Containers on HPC

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## Best Practice: Containers

### What is the Best Practice?

Providing a container solution that supports user container images and satisfies security requirements of your site.

### Why is it needed?

To provide a common framework that simplifies the deployment, update, and scaling of user applications while improving environment consistency and application portability, ease of use, installation, and configuration.

### Who does it impact and when?

**Site admins:** easier software updates, multiple software versions not affecting the software stack on the system, no-reboot-necessary software updates.  
**Users:** consistent environment for applications; customization of software.

### Why is this a Best Practice?

Consistent with larger community. Allows testing on an individual (image) basis without affecting other software and users.
Containers: Isolated Environments for Applications

Individual
- Docker
- Docker Compose
- Singularity
- Podman

Orchestration
- Docker Swarm
- Kubernetes
- Apache Mesos

Infrastructure Management
- OpenStack Magnum

HPC-aware
- Singularity
- Charliecloud
- Shifter
- Podman
Docker

+ The most popular container solution
+ Streamlined experience defining, creating, and using container images
  – Requires privileged permissions
  – Runs a separate daemon process in the background

Docker Compose

• Tool for defining and running multi-container Docker applications
• Uses Docker images / containers
Singularity

+ Alternative to Docker
+ Can be used with unprivileged permissions
+ Doesn't require a separate daemon process
+ Has its own image format but can also import Docker images
+ Has its own image registry but can also work with DockerHub
  - Has a security issue that isn’t patched on Cray XE/XK systems (Blue Waters). Patched on Cray XC systems.
Podman

- Supports OCI, Docker, and other image formats
- Multiple means to download images
- Rich container image management
- Full management of container lifecycle

Charliecloud

- Fully unprivileged workflow
- Works with Linux filesystem tree
Docker Swarm

- Container orchestration tool
- Uses Docker images/containers

Kubernetes

- Alternative to Docker Swarm
- Major use in Cloud and {AI, ML, DL} computing.

Magnum

- Container Infrastructure Management tool
- Makes orchestration tools aware of each other
Shifter

- Designed for HPC
- Works with Docker images, DockerHub, custom image registries
- Supports private Docker images
- Supports local images
- Supports custom “modules” to help specialize images for local system
- [Blue Waters]: Added support for *private* local images
- [Blue Waters]: Enabled metadata manipulations for local images
- [Blue Waters]: Added support for primary owners of private local images
- [Blue Waters]: MPI in images can be installed with package managers
HPC-aware Container Solutions: Final Remarks

- Linux kernel support is **critical**
- Direct access to the underlying hardware is **very important**
  - GPUs (CUDA), MPI, other specialized hardware
- User experience is **important**
  - Docker images and containers. Docker Hub
  - Intuitive interaction with images
  - Integration with site’s workload manager and scheduler
- Private images **might be important**
- Admin support is **required**
Q&A