

HPC Software Environment in ASPIRE 2A

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About Myself

■ Work in NSCC

- HPC application benchmarking and performance evaluation.
- HPC software support.
- ASPIRE 2A system HPC software build and installation.

■ Research Interest

- Parallel algorithms for multi-core CPU and GPU.
- Cache performance optimization.
- Adaptive scheduling algorithms.

ASPIRE 2A HPC Software Environment

System	Development	Library	Profiling & Debugging	Application
Workload Manager Altair PBS Pro	Cray Programming Environment AMD AOCC GNU GCC HPE CCE Intel oneAPI NVHPC	MPI Libraries Cray MPICH OpenMPI Scientific Libraries AMD AOCL BLIS Cray LibSci FFTW GSL Intel MKL PETSc I/O Libraries HDF5 NetCDF	ARM Forge Cray Stat gdb4hpc Perftools Valgrind4hpc	AI Tensorflow PyTorch Simulation BerkeleyGW GROMACS LAMMPS Mumax3 OpenFOAM Nek5000 Quantum ESPRESSO Nektar++ WRF
Remote Visualization Altair Access	Programming Nvidia CUDA Go Python Java Julia Octave R		Bio Tools ABYSS BEAST bedtools BWA bowtie2 GATK BLAST+ SAMtools	Applications and Tools Anaconda3 FCM GNU Parallel FFmpeg MRtrix3 NCL RELION Ncview Tmod Velvet
Container Singularity *Kubernetes with Docker			Workflow Cylc Rose Nextflow	
Parallel File System GPFS Lustre				
Operating System Red Hat Enterprise Linux 8				

Cray Programming Environment (CPE)

Choice of toolchains

- PrgEnv-aocc
- PrgEnv-cray
- PrgEnv-gnu
- PrgEnv-intel
- PrgEnv-nvhpc

```
$ module list
Currently Loaded Modulefiles:
  1) craype-x86-rome          5) cce/13.0.2                9) cray-pals/1.1.6
  2) libfabric/1.11.0.4.125  6) craype/2.7.15            10) PrgEnv-cray/8.3.3
  3) craype-network-ofi     7) cray-dsmml/0.2.2
  4) perftools-base/22.04.0  8) cray-mpich/8.1.15
$ cc main.c
$ cc --version
Cray clang version 13.0.2 (a5f4c8bb61d2be51079c8815e5195c7827c51639)
Target: x86_64-unknown-linux-gnu
Thread model: posix
InstalledDir: /opt/cray/pe/cce/13.0.2/cce-clang/x86_64/share/../bin
$
```

Choice of compatible sets of libraries

	Set 1 (Current)	Set 2	Set 3
HPE CCE	13.0.2	11.0.1	9.0.0
Cray LibSci	21.08.1.2	20.09.1	19.06.1
FFTW	3.3.8.13	3.3.8.8	3.3.8.3
HDF5	1.12.1.1	1.12.0.0	1.10.5.0
NetCDF	4.8.1.1	4.7.4	4.6.3.0

Software Modules and Organization

- /app/apps/<NAME>/<VERSION>

 - /app/apps/lammps/23June2022

 - /app/apps/tensorflow/2.8.1-py3

WORK IN PROGRESS !!!

- /app/libs/<NAME>/<VERSION>

 - /app/libs/aocl/3.1.0-gcc11.1

 - /app/libs/cudnn/11.6-8.4.0.27

- /app/apps/containers/<NAME>/

 - /app/apps/containers/gromacs/gromacs-nvidia-2021.3.sif

 - /app/apps/containers/pytorch/pytorch-nvidia-22.04-py3.sif

- /app/envs/

 - Conda and Python environments.

