

Run HPC simulation workflows in Microsoft Azure

Tejas Karmarkar
Principal Program Manager
Azure Compute
tejaskar@Microsoft.com

Topics

What is HPC?

- What type of workloads you can run in Azure?
- Target industries

Typical technology stack

- Technical prerequisites to run HPC workloads

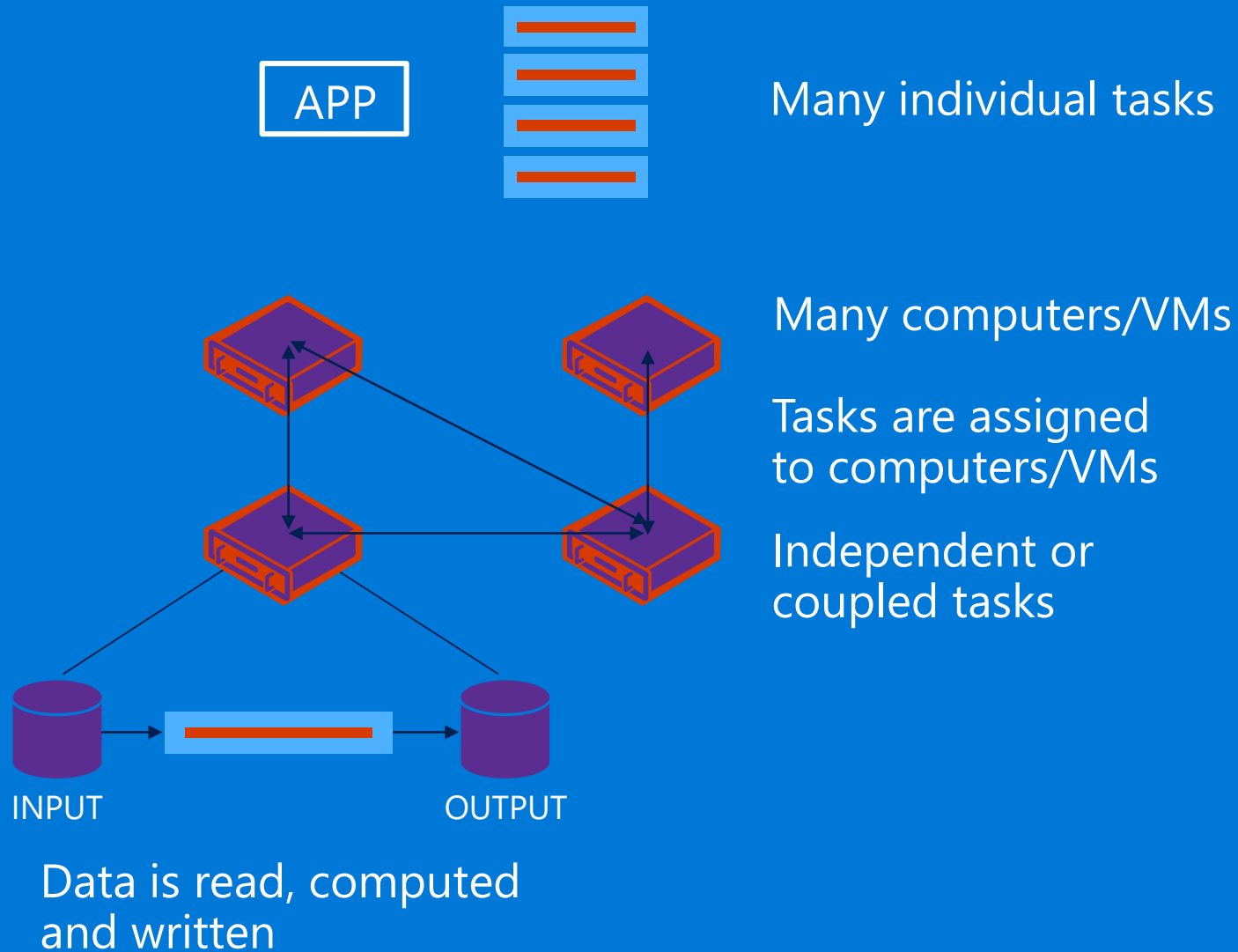
Azure core HPC technologies

- HPC compute VMs, HPC GPU VMs, RDMA networking, Azure Batch, HPC PACK, Premium storage etc.

How to run HPC workloads in Azure?

- Demo of how to run simulation applications on VMs
- Demo of cloud burst environment with a third party scheduler/workload manager
- Demo of Simulation in the cloud: SaaS service built on Azure
- HPC applications in the marketplace

What is Big Compute HPC ?



Uses:

Financial risk
Oil and gas production
Climate & hydrology
Science and research
Genomics & pharma
Image analysis & processing
Video & audio transcoding
Engineering stress analysis
Automobile crash simulation
Test and build execution

Two Types of Applications

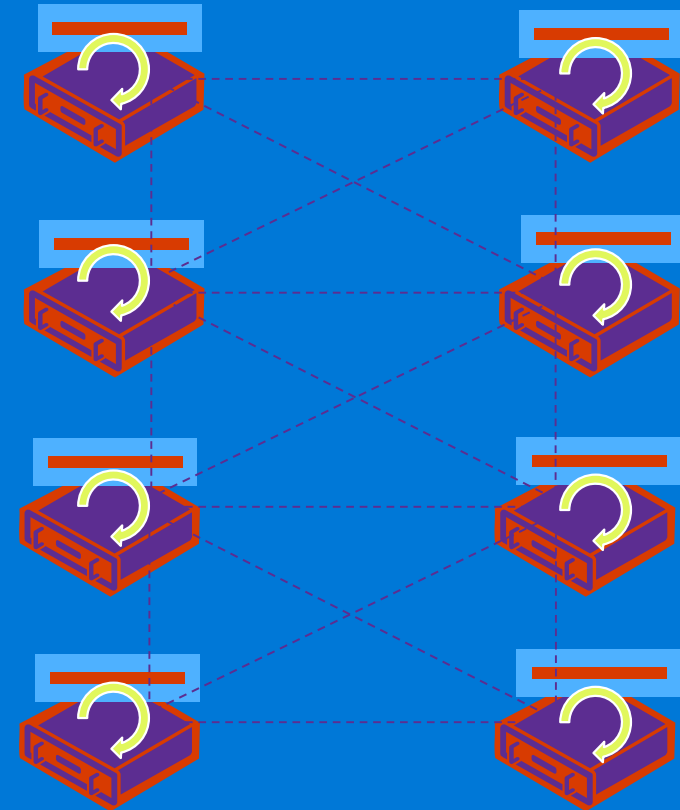
Embarrassingly parallel:

- VMs don't need to talk to each other, or very little cross-node communication
- Usually a parameter sweep, a job splitting, or a search/comparison through data
- Examples: Monte Carlo simulations, image/video rendering, genetic algorithms, sequence matching, file processing

Tightly coupled:

