

Introduction

5th High Performance Container Workshop - ISC19

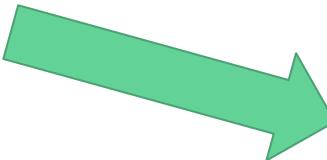
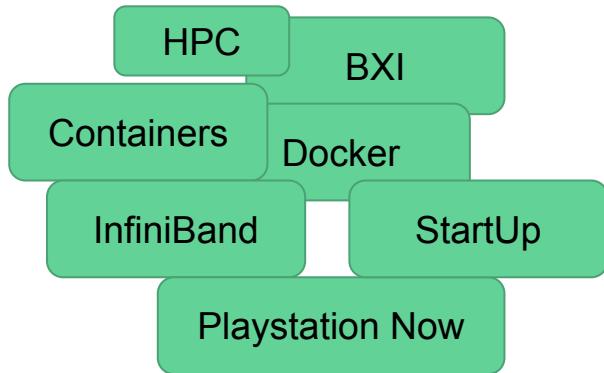
Welcome!

This workshop aims to provide you with a comprehensive overview of all-things-containers.

It's about the audience - so please engage and ask questions.

First up: Short segment, so that every speaker has the opportunity to get his About Me / About my Company' slides out of the way.

About Me



AWS
Spot/HPC

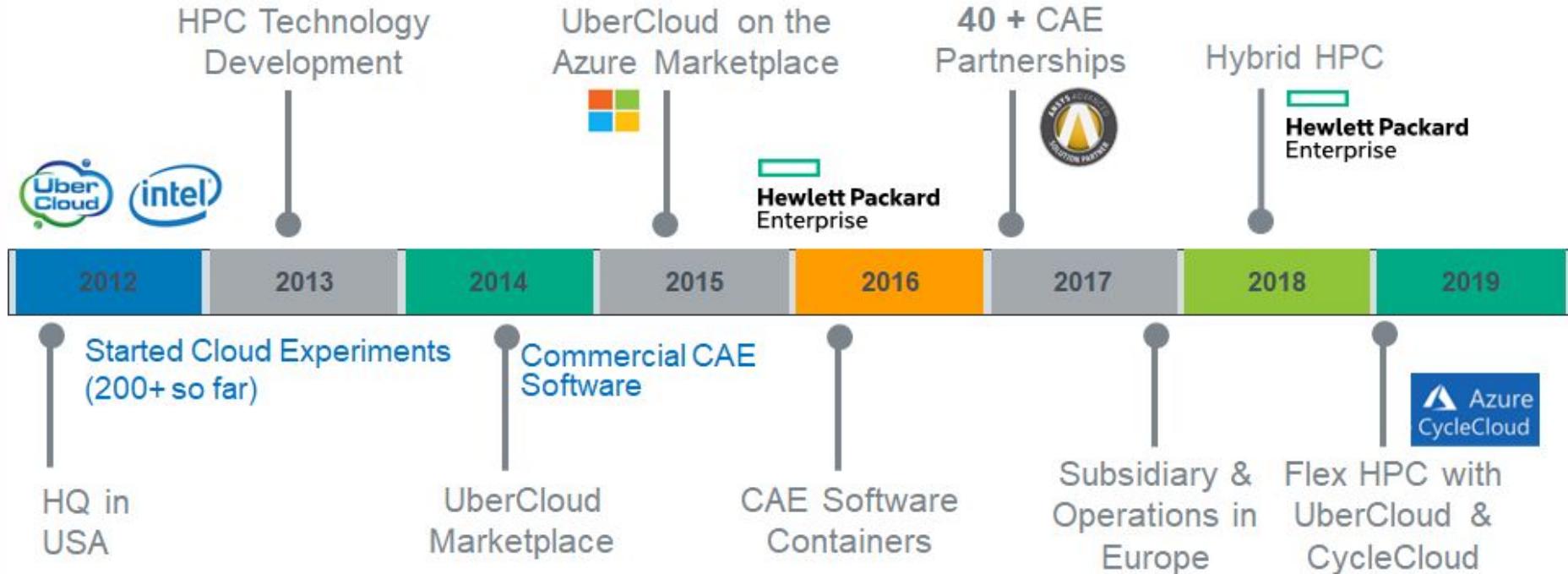
Christian Kniep
christian@qnib.org



UberCloud Containers on Kubernetes



Brief History of UberCloud



References and Awards

50+ ISV Partnerships



Customers

3 of the 10 Largest
IT Companies

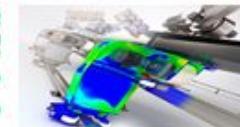


2012
2019 7 Years

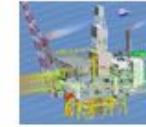
USA Germany
Turkey India Global Service

200+ Engineering Case Studies

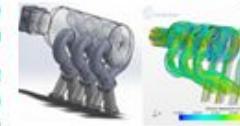
6 Industries to Focus



Manufacturing



Oil & Gas



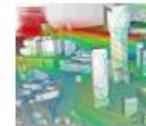
Automotive



Life Sciences

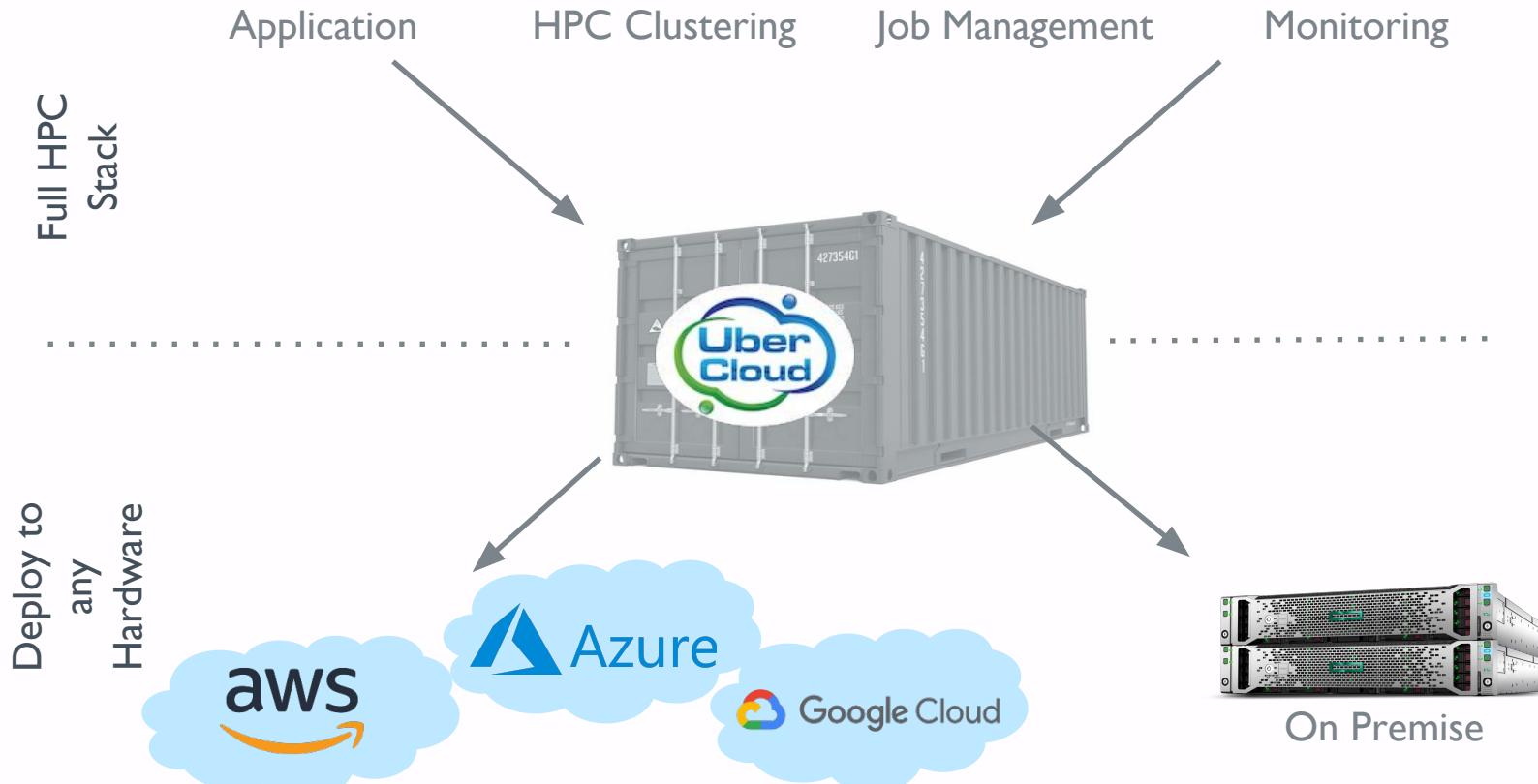


Electronics



Engineering Services

Why / How we use UberCloud Containers



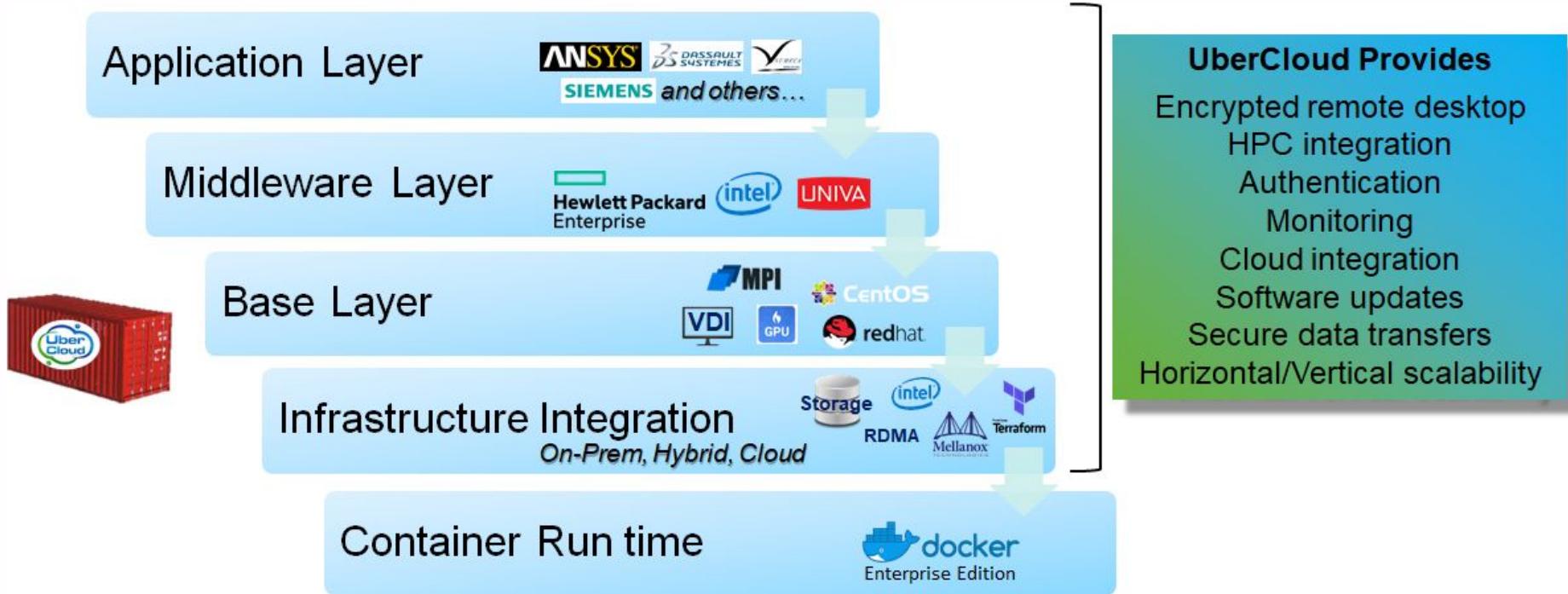
UberCloud Containers provide:



- OCI compliant images containing all what an Engineer requires
