



NIMBIX

Supercomputing made super human

5 Years of Containerized HPC in the Cloud: Past, Present, and Future

Leo Reiter, CTO and Vice President of Software Engineering,
Nimbix

What Are Containers?

Linux containers

- Abstraction – not actually “things”
- “Inter-modal” Method for packaging, distributing, and deploying applications and dependencies onto arbitrary infrastructure
 - VM’s, PC’s, servers, clusters, etc.
 - Consistency and integrity across platforms
 - Repeatable mechanisms
- VM’s useful in some cases, but no longer needed
 - VM’s are not compatible with HPC!

“Demystified” ...



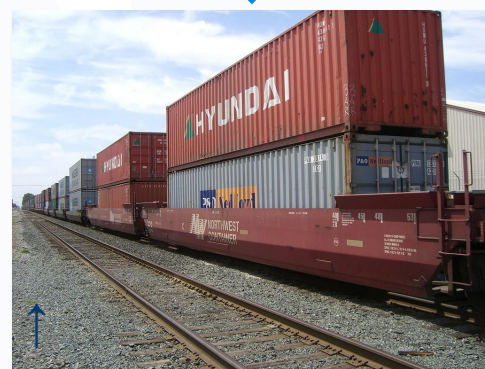
Application
n



Container

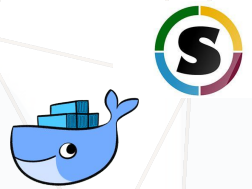


Platform



Runtime
e

Container Ecosystem: Explained



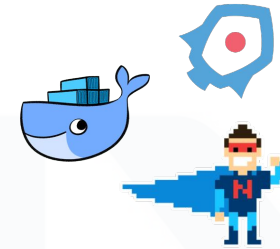
Formats



Registries

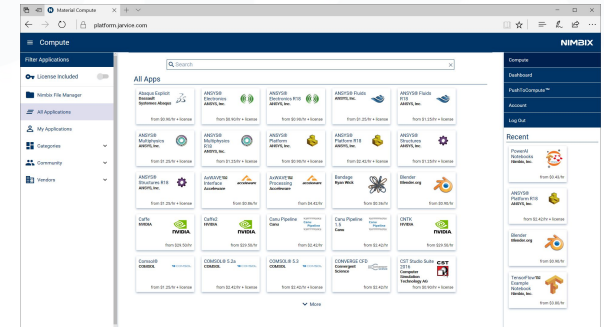
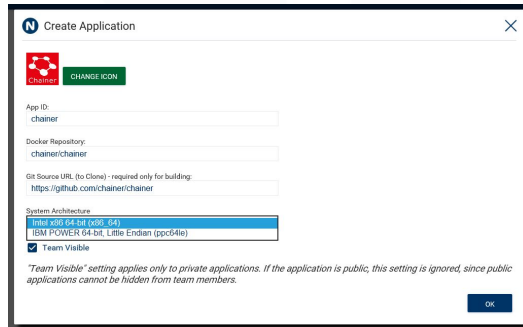
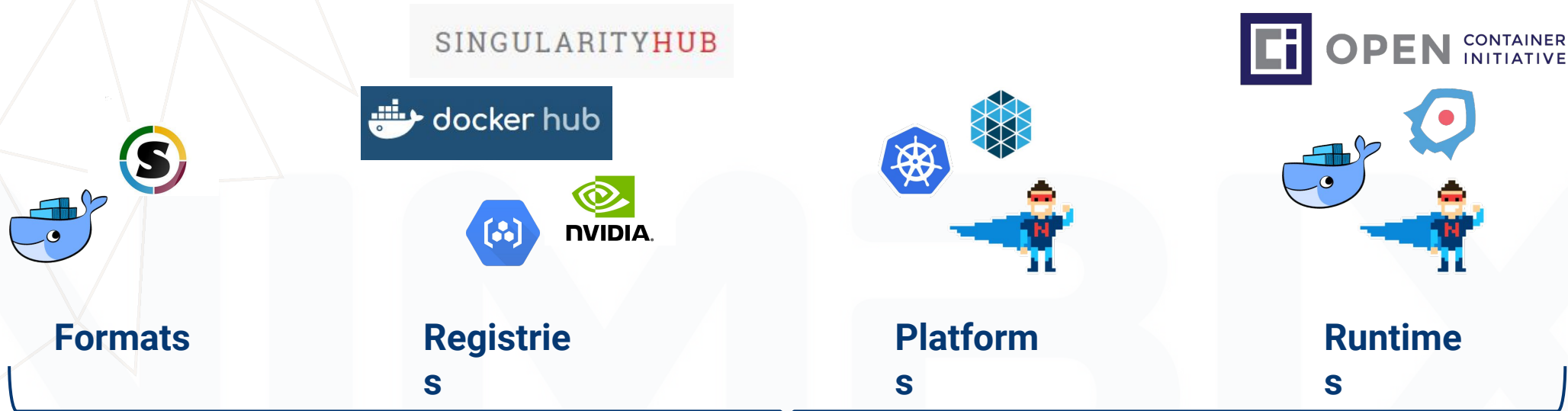