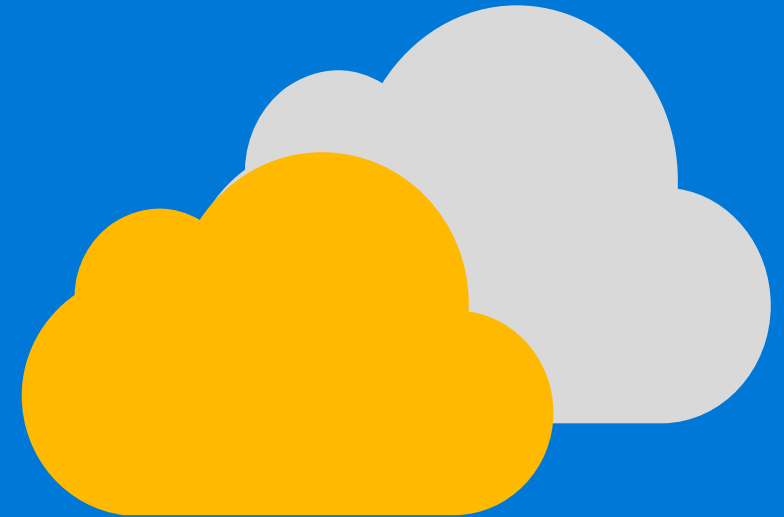
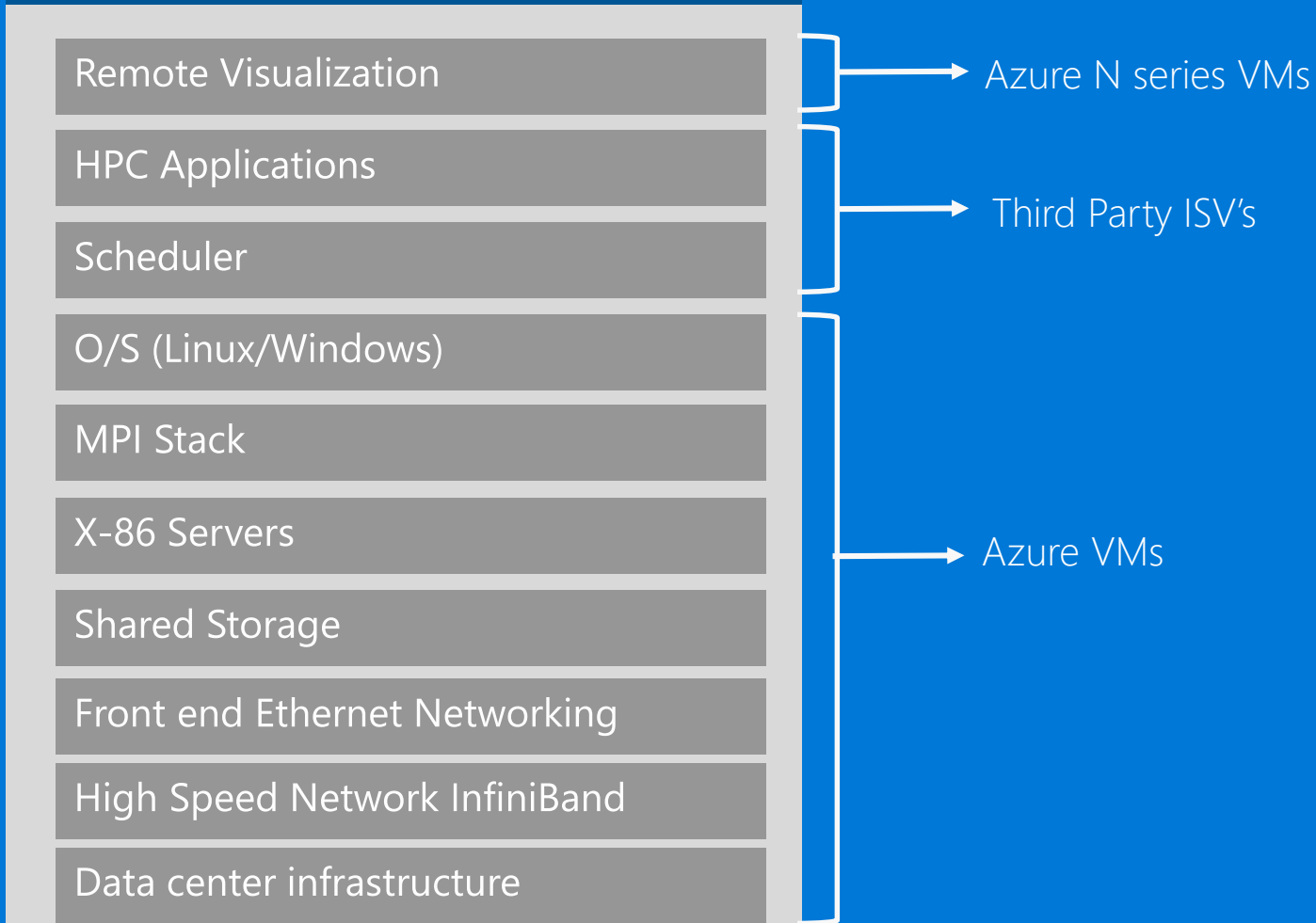
- Nodes need to talk to each other constantly
- Requires a fast interconnection network (low latency and high throughput)
- Examples: automotive crash simulation, fluid dynamics, climate modeling, reservoir simulation, manufacturing design

→ Now possible in cloud with HPC VMs with RDMA on Azure



HPC Value Chain and Technology Stack

Typical HPC technology stack



Applications on Azure

- Intersect (Schlumberger)
- NAMD
- LS-DYNA
- FLUENT
- STAR-CCM+
- RADIOSS
- ACU-SOLVE
- OPENFOAM
- PAM-CRASH
- LANDMARK (Halliburton)
- ABAQUS
- MSC NASTRAN
- OPTISTRUCT

• Preferred Scheduler

- PBS-PRO/COMPUTE MANAGER
- HPC-PACK

• MPI-SUPPORT

- Intel MPI
- MS-MPI on Windows

• Parallel file systems

- Intel Lustre

• OS SUPPORT

- SLES 12 SP1, CENTOS 6.5, 7.1 & Redhat coming soon
- WINDOWS SERVER 2012, R2, 2008 R2

Technical Pre-requisites to a run HPC jobs

High performance VMs

- High performance, High bandwidth low latency VM's for tightly coupled workloads
- High frequency VM's for high performance without low latency network

Shared Storage

- Parallel file system for global scratch or NFS share

Password-less SSH between the compute nodes

- SSH key shared across compute nodes for seamless communication

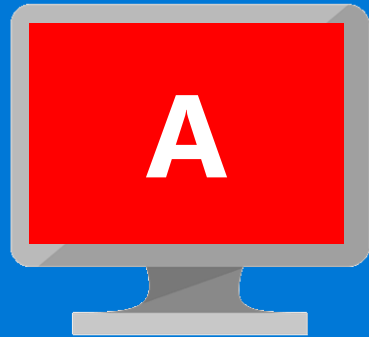
Vnet set up

- Recommended set up to controls IP range for connectivity to on-prem infrastructure

Scheduler

- Useful if more than one user going to access HPC service in the cloud

High performance VMs



A8-A11
E5-2670 Sandy Bridge processor
2.6 GHz, 112 Gb memory
QDR InfiniBand with 32 Gbps intra-node connectivity
3.2 Microseconds latency
High bandwidth frontend Ethernet
40 GB local HDD

New



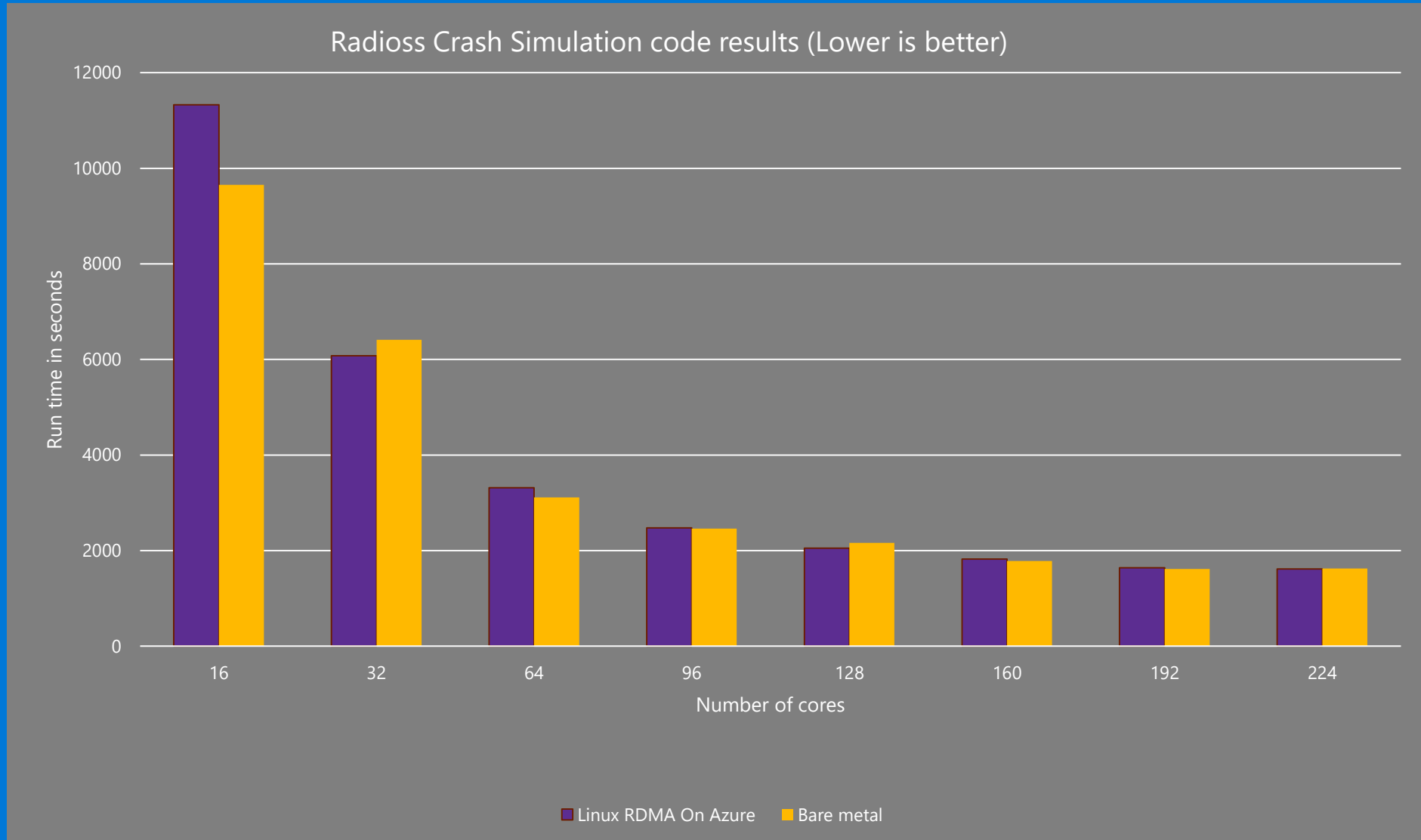
H-series
Fastest VM's in the public cloud
E5-2667 V3 Haswell processor
3.2 GHz, Up to 224 Gb memory
FDR InfiniBand with 56 Gbps intra-node connectivity
2.6 Microseconds latency
High bandwidth frontend Ethernet
2 TB of local SSD

