# **Survey of HPC Container Tools**

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#### About

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  - Club Tennis









#### About

- Rachel
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  - Major: Computer Science BS
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#### What are Containers?

- Standard unit of code that packages up software and all its dependencies so that the application can be run quickly and reliably on multiple systems
- Podman, Singularity, Charliecloud, Sarus, Shifter



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### Why do Containers Matter to HPC?

- Portable
  - Ease of transporting software and its dependencies to different systems
- Lightweight
  - Containers are very lightweight compared to VMs
    - Containers use a fraction of the memory required to boot an OS
- Scalable
  - Can distributed to many nodes easily
  - HPC workloads can face a spike in data processing requirements
- Reproducible



## Why Not Docker?

- The Docker Runtime doesn't work well in HPC because....
  - Multitenancy
  - Networking
- Docker/OCI Compatible Containers can be run in HPC, just not with the Docker runtime









 Install and properly configure container runtimes optimized for HPC

 Run rootless containers using Singularity, Charliecloud, Sarus, Podman, and Shifter

Configure MPI to work with containers





#### **Roadmap: What We Compared**

 MVAPICH2 Library performance vs OpenMPI Library performance

Container performance vs Host System performance

Singularity vs Charliecloud performance





#### **MVAPICH2 vs. OpenMPI Runtimes**

MVAPICH2 performed significantly faster than OpenMPI for small and large message sizes







#### **Container vs. Host MPIBench Runtimes**

 Containers installed with MVAPICH2 were slower than the host system with MVAPICH2









#### **Container vs. Host MPIBench Runtimes**

• OpenMPI showed consistent results inside and outside Charliecloud/Singularity containers

















**Singularity vs. Charliecloud** 

performance of MPIBench inside







## Challenges

- Sarus
  - Not using the interconnect properly led to high runtimes
- Running Podman Containers stored on NFS
  - Setting up rootless podman to work with NFS
    - Stores images in an NFS based home directory
    - Podman containers cannot run on NFS so you must copy container storage over to each compute node manually
- Establishing MPI and Slurm Compatability
  - Configuring Slurm, OpenMPI, and MVAPICH2 to work with PMI support
  - We had to install OpenMPI and MVAPICH2 from Source not from the package manager
- Installing Shifter
  - Shifter uses Python 2.7 so it could not be installed on CentOS 8



#### **Future Work**

- Shifter
  - Testing runtimes
- Podman
  - Slurm and MPI compatibility
- Sarus high-speed infiniband interface
  - rather than ethernet
- E4s-cl Project
  - Extreme Scale Scientific Software Stack container launcher (e4s-cl)
  - a tool used to run MPI applications in containers
  - Use it to run MPI benchmarks inside the container





- <u>https://www.redhat.com/sysadmin/rootless-podman-nfs</u>
- <u>https://podman.io/</u>
- <u>https://www.docker.com/resources/what-container</u>
- <u>https://chrisshort.net/docker-inc-is-dead/</u>
- <u>https://id.pinterest.com/pin/639792690799904646/?amp\_client\_id=CLIENT\_ID()</u> <u>&mweb\_unauth\_id={{default.session}}&amp\_url=https%3A%2F%2Fid.pinterest.co</u> <u>m%2Famp%2Fpin%2F639792690799904646%2F&from\_amp\_pin\_page=true</u>
- <u>https://sarus.readthedocs.io/en/stable/</u>
- <u>https://hpc.github.io/charliecloud/</u>
- <u>https://containerjournal.com/topics/container-management/containers-hpc-mutually-beneficial/</u>
- <u>https://www.netapp.com/devops-solutions/what-are-containers/</u>
- <u>https://cloud.google.com/containers</u>



#### Questions



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