Microsoft

Best Practices for Running HPC Applications on Microsoft Azure using MVAPICH2

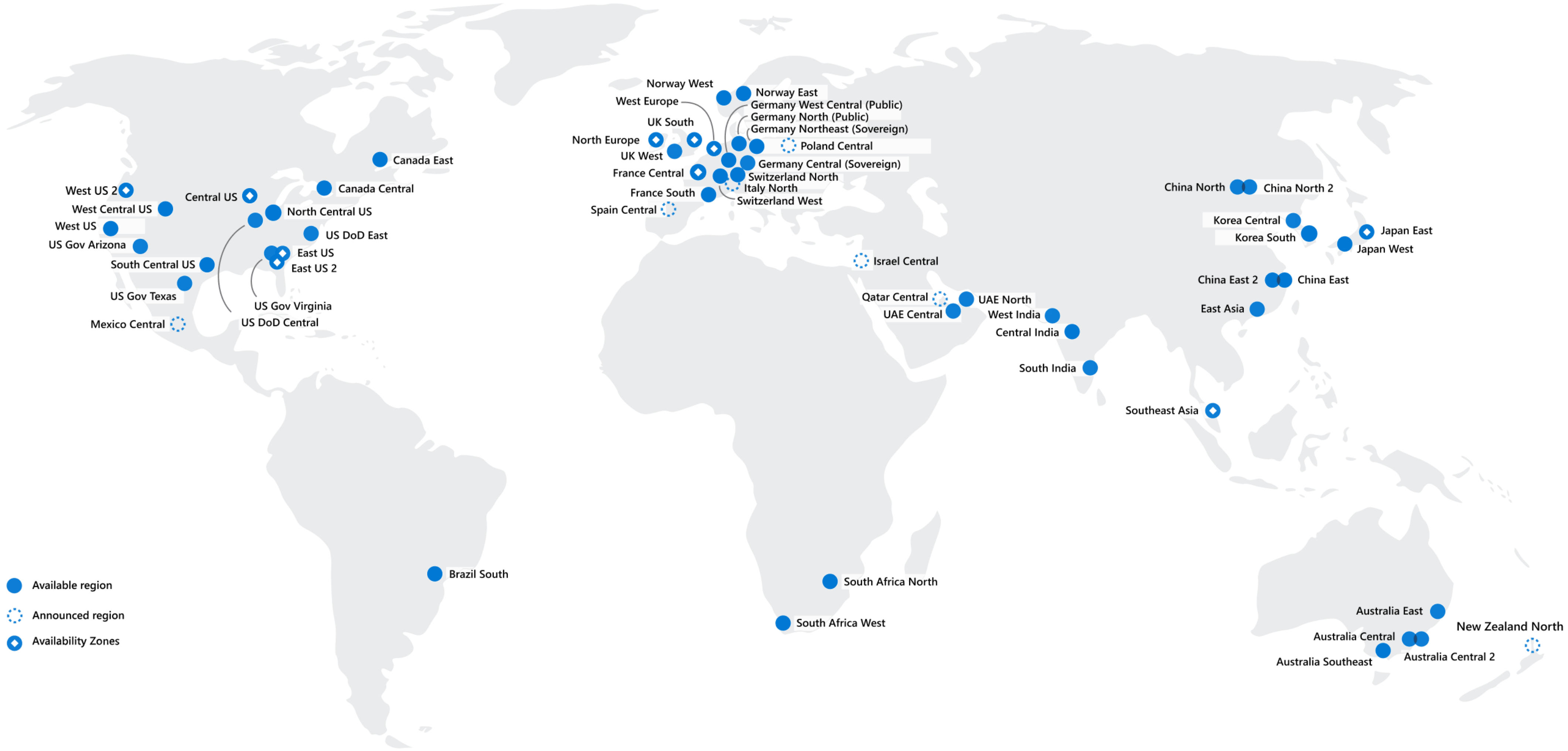
Jithin Jose, Jon Shelley
Azure HPC Team

MVAPICH User Group Meeting 2020

Agenda

- ✓ Overview of Microsoft Azure
- ✓ Azure HPC Offerings
- ✓ HPC Software Ecosystem
- ✓ HPC Deployment Models and Demo
- ✓ Performance Characteristics
- ✓ Best Practice Recommendations

Microsoft Azure



- ✓ **Cost**
- ✓ **Global Scale**
- ✓ **Performance**
- ✓ **Security**
- ✓ **Speed**
- ✓ **Productivity**
- ✓ **Reliability**

HPC Fleet in Azure

H-Series (InfiniBand)

- H16r (FDR)
- HB60rs (EDR)
- HC44rs (EDR)
- **HB120rs_v2** (HDR)