New

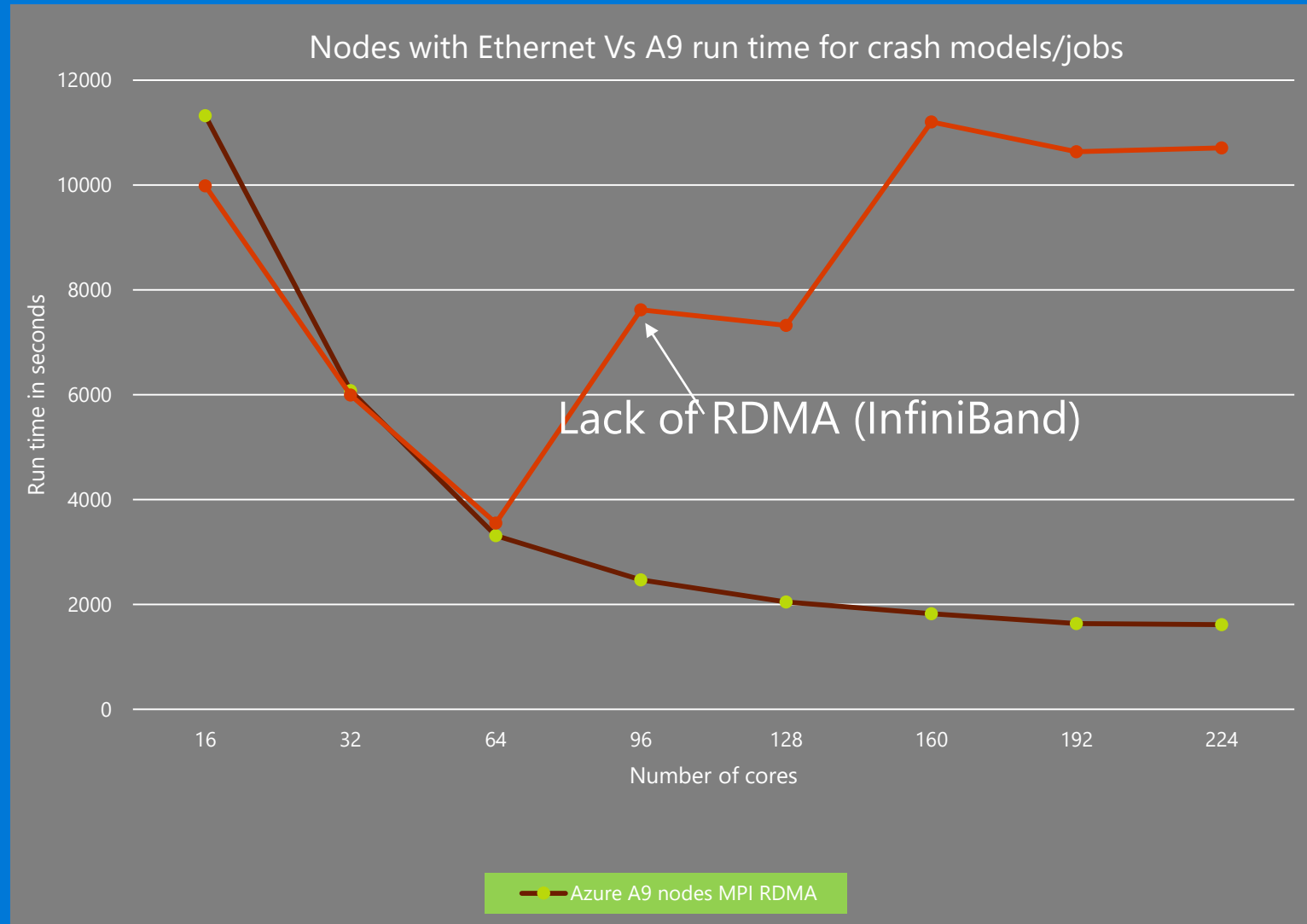


N-series
NVidia M 60 and K80 GPU's
High bandwidth frontend Ethernet
Up to 2 TB of local SSD

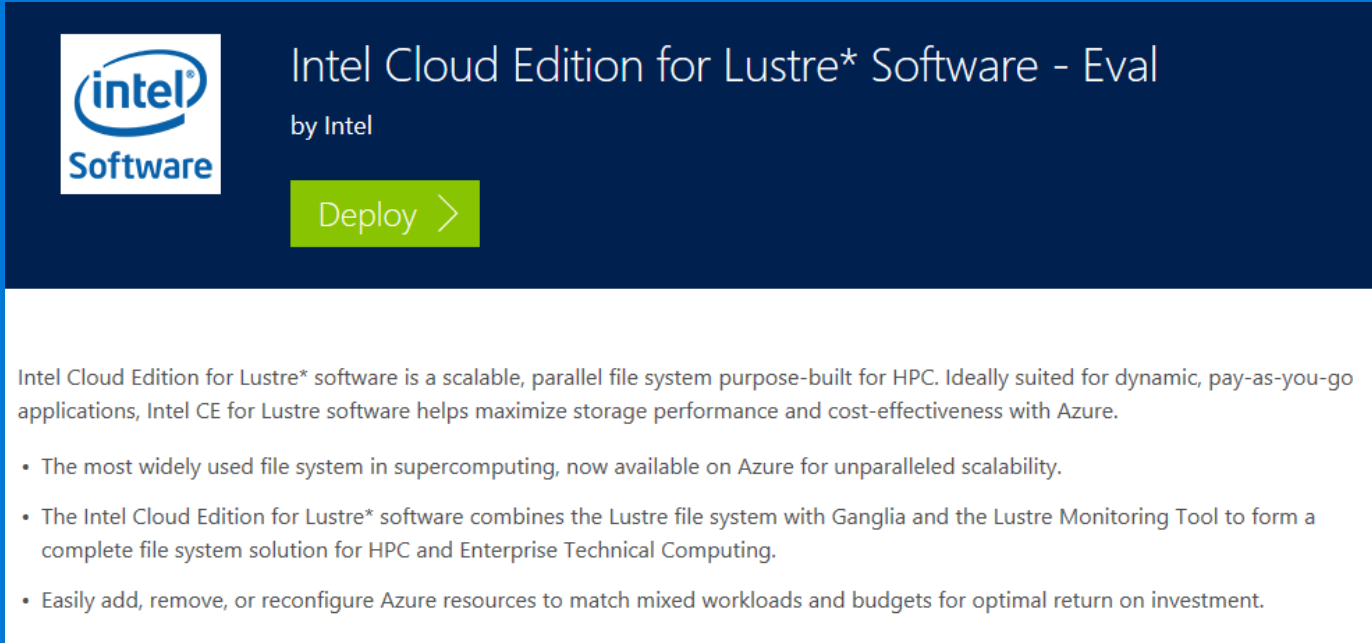
Why InfiniBand RDMA matters?