Platforms



Runtimes

Container Solution: Complete



JARVIC
E

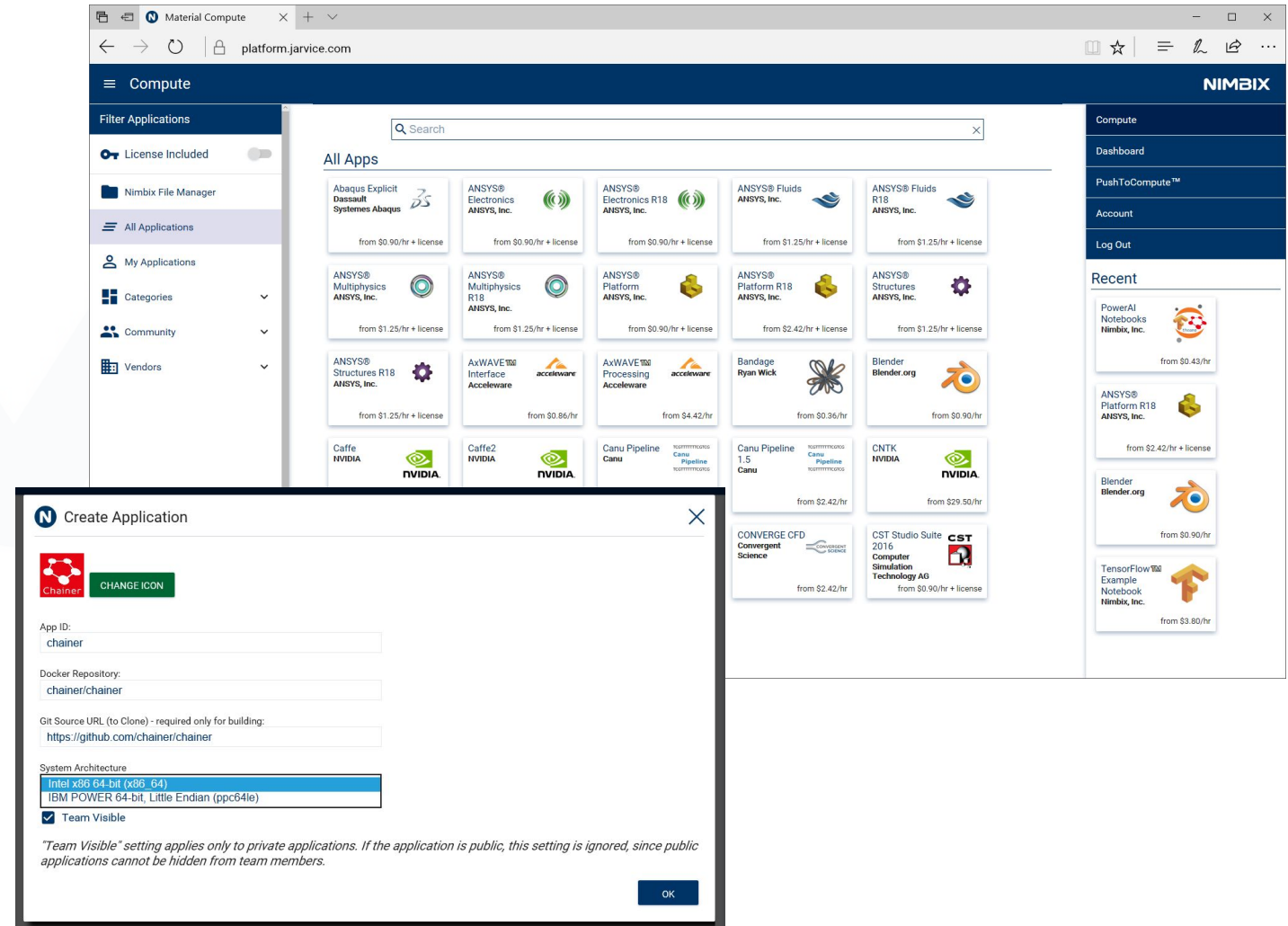
JARVICE

A purpose built container-native cloud operating system and application delivery platform for accelerated and high performance computing.

Powers the Nimbix Cloud, now available on-premises.

Introduced containerized HPC and ML/DL, at scale to the world.

In production since 2013.



What is Containerized HPC?



What is Containerized HPC?

- ✓ Bare-metal – no hypervisors
 - HPC and virtualization don't mix!



What is Containerized HPC?

- ✓ Bare-metal – no hypervisors
 - **HPC and virtualization don't mix!**
- ✓ Large scale, no bottlenecks
 - Tightly coupled algorithm support for existing MPI and next-gen DDL
 - **Low latency fabric support**



What is Containerized HPC?



- ✓ Bare-metal – no hypervisors
 - **HPC and virtualization don't mix!**
- ✓ Large scale, no bottlenecks
 - Tightly coupled algorithm support for existing MPI and next-gen DDL
 - **Low latency fabric support**
- ✓ Accelerated and Heterogeneous
 - x86, POWER, GPUs, FPGAs, multi-core, “many-core” - **all of the above**

What is Containerized HPC?



- ✓ Bare-metal – no hypervisors
 - **HPC and virtualization don't mix!**
- ✓ Large scale, no bottlenecks
 - Tightly coupled algorithm support for existing MPI and next-gen DDL
 - **Low latency fabric support**