N-Series (NVIDIA GPU + InfiniBand)*

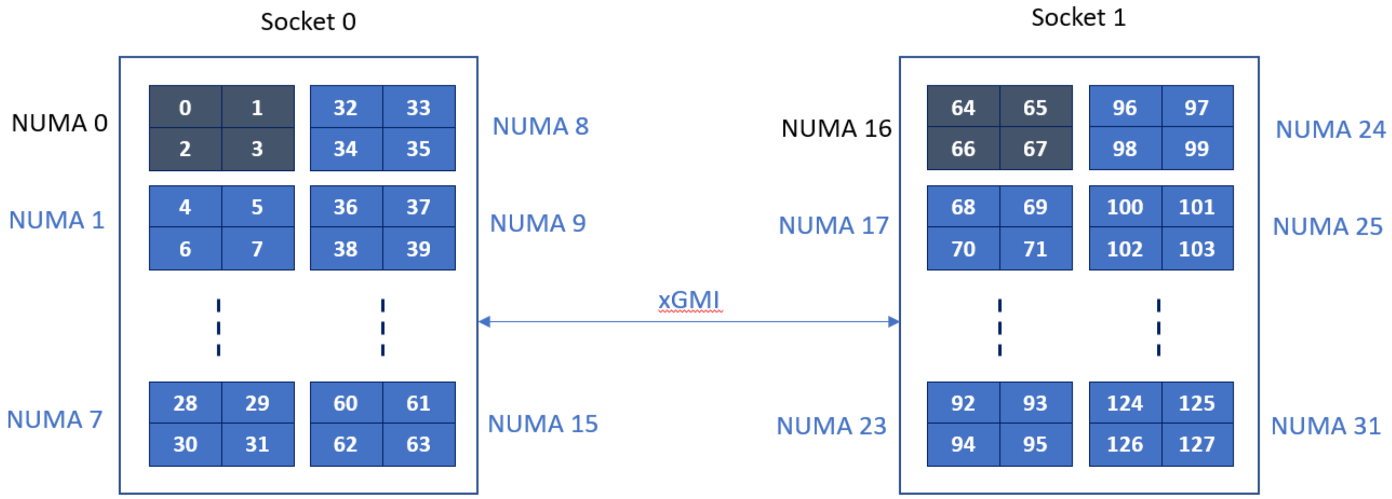
- NC24r (2 x NVIDIA K80 + FDR)
- NC24rs_v2 (4 x NVIDIA P100 + FDR)
- NC24rs_v3 (4 x NVIDIA V100 + FDR)
- ND24rs (4 x NVIDIA P40 + FDR)
- **ND40rs_v2** (8 x NVIDIA V100, EDR)

- SKU Name indicates core count
- "r" indicates RDMA support
- "s" indicates Premium Storage support

*GPU-only sizes not listed

HB120rs_v2 VM Instances

- AMD Rome
- VM Cores: 120
- Clock Speed: 3.3 GHz
- Memory Bandwidth: 340 GB/sec
- Memory: 480 GB (4GB/core)
- Local Disk: 900 GB NVMe
- NVIDIA Mellanox InfiniBand Network: 200 Gbps HDR (SR-IOV)



Socket 0

NUMA 0: 0 1 2 3

NUMA 8: 32 33 34 35

NUMA 1: 4 5 6 7

NUMA 9: 36 37 38 39

NUMA 7: 28 29 30 31

NUMA 15: 60 61 62 63

xGMI

Socket 1

NUMA 16: 64 65 66 67

NUMA 24: 96 97 98 99

NUMA 17: 68 69 70 71

NUMA 25: 100 101 102 103

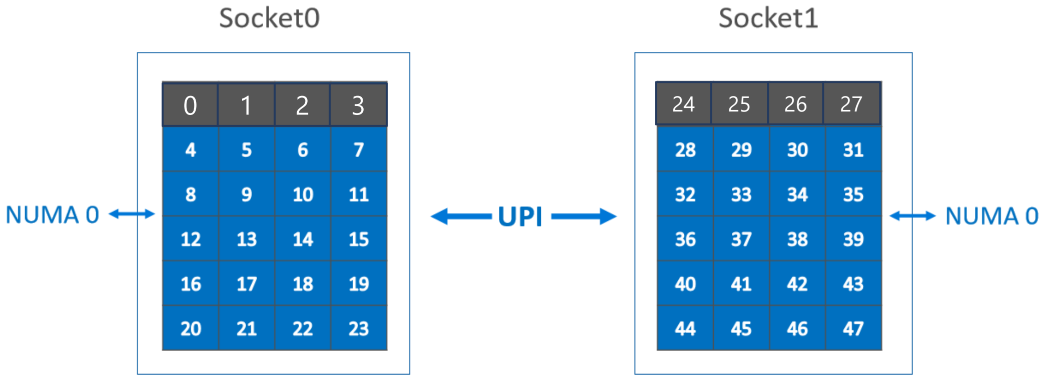
NUMA 23: 92 93 94 95

NUMA 31: 124 125 126 127

Hypervisor Reserved Cores:
0-3, 64-67

VM Cores:
4-63, 68-127

ND40rs_v2 VM Instances



0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15
16	17	18	19
20	21	22	23

24	25	26	27
28	29	30	31
32	33	34	35
36	37	38	39
40	41	42	43
44	45	46	47

**Hypervisor Reserved Cores:
0-3, 24-27**

**VM Cores:
4-23, 28-47**

- Intel Skylake
- VM Cores: 40
- Memory: 672 GB
- NVIDIA Mellanox InfiniBand Network: 100 Gbps EDR (SR-IOV)
- 8 x NVIDIA V100 NVIDIA NVLINK connected GPUs
  - 32 GB GPU memory per GPU

Network Features

- **HB, HC, NDv2:** ConnectX·5
  - EDR 100Gb/s NVIDIA Mellanox InfiniBand
  - Up to 200M messages/second

- **HBv2:** ConnectX·6
  - HDR 200Gb/s NVIDIA Mellanox InfiniBand
  - Up to 215M messages/second