Why InfiniBand RDMA matters?



Shared Storage: Lustre or NFS



The image shows a screenshot of the Intel Cloud Edition for Lustre* Software - Eval page. It features the Intel Software logo, a 'Deploy >' button, and a description of the software as a scalable, parallel file system for HPC. Below the description are three bullet points highlighting its features: scalability, integration with Ganglia and the Lustre Monitoring Tool, and the ability to easily add, remove, or reconfigure Azure resources.

Intel Cloud Edition for Lustre* Software - Eval
by Intel

[Deploy >](#)

Intel Cloud Edition for Lustre* software is a scalable, parallel file system purpose-built for HPC. Ideally suited for dynamic, pay-as-you-go applications, Intel CE for Lustre software helps maximize storage performance and cost-effectiveness with Azure.

- The most widely used file system in supercomputing, now available on Azure for unparalleled scalability.
- The Intel Cloud Edition for Lustre* software combines the Lustre file system with Ganglia and the Lustre Monitoring Tool to form a complete file system solution for HPC and Enterprise Technical Computing.
- Easily add, remove, or reconfigure Azure resources to match mixed workloads and budgets for optimal return on investment.

• Leverage Premium Storage with Ds series VMs with P30 disk

Ready to deploy ARM template that can launch 1600 core cluster in 10 minutes

Create large storage volumes shared across single name space

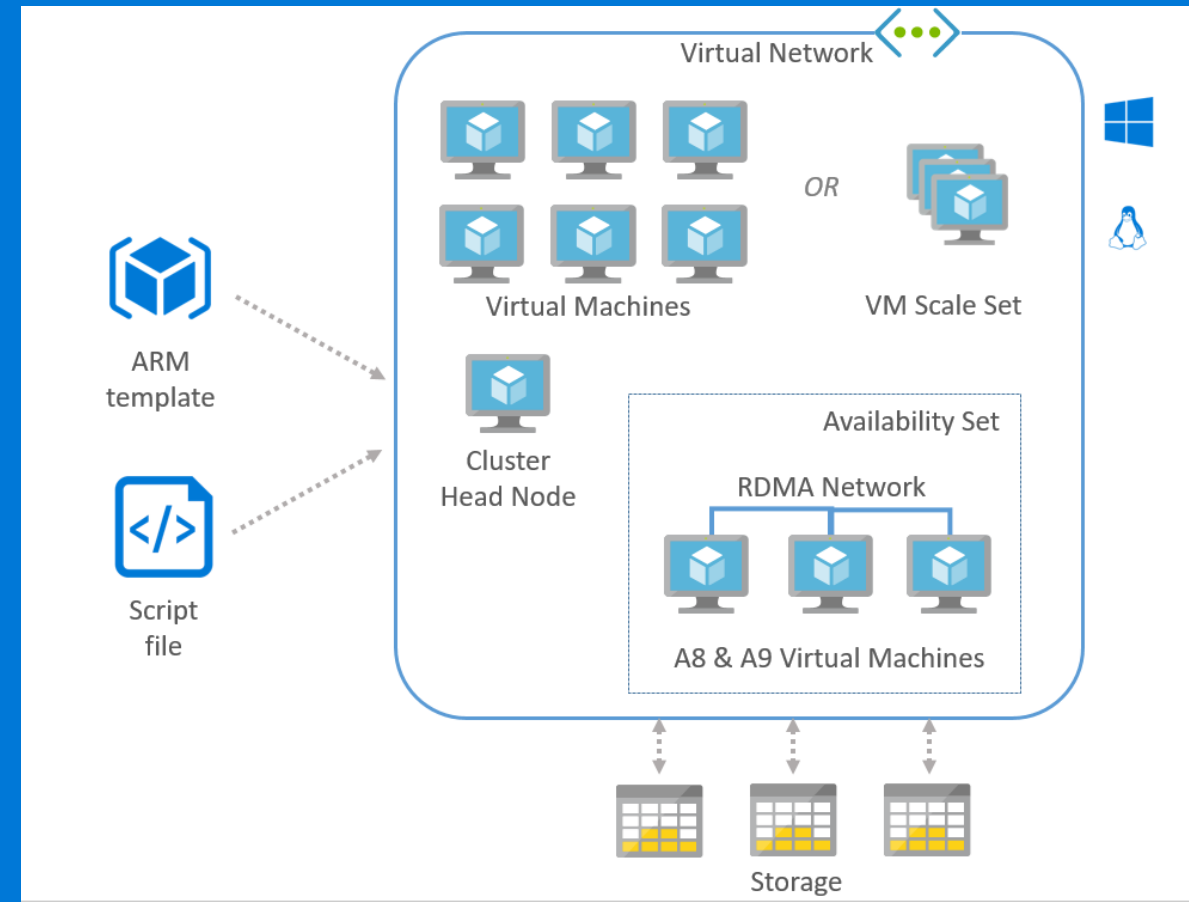
<https://azure.microsoft.com/en-us/marketplace/partners/intel/lustre-cloud-edition-evaleval-lustre-2-7/>

Password less SSH between the compute nodes

- Use the script from GitHub or write your own bash script
https://github.com/tanewill/utils/blob/master/user_authentication.sh

Vnet set up

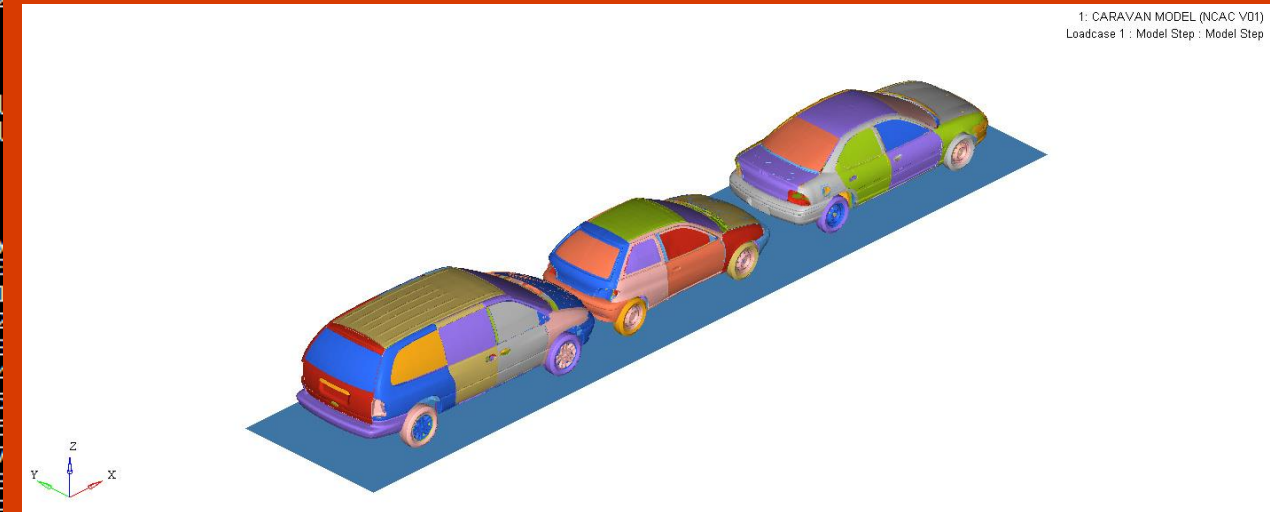
- Recommended set-up to controls IP range for connectivity to on-prem infrastructure



Demo: How to run HPC workloads in Azure?

