Boosting the Performance of HPC Applications with MVAPICH

A Tutorial at MUG’23

Presented by

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The MVAPICH Team
The Ohio State University

http://mvapich.cse.ohio-state.edu/
Overview of the MVAPICH Project

• High Performance open-source MPI Library
• Support for multiple interconnects
  – InfiniBand, Omni-Path, Ethernet/iWARP, RDMA over Converged Ethernet (RoCE), AWS EFA, OPX, Broadcom RoCE, Intel Ethernet, Rockport Networks, Slingshot 10/11
• Support for multiple platforms
  – x86, OpenPOWER, ARM, Xeon-Phi, GPGPUs (NVIDIA and AMD)
• Started in 2001, first open-source version demonstrated at SC ‘02
• Supports the latest MPI-3.1 standard
• http://mvapich.cse.ohio-state.edu
• Additional optimized versions for different systems/environments:
  – MVAPICH2-X (Advanced MPI + PGAS), since 2011
  – MVAPICH2-GDR with support for NVIDIA (since 2014) and AMD (since 2020) GPUs
  – MVAPICH2-MIC with support for Intel Xeon-Phi, since 2014
  – MVAPICH2-Virt with virtualization support, since 2015
  – MVAPICH2-EA with support for Energy-Awareness, since 2015
  – MVAPICH2-Azure for Azure HPC IB instances, since 2019
  – MVAPICH2-X-AWS for AWS HPC+EFA instances, since 2019
• Tools:
  – OSU MPI Micro-Benchmarks (OMB), since 2003
  – OSU InfiniBand Network Analysis and Monitoring (INAM), since 2015
• Used by more than 3,325 organizations in 90 countries
• More than 1.70 Million downloads from the OSU site directly
• Empowering many TOP500 clusters (Jun ‘23 ranking)
  – 7th, 10,649,600-core (Sunway TaihuLight) at NSC, Wuxi, China
  – 21st, 448,448 cores (Frontera) at TACC
  – 36th, 288,288 cores (Lassen) at LLNL
  – 49th, 570,020 cores (Nurion) in South Korea and many others
• Available with software stacks of many vendors and Linux Distros (RedHat, SuSE, OpenHPC, and Spack)
• Partner in the 21st ranked TACC Frontera system
• Empowering Top500 systems for more than 16 years
Architecture of MVAPICH Software Family for HPC and DL/ML

High Performance Parallel Programming Models

- Message Passing Interface (MPI)
- PGAS (UPC, OpenSHMEM, CAF, UPC++)
- Hybrid --- MPI + X
  (MPI + PGAS + OpenMP/Cilk)

High Performance and Scalable Communication Runtime

Diverse APIs and Mechanisms

- Point-to-point Primitives
- Collectives Algorithms
- Job Startup
- Energy-Awareness
- Remote Memory Access
- I/O and File Systems
- Fault Tolerance
- Virtualization
- Active Messages
- Introspection & Analysis

Support for Modern Networking Technology
(InfiniBand, iWARP, RoCE, Omni-Path, Elastic Fabric Adapter)

- Transport Protocols
  - RC
  - SRD
  - UD
  - DC

- Modern Features
  - UMR
  - ODP
  - SR-IOV
  - Multi Rail

Support for Modern Multi-/Many-core Architectures
(Intel-Xeon, OpenPOWER, Xeon-Phi, ARM, NVIDIA/AMD GPGPU)

- Transport Mechanisms
  - Shared Memory
  - CMA
  - IVSHMEM
  - XPMEM

- Modern Features
  - Optane*
  - NVLink
  - CAPI*

* Upcoming
Production Quality Software Design, Development and Release

• Rigorous Q&A procedure before making a release
  - Exhaustive unit testing
  - Various test procedures on diverse range of platforms and interconnects
  - Test 19 different benchmarks and applications including, but not limited to
    • OMB, IMB, MPICH Test Suite, Intel Test Suite, NAS, Scalapak, and SPEC
    - Spend about 18,000 core hours per commit
  - Performance regression and tuning
  - Applications-based evaluation
  - Evaluation on large-scale systems

• All versions (alpha, beta, RC1 and RC2) go through the above testing
Automated Procedure for Testing Functionality

- Test OMB, IMB, MPICH Test Suite, Intel Test Suite, NAS, Scalapak, and SPEC
- Tests done for each build done build “buildbot”
- Test done for various combinations of environment variables meant to trigger different communication paths in MVAPICH
Scripts to Determine Performance Regression

• Automated method to identify performance regression between different commits
• Tests different MPI primitives
  – Point-to-point; Collectives; RMA
• Works with different
  – Job Launchers/Schedulers
    • SLURM, PBS/Torque, JSM
  – Works with different interconnects
• Works on multiple HPC systems
• Works on CPU-based and GPU-based systems
Deployment Solutions: RPM and Debian Deployments

- Provide customized RPMs for different system requirements
  - ARM, Power8, Power9, x86 (Intel and AMD)
  - Different versions of Compilers (ICC, PGI, GCC, XLC, ARM), CUDA, OFED/Intel IFS
Deployment Solutions: Spack Workflow

1. Create a new package
2. Edit package.py
3. Specify variants and dependencies
4. Functions to convert variants to build options
5. Convert installation to portable spack binaries
6. Create a local http mirror
7. Initialize gpg keys
8. Unit test installation locally
9. Test and Verify with binary from mirror
10. Raise Pull Request for package.py
11. Test and Verify with upstream
12. Release Announcement

Deployment Solutions: Spack Workflow
Deployment Solutions: Installation and Setup MVAPICH from Spack

Install Spack

$ git clone https://github.com/spack/spack.git
$ source ~/spack/share/spack/setup-env.sh

Installing MVAPICH (From Source)

$ spack info mvapich
$ spack install mvapich@3.0a %gcc@8.3.0 (or other available compiler on the system)
$ spack find -l -v -p mvapich
Deployment Solutions: MVAPICH2-X or MVAPICH2-GDR

Add the required mirrors

$ spack mirror add MVAPICHx http://mvapich.cse.ohio-state.edu/download/mvapich/spack-mirror/MVAPICHx

$ spack mirror add MVAPICH2-GDR http://mvapich.cse.ohio-state.edu/download/mvapich/spack-mirror/MVAPICH2-GDR

Trust the public key used to sign the packages

$ wget http://mvapich.cse.ohio-state.edu/download/mvapich/spack-mirror/MVAPICHx/build_cache/public.key

$ spack gpg trust public.key
Deployment Solutions: MVAPICH2-X or MVAPICH2-GDR from Spack

List the available binaries in the mirror

$ spack buildcache list -L -v -a

Install MVAPICH2-X and MVAPICH2-GDR

$ spack install MVAPICHx@2.3%gcc@4.8.5 distribution=mofed4.6 feature=advanced-xpmem
  pmi_version=pmi1 process_managers=mpirun target=x86_64

$ spack install MVAPICH2-GDR@2.3.3~core_direct+mcast~openacc distribution=mofed4.5
  pmi_version=pmi1 process_managers=mpirun ^cuda@9.2.88 target=x86_64

Supported CUDA Versions

- ^cuda@9.2.88, ^cuda@10.1.243, ^cuda@10.2.89
Designing (MPI+X) for Exascale

• Scalability for million to billion processors
  – Support for highly-efficient inter-node and intra-node communication (both two-sided and one-sided)

• Scalable Collective communication
  – Offloaded
  – Non-blocking
  – Topology-aware

• Balancing intra-node and inter-node communication for next generation multi-/many-core (128-1024 cores/node)
  – Multiple end-points per node

• Support for efficient multi-threading

• Integrated Support for GPGPUs and Accelerators

• Fault-tolerance/resiliency

• QoS support for communication and I/O

• Support for Hybrid MPI+PGAS programming
  • MPI + OpenMP, MPI + UPC, MPI + OpenSHMEM, CAF, MPI + UPC++...

