Boosting the Performance of HPC Applications with MVAPICH2

A Tutorial at MUG’22

Presented by

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The MVAPICH Team
The Ohio State University

http://mvapich.cse.ohio-state.edu/
Overview of the MVAPICH2 Project

• High Performance open-source MPI Library
• Support for multiple interconnects
  – InfiniBand, Omni-Path, Ethernet/iWARP, RDMA over Converged Ethernet (RoCE), AWS EFA, Rockport Networks, and Slingshot10/11, Broadcom, Cornelis Networks OPX
• 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 3,275 organizations in 90 countries
• More than 1.61 Million downloads from the OSU site directly
• Empowering many TOP500 clusters (June ‘22 ranking)
  – 6th, 10,649,600-core (Sunway TaihuLight) at NSC, China
  – 16th, 448, 448 cores (Frontera) at TACC
  – 30th, 288,288 cores (Lassen) at LLNL
  – 42nd, 570,020 cores (Nurion) in South Korea and many more
• Available with software stacks of many vendors and Linux Distros (RedHat, SuSE, OpenHPC, and Spack)
• Partner in the 16th ranked TACC Frontera system
• Empowering Top500 systems for more than 20 years
Architecture of MVAPICH2 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 different combinations of environment variables meant to trigger different communication paths in MVAPICH2

Summary of all tests for one commit

Summary of an individual test

Details of individual combinations in one test
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: Installation and Setup MVAPICCH2 from Spack

Install Spack

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

Installing MVAPICCH2 (From Source)

$ spack info mvapich2
$ spack install mvapich2@2.3.7 %gcc@8.3.0
$ spack find -l -v -p mvapich2
Currently only for gcc@4.8.5

$ spack compiler find

Add the required mirrors

$ spack mirror add mvapich2x http://mvapich.cse.ohio-state.edu/download/mvapich/spack-mirror/mvapich2x

$ 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/mvapich2x/build_cache/public.key

$ spack gpg trust public.key
List the available binaries in the mirror

$ spack buildcache list -L -v -a

Install MVAPICH2-X and MVAPICH2-GDR

$ spack install mvapich2x@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
## MVAPICH2 Software Family

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<td>Advanced MPI features (SRD and XPMEM) with support for Amazon Elastic Fabric</td>
<td>MVAPICH2-X-AWS</td>
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<td>Adapter (EFA)</td>
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<tr>
<td>Optimized MPI for clusters with NVIDIA GPUs and for GPU-enabled Deep Learning</td>
<td>MVAPICH2-GDR</td>
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<tr>
<td>Applications</td>
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<td>Energy-aware MPI with Support for InfiniBand, Omni-Path, Ethernet/iWARP and,</td>
<td>MVAPICH2-EA</td>
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<td>RoCE (v1/v2)</td>
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<td>MPI Energy Monitoring Tool</td>
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MVAPICH2 2.3.7

- Released on 03/02/2022
- Major Features and Enhancements
  - Added support for systems with Rockport's switchless networks
    - Added automatic architecture detection
    - Optimized performance for point-to-point operations
  - Added support for the Cray Slingshot 10 interconnect
  - Enhanced support for blocking collective offload using Mellanox SHARP
    - Scatter and Scatterv
  - Enhanced support for non-blocking collective offload using Mellanox SHARP
    - Iallreduce, Ibarrier, Ibcast, and Ireduce
  - Enhanced collective tuning for several systems
  - Add support for GCC compiler v11
  - Add support for Intel IFX compiler
  - Update hwloc v1 code to v1.11.14 & hwloc v2 code to v2.4.2
Overview of MVAPICH2 Features

• Process Mapping and Point-to-point Intra-node Protocols
• Collectives
Process Mapping support in MVAPICH2

- Preset Binding Policies
  - bunch (Default)
  - scatter
  - hybrid
  - core (Default)
  - socket
  - numanode

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

MVAPICH2 detects processor architecture at job-launch
Preset Process-binding Policies – Bunch

• “Core” level “Bunch” mapping (Default)
  - MV2_CPU_BINDING_POLICY=bunch

• “Socket/Numanode” level “Bunch” mapping
  - MV2_CPU_BINDING_LEVEL=socket MV2_CPU_BINDING_POLICY=bunch
Preset Process-binding Policies – Scatter

