

PROPEL ACADEMIC BREAKTHROUGHS WITH RESEARCH IT INNOVATION

The fastest path to the greatest research breakthroughs relies in part on the quality of tools at the researchers' disposal. This makes the mission of system admins, who support researchers at universities, pivotal for gaining accurate scientific insights.

High-performance computing (HPC) is a critical tool for advancing research and discovery, and it's growing at an astronomical rate.

But research IT teams face bottleneck challenges in workflow components, like application deployment. Container technology, such as through NVIDIA'S NGC, can bypass these bottlenecks and give IT teams rich opportunities to streamline workflows and enable future discoveries.

Deploying Applications in HPC Environments Is Complex

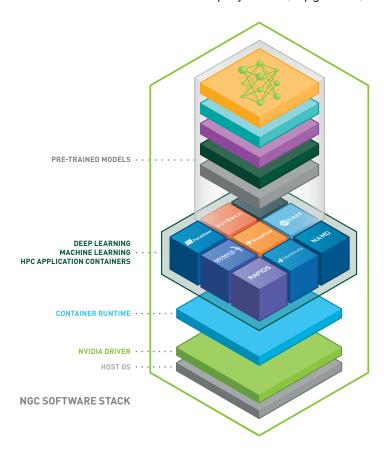
HPC applications rely on the installation of various dependencies, including libraries, drivers, MPI, and network protocols. This makes upgrading or introducing an application a time-intensive process: System admins have to identify, implement, or upgrade any missing dependencies while ensuring that the existing network of applications doesn't break. As a result, researchers have to wait longer to get an application's most updated features.

Addressing the Bare-Metal Install Challenges with Containers

A container packages the application and all of its dependencies, providing an environment for the application to run properly. It's agnostic to the underlying hardware or other system software, which means system admins don't have to worry about breaking the dependency networks.

NGC—the Container Registry for GPU-Powered HPC Systems

NVIDIA's NGC container registry offers GPU-optimized deep learning frameworks, HPC and visualization applications, machine learning algorithms, and pre-trained models. NGC containers are designed to run on systems powered with NVIDIA Pascal $^{\text{TM}}$, NVIDIA Volta, and NVIDIA Turing $^{\text{TM}}$ GPUs. NGC streamlines software deployments, upgrades, accessibility, and utilization in a number of ways:



- > **Updated monthly:** Frameworks are constantly optimized for performance, and key frameworks like TensorFlow, PyTorch, and MxNet are updated monthly.
- > **Scalable performance:** HPC containers, including NAMD, GROMACS, LAMMPS, and MILC, provide scalable performance across multiple GPUs and nodes to deliver faster simulations.
- > Supports Singularity: While NGC containers are Docker-based, they've been tested and documented to run on Singularity.
- > Runs anywhere: Containers are portable and flexible across systems. University clusters can't always handle very large simulations, but containers can be easily deployed by a cloud platform like AWS.
- > Run multiple versions simultaneously: NGC hosts various versions of containerized applications so that different users can run different versions on the same system without causing dependency conflicts.
- > Reproducible results: Researchers often want reproducible results across different systems to publish their papers. Unlike bare-metal installs, container applications can run in the same environment across different systems.

NGC in Research

Container technology is being rapidly adopted for a wide variety of subject areas, from molecular dynamics to quantum chemistry to visualization. In fact, top education and research facilities in the country, such as Clemson University and the University of Arizona, are already using NGC to strengthen their research IT services.