- ✓ Accelerated and Heterogeneous
 - x86, POWER, GPUs, FPGAs, multi-core, “many-core” - **all of the above**
- ✓ Workflow-oriented
 - Not machines, not microservices – **just answers**

3 Containerized HPC Myths...



3 Containerized HPC Myths...

Myth #1:
Containers are not
bare-metal!



3 Containerized HPC Myths...

Myth #1:
Containers are not
bare-metal!



Yes they
are.

3 Containerized HPC Myths...

Myth #1:
Containers are not
bare-metal!



Yes they are.
In the Nimbix
Cloud!



3 Containerized HPC Myths...

Myth #2:
Containers are hard to
make!



3 Containerized HPC Myths...

Myth #2:
Containers are hard to
make!



No they're
not!

3 Containerized HPC Myths...

Myth #2: Containers are hard to make!



<https://github.com/nimbix/app-hpctest/bb/master/Dockerfile>

7 lines (4 sloc) | 191 Bytes

```
1 FROM jarvice/base-centos-torque:6.0.4
2
3 RUN yum -y install nano vim emacs man && yum clean all
4 COPY 01-openmpi-path.sh /etc/profile.d/01-openmpi-path.sh
5 COPY AppDef.json /etc/NAE/AppDef.json
6
```



<http://singularity.lbl.gov/docs-recipes>

```
Bootstrap: docker
From: ubuntu

%help
Help me. I'm in the container.

%setup
    touch ${SINGULARITY_ROOTFS}/tacos.txt
    touch avocados.txt
```

**No they're
not!**

3 Containerized HPC Myths...

Myth #3:
My code is not container
native!



3 Containerized HPC Myths...

Myth #3:
My code is not container
native!