• Virtualization

• Energy-Awareness
## MVAPICH Software Family

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<td>MVAPICH</td>
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<td>Advanced MPI features/support (UMR, ODP, DC, Core-Direct, SHArP, XPMEM), OSU</td>
<td>MVAPICH2-X</td>
</tr>
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<td>INAM (InfiniBand Network Monitoring and Analysis), PGAS (OpenSHMEM, UPC, UPC++</td>
<td></td>
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<tr>
<td>and CAF), MPI+PGAS (OpenSHMEM, UPC, UPC++, and CAF) with IB and RoCE (v1/v2)</td>
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</tr>
<tr>
<td>Optimized MPI for clusters with NVIDIA GPUs and for GPU-enabled Deep Learning</td>
<td>MVAPICH2-GDR</td>
</tr>
<tr>
<td>Applications</td>
<td></td>
</tr>
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<td>Advanced MPI with unified MVAPICH2-GDR and MVAPICH2-X features for HPC, DL,</td>
<td>MVAPICH-PLUS</td>
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<tr>
<td>ML, Big Data and Data Science applications</td>
<td></td>
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MVAPICH 3.0

• Beta version released 05/10/2023
• Major Features and Enhancements
  – Based on MPICH 3.4.3
  – Support for OFI and UCX network libraries through MPICH netmod interface
  – MVAPICH enhanced collective designs
  – Support for Cray Slingshot 11 network
  – Improved CVAR interface for consistency and performance
  – Support for SHARP
Overview of MVAPICH Features

• Process Mapping and Point-to-point Intra-node Protocols
• Enhanced Collective Communication Designs
• MVAPICH 3.0 New Features
Process Mapping support in MVAPICH

Preset Binding Policies
- spread (Default)
- bunch
- scatter
- hybrid

User-defined binding
- MPI rank-to-core binding

Policy

Granularity

MVAPICH detects processor architecture at job-launch
Preset Process-binding Policies – Bunch

- "Core" level "Bunch" mapping
  - \texttt{MVP\_CPU\_BINDING\_POLICY=\textit{bunch}}

- "Socket/Numanode" level "Bunch" mapping
  - \texttt{MVP\_CPU\_BINDING\_LEVEL=socket MVP\_CPU\_BINDING\_POLICY=\textit{bunch}}
Preset Process-binding Policies – Scatter

- "Core" level "Scatter" mapping
  - MVP_CPU_BINDING_POLICY=scatter

- "Socket/Numanode" level "Scatter" mapping
  - MVP_CPU_BINDING_LEVEL=socket MVP_CPU_BINDING_POLICY=scatter
Process and thread binding policies in hybrid MPI+Threads

- A new process binding policy – “hybrid”
  - \texttt{MVP\_CPU\_BINDING\_POLICY} = hybrid

- A new environment variable for co-locating Threads with MPI Processes
  - \texttt{MVP\_THREADS\_PER\_PROCESS} = \(k\)
  - Automatically set to \texttt{OMP\_NUM\_THREADS} if OpenMP is being used
  - Provides a hint to the MPI runtime to spare resources for application threads.

- New variable for threads bindings with respect to parent process and architecture
  - \texttt{MVP\_HYBRID\_BINDING\_POLICY} = \{bunch | scatter | linear | compact | spread | numa\}
    - Linear – binds MPI ranks and OpenMP threads sequentially (one after the other)
      - Recommended to be used on non-hyper threaded systems with MPI+OpenMP
    - Compact – binds MPI rank to physical-core and locates respective OpenMP threads on hardware threads
      - Recommended to be used on multi-/many-cores e.g., KNL, POWER8, and hyper-threaded Xeon, etc.
Binding Example in Hybrid (MPI+Threads)

- MPI Processes = 4, OpenMP Threads per Process = 4
- MVP_CPU_BINDING_POLICY = hybrid
- MVP_THREADS_PER_PROCESS = 4
- MVP_THREADS_BINDING_POLICY = compact

- Detects hardware-threads support in architecture
- Assigns MPI ranks to physical cores and respective OpenMP Threads to HW threads
Binding Example in Hybrid (MPI+Threads) ---- Cont’d

• MPI Processes = 4, OpenMP Threads per Process = 4
• MVP_CPU_BINDING_POLICY = hybrid
• MVP_THREADS_PER_PROCESS = 4
• MVP_THREADS_BINDING_POLICY = linear

• MPI Rank-0 with its 4-OpenMP threads gets bound on Core-0 through Core-3, and so on
Binding Example in Hybrid (MPI+Threads) ---- Cont’d

• MPI Processes = 16
• Example: AMD EPYC 7551 processor with 8 NUMA domains
• MVP_CPU_BINDING_POLICY = hybrid
• MVP_HYBRID_BINDING_POLICY = numa
User-Defined Process Mapping

• User has complete-control over process-mapping

• To run 4 processes on cores 0, 1, 4, 5:
  - $ mpirun_rsh -np 4 -hostfile hosts MVP_CPU_MAPPING=0:1:4:5 ./a.out

• Use ‘,’ or ‘-’ to bind to a set of cores:
  - $mpirun_rsh -np 64 -hostfile hosts MVP_CPU_MAPPING=0,2-4:1:5:6 ./a.out

• Is process binding working as expected?
  - MVP_SHOW_CPU_BINDING=1
    • Display CPU binding information
    • Launcher independent
    • Example
      - MVP_SHOW_CPU_BINDING=1 MVP_CPU_BINDING_POLICY=scatter
        --------------CPU AFFINITY--------------
        RANK:0 CPU_SET: 0
        RANK:1 CPU_SET: 8

• Refer to Running with Efficient CPU (Core) Mapping section of MVAPICH user guide for more information
  • http://mvapich.cse.ohio-state.edu/static/media/mvapich/MVAPICH-userguide.html#x1-650006.5
Collective Communication in MVAPICH

Run-time flags:
- All shared-memory based collectives: MVP_USE_SHMEM_COLL (Default: ON)
- Hardware Mcast-based collectives: MVP_USE_MCAST (Default: OFF)
- XPMEM-based collectives are available in MVAPICH2-X

Designed for Performance & Overlap
Hardware Multicast-aware MPI_Bcast on TACC Frontera

- MCAST-based designs improve latency of MPI_Bcast by up to 2X at 2,048 nodes
- Use MVP_USE_MCAST=1 to enable MCAST-based designs
MPI_Scatter - Benefits of using Hardware-Mcast

- Enabling MCAST-based designs for MPI_Scatter improves small message up to 75%

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVP_USE_MCAST = 1</td>
<td>Enables hardware Multicast features</td>
<td>Disabled</td>
</tr>
<tr>
<td>--enable-mcast</td>
<td>Configure flag to enable</td>
<td>Enabled</td>
</tr>
</tbody>
</table>

- Refer to Running Collectives with Hardware based Multicast support section of MVAPICH user guide for more information
- [http://mvapich.cse.ohio-state.edu/static/media/mvapich/MVAPICH-userguide.html#x1-730006.9](http://mvapich.cse.ohio-state.edu/static/media/mvapich/MVAPICH-userguide.html#x1-730006.9)
Offloading with Scalable Hierarchical Aggregation Protocol (SHArP)

- Management and execution of MPI operations in the network by using SHArP
  - Manipulation of data while it is being transferred in the switch network
- SHArP provides an abstraction to realize the reduction operation
  - Defines Aggregation Nodes (AN), Aggregation Tree, and Aggregation Groups
  - AN logic is implemented as an InfiniBand Target Channel Adapter (TCA) integrated into the switch ASIC *
  - Uses RC for communication between ANs and between AN and hosts in the Aggregation Tree *

* Bloch et al. Scalable Hierarchical Aggregation Protocol (SHArP): A Hardware Architecture for Efficient Data Reduction

More details in the tutorial "SHARPv2: In-Network Scalable Streaming Hierarchical Aggregation and Reduction Protocol" by Devendar Bureddy (NVIDIA/Mellanox)
Performance of Blocking Collectives with In-Network Computing

**Optimized SHARP designs in MVAPICH2-X**

*Up to 9X* performance improvement with SHARP over MVAPICH2-X default for 1ppn MPI_Barrier, *6X* for 1ppn MPI_Reduce and *5X* for 1ppn MPI_Allreduce


*Optimized Runtime Parameters: MVP_ENABLE_SHARP = 1*
Performance of Reduction Collectives with Streaming Aggregation

More information in Short Talk by Bharath Ramesh titled "Designing In-Network Computing Aware Reduction Collectives in MPI" on August 21st, 4PM - 5:30PM
Non-blocking Collectives Support with In-Network Computing

• With SHARP:
  - Flat scaling in terms of overall time
  - High overlap between computation and communication

Platform: Dual-socket Intel(R) Xeon(R) Platinum 8280 CPU @ 2.70GHz nodes equipped with Mellanox InfiniBand, HDR-100 Interconnect
Benefits of SHARP Allreduce at Application Level