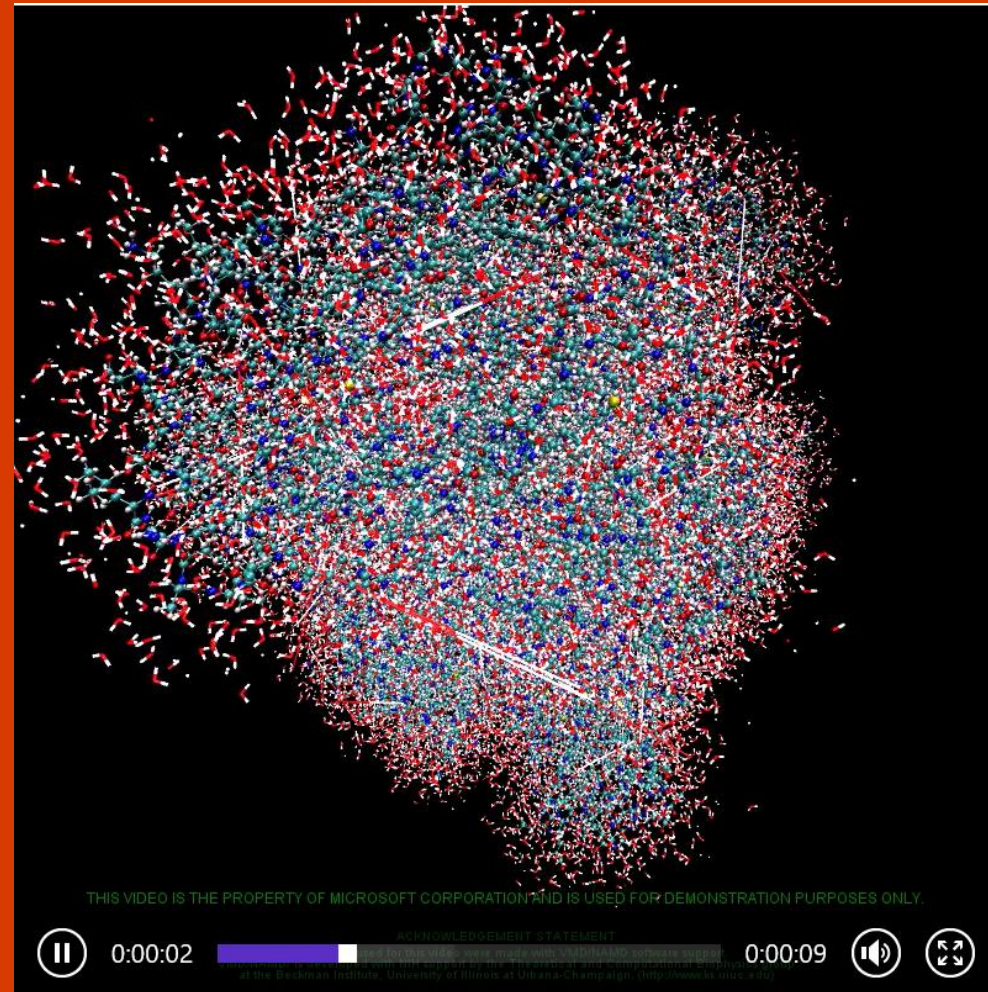
- Demo of how to run simulation applications on a VMs

```
cars 3cars.tar.gz car2car-ver10.tar Caravan2m-ver10 jama neon_refined_revised r
ejask@rdmafinal11:~/demo_models> cd neon_refined_revised/
ejask@rdmafinal11:~/demo_models/neon_refined_revised> ls
cars_shell2_150ms.k d3dump01.0010 d3hsp_32 disk8.0417 host1
dptmp d3dump01.0011 d3hsp_512 disk8.0418 host_12
g_switch d3dump01.0012 d3hsp_64 disk8.0419 host2
inout0000 d3dump01.0013 d3hsp_ff_test disk8.0420 host48
inout0001 d3dump01.0014 d3plot disk8.0421 host64
inout0002 d3dump01.0015 d3plot01 disk8.0422 hostfil
inout0003 d3dump01.0208 d3plot02 disk8.0423 host_pl
inout0004 d3dump01.0209 d3plot03 disk8.0424 hosts
inout0005 d3dump01.0210 d3thdt disk8.0425 hostt
inout0006 d3dump01.0211 disk8.0208 disk8.0426 input
inout0007 d3dump01.0212 disk8.0209 disk8.0427 kill_by
inout0008 d3dump01.0213 disk8.0210 disk8.0428 mes0000
inout0010 d3dump01.0214 disk8.0211 disk8.0429 mes0001
inout0014 d3dump01.0215 disk8.0212 disk8.0430 mes0002
inout0015 d3dump01.0216 disk8.0213 disk8.0431 mes0003
ore d3dump01.0217 disk8.0214 dyna_3car.sh mes0004
d3dump01.0000 d3dump01.0218 disk8.0215 dynademo.sh mes0005
d3dump01.0001 d3dump01.0219 disk8.0216 dynarun_48.sh mes0006
d3dump01.0002 d3dump01.0220 disk8.0217 dynarun_64.sh mes0007
d3dump01.0003 d3dump01.0221 disk8.0218 dynarun.sh mes0008
d3dump01.0004 d3dump01.0222 disk8.0219 dynarun_test2.sh mes0009
d3dump01.0005 d3dump01.0223 disk8.0220 dynarun_test.sh mes0010
d3dump01.0006 d3full01 disk8.0221 fort.13 mes0011
d3dump01.0007 d3hsp_128 disk8.0222 fort.59 mes0012
d3dump01.0008 d3hsp_16 disk8.0223 GBBP_Dyna_Testing-Cargo.k mes0013
d3dump01.0009 d3hsp_256 disk8.0416 glstat mes0014
ejask@rdmafinal11:~/demo_models/neon_refined_revised>
```



Demo: How to run HPC workloads in Azure?

- Molecular dynamics modeling application running on PaaS Windows HPC instances using HPC PACK and MS-MPI



Simulation and Analytics in Azure

"We have high-performance computing power with Azure that we can scale up only when we need it. Compared to building a \$200,000 infrastructure and keeping it running 24 hours a day, there's really no question."

—David Hood,
Engineer and Data Scientist,
Hendrick Motorsports



Simulation and Analytics in Azure

Business transformation in Motorsports

Challenge

- Make better decisions on car setup and race strategy through simulation and data analysis
- Desktop to garage to racetrack