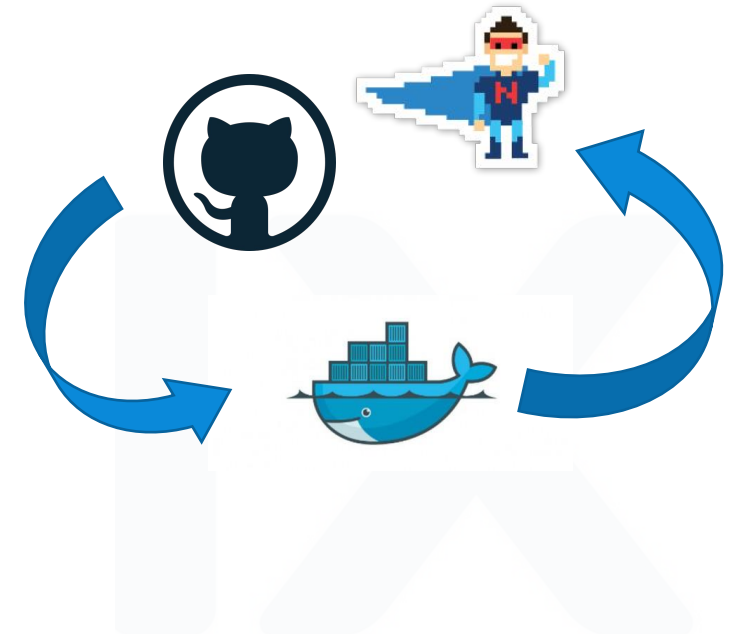


That's
okay.

3 Containerized HPC Myths...

Myth #3: My code is not container

 Abaqus Explicit from \$0.90/hr + license	 ANSYS Electronics from \$0.90/hr + license	 ANSYS Fluids R18 from \$0.90/hr + license	 ANSYS Fluids R18 from \$1.25/hr + license	 ANSYS Fluids R18 from \$1.25/hr + license	 Meep from \$1.25/hr	 M8bytes from \$0.90/hr	 MSC Nastran from \$0.68/hr + license	 MXNet from \$29.50/hr	 myapp from \$0.36/hr
 ANSYS Multiphysics R18 from \$1.25/hr + license	 ANSYS Platform R18 from \$1.25/hr + license	 ANSYS Platform R18 from \$0.90/hr + license	 ANSYS Platform R18 from \$0.36/hr + license	 ANSYS Platform R18 from \$1.25/hr + license	 Neural Style from \$0.36/hr	 Nimble File Manager from \$0.36/hr	 NVIDIA DIGITS 3 from \$0.90/hr	 NVIDIA DIGITS 4 from \$0.90/hr	 NVIDIA DIGITS 5 from \$0.90/hr
 ANSYS Structures R18 from \$1.25/hr + license	 AxiWave from \$0.86/hr	 AxiWave Processing Accelerator from \$4.42/hr	 Bandage from \$0.36/hr	 BioBuilds from \$0.43/hr	 NVIDIA DIGITS 5 for IBM POWER8 from \$0.36/hr	 NVIDIA Iray from \$1.10/hr	 OpenSCAD from \$0.36/hr	 PacBio SMRT Portal from \$2.42/hr	 ParaView from \$2.50/hr
 Blender from \$0.90/hr	 Caffe from \$29.50/hr	 Caffe2 from \$29.50/hr	 Canu Pipeline from \$2.42/hr	 Canu Pipeline from \$2.42/hr	 PowerAI from \$3.80/hr	 PowerAI Example Notebooks from \$0.43/hr	 prestackPro from \$2.42/hr + license	 PyTorch from \$29.50/hr	 Qin & Offshoot from \$11.25/hr
 Canu Pipeline 1.6 from \$2.42/hr	 CNTK from \$29.50/hr	 Cortado from \$1.25/hr + license	 COMSOL 5.2a from \$2.42/hr + license	 COMSOL 5.3 from \$2.42/hr + license	 Quartus Prime & SDK for OpenCL 18.1 from \$0.36/hr + license	 Quartus Prime & SDK for OpenCL 18.1 from \$0.36/hr	 Quartus Prime & SDK for OpenCL 18.1 from \$0.36/hr	 RealityServer from \$1.90/hr	 SDAccel Development Xilinx from \$1.50/hr
 CONVERGE CFD from \$2.42/hr	 CST Studio Suite 2017 from \$1.25/hr + license	 CUDA 9.0 + cuDNN 7 from \$29.50/hr	 Database Acceleration Demo Xilinx from \$3.00/hr	 DIGITS from \$29.50/hr	 SDAccel Runtime Xilinx from \$0.00/hr	 SIMULIA Abacus from \$2.42/hr + license	 STAR-CCM+ from \$1.25/hr	 STAR-CCM+ from \$1.25/hr	 STAR-CCM+ from \$1.25/hr
 Dog Classification Demo for POWER8 from \$4.95/hr	 DriverlessAI 1.0.0 from \$1.06/hr	 EnLight from \$0.90/hr	 FENSAP-ICE 17.2 from \$2.42/hr + license	 H2o3 from \$0.36/hr	 TensorFlow from \$29.50/hr	 TensorFlow Example Notebooks from \$3.80/hr	 Theano from \$29.50/hr	 Torch from \$29.50/hr	 Torch/Quasimodo with OpenMPI for POWER8 from \$4.95/hr
 H2o3 for POWER8 from \$0.43/hr	 Hadoop with ROMA from \$0.90/hr	 HPG Test Environment from \$2.42/hr	 IBM PowerAI ML/DL and COOL from \$3.80/hr	 Kinetics 6.0 for POWER8 from \$18.15/hr	 Ubuntu Linux for Intel from \$0.36/hr	 Ubuntu Linux for POWER8 from \$0.43/hr	 Vault Migration Assistant from \$0.36/hr	 Xilinx AlexNet Test Drive Xilinx from \$3.00/hr	
 LSTC LS-DYNA 18.1 from \$2.42/hr	 LSTC LS-PrePost 18.1 from \$1.25/hr	 Machine Learning Developer Environment from \$0.36/hr	 MATLAB Distributed Cluster Server from \$2.42/hr + license	 MATLAB R2017a from \$2.42/hr + license					