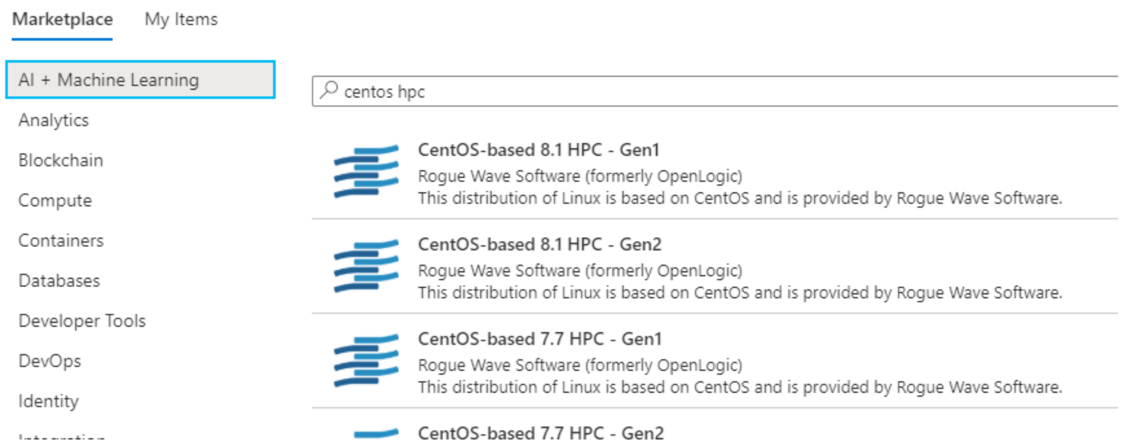
- Dynamically Connected Transport (DCT)
  - Reliable and scalable transport
  - Lesser Memory footprint
- Hardware collectives (hcoll)
  - Collectives offload framework
  - Asynchronous execution
  - Supports blocking/non-blocking collectives
- UD multicast (MCAST)
  - Unreliable datagram (UD) based multicast
  - Create a mcast group and broadcast
- Hardware Tag Matching
- Reliability/Congestion Control
  - SHIELD, Adaptive Routing

Outline

- ✓ Overview of Microsoft Azure
- ✓ Azure HPC Offerings
- ✓ **HPC Software Ecosystem**
- ✓ HPC Deployment Models and Demo
- ✓ Performance Characteristics
- ✓ Best Practice Recommendations

HPC Software Ecosystem

- Out-of-the Box CentOS-HPC VM Images
  - NVIDIA Mellanox OFED
  - MPI Libraries
    - Includes **MVAPICH2, MVAPICH2X-Azure**
  - HPC Libraries
  - Optimization Configurations
  - All recipes in GitHub repository
    - https://github.com/Azure/azhpc-images/



centos hpc

CentOS-based 8.1 HPC - Gen1
Rogue Wave Software (formerly OpenLogic)
This distribution of Linux is based on CentOS and is provided by Rogue Wave Software.

CentOS-based 8.1 HPC - Gen2
Rogue Wave Software (formerly OpenLogic)
This distribution of Linux is based on CentOS and is provided by Rogue Wave Software.

CentOS-based 7.7 HPC - Gen1
Rogue Wave Software (formerly OpenLogic)
This distribution of Linux is based on CentOS and is provided by Rogue Wave Software.

CentOS-based 7.7 HPC - Gen2

- Or, BYO Software Stack
  - Any Linux/Windows OS flavor
  - Build/Configure custom HPC Software stack
  - Prepare custom image

MVAPICH2-X Azure

- Available in all Azure CentOS-HPC images

- Feature Highlights:
  - Enhanced tuning for point-to-point and collectives
  - XPMEM Support
  - DC Support
  - Cooperative Protocol
  - Hybrid RC/UD Support

Outline

- ✓ Overview of Microsoft Azure
- ✓ Azure HPC Offerings
- ✓ HPC Software Ecosystem
- ✓ **HPC Deployment Models and Demo**
- ✓ Performance Characteristics
- ✓ Best Practice Recommendations

Prerequisites:

- Azure Account
- Azure Subscription
- Sufficient Quota
  - # Cores
  - Specific to Region/ SKU Type

Deployment Options:

- AzureHPC Scripts
  - Deployment Scripts tailored for HPC needs
- CycleCloud
  - HPC Workload manager
- Azure Batch
  - Cloud scale job scheduling and Compute Management
- ARM Templates
  - Azure Resource Manager Templates

Setting up Azure HPC Scripts

- Prerequisites for AzureHPC
  - Azure CLI
    - https://docs.microsoft.com/cli/azure/install-azure-cli
  - Other utilities: bash, jq and ssh

- Can be invoked from:
  - Azure Cloud Shell
  - Linux VM
  - Windows Ubuntu Shell

- Detailed instructions:
  - https://github.com/Azure/azurehpc/blob/master/README.md

