

Linux Containers for HPC

2023 Update

Holger Gantikow

Juli 2023



Agenda

01. whoami

02. Intro

03. Container 101

04. Container Use Cases

05. Nimbix

06. Conclusion

01. whoami





Holger Gantikow

Senior IT Consultant / IT Landscape Architect at science + computing ag

Stuttgart Region · [Contact info](#)

About

Diploma Thesis "Virtualisierung im Kontext von Hochverfügbarkeit" / "Virtualization in the context of High Availability , IT-Know-How, Experience with Linux, especially Debian&Red Hat, Windows, Mac OS X, Solaris, *BSD, HP-UX, AIX, Computer Networking, Network Administration, Hardware, Asterisk, VoIP, Server Administration, Cluster Computing, High Availability, Virtualization, Python Programming, Red Hat Certified System Administrator in Red Hat OpenStack

Current fields of interest:

Virtualization (Xen, ESX, ESXi, KVM), Cluster Computing (HPC, HA), OpenSolaris, ZFS, MacOS X, SunRay ThinClients, virtualized HPC clusters, Monitoring with Check_MK, Admin tools for Android and iOS, Docker, Rkt, Singularity, Shifter, uDocker, Charliecloud + Container in general (as well as HPC usage), Linux 3D VDI (HP RGS, NiceDCV, VMware Horizon, Citrix HDX 3D Pro)

Specialties: Virtualization: Container, KVM, Xen, VMware products, Citrix XenServer, HPC, SGE, author for Linux Magazin (DE and EN), talks on HPC, virtualization, container, admin tools for Android and iOS, Remote Visualization



Experience



science + computing ag - an Atos Company

14 yrs 9 mos

- Senior IT Consultant / CAE IT Landscape Architect
Jul 2022 - Present · 1 yr
Baden-Württemberg, Germany
- Senior Systems Engineer
Apr 2009 - Oct 2022 · 13 yrs 7 mos
- System Engineer
2009 - Oct 2022 · 13 yrs 10 mos
- Graduand
Oct 2008 - Mar 2009 · 6 mos

Education



Paderborn University

GOLD for Technology Leaders, Software Innovation Campus (SICP)
Sep 2022

Successfully completed the Atos Group Talent program "GOLD for Technology Leaders", with the Cambridge University's Institute for Manufacturing (IfM) ...see more



University of Cambridge

GOLD for Technology Leaders, Department of Engineering, Institute for Manufacturing (IfM)
Sep 2022

Successfully completed the Atos Group Talent program "GOLD for Technology Leaders", with the Cambridge University's Institute for Manufacturing (IfM) ...see more



Hochschule Furtwangen

Dipl. Inform. (FH), Coding, HPC, Clustering, Unix stuff :-)
2003 - 2009

Find me on LinkedIn & Xing – feel free to reach out!

Quick Facts

Focus on technical & scientific computing with 30 years of expertise

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



found in 1989
as a university spin-off



science + computing

dedicated unit for
high-end & business
critical IT-Services

FY2020

€ 40.4M
external revenue

Atos

accompanied by Atos /
Bull Advanced
Computing Solutions



Tübingen



Berlin



Munich



Düsseldorf



Timișoara



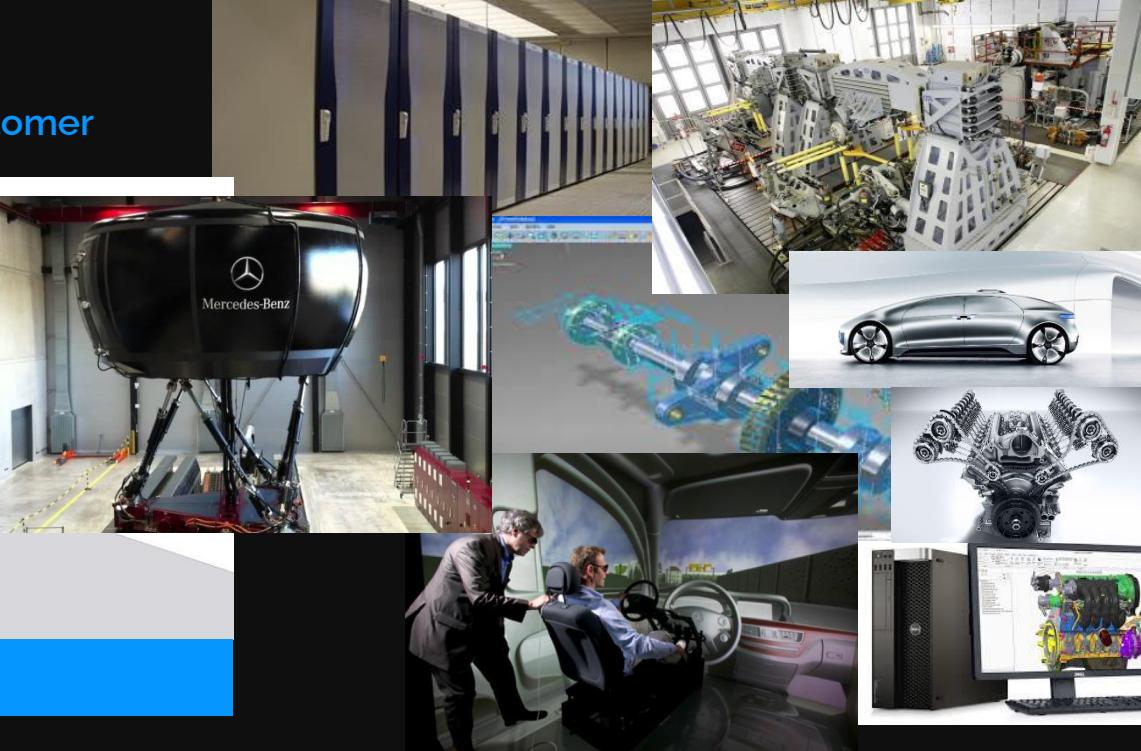
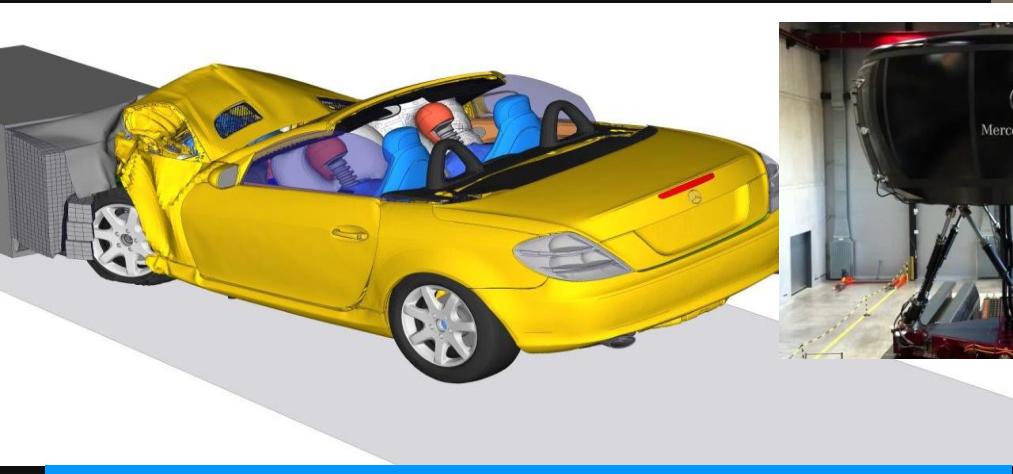
Brașov

EVIDEN

Starting Summer 2023

HPC Services

Operation and Projects close to the Customer



Our job and expertise

- *Operations of large scale heterogenous environments*
 - *Consulting projects in challenging environments*
 - *R&D + (Co-)Innovation projects*
 - *Automation*
 - *Close collaboration and customer-centric solutions*
-
- ▶ CAD / CAE / CAT, Virtual Reality
 - ▶ Driver Assistance Systems / Autonomous Driving
 - ▶ 3D accelerated Linux Engineering Work Places
 - ▶ Virtualization, Ways to the Cloud, Hybrid HPC
 - ▶ Data Management, Backup

Wir sind bei der science + computing immer wieder auf der Suche nach...

- Systems Engineers CAE/Linux
- Linux / IT / HPC Consultants (CAE/Linux)
- Systems Engineers Cloud
- HPC Performance Engineers
- Database Engineers
- Software Engineers
- Praktika, Abschlussarbeiten, Werkstudent:innen...

- Aktuelle Angebote unter
jobs.atos.net – Filter beachten

Country/Region	City	Experience Level
All	Tübingen	All
Brand	Job Area	
All	All	

- Gerne auch **initiativ** via Mail anfragen!
 - holger.gantikow@atos.net

The screenshot shows the Atos jobs website interface. At the top, there's a navigation bar with 'Language' and 'Sign In' options. Below it, the Atos logo and 'WORKING AT ATOS' are displayed. The main area has two search fields: 'Search by Keyword' and 'Search by Location'. A 'VIEW JOBS' button is visible. Below these, there's a brief introduction: "Hello, let's start by helping you get to know Atos. We are the global leader in secure and decarbonized digital with 110,000 employees in 73 countries and an annual revenue of € 12 billion. We are proud to work together with companies and industries around the world." Further down, there's another section titled "Getting to know Atos" with a video thumbnail and a text about the company's values and future focus.

Atos

WORKING AT ATOS

Search by Keyword Search by Location

VIEW JOBS

Hello, let's start by helping you get to know Atos. We are the global leader in secure and decarbonized digital with 110,000 employees in 73 countries and an annual revenue of € 12 billion. We are proud to work together with companies and industries around the world.

We are a European number one in Cloud, digital security and High-Performance Computing, not to mention AI, IoT, big data & analytics, edge computing and sustainability, we are busy shaping the future of the information space with our clients. Being the worldwide Information Technology Partner for the Olympic & Paralympic Games is something we pride ourselves on and we operate under the brands Atos and AtosSyntel. Atos is a SE (Societas Europaea), listed on the CAC40 Paris stock index.

Helping design the future of the information space is our core purpose. The expertise of our people and the services we support contribute to the development of knowledge, education and research in a multicultural approach leading the way in the development of scientific and technological excellence. Across the world, the group enables its customers and employees, and members of societies at large to live, work and develop sustainably, in a safe and secure information space.

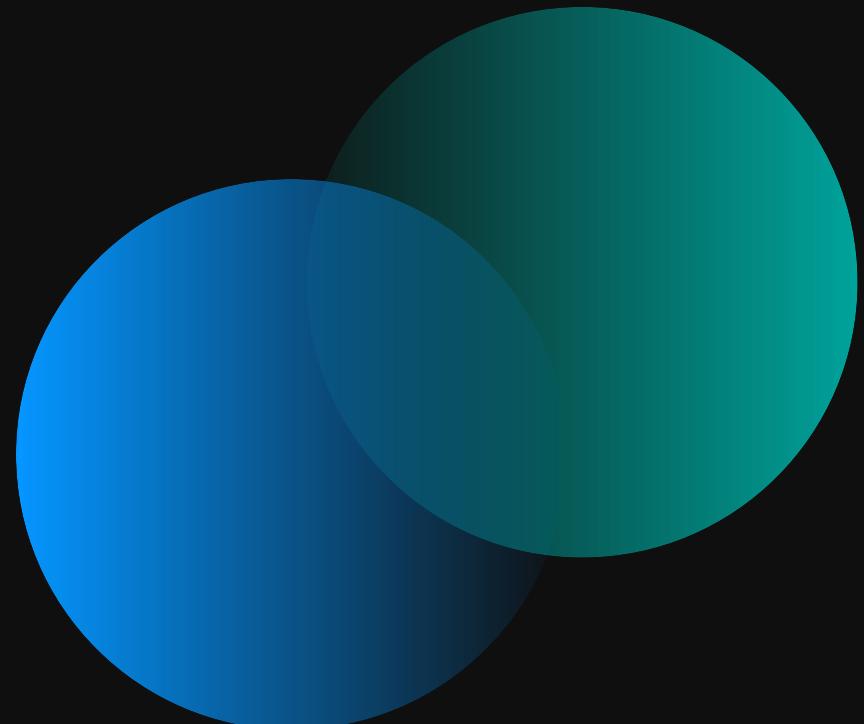
Getting to know Atos

Atos The Future is Our Choice

Here at Atos, we inspire candidates and our people to make the right choices, collectively and individually, to shape the future of the information space, the future of our organization and their own future. We value the diversity of our peoples' backgrounds and skills to make choices that will have positive economic, social and ethical impacts on business and humanity tomorrow.