- Ready to deploy in different Cloud Environments (Azure, AWS, GCP, Oracle Cloud) and on-premise environments without any changes
- Out of the box HPC layers with MPI, Devices, Storage, and Visualization capabilities
- Fully interactive GUI Nodes with engineering applications preconfigured
- GPU Support for visualization and computation
- Tight integration with batch scheduling system without manual configuration requirements
- Seamless Hybrid HPC and Bursting capabilities



UberCloud HPC Containers



Kubernetes: One way to orchestrate UberCloud

- The de-facto standard container orchestration platform which is supported by many companies (Google, Amazon, Microsoft, RedHat, Pivotal, ...)
- Many organisations introduce Kubernetes in their IT environment either on-premises or in cloud. It is a known technology for Administrators and IT.
- UberCloud HPC containers make it simple for Engineers and administrators to run Applications like Comsol, Ansys, ... in existing Kubernetes environments.

Alternatively: Orchestrating through Job Schedulers (like Univa Grid Engine), Atrio Composable Cloud, custom Infrastructure as Code implementations.

Why UberCloud Containers on Kubernetes?

- ★ Speed up HPC adaptation
- ★ Maximize resource usage
- ★ Secure environment
- ★ No learning required - full GUI with virtual desktop
- ★ Wide availability of Kubernetes expertise in IT