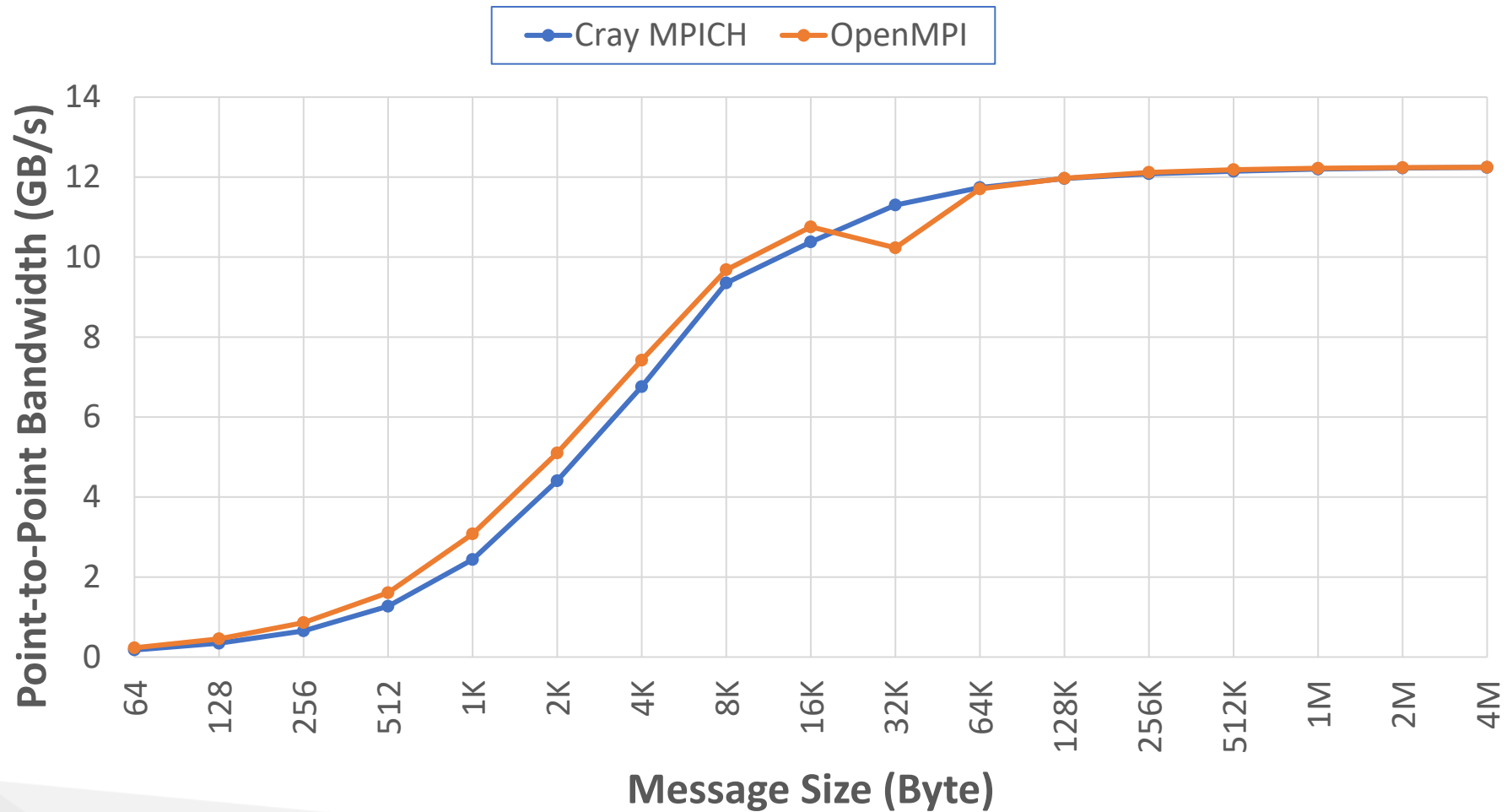
Software Modules and Organization

```
----- /app/apps/modulefiles -----
abyss/2.3.2                gcc/11.3.0-nscc          ncbi-blast/2.13.0       pytorch/1.11.0-py3
anaconda2/2019.10         gcc/12.1.0-nscc          ncl/6.6.2               pytorch/1.11.0-py3-gpu
anaconda3/2021.11        go/1.18.1                nco/5.0.6                qe/7.0
aocc/3.2.0                grace/5.1.25            ncview/2.1.7            r/4.2.0
arm-forge/21.1.2(default) gromacs/2021.4-cuda-hpe  nek5000/19.0            relion/3.1.3
bazel/4.2.2                gromacs/2021.4-hpe      nektar/5.2.0            rose/2019.01.5
bcftools/1.15.1          gromacs/2022.1          nextflow/22.04.0        sambamba/0.8.2
beast/1.10.4              gromacs/2022.1-gpu      numactl/2.0.14          samtools/1.15.1
beast/2.6.7                intel/2022.0.2          nvhpc/22.3(default)     singularity/3.10.0
bedtools/2.30.0          java/18.0.1.1-jdk        octave/7.1.0            sorflow/1.15.5-hpe
berkeleygw/3.0.1         julia/1.7.2              openfoam/2112           sorflow/1.15.5-hpe-gpu
bowtie/2.4.5              julia/1.7.2-hpe         openfoam/2112-hpe      sorflow/2.7.0-hpe
bwa/0.7.17                lammps/23June2022        openmpi/4.1.2-hpe     sorflow/2.7.0-hpe-gpu
cdo/2.0.5                  lammps/29Sep2021        python/2.7.18          sorflow/2.8.1-py3
cmake/3.23.1              lammps/29Sep2021        python/3.7.13          tensorflow/2.8.1-py3-gpu
cuda/10.0                  miniconda3/py38_4.8.3(default) python/3.7.13          velvet/1.2.10
cuda/11.2                  miniconda3/py39_4.11.0  python/3.8.13          wrf/4.2.2-hpe
cuda/11.6.2(default)     mrtrix/3.0.3            python/3.9.12          wrf/4.4
cylc/7.9.6                 mumax/3.10-gpu          python/3.10.4          xios/1.0.703
eccodes/2.16.0            mvapich/2.3.7-hpe       pytorch/1.11.0-hpe    xios/2.5
fcm/2021.05.0             nasm/2.15.05            pytorch/1.11.0-hpe-gpu xios/r2331
ffmpeg/5.0.1              nccl/11.6-2.12.10-1     xxdiff/4.0.1
gatk/4.2.6.1              nco/5.0.6                xios/2.5
gcc/8.5.0-nscc            ncbi-blast/2.13.0       xios/r2331
gcc/11.2.0-nscc           ncl/6.6.2                xxdiff/4.0.1
                           nco/5.0.6
                           ncview/2.1.7
                           nek5000/19.0