Avg DDOT Allreduce time of HPCG

SHARP support available since MVAPICH 2.3a

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<tr>
<td>MVP_ENABLE_SHARP=1</td>
<td>Enables SHARP-based collectives</td>
<td>Disabled</td>
</tr>
<tr>
<td>--enable-sharp</td>
<td>Configure flag to enable SHARP</td>
<td>Disabled</td>
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More details in the talk "Benefits of Streaming Aggregation with SHARPv2 in MVAPICH, Bharath Ramesh, The Ohio State University on Tuesday (08/24/2020) from 4:30 PM - 5:30 PM EDT

- Refer to Running Collectives with Hardware based SHARP support section of MVAPICH user guide for more information
- [http://mvapich.cse.ohio-state.edu/static/media/mvapich/MVAPICH-userguide.html#x1-1050006.27](http://mvapich.cse.ohio-state.edu/static/media/mvapich/MVAPICH-userguide.html#x1-1050006.27)
Performance Evaluation – Micro-benchmarks on Broadcom RoCE

- Experimental results from Dell Bluebonnet
- Up to 20% reduction in small message point-to-point latency
- From 0.1x to 2x increase in bandwidth
- Up to 12.4x lower MPI_Allreduce latency
- Up to 5x lower MPI_Scatter latency
Performance Evaluation – Applications on Broadcom RoCE

- Reduce up to 45% execution time of CP2K H2O-dft-Is (NREP4)
- Reduce up to 7% execution time of WRF CONUS 3KM

More information in Short Talk by Shulei Xu titled “High Performance & Scalable MPI library over Broadcom RoCEv2” on August 21st, 4PM – 5:30PM
MVAPICH 3.0 - OFI and UCX Support

• Support a broad range of interconnects with widely used libraries
  - Configure with `--with-device=ch4:ofi` or `--with-device=ch4:ucx`

• Runtime provider selection via CVARs
  - `MPIR_CVAR_OFI_USE_PROVIDER=<prov>`

• System default, embedded, or custom installation of OFI/UCX
  - Configure with `--with-libfabric=embedded` or `--with-libfabric=<path>`
  - Configure with `--with-ucx=embedded` or `--with-ucx=<path>`

• Enhanced MVAPICH collective designs available on all supported networks
Upcoming/Planned Features

• MVAPICH custom ch4 netmod
• Enhanced pt2pt support for IB/RoCE systems
• Enhanced launcher
MPI Level Latency on Slingshot 11

- **2us** inter-node point-to-point latency for small messages

Interconnect: Cray HPE Slingshot 11
Library: MVAPICH 3.0a
CPU: AMD EPYC 7763 (milan) Processor
MPI Level Bandwidth on Slingshot 11

- **23,985 MB/s** uni-directional peak bandwidth
- **42,034 MB/s** bi-directional peak bandwidth

Interconnect: Cray HPE Slingshot 11 (200 Gbps)
Library: MVAPICH 3.0a
CPU: AMD EPYC 7763 (milan) Processor
MVAPICH-3.0a+OPX vs MVAPICH-2.3.7+PSM2 (Early Performance Results)

**OSU_BIBW (2 Nodes, 1 PPN)**

- **MVAPICH2-2.3.7-PSM**
- **MVAPICH2-3.0a-OPX**

**OSU_BW (2 Nodes, 1 PPN)**

- **MVAPICH2-2.3.7-PSM**
- **MVAPICH2-3.0a-OPX**

**OSU_Latency (2 Nodes, 1 PPN)**

- **MVAPICH2-2.3.7-PSM**
- **MVAPICH2-3.0a-OPX**

**OSU_MBW_MR (2 Nodes)**

- **MVAPICH2-2.3.7-PSM**
- **MVAPICH2-3.0a-OPX**

**System:** Intel Xeon Bronze (Skylake) 3106 CPU @ 1.70GHz (4 nodes, 16 cores/node, 8 x 2 sockets) with Omni-Path 100Gbps
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MPI + CUDA - Naive

- Data movement in applications with standard MPI and CUDA interfaces

**At Sender:**
```
cudAmemcpy(s_hostbuf, s_devbuf, ...);
MPI_Send(s_hostbuf, size, ...);
```

**At Receiver:**
```
MPI_Recv(r_hostbuf, size, ...);
cudAmemcpy(r_devbuf, r_hostbuf, ...);
```

*High Productivity and Low Performance*
MPI + CUDA - Advanced

- Pipelining at user level with non-blocking MPI and CUDA interfaces

**At Sender:**

```c
for (j = 0; j < pipeline_len; j++)
    cudaMemcpyAsync(s_hostbuf + j * blk, s_devbuf + j * blksz, ...);
for (j = 0; j < pipeline_len; j++) {
    while (result != cudaSuccess) {
        result = cudaStreamQuery(...);
        if(j > 0) MPI_Test(...);
    }
    MPI_Isend(s_hostbuf + j * block_sz, blksz, ...);
}
MPI_Waitall();
```

<<Similar at receiver>>

**Low Productivity and High Performance**
GPU-Aware (CUDA-Aware) MPI Library: MVAPICH-GPU

- Standard MPI interfaces used for unified data movement
- Takes advantage of Unified Virtual Addressing (>= CUDA 4.0)
- Overlaps data movement from GPU with RDMA transfers

**At Sender:**

\[
\text{MPI\_Send}(s\_devbuf, \text{size}, \ldots);
\]

**At Receiver:**

\[
\text{MPI\_Recv}(r\_devbuf, \text{size}, \ldots);
\]

*High Performance and High Productivity*
GPU-Aware MPI: MVAPICH2-GDR 1.8-2.3.7 Releases

• GPU-aware MPI:
  − CUDA-aware MPI: Support for MPI communication from NVIDIA GPU device memory
  − ROCm-aware MPI: Support for MPI communication between AMD GPUs (from MVAPICH2-GDR 2.3.5+)

• High performance RDMA-based inter-node point-to-point communication (GPU-GPU, GPU-Host and Host-GPU)

• High performance intra-node point-to-point communication for multi-GPU adapters/node (GPU-GPU, GPU-Host and Host-GPU)

• Taking advantage of CUDA IPC (available since CUDA 4.1) in intra-node communication for multiple GPU adapters/node

• Optimized and tuned collectives for GPU device buffers

• MPI datatype support for point-to-point and collective communication from GPU device buffers

• Unified memory
MVAPICH2-GDR: Pre-requisites for OpenPOWER & x86 Systems

• MVAPICH2-GDR 2.3.7 requires the following software to be installed on your system:
  1. Mellanox OFED 3.2 and later
  2. NVIDIA Driver 367.48 or later
  3. NVIDIA CUDA Toolkit 7.5 and later
  4. NVIDIA Peer Memory (nv_peer_mem) module to enable GPUDirect RDMA (GDR) support

• Strongly Recommended for Best Performance
  5. GDRCOPY Library by NVIDIA: https://github.com/NVIDIA/gdrcopy

• Comprehensive Instructions can be seen from the MVAPICH2-GDR User Guide:
  - http://mvapich.cse.ohio-state.edu/userguide/gdr/
MVAPICH2-GDR: Download and Setup on OpenPOWER & x86 Systems

• Simple Installation steps for both systems
• Pick the right MVAPICH2-GDR RPM from Downloads page:
  – http://mvapich.cse.ohio-state.edu/downloads/
  – e.g. http://mvapich.cse.ohio-state.edu/download/mvapich/gdr/2.3/mofed4.5/MVAPICH2-GDR-mcast.cuda10.0.mofed4.5.gnu4.8.5-2.3.7-1.el7.x86_64.rpm
  (== <mv2-gdr-rpm-name>.rpm)

$ wget http://mvapich.cse.ohio-state.edu/download/mvapich/gdr/2.3/<mv2-gdr-rpm-name>.rpm

Root Users:
$ rpm -Uvh --nodeps <mv2-gdr-rpm-name>.rpm

Non-Root Users:
$ rpm2cpio <mv2-gdr-rpm-name>.rpm | cpio – id

• Contact MVAPICH help list with any questions related to the package
  mvapich-help@cse.ohio-state.edu
ROCE and Optimized Collectives Support

- RoCE V1 and V2 support
- RDMA_CM connection support
- CUDA-Aware Collective Tuning
  - Point-point Tuning (available since MVAPICH2-GDR 2.0)
    - Tuned thresholds for the different communication patterns and features
    - Depending on the system configuration (CPU, HCA and GPU models)
  - Tuning Framework for GPU based collectives
    - Select the best algorithm depending on message size, system size and system configuration
    - Support for Bcast and Gather operations for different GDR-enabled systems
- Available since MVAPICH2-GDR 2.2RC1 release
MVAPICH2-GDR 2.3.7