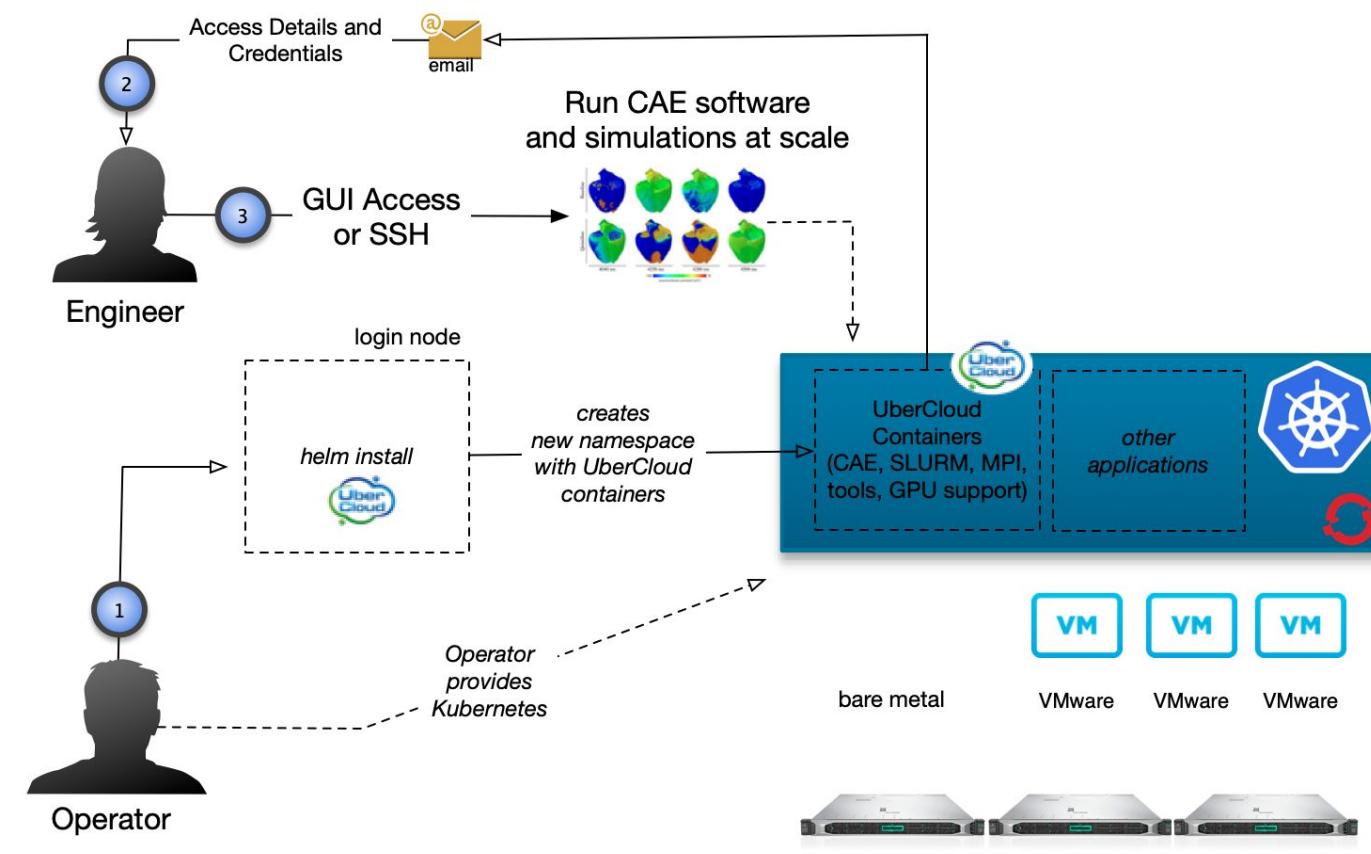
- Enable Kubernetes to run HPC workloads
- Exploit under-utilized powerful resources in pre-existing Kubernetes environments
- Engineers can be 10-times faster executing simulations when using more powerful resources
- Always run the latest software with the newest security patches. No worries about updates.
- Disposable and dynamically requestable resources - get only charged for resources when you actually use it
- No complex setup required
- Accepted solution by IT - common understanding of the container technology

UberCloud Containers address these gaps

- Kubernetes lacks HPC scheduler capability
- Kubernetes has no license orchestration
- Kubernetes does not provide native MPI support
- Kubernetes lacks devices and controllers needed for engineering software and HPC



How?



An HTC Case on OpenShift + UberCloud Containers

Hewlett Packard Enterprise



Mixed OpenShift setup (virtualized and bare metal):

1 ESXi host serving 3 VMs for the OpenShift control plane
(HPE ProLiant DL360 Gen10)

2 VMs + 1 bare metal host for running UberCloud containers in OpenShift
(HPE Apollo 6500 Gen10)

Kubernetes: OpenShift v3.10 / Kubernetes 1.10

Workload: MPI jobs (shared memory and distributed memory)

Application: OpenFoam with Motorbike model

Workload Management: UberCloud containers running containerized slurm workload manager

Results: Successfully run single node and multi-node jobs in a distributed UberCloud container setup running all workload (job submission + job execution).

Hewlett Packard Enterprise



kubernetes

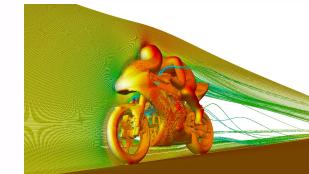


The UberCloud



slurm
workload manager

Open ∇ FOAM



Thank you

burak@TheUberCloud.com





HPCW: NVIDIA

CJ Newburn, Principal Architect for HPC

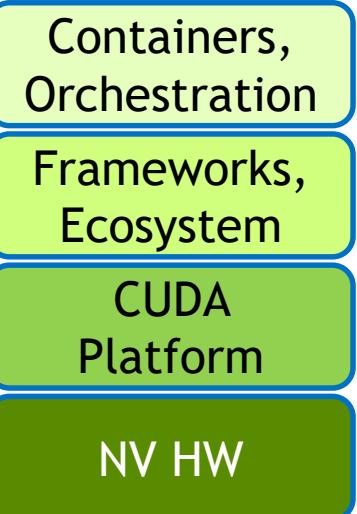
NVIDIA OVERVIEW

- Containers and HPC
- What NVIDIA is doing
- NVIDIA GPU Cloud

WHY CONTAINER TECHNOLOGIES MATTER TO HPC

Good for the community, good for NVIDIA

- Democratize HPC
 - Easier to develop, deploy (admin), and use
- Good for the community, good for NVIDIA
 - **Scale** → HPC; more people enjoy benefits of our scaled systems
 - Easier to deploy → less scary, less complicated → **more GPUs**
 - Easier to get all of the right ingredients → **more performance** from GPUs
 - Easier **composition** → HPC spills into adjacencies



WHAT NVIDIA IS DOING

Earning a return on our investment

- Container images, scripts, and industry-specific pipelines in **NGC** registry
 - Working with developers to tune scaled performance
 - Validating containers on NGC and posting them in registry
 - Used by an increasing number of data centers
- Making creation and optimization automated and robust with **HPCCM** ([blog](#))
 - Used for every new HPC container in NGC, broad external adoption
 - Apply best practices with building blocks, favor our preferred ingredients, small images
- Moving the broader **HPC community** forward
 - CUDA enabling 3rd-party runtimes and orchestration layers
 - Identifying and addressing technical challenges in the community

NGC: GPU-OPTIMIZED SOFTWARE HUB

Simplifying DL, ML and HPC Workflows

INDUSTRY SOLUTIONS

SMART CITIES

Parking Management Traffic Analysis
DeepStream SDK

MEDICAL IMAGING

Organ Segmentation
Clara SDK

DEEP LEARNING MODEL SCRIPTS

Classification Translation Text to Speech Recommender ...



