Demystifying HPC for Biomedical Research

With a drive to bring personalised medicine from science fiction to science fact, the CompBioMed Centre of Excellence focuses their training efforts towards bridging the gap between High Performance Computing (HPC) and the computational science of biomolecules.

Business Need

With social distancing restrictions inhibiting traditional models of on-site education, the CompBioMed team was looking for innovative ways to keep the education program moving forward. Through their Associate Partnership with Alces Flight they identified utilising cloud HPC as a means to develop flexible, scalable, and affordable training models.

Solution

CompBioMed Core Partners UCL and the University of Sheffield came together with Alces Flight to build the nUCLeus cloud HPC cluster environment. Utilising Alces Flight Center as a central hub for all computing information the teams worked in tandem to build out an unfederated cloud cluster environment focused on training using the QIIME2 application. The end result of this work is a complete cloud foundation for continued biomedical training initiatives, including exascale.

"Having a managed cluster environment that is able to work across cloud platforms is ideal when looking to train researchers in HPC foundations. Our initiatives, which are global and cover incoming exascale requirements, mean we not only need to be easily accessible but also flexible, scalable and sensitive to budgetary requirements. nUCLeus achieves all this and more."

Andrea Townsend-Nicholson,
Professor of Biochemistry & Molecular Biology
University College London (UCL)

Benefits

- Centralized management of computational resources.
- Complete flexibility in design of the nUCLeus cloud cluster environment.
- Ability to optimise both performance and cost of resources.
- Capability to build multiple training intitiatives as well as evolve prior courses as requirements change.

Solution at a glance

- Cloud HPC solutions
- Managed HPC Services
- Training and Education

CompBioMed Core Partners::

The University Of Sheffield.

UCL

CompBioMed Partners UCL and the University of Sheffield had begun planning their collaborative training in HPC foundations for 2020, when the COVID-19 pandemic struck. Instead of delaying the work the team chose to look at novel approaches in HPC education, specifically, what cloud could do to build up a flexible, scalable training model that could be evolved into a key component for upcoming exascale initiatives.

CompBioMed is a European Commission Horizon 2020-funded Center of Excellence focused on the use and development of computational methods for biomedical applications. "Computer-based modelling and simulation is already established in the physical sciences and engineering," explains Andrea Townsend-Nicholson, Professor of Biochemistry & Molecular Biology at UCL, "With biomedicine, this capability is now beginning to advance towards maturity. We are developing predictive models in health and disease that are becoming relevant to clinical practice. As such, we have been delivering foundational training for HPC in biosciences in order to bring medical students along the journey towards our long-term goal of developing personalised medicine."

The path to creating an in silico - or virtual - human requires the capability to train incoming students on core HPC practices as well as transitioning them from desktop application work to engaging with complex cluster environments. Usually, consortia members collaborate and launch courses utilising on-premises HPC clusters. With the pandemic, holding events like these became impractical - so the team considered a novel approach. "We wanted something the consortia could have access to that could be used remotely, could be flexible and would be able to scale sufficiently to meet a range of objectives. That's when we decided to look at the cloud."

Building nUCLeus
In order for a cloud course to work there were several key components required. First, locating students who would be excited at the prospect of working in cloud HPC. "We chose to work with medical students who self-selected into supercomputing applications of relevance to medicine, as we wanted to encourage the open discourse needed to build a solid foundation of work," said Andrew Narracott, Senior Lecturer, at the University of Sheffield. "We also required a collaborative model of teaching and we

needed to ensure that the cluster environment we built would process at an active pace outside of class so we could keep an eye on budget." The team chose to focus on the QIIME2 application as it is non-compute intensive, lending itself to being relatively easy to teach and to process in the cloud. "It was important to have a cluster environment that could be optimised to QIIME2", explains Art Hoti, Masters Student at UCL. "Being able to keep records of the configurations and templates that worked is essential for the course to be re-used in future and we can use our efforts to focus on improvements. Thankfully, the team at Alces Flight made it possible for us."

Ready for Flight
The team at Alces provide a managed HPC cluster service for nUCLeus - designed entirely around building and maintaining a cost-effective persistent core of information that can be enabled, modified and scaled to meet whatever course requirements come CompBioMed's way. "nUCLeus needs to be unfederated, which means that the cluster environment can be tailored to whichever cloud platform can provide CompBioMed the best options for teaching," said Cristin Merritt, Cloud HPC Program Manager for Alces Flight. "CompBioMed has different partners with a shared set of goals that need to be tailored to location and to the trainees' level of HPC education. By using the Alces Flight Center service, they keep all information in one location and launch courses as needed. This ensures their time is spent more on delivering quality coursework while the cloud resource is managed efficiently and cost-effectively."

The initial nUCLeus launch reached full enrolment capacity at the University of Sheffield and allowed four students to achieve contributing author status for work in HPC Education at the 2020 international Supercomputing conference (SC'20). nUCLeus is now in preparation for its next course launch in 2021, as well as undergoing development as part of future exascale training initiatives.

"Using Flight Center to manage the optimisation tests was key in progressing the development of nUCLeus for QIIME2. We know what does and doesn't work and can use this information to speed up the launch of the next iteration of the class."

Art Hoti,
4th Year MSci in Biochemisty
UCL

"Managing twenty students virtually took significant collaborative effort. For us, knowing Alces Flight was there to handle the cluster requirements meant we could focus our efforts on our area of expertise: delivering excellent teaching to our students."

Andrew Narracott,
Senior Lecturer
University of Sheffield

Technology

Products

Flight for Managed Environments

Alces Flight Center

Platform

Unfederated (built for public cloud with option for on-premises)

alcesflight