- Released on 05/27/2022
- Major Features and Enhancements
  - Based on MVAPICH 2.3.7
  - Enhanced performance for GPU-aware MPI_Alltoall and MPI_Alltoallv
  - Added automatic rebinding of processes to cores based on GPU NUMA domain
    * This is enabled by setting the env MVP_GPU_AUTO_REBIND=1
  - Added NCCL communication substrate for various non-blocking MPI collectives
    * MPI_Allreduce, MPI_Reduce, MPI_Allgather, MPI_Allgatherv, MPI_Alltoall, MPI_Alltoallv, MPI_Scatter, MPI_Scatterv, MPI_Gather, MPI_Gatherv, and MPI_Bcast
  - Enhanced point-to-point and collective tuning for AMD Milan processors with NVIDIA A100 and AMD MI100 GPUs
  - Enhanced point-to-point and collective tuning for NVIDIA DGX-A100 systems
  - Added support for Cray Slingshot-10 interconnect
  - Added support for 'on-the-fly' compression of point-to-point messages used for GPU-to-GPU communication
    * Applicable to NVIDIA GPUs
  - NCCL communication substrate for various MPI collectives
    * Support for hybrid communication protocols using NCCL-based, CUDA-based, and IB verbs-based primitives
  - Full support for NVIDIA DGX, NVIDIA DGX-2 V-100, and NVIDIA DGX-2 A-100 systems
  - Enhanced architecture detection, process placement and HCA selection
  - Enhanced intra-node and inter-node point-to-point tuning
  - Enhanced collective tuning
  - Introduced architecture detection, point-to-point tuning and collective tuning for ThetaGPU @ANL
  - Enhanced point-to-point and collective tuning for NVIDIA GPUs on Frontera @TACC, Lassen @LLNL, and Sierra @LLNL
  - Enhanced point-to-point and collective tuning for Mi50 and Mi60 AMD GPUs on Corona @LLNL
  - Added several new MPI_T PVARs
  - Added support for CUDA 11.3
  - Added support for ROCm 4.1
  - Enhanced output for runtime variable MVP_SHOW_ENV_INFO
  - Tested with Horovod and common DL Frameworks
    * TensorFlow, PyTorch, and MXNet
  - Tested with MPI4Dask 0.2
    * MPI4Dask is a custom Dask Distributed package with MPI support
  - Tested with MPI4cuML 0.1
    * MPI4cuML is a custom cuML package with MPI support
  - Applicable to NVIDIA GPUs
# Tuning GDRCOPY Designs in MVAPICH2-GDR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Significance</th>
<th>Default</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVP_USE_GDRCOPY</td>
<td>• Enable / Disable GDRCOPY-based designs</td>
<td>1</td>
<td>(Enabled)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• Always enable</td>
</tr>
<tr>
<td>MVP_GDRCOPY_LIMIT</td>
<td>• Controls messages size until which GDRCOPY is used</td>
<td>8 KByte</td>
<td>• Tune for your system</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• GPU type, host architecture. Impacts the eager performance</td>
</tr>
<tr>
<td>MVP_GPUDIRECT_GDRCOPY_LIB</td>
<td>• Path to the GDRCOPY library</td>
<td>Unset</td>
<td>• Always set</td>
</tr>
<tr>
<td>MVP_USE_GPUDIRECT_D2H_GDRCOPY_LIMIT</td>
<td>• Controls messages size until which GDRCOPY is used at sender</td>
<td>16Bytes</td>
<td>• Tune for your systems</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• CPU and GPU type</td>
</tr>
</tbody>
</table>

* Refer to Tuning and Usage Parameters section of MVAPICH2-GDR user guide for more information
* [http://mvapich.cse.ohio-state.edu/userguide/gdr/#_tuning_and_usage_parameters](http://mvapich.cse.ohio-state.edu/userguide/gdr/#_tuning_and_usage_parameters)
# Tuning Loopback Designs in MVAPICH2-GDR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Significance</th>
<th>Default</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVP_USE_GPUDIRECT_LOOPBACK</td>
<td>• Enable / Disable LOOPBACK-based designs</td>
<td>1 (Enabled)</td>
<td>• Always enable</td>
</tr>
<tr>
<td>MVP_GPUDIRECT_LOOPBACK_LIMIT</td>
<td>• Controls messages size until which LOOPBACK is used</td>
<td>8 KByte</td>
<td>• Tune for your system</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• GPU type, host architecture and HCA. Impacts the eager performance</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• Sensitive to the P2P issue</td>
</tr>
</tbody>
</table>

- Refer to [Tuning and Usage Parameters](http://mvapich.cse.ohio-state.edu/userguide/gdr/#_tuning_and_usage_parameters) section of MVAPICH2-GDR user guide for more information
# Tuning GPUDirect RDMA (GDR) Designs in MVAPICH2-GDR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Significance</th>
<th>Default</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVP_USE_GPUDIRECT</td>
<td>• Enable / Disable GDR-based designs</td>
<td>1 (Enabled)</td>
<td>• Always enable</td>
</tr>
<tr>
<td>MVP_GPUDIRECT_LIMIT</td>
<td>• Controls messages size until which GPUDirect RDMA is used</td>
<td>8 KByte</td>
<td>• Tune for your system</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• GPU type, host architecture and</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CUDA version: impact pipelining overheads and P2P bandwidth bottlenecks</td>
</tr>
<tr>
<td>MVP_USE_GPUDIRECT_RECEIVE_LIMIT</td>
<td>• Controls messages size until which 1 hop design is used (GDR Write at the receiver)</td>
<td>256KBytes</td>
<td>• Tune for your system</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>• GPU type, HCA type and configuration</td>
</tr>
</tbody>
</table>

- Refer to [Tuning and Usage Parameters](http://mvapich.cse.ohio-state.edu/userguide/gdr/#_tuning_and_usage_parameters) section of MVAPICH2-GDR user guide for more information
MVAPICH2-GDR with CUDA-aware MPI Support

**GPU-GPU Inter-node Latency**
- MV2-(NO-GDR)
- MV2-GDR 2.3

**GPU-GPU Inter-node Bandwidth**
- MV2-(NO-GDR)
- MV2-GDR-2.3

**Message Size (Bytes)**
- 0 1 2 4 8 16 32 64 128 256 512 1K 2K 4K 8K

**GPU-GPU Inter-node Bi-Bandwidth**
- MV2-(NO-GDR)
- MV2-GDR-2.3

**Message Size (Bytes)**
- 0 1 2 4 8 16 32 64 128 256 512 1K 2K 4K 8K

- **1.85us**
- **10x**
- **9x**
- **11X**

**Intel Haswell (E5-2687W @ 3.10 GHz) node - 20 cores**
- NVIDIA Volta V100 GPU
- Mellanox Connect-X4 EDR HCA
- CUDA 9.0
- Mellanox OFED 4.0 with GPU-Direct-RDMA
MPI Datatype support in MVAPICH

• Datatypes support in MPI
  - Operate on customized datatypes to improve productivity
  - Enable MPI library to optimize non-contiguous data

At Sender:

\[
\text{MPI} \_\text{Type} \_\text{vector} \ (n\_blocks, n\_elements, \text{stride}, \text{old\_type}, \&\text{new\_type}); \\
\text{MPI} \_\text{Type} \_\text{commit} \ (&\text{new\_type}); \\
\ldots \\
\text{MPI} \_\text{Send} (s\_buf, \text{size}, \text{new\_type}, \text{dest}, \text{tag}, \text{MPI}\_\text{COMM}\_\text{WORLD});
\]

• Inside MVAPICH
  - Use datatype specific CUDA Kernels to pack data in chunks
  - Efficiently move data between nodes using RDMA
  - In progress - currently optimizes vector and hindexed datatypes
  - Transparent to the user

MVAPICHE2-GDR: Enhanced Derived Datatype

- Kernel-based and GDRCOPY-based one-shot packing for inter-socket and inter-node communication
- Zero-copy (packing-free) for GPUs with peer-to-peer direct access over PCIe/NVLink

Platform: Nvidia DGX-2 system
(NVIDIA Volta GPUs connected with NVSwitch), CUDA 9.2

Improved 3.4X

Platform: Cray CS-Storm
(16 NVIDIA Tesla K80 GPUs per node), CUDA 8.0
Enhanced DDT Support: HCA Assisted Inter-Node Scheme (UMR)

- Comparison of UMR based DDT scheme in MVAPICH2-GDR-Next with OpenMPI 4.1.3, MVAPICH2-GDR 2.3.6
- 1 GPU per Node, 2 Node experiment. Speed-up relative to OpenMPI
- Uses nested vector datatype for 4D face exchanges.