50+ Containers
DL | ML | HPC



35 Models



Simplify Deployments



Innovate Faster



Deploy Anywhere

THE DESTINATION FOR GPU-OPTIMIZED SOFTWARE

HPC	Deep Learning	Machine Learning	Inference	Visualization	Infrastructure
BigDFT	Caffe2	Dotscience	DeepStream	CUDA GL	Kubernetes on NVIDIA GPUs
CANDLE	Chainer				
CHROMA*	CT Organ Segmentation	H2O Driverless AI	DeepStream 360d	Index*	
GAMESS*	CUDA	Kinetica	TensorRT	ParaView*	
GROMACS	Deep Cognition Studio	MapR	TensorRT Inference Server	ParaView Holodeck	
HOOMD-blue*	DeepStream 360d	MATLAB		ParaView Index*	
LAMMPS*	DIGITS			ParaView Optix*	
Lattice Microbes	Kaldi	OmniSci (MapD)		Render server	
Microvolution	Microsoft Cognitive Toolkit	RAPIDS		VMD*	
MILC*	MXNet				
NAMD*	NVCaffe				
Parabricks	PaddlePaddle				
PGI Compilers	PyTorch				
PIConGPU*	TensorFlow*				
QMCPACK*	Theano				
RELION	Torch				
	TLT Stream Analytics IVA				

*Multi-node HPC containers
New since SC18

NGC registration not required as of Nov'18

10 containers

SOFTWARE ON THE NGC CONTAINER REGISTRY

48 containers

October 2017

-March 2019

CUDA CONTAINERS ON NVIDIA GPU CLOUD

- CUDA containers available from NGC Registry at nvcr.io/nvidia/cuda

- Three different flavors:

Base

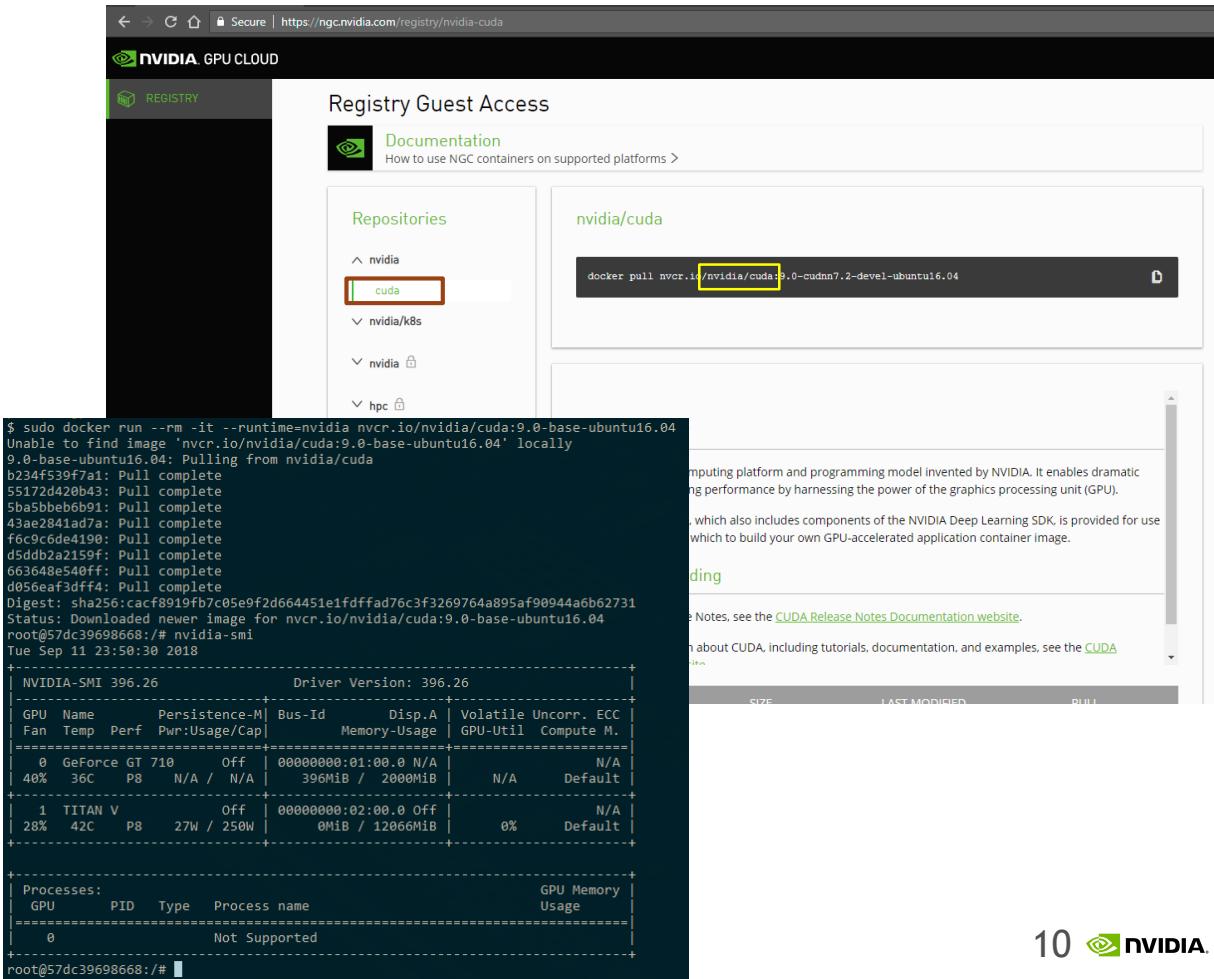
- Contains the minimum components required to run CUDA applications

Runtime

- Contains *base* + CUDA libraries (e.g. cuBLAS, cuFFT)

Devel

- Contains *runtime* + CUDA command line developer tools. Some *devel* tags also include cuDNN





Sylabs Intro - 10 min

20 June 2019

Michael Bauer - HPC Container Workshop ISC19



Sylabs provides licensing, enterprise level support, professional services, cloud functionality, and value-added plugins for the Singularity container runtime

Sylabs also drives the development efforts of the Open Source Singularity Project along with orchestration and resource management systems to support compute driven workflows, such as in Artificial Intelligence, Security and Data Science fields

SingularityPRO

Enterprise Grade Support

- Sylabs sponsors and productizes Singularity, and are uniquely qualified to provide the top tier of support
- Sylabs employs key members of the open source developer community
- SingularityPRO is provided as a pre-built binary, no need to build from source
- Available via per node, system, or site licenses for an easy on-ramp to adoption and system management (to include cloud and desktop/workstation)