- “Core” level “Scatter” mapping
  - `MV2_CPU_BINDING_POLICY=scatter`

- “Socket/Numanode” level “Scatter” mapping
  - `MV2_CPU_BINDING_LEVEL=socket MV2_CPU_BINDING_POLICY=scatter`
Process and thread binding policies in hybrid MPI+Threads

• A new process binding policy – “hybrid”
  - MV2_CPU_BINDING_POLICY = hybrid

• A new environment variable for co-locating Threads with MPI Processes
  - MV2_THREADS_PER_PROCESS = k
  - Automatically set to 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
  - MV2_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
- MV2_CPU_BINDING_POLICY = hybrid
- MV2_THREADS_PER_PROCESS = 4
- MV2_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
- MV2_CPU_BINDING_POLICY = hybrid
- MV2_THREADS_PER_PROCESS = 4
- MV2_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
• MV2_CPU_BINDING_POLICY = hybrid
• MV2_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 MV2_CPU_MAPPING=0:1:4:5 ./a.out

• Use ‘,’ or ‘-’ to bind to a set of cores:
  – $mpirun_rsh -np 64 -hostfile hosts MV2_CPU_MAPPING=0,2-4:1:5:6 ./a.out

• Is process binding working as expected?
  – MV2_SHOW_CPU_BINDING=1
    • Display CPU binding information
    • Launcher independent
    • Example
      – MV2_SHOW_CPU_BINDING=1 MV2_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 MVAPICH2 user guide for more information
• http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#x1-650006.5
Collective Communication in MVAPICH2

Run-time flags:
- All shared-memory based collectives: MV2_USE_SHMEM_COLL (Default: ON)
- Hardware Mcast-based collectives: MV2_USE_MCAST (Default: OFF)
- CMA and XPMEM-based collectives are 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 MV2_USE_MCAST=1 to enable MCAST-based designs
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>MV2_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 MVAPICH2 user guide for more information.

http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-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 *

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

* Bloch et al. Scalable Hierarchical Aggregation Protocol (SHArP): A Hardware Architecture for Efficient Data Reduction
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: MV2_ENABLE_SHARP = 1
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 MVAPICH2 2.3a

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<tr>
<td>MV2_ENABLE_SHARP=1</td>
<td>Enables SHARP-based collectives</td>
<td>Disabled</td>
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<tr>
<td>--enable-sharp</td>
<td>Configure flag to enable SHARP</td>
<td>Disabled</td>
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</table>

More details in the talk "Benefits of Streaming Aggregation with SHARPv2 in MVAPICH2, 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 MVAPICH2 user guide for more information
• [http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#x1-1050006.27](http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#x1-1050006.27)
MVAPICH2-3.0a

- Released on 08/15/2022
- Based on MPICH 3.4.3
- Added support for the ch4:ucx and ch4:ofi devices
- Support for MVAPICH2 enhanced collectives over OFI and UCX
- Added support for the Cray Slingshot 11 interconnect over OFI
  - Supports Cray Slingshot 11 network adapters
- Added support for the Cornelis OPX library over OFI
  - Supports Intel Omni-Path adapters
- Added support for the Intel PSM3 library over OFI
  - Supports Intel Columbiaville network adapters
- Added support for IB verbs over UCX
  - Supports IB and RoCE network adapters
Features of 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 MVAPICH2 collective designs
Upcoming/Planned Features

- MVAPICH2 custom ch4 netmod
- Enhanced pt2pt support for IB/RoCE systems
- GPU support
- Enhanced launcher
MPI Level Latency on Broadcom RoCE

• 3.88us inter-node point-to-point latency for small messages

Interconnect : InfiniBand EDR 100Gbps with Broadcom NetXtreme RoCE HCAs
Library : MVAPICH2 3.0a
CPU : 2 GHz AMD EPYC 7662 64-Core Processor
MPI Level Latency on Broadcom RoCE

- **12,171 MB/s** uni-directional peak bandwidth
- **24,394 MB/s** bi-directional peak bandwidth

Interconnect: InfiniBand EDR 100Gbps with Broadcom NetXtreme RoCE HCAs
Library: MVAPICH2 3.0a
CPU: 2 GHz AMD EPYC 7662 64-Core Processor
**MPI Level Latency on Slingshot 11**

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

Interconnect : Cray HPE Slingshot 11
Library : MVAPICH2 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 : MVAPICH2 3.0a
CPU : AMD EPYC 7763 (milan) Processor
MVAPICH2-3.0a+OPX vs MVAPICH2-2.3.7+PSM2 (Early Performance Results)

