SINGULARITY USER GROUP

March 12-13, 2019

AGENDA

Presented By
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Tuesday, March 12, 2019

8:00 – 8:30	**Registration and Continental Breakfast**
8:30 – 8:45	**Welcome** Shawn Strande, San Diego Supercomputer Center
8:45 – 9:15	**Opening Keynote** **Singularity: Past, Present, and Future!** Gregory Kurtzer, CEO, Sylabs Inc.
9:15 – 10:15	**Morning Hands-on Session** **Creating and Running Software Containers with Singularity** Eduardo Arango, Software Engineer, Sylabs Inc.
10:15 – 10:30	**Break**
10:30 – 11:00	**What's New in Singularity 3.0** Dave Godlove, Product Manager, Sylabs Inc.
11:00 – 11:30	**LiCO and Singularity - Driving the Convergence of HPC & AI** JJ Falkanger, Sr. AI Software & Solutions Manager, Lenovo
11:30 – 12:00	**System Telemetry and I/O Profiling for Cloud Migration and Containers** Rosemary Francis, CEO, Ellexus
12:00 – 12:45	**Lunch**
12:45 – 1:15	**Combining VMware vSphere w/ Singularity Containers Brings Together the Best of Both Worlds** Mohan Potheri, Solutions Lab & HPC Solutions Architect, VMware
1:15 – 1:45	**PMIx: Bridging the Container Boundary** Ralph Castain, Principal Engineer, Intel
1:45 – 2:15	**Using Singularity Containers for Research Workflows and Reproducible Science** BJ Lougee, CI Engineer, Federal Reserve Bank of Kansas City
2:15 – 2:45	**AI Augmented HPC on Rescale and Singularity** Riaz Liyakath, Solutions Architect, Rescale
2:45 – 3:00	**Break**
3:00 – 3:30	**Best Practices for Containerizing InfiniBand** Parav Pandit, Staff Engineer, Mellanox Technologies
3:30 – 4:00	**From Containerizing Testbeds for HPC Applications to Exascale Supercontainers** Andrew Younge, Computer Scientist, Sandia National Laboratories
4:00 – 4:30	**FuncX: A Function Serving Platform for HPC** Ryan Chard, Argonne Scholar (postdoc), Argonne National Laboratory
4:30 – 5:00	**Highly Distributed, High Performance Application Scheduling with HashiCorp Nomad** Jake Lundberg, Senior Solutions Engineer, HashiCorp

Tuesday, March 12, 2019 (cont'd)

5:00 – 5:30	**Enabling Generalized GPU Support in Singularity** Derek Bouius, Product Manager, AMD
5:30 - 8:00	**Evening Reception & Grand Prize Raffle** (sponsored by Lenovo)

Wednesday, March 13, 2019

8:00 – 8:30	**Continental Breakfast**
8:30 – 9:00	**Building a Testing Infrastructure for Singularity - A Complex CGO Project** Eduardo Arango, Software Engineer, Sylabs Inc.
9:00 – 9:30	**Managing Large-Scale Cosmology Simulations with Parsl and Singularity** Rick Wagner, Globus
9:30 – 10:00	**Using Singularity Containers to Enable Scalable Interactive Workflows on Harvard Odyssey HPC Cluster** Francesco Pontiggia, Harvard FAS Research Computing
10:00 – 10:30	**NVIDIA HPC Container Efforts: An Overview** Adam Simpson, Systems Software Engineer, NVIDIA
10:30 – 10:45	**Break**
10:45 – 11:15	**Simplify Your Containers with Spack!** Gregory Becker, Computer Scientist, Lawrence Livermore National Laboratory
11:15 – 11:45	**Kubernetes the Next Research Program** Bob Killen, Senior Research Cloud Administrator, University of Michigan
11:45 – 12:15	**Singularity on Summit** Adam Carlyle, Senior Software Engineer, Oak Ridge National Laboratory Jack Morrison, HPC Engineer, Oak Ridge National Laboratory
12:15 – 1:00	**Lunch**
1:00 – 1:30	**Status Update on the Integration of Singularity and Kubernetes** Michael Bauer, Software Engineer, Sylabs Inc.
1:30 – 2:00	**Managing and/or Orchestrating Containerized Workloads?** Ian Lumb, Technical Writer, Sylabs Inc.
2:00 – 2:30	**Singularity and High Throughput Computing** Dave Dykstra, Fermilab
2:30 – 3:00	**Providing a National Software Repository for Interactive HPC** Lance Wilson, Characterisation Virtual Laboratory (CVL) Coodinator & Senior HPC Consultant, Jafar Lie-Monash University
3:00 – 3:15	**Break**
3:15 – 3:45	**Closing Keynote** **Enabling Scientific Computing with Singularity Containers on SDSC Comet** Shawn Strande & Mahidhar Tatineni, San Diego Supercomputer Center
3:45 – 4:30	**Town Hall**

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Featured Speakers

Tuesday March 12, 2019

8:45 - 9:15 am

Opening Keynote

Singularity: Past, Present, and Future!