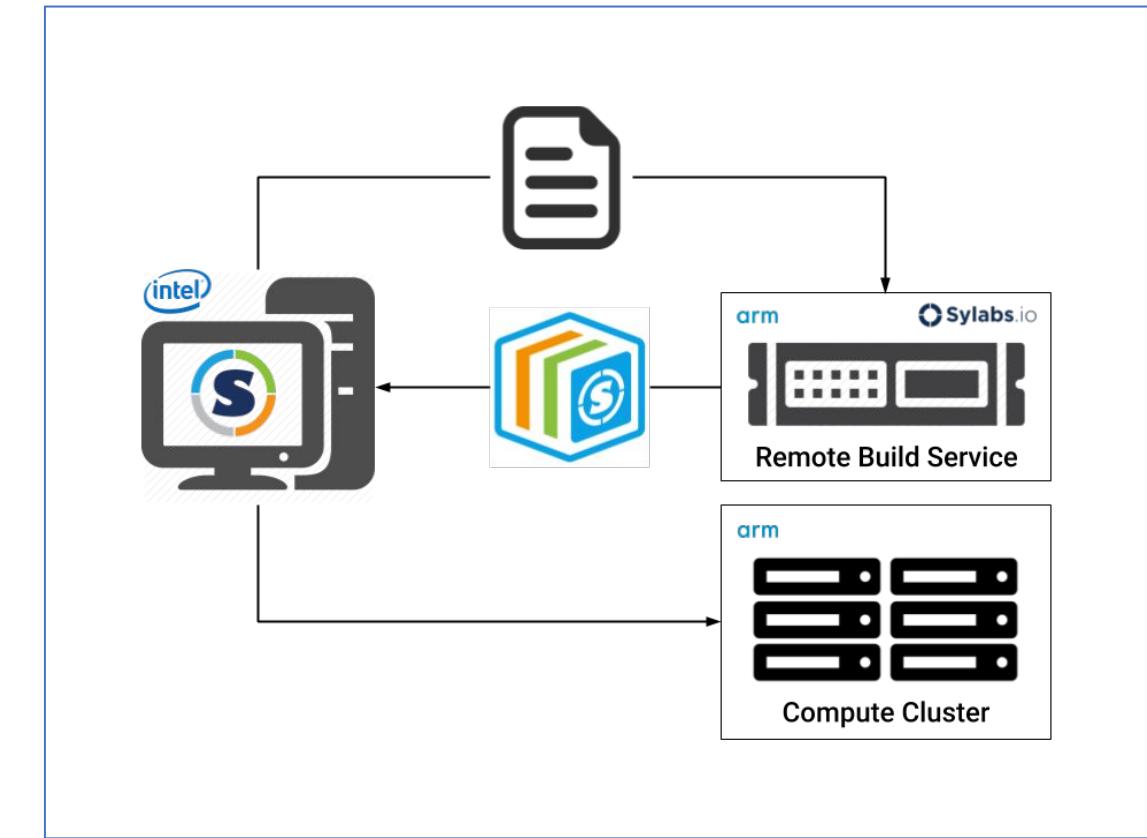
To Summarize SingularityPRO differences

- Enterprise Grade Support
- Backporting of security and bug fixes
- Influence on feature development and timelines
- Extra functionality via custom plugin development

Singularity Container Services

Sylabs

Singularity Container Services:

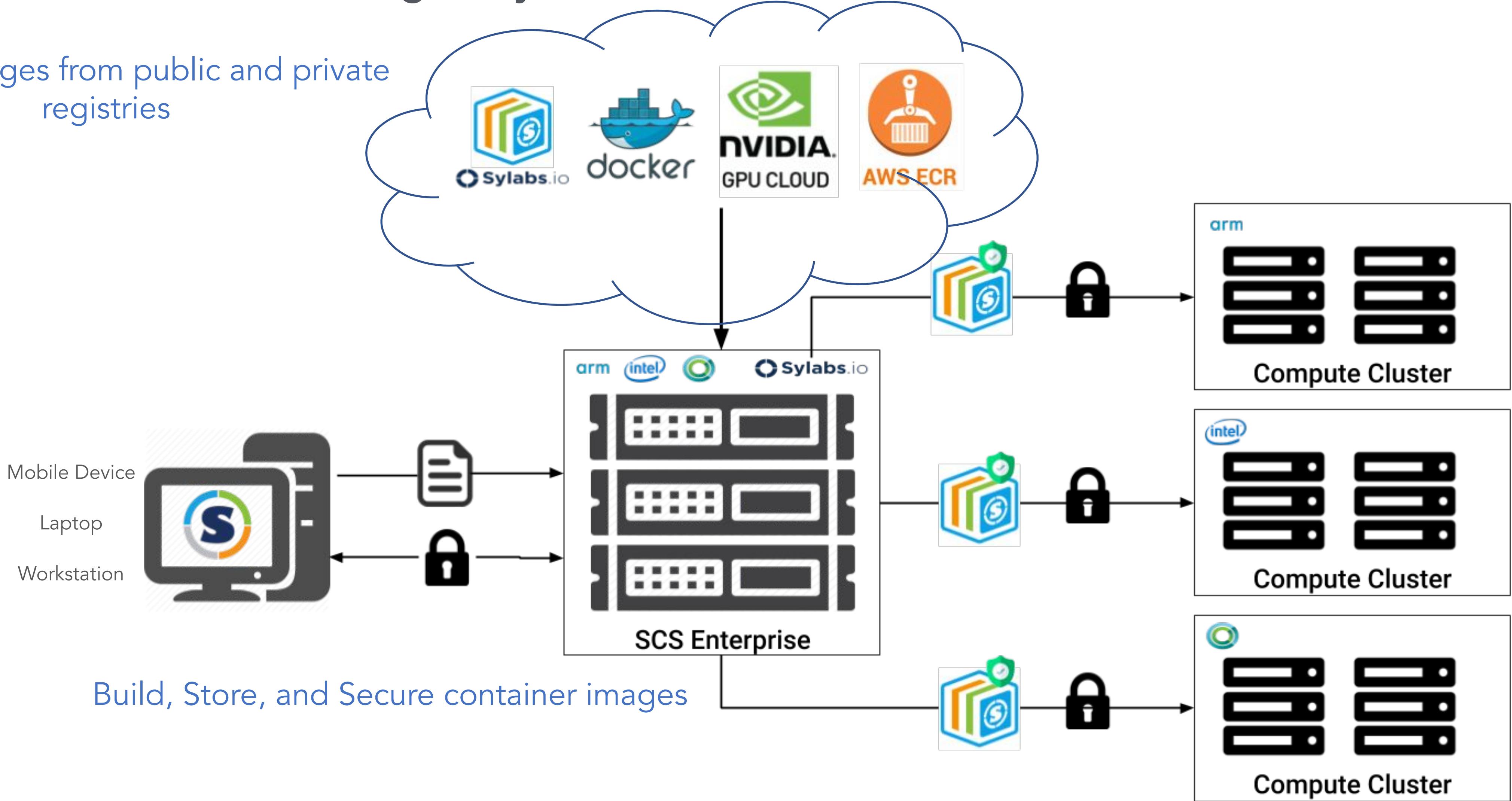


- Key Management Platform to cryptographically validate signed images; provides management, storage and distribution of PGP public keys
- Container Library provides centralized storage and management capability for signed and encrypted SIF files
- Remote Build Services provide a platform for unprivileged users to create secure compliant SIF images without requiring privilege escalation across hardware platforms

Available now OnPrem and VPC in 2H2019 <https://cloud.sylabs.io>

Singularity Container Services

Retrieve images from public and private registries



Who am I ?

