Enabling User-Defined Software Stacks with Charliecloud

Using a container approach enabled by Charliecloud, a program developed at Los Alamos National Laboratory, you can package your own software stacks and use them across multiple platforms, including on NAS systems.

The software stacks provided by NAS, which are available in the /nasa directory and the system directories (such as /usr/bin, /usr/lib, /usr/local/bin, and /usr/local/lib), meet the needs of most users most of the time. However, in some cases, you might want to use your own software stack that is not available on NAS systems (either because it is not compatible with the NAS default system image—currently, SLES 12 SP3—or because it would require a disproportionate effort to create and maintain by the system administrators). In order to use your own, customized software stack on NAS systems, you can build a container image using Charliecloud.

Using Charliecloud

A container image is an executable package that includes everything needed to run an application, including the code, a runtime, libraries, environment variables, and configuration files. Using a user-namespace implementation, the filesystem tree of a Charliecloud container image is independent of that of the host image. For example, a container has its own root (/) directory and system directories, such as /usr/bin and /usr/lib, that are separate from those of a Pleiades host. This allows you full control of the container.

This functionality addresses the following needs, as stated in this list from the Charliecloud documentation:

- Software dependencies that are numerous, complex, unusual, differently configured, or simply newer/older than what the center (NAS) provides;
- Build-time requirements unavailable within the center (NAS), such as relatively unfettered internet access;
- Validated software stacks and configuration to meet the standards of a particular field of inquiry;
- Portability of environments between resources, including workstations and other test and development systems not managed by the center (NAS);
- Consistent environments, even archivally so, that can be easily, reliably, and verifiably reproduced in the future; and/or
- Usability and comprehensibility

Creating a Charliecloud Container Image

To create a user-defined software stack, you typically start with a base system image—such as SLES, Ubuntu, Debian, or CentOS. For your convenience, there is currently a CentOS 7 base image available on Pleiades that you can use to build your container image. If you prefer, you can build a container image on your own workstation, using the Docker platform. Both methods are described in the following articles:

- Build a Container Image on Pleiades with the NAS-Provided CentOS 7 Base Image
- Build a Container Image on Your Own Workstation Using Docker

Note: Building a container image on your own workstation requires root privileges.

Running a Charliecloud Container Image

You can bring your container image to many platforms where Charliecloud is installed. Running your image does not require root privilege. See the following article to learn how to run your container image on Pleiades:
Running a Charliecloud Container Image on Pleiades

References

For more information about Charliecloud and Docker, see the following publications:

- Charliecloud Documentation
- Docker Documentation
- Charliecloud: Unprivileged containers for user-defined software stacks in HPC (SC17 technical paper)