Reducing the Barrier of Entry for GPU Accelerated Workflows using Open OnDemand and Charliecloud Containers in HPC

Abhinav Kotta
Cornell University
abhinavkotta.io@gmail.com

Beamlak Bekele
University of Maryland Baltimore County
bekbeamlak@gmail.com

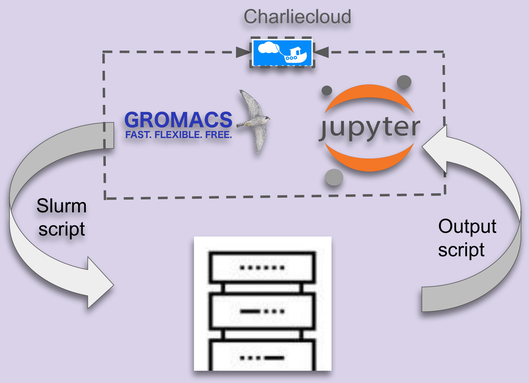
Kelsey Tirado
Rochester Institute of Technology
kelseytirado3@gmail.com

Mentors:
Jordan Ogas, Hunter Easterday, Angelica Loshak, and Andres Quan

Background

- HPC systems enable powerful simulations but require complex command line skills to complete the job.
- LANL lacks an accessible framework for integrating scientific workflows.
- Time spent learning HPC tools can instead be used to focus on core parts of experiments.

Overview

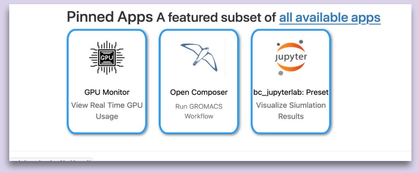


1. The integration of Open OnDemand, JupyterLab, Charliecloud, GROMACS, and OpenComposer enables an accessible HPC workflow.
2. Simulations run in Charliecloud containers and are submitted as GPU jobs across two nodes.
3. Post-processing is done in JupyterLab using Python to visualize molecular trajectories.

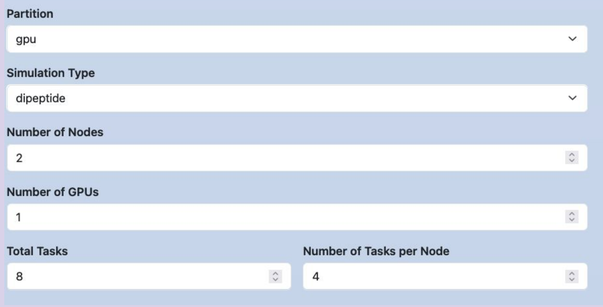
Key Takeaways

- OOD provides a web-based, non-command line interface to users.
- Job Composer provides a complete, sharable, repeatable turnkey simulation campaign for users.
- All non-OOD software stack elements containerized and abstracted from users.

GROMACS GPU Workflow



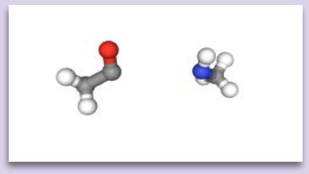
Starting on the fully customizable dashboard a user can easily navigate to the GROMACS workflow through the custom Open Composer application. The simulation is readily available for use. Select the dipeptide option and the sbatch script is automatically loaded in



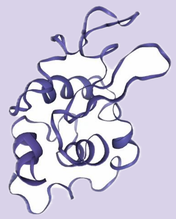

```
#SBATCH --ntasks-per-node=4
#SBATCH -N2
#SBATCH --output=/home/admin/output.log
#SBATCH --error=/home/admin/error.log
 cd /home/admin/GROMACS_workflow/dipeptide_simulation
PATH=/home/admin/charliecloud/bin:$PATH
cat << 'EOC' > container.sh
export GMX_ENABLE_DIRECT_GPU_COMM=1
export GMX_GPU_PME_DECOMPOSITION=1
export NVSHMEM_BOOTSTRAP=MPI
export GMXLIB=/usr/local/share/GROMACS/top
```

Visualization

Once The job is complete the user launches a Jupyter Notebook which visualises the results. All the necessary code is preloaded into the application to allow for visualization of the data



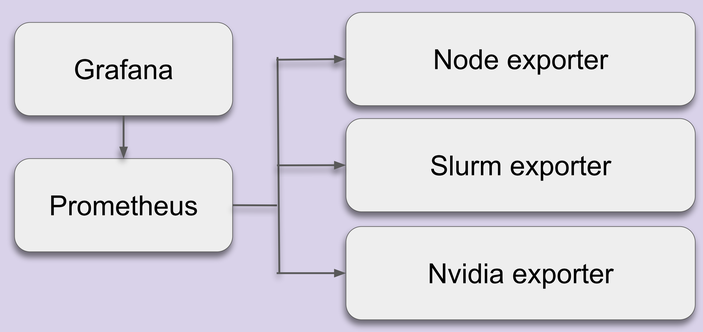
Trajectory of dipeptide molecules through a solvent



Generated image showing a protein (lysozyme) in a box of water, with ions

Monitoring

Grafana monitoring for allocated resources per active job




```
================ gu01 ====================
Warning: Permanently added 'gu01' (ED25519) to the list of known hosts.
Tue Jul 22 14:18:40 2025
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 575.57.08              Driver Version: 575.57.08      CUDA Version: 12.9     |
|-----------------------------------------+------------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id          Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |           Memory-Usage | GPU-Util  Compute M. |
|                                         |                        |               MIG M. |
|=========================================+========================+======================|
|   0  NVIDIA A2                      Off |   00000000:3D:00.0 Off |                    0 |
|  0%   45C    P0              26W /   60W |    2084MiB /  15356MiB |     55%      Default |
|                                         |                        |                  N/A |
+-----------------------------------------+------------------------+----------------------+
```

Real time GPU monitoring showing raw logs from the compute nodes that are running an active job

Future Works

- Replace Open Composer with a fully custom made application encased in Open OnDemand environment
- Offer other scientific softwares through Open Composer
- Make the GPU app more interactive
- Integrate an automatic job submission functionality for repeatable runs

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