AWS HPC Specialist Solutions Architect

Based out of Paris

Previously:

HPC Services CTO @ATOS

HPC Support Mgr @Bull

And a few other stuffs

Enjoy moving **Snowballs** around Paris on a bicycle



AWS Global Infrastructure

21 Geographical Regions, 1 Local Region, 66 Availability Zones, 180 POPs

Region and Availability Zones (AZs)

GovCloud (US)  Europe

US-East (3), US-West (3) Frankfurt (3)

Ireland (3)

US West

Oregon (4)
Northern California (3)

London (3)

Paris (3)

Stockholm (3)

US East

N. Virginia (6), Ohio (3)
Asia Pacific

Singapore (3), Sydney (3),
Tokyo (4), Osaka-Local (1)*

Canada

Central (2)

Seoul (3), Mumbai (3),
Hon Kong (3)

China

South America
São Paulo (3)

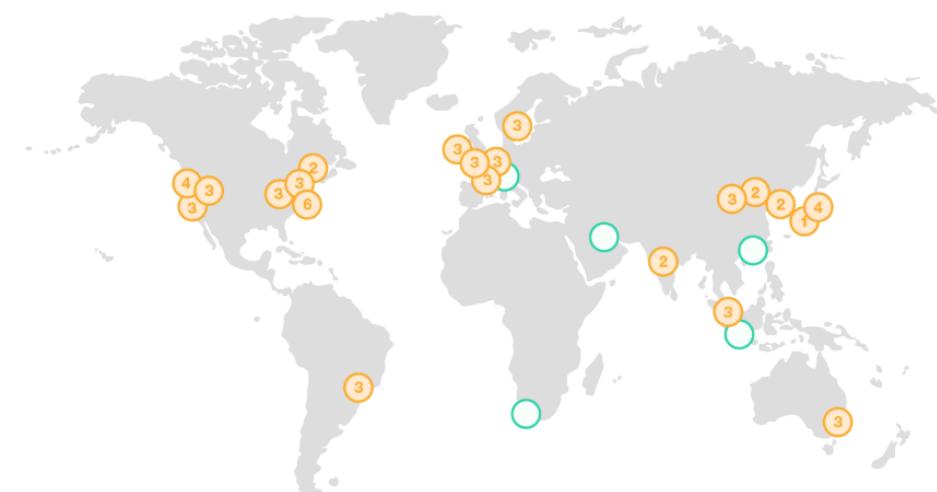
Beijing (2), Ningxia (3)

Future Announced Regions

Bahrain (3), Cape Town (3), Jakarta (3), Milan (3)



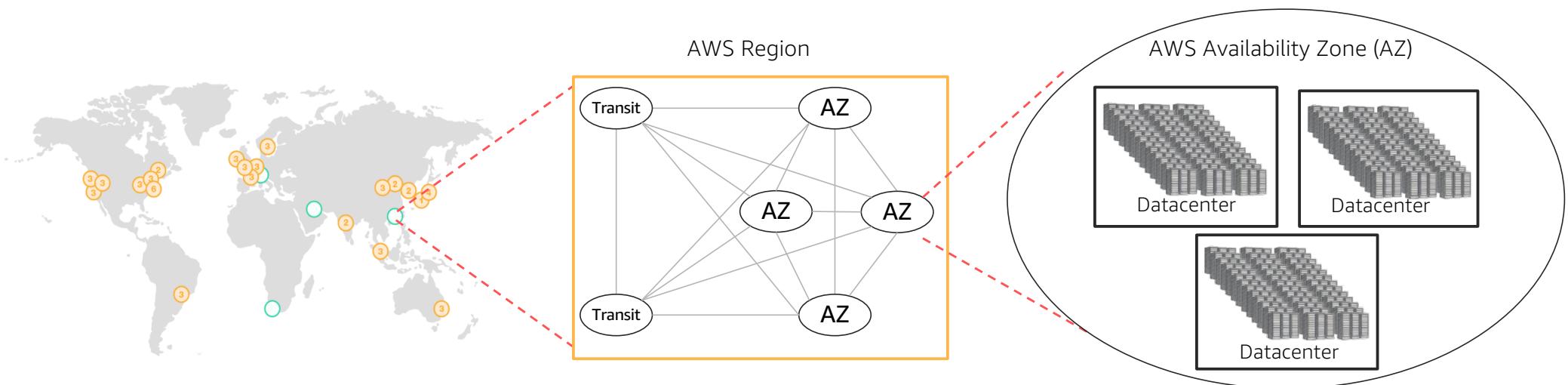
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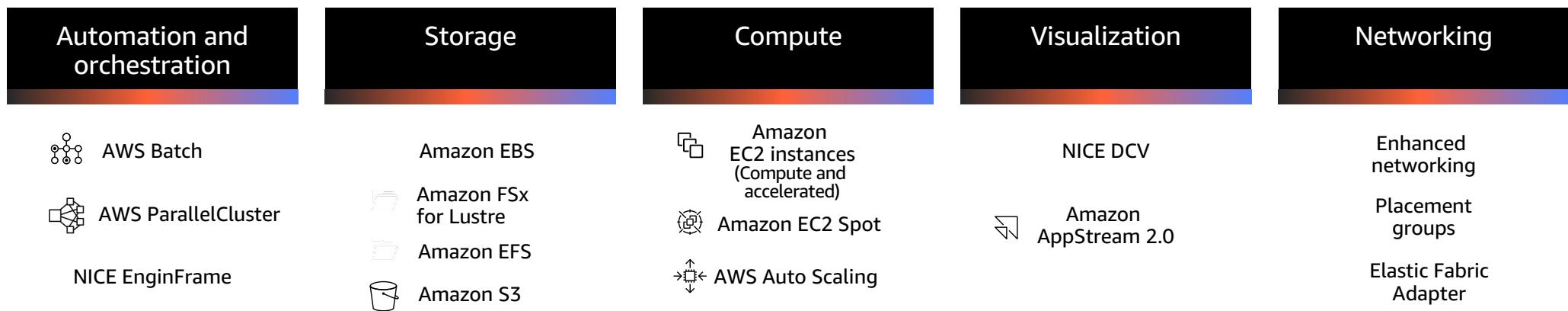
<https://www.infrastructure.aws/>

AWS Region Overview

AWS Regions are comprised of multiple AZs for high availability, high scalability, and high fault tolerance.
Applications and data are replicated in real time and consistent in the different AZs



HPC on AWS solution components



Mellanox - Introduction

Dror Goldenberg

ISC Container Workshop Frankfurt, June 2019







SUPERCONNECTING

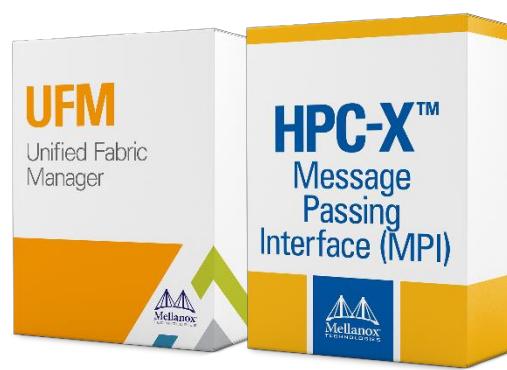
the #1 Supercomputers



ConnectX[®] 6



Mellanox
Quantum



HPC-X[™]