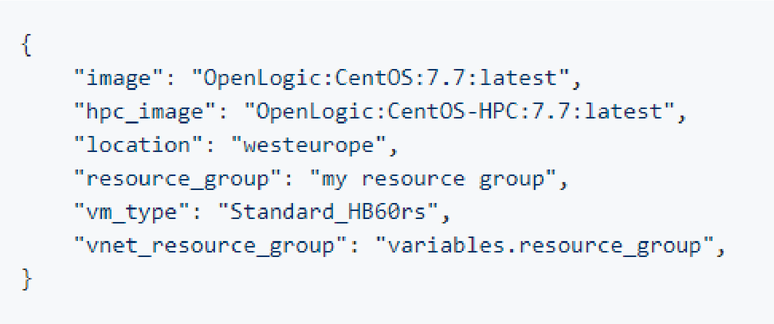
AzureHPC for Deployment

- Install AzureHPC

```
source ~/azurehpc/install.sh
```

- Initialize/Configure Cluster

```
 azhpc-init -c $azhpc_dir/examples/simple_hpc_pbs -d hbv2_cluster
# Update config.json
#   Select SKU type, instance count, region, etc.
```



```
{
    "image": "OpenLogic:CentOS:7.7:latest",
    "hpc_image": "OpenLogic:CentOS-HPC:7.7:latest",
    "location": "westeurope",
    "resource_group": "my resource group",
    "vm_type": "Standard_HB60rs",
    "vnet_resource_group": "variables.resource_group",
}
```

- Deploy Cluster

```
azhpc-build
```

- Connect to your Azure Cluster

```
azhpc-connect -u hpcadmin headnode
```

Demo: Deploy an HPC Cluster on Azure

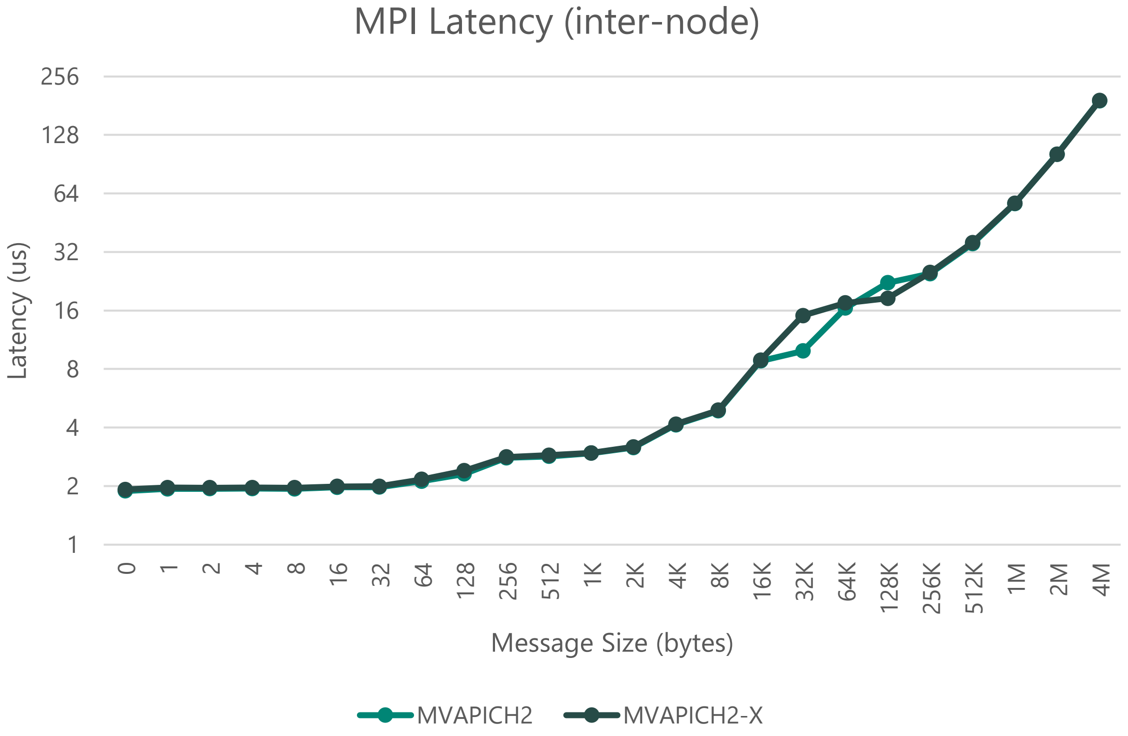
Outline

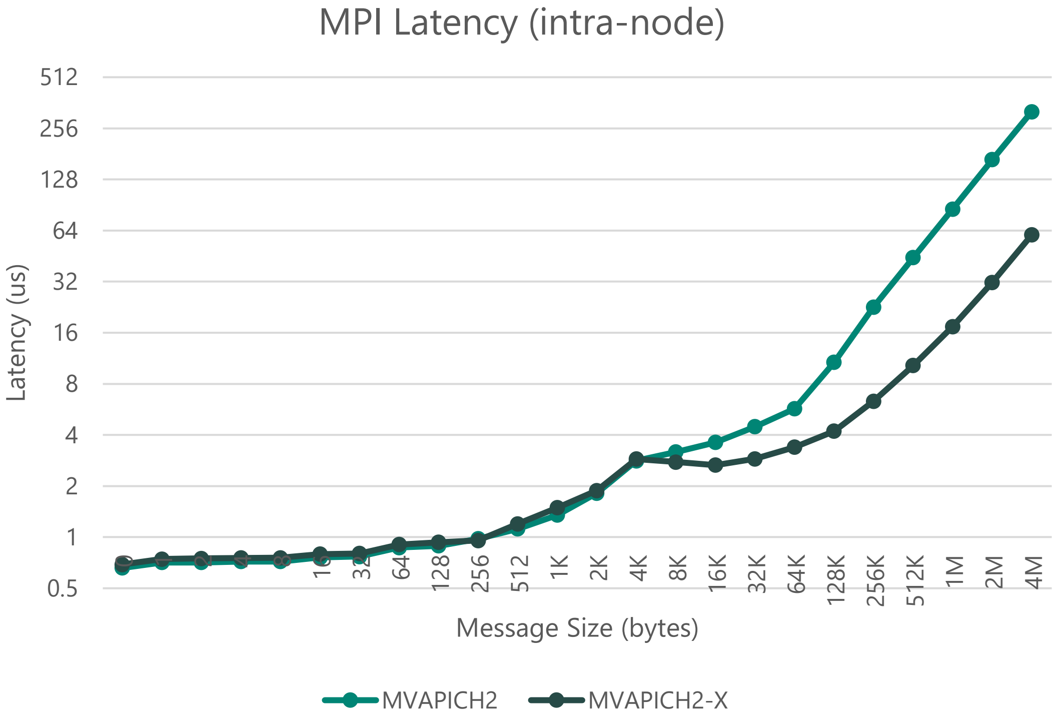
- ✓ Overview of Microsoft Azure
- ✓ Azure HPC Offerings
- ✓ HPC Software Ecosystem
- ✓ HPC Deployment Models and Demo
- ✓ **Performance Characteristics**
- ✓ Best Practice Recommendations