#TheFutureIsOurChoice

02. Intro



Customers' Innovation is driven by HPC (High Performance Computing)



Customer's Hot Topics

CAE Cloudification, HPCaaS, Container

CAE Cloudification

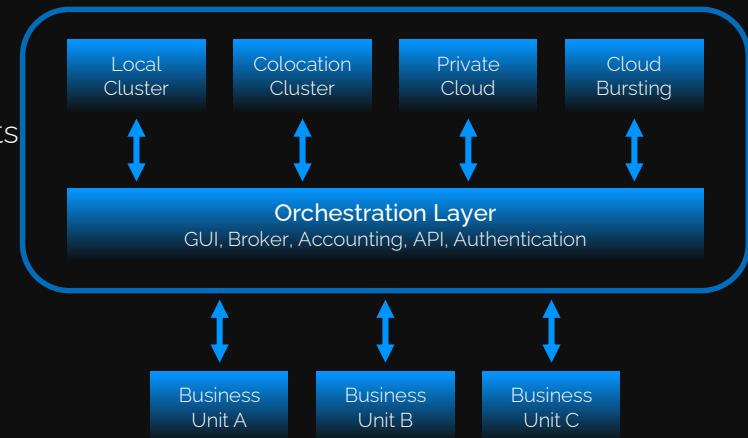
- Design and implementation of hybrid HPC environments.
- Customization of technical workflows to overcome limited cloud capabilities
- Development of solutions for asynchronous data transfer
- Optimization of total cost of ownership / bursting scenarios

HPC & CAE as a Service

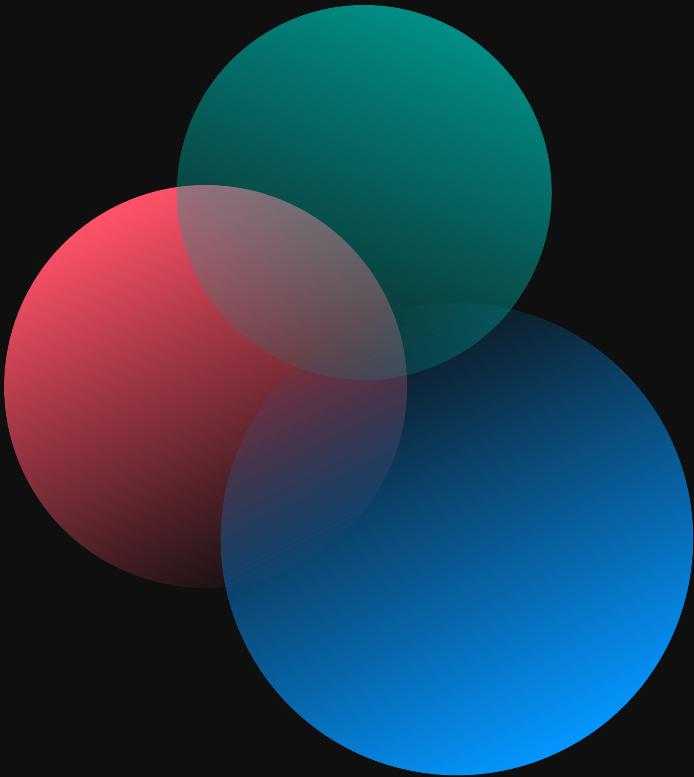
- Reduce project management and multi-provider management efforts
- Create private cloud CAE platforms

Containers for CAE/HPC

- Driver for many commercial use cases
 - Multi-site HPC Grids, K8s, Cloud HPC, Security, Standardization



03. Container 101



What is a container?

Wörterbuch

Nach einem Begriff suchen

Con·tai·ner

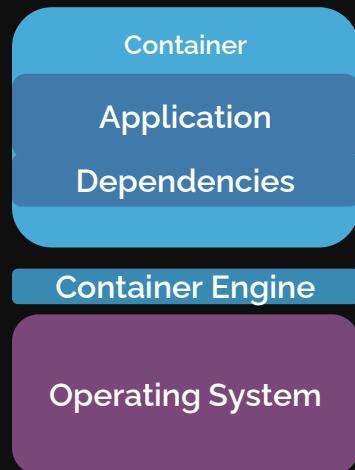
Substantiv, maskulin [der]

1. der rationelleren und leichteren Beförderung dienender [quaderförmiger] großer Behälter [in standardisierter Größe]
"fahrbare Container"
2. **VERLAGSWESEN**
Schachtel, Karton zum Versand von Büchern

Ähnlich

1. Behälter, Bunker, Großbehälter
2. Box, Karton, Schachtel, Drucke

Übersetzungen, Wortherkunft und weitere Definitionen



- Standardized packaging unit to simplify handling - has revolutionized transport
- Same in IT: standardized unit of applications + dependencies.
- Often offers advantages in distribution and operation
- Requires a container engine/runtime + underlying operating system (usually Linux)
- Differentiation *container image* + *container*

Container Image vs Container

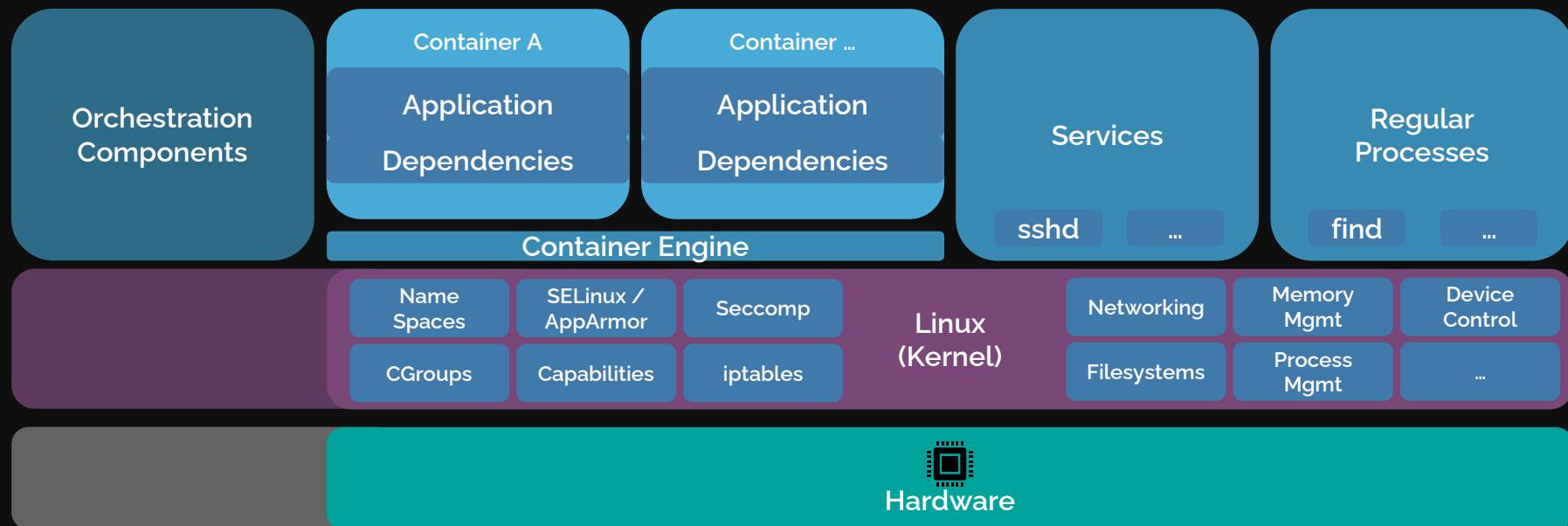


Notes

- **Containers Image** = Package containing *software, libraries and other dependencies* to run it.
- **Container** = Instantiated *container image*. Needs a *container engine + underlying OS*
- **Container Engine** often aka *Container Runtime* = “*Thing that starts the container*”
 - **Engine**: *Tooling around the runtime*. **Runtime**: *spawns the container*
- **Container Image Registry** = ~ “*App Store for Container Images*”
- Container images can be provided *locally* – or typically by using a **container registry**

Container + Linux

Containers rely a lot on existing kernel infrastructure



- Containers require a *container runtime environment* to operate
- Containers use many (already existing) Linux kernel features
- Orchestration components are often added to the mix

Container Base Technologies

Container = Namespaces + Control Groups

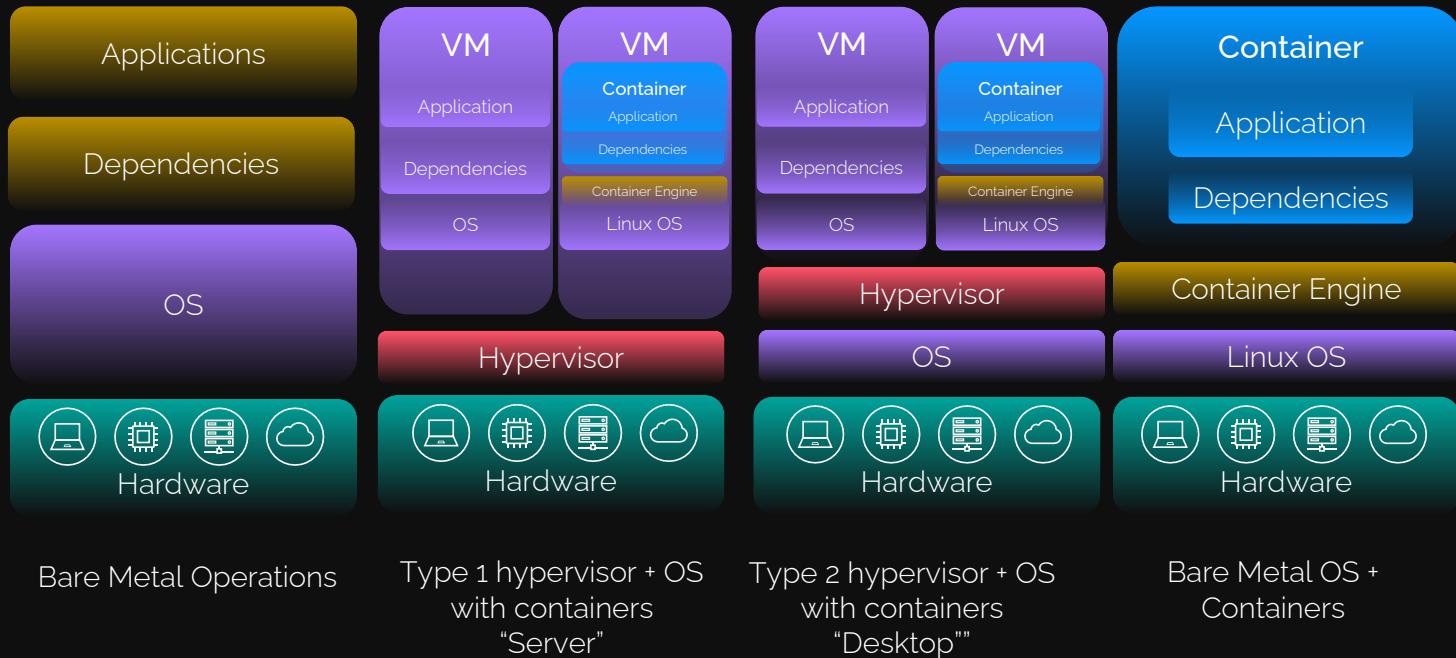
Both features of the Linux Kernel

- Namespaces: Some sub systems ns-aware - isolated operation.
- Cgroups: Some resources limitable - prevention of excessive utilization