Strategy

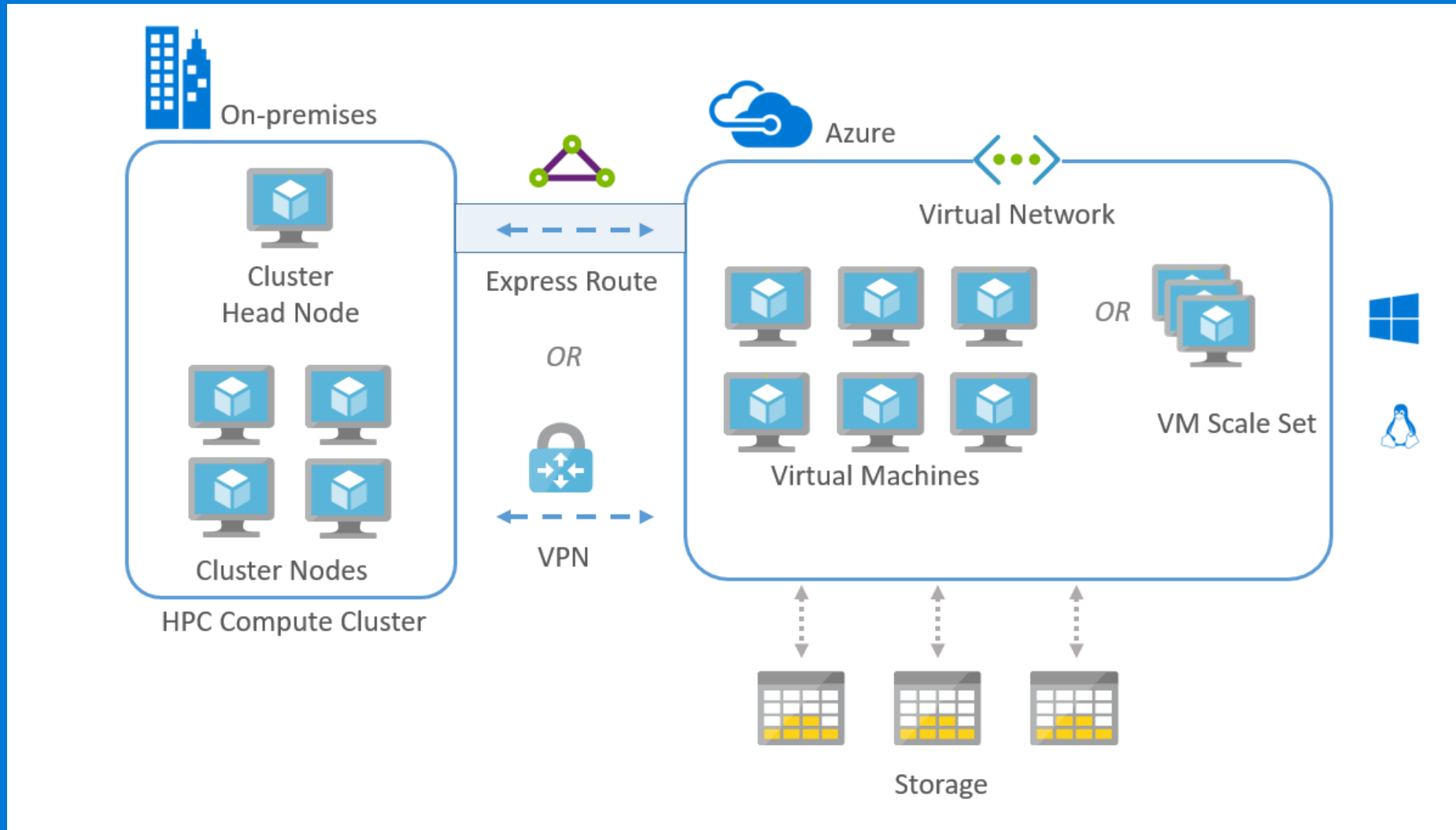
- CFD in Azure to model airflow
- Azure Machine Learning and Cortana Analytics for race strategy

Results

- CFD results in half the time
- Highly accurate models for fuel and tires
- Tools for the simulator at race day



How to run HPC in a burst scenario?



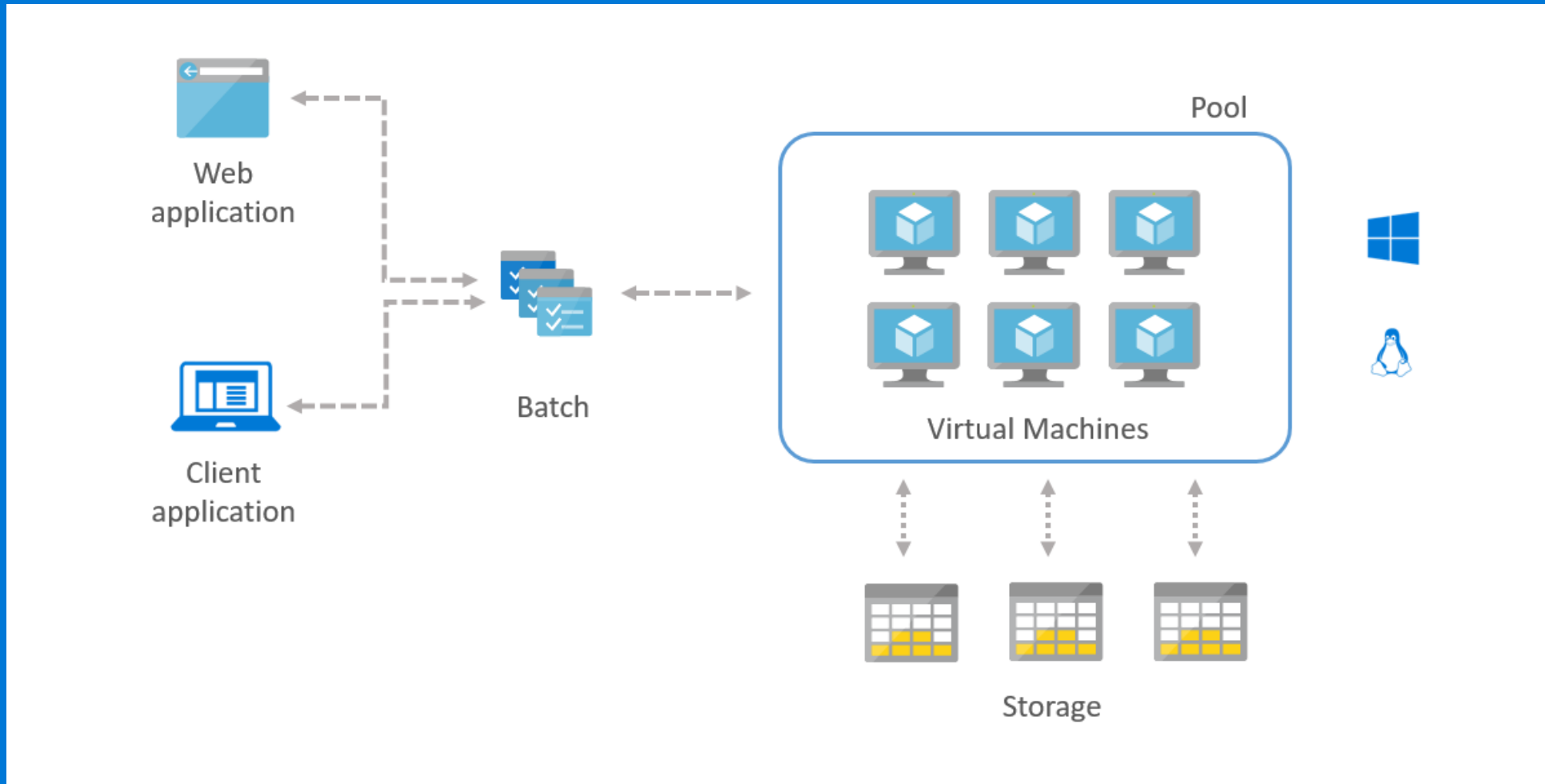
Demo: How to run a burst scenario?

- Demo of cloud burst environment with a third party scheduler/workload manager?
- Using Altair PBS-PRO/Compute Manager