Experiment Setup

- HBv2 VM Instances
- CentOS 7.7 HPC Image
- MPI Libraries
  - MVAPICH2 2.3.4
  - MVAPICH2-X 2.3
- NVIDIA Mellanox OFED 5.1

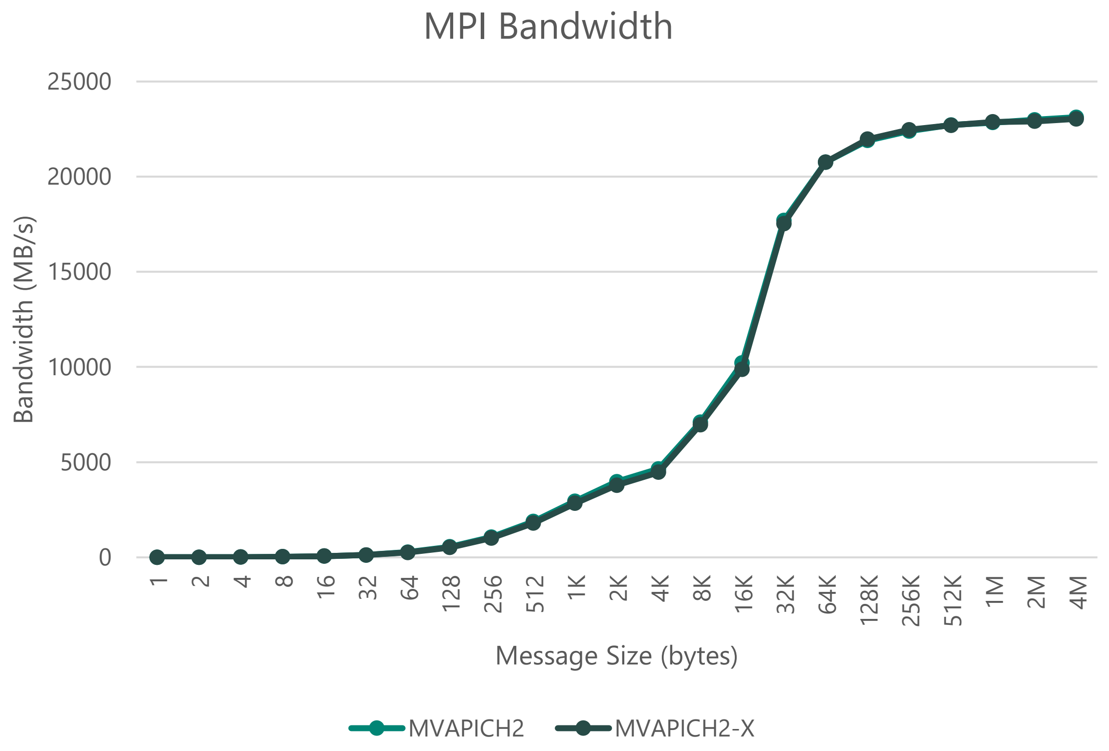
MPI Latency

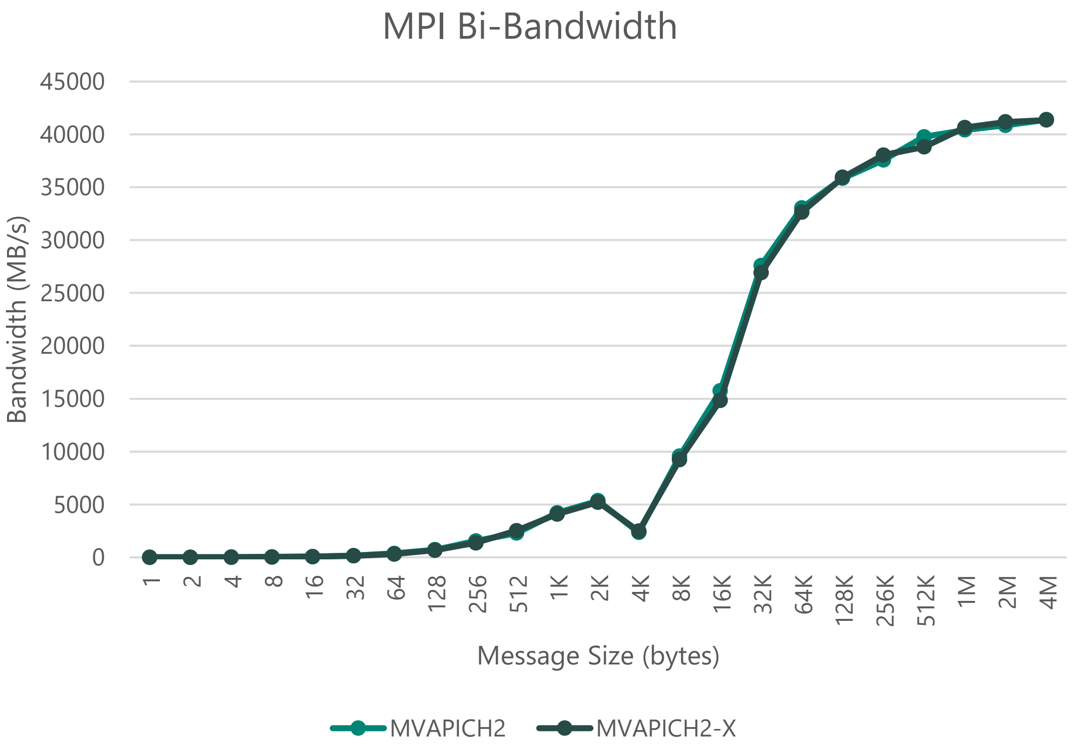




- MVAPICH2, MVAPICH2-X achieves < 2us latencies