Gregory Kurtzer, CEO, Sylabs Inc.

Gregory M. Kurtzer is the CEO and founder of Sylabs Inc., the company behind the open source container project, Singularity. Sylabs caters to the needs of EPC (Enterprise Performance Computing) supporting traditional simulation, compute, and AI use-cases. Previously, Greg has spent most of his career enabling massive scale compute focused use cases where he created and led various open source projects along that mission, including the Warewulf cluster management toolkit, CentOS Linux, and most recently, the container system Singularity.

9:15 - 10:15 am

Morning Hands-on Session

Creating and Running Software Containers with Singularity

Eduardo Arango, Software Engineer, Sylabs Inc.

Eduardo Arango is a Software engineer at Sylabs Inc. Currently a PhD student at Universidad del Valle, Colombia, on Cloud computing architecture. His areas of research are High Performance Computing, linux containers, Distributed Systems, and cloud computing. Eduardo is a software engineer at Sylabs inc, the company behind the Singularity OSS project, working on quality assurance and the test infrastructure for the singularity project, Nomad integration with Singularity runtime, and also a Singularity OSS maintainer.

10:30 - 11:00 am

What's New in Singularity 3.0

Dave Godlove, Product Manager, Sylabs Inc.

Singularity 3.0 represents a complete re-write of the Singularity source code in Go and adds many new features. The Singularity Image Format (SIF) is now the default image format. This flexible and extensible image format will allow for many future innovations, and it already enables cryptographic signing to produce and verify trusted containers. Network virtualization is now provided by cni plugins, the same network solution used by Kubernetes. There are many new security-related features, allowing admins to have fine grained control over privileged operations carried out by users with containers. Singularity 3.0 also introduces native support for c-groups, so that users no longer need to rely on resource managers to limit container resources. It's now easier than ever to work with Docker and OCI images in Singularity thanks to a few new bootstrap agents. And finally, 3.0 introduces the Singularity Container Services (SCS), a whole suite of cloud tools designed to help you build, distribute, and find trusted containers with ease. Singularity 3.1 adds the new ability to expose a SIF container to the host as an OCI compliant image bundle, and to run containers via an OCI compliant runtime variant within Singularity. This enables integrations between Singularity and other tools such as Kubernetes. In this talk we will briefly discuss the new features of Singularity with short illustrative demonstrations.

Dave Godlove is the Product Manager at Sylabs Inc. He has a Ph.D. in Neuroscience, and spent several years as a researcher at the National Institutes of Health. While there, he took a position helping to administer Biowulf, the NIH intramural HPC resource. He ultimately became a vocal advocate for containers in HPC, helped to develop early versions of Singularity, and became a founding member of Sylabs Inc. Today, he coordinates development effort across and within Sylabs projects, manages the Singularity release cycle, and is an active member of the open source community.

Featured Speakers

Tuesday March 12, 2019

11:00-11:30 am

LiCO and Singularity - Driving the Convergence of HPC & AI

JJ Falkanger, Sr. AI Software & Solutions Manager, Lenovo

Scientific researchers and commercial enterprises have been increasingly applying high performance computing (HPC) and artificial intelligence (AI) techniques for drivinginsights and business value, often in the same computing environment. This convergence demands flexible tools to effectively utilize the resources and workflows. Lenovo Intelligent Computing Orchestration (LiCO) provides an intuitive web-based interface for managing and deploying both AI and HPC workloads on the same cluster. Built upon an OpenHPC management stack, LiCO enables even inexperienced users to utilize cluster resources, thanks to Singularity container management and job template integration. This session covers the capabilities of LiCO, and the many benefits for users Singularity provides as part of the architecture.

J.J. Falkanger is Senior AI Software and Solutions Manager for the Lenovo Data Center Group, responsible for driving scale-out solutions to market that enable clients to increase business value with AI and HPC. Prior to joining Lenovo, J.J. was with IBM where he led competitive research and client engagements in Cloud Management, and was Sr. Product Marketing Manager for the iDataPlex and NeXtScale products in System x.

11:30 am-12:00 pm

System Telemetry and I/O Profiling for Cloud Migration and Containers

Rosemary Francis, CEO, Ellexus

Many organisations are looking to move their compute architectures to the cloud and into new technologies such as containerisation. However, dependence of legacy systems and large amounts of shared storage can make it hard to migrate to more flexible compute environments. Without a clear list of dependencies, for example, it can take a lot of time to containerise applications and to size storage appropriately for the application in the new environment.