Platform: ThetaGPU (NVIDIA DGX-A100) (NVIDIA Ampere GPUs connected with NVSwitch), CUDA 11.0

MVAPICH2-GDR: “On-the-fly” Compression – Motivation

- For HPC and data science applications on modern GPU clusters
  - With larger problem sizes, applications exchange orders of magnitude more data on the network
  - Leads to significant increase in communication times for these applications on larger scale (AWP-ODC)
  - On modern HPC systems, there is disparity between intra-node and inter-node GPU communication bandwidths that prevents efficient scaling of applications on larger GPU systems
  - CUDA-Aware MPI libraries saturate the bandwidth of IB network

![Disparity between intra-node and inter-node GPU communication on Sierra OpenPOWER supercomputer](image)

![Saturated bandwidth at large message size](image)

Install Supporting Libraries for “On-the-fly” Compression Support

• MPC
  - Installation (Built-in with MVAPICH2-GDR)
  - Runtime parameters
    MVP_USE_CUDA=1 MVP_USE_COMPRESSION=1 MVP_COMPRESSION_ALGORITHM=1

• ZFP
  - Installation
    >git clone git@scm.nowlab.cse.ohio-state.edu::zhou.2595/zfp_compression.git --branch MPI-on-the-fly
    >cd zfp_compression && mkdir build && cd build
    >module load cuda/<CUDA_VERSION>
    >cmake .. -DCMAKE_INSTALL_PREFIX=PATH_TO_ZFP/zfp -DZFP_WITH_CUDA=ON
    >make -j8 && make install
  - Runtime parameters
    export LD_LIBRARY_PATH="PATH_TO_ZFP/zfp/lib64:$LD_LIBRARY_PATH"
    MVP_USE_CUDA=1 MVP_USE_COMPRESSION=1 MVP_COMPRESSION_ALGORITHM=2
## Tuning “On-the-fly” Compression Support in MVAPICH2-GDR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Default value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVP_USE_COMPRESSION</td>
<td>0</td>
<td>Enable compression</td>
</tr>
</tbody>
</table>
| MVP_COMPRESSION_ALGORITHM                      | 1             | 1: Use MPC compression  
2: Use ZFP compression |
| MVP_COMPRESSION_THRESHOLD                      | 524288        | Threshold of using compression for inter-node pt2pt GPU communication |
| MVP_COMPRESSION_THRESHOLD_INTRA                | 524288        | Threshold of using compression for intra-node pt2pt GPU communication |
| MVP_COMPRESSION_DIMENSION                      | Depends on compression library | Dimensionality of input data  
[1, 31]: For MPC compression  
1: For ZFP compression |
| MVP_COMPRESSION_ZFP_RATE                       | 8             | Compressed bits/value  
[1, 32]: For ZFP compression only |
“On-the-fly” Compression Support in MVAPICH2-GDR

- Weak-Scaling of HPC application **AWP-ODC** on Lassen cluster (V100 nodes)
- MPC-OPT achieves up to +18% GPU computing flops, -15% runtime per timestep
- ZFP-OPT achieves up to +35% GPU computing flops, -26% runtime per timestep

![Graph](image)

Performance of All-to-All with Online Compression

• Improvement compared to MVAPICH2-GDR-2.3.7 with Point-to-Point compression
  - 3D-FFT: Reduce All-to-All runtime by up to 29.2% with ZFP(rate: 24) on 64 GPUs
  - DeepSpeed benchmark: Reduce All-to-All runtime by up to 35.8% with ZFP(rate: 16) on 32 GPUs


Available in MVAPICH2-GDR 2.3.7
Collectives Performance on DGX2-A100 – Small Message

Allgather (4 nodes, 8 ppn, 32 GPUs)

Latency (us)

Size (bytes)

Reduce (4 nodes, 8 ppn, 32 GPUs)

Latency (us)

Size (bytes)

Bcast (4 nodes, 8 ppn, 32 GPUs)

Latency (us)

Size (bytes)

Allreduce (4 nodes, 8 ppn, 32 GPUs)

Latency (us)

Size (bytes)
Collectives Performance on DGX2-A100 – Large Message

**Allgather (4 nodes, 8 ppn, 32 GPUs)**

**Bcast (4 nodes, 8 ppn, 32 GPUs)**

**Reduce (4 nodes, 8 ppn, 32 GPUs)**

**Allreduce (4 nodes, 8 ppn, 32 GPUs)**
Highly Efficient Optimized Alltoall(v) Communication

Propose an optimized Alltoall(v) design to overlap inter (sendrecv-based) and intra-node (IPC-based) communication.

**Alltoall latency on 1 node (8 GPUs)**

**Alltoall latency on 16 nodes (128 GPUs)**

**heFFT throughput (alltoally) on 1 node (8 GPUs)**

**heFFT throughput (alltoally) on 16 node (128 GPUs)**


Available in MVAPICH2-GDR v2.3.7
MVAPICH-Plus 3.0

• Latest Alpha Release 07/19/2023

• Major Features and Enhancements
  – Based on MVAPICH 3.0
  – Supports all networks types supported by
  – Support for AMD and NVIDIA GPUs
  – Support for MVAPICH enhanced GPU Collectives

• Upcoming Beta Release
  – Support for enhanced GPU pt2pt operations
    • GDRCOPY and IPC

• Upcoming:
  – Combined features of MVAPICH2-X and MVAPICH2-GDR
  – Enhanced designs to leverage next generation Exascale systems
    • Frontier, El Capitan
MVAPICH-PLUS with GDRCopy Design on AMD GPUs

Latency:

Latency (Small Messages)

Latency for small Messages (with MI100 on MRI)

TIOGA - AMD MI100 GPUs

AMD GPUs on MRI
MVAPICH-PLUS GPU Optimized for Collectives - NVIDIA + IB

**MPI_Gather:**

**MPI_Scatter:**

**MPI_Alltoall:**

NVIDIA A100 GPUs (8 GPUS – 4 Nodes, 2 GPUS per Node) + CUDA 12.0
MVAPICH-PLUS GPU Optimized for Collectives – AMD + Slingshot-11

- **MPI_Gather:**
  - Latency (us): 10.67
  - Message Size: 1K
  - Latency (us): 43.68
  - Message Size: 2K

- **MPI_Scatter:**
  - Latency (us): 29.78
  - Message Size: 1K
  - Latency (us): 65.4
  - Message Size: 2K

- **MPI_Alltoall:**
  - Latency (us): 78.96
  - Message Size: 1K
  - Latency (us): 284.63
  - Message Size: 2K

AMD MI250 GPUs (16 GPUs – 2 Nodes, 8 GPUs per Node) + ROCm 5.1.0
Applications-Level Tuning: Compilation of Best Practices

• MPI runtime has many parameters
• Tuning a set of parameters can help you to extract higher performance
• Compiled a list of such contributions through the MVAPICH Website
  – http://mvapich.cse.ohio-state.edu/best_practices/

• Initial list of applications
  – Amber
  – HoomDBlue
  – HPCG
  – Lulesh
  – MILC
  – Neuron
  – SMG2000
  – Cloverleaf
  – SPEC (LAMMPS, POP2, TERA_TF, WRF2)

• Soliciting additional contributions, send your results to mvapich-help at cse.ohio-state.edu.
• We will link these results with credits to you.
Case Study: GROMACS – Impact of Tuning Transport Protocol

Experimental Setup

• Platform:
  – Broadcom RoCEv2 Thor Adapter
  – 64 Nodes x 2 x AMD EPYC 7713 64-Core Processor

• Application:
  – GROMACS v2022.3
  – Dataset: 3000k-atoms dataset

• Raw run lines:
  – OpenMPI 4.1.3 + UCX 1.14
    `export OMPI_PARAM="--mca pml ucx --mca osc ucx --mca spml ucx --mca btl ^vader,tcp,openib,uct -x UCX_NET_DEVICES=bnxt_re0:1 -x UCX_IB_GID_INDEX=3 -x UCX_TLS=self,sm,rc_v"
    mpirun --hostfile $HOSTFILE $OMPI_PARAM gmx_mpi mdrun -ntomp 1 -s $GROMACS_BENCHMARK -deffnm md -nsteps 10000`