Namespace	Description	Controller	Description
pid	Process ID	blkio	Access to block devices
net	Network Interfaces, Routing Tables, ...	cpu	CPU time
ipc	Semaphores, Shared Memory, Message Queues	devices	Device access
mnt	Root and Filesystem Mounts	memory	Memory usage
uts	Hostname, Domainname	net_cls	Packet classification
user	UserID and GroupID	net_prio	Packet priority

Virtualization with Containers

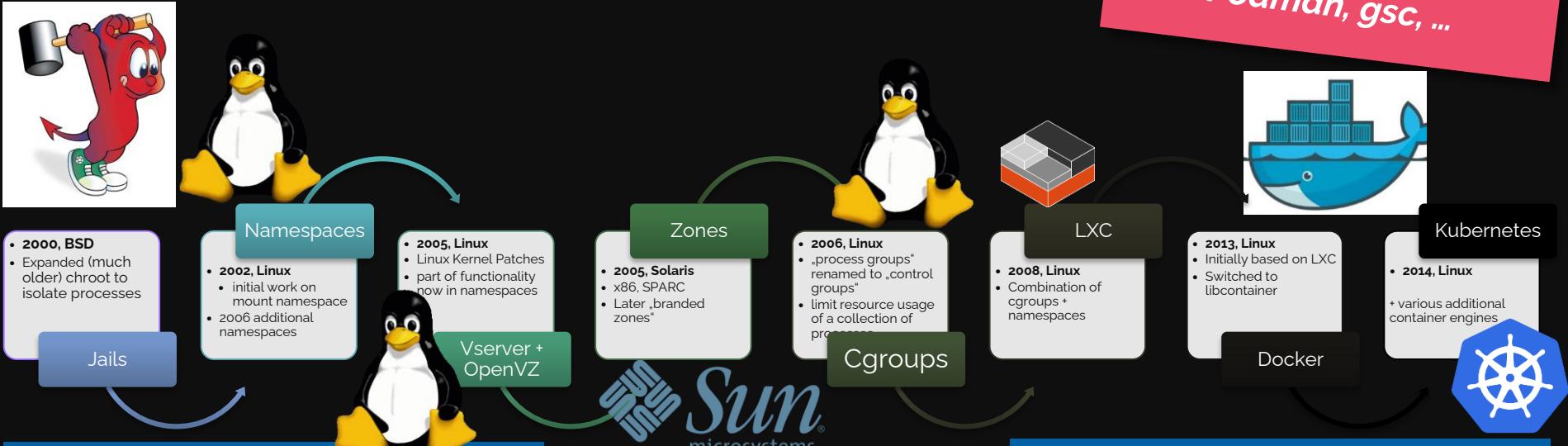
Stack: Bare Metal + Hypervisor + Containers



Evolution of OS-level Virtualization

Containers not just around since yesterday

+*gVisor, SCONE, Kata, Podman, gsc, ...*



HPC Container Runtimes

2015 Charliecloud (Jun)



2015 Shifter (Aug)

2016 Singularity 1.0 (Apr)

2016 udocker (Jul)

2019 Sarus 1.0 (Nov)

Hypervisor-based virtualization

1999 VMware Workstation 1.0

2001 ESX 1.0 & GSX 1.0

2003 Xen 1st public release

2006 KVM (2.6.10)

Container for Quick Solutions From Zero to Hero

- Fast ramp-up of specialized applications
 - Databases, ...
 - Programming environments
 - Machine Learning Stack
 - IoT (sensor board example)
- Easy sharing
- No lengthy installation manuals
 - "Take my image and run this".
- Other environment: Ubuntu on RHEL Ubuntu, ...



GreenNose@HFU Sensor Board



Source: <http://img.youtube.com/vi/KJRMjUzlHI8/o.jpg>

The Docker Hub search results for 'official & operating_system=linux & architecture=amd64' are displayed. The results include:

- couchbase**: Official Image. Updated a month ago. Couchbase Server is a NoSQL document database with a distributed architecture. Container, Linux, x86-64, Storage, Application Frameworks.
- alpine**: Official Image. Updated 2 months ago. A minimal Docker image based on Alpine Linux with a complete package index and only 5 MB in size. Container, Linux, PowerPC 64 LE, x86-64, riscv64, IBM Z, ARM, ARM 64, 386, Featured Images, Base Images, Operating Systems.
- busybox**: Official Image. Updated 3 days ago. Busybox base image. Container, Linux, ARM, x86-64, ARM 64, PowerPC 64 LE, IBM Z, 386, riscv64, mips64le, Base Images.
- python**: Official Image. Updated a day ago. Python is an interpreted, interactive, object-oriented, open-source programming language. Container, Linux, Windows, 386, x86-64, PowerPC 64 LE, ARM 64, IBM Z, mips64le, ARM, Programming Languages.
- nginx**: Official Image. Updated a day ago. Official build of Nginx. Container, Linux, ARM, 386, x86-64, mips64le, IBM Z, PowerPC 64 LE, ARM 64, Application Infrastructure.
- ubuntu**: Official Image. Updated 11 hours ago. Ubuntu is a Debian-based Linux operating system based on free software. Container, Linux, ARM 64, x86-64, IBM Z, ARM, 386, riscv64, PowerPC 64 LE, Base Images, Operating Systems.
- postgres**: Official Image. Updated 16 days ago. The PostgreSQL object-relational database system provides reliability and data integrity. Container, Linux, IBM Z, mips64le, 386, PowerPC 64 LE, ARM 64, x86-64, ARM, Databases.
- httpd**: Official Image. Updated 20 days ago. The Apache HTTP Server Project. Container, Linux, mips64le, PowerPC 64 LE, 386, ARM, x86-64, ARM 64, IBM Z, Application Infrastructure.

Containers in Everyday IT

Hybrid Cloud, DevOps, HPC, ...

Hybrid Cloud

- Simplified application deployment, scaling

DevOps - bringing developers (Dev) and operations team (Ops) together

- Containers are great for streamlining DevOps workflows

- Ops roll out applications that Dev has developed - doesn't always have to work out... - "Works on my machine"
 - Easier with containers - as application already has dependencies with in package

- Creation of images usually combined with CI/CD pipelines (Jenkins, ...)

- Automatic creation of images that are uploaded to a registry

- Consistency for development, test and production environments.

- Everyone works with the same consistent container environment

- Simplify updates

- Rollbacks to working state by redeploying an earlier working version

HPC - Containers are also gaining adoption in HPC, motivation:

"portability" (grid-like environment), user-supplied software stack, low overhead, ...



Further Reading

Container and Kubernetes, Market Dynamics Report, 2021

TOP BARRIERS TO WIDER ADOPTION OF CONTAINERS



n = 574

USAGE AND HOSTING OF KUBERNETES

Do you use Kubernetes ?

Yes 54%	65% In a virtual machine
No 46%	47% In the cloud
	35% Locally
	20% On my own PC
	1% I don't know

n = 338



Technical Benefits of Containers

Innovation	39%
Modernization	36%
Support for hybrid IT operations	34%
Scalable operations	34%
Improved productivity	34%
Cloud adoption	33%
Portability	32%

n = 345

For supply chain automated services	28%
n = 524	

Usage of Containers

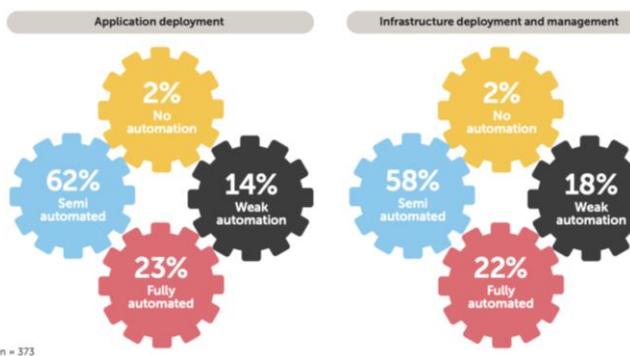
To simplify the integration or consistency of internal systems	43%
To autoscale solutions that have no internal scaling mechanisms	35%
Development and delivery of commercial solutions for external customers	32%
To deliver common reusable features across the organization	31%
To distribute internal shared resources	29%
For supply chain automated services	28%

Business Benefits of Containers

Cloud adoption	33%
Innovation	31%
Scalable operations	30%
Modernization	29%
Improved productivity	29%
Cost savings	29%
Portability	29%
Support for hybrid IT operations	24%

n = 574

DEPLOYMENT AUTOMATION MATURITY OF RESPONDENTS



n = 373

Why scientists + the HPC community love Containers

And so should you!



Mobility / Portability

- Compute resources are flexible
 - Laptop
 - Workstation
 - HPC
 - Cloud
- Encapsulated SW stack



User-supplied applications

- Growing demand
- Helps with contradictory requirements
- "Works on my machine"
- Novel applications
 - Latest Ubuntu vs Enterprise Linux
- Legacy code
 - Fortran @CentOS5



Reproducibility

- Collaboration
- Passing on the SW environment
- Simplifies reproducibility
- Defined SW stack in container („immutability“)
- Standardization



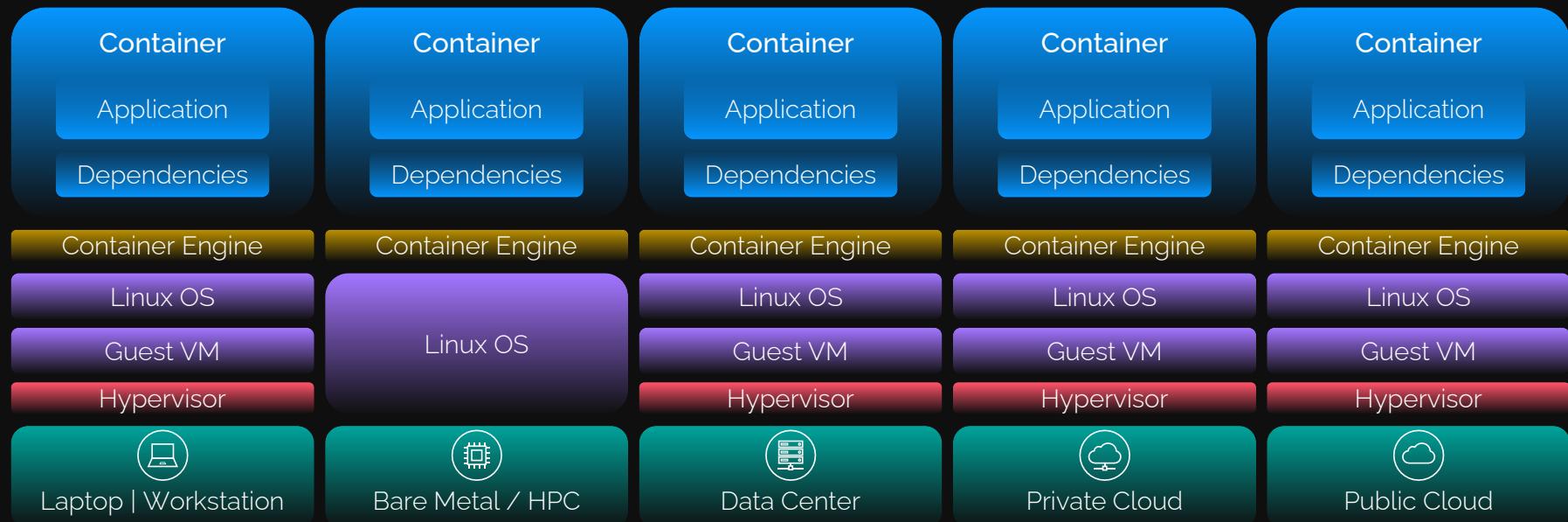
Performance

- Very low overhead
- Performance close to bare metal
- Lots of research on the subject, including our own

Container Technology

The promise of portability

- "Containers enable portability across platforms"
- Singularity talks about "Mobility of Compute"



Portability

Why is it harder in HPC?