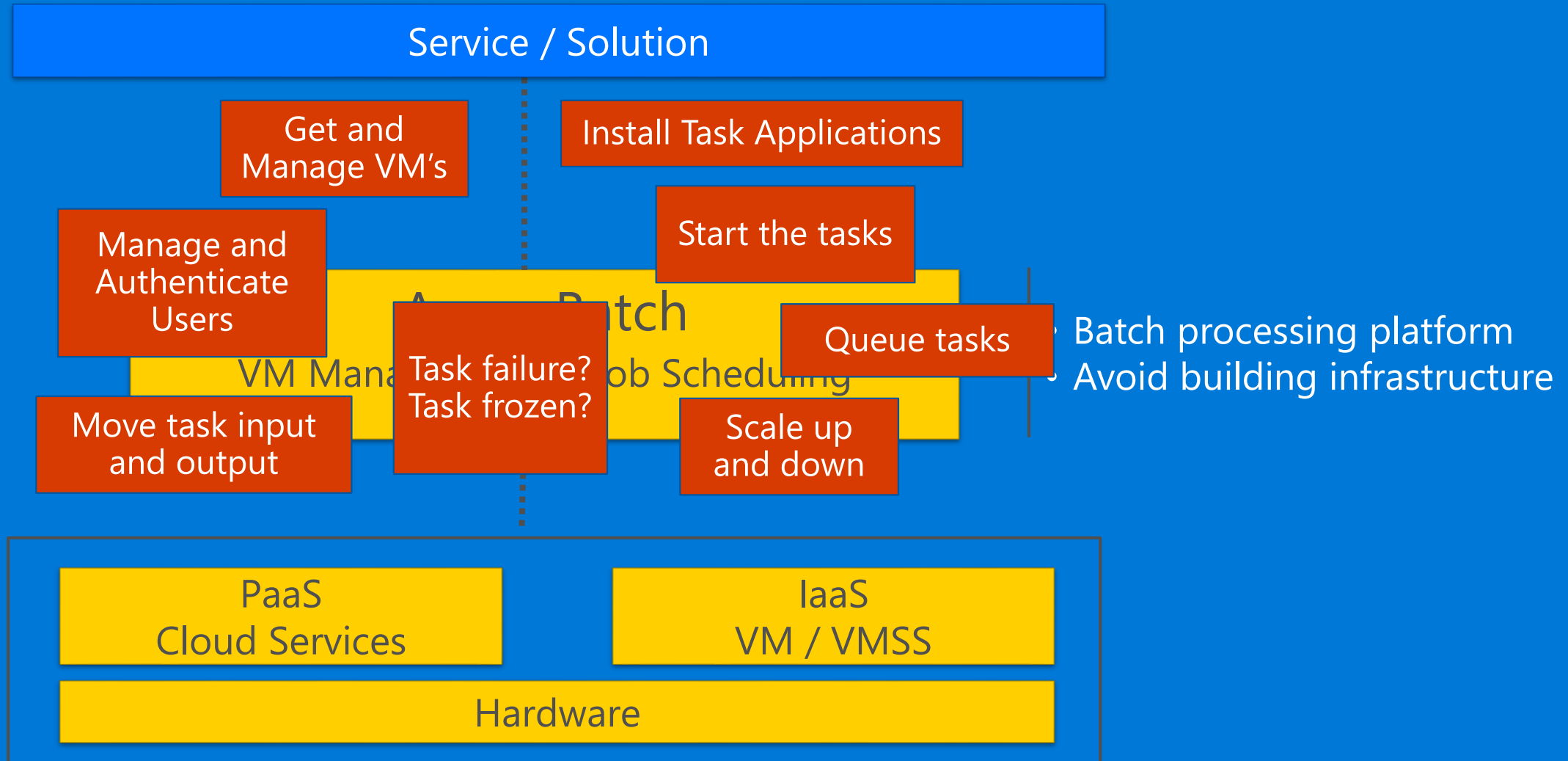


How to run HPC workloads in a SaaS scenario?

- Develop a simulation service on Azure infrastructure or Azure batch



Azure Batch and compute stack



Azure Batch

Cloud enable applications

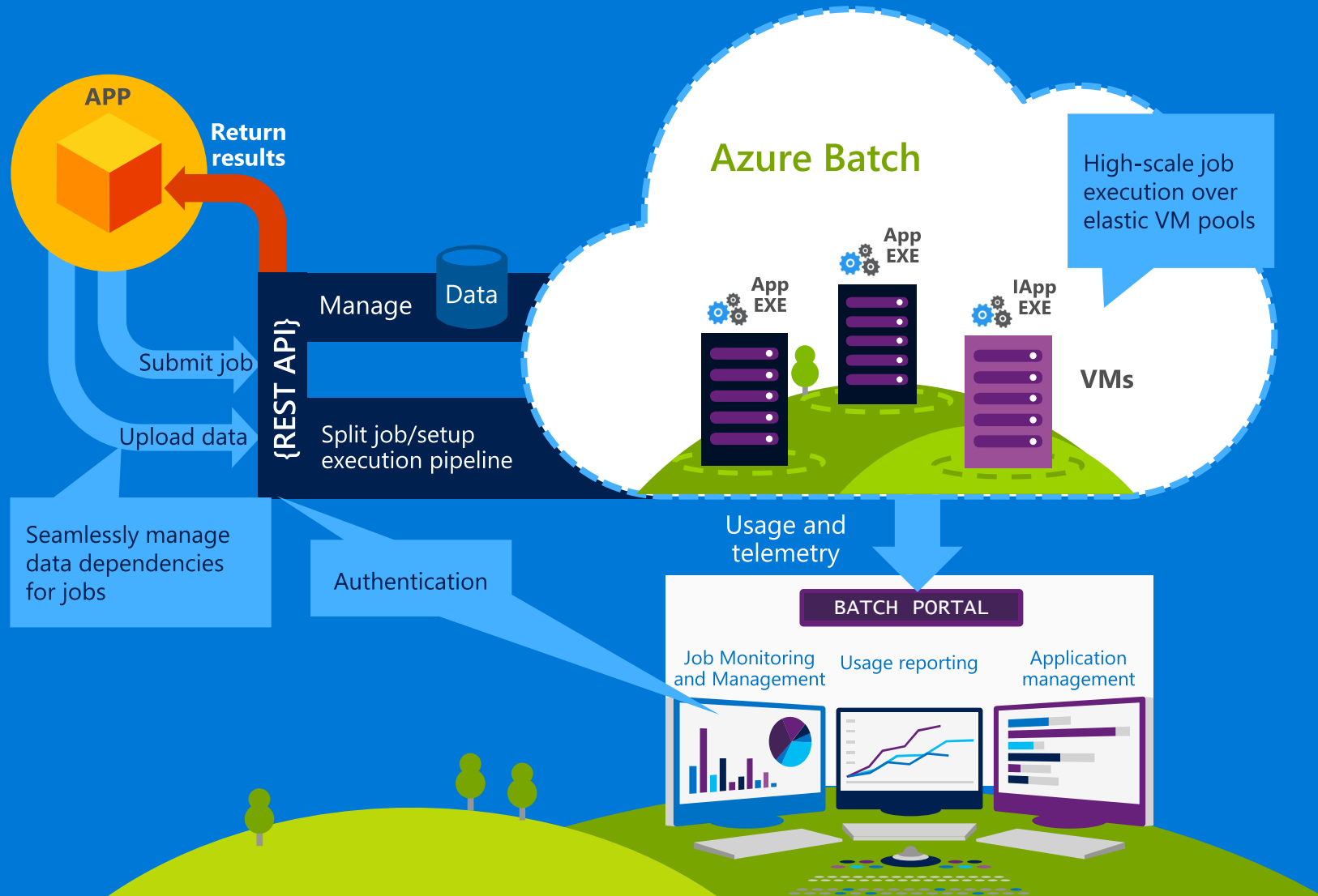
Run the applications you use on workstations and clusters today

Run at scale

Batch starts a pool of compute VMs when you're ready to run a job and turns them off when you're done

Manage delivery

Manage who can access it, how many resources they can use, and ensure requirements such as encryption are met



Demo: SaaS service built on Azure

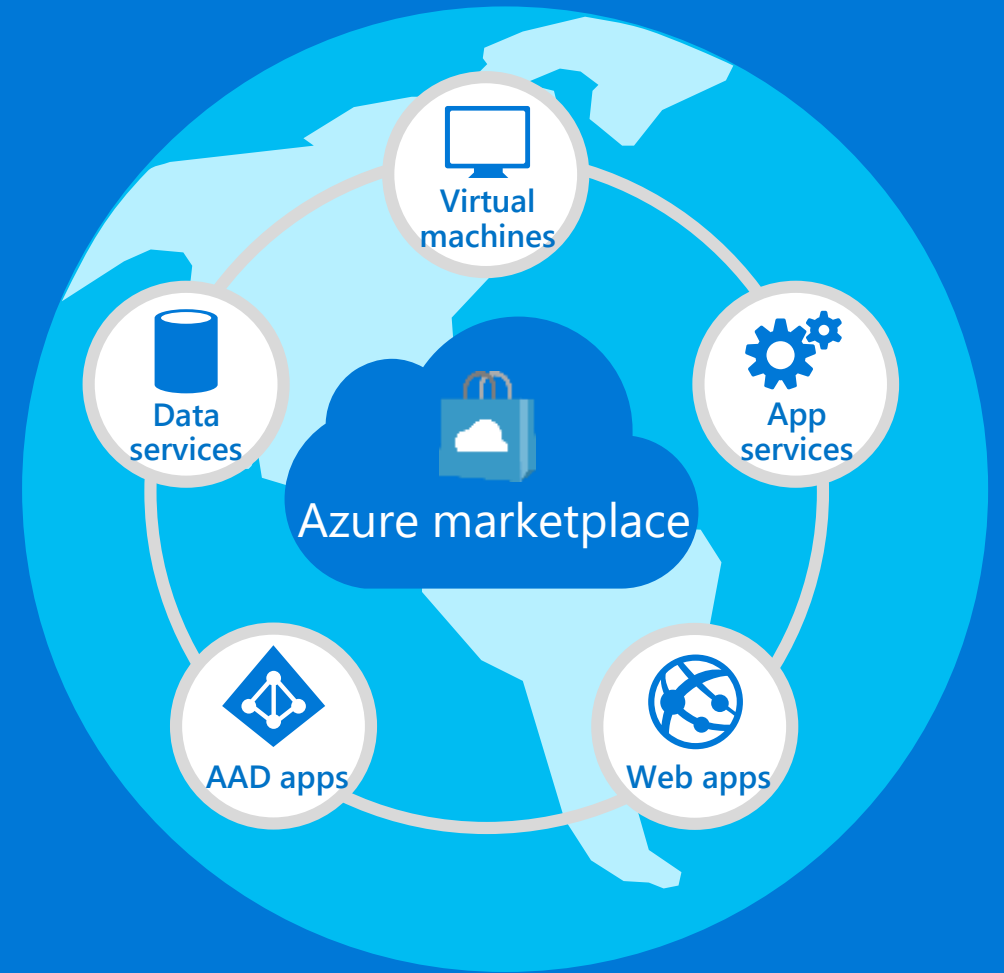
- Simulations in the cloud: SaaS service built on Azure
- Using d3VIEW service