  – MVAPICH2-2.3.7-Broadcom
    `mpirun_rsh --export-all -np $NP -ppn $PPN run_mpi gmx_mpi mdrun -ntomp 1 -s $GROMACS_BENCHMARK -deffnm md -nsteps 10000`
Case Study: GROMACS – Impact of Tuning Transport Protocol

First experiment – Unoptimized version

- Strong scaling the GROMACS application performance
- We are measuring the nanoseconds of simulated time per day
  - Higher is better
- Degradation observed beyond 1K MPI processes
- This is the unoptimized MVAPICH2-2.3.7 version
- Need to use TAU to see what MPI calls are causing the degradation
Case Study: GROMACS – Performance Engineering with TAU Diagnosis and workaround found

- Investigate UD communication (read progress poll)
- Use RC to get the desired lead in performance
- Gains:
  - 2.5x improvement over MVAPICH baseline
  - 15% compared to OpenMPI default RC
- Update the following parameter for GROMACS runs
  MV2_HYBRID_ENABLE_THRESHOLD = 8192
  this will enable UD-hybrid communication after the 8192 threshold*

*For more details check user-guide: https://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#:~:text=use%20any%20HugePages,-,11.110,-MV2_HYBRID_ENABLE_THRESHOLD
Case Study: 3D Stencil – Impact of Tuning Eager Threshold

Experimental Setup

- **Platform:**
  - Broadcom RoCEv2 Thor Adapter
  - 64 Nodes x 2 x AMD EPYC 7713 64-Core Processor

- **Application:**
  - 3D Stencil HPC Benchmark
  - Dataset: 3000k-atoms dataset

- **Raw run lines:**
  - MVAPICH2-2.3.7-Broadcom
    
    mpirun_rsh -np $NP -ppn $PPN ./3Dstencil_overlap 8 8 8 1000
Case Study: 3D Stencil – Impact of Tuning Eager Threshold
First experiment – Unoptimized version

- Execution time tests on 2 Nodes x 128 PPN (512 ranks)
- We are measuring the latency
  - Lower is better
- Degradation observed at 256K message
- This is the unoptimized MVAPICH2-2.3.7 version
- Need to use TAU to see
  - what MPI calls are causing the degradation
  - What is the dominant communication pattern
Case Study: 3D Stencil – Impact of Tuning Eager Threshold
Diagnosis and workaround found

- Diagnosis: more time is spent in inter-node pt-to-pt Rendezvous communication
- Solution: Use pt-to-pt eager communication
- Gains:
  - 2x reduction in latency
- Update the following parameter for the 3D Stencil runs

`MV2_IBA_EAGER_THRESHOLD = 524288`
this will enable inter-node eager communication until the specified message size*

*For more details check user-guide:

https://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#:~:text=for%20the%20job,-MV2_IBA_EAGER_THRESHOLD
MVAPICH – Future Roadmap and Plans for Exascale

• Performance and Memory scalability toward 1M-10M cores
• Hybrid programming (MPI + OpenSHMEM, MPI + UPC, MPI + CAF ...)
  • MPI + Task*
• Enhanced Optimization for GPUs and FPGAs*
• Taking advantage of advanced features of Mellanox InfiniBand
  • Tag Matching*
  • Adapter Memory*
• Enhanced communication schemes for upcoming architectures
  • NVLINK*
  • InfiniFabric*
  • Bluefield-3*
• Extended topology-aware collectives
• Extended Energy-aware designs and Virtualization Support
• Extended Support for MPI Tools Interface (as in MPI 3.0)
• Extended FT support
• Support for * features will be available in future MVAPICH Releases
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- A. Ruhela
- J. Vienne
- H. Wang
Thank You!

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Network-Based Computing Laboratory

http://nowlab.cse.ohio-state.edu/

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http://hibd.cse.ohio-state.edu/

The High-Performance Deep Learning Project
http://hidl.cse.ohio-state.edu/
Analyzing the Capabilities of Your System Using OSU Microbenchmarks

A Tutorial at MUG’23

Presented by

Hari Subramoni, Aamir Shafi, and Akshay Paniraja Guptha

The MVAPICH Team

The Ohio State University

http://mvapich.cse.ohio-state.edu/
OSU Micro Benchmarks v7.2

- New features since MUG'22
  - Add MPI-4 session based initialization support to the following benchmarks.
    - Pt2pt, Collective, One-sided, Neighborhood
  - Add MPI_IN_PLACE support for following blocking and non-blocking collectives.
  - Add an option to set root rank for rooted blocking and non-blocking collectives.
  - Add new blocking and non-blocking neighborhood collective benchmarks with support for CPU buffers.
  - Add new benchmarks for point-to-point persistent communication primitives.
  - Add PAPI support for the following MPI benchmarks.
    - Pt2pt, Collective, One-sided
  - Add support for benchmarking non-blocking Reduce-Scatter.
  - Add graphing support to the following MPI benchmarks.
    - Pt2pt, Collective, One-sided
  - Add support for benchmarking blocking Alltoallw.
  - Add support for derived data types in MPI pt2pt benchmarks.
  - Extend collective and point-to-point benchmarks to support different MPI datatypes.
  - Add support for derived data types in MPI blocking and non-blocking collective benchmarks
OMB Releases since MUG’22

- OSU Micro Benchmarks v6.1 (09/16/2022)
- OSU Micro Benchmarks v6.2 (10/25/2022)
- OSU Micro Benchmarks v7.0 (11/10/2022)
- OSU Micro Benchmarks v7.1 (04/06/2023)
- OSU Micro Benchmarks v7.2 (07/10/2023)
OMB New Features

- Major Feature Enhancements
  - Support for Derived Data Types
  - Support for Plotting
  - Support for PAPI Counters
  - Support for Neighborhood Collectives
  - Support for MPI Datatypes
  - Support for MPI-4 Sessions
- Support for New Benchmarks
  - pt2pt persistent communication primitives
  - osu_alltoallw
  - osu_ireduce_scatter

- Minor Feature Enhancements
  - Support for MPI_IN_PLACE
  - Support to change root rank in rooted collectives
Using Derived Data Types (DDT) in OMB

OMB benchmarks now support derived data types enabled using ‘-D’ option.

- **Contiguous**
  - `-Dcont`
  - E.g. `./osu_allgather -Dcont`

- **Vector**
  - `-Dvect:[stride]:[block_length]`
  - E.g. `./osu_allgather -Dvect:6:4`
    - Stride: 6
    - Block_length: 4

- **Indexed**
  - `-Dindx:[ddt file path]`

Sample Output/Input for DDT Support

- `.osu_allgather -Dvect:4:2`

- Indexed DDT parameters can be configured in a file as shown below.

- `.osu_allgather -Dindx:$OMB_HOME/c/util/ddt_sample.txt`

Sample indexed DDT config file:

```
#This is a comment
#Values must be number of elements.
#Displacement, Block Length
2, 10
12, 5
20, 4
```

Sample table:

<table>
<thead>
<tr>
<th>Size</th>
<th>Avg Latency(us)</th>
<th>Transmit Size</th>
<th>Actual number of bytes transferred</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.45</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>1.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>2.06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>2.30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>2.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>256</td>
<td>2.93</td>
<td></td>
<td></td>
</tr>
<tr>
<td>512</td>
<td>3.62</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1024</td>
<td>4.00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2048</td>
<td>8.39</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4096</td>
<td>14.51</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8192</td>
<td>27.02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16384</td>
<td>52.86</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32768</td>
<td>117.76</td>
<td></td>
<td></td>
</tr>
<tr>
<td>65536</td>
<td>229.63</td>
<td></td>
<td></td>
</tr>
<tr>
<td>131072</td>
<td>439.85</td>
<td></td>
<td></td>
</tr>
<tr>
<td>262144</td>
<td>838.70</td>
<td></td>
<td></td>
</tr>
<tr>
<td>524288</td>
<td>1665.82</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1048576</td>
<td>3193.65</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Enabling Plotting Support in OMB

• Graphs of latency/bandwidth across iterations can now be plotted directly from OMB.

• Depends on ‘gnuplot’ to plot graphs.
  – If not in PATH, configure with --with-gnuplot=<path to gnuplot install dir>

• Depends on ‘convert’ to get output in pdf format.
  – If not in PATH, configure with  --with-convert=<path to ImageMagick install dir>.