- MVAPICH2-X offers better large message latencies for intra-node transfers (XPMEM)

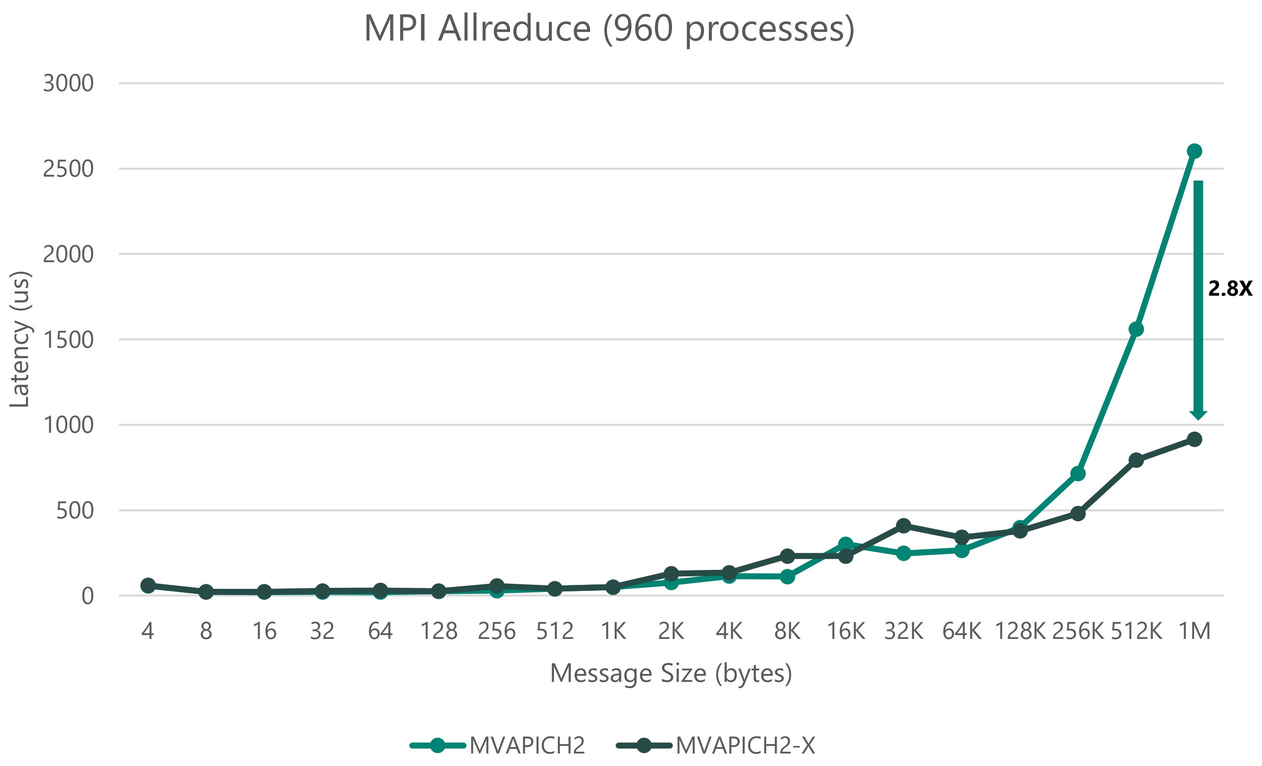
MPI Bandwidth / Bi-Bandwidth





- MVAPICH2, MVAPICH2-X close to line rates
- Both uses same inter-node protocols
- RPUT Rendezvous protocol (`MV2_RNDV_PROTOCOL=RPUT`)

