CaRCC Researcher-Facing Call, 2023-08-10

Evolution of Containers for HPC

Speaker:David Godlove, Solutions Architect, CIQ

Abstract:

In this session, Dave Godlove (Solutions Architect) will provide an update on the ongoing evolution of containers for HPC. We'll discuss the transition from Singularity to Apptainer as a project supported by the Linux Foundation. Then we'll turn attention to leveraging fake root permissions using the User namespace and running containers in "rootless mode". We'll also briefly discuss new recommendations for running containers in parallel and strategies for securing pre-built base containers. Finally, we will discuss job orchestration for containers in HPC. This presentation will be followed by a community discussion.

Please Note:

- ***We will record this call and post shortly thereafter on CaRCC's YouTube channel.***
- ***We expect all persons on the call to adhere to CaRCC's Code of Conduct.***

Connection Details

https://utah.zoom.us/my/carcc?pwd=TjFuR3VVM2d5eE5zWnEvWWxDTFBCUT09

Meeting ID: 824 051 8198
Password: 31415926

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Agenda

- Welcome + Introduction to CaRCC
  - Researcher-Facing Track description
  - CaRCC is your community for research computing and data professionals. Please see this brief overview; more information on activities on our Groups web pages.
  - If you have questions about CaRCC or are interested in becoming more involved, please contact:
    - rf-coordinators@carcc.org for R-F-related activities, or
    - getstarted@carcc.org or getinvolved@carcc.org for other CaRCC work
  - We expect all persons on the call to adhere to CaRCC's Code of Conduct.
- Topic of the month:
  - Presenter: David Godlove, Solutions Architect, CIQ
  - *Abstract - In this session, Dave Godlove (Solutions Architect) will provide an update on the ongoing evolution of containers for HPC. We'll discuss the transition from Singularity to Apptainer as a project supported by the Linux Foundation. Then we'll turn attention to leveraging fake root permissions using the User namespace and running containers in "rootless mode". We'll also briefly discuss new recommendations for running containers in parallel and strategies for securing pre-built base containers. Finally, we will discuss job orchestration for containers in HPC. This presentation will be followed by a community discussion.*
- Open Discussion
- Announcements
  - August 16th @ 12:00 pm EDT - Emerging Centers
    - Centre for High Performance Computing, South Africa
  - August 17th @ 1:00 pm EDT - Systems-Facing
    - Cluster Resource Management software and solutions - Part 2 (Part 1 was June call)
  - **September 14th - NEXT Researcher Facing Call**
    - Library Research Support perspective - Call details pending.

Sign-In (Name / Affiliation /Email)

Note: please follow the suggested sign-in format so our evolving data science intelligence routines won't trip up and forget to enter you in our $1m sweepstakes.

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Max attendee count - Sign in 36 above - 55 max on Zoom

Notes from the call

Slides

[Intro slides]
[David Godlove CIQ]

Notes - Topics Covered
Singularity is Apptainer!

- Leveraging the User Namespace
- New recommendations for containerized MPI
- Increased adoption of ORAS (for Software Supply Chain)
- Container Orchestration (for jobs, from an HPC perspective)

Questions

- If you do an "ls -ln" in the non-containerized environment vs. the container environment, you'll see the uid # mapping.
- Is this available in any version of apptainer? If not, which version we would need?
    - It was in Apptainer 1.1.0 when the user name spaces were set as default, that was about fall last year, but it was non-default before that
- The unprivileged install looks like it only works on certain distributions? What about Ubuntu/Debian?
- Spack, EZbuild and ?? there was a third mentioned I haven't heard of prior
- How does Fuzzball differ from Jobs in K8s
- Do you have example workflow / yaml files? And could this be adapted for ‘pleasantly parallelized’ workflows? Ah! I see ‘task array’ in there

Chat Comments

I think the work presented by Sgambati and Anderson (INL) at PEARC23 is also useful here:

> Matthew Sgambati and Matthew Anderson. 2023. Software Quality Assurance for High Performance Computing Containers. In Practice and Experience in Advanced Research Computing (PEARC ’23), July 23–27, 2023,Portland, OR, USA. ACM, New York, NY, USA, 12 pages. https://doi.org/10.1145/3569951.3593596