• Support enabled with  -G, --graph [tty,png,pdf]
  E.g: ./osu_allgather -Gtty,png
  ./osu_allgather -Gpng
Sample Plot Outputs from OMB

- **Terminal plot** – basic plot with necessary information.
- **png, pdf** – detailed plots with 3D plots for smaller and large message sizes.

Terminal output of iterations(X) vs latency(Y) (-Gtty)

PNG/PDF output of iterations(X) vs latency(Y) (-Gpng,pdf)

PNG/PDF 3D output across message sizes (-Gpng,pdf)
Enabling PAPI Support in OMB

• OMB now supports Performance Application Programming Interface (PAPI) used for collecting performance counter information from various hardware and software components.

• Configured with --enable-papi --with-papi=<PAPI install path>

• -P, --papi [EVENTS]:[PATH] Enable PAPI support
  – [EVENTS] //Comma separated list of PAPI events
  – [PATH] //PAPI output file path
Using PAPI with OMB

- E.g: ./osu_allreduce -PPAPI_L1_DCM,PPAPI_TLB_DM,PPAPI_FML_INS:papi.out

| Size: 1 |
|-----------------|-----------------|
| PAPI Event Name | Rank:0 | Rank:1 |
| PAPI_L1_DCM     | 14433 | 33553 |
| PAPI_TLB_DM     | 13560 | 11195 |
| PAPI_FML_INS    | 2000  | 2000  |

Size: 2

<table>
<thead>
<tr>
<th>PAPI Event Name</th>
<th>Rank:0</th>
<th>Rank:1</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAPI_L1_DCM</td>
<td>14304</td>
<td>13204</td>
</tr>
<tr>
<td>PAPI_TLB_DM</td>
<td>13726</td>
<td>12322</td>
</tr>
<tr>
<td>PAPI_FML_INS</td>
<td>2000</td>
<td>2000</td>
</tr>
</tbody>
</table>

Size: 4

<table>
<thead>
<tr>
<th>PAPI Event Name</th>
<th>Rank:0</th>
<th>Rank:1</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAPI_L1_DCM</td>
<td>14743</td>
<td>14561</td>
</tr>
<tr>
<td>PAPI_TLB_DM</td>
<td>13521</td>
<td>12737</td>
</tr>
<tr>
<td>PAPI_FML_INS</td>
<td>2000</td>
<td>2000</td>
</tr>
</tbody>
</table>

Sample PAPI output file(papi.out).
Support for Neighborhood Collectives in OMB

**Cartesian**

- 
  - N cart:<num of dimensions:radius>
  
  E.g: ./osu_neighbor_allgather -N cart:2:1

**Cartesian Neighborhood**

**Graph**

- 
  - N graph:<adjacency graph file>

**Graph Neighborhood**

Image Source: [https://cvw.cac.cornell.edu/mpiadvtopics/process-topologies/neighborhood-collectives](https://cvw.cac.cornell.edu/mpiadvtopics/process-topologies/neighborhood-collectives)
Running Neighborhood Collectives in OMB

- ./osu_neighbor_allgather -N cart:2:1

```
Dimensions size = 4 4
Time took to create topology graph:52.01 us.

# DSU MPI Neighborhood Allgather Latency Test v7.2
# Datatype: MPI_CHAR.
# Size  Avg Latency(us)
1  3.95
2  4.00
4  4.05
8  4.10
16 4.11
32 4.87
64 5.43
128 7.10
256 7.53
512 5.96
1024 7.88
2048 12.89
4096 12.45
8192 24.95
16384 74.66
32768 37.60
65536 61.97
131072 103.27
262144 280.24
524288 703.98
1048576 2491.98
```

- ./osu_neighbor_allgather -N
  graph:$OMB_HOME/c/util/nhbrhd_graph.adj

```
#This is a comment
#All values are ranks of the process
#Source, Destination
2, 0
0, 1
1, 2
2, 3
1, 3
0, 3

Sample adjacency graph file.
```
Using MPI Data Types with OMB

- OMB now supports the following MPI datatypes,
  - MPI_CHAR
  - MPI_FLOAT
  - MPI_INT
- MPI Data Type can be set using ‘-T’ option.
  - -T<all,mpi_char,mpi_int,mpi_float>
  - E.g: ./osu_allgather -T mpi_int

- ./osu_allgather -T all -m :64

<table>
<thead>
<tr>
<th>Size</th>
<th>Avg Latency(us)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.86</td>
</tr>
<tr>
<td>2</td>
<td>2.83</td>
</tr>
<tr>
<td>4</td>
<td>4.20</td>
</tr>
<tr>
<td>8</td>
<td>4.71</td>
</tr>
<tr>
<td>16</td>
<td>5.28</td>
</tr>
<tr>
<td>32</td>
<td>6.49</td>
</tr>
<tr>
<td>64</td>
<td>8.63</td>
</tr>
</tbody>
</table>

# OSU MPI Allgather Latency Test v7.2
# Datatype: MPI_CHAR.
<table>
<thead>
<tr>
<th>Size</th>
<th>Avg Latency(us)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.91</td>
</tr>
<tr>
<td>8</td>
<td>4.33</td>
</tr>
<tr>
<td>16</td>
<td>5.09</td>
</tr>
<tr>
<td>32</td>
<td>6.38</td>
</tr>
<tr>
<td>64</td>
<td>8.39</td>
</tr>
</tbody>
</table>

# Datatype: MPI_FLOAT.
<table>
<thead>
<tr>
<th>Size</th>
<th>Avg Latency(us)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.79</td>
</tr>
<tr>
<td>8</td>
<td>4.33</td>
</tr>
<tr>
<td>16</td>
<td>4.86</td>
</tr>
<tr>
<td>32</td>
<td>6.11</td>
</tr>
<tr>
<td>64</td>
<td>8.29</td>
</tr>
</tbody>
</table>
Additional features in OMB

• MPI_IN_PLACE support
  – OMB not supports running benchmarks with MPI_IN_PLACE enabled by passing ‘-l’ options.
  – E.g: ./osu_allgather --in-place

• MPI-4 session
  – Currently MPI-4 standards describes support for mpi://WORLD, mpi://SELF. Since most OMB benchmarks require more than one process, mpi://WORLD is set as default when running with MPI session support.
  – Enabled by passing ‘-l’ option.

• Set root rank
  – OMB benchmarks support setting root rank for rooted collectives using ‘-k’ option.
    • Fixed
      – Root rank is fixed for all iterations of the benchmark.
      E.g: ./osu_reduce -k fixed:1
    • Rotate
      – Root rank varies in a cyclic manner for each iteration on the benchmark.
      E.g: ./osu_reduce -k rotate
Funding Acknowledgments

Funding Support by

![Logos of various sponsors]

Equipment Support by

![Logos of various sponsors]
Acknowledgments to all the Heroes (Past/Current Students and Staffs)

**Current Students (Graduate)**
- K. Al Attar (Ph. D.)
- N. Alnaasan (Ph.D.)
- Q. Anthony (Ph.D.)
- C.-C. Chun (Ph.D.)
- T. Chen (Ph. D.)
- N. Contini (Ph.D.)

**Current Students (Graduate)**
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**Past Students**
- A. Awan (Ph.D.)
- A. Augustine (M.S.)
- P. Balaji (Ph.D.)
- M. Bayatpour (Ph.D.)
- R. Biswas (M.S.)
- S. Bhagvat (M.S.)
- A. Bhat (M.S.)
- D. Buntinas (Ph.D.)
- L. Chai (Ph.D.)
- B. Chandrasekharan (Ph.D.)
- S. Chakraborthy (Ph.D.)
- N. Dandapanthula (M.S.)
- V. Dhanraj (M.S.)
- C.-H. Chu (Ph.D.)

**Past Post-Docs**
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- X. Besseron
- M. S. Ghazimirsaeed

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- V. Dhanraj (M.S.)
- C.-H. Chu (Ph.D.)