This presentation will use industry case studies to show attendees how they can get a clear picture of their shared storage requirements in order to develop an informed go-to-cloud and containerisation strategy with I/O profiling tools from Ellexus and Singularity containers. By using system telemetry, attendees will gain an understanding of how to manage hybrid cloudarchitectures. We will describe techniques and best-practices for use by small teams, for corporation-wide infrastructure strategy or those just starting to look at Singularity.

Rosemary obtained her PhD in Computer Architecture from the Cambridge University Computer Lab after studying computer science at Newnham College. After working in the chip design industry, Rosemary founded Ellexus to help manage the complex tool chains needed for semiconductor design. Since then Ellexus has evolved to become the I/O profiling company, providing unique application and cluster monitoring tools to high performance computing organisations around the world. Rosemary is on the board of IdeaSpace, is a member of the Raspberry Pi Foundation and is a frequent speaker at both IEEE and Cambridge University as well as at business events around the world.

Featured Speakers

Tuesday March 12, 2019

12:45-1:15 pm

Combining VMware vSphere w/ Singularity Containers Brings Together the Best of Both Worlds

Mohan Potheri, Solutions Lab & HPC Solutions Architect, VMware

VMware vSphere provides excellent capabilities for isolating workloads and sharing HW. Singularity containers are an excellent packaging mechanism for applications. We will look at how vSphere virtual machines and Singularity can be combined effectively for sharing GPUs in machine learning applications. We will discuss some experiments we have done in image processing and the 3X gains we saw in processing throughput by using this solution.

Mohan Potheri is VCDX#98 and has more than 20 years in IT infrastructure, with in depth experience on VMWARE virtualization. He currently focuses on evangelization of “High Performance Computing” and “Big Data” Virtualization on vSphere. He has extensive experience with high performance & business critical applications across UNIX, Linux and Windows environments. Mohan Potheri is an expert on HPC virtualization and has been a speaker in multiple VMWORLD and HPC events. Prior to VMWARE, Mohan worked at many large enterprises where he has engineered fully virtualized HPC environments. He has planned, designed, implemented and managed robust highly available, DR compliant HPC environments in UNIX and x86 environments.

1:15-1:45 pm

PMIx: Bridging the Container Boundary

Ralph Castain, Principal Engineer, Intel

High-Performance Computing (HPC) applications have historically executed in static resource allocations, using programming models that ran independently from the resident system management stack (SMS). The Process Management Interface - Exascale (PMIx) community is committed to establishing scalable workflow orchestration by defining an abstract set of interfaces by which not only applications and tools can interact with the resident SMS, but also the various SMS components can interact with each other. PMIx has been widely adopted by both HPC programming libraries (e.g., MPI, OpenSHMEM) and SMS vendors (e.g., Slurm, JSM, PBSPro), and work is underway to extend support into non-HPC areas (e.g., Spark, Kubernetes). This presentation will provide an overview of the project and how it impacts the container community, and introduce a new community project (Epyx) specifically tailored to supporting containers in PMIx-enabled environments.

Dr. Ralph Castain is a Principal Engineer at Intel. He founded and leads the Process Management Interface-Exascale (PMIx) community (https://pmix.org), a consortium of industry, government, and academia members spanning the general HPC arena, specifically focused on orchestration of applicationlaunch and execution. He also aided initial development of Singularity container system and led two different efforts to integrate MPI support with Hadoop. Dr. Castain received his B.S. degree in physics from Harvey Mudd College and multiple graduate level degrees (M.S. in solid-state physics, M.S.E.E. degree in robotics, and Ph.D. in nuclear physics) from Purdue University. He has served in government, academia, and industry for over 35 years as a contributing scientist and business leader in fields ranging from HPC to nuclear physics, particle accelerator design, remote sensing, autonomous pattern recognition, and decision analysis. Dr. Castain has advised the National Science Foundation on the Partnership for a New Generation Vehicle program, created and led the first Electronics/VLSI section of the International Neural Network Society, and served on the program committees of several prominent international conferences.

Featured Speakers

Tuesday March 12, 2019

1:45-2:15 pm

Using Singularity Containers for Research Workflows and Reproducible Science

BJ Lougee, CI Engineer, Federal Reserve Bank of Kansas City

Moving a researcher's project between different cyber infrastructures can prove to be challenging without the use of containerization. What is worse is having to keep track of changes to a researcher's workflow (like code libraries or developed code) over a research project. After a researcher has completed their project and submitted their work for publication, others may not have the tools necessary to reproduce their research. This presentation will discuss using Singularity in a researcher's workflow that is simple and easy to use and could help advance reproducible science.