- Portability depends on the application
- Results from host/environment dependencies

	Tensorflow	Tensorflow with GPU	Solver with GPU Support	Typical CAE Solver
Node	Single	Single	Single	Multi
Storage / Scratch	Volume	Volume	Shared	Shared
Devices required	-	GPU	GPU	Infiniband
Other				MPI & Slurm
Runtime	Enterprise	NVIDIA-docker	Enterprise/HPC	HPC

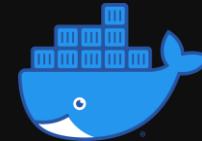
Dependencies and required effort

Container Engines

Not all containers are created equal

Even though everything is called a container, the degree of isolation varies

- Depending on origin (enterprise/HPC container engine) different degree of isolation mechanisms:
"As much isolation as possible vs as little as necessary."
 - *chroot vs namespaces, Cgroups, Seccomp, AppArmor/SELinux, ...*
 - *Background: n containers / host vs 1 container / host*
- Isolation can often be activated for HPC engines or deactivated for enterprise engines.
- Approximate classification of the isolation on the basis of the available features*:



chroot

Isolation (Workloads among themselves + Host)
*(*simplified representation)*

Virtual Machine

Container Engine Diversity

Quick Summary



Docker (2013)

- Without a chance in HPC, fading in importance:
 - Dockershim in Kubernetes (aka "K8s drops Docker").
 - Sale of Enterprise to Mirantis, focus on Hub + Desktop



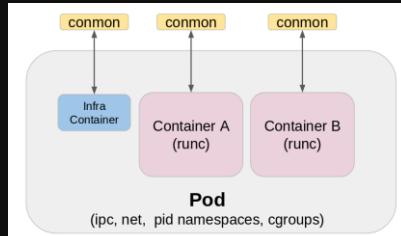
Singularity (2015)

- The most popular and widespread HPC container engine
- Additional own flat image format (SIF) - potentially more performant
- Singularity (Sylabs) vs Apptainer (CIQ / Linux Foundation)**
- 11/22:** Will encapsulate OCI images in SIF in the future



Podman (2017)

- Support by Red Hat
- Migration: "alias docker=podman" and "podman-compose"
- Rootless container, buildah for building images
- Supports pod concept -> simplified way to K8s from local tests
- 07/2022: Support SIF Images**
- 11/2022 NERSC's podman-hpc**



Container Engine Diversity

The lesser known HPC Container Engines



Shifter (2015)

- Docker images on Cray, focus on image workflow.
- *"Liked the container concept, but not the technology"*
- Maintenance only (due to NERSC's podman strategy)



Charliecloud (2015)"

- Use of user namespaces. Compact (800 LOCs)
- Usable as Uboot (LRZ), but rough - own commands, image conversion

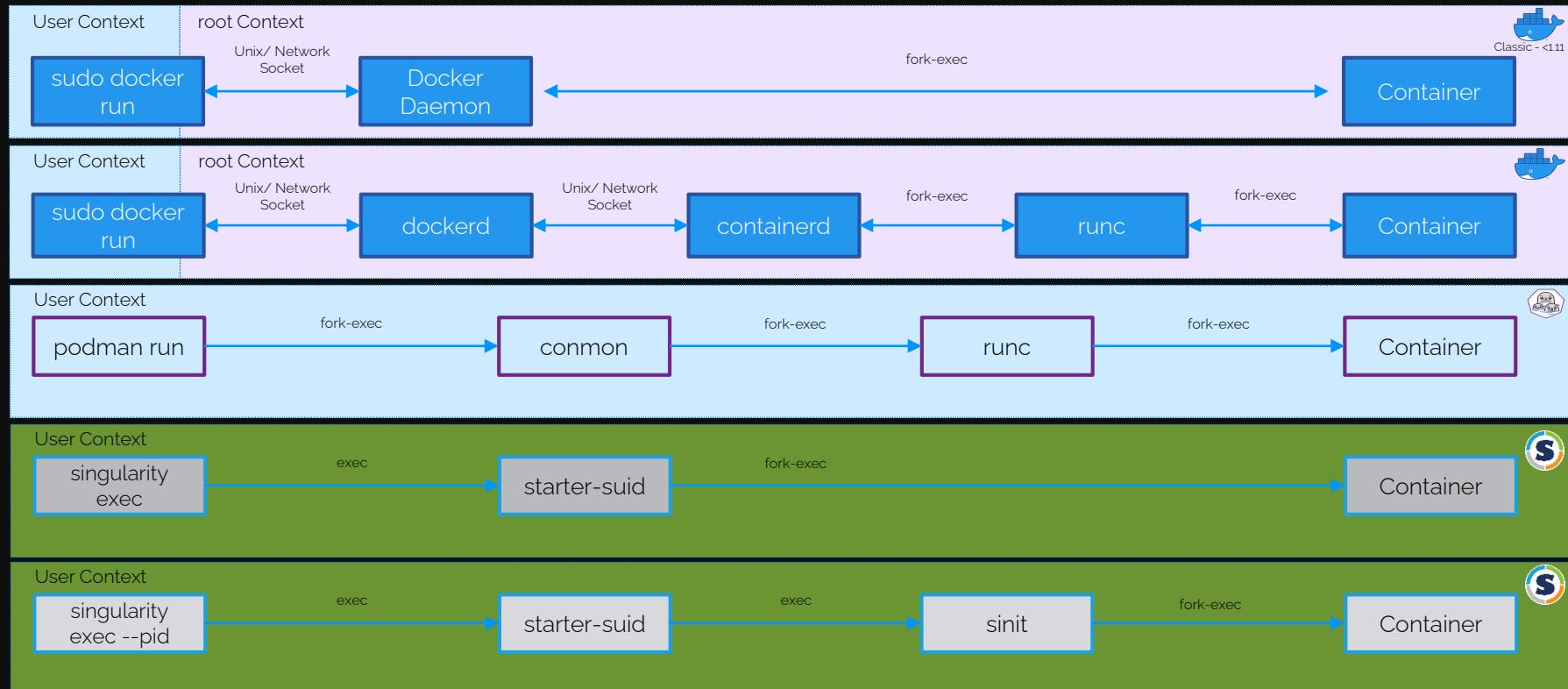


Sarus (2019)

- Developed at CSCS – focus: full OCI Support
- Providing of useful features via OCI Hooks (NVIDIA Container Toolkit, Native MPI, Native glibc, SSH, Slurm global sync hook,...)

Container Engines

From container engine call to running Container



Container Technologies

Standards

- Despite Docker's fading importance:
 - Co-created Open Container Initiative (OCI) *specifications* *image*, *runtime*, *distribution* will outlast
- All engines support *OCI images* - switching engines is relatively easy
- Many engines now rely on *runc* as runtime
 - Docker, Podman, Sarus
 - *runc* is the reference implementation of the OCI runtime-specification
 - Availability of *crun* as a replacement (reasons: Go vs C implementation, cgroups v2, performance)
 - Hooks support to extend core functionality defined in runtime spec

The Agony of Choice

Singularity vs. Podman vs. Others

- **Singularity is appropriate when**
 - The containerized workload is to be integrated into the environment as transparently as possible, including HPC-specific elements.
 - SIF image should not be stored in registry but in a share, directly executable, no "import"
- **Podman is advisable when**
 - The integration effort plays a subordinate role
 - Rootless limitations (work in progress) do not come into play
 - *Stronger isolation* is desired and feasible
 - A homogeneous setup for different workloads is desired + *single vendor strategy* if applicable
- **Further Findings**
 - Docker unfit for HPC
 - Sarus is still interesting, but low adoption and small developer group
 - Performance differences negligible
 - Future belongs to Podman – see also

Scaling Podman on Perlmutter

SC22 CANOPIE Container Workshop

2022 IEEE/ACM 4th International Workshop on Containers and New Orchestration Paradigms for Isolated Environments in HPC (CANOPIE-HPC)

Scaling Podman on Perlmutter: Embracing a community-supported container ecosystem

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Abstract—Containers have provided a popular new paradigm for managing software and services in HPC. The use of containers has brought many more difficult challenges, security, and performance requirements; consequently several custom HPC container runtimes have emerged from the community. In this paper we describe the challenges and opportunities both for HPC container runtimes and for users. In this paper we describe work at NERSC to add Podman, an OCI-compliant container runtime developed by Red Hat, Inc., for use in HPC. Podman has several key features which make it appropriate for use in HPC. Rootless container mode addresses security concerns, it has a standardized command interface which will be familiar to users of Docker, and it is designed to be fast and reliable, and it is open-source and community supported. Additional innovations at NERSC have enabled Podman to achieve the goal of scaling behaviors specific to HPC applications. Containers

Index Terms—High-Performance Computing, Containers

Container-based software deployment models have flourished in recent years across the computing industry, both on-premises and in the cloud [12]. Enabled by the combination of advances in compute and memory in the Linux kernel, containers provide a lightweight method of producing isolated software environments. Containers have played a key role in enterprise cloud technologies such as Kubernetes, and have enabled innovations in deployment and cloud computing instances. These container and infrastructure innovations have understandably bled into the world of high performance computing (HPC), where both center staff and users are eager to leverage all the benefits containers have to offer.

The current HPC container landscape currently includes several different container runtime technologies and often differs based on the center. Importantly, these frameworks are not typically used outside of HPC. Today, Podman/Singularity are the respective build/runtime solutions at OLCF [3] and Sandia [4], CharlieCloud [5], [6] is the build and runtime

solution at LANL, Singularity is the runtime solution at LLNL [7], [8], Singularity [10] is the runtime solution at ETH Zurich [9], and Podman is the production runtime solution at NERSC [11], [12]. This varied landscape can be difficult for users who must adapt their containerized applications for each new kind of container runtime (which can be non-trivial), and it is for this reason that this wide array of choices exists. In an attempt to reduce the fragmentation in the community and tack towards a more widely-used framework, our goal is to satisfy HPC-specific use cases with a more general purpose and widely used container implementation by adapting Podman. Redefining Podman's behavior in an HPC system with a production-class container runtime, adding HPC-specific capabilities to Podman could have larger impacts as the wider cloud industry looks to make singularity capable of running in HPC.

L INTRODUCTION

Podman (Podman [13] is an Open Container Initiative (OCI) compliant container ecosystem developed and actively supported by Red Hat, Inc. that provides full build and runtime capabilities. Podman 1.0 was released in 2019 [14] and it is now the default container runtime in Red Hat Linux. Podman is near-CLI-compatible with Docker. The main benefit that makes Podman desirable from an HPC perspective is that it can be run in *rootless* mode [15], which addresses many of the security and long-term issues associated with root access in containers. The container root is set according to a hostnamespace mapping, giving the user what feels like full root access within their container, but what is really an isolated, limited-privilege environment. All user-facing Podman capabilities at NERSC will run exclusively in rootless mode on our Perlmutter system, which is discussed in detail in Section V-A.

II. BACKGROUND AND MOTIVATION

Containers can provide a few major advantages to HPC users. First, several studies have demonstrated that containers can help provide fast and reliable performance with effectively

NERSC

- Very large scale HPC site (Perlmutter #5/#8 @Top500)
- uses **Shifter** as production runtime
- Goal: satisfy HPC-specific use cases with a more general purpose and widely used container implementation by adapting **Podman**
- Added HPC-specific capabilities in collab. with Red Hat

Why Podman?

- large community, build capabilities with same tooling, fuse-overlay mount for writeable images, SIF image support, rootless containers, network isolation, OCI compliant

-> Growing interest in Podman in the HPC community

Kubernetes

Kubernetes (K8s)

If one says containers, he typically means Kubernetes



State-of-the-art Open-source system for **automating deployment, scaling, and management** of containerized applications - aka "Container Orchestration"

Commercial representatives

- Red Hat OpenShift, SUSE Rancher, ...