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- S. Sur
- X. Lu

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- S. Sur
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**Past Senior Research Associate**
- J. Hashmi

**Past Programmers**
- A. Reifsteck
- D. Bureddy
- J. Perkins
- B. Seeds

**Past Research Specialist**
- M. Arnold
- J. Smith

**Current Research Scientists**
- M. Abduljabbar
- A. Shafi

**Current Students (Undergrads)**
- T. Chen

**Current Research Scientists**
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- A. Shafi

**Current Students (Undergrads)**
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Thank You!

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Network-Based Computing Laboratory

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https://twitter.com/mvapich

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http://mvapich.cse.ohio-state.edu/

The High-Performance Big Data Project
http://hibd.cse.ohio-state.edu/

The High-Performance Deep Learning Project
http://hidl.cse.ohio-state.edu/
# MVAPICH Software Family

<table>
<thead>
<tr>
<th>Requirements</th>
<th>Library</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI with Support for InfiniBand, Omni-Path, Ethernet/iWARP and, RoCE (v1/v2)</td>
<td>MVAPICH</td>
</tr>
<tr>
<td>Advanced MPI features/support (UMR, ODP, DC, Core-Direct, SHArP, XPMEM), OSU INAM (InfiniBand Network Monitoring and Analysis), PGAS (OpenSHMEM, UPC, UPC++, and CAF), MPI+PGAS (OpenSHMEM, UPC, UPC++, and CAF) with IB and RoCE (v1/v2)</td>
<td>MVAPICH2-X</td>
</tr>
<tr>
<td>Optimized MPI for clusters with NVIDIA GPUs and for GPU-enabled Deep Learning Applications</td>
<td>MVAPICH2-GDR</td>
</tr>
<tr>
<td>Advanced MPI with unified MVAPICH2-GDR and MVAPICH2-X features for HPC, DL, ML, Big Data and Data Science applications</td>
<td>MVAPICH-PLUS</td>
</tr>
</tbody>
</table>
**MVAPICH2-X for MPI and Hybrid MPI + PGAS Applications**

High Performance Parallel Programming Models

<table>
<thead>
<tr>
<th>MPI</th>
<th>PGAS</th>
<th>Hybrid --- MPI + X</th>
</tr>
</thead>
<tbody>
<tr>
<td>Message Passing Interface</td>
<td>(UPC, OpenSHMEM, CAF, UPC++)</td>
<td>(MPI + PGAS + OpenMP/Cilk)</td>
</tr>
</tbody>
</table>

High Performance and Scalable Unified Communication Runtime

Diverse APIs and Mechanisms

- Optimized Point-to-point Primitives
- Remote Memory Access
- Active Messages
- Collectives Algorithms (Blocking and Non-Blocking)
- Scalable Job Startup
- Fault Tolerance
- Introspection 
  & Analysis with OSU INAM

Support for Modern Networking Technologies

- (InfiniBand, iWARP, RoCE, Omni-Path...)

Support for Modern Multi-/Many-core Architectures

- (Intel-Xeon, OpenPower...)

- Current Model – Separate Runtimes for OpenSHMEM/UPC/UPC++/CAF and MPI
  - Possible deadlock if both runtimes are not progressed
  - Consumes more network resource

- Unified communication runtime for MPI, UPC, UPC++, OpenSHMEM, CAF
  - Available with since 2012 (starting with MVAPICH2-X 1.9)
  - [http://mvapich.cse.ohio-state.edu](http://mvapich.cse.ohio-state.edu)
# MVAPICH2-X Feature Table

<table>
<thead>
<tr>
<th>Features for InfiniBand (OFA-IB-CH3) and RoCE (OFA-RoCE-CH3)</th>
<th>Basic</th>
<th>Basic-XP MEM</th>
<th>Intermediate</th>
<th>Advanced</th>
</tr>
</thead>
<tbody>
<tr>
<td>Architecture Specific Point-to-point and Collective Optimizations for x86, OpenPOWER, and ARM</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Optimized Support for PGAS models (UPC, UPC++, OpenSHMEM, CAF) and Hybrid MPI+PGAS models</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>CMA-Aware Collectives</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Optimized Asynchronous Progress*</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>InfiniBand Hardware Multicast-based MPI_Bcast*</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>OSU InfiniBand Network Analysis and Monitoring (INAM)**</td>
<td></td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>XPMEM-based Point-to-Point and Collectives</td>
<td></td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Direct Connected (DC) Transport Protocol**</td>
<td></td>
<td>✓</td>
<td>✓</td>
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</tr>
<tr>
<td>User mode Memory Registration (UMR)**</td>
<td></td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>On Demand Paging (ODP)**</td>
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<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Core-direct based Collective Offload**</td>
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<td>✓</td>
<td>✓</td>
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<tr>
<td>SHARP-based Collective Offload*</td>
<td></td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

- *indicates disabled by default at runtime. Must use appropriate environment variable in MVAPICH2-X user guide to enable it.
- +indicates features only tested with InfiniBand network
Overview of MVAPICH2-X Features

• Direct Connect (DC) Transport
  - Available from MVAPICH2-X 2.3rc1 onwards

• CMA-based Collectives
  - Available from MVAPICH2-X 2.3rc1 onwards

• Optimized Asynchronous Progress
  - Available from MVAPICH2-X 2.3rc1 onwards

• XPMEM-based Reduction Collectives
  - Available from MVAPICH2-X 2.3rc1 onwards

• XPMEM-based Non-reduction Collectives
  - Available from MVAPICH2-X 2.3rc2 onwards
Impact of DC Transport Protocol on Neuron

- Up to 76% benefits over MVAPICH for Neuron using Direct Connected transport protocol at scale
  - VERSION 7.6.2 master (f5a1284) 2018-08-15
- Numbers taken on bbpv2.epfl.ch
  - Knights Landing nodes with 64 ppn
  - ./x86_64/special -mpi -c stop_time=2000 -c is_split=1 parinit.hoc
  - Used “runtime” reported by execution to measure performance
- Environment variables used
  - MVP_USE_DC=1
  - MVP_NUM_DC_TGT=64
  - MVP_SMALL_MSG_DC_POOL=96
  - MVP_LARGE_MSG_DC_POOL=96
  - MVP_USE_RDMA_CM=0

Available from MVAPICH2-X 2.3rc2 onwards

More details in talk
“Building Brain Circuits: Experiences with shuffling terabytes of data over MPI”, by Matthias Wolf at MUG’20
https://www.youtube.com/watch?v=TFi8O3-Hznw
Optimized CMA-based Collectives for Large Messages

- Significant improvement over existing implementation for Scatter/Gather with 1MB messages (up to $4x$ on KNL, $2x$ on Broadwell, $14x$ on OpenPower)
- New two-level algorithms for better scalability
- Improved performance for other collectives (Bcast, Allgather, and Alltoall)


Available since MVAPICH2-X 2.3b
Benefits of Asynchronous Progress Design: Broadwell + InfiniBand

**P3DFFT**

- Up to **27%** performance improvement in P3DFFT application with 112 processes
- Up to **26%** performance improvement in P3DFFT application with 224 processes
- Up to **33%** performance improvement in P3DFFT application with 448 processes

**High Performance Linpack (HPL)**

- Higher is better
- Memory Consumption = 69%
- Up to **29%** performance improvement in HPL application with 896 processes


Available since MVAPICH2-X 2.3rc1

Network Based Computing Laboratory
**Shared Address Space (XPMEM)-based Collectives Design**

**OSU_Allreduce (Broadwell 256 procs)**

- “**Shared Address Space**”-based true zero-copy Reduction collective designs in MVAPICH
- Offloaded computation/communication to peers ranks in reduction collective operation
- Up to **4X** improvement for 4MB Reduce and up to **1.8X** improvement for 4M AllReduce

---

**OSU_Reduce (Broadwell 256 procs)**

Available since MVAPICH2-X 2.3rc1

---

*J. Hashmi, S. Chakraborty, M. Bayatpour, H. Subramoni, and D. Panda, Designing Efficient Shared Address Space Reduction Collectives for Multi-/Many-cores, International Parallel & Distributed Processing Symposium (IPDPS ’18), May 2018.*
Performance of Non-Reduction Collectives with XPMEM

- 28 MPI Processes on single dual-socket Broadwell E5-2680v4, 2x14 core processor

![Graph showing performance of non-reduction collectives with XPMEM for Broadcast and Gather operations.]

- Broadcast latency is reduced by 5X over OpenMPI.
- Gather latency is reduced by 3X over OpenMPI.
Application Level Benefits of XPMEM-based Designs

**Intel XeonCPU E5-2687W v3 @ 3.10GHz (10-core, 2-socket)**

- Up to **20%** benefits over IMPI for CNTK DNN training using AllReduce
- Up to **27%** benefits over IMPI and up to **15%** improvement over MVAPICH for MiniAMR application kernel