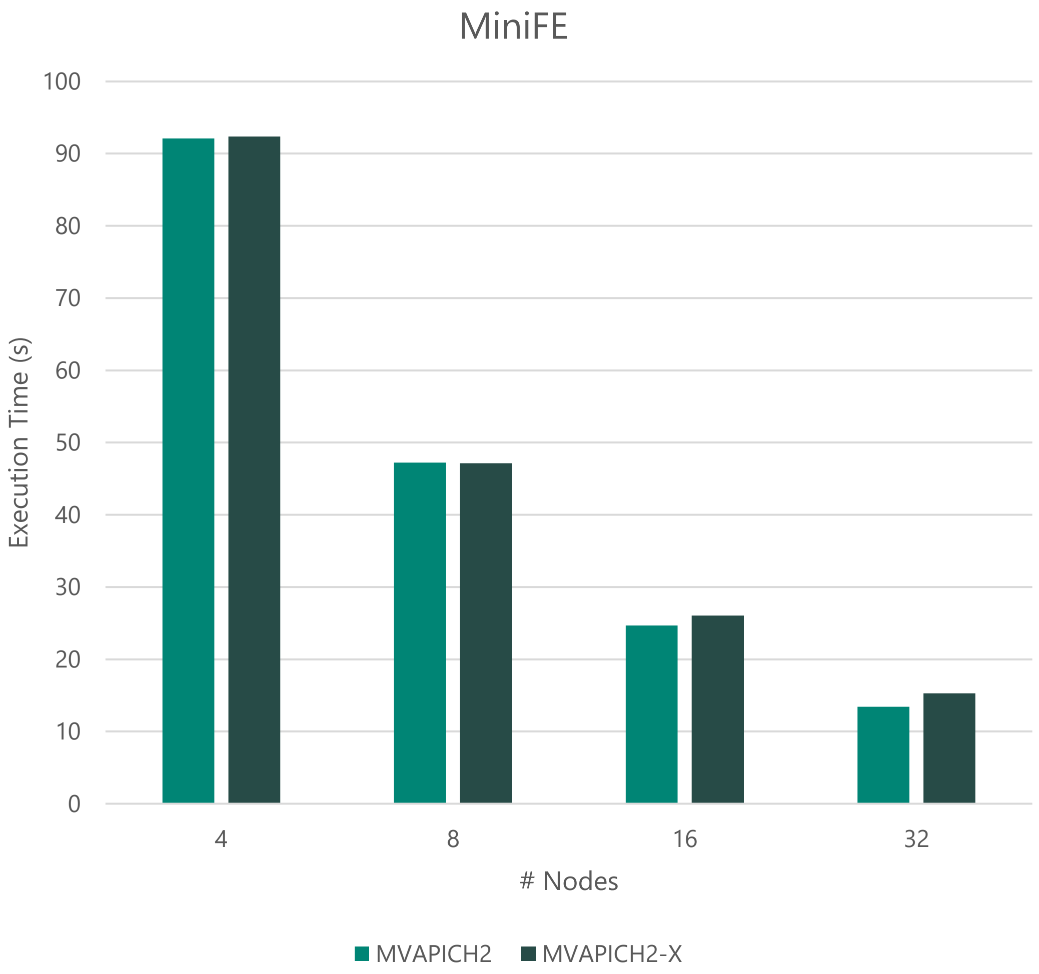
MPI Allreduce



- MVAPICH2-X XPMEM Collectives offers better large message allreduce latencies
- 16 HBv2 nodes, 120 PPN