Also available at the Hyperscaler of your choice

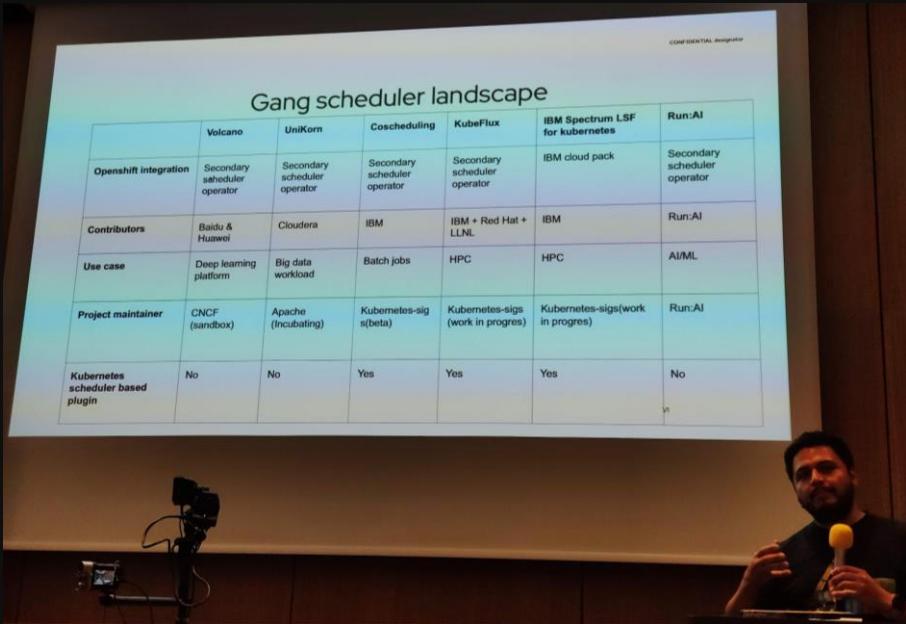
- AKS@Azure, EKS@AWS, GKE@GCP

However...



Kubernetes and HPC

Much harder than it sounds



Source: ISC 2022 – High Performance Container Workshop – Kubernetes + HPC – Eduardo Arango

Kubernetes was primarily designed with **cloud native scalable services** in mind

- Typical HPC applications behave differently
 - No dynamic auto-scaling
 - Use of MPI
 - Requirements for HPC interconnects (Infiniband, ...)
 - ...
- **Ongoing efforts** to make K8s **HPC-aware**
 - Variety of gang schedulers for HPC/Batch/AI+ML
 - MPI Operator
- **Nimbix invested lots of effort** to bring the two worlds together

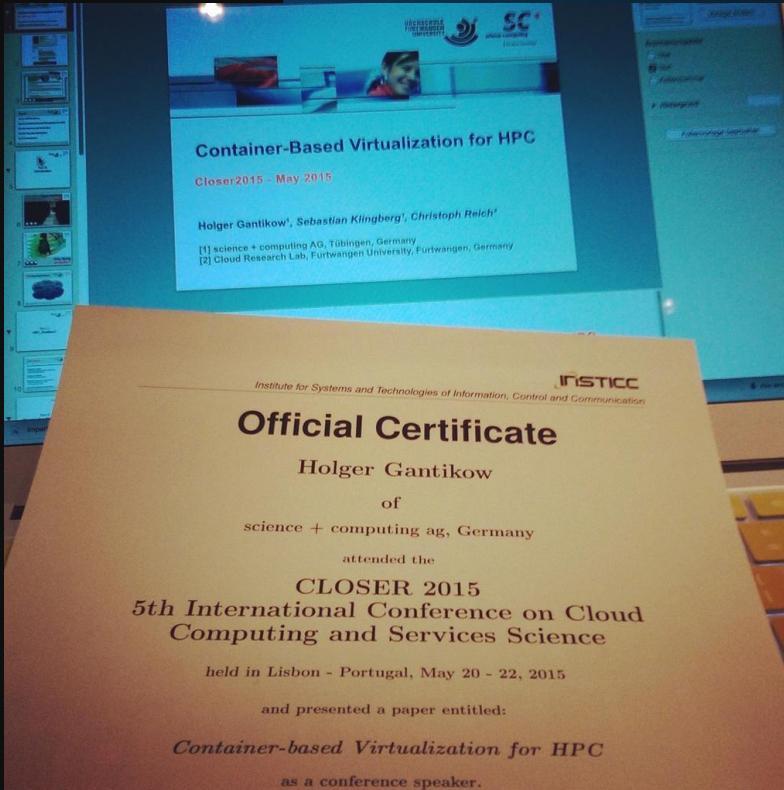
04. Use Cases in HPC

Aka *We and Containers*



Containers?

Not a new topic for us



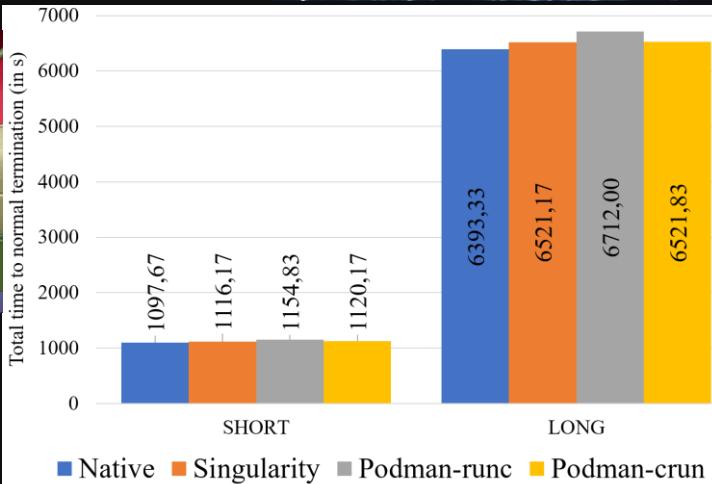
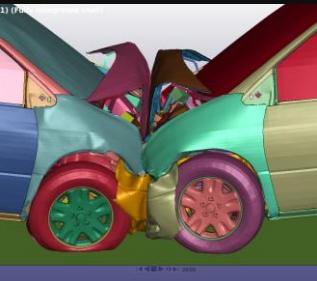
- Publications : 7
- Final Theses: 7
- Interns: 4
- Focus: Security, HPC

Rootless containers with Podman for HPC (2020)

Based on *elapsed time to normal termination* reported by LS-DYNA

All container runtimes introduce a certain amount of overhead (1,85% - 5,10%)

- Overhead **might be negligible** over benefits
 - 2/3 runtimes add <= 2,04% overhead
- Singularity causes smallest overhead**
- Diff. Singularity vs Podman-crun **minimal**
 - 1,61%-1,62% for long runs
- Performance of runc is noticeably (s)lower compared to crun / Singularity**



Gantikow, H., Walter, S., & Reich, C. (2020). Rootless Containers with Podman for HPC. In High Performance Computing (pp. 343–354). Springer International Publishing.

http://dx.doi.org/10.1007/978-3-030-59851-8_23

Where are we coming from?

Developments for Enterprise HPC Users (focus on CAE/Automotive)*

- **2021 Summary:**
 - Started to listen, interested, but container adoption rate far behind research sites
 - Mostly due to UDSS being no use-case – ops installs all the software...
 - Containers mostly seen with specific offerings (Nimbix, UberCloud, ...)
- **2022 Summary:**
 - Growing interest, recognized potential benefits of containers
 - Drivers: Multi-site HPC Grids, co-usage of K8s-based resources, cloud
 - + additional non-traditional workloads, specific interests
 - Growing interest in Podman for new installations (single vendor strategy?)
 - Singularity (at least for new installations) declining (Singularity vs Apptainer did not help)
- **Since then:**
 - Extended PoCs
 - Starting to think beyond “just put this in a container”
 - Lifecycle topics, run complex(er) workflows + SBOMs, security benefits



For more details see ISC 2021/2022/2023 talks

Reasons for low adoption for ISVs

And what to do about it?

- Lack of financial incentive
 - Customer needs our SW, will not pay more if containerized
- Don't fix it, if it ain't broken (enough)
 - Working software distribution model in place
 - Issues they had to solve predate containers – found "ways"
- Don't have a common specification to satisfy all customers
 - Environment dependencies, workflows, ...
- Increased effort + responsibilities, update frequency
 - As base layers would also be part of the shipped package

Recommendation to get started:



Pick one workload / container image to start with



Use Dockerfile to define the image, test various runtimes based on needs



Solve for not one time build but also for long term maintenance



Move to the next workload, at each step introduce one additional complexity



Share your experience with your software vendor and others in the community



Container Infrastructure

POC in Multi-Site HPC Environment

Holger Gantikow
CAE IT Landscape Architect

POC Container Infrastructure

POC Automotive Customer

Container Manufaktur



CI/CD Pipeline



Container Registry



Security Scanning

- \$CUSTOMER uses a geographically distributed HPC environment with diverse resources.
 - Platforms: Onprem HPC, onprem "cloud native" environment, DataCenter in Scandinavia, Hyperscaler.

Focus of the project

- Deployment of Container Engine on different platforms (Singularity)
- Infrastructure for building, deploying and maintaining images for the different platforms
 - Jenkins CI/CD, Harbor Registry - automated build + replication to different locations
- Improve application deployment in the different environments
 - Image push vs SW share rsync (direct transfer image to Scandinavia 8min vs share sync overnight)
- Provision of images for typical CAE workloads for the different target environments
 - LS-Dyna, Abaqus, StarCCM, specific coupled application
- Enabling Bring your own Environment (BYOE) for power users (future outlook)
 - Encapsulation of self-developed SW / tools / workflows
- Starting points for future initiatives: Security scanning, software bill of material (SBOM)



Validation & Certification

Group-wide CAE Images

Holger Gantikow
CAE IT Landscape Architect



Validation + Certification Group-wide CAE Images

Supported by us

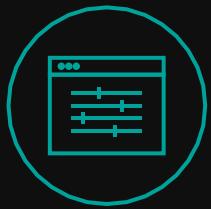


Image Build

- CAE images with ISV code get built using a CI/CD pipeline – or provided by the ISV

Validation

- Need to undergo validation based on company wide policies regarding SW (network connections, ...)

Testing

- Test users have to verify that the application is behaving as expected

Certification

- CAE SW image gets certified for productive use

Availability

- Image made available group wide

Security in HPC with Containers

Online, December 2021

Software Bill of Material

Aka "What is running on my cluster?"

Hard to keep track of software used on a large-scale system

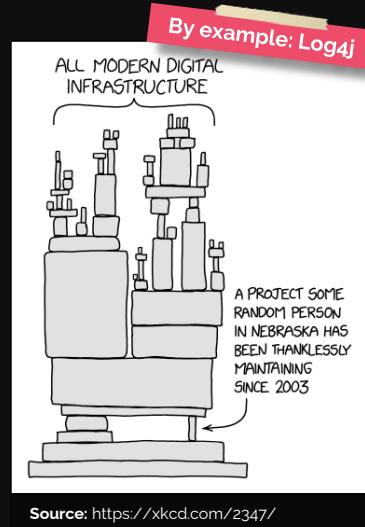
- Lots of different applications, with numberless dependencies
- Especially hard when SW is provided beyond `rpm/apt/apk` (`pip`, `jars`, `go modules`, ...)

Hard to answer questions like

- What software is outdated / has vulnerabilities?
- What software relies on a specific buggy library version that impacts the results?