                           nektar/5.2.0
                           nextflow/22.04.0
                           numactl/2.0.14
                           nvhpc/22.3(default)
                           octave/7.1.0
                           openfoam/2112
                           openfoam/2112-hpe
                           openmpi/4.1.2-hpe
                           python/2.7.18
                           python/3.7.13
                           python/3.8.13
                           python/3.9.12
                           python/3.10.4
                           pytorch/1.11.0-hpe
                           pytorch/1.11.0-hpe-gpu
                           pytorch/1.11.0-py3
                           pytorch/1.11.0-py3-gpu
                           qe/7.0
                           r/4.2.0
                           relion/3.1.3
                           rose/2019.01.5
                           sambamba/0.8.2
                           samtools/1.15.1
                           singularity/3.10.0
                           sorflow/1.15.5-hpe
                           sorflow/1.15.5-hpe-gpu
                           sorflow/2.7.0-hpe
                           sorflow/2.7.0-hpe-gpu
                           sorflow/2.8.1-py3
                           tensorflow/2.8.1-py3-gpu
                           velvet/1.2.10
                           wrf/4.2.2-hpe
                           wrf/4.4
                           xios/1.0.703
                           xios/2.5
                           xios/r2331
                           xxdiff/4.0.1
----- /app/libs/modulefiles -----
aocl/3.1.0-aocc3.2        eigen/3.3.9              gsl/2.7.1-hpe           openjpeg/1.5.2
aocl/3.1.0-gcc11.1       eigen/3.4.0              hdf5/1.10.5             openjpeg/2.4.0
atlas/3.10.3-hpe         fftw/3.3.10-gcc11        hdfs/1.10.5            petsc/3.16.5-hpe
beagle-lib/3.1.2-gcc11   g2clib/1.6.0             jasper/1.900.1         proj/4.9.3
beagle-lib/3.1.2-gcc11-cuda11 gdal/2.2.4              jasper/2.0.14          proj/8.1.1
blis/0.8.1-hpe           gdal/2.4.4              jpeg/9c                 sparsehash/2.0.4-gcc11
cudnn/10.0-7.6.5.32     geos/3.10.1             mkl/2022.0.2           szip/2.1.1
cudnn/11.2-8.1.1.33     grib_api/1.25.0         nccl/11.6-2.12.10-1   udunits/2.2.26
cudnn/11.6-8.4.0.27     gsl/2.7.1-gcc11         oasis3-mct/2.8
$
```