Highest Performance HDR 200G InfiniBand

Accelerating All Levels of HPC / AI Frameworks



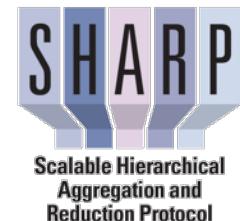
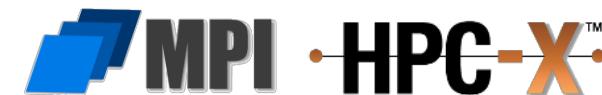
Application

- Data Analysis
- Real Time
- Deep Learning



Communication

- Mellanox SHARP In-Network Computing
- MPI Tag Matching
- MPI Rendezvous
- Software Defined Virtual Devices



Network

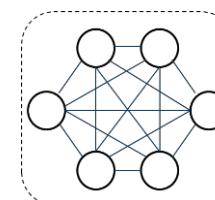
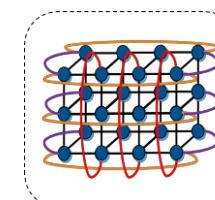
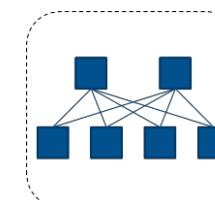
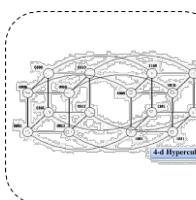
- Network Transport Offload
- RDMA and GPU-Direct RDMA
- SHIELD (Self-Healing Network)
- Enhanced Adaptive Routing and Congestion Control

GPUDirect



Connectivity

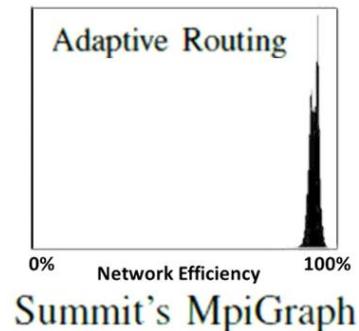
- Multi-Host Technology
- Socket-Direct Technology
- Enhanced Topologies



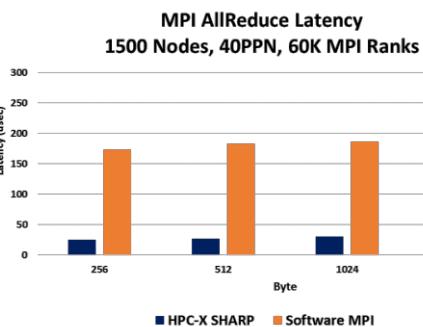
Highest Performance and Scalability for Exascale Platforms



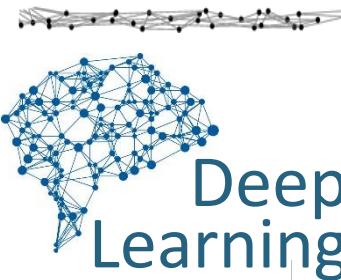
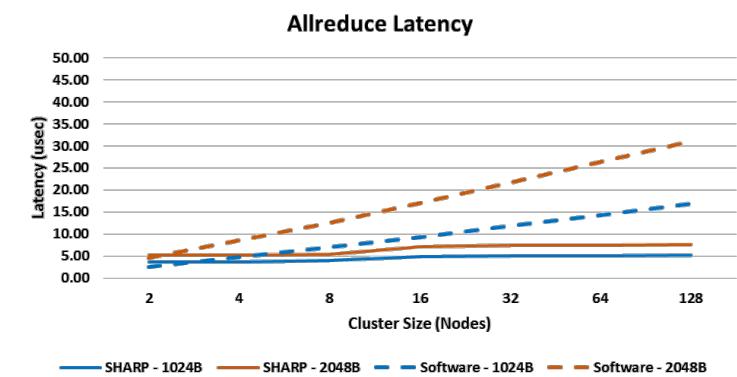
96%
Network Utilization