That's okay.
Neither are most of
these!

How JARVICE Helps Get There

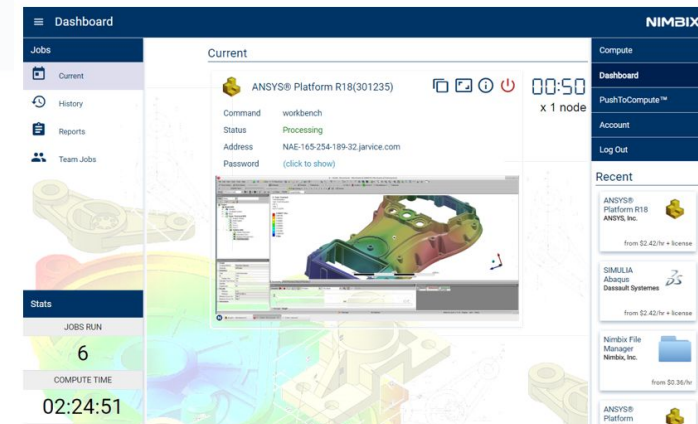
Traditional App

- Turn-key HPC-ready environment with MPI, IB drivers, SSH, on either Ubuntu or CentOS (RHEL)
- Seamless access to state of the art acceleration
- Batch and interactive modes, including transparent 3D OpenGL hardware acceleration

```
~ % mpirun -machinefile /etc/JARVICE/nodes /usr/local/bin/solver ...
```

Container-native App

- Fastest container runtime engine with the fastest starts
- Seamless access to state of the art acceleration
- Secure remote access with graphical desktop capabilities and SSH



The screenshot shows the NIMBIX website with a navigation bar at the top containing links like 'HOME', 'ABOUT', 'CONTACT', 'SOLUTIONS', 'SERVICES', and 'PARTNERS'. The main content area features several product cards:

- 2017 2 SDAccel Runtime**: A Xilinx 2017.2 FPGAs runtime environment for 4.0 DSA's.
- ANSYS® Electronics R18**: From \$3,500/hr + license. ANSYS electronics solutions help you design innovative elect...
- ANSYS® Electronics R19**: From \$3,500/hr + license. ANSYS electronics solutions help you design innovative elect...
- ANSYS® Fluent 16.0**: From \$1,250/hr + license. Predicting and controlling fluid flow is critical in optimiz...
- Abaqus Explicit**: Dassault Systemes Abaqus. From \$3,900/hr + license. Abaqus/Explicit is a finite element analysis product that is...