WORK IN PROGRESS !!!

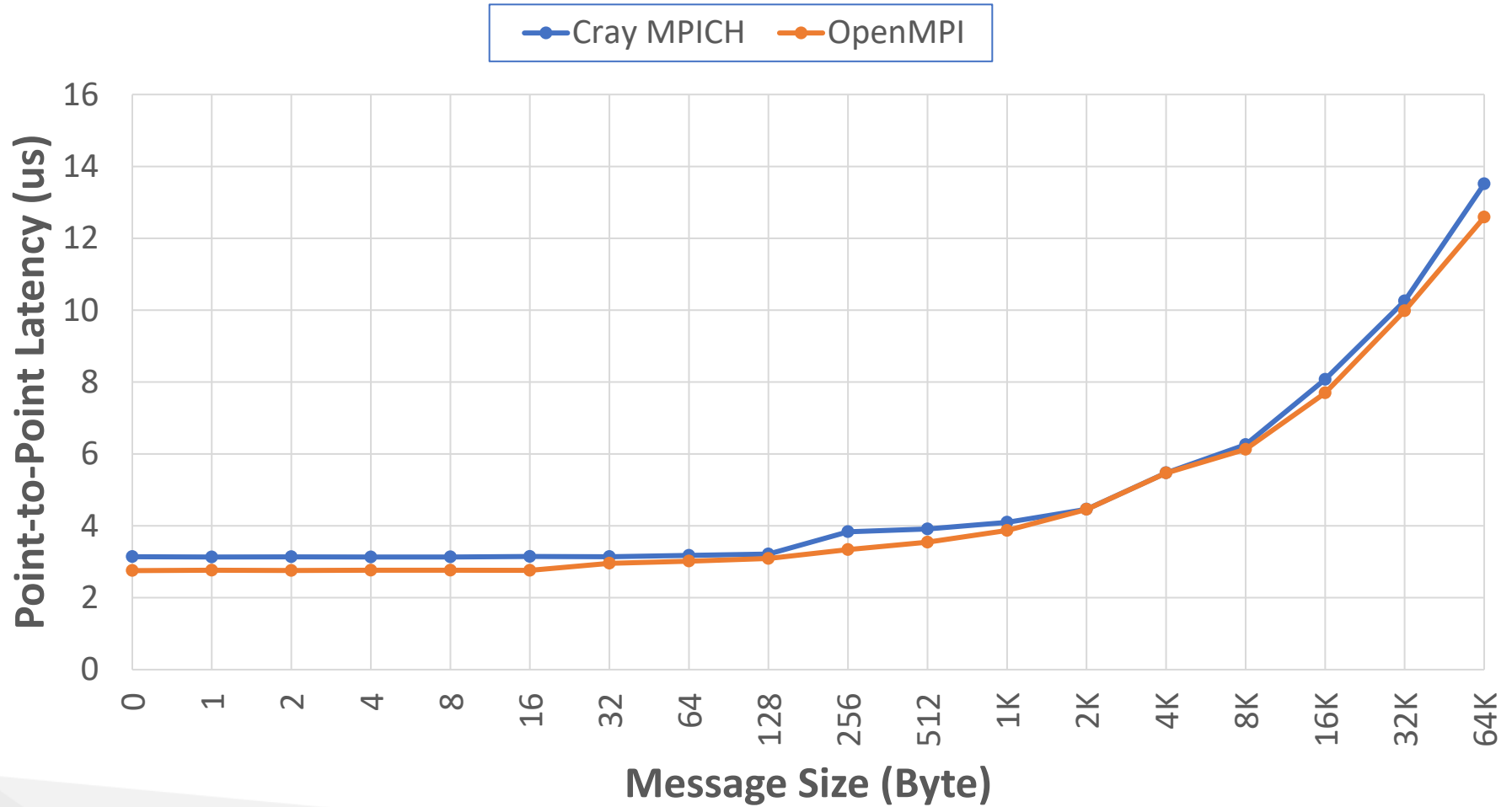
Cray MPICH vs OpenMPI

OSU MPI Bandwidth Test v5.8



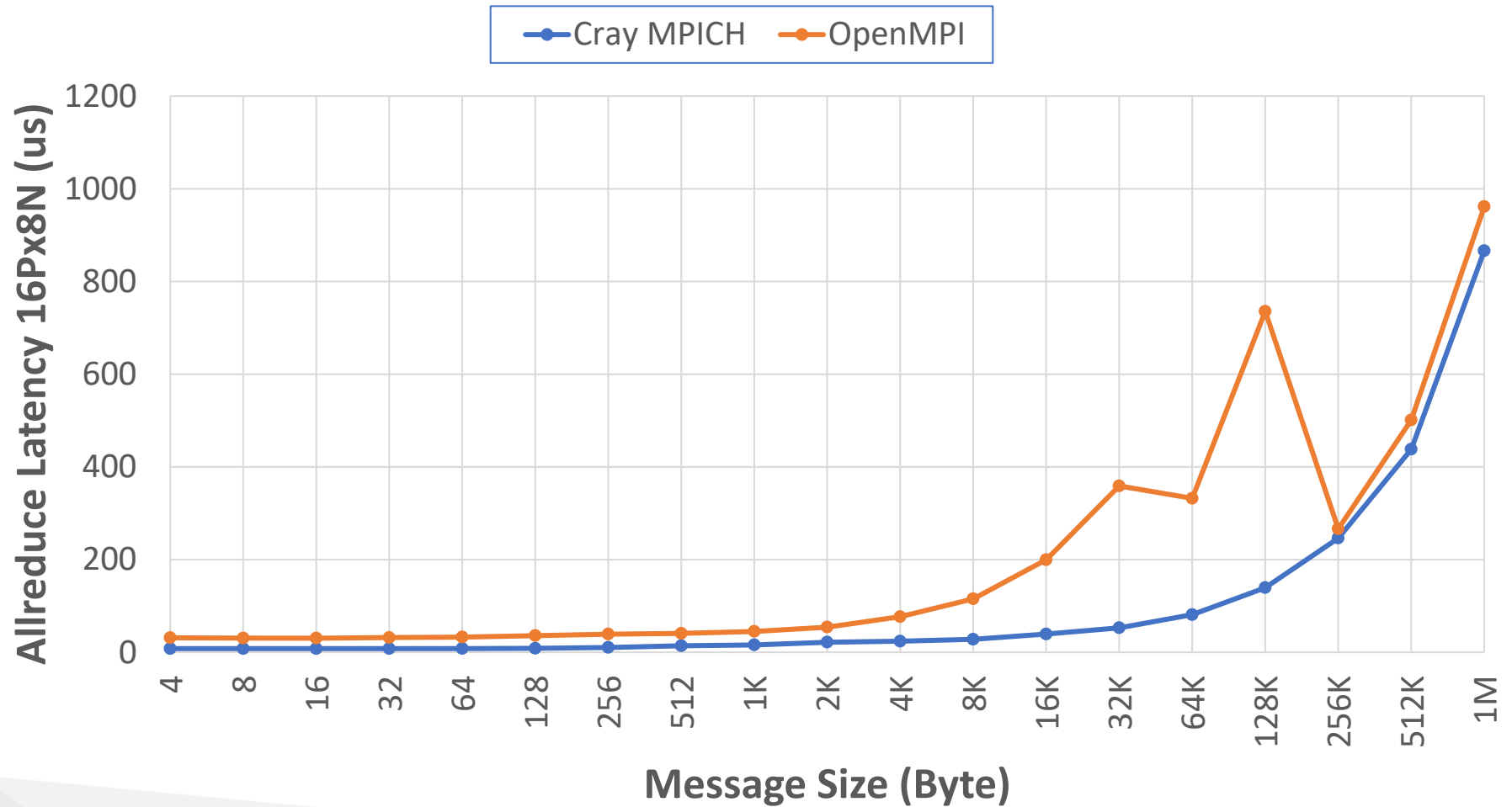
Cray MPICH vs OpenMPI

OSU MPI Latency Test v5.8



Cray MPICH vs OpenMPI

OSU MPI Allreduce Latency Test v5.8



- MPICH ABI (Application Binary Interface)
- Enable interoperability between different MPICH derivatives.
e.g. Cray MPICH, Intel MPI and MVAPICH
- Possible to build HPC software in containers with ANL MPICH.
- Run natively with Cray MPICH via MPICH ABI.

Q&A

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Thank You