Gets much easier when relying on containers as sole source of software

- Software used = Host Software + Container image content



OSS software solutions to support this (examples later)

- Various package formats / SW sources, details like Maintainers, Licences, Checksums of files, ...
- Should be integrated with image release process / registry ("Container App Store")

Software Solution – vulnerability static analysis

Standalone, Integrated in Image Registry

Rep: Clair, Syft / Grype, Trivy

- Native support for OCI images
- Singularity Image Format mostly possible (with workaround)
- Mostly standalone scanners, often also integrable in container registry
- Work according to identical principle

Scanning simple, decision how to proceed complicated

- Deactivate image?
- Rebuild image?
- Use in strongly isolated environment?

```
holgrrr@nuci:~$ grype docker.elastic.co/logstash/logstash:7.11.1 | grep -i log4j | grep -i critical
✓ Vulnerability DB [no update available]
✓ Parsed image
✓ Cataloged packages [605 packages]
✓ Scanned image [813 vulnerabilities]
log4j-api 2.11.1 2.15.0 GHSA-jfh8-c2jp-5v3q Critical
log4j-api 2.11.1 CVE-2021-44228 Critical
log4j-api 2.9.1 GHSA-jfh8-c2jp-5v3q Critical
log4j-api 2.9.1 CVE-2021-44228 Critical
log4j-api 2.13.3 GHSA-jfh8-c2jp-5v3q Critical
log4j-api 2.13.3 CVE-2021-44228 Critical
log4j-core 2.9.1 2.15.0 GHSA-jfh8-c2jp-5v3q Critical
log4j-core 2.9.1 CVE-2021-44228 Critical
log4j-core 2.13.3 GHSA-jfh8-c2jp-5v3q Critical
log4j-core 2.13.3 CVE-2021-44228 Critical
log4j-slf4j-impl 2.13.3 2.9.1 CVE-2021-44228 Critical
log4j-slf4j-impl 2.13.3 2.9.1 CVE-2021-44228 Critical
log4j-slf4j-impl 2.13.3 2.13.3 CVE-2021-44228 Critical
holgrrr@nuci:~$
```

[0 bash] 1 bash 2 bash | @nuci | 1,40 1,14 0,95 | 2021-12-16 0:40

Vulnerability	Severity	CVSS3	Package	Current version	Fixed in version	Listed in CVE Allowlist
CVE-2019-1010022	High	7.8	glibc	2.17-323.el7_9		No
CVE-2019-1010022	High	7.8	glibc-common	2.17-323.el7_9		No
CVE-2021-43527	High	7.8	nss	3.53.1-3.el7_9	3.67.0-4.el7_9	No
CVE-2021-43527	High	7.8	nss-sysinit	3.53.1-3.el7_9	3.67.0-4.el7_9	No
CVE-2021-43527	High	7.8	nss-tools	3.53.1-3.el7_9	3.67.0-4.el7_9	No
CVE-2021-45046	High	7.8	org.apache.logging.log4j-api	2.13.3	2.16.0	No
CVE-2021-44228	High	7.8	org.apache.logging.log4j-core	2.13.3	2.15.0	No

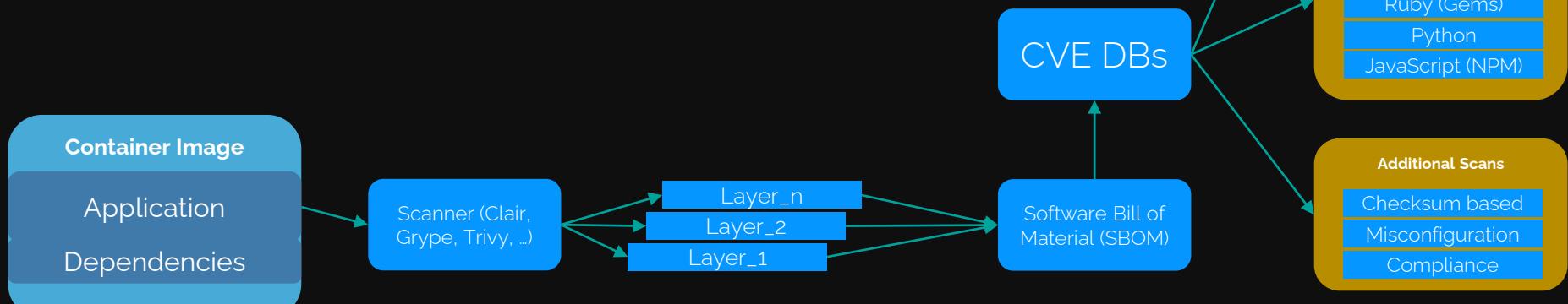
How an image scanner works

Divide et impera – divide & conquer

Procedure for all layers in a container image

- Create a Bill of Material (BoM)
- Check BoM with SW vendor for common vulnerabilities and exposures (CVEs)
- Linux Distro, Ruby, Java, JavaScript, Python, ...
- Create a report

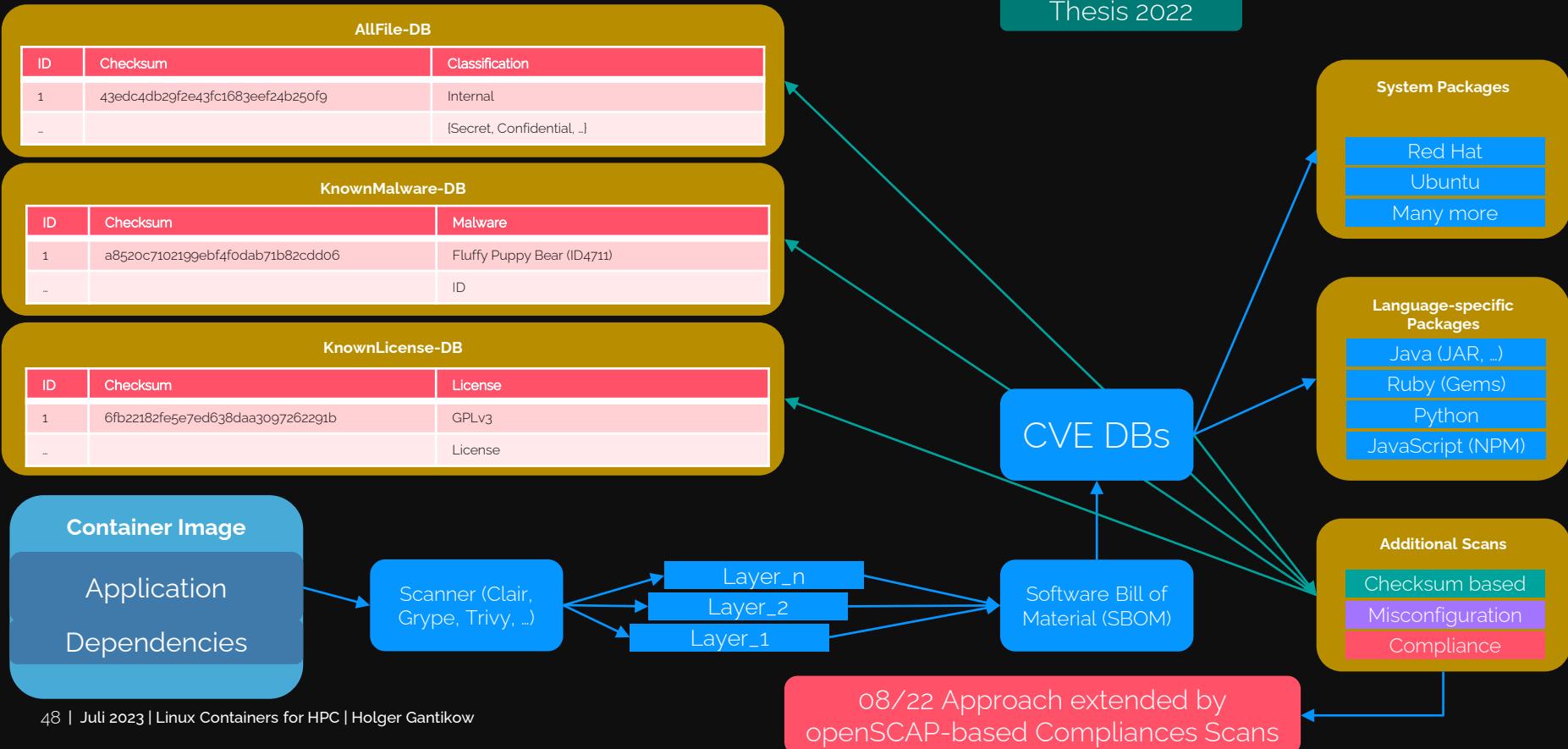
Other approaches can be integrated (compliance, configuration, checksums, ...)



Checksum approach: Connection to Data Classification

Policy: */Images Containing Files with Classification > Public -> only allowed onPrem*

Thesis 2022



Last Student Final Theses

2022/2023



Orchestrating modern workloads

- Usability of HPC, AI/ML, Data Analytics workloads with K8s
- Evaluation of different gang schedulers



Security of containerized workloads

- Untrusted code in security-aware environment
- Seccomp, sidecar containers, ...
- Integration with Nimbix (?)



Container-based confidential computing

- Intel SGX, Trusted Execution Environments
- Unmodified code running in secure enclaves
- Gramine, Gramine Shielded Containers

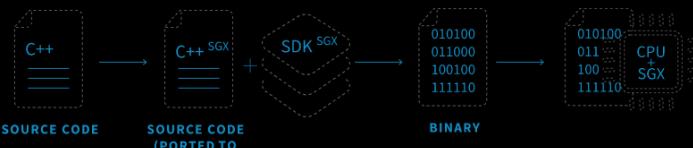
Gramine & gramine Shielded Containers

Few more details

- <https://gramineproject.io/>
- <https://gramine.readthedocs.io/projects/gsc/en/latest/>

Intel SGX integration made simple

Regular integration of Intel SGX



Integration of Intel SGX with Gramine



Applications can benefit from confidentiality and integrity guarantees of Intel SGX, but developers need to be very skilled for effective partitioning and code modification for Intel SGX environment.

Gramine runs unmodified applications inside Intel SGX. It supports dynamically loaded libraries, runtime linking, multi-process abstractions, and file authentication. For additional security, Gramine performs cryptographic and semantic checks at untrusted host interface. Developers provide a manifest file to configure the application environment and isolation policies, Gramine automatically does the rest.

gsc - Gramine Shielded Containers

Synopsis

gsc COMMAND [OPTIONS] ...

Description

Docker containers are widely used to deploy applications in the cloud. Using Gramine Shielded Containers (GSC) we provide the infrastructure to deploy Docker containers protected by Intel SGX enclaves using the Gramine Library OS.

Ad by EthicalAds • Host these ads

The gsc tool transforms a Docker image into a new image (called `gsc-<image-name>`) which includes the Gramine Library OS, manifest files, Intel SGX related information, and executes the application inside an Intel SGX enclave using the Gramine Library OS. It follows the common Docker approach to first build an image and subsequently run a container of an image. At first a Docker image has to be graminized via the `gsc build` command. When the graminized image should run within an Intel SGX enclave, the image has to be signed via a `gsc sign-image` command. Subsequently, the image can be run using `docker run`.

Self Service Portals

Based on the plans for LUMI-K

Containers in LUMI - LUMI-K (future)

The screenshot shows a web interface for installing various software packages. The top navigation bar includes 'UNINETT', 'Library', 'My applications', and 'Påkvarande'. A search bar at the top right contains the text 'researchlab'. Below the search bar, there is a 'Filter packages...' dropdown. The main area displays several packages with their versions and descriptions:

- deep-learning-tools** 0.5.7 (researchlab): GPU enabled, Jupyter notebook. Buttons: Install, Uninstall.
- jupyter** 0.6.0 (researchlab): Apache Spark, Data. Buttons: Install, Uninstall.
- jupyterhub** 0.9.12 (researchlab): Jupyter notebook variant. Buttons: Install, Uninstall.
- minio** 0.2.6 (researchlab): File sharing, Cloud storage. Buttons: Install, Uninstall.
- rstudio** 0.10 (researchlab): R Studio. Buttons: Install, Uninstall.
- spark** 0.76 (researchlab): Distributed computing. Buttons: Install, Uninstall.

