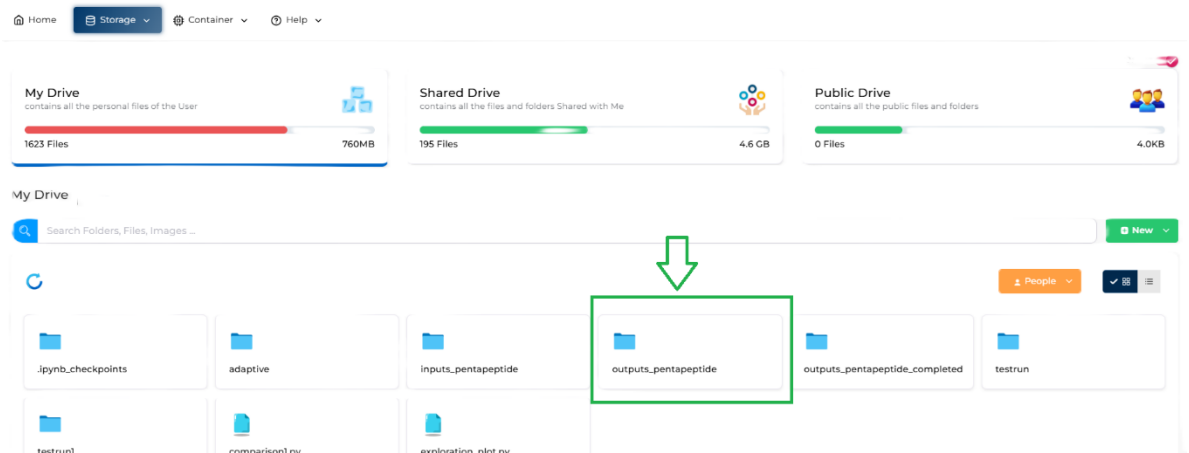
  o Inside the main output folder, would be sub-folders with information of every cycle of adaptive sampling
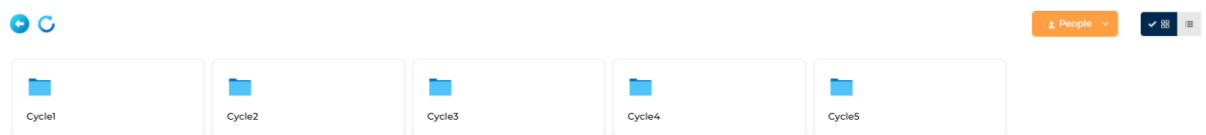
  o Inside every sub-folder would be the information on the frames selected for every run in that particular cycle. The simulation data for each of the runs would be written in the individual "Run1/2/3/4/5" folders.

Run1	Run2	Run3	Run4	Run5	.all_traj.xtc_offsets.lock
.all_traj.xtc_offsets.npz	5unexplored_KDE.csv	5unexplored_KDE_seperated.csv	aligned_merged1.xtc	all_traj.xtc	combine.in
cpp.log	input_for_cycle2.txt				