OSU_BIBW (2 Nodes, 1 PPN)

Message size (bytes)

Bandwidth (MB/s)

MVAPICH2-2.3.7-PSM  MVAPICH2-3.0a-OPX

OSU_BW (2 Nodes, 1 PPN)

Message size (bytes)

Bandwidth (MB/s)

MVAPICH2-2.3.7-PSM  MVAPICH2-3.0a-OPX

OSU_Latency (2 Nodes, 1 PPN)

Message size (bytes)

Latency (microseconds)

MVAPICH2-2.3.7-PSM  MVAPICH2-3.0a-OPX

OSU_MBW_MR (2 Nodes)

Message size (bytes)

Messages per second

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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MVAPICH2-X for MPI and Hybrid MPI + PGAS Applications

- **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

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<th>Features for InfiniBand (OFA-IB-CH3) and RoCE (OFA-RoCE-CH3)</th>
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<th>Basic-XPMEM</th>
<th>Intermediate</th>
<th>Advanced</th>
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<tr>
<td>Architecture Specific Point-to-point and Collective Optimizations for x86, OpenPOWER, and ARM</td>
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<tr>
<td>Optimized Support for PGAS models (UPC, UPC++, OpenSHMEM, CAF) and Hybrid MPI+PGAS models</td>
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<td>CMA-Aware Collectives</td>
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<td>Optimized Asynchronous Progress*</td>
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<td>InfiniBand Hardware Multicast-based MPI_Bcast*+</td>
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<td>Direct Connected (DC) Transport Protocol**</td>
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</tr>
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<td>On Demand Paging (ODP)**</td>
<td>☑️</td>
<td>☑️</td>
<td>☑️</td>
<td>☑️</td>
</tr>
<tr>
<td>Core-direct based Collective Offload**</td>
<td>☑️</td>
<td>☑️</td>
<td>☑️</td>
<td>☑️</td>
</tr>
<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

• **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 MVAPICH2 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
  - MV2_USE_DC=1
  - MV2_NUM_DC_TGT=64
  - MV2_SMALL_MSG_DC_POOL=96
  - MV2_LARGE_MSG_DC_POOL=96
  - MV2_USE_RDMA_CM=0

**Overhead of RC protocol for connection establishment and communication**

**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 the New Asynchronous Progress Design: Broadwell + InfiniBand

**P3DFFT**

<table>
<thead>
<tr>
<th>Number of Processes</th>
<th>Time per loop in seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>112</td>
<td>MVAPICH2 Async 27%</td>
</tr>
<tr>
<td>224</td>
<td>MVAPICH2 Default 26%</td>
</tr>
<tr>
<td>448</td>
<td>IMPI 2019 Default 33%</td>
</tr>
</tbody>
</table>

Lower is better

**High Performance Linpack (HPL)**

<table>
<thead>
<tr>
<th>Number of Processes</th>
<th>Performance in GFLOPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>224</td>
<td>MVAPICH2 Async 8%</td>
</tr>
<tr>
<td>448</td>
<td>MVAPICH2 Default 12%</td>
</tr>
<tr>
<td>896</td>
<td>IMPI 2019 Default 29%</td>
</tr>
</tbody>
</table>

Higher is better

Memory Consumption = 69%

Up to 33% performance improvement in P3DFFT application with **448 processes**

Up to 29% performance improvement in HPL application with **896 processes**


Available since MVAPICH2-X 2.3rc1
**Shared Address Space (XPMEM)-based Collectives Design**

- "Shared Address Space"-based true zero-copy Reduction collective designs in MVAPICH2
- 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

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

- **Broadcast**
  - Intel MPI 2018
  - OpenMPI 3.0.1
  - MV2X-2.3rc1 (CMA Coll)
  - MV2X-2.3rc2 (XPMEM Coll)
  - Latency (us)
  - Message Size (Bytes)
  - 5X over OpenMPI

- **Gather**
  - Intel MPI 2018
  - OpenMPI 3.0.1
  - MV2X-2.3rc1 (CMA Coll)
  - MV2X-2.3rc2 (XPMEM Coll)
  - Latency (us)
  - Message Size (Bytes)
  - 3X over OpenMPI

- **28 MPI Processes** on single dual-socket Broadwell E5-2680v4, 2x14 core processor
Application Level Benefits of XPMEM-based Designs