HPC applications in the Azure marketplace

The Azure marketplace brings the quality, choice, and strength of the Azure partner ecosystem to customers around the world

- Simple deployment for pre-packaged solution
- A unified location for Azure based offerings from Microsoft and partners
- Thousands of offers
- Integrated platform experience Streamlined configuration, deployment, and management
- Fortune 500 and SMB customers across 86 global markets



Azure Marketplace Solution: UberCloud



OpenFOAM v2.3 on CentOS v6 MARKETPLACE

azure.microsoft.com/marketplace/partners/ubercloud/openfoam-v2dot3-centos-v6/

OpenFOAM v2



STAR-CCM+ v10 MARKETPLACE

azure.microsoft.com/marketplace/partners/ubercloud/star-ccm-v10-04/

STAR-CCM+ v10 integrated engineering simulation software on Microsoft Azure gives you the additional compute power you need to solve your complex simulations



STAR-CCM+ v10 with HEEDS MDO v2015 MARKETPLACE

azure.microsoft.com/marketplace/partners/ubercloud/star-ccm-v10-06-heeds-mdo-v2015/

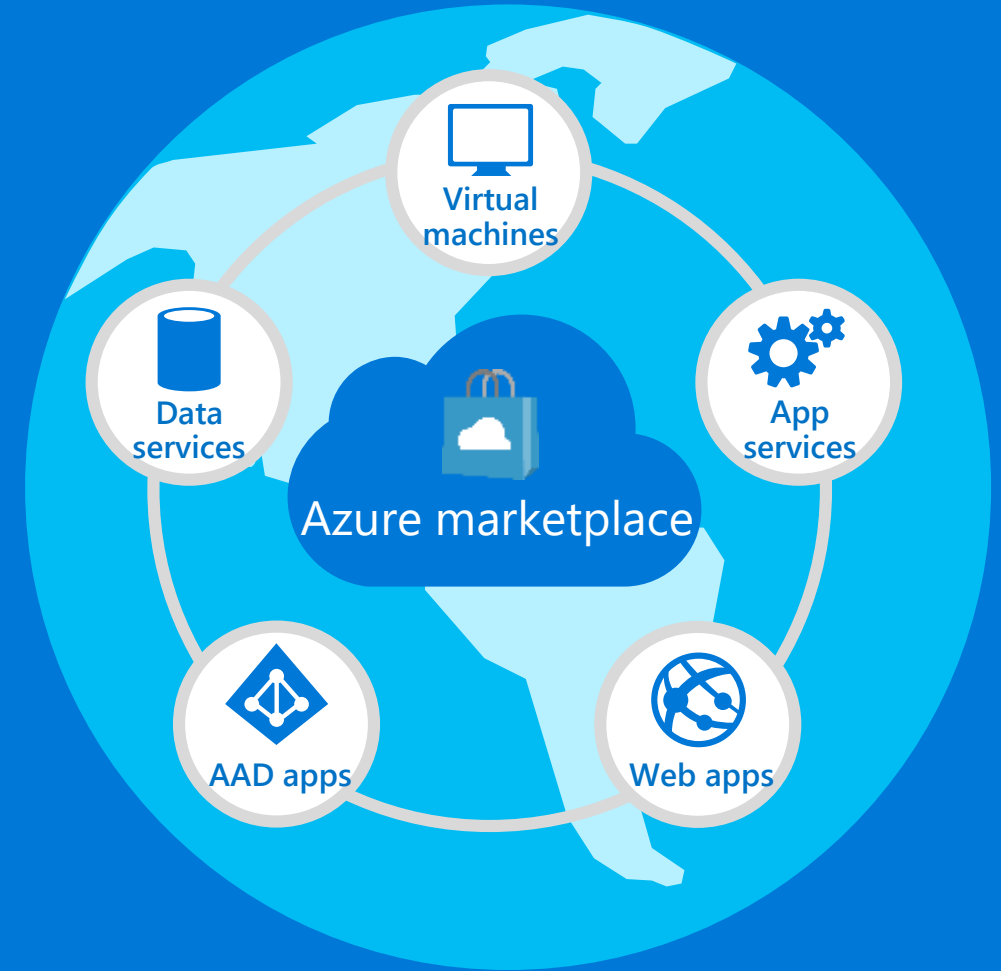
STAR-CCM+ v10 integrated engineering simulation software on Microsoft Azure gives you the additional compute power you need to solve your complex simulations



COMSOL Multiphysics v5.2 MARKETPLACE

azure.microsoft.com/marketplace/partners/ubercloud/comsol-multiphysics-v5-2/

COMSOL Multiphysics® cross-disciplinary product development suite on Microsoft Azure gives you the additional compute power you need to solve your complex simulations





Expanding customers' computational horizons

"We envision a future where game-changing innovations in advanced industries and scientific disciplines can come from anywhere, not just the major research institutions and large corporations with HPC resources of their own. UberCloud, Microsoft Azure, and Intel have leveled CFD's playing field, so anyone with an interest and a problem to solve can work on it."

Luboš Pírk, Co-founder & Managing Director, CFD support Ltd.



Conclusion

Multiple options available to run your HPC applications in Azure

On VMs DIY

Customers setting up separate cloud environment for additional capacity and new workloads

Burst

Burst to cloud for more capacity
Utilize existing scheduler to burst to Azure and use compute on demand

SaaS

ISV's and Managed service providers launch their own SaaS solutions. Pay for compute and application software per hour

Marketplace

Utilize the scale of Azure Applications and compute capacity sold through Azure marketplace

Visit us at

<http://simulation.azure.com>

Free IT Pro resources

To advance your career in cloud technology

Plan your
career path

Microsoft IT Pro Career Center
www.microsoft.com/itprocareercenter

Get started
with Azure

Microsoft IT Pro Cloud Essentials
www.microsoft.com/itprocloudessentials

Demos and
how-to videos

Microsoft Mechanics
www.microsoft.com/mechanics

Connect with peers
and experts

Microsoft Tech Community
<https://techcommunity.microsoft.com>

Free IT Pro resources

To advance your career in cloud technology

Plan your
career path

IT Pro Career Center

<http://www.microsoft.com/itprocareercenter>

Get started
with Azure

IT Pro Cloud Essentials

<https://www.microsoft.com/itprocloudessentials>

Demos and
how-to videos

Microsoft Mechanics

<https://www.microsoft.com/mechanics>

Connect with
peers and experts

Ask questions, get answers, exchange ideas

<https://techcommunity.microsoft.com>

Azure Solutions

Get started with Azure Solutions today

<http://azure.com/solutions>

Azure monthly
webinar series

Join live or watch on-demand

<http://aka.ms/AzureMonthlyWebinar>

Please evaluate this session
Your feedback is important to us!



From your PC or Tablet visit MyIgnite at
<http://myignite.microsoft.com>

From your phone download and use the Ignite
Mobile App by scanning the QR code above or
visiting <https://aka.ms/ignite.mobileapp>

