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Title: Reducing HPC Barrier of entry for GPU accelerated workflows using Open OnDemand and Charliecloud containers

**Abstract:**

High performance computing (HPC) accelerates scientific research and discovery but requires proficiency with the Linux command line, the job scheduler, scripting, and software environment management. These requisite skills often prove to be a barrier of entry, preventing a broader range of researchers from leveraging HPC resources. We lower this barrier with established tools behind a single, browser-based interface: Open OnDemand (OOD) for cluster web access and job submission, Charliecloud for lightweight unprivileged containers, and Slurm for resource scheduling. Through OOD we deliver a ready-to-use workflow for GROMACS molecular dynamics simulation campaigns. Users launch pre-built Charliecloud containers that encapsulate the entire scientific software stack, establishing consistency across same-architecture systems and eliminating the need for environment modification. A custom Open Composer app lets researchers graphically assemble, save, and relaunch complete GPU accelerated GROMACS pipelines, replacing more than 30 shell commands with a few clicks. Jupyter Notebook with NGLView provides in-browser, 3D visualization of trajectories, while our integrated custom GPU Monitoring and Grafana dashboards give real-time comprehensive, numerical, and visual analysis about job resource usage. This system gives scientists the ability to quickly develop and iterate over personal and shared workflows, removing the need to master the job scheduler, Linux commands, and writing custom job scripts. Our integration of OOD, reduces the time to science for a broader scientific audience by abstracting HPC system mechanics.