On the right side, there is a sidebar with a 'FILTER' section containing radio buttons for 'All', 'On-demand', and 'Licensed'. Below this is a 'CATEGORIES' section with a list of categories: AI, Bioinformatics, Computer Aided Design, Data Science, IBM POWER, Machine Learning, NVIDIA DGX, Oil and Gas, and Rendering.

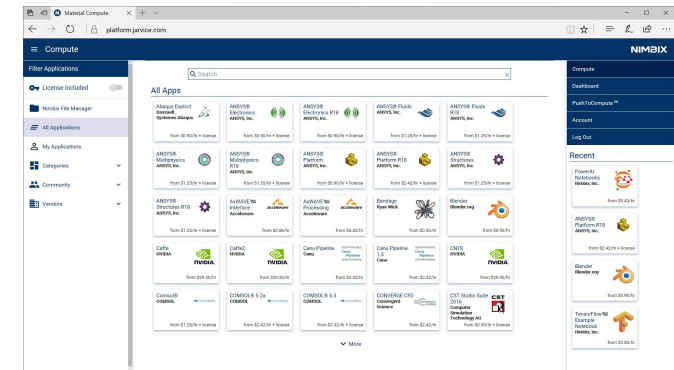
Containerized workflows

NACC 2012

- Extensible/scale-out SOA
- Container-native
- PaaS "v2"

2016
PushToCompute™

Docker and Singularity PaaS “v3”



Stuff We Invented Along the Way

Reconfigurable Cloud Computing

- Application-defined workflows
- Processing API
- Bare-metal for cloud HPC
- Seamless programming/setup/teardown of accelerators including GPUs and FPGAs in the cloud

Dynamic creation and execution of containerized applications in cloud computing

- End-to-end orchestration and scheduling of workflows using Linux containers in cloud computing

JARVICE 3 + Kubernetes

JARVICE 3 brings end to end HPC application development, deployment, and scaling capabilities to Kubernetes!

- Same benefits enjoyed in the Nimbix Public Cloud now available on single tenant and on premises clusters via the Kubernetes API
- HPC and distributed deep learning (DDL), side by side with Enterprise microservices and web apps
- Bare-metal or virtualized, or both
- Hundreds of commercial and open source turn-key workflow from Nimbix Public Cloud, ready to run

How We Brought HPC to Kubernetes

- Tightly coupled workflows, capable of running MPI style applications in a turn-key manner
- Distributed container cache for very large HPC containers
 - Essential innovation of PushToCompute™
- Nimbix Public Cloud service catalog 100% compatibility
- x86 and IBM POWER are equal citizens and runtime selectable by application workflows

A composite image of Earth from space. The top half shows a bright sun rising over the horizon, casting a glow over the clouds. The bottom half shows the Earth at night, with city lights visible as yellow and white specks against the dark blue of the oceans and landmasses. The text "What About the Next 5 Years?" is centered in white.

What About the Next 5 Years?

What About the Next 5 Years?

- Very soon: Federated, exascale capabilities across multiple clouds under tenant control, with seamless end-user interface

What About the Next 5 Years?

- Very soon: Federated, exascale capabilities across multiple clouds under tenant control, with seamless end-user interface
- Down the road: Data-driven workflows, for exploratory computing, including data-driven “pipelines” for scientific data processing

What About the Next 5 Years?

- Very soon: Federated, exascale capabilities across multiple clouds under tenant control, with seamless end-user interface
- Down the road: Data-driven workflows, for exploratory computing, including data-driven “pipelines” for scientific data processing
- Not-too-distant future: ML/DL-driven platform optimization for cost and/or performance

What About the Next 5 Years?

- Very soon: Federated, exascale capabilities across multiple clouds under tenant control, with seamless end-user interface
- Down the road: Data-driven workflows, for exploratory computing, including data-driven “pipelines” for scientific data processing
- Not-too-distant future: ML/DL-driven platform optimization for cost and/or performance
- Eventually: time travel, cold fusion, world peace

Thank You

Questions? Comments? Thoughts?