BJ Lougee is a computer scientist and cyberinfrastructure engineer and practitioner in the Center for the Advancement of Data and Research in Economics (CADRE) at the Federal Reserve Bank of Kansas City. He is also the XSEDE Campus Champion Deputy Director for Region 4

2:15-2:45 pm

AI Augmented HPC on Rescale and Singularity

Riaz Liyakath, Solutions Architect, Rescale

The current approach used in the engineering design community has been to use a Simulation Driven Product Development approach where Computer Aided Engineering (CAE) softwares are used for design analysis and virtual prototyping. However, the design of experiments and optimization process used today is tedious and involves running a lot of CAE simulations as well as requiring manual tweaking of design parameters by engineers to come up with a design which is ready for manufacturing. Luckily with the advance of containerization and cloud computing, manufacturing company can now take full advantage of artificial intelligence (AI) to accelerate innovation. In this presentation, we demonstrate using an industry example how Rescale provides a single HPC environment to:

- harvest all the simulation input data necessary to train a deep learning algorithms
- iterate efficiently with container to develop and validate your DL algorithm.
- deploy containers to the enterprise and execute it anywhere on-premise or in the cloud with consistency.

3:00-3:30 pm

Best Practices for Containerizing InfiniBand

Parav Pandit, Staff Engineer, Mellanox Technologies

InfiniBand is the leading interconnect accelerating HPC applications, delivers high bandwidth, low latency, RDMA and In-Network Computing advantages. The InfiniBand technology enables to bypasses the kernel, and offloads the network transport to the Host Channel Adapter (HCA). In the case of non-RDMA networks, when using containerized application, only system call level ABI compatibility needed between the Linux kernel and the container. However, a containerized application which uses RDMA, needs to ensure ABI compatibility between (a) application and kernel, (b) kernel and HCA and (c) user space stack and HCA. This talk highlights some of the best practices for InfiniBand in such environment. In this talk we will also discuss how to containerize InfiniBand for Singularity platform in an easy manner.

Parav contributes to linux kernel rdma and networking subsystem, container orchestrations tools, netlink go library. At Mellanox he contributes in software architecture, design and integrating rdma solutions with cloud, database, hpc users. Parav brings experience in rdma, networking, virtualization, hyper converged storage and NVMe fabrics.

3:30-4:00 pm

From Containerizing Testbeds for HPC Applications to Exascale Supercontainers

Andrew Younge, Computer Scientist, Sandia National Laboratories

As the code complexity of HPC applications expand, development teams continually rely upon detailed software operation workflows to enable automation of building and testing their application. These development workflows can become increasingly complex and, as a result, difficult to maintain when the target platforms' environments are increasing in architectural diversity and continually changing. Recently the advent of containers in industry have demonstrated the feasibility of such workflows, and the latest support for containers in HPC environments makes them now attainable for application teams. Fundamentally, containers have the potential to provide a mechanism for simplifying workflows for development and deployment, which could improve overall build and testing efficiency for many teams.

This talk will provide an overview of the current strategy for utilizing containers in HPC, starting at Sandia and expanding to the broader DOE Exascale ecosystem. This first includes the initial efforts for running Singularity on testbed clusters, expanding to Singularity deployments on DOE/NNSA production supercomputing resources. From here, the ECP Supercomputing Containers Project (aka ECP Sueprcontainers) will be introduced, which represents a consolidated effort across the DOE and NNSA to use a multi-level approach to accelerate adoption of container technologies. This project will investigate container scalability, interoperability, and ensure a high level of integration future HPCsystems and application teams. Effectively, we hope to ensure container runtimes like Singularity will be well poised to take advantage of the first Exascale supercomputers across the DOE.

Andrew Younge is a Computer Scientist at Sandia National Laboratories with the Scalable System Software group. His research interests include High Performance Computing, Virtualization, Distributed Systems, and energy efficient computing. The central focal point of Andrew's work is to improve the usability and efficiency of supercomputing system software. He has a Ph.D in Computer Science from Indiana University, where he was the Persistent Systems fellow and a member of the FutureGrid project, an NSF-funded experimental Cloud testbed. Over the years, Andrew has held visiting positions at the MITRE Corporation, the University of Southern California / Information Sciences Institute, and the University of Maryland, College Park. He received his Bachelors and Masters of Science from the Computer Science Department at Rochester Institute of Technology (RIT) in 2008 and 2010, respectively.