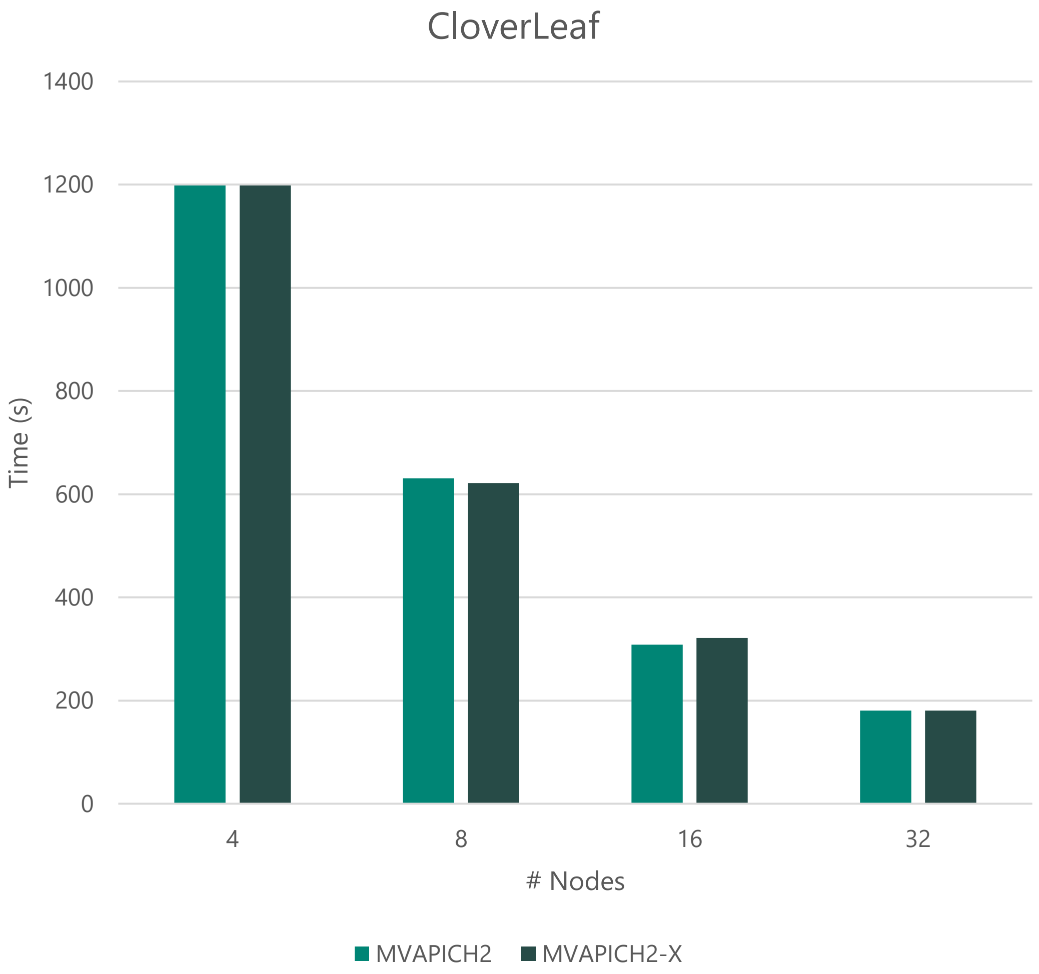
MiniFE

- Finite Element Mini-Application
- Proxy application for unstructured implicit FE codes
- Strong scaling experiment
- Version: openmp-opt
- Problem Size
  - nx=1024, ny=1024, nz=1024



CloverLeaf

- Hydrodynamics mini0app to solve compressible Euler equations in 2D
- Version: CloverLeaf_MPI
- DataSet: clover_bm256.in
  - x_cells: 15360, y_cells: 15360
  - Steps: 2955



Outline

- ✓ Overview of Microsoft Azure
- ✓ Azure HPC Offerings
- ✓ What’s unique
- ✓ HPC Software Ecosystem
- ✓ HPC Deployment Models and Demo
- ✓ Performance Characteristics
- ✓ **Best Practice Recommendations**

Prerequisite for InfiniBand support

- If using VMs:
  - Use single Availability Set for all VMs
    - Logical Grouping of Virtual Machines
  - All VMs in Availability Set will have same PKEY (InfiniBand partition key)

- If using Virtual Machine Scale Set (VMSS):
  - All VMs in VMSS will have same PKEY
  - VMSS:
    - Set of VM instances
    - Supports flexible scale up/scale down

- Check PKEY

```
$ cat /sys/class/infiniband/mlx5_0/ports/1/pkeys/0
$ 0x801d
```

Best Practices: Guest Agent Configuration

- Minimal Guest Agent Configuration
  - `"Extensions.GoalStatePeriod": 300`
  - `"OS.EnableFirewallPeriod": 300`
  - `"OS.RemovePersistentNetRulesPeriod": 300`
  - `"OS.RootDeviceScsiTimeoutPeriod": 300`
  - `"OS.MonitorDhcpClientRestartPeriod": 60`
  - `"Provisioning.MonitorHostNamePeriod": 60`

- For extremely sensitive workloads:
  - eg:

```
sudo systemctl disable waagent
<run hpc job>
sudo systemctl enable waagent
```

Best Practices: Large Scale Jobs

- Use Scalable Transports
  - **Dynamic Connected Transport (DCT)**
    - Highly scalable, and supports all features of RC
    - Lesser memory footprint
    - `Eg: MV2_USE_DC=1`
  - **Hybrid RC/UD Transports**
    - RC for frequently communicating pairs
    - Lesser memory footprint, Avoids QP Thrashing
    - `Eg: MV2_USE_UD_HYBRID`
- Enable Adaptive Routing (AR)
  - AR is enabled in all non-zero Service Levels (SL)
  - To make use of AR, specify SL during job launch
    - `Eg: MV2_DEFAULT_SL=1`

Best Practices: NUMA Awareness

- NUMA Affinity
  - SKU/Workload Specific
  - Bind to NUMA node closer to NIC
  - `Eg: MV2_CPU_MAPPING=X`

- NUMA Binding
  - Workload specific (`MV2_CPU_BINDING=numanode`)

- NUMA Aware Collectives
  - NUMA Hierarchy

Best Practices: MVAPICH2 Protocols/Thresholds

- Internode:
  - RPUT protocol for Rndv Transfers
    - `MV2_RNDV_PROTOCOL=RPUT`

- Intra-node
  - Enable XPMEM (MVAPICH2-X)
    - `MV2_SMP_USE_XPMEM=1`
  - Enable XPMEM for Collectives
    - `MV2_SMP_USE_XPMEM=1  MV2_USE_XPMEM_COLL=1`

Pointers

- AzureHPC Deployment Scripts
  - https://github.com/Azure/azurehpc

- Azure HPC/GPU VM Sizes
  - https://docs.microsoft.com/azure/virtual-machines/sizes-hpc
  - https://docs.microsoft.com/azure/virtual-machines/sizes-gpu

- HPC Marketplace Images
  - https://techcommunity.microsoft.com/t5/azure-compute/azure-hpc-vm-images/ba-p/977094

- MVAPICH2 on Azure
  - https://techcommunity.microsoft.com/t5/azure-compute/mvapich2-on-azure-hpc-clusters/ba-p/1404305

- Adaptive Routing on Azure HPC
  - https://techcommunity.microsoft.com/t5/azure-compute/adaptive-routing-on-azure-hpc/ba-p/1205217

Thank You!

jijos@microsoft.com, joshelle@microsoft.com
Microsoft