7X
Better

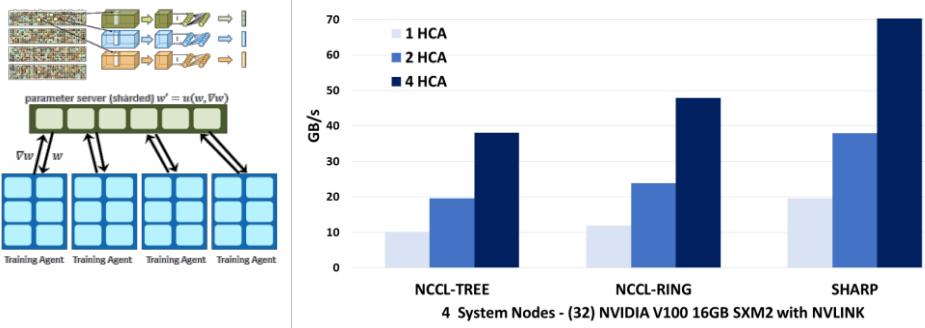


Flat
Latency

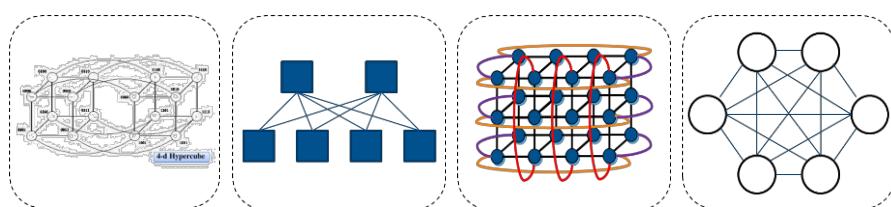


2X
Better

Mellanox SHARP with NCCL 2.4



5000X
Better



XDR 1000G

NDR 400G

HDR 200G



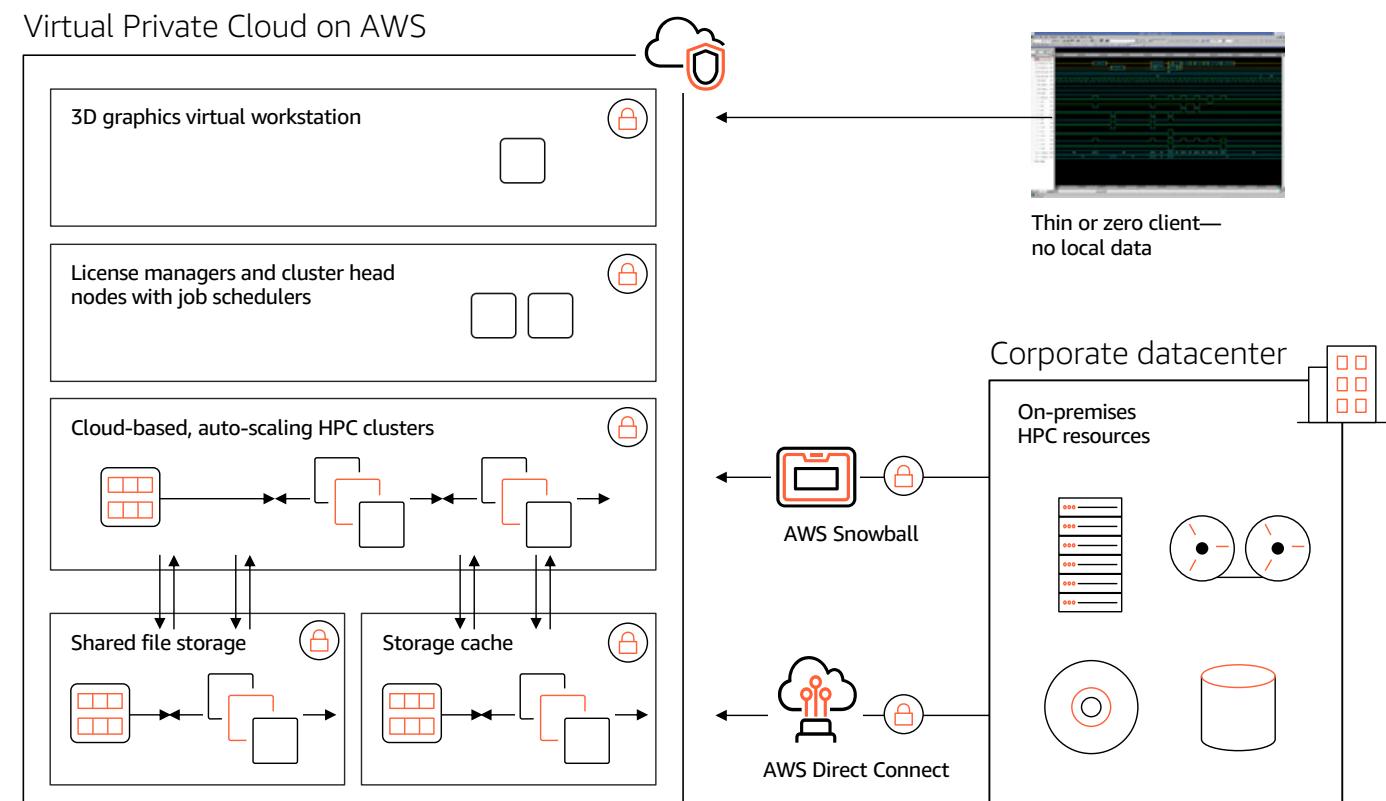
Thank You!

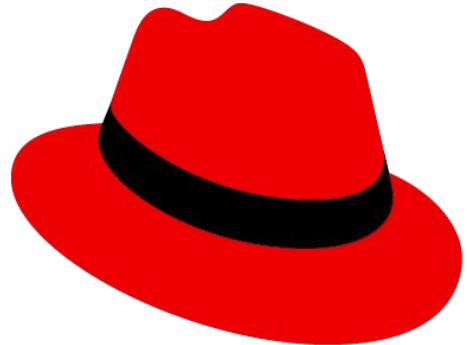


High Performance Computing (HPC) on AWS

On AWS, secure and well-optimized HPC clusters can be automatically created, operated, and torn down in just minutes

- Machine learning and analytics
- Amazon S3 and Amazon Glacier
- Third-party IP providers and collaborators





Red Hat

Valentin Rothberg
Container-Runtimes Team

Today...

I will not be talking about products,
but about projects.

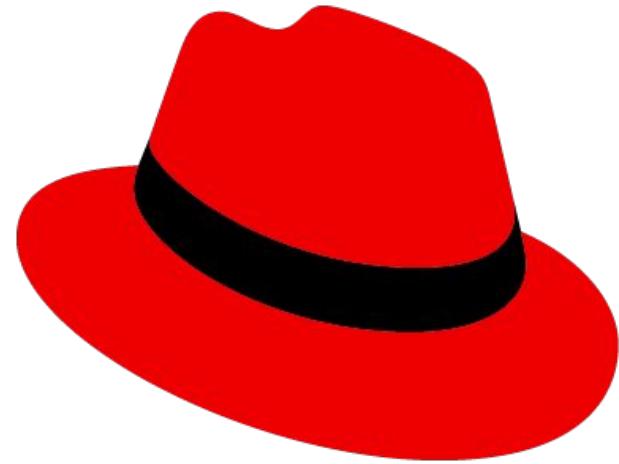
No Kubernetes, no OpenShift,
but the layers below them.

Everything started with Docker

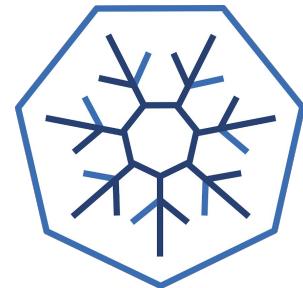


Red Hat's Philosophy

- No *one-size-fits-all* solution
- Have dedicated and *specialized* tools
 - Compatibility
 - Open standards
 - Open development
 - Open source
 - Interoperability to enable more use cases

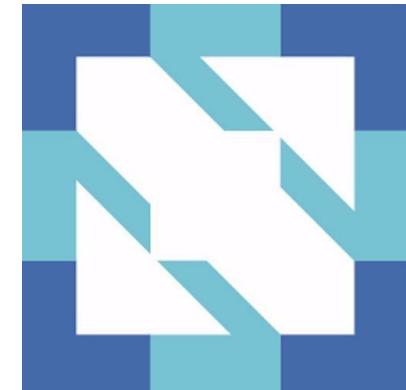


CRI-O



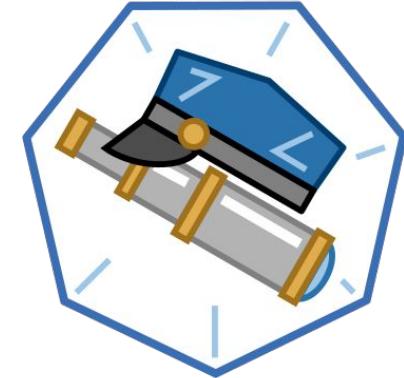
cri-O

- OCI-based Kubernetes Runtime
 - *The only use case is Kubernetes*: nothing more nothing less
- CNCF project since April 2019
- Supports all OCI compatible container images
 - Including all older Docker formats
- Supports any container registry
- Supports all OCI container runtimes
- 100+ contributors, 90+ releases, 1500+ per PR
- Collaboration across the industry (Red Hat, SUSE, Intel, IBM, lyft)



More tools, more use cases

- **Skopeo**: image distribution and management
- **Podman**: container and pod execution and management
- **Buildah**: building container images
- All share the same libraries and are developed at github.com/containers
- Collaboration across the industry and across Linux distributions



podman



buildah

Workshop Overview

5th High Performance Container Workshop - ISC19

Segments

The workshop is split into different segments to shed light on various aspects.

- Runtime
- Build
- Distribution
- Orchestration/Scheduling
- HPC Specifics
- Use-cases / Conclusions / Open Discussion

Segments Structure

1. The segments will be kicked off by a set of lightning talks (around 5 minutes each).

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3. If you are enthusiastic about a certain topic - volunteer to become a panelist. The panel is not locked down.

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3. If you are enthusiastic about a certain topic - volunteer to become a panelist.
The panel is not locked down.
4. The Catch-Box microphone is used for audience question.
Please wait until you got it.