4:00-4:30 pm

FuncX: A Function Serving Platform for HPC

Ryan Chard, Argonne Scholar (postdoc), Argonne National Laboratory

There is a growing need to support the execution of short-duration tasks on High Performance Computing (HPC) infrastructure. To address this need we have developed FuncX: a function serving platform that is designed to provide on-demand execution of stateless functions directly from existing HPC infrastructure. FuncX aims to remove the barriers that exist between functions and large-scale computing infrastructure by simplify execution of function-based workloads, enabling integration of HPC capabilities in applications and analysis pipelines, and ultimately increasing the usability of computing infrastructure. FuncX uses the Parsl scripting library to provide low-latency, scalable, and reliable execution of tasks across heterogeneous computing environments. It securely isolates function executions within containerized Singularity execution environments and leverages Globus, as an identity and access management framework and to automate the movement of functions and data. In this talk I will describe the use cases that have motivated the development of FuncX, present the design of the FuncX execution framework, and present the prototype implementation and early experiences using the system. *(continued on the following page)*

Ryan Chard is a Maria Goeppert Mayer Fellow in the Data Science and Learning division at Argonne National Laboratory. His research focuses on scientific data management and research automation systems. In particular he works on Globus Automate to streamline data analysis pipelines, DLHub to serve machine learning models on-demand, and most recently, FuncX to enable function serving on HPC.

4:30-5:00 pm

Highly distributed, high performance application scheduling with HashiCorp Nomad

Jake Lundberg, Senior Solutions Engineer, Hashicorp

This talk will cover why application schedulers are necessary, a high level overview of Nomad as an application scheduler and some examples of our customers using Nomad for highly distributed batch processing.

Jake Lundberg is a Senior Solutions Engineer for HashiCorp and a recovering Systems Administrator. When not helping customers automate all the things, he enjoys spending time with his family, riding his bike, long walks on the beach and talking about himself in third person.

5:00-5:30 pm

Enabling Generalized GPU Support in Singularity

Derek Bouius, Product Manager, AMD

Walk through design and code changes needed to enable general graphics card support for use in Singularity containers. Discuss some of the challenges of supporting dedicated acceleration devices in a server environment and highlight solutions using Singularity containers.

Derek Bouius is a product manager at AMD and is responsible for the GPU computing software roadmap targeting AI and HPC workloads.

Featured Speakers

Wednesday, March 13, 2019

8:30-9:00 am

Building a Testing Infrastructure for Singularity - a Complex CGO Project

Eduardo Arango, Software Engineer, Sylabs Inc.

After a major project re-write from a code base Bash/Python/C to CGO, our team faced a new and interesting challenge, building a test suite in Go. As a team we decided that moving away from bash scripts to a formal language will give us better reproducibility, more test complexity (test tables), mock services, and std libraries for config files and crypto keys. This talk will share the experience of building a test infrastructure for a CGO, and will highlight the challenges we faced, and how we overcome them with Go std libraries and Go test tools.

Eduardo Arango is a Software engineer at Sylabs Inc. Currently a PhD student at Universidad del Valle, Colombia, on Cloud computing architecture. His areas of research are High Performance Computing, linux containers, Distributed Systems, and cloud computing. Eduardo is a software engineer at Sylabs inc, the company behind the Singularity OSS project, working on quality assurance and the test infrastructure for the singularity project, Nomad integration with Singularity runtime, and also a Singularity OSS maintainer.

9:00-9:30 am

Managing large-scale cosmology simulations with Parsl and Singularity

Rick Wagner, Globus

In preparation for the Large Synoptic Survey Telescope (LSST), we are working with dark energy researchers to simulate images that are similar to the raw exposures that will be generated from the telescope. To do so, we use the imSim software package (https://github.com/LSSTDESC/imSim) to create images based on catalogs of astronomical objects and by taking into account effects of the atmosphere, optics, and telescope. In order to produce data comparable to what the LSST will create, we must scale the imSim workflow to process tens of thousands of instance catalogs, each containing millions of astronomical objects, and to simulate the output of the LSST's 189 LSST's 189 CCDs, comprising 3.1 gigapixels of imaging data. To address these needs, we have developed a Parsl-based workflow that coordinates the execution of imSim on input instance catalogs and for each sensor. We package the imSim software inside a Singularity container so that it can be developed independently, packaged to include all dependencies, trivially scaled across thousands of computing nodes, and seamlessly moved between computing systems. The Parslworkflow is responsible for processing instance catalogs, determining how to pack simulation workloads onto compute nodes, and orchestrating the invocation of imSim in the Singularitycontainers deployed to each node. To date, the simulation workflow has consumed more than 30M core hours using 4K nodes (256K cores) on Argonne's Theta supercomputer and 2K nodes (128K cores) on NERSC's Cori supercomputer. The use of Singularity not only enabled efficient scaling and seamless conversion to support other container technologies, but it was also an integral part of our development process. It significantly simplified the complexity of developing and managingthe execution of a workflow as part of a multi-institution collaboration and furthermore it removed much of the difficulties associated with execution on heterogeneous supercomputers.