At the bottom left, it says 'Uninett AS'.

LUMI



Containers in LUMI - LUMI-K (future)

The screenshot shows a 'Service Catalog' interface with a 'Browse Catalog' section. The catalog lists various container configurations under different categories:

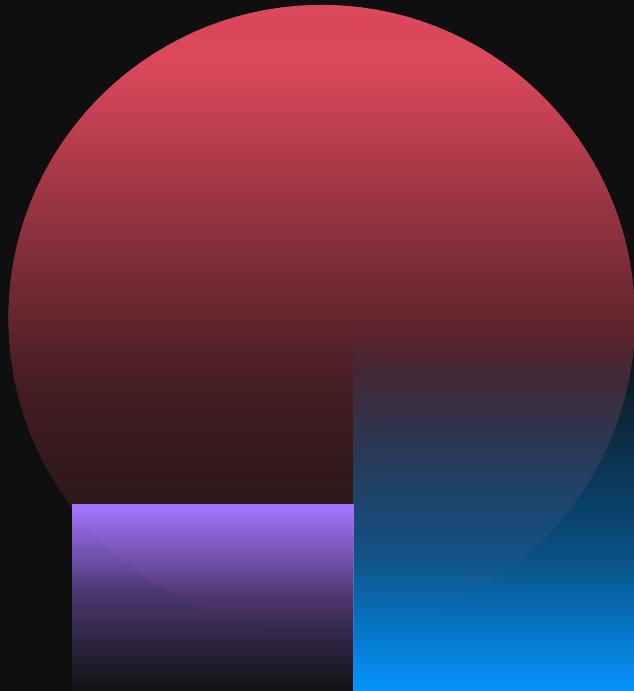
- .NET**: .NET Core, .NET Core + PostgreSQL (Persistent), .NET Core Example, .NET Core Runtime Example, 3scale gateway.
- Apache**: amp-apicast-wildcard-router, amp-pvc, Apache Airflow, Apache HTTP Server (httpd).
- PHP**: Apache Spark, CakePHP + MySQL, CakePHP + MySQL (Ephemeral), Dancer + MySQL, Dancer + MySQL (Ephemeral).
- Python**: Django + PostgreSQL, Django + PostgreSQL (Ephemeral), Jenkins, Jenkins (Ephemeral), JupyterHub (Github OAuth).
- Others**: jupyterhub (Native Authentication), MariaDB, MariaDB (Ephemeral), Minio Object Store, MLflow.

On the right side, there is a sidebar for 'My Projects' showing a list of 48 projects and a 'Recently Viewed' section with icons for .NET, Python, and Java.

- LUMI: #3 Top500 (06/2022)
 - Future: "Cloud partition based on Kubernetes (LUMI-K)"
 - K8s Cluster running service containers
 - Could also be implemented with Nimbix

05. Nimbix

Nimbix Supercomputing Suite



Atos Nimbix

Leading-Edge CAE as a Service



Atos Acquires HPC Cloud Platform Provider Nimbix

July 27, 2021 by [staff](#)

Last month, Agnès Boudot, SVP, head of HPC & Quantum at Atos, told us — without sharing details — that the company's global strategy includes expansion into the U.S. market. At least part of that strategy was revealed today with the news that [Atos](#) has acquired long-time high-performance computing cloud platform provider [Nimbix](#).



A photograph of several server racks in a data center. The background is filled with a digital grid of binary code (0s and 1s) in blue and white, creating a futuristic, high-tech feel.

Digging into the Atos-Nimbix Deal: Big US HPC and Global Cloud Aspirations. Look out HPE?
By John Russell



Episode 339: Atos Acquires Nimbix

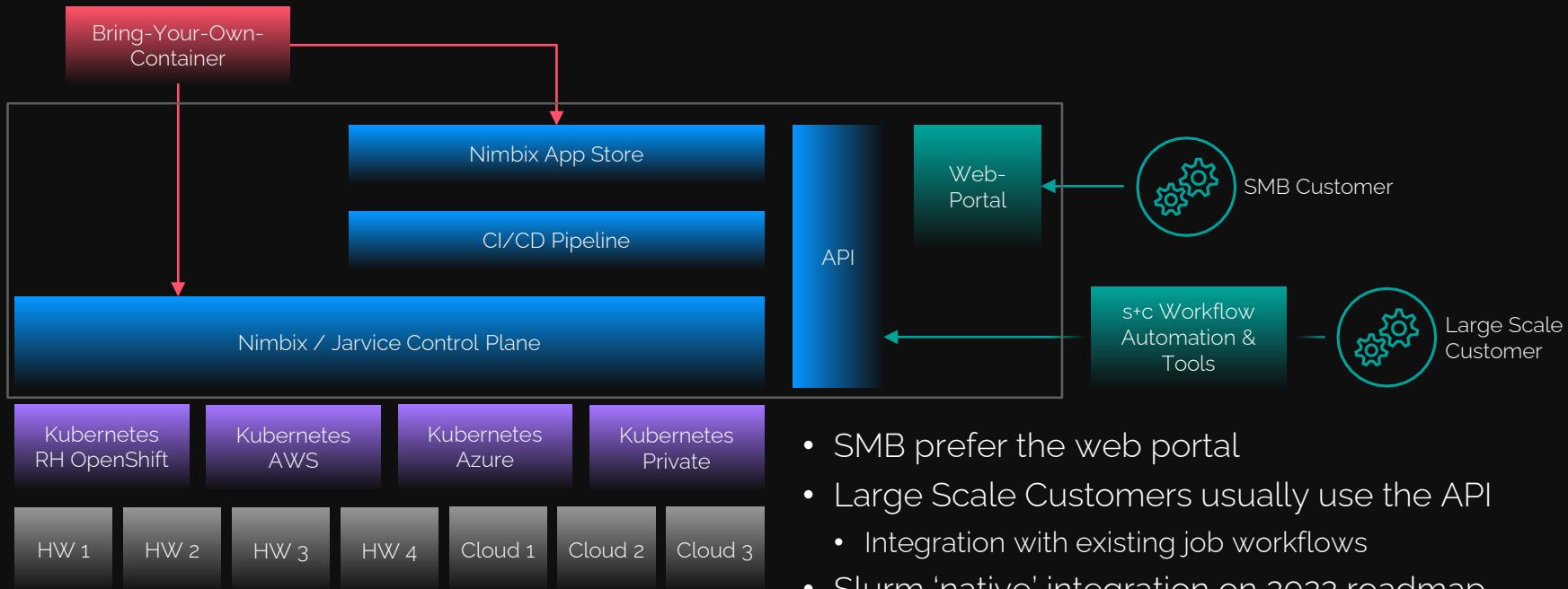
Nimbix JARVICE™

is a container-based solution for multi-site, multi-cloud HPC workloads with an integrated App marketplace and ready to use click-to-run workflows of typically used simulation applications and community AI tools.

Nimbix™

HPC in Kubernetes – simplified architecture

Nimbix enables HPC with containers on Kubernetes based infrastructure



HyperHub

Ready to run commercial + popular community applications

The screenshot shows the HyperHub application interface. On the left, a sidebar titled "Compute" contains a "Filter Applications" section with options like "License Included" (unchecked), "File Manager", and "All Applications" (which is circled in red). Below this are "My Applications", "Categories", and "Vendors". The main area displays a grid of application cards. Some visible cards include:

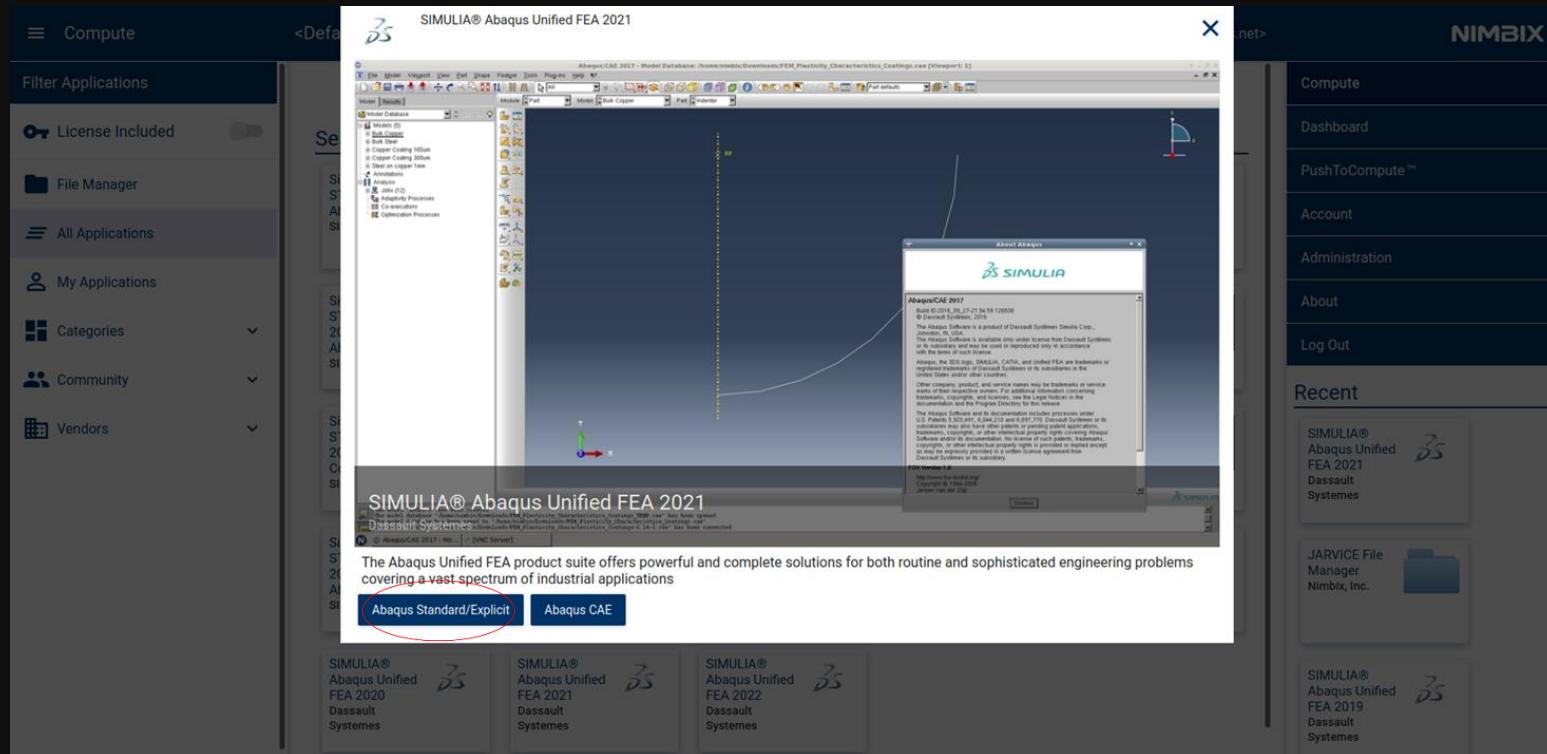
- ANSYS® Platform R19.2 ANSYS, Inc. from \$1.00/hr + license
- ANSYS® Structures 2019 R1 ANSYS, Inc. from \$1.00/hr + license
- ANSYS® Structures 2019 R2 ANSYS, Inc. from \$1.00/hr + license
- ANSYS® Structures 2019 R3 ANSYS, Inc. from \$1.00/hr + license
- ANSYS® Structures 2020 R1 ANSYS, Inc. from \$1.00/hr + license
- Ansys® Structures 2020 R2 ANSYS, Inc. from \$1.00/hr + license
- Ansys® Structures 2021 R1 ANSYS, Inc. from \$1.00/hr + license
- Ansys® Structures 2021 R2 ANSYS, Inc. from \$1.00/hr + license
- Ansys® Structures 2022 R1 ANSYS, Inc. from \$1.00/hr + license
- Ansys® Structures R19.2 ANSYS, Inc. from \$1.00/hr + license
- b2com [SDR-HDR Converter] b2com / Accelize from \$1.00/hr
- Blender® Blender Foundation from \$1.00/hr
- Canu Pipeline 1.5 Canu from \$1.00/hr
- Canu Pipeline 1.6 Canu from \$1.00/hr
- Canu Pipeline 1.7.1 Canu from \$1.00/hr
- Canu Pipeline 1.8 Canu from \$1.00/hr
- CentOS Linux desktop Nimbix, Inc. from \$1.00/hr
- COMSOL® 5.4 COMSOL Inc. from \$1.00/hr + license
- COMSOL® 5.5 COMSOL Inc. from \$1.00/hr + license
- COMSOL® 5.6 COMSOL Inc. from \$1.00/hr + license
- CUDA 9.1 (Ubuntu) NVIDIA from \$1.00/hr
- FFmpeg fffmpeg.org from \$1.00/hr
- GNU Octave Nimbix, Inc. from \$1.00/hr
- H2o3 h2o.ai from \$1.00/hr
- H2o3 3.20.0.7 Ubuntu16 x64, 64 h2o.ai from \$1.00/hr
- HPC Test Environment Nimbix, Inc. from \$1.00/hr
- HPC Test Environment with Slurm 20.11.7 Nimbix, Inc. from \$1.00/hr
- JARVICE File Manager Nimbix, Inc. from \$1.00/hr
- Keysight ADS Keysight Technologies, Inc. from \$1.00/hr + license
- Keysight ADS 2020 Update 1 Keysight Technologies, Inc. from \$1.00/hr + license
- Keysight EMPro Keysight Technologies, Inc. from \$1.00/hr + license
- MATLAB® R2020b MathWorks from \$1.00/hr + license
- MATLAB® R2021a MathWorks from \$1.00/hr + license
- Kerisight ADS 2020 Update 2 Keysight Technologies, Inc. from \$1.00/hr + license
- Kerisight EMPro 2020 Keysight Technologies, Inc. from \$1.00/hr + license
- MATLAB® R2021a MathWorks from \$1.00/hr + license
- MATLAB® R2022a MathWorks from \$1.00/hr + license
- SIMULIA® Abaqus Unified FEA 2022 Dassault Systems from \$1.00/hr + license