Featured Speakers

Wednesday, March 13, 2019

9:30-10:00 am

Using Singularity containers to enable scalable interactive workflows on Harvard Odyssey HPC cluster

Francesco Pontiggia, Harvard FAS Research Computing

Harvard FAS Research Computing has recently deployed a web-portal to allow users to run on the HPC cluster Odyssey interactive GUI jobs,including remote desktop sessions, notebook oriented workflows, GUI desktop software and other applications with a web-based frontend like for example RStudio server. Trying to deploy and run those applications out of our standard cluster software repository resulted in numerous challenges.

We encountered substantial difficulties in terms of ease of development and we faced compatibility issues with some specific software packages not designed to run in multi-tenant HPC environments. Moreover we faced severe limitations in the application startup performance, due to some aspect of our storage infrastructure not originally designed to support those type of workflows. While a slow startup is not a particularly relevant factor in the context of typical batch jobs run on our system, it becomes an important factor in negatively impacting the user experience when scheduling and accessing interactive applications.

Using Singularity containers proved crucial for an efficient deployment of our new portal. It gave us flexibility in the application development and allowed us to circumvent intrinsic limitations of specific applications. Moreover the use of containers allowed us to leverage our high performance lustre storage, particularly suited fast read access of large size files, allowing a significant performance boost in the applications startup time.

10:00-10:30 am

NVIDIA HPC Container Efforts: An Overview

Adam Simpson, Systems Software Engineer, NVIDIA

The NVIDIA GPU Cloud, NGC, is a hub providing performance-optimized application containers which can be deployed on NVIDIA GPU-powered desktops, data center servers, and cloud services. This talk will cover engineering challenges that NVIDIA has faced in deploying such containers to NGC, and their solutions. Focus areas will including NVIDIA GPU access within containers, multi-node distributed containers, cluster integration, and performance portable optimization strategies.

Adam Simpson is a systems software engineer at NVIDIA working to build and deploy HPC containers targeting the NVIDIA GPU Cloud(NGC). Before joining NVIDIA Adam worked for Oak Ridge National Laboratory supporting DoE leadership compute resources.

10:45-11:15 pm

Simplify Your Containers with Spack!

Gregory Becker, Computer Scientist, Lawrence Livermore National Laboratory

Spack is an open-source package manager for HPC. Its simple, templated Python DSL allows the same package to be built in many configurations, with different compilers, flags, dependencies, and dependency versions. Spack allows HPC end users to automatically build any of over 3,000 community-maintained packages, and it enables software developers to easily manage large applications with hundreds of dependencies. These capabilities also enable Spack to greatly simplify HPC container builds.

This presentation will give an overview of Spack, including recent developments and a number of items on the near-term roadmap. We will focus on container use cases of interest to the Singularity community, including: optimized binary packages, improved developer workflows with Spack environments, and better support for large-scale HPC facility deployment. We will also discuss how Spack can be used to simplify container recipes, and some ideas for making Spack automatically generate multi-stage container builds.

Gregory Becker is a computer scientist at Lawrence Livermore National Laboratory. His focus is on bridging the gap between research and production software at LLNL. His work in software productization has led him to work on Spack, a package manager for high performance computing, as well scalable I/O formats for performance tools. Gregory has been at LLNL since 2015. He received his B.A. in Computer Science and Mathematics from Williams College in 2015.

11:15-11:45 am

Kubernetes the next research program

Bob Killen, Senior Research Cloud Administrator, University of Michigan

Kubernetes has become the defacto standard as a platform for container orchestration. Its ease of extending and many integrations has paved the way for a wide variety of data science and research tooling to be built on top of it.

From all encompassing tools like Kubeflow that make it easy for researchers to build end-to-end Machine Learning pipelines to specific orchestration of analytics engines such as Spark;Kubernetes has made the deployment and management of these things easy. This presentation will showcase some of the larger research tools in the ecosystem and go into how Kubernetes has enabled this easy form of application management.

Bob is a Research Cloud Administrator with the Advanced Research Computing Technology Services (ARC-TS) group at the University of Michigan. He has been with the University for more than 15 years, serving in various capacities within the Health System and ARC-TS. As a Cloud Native Computing Foundation Ambassador, Bob has worked towards improving High Performance Computing, Machine Learning, and other Computational Research initiatives by integrating them with Cloud Native practices and tooling. He is passionate about Academic Outreach, and is an outspoken advocate of both Open Source and Open Science.