The right sidebar includes sections for "Compute", "Dashboard" (which is circled in red), "PushToCompute™", "Account", "About", "Log Out", and "Recent" (which lists TensorFlow, OpenFOAM, JARVICE, and SIMULIA).

- Point-and-click workflows, Support for GPU, IB, EFA, Extendable

Abaqus

Let's start a job!



Abaqus

Insert input data, Resource selection – will be *scaled up on demand*

SIMULIA® Abaqus Unified FEA 2021

Abaqus Standard/Explicit
Run a Standard or Explicit analysis on an input file

GENERAL OPTIONAL STORAGE PREVIEW SUBMISSION

Machine

Machine type: DEMO; 7 core, 32GB RAM (CPU Only) t2.2xlarge (n4)

Cores: 14 (7 to 1792)
2 nodes, 60GB RAM

Parameters

input file (*.inp): /Abaqus-Job/abaqus_static.inp

Version: 2021 (Abaqus version)

SUBMIT

NIMBIX

- Compute
- Dashboard
- PushToCompute™
- Account
- Administration
- About
- Log Out

Recent

- SIMULIA® Abaqus Unified FEA 2021 Dassault Systems
- JARVICE File Manager Nimbix, Inc.
- SIMULIA® Abaqus Unified FEA 2019 Dassault Systems

Abaqus

Job starts processing

The screenshot shows the Nimbix cloud computing interface. On the left, there's a sidebar with 'Jobs' (Current, History, By Label, Reports) and 'Stats' (My stats, JOBS RUN: 8, COMPUTE: \$, TIME: 01:45:34). The main area is titled 'Current' and shows a job named 'SIMULIA® Abaqus Unified FEA 2022(364)'. The job status is 'Processing' (highlighted with a red circle), and it's utilizing 0% CPU and 0.07 of 320GB memory across 2 nodes. Below the status, there's a terminal window displaying Abaqus startup logs. To the right, there's a vertical navigation bar with 'Compute', 'Dashboard', 'PushToCompute™', 'Account', 'About', and 'Log Out'. A 'Recent' section lists various services: TensorFlow (CPU only - Community version, tensorflow.org), OpenFOAM® 7 (OpenCFD Ltd, from \$1.00/hr), JARVICE File Manager (Nimbix, Inc., N logo), and SIMULIA® Abaqus Unified FEA 2022 (Dassault Systems, from \$1.00/hr + license).

Dashboard demo-nimbix-eu-eks-downstream-01 Demo User <demo01.nimbix@science-computing.de>

Jobs

- Current
- History
- By Label
- Reports

Current

SIMULIA® Abaqus Unified FEA 2022(364)

Command Analysis

Status Processing

Utilization CPU: 0% MEM: 0.07 of 320GB

Address none

Click to copy password to clipboard

```

INIT[1]: Waiting for job configuration before executing application...

INIT[1]: hostname: jservice-job-364-cmz94

INIT[1]: Configuring systemd to start JARVICE ping-based health check

INIT[57]: HOME=/home/nimbix

#####
#  

# INFO: Using license Server: http://10.95.50.1.lic.nimbix.net/  

# Parallel execution enabled in 24 processes(4)  

Generating SSH2 RSA host key: [1]60G[0]0:32m OK [0]0:39m  

Generating SSH2 ECDSA host key: [1]60G[0]0:32m OK [0]0:39m  

Generating SSH2 ED25519 host key: [1]60G[0]0:32m OK [0]0:39m  

INFO: Running Abaqus with input file abaqus.inp  

INFO: Job label: abaqus static-20220615073629-XS2Q-jservice-abaqus2022-demo_user  

Analysis initiated from SIMULIA established products  

Abaqus Job abaqus static-20220615073629-XS2Q-jservice-abaqus2022-demo_user_1_si  

Abaqus 2022
  
```

Compute

Dashboard

PushToCompute™

Account

About

Log Out

Recent

- TensorFlow (CPU only) - Community version tensorflow.org
- OpenFOAM® 7 (OpenCFD Ltd, from \$1.00/hr)
- JARVICE File Manager (Nimbix, Inc., N logo)
- SIMULIA® Abaqus Unified FEA 2022 (Dassault Systems, from \$1.00/hr + license)

Nimbix Supercomputing Suite

Global Elastic HPC & Supercomputing as-a-Service

3 Supercomputing "as-a-Service" Consumption Models



Elastic

Pay-as-you-go, on-demand, secure and scalable supercomputing through a single user interface.



Dedicated

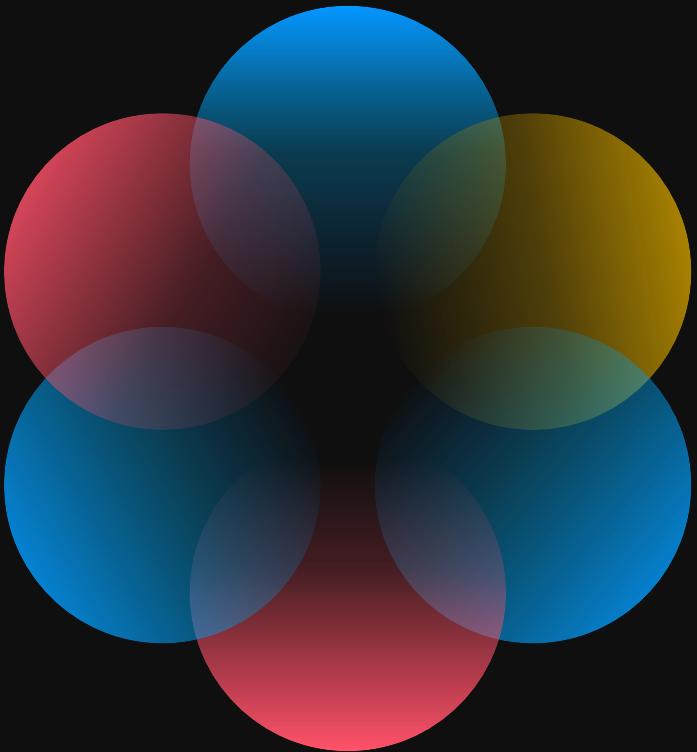
Leverage powerful dedicated HPC servers as "Bare Metal as-a-Service" for the best of infrastructure and on-demand scalability, convenience, and agility.



Federated

Federated Supercomputing-as-a-Service offers a unified service console to manage all compute zones and regions in a public or private HPC, AI, and supercomputing federation

06. Conclusion



Containers from the big player perspective (CAE focus)

Certification + Standardization, Off-premises Resources, SBOM, Security as drivers



Certification + Standardization

- Build based on a build file
- Defined frozen stack for use in the future as OS-base evolves
- Application + dependencies library setup as one package
- Defined stack for a project (standardized + documented)
- Possibility to share the image
- Possibility to define deviation in additional layer



Off-premises Resources

- Decoupling containers from host OS - RHEL vs SLES vs Ubuntu*
- Use of resources with different SW configuration (library setup)*
- Deployment of applications in environments under foreign administrative sovereignty (easier handling with containers)



Software Bill of Material

- Topic from last year
- What's running on my cluster?
- Which applications are affected by CVE XYZ?
- What dependencies does application X have?
- Which setup do I actually use to compute project Y?



Security Aspects

- Streamline some processes regarding new applications
- Beyond: improve status quo of HPC security with containers, fields of interest:
 - Signed Images
 - Seccomp Profiles
 - Security Monitoring
 - Behavioral Monitoring
 - -> Mostly „future use“

Current challenges in adoption

ISVs, Registries at Scale, „FUD“ + Future Topics



Still no ISV images

- Short version: ISVs...
- have established mechanisms to distribute applications
- don't feel enough pressure?
- are not container-aware?
Containers might be used internally though
- fear shift in responsibility? –
base layers part of the distributed artifact (CVEs, ...) –
more frequent releases needed



Registries at Scale

- Best practices for registry setup – especially in distributed environments
- Mirroring / caching / pull through
- How many registries per cluster



„FUD“*, MPI, SUB*-Mapping

- Some operators like to disable user namespaces support
- Which breaks usability of some container runtimes...
- MPI compatibility – injecting host MPI typically not an option
- Subuid/gid-Mapping problematic
- UID in the Kernel should equal the actual UID, license server...



Potential Challenges + Future Topics

- Automated (re)builds
- Reproducibility in builds
- Image signing
- Fat vs multiple small images - Dealing with site specifics + Complex workflows involving multiple applications / tools
- Performance-optimized images – less of a topic, as image build is around ISV provided code
- Moving towards K8s

Conclusion

Container all the things?

- **Containers have become established in the last few years and will remain so**
 - Some customers are already thinking about containerizing 100% of CAE applications (Desktop+HPC)
 - Much (OCI specs) now standardized, HPC engines can run OCI images, Podman learns SIF
 - Performance overhead minimal
 - No longer only vehicle for historical SW on new OS, also standard in the domain of AI/ML
- **Paving the way for better use of resources in distributed environments**
 - The less host dependencies the more portable (MPI, Infiniband, Omnipath, ...)
- **Currently practically no container images through the ISVs - self-build or image-aaaS**
- **Reasonable approach: mapping in CI/CD pipelines and corresponding infrastructure**
 - Enables automated build per target environment
- **Containers provide opportunity to improve security of HPC environment**
 - What is running in the environment? What of it has security vulnerabilities? What SW is being used at all?
- **Nimbix approach highly interesting for very many customers**
 - Especially when cloud resources or Kubernetes setups are to be connected.

WIR WÜLLEN CONTINUUM

Thank you!

For more information please contact:

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