11:45 am-12:15 pm

Singularity on Summit

Adam Carlyle, Senior Software Engineer, Oak Ridge National Laboratory
Jack Morrison, HPC Engineer, Oak Ridge National Laboratory

Leadership computing systems traditionally have been designed for the execution of parallel simulations with the assumptions that these applications optimized will have an optimal access to the network and other hardware resources such as accelerators in order to guarantee maximum performance. However, this approach imposes application teams to adapt their codes to the target platforms, sometimes leading to major investments in terms of time and manpower when a new systems is delivered.

A natural way to try to address this limitation and potentially limit the cost to support a new computing platform is to let application teams define, instantiate and run their customized environments. Historically, virtual machines were considered to achieve that goal but were proven to impose an execution overhead that was too high for HPC workloads. Fortunately, the venue of new technologies such as containers have proven a drastically lower execution overhead (at the cost of some isolation capabilities, e.g., the kernel is shared by the host and the guests) without imposing overbearing limitations on the customization of execution environments.

In this study, we present our experience with supporting Singularity on leadership computing systems at ORNL, from the creation of images to the execution of Singularity containers for the execution of MPI applications, highlighting its benefits and limitations.

Adam is a Senior Software Engineer at the Oak Ridge Leadership Computing Facility. He oversees a small team of software engineers tasked with writing and maintaining a broad array of applications and operational services that impact the OLCF's end-user community.

Jack is an HPC Engineer in the User Assistance Group at the Oak Ridge Leadership Computing Facility. He provides technical support to the OLCF's user base, and focuses on providing tools to simplify the user experience.

1:00-1:30 pm

Status Update on the Integration of Singularity and Kubernetes

Michael Bauer, Software Engineer, Sylabs Inc.

Singularity 3.1.0 introduced integration with Kubernetes via two efforts: an OCI engine on the Singularity side, and a CRI implementation called singularity-cri. The singularity-cri project was recently tagged with its first and second alpha releases, paving the way towards Singularity + Kubernetes in production. An update on these projects will be provided in this talk

Michael is a software engineer at Sylabs who has been involved with the Singularity project for almost three years. He currently is the technical leader of the Singularity project, and helps direct some of the other core container projects that Sylabs maintains

1:30-2:00 pm

Managing and/or Orchestrating Containerized Workloads?

Ian Lumb, Technical Writer, Sylabs, Inc.

In those compute clusters that have been used traditionally for High Performance Computing (HPC), requirements for the management of workload have been addressed for more than two decades. Through dependencies involving two or more 'jobs', workload managers (WLMs) have some innate ability to allow for workflows, though this requirement is increasingly better serviced by 'external' capabilities - e.g., Nextflow is representative of possibilities that can be well addressed today. Even in isolation from other types, there is an emerging set of requirements that seek to execute HPC workloads via containers. For the most part, this is also well addressed by WLMs in traditional HPC compute clusters. What is less clear, however, are the full complement of requirements that relate to the execution of HPC or Enterprise Performance Computing (EPC) workloads via containers orchestrated by Kubernetes. Whereas Kubernetes' simplistic complement of build-in scheduling policies may adequately address the requirements typical of microservices based deployments, it is evident that the needs of HPC and EPC workloads are not being addressed. And as hybrid use cases involving some combination of services alongside HPC or EPC workloads, unmet requirements manifest as an ever-widening gap. With the recent alpha release availability of the Singularity Container Runtime Interface (CRI), there now exists new possibilities for HPC and EPC workloads for orchestration via Kubernetes. Beyond supporting native passthrough involving the built-in scheduler for Kubernetes, work on the Singularity CRI has motivated other possibilities - other possibilities that would allow WLMs like Slurm to be utilized in a Kubernetes context. After briefly reviewing the traditional case for WLMs in HPC clusters, emphasis shifts to the possibilities and probabilities for applications containerized via Singularity in a Kubernetes container cluster.

Although Ian's been making his way around the HPC solution stack for over 20 years, this is the first time he's been contained by it. In turn, Ian actively seeks to containerize HPC, Data Science and Machine Learning via Singularity through a combination of words and technology.

2:00-2:30 pm

Singularity and High Throughput Computing

Dave Dykstra, Fermilab

Singularity is used heavily in production by multiple High Energy Physics (HEP) projects (the LHC's CMS, the Open Science Grid Virtual Organization, and several Fermilab projects) on hundreds of thousands of CPU cores worldwide based on High Throughput Computing (HTC, also known as grid computing). Many more projects are making plans to also use it. The HEP projects rely on singularity for both controlling the software environment and for isolating jobs from end users that are run by unprivileged pilot jobs. They exclusively use the singularity sandbox mode, with images unpacked in the CernVM FileSystem (CVMFS) which securely distributes the images by means of a very efficient on-demand caching infrastructure. They are currently rolling out a conversion to using non-setuid singularity, based on RHEL 7.6 which introduced full support for unprivileged namespaces. This talk will introduce the Singularity User Group to this important singularity user community. *(continued on the following page)*

Dave Dykstra has worked for the Scientific Computing Division at Fermilab since 2006 and has been a big supporter of open source for much longer than that. He began his career at AT&T Teletype writing embedded software to run computer terminals, and later got his PhD in Computer Science from the University of Illinois. At Bell Labs he ran a system called Exptools that made both internal and open source software widely available and updated throughout the company. For part of that time he was also the primary maintainer of the popular open source tool 'rsync'. Currently at Fermilab he supports software widely used by LHC experiments and the Open Science Grid, in particular Singularity, the CernVM Filesystem, squid, and a system called Frontier that distributes and caches database lookups for the two biggest LHC experiments CMS and ATLAS. He also supports Singularity for EPEL and Fedora.

2:30-3:00 pm

Providing a national software repository for interactive HPC

Lance Wilson, Characterisation Virtual Laboratory (CVL) Coordinator & Senior HPC Consultant, Jafar Lie-Monash University

The characterisation community within Australia has been working towards a federated analytics platform to provide researchers with the tools, compute and storage needed to make the most of national investments in instruments. The current user base is ~1000 across disciplines from neuroscience to neutron and synchrotron science. One of the highlighted needs was for consistency between software stacks provided on different HPC systems. The initial work has been an extension of the existing container first philosophy on the MASSIVE HPC facility (Goscinski, 2014) which provides the Characterisation Virtual Laboratory (https://www.cvl.org.au). The repository for the build files is public (https://github.com/Characterisation-Virtual-Laboratory/CharacterisationVL-Software) and is run in the same way as a software development project. In addition to the build files being public, the repository is linked to singularity hub (https://singularity-hub.org/collections/1396), such that the containers are easily available to anyone in the characterisation research community. The containers are a diverse mix of single applications through to workflows, highly dependent on the intended use by the research community. Containers have also simplified aspects of user support, for single applications that are particularly difficult to install on complex HPC systems. It has also created a new support aspect in workflows or software aggregation tools, where the expectation from the software developers is that they are installed locally in the path. Overall however software support is now more convenient for both the administrators and researchers especially where we partner with software developers to provide containers.

Dr Lance Wilson is the coordinator of the Characterisation Virtual Laboratory, a specialist national program for imaging and visualization on Australian high performance computing facilities, and an Senior HPC Consultant at the Monash e-Research Centre a role in which he promotes effective and creative applications of technology in research.
Dr Wilson's research career has spanned the full breadth of mechanical and medical engineering, with a strong experimental focus. Research equipment instrumentation was a strong activity, especially in the design and testing of orthopaedic implants for multinational medical device companies. Later in his research career the focus shifted to more simulation and analysis of medical imaging to inform the experimental activities. He holds a PhD in Mechanical Engineering with strong interests in all areas of characterisation, in both experimental and computational aspects.

3:15-3:45 pm

Enabling Scientific Computing with Singularity Containers on SDSC Comet

Shawn Strande & Mahidhar Tatineni, San Diego Supercomputer Center

For over 30 years, the San Diego Supercomputer Center has been providing high-performance computing and data resources to the national community. Along with expertise in scientific computing, data science, and high-performance networking, SDSC has played an instrumental role in facilitating research across virtually every domain and enabling breakthrough discoveries. In this talk, we look at how SDSC has evolved to meet emerging needs of the community and how tools like Singularity have become an essential part of the strategy for serving an ever-larger and more diverse user community and research agenda.

Shawn Strande is the Deputy Director of SDSC. He holds Bachelor's and Master's Degrees in Aeronautical Engineering. He has worked in high-performance computing for most of the last 35 years, with stints at NASA Ames Research Center, the National Center for Atmospheric Research, and a number of private sector companies. In his current role he helps the center develop large funding proposals, and oversees the Comet project.

Mahidhar Tatineni received his M.S. & Ph.D. in Aerospace Engineering from UCLA. He currently leads the User Services group at SDSC. He has worked on many NSF funded optimization and parallelization research projects such as petascale computing for magnetosphere simulations, MPI performance tuning frameworks, hybrid programming models, topology aware communication and scheduling, big data middleware, and application performance evaluation using next generation communication mechanisms for emerging HPC systems.