CNTK AlexNet Training
(B.S=default, iteration=50, ppn=28)

- 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 MVAPICH2 for MiniAMR application kernel

MiniAMR (dual-socket, ppn=16)

- Intel MPI
- MVAPICH2
- MVAPICH2-XPMEM
## MVAPICH2 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>MVAPICH2</td>
</tr>
<tr>
<td>Optimized Support for Microsoft Azure Platform with InfiniBand</td>
<td>MVAPICH2-Azure</td>
</tr>
<tr>
<td>Advanced MPI features/support (UMR, ODP, DC, Core-Direct, SHArP, XPMEM), OSU INAM (InfiniBand Network Monitoring and Analysis),</td>
<td>MVAPICH2-X</td>
</tr>
<tr>
<td>Advanced MPI features (SRD and XPMEM) with support for Amazon Elastic Fabric Adapter (EFA)</td>
<td>MVAPICH2-X-AWS</td>
</tr>
<tr>
<td>Optimized MPI for clusters with NVIDIA and AMD GPUs and for GPU-enabled Deep Learning Applications</td>
<td>MVAPICH2-GDR</td>
</tr>
<tr>
<td>Energy-aware MPI with Support for InfiniBand, Omni-Path, Ethernet/iWARP and, RoCE (v1/v2)</td>
<td>MVAPICH2-EA</td>
</tr>
<tr>
<td>MPI Energy Monitoring Tool</td>
<td>OEMT</td>
</tr>
<tr>
<td>InfiniBand Network Analysis and Monitoring</td>
<td>OSU INAM</td>
</tr>
<tr>
<td>Microbenchmarks for Measuring MPI and PGAS Performance</td>
<td>OMB</td>
</tr>
</tbody>
</table>
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: MVAPICH2-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:

MPI_Send(s_devbuf, size, ...);

At Receiver:

MPI_Recv(r_devbuf, size, ...);

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/
Simple Installation steps for both systems

Pick the right MVAPICH2-GDR RPM from Downloads page:

- [http://mvapich.cse.ohio-state.edu/downloads/](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.cudait0.0.mofed4.5.gnu4.8.5-2.3.7-1.elit.x86_64.rpm](http://mvapich.cse.ohio-state.edu/download/mvapich/gdr/2.3/mofed4.5/mvapich2-gdr-mcast.cudait0.0.mofed4.5.gnu4.8.5-2.3.7-1.elit.x86_64.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 MVAPICH2 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 MV2_GPU_AUTO_REBIND=1
  - Added NCCL communication substrate for various non-blocking MPI collectives
    - MPI_Allreduce, MPI_Ireduce, 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
    - MPI_Allreduce, MPI_Reduce, MPI_Allgather, MPI_Allgatherv, MPI_Alltoall, MPI_Alltoallv, MPI_Scatter, MPI_Scatterv, MPI_Gather, MPI_Gatherv, and MPI_Bcast
  - 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 MV2_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
## 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>MV2_USE_GDRCOPY</td>
<td>• Enable / Disable GDRCOPY-based designs</td>
<td>1 (Enabled)</td>
<td>• Always enable</td>
</tr>
<tr>
<td>MV2_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>MV2_GPUDIRECT_GDRCOPY_LIBRARY</td>
<td>• Path to the GDRCOPY library</td>
<td>Unset</td>
<td>• Always set</td>
</tr>
<tr>
<td>MV2_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](http://mvapich.cse.ohio-state.edu/userguide/gdr/#_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>MV2_USE_GPUDIRECT_LOOPBACK</td>
<td>Enable / Disable LOOPBACK-based designs</td>
<td>1 (Enabled)</td>
<td>Always enable</td>
</tr>
<tr>
<td>MV2_GPUDIRECT_LOOPBACK_LIMIT</td>
<td>Controls messages size until which LOOPBACK is used</td>
<td>8 KByte</td>
<td>Tune for your system, GPU type, host architecture and HCA. Impacts the eager performance. Sensitive to the P2P issue</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 GPUsDirect 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><strong>MV2_USE_GPUDIRECT</strong></td>
<td>• Enable / Disable GDR-based designs</td>
<td>1 (Enabled)</td>
<td>• Always enable</td>
</tr>
<tr>
<td><strong>MV2_GPUDIRECT_LIMIT</strong></td>
<td>• Controls messages size until which GPUsDirect RDMA is used</td>
<td>8 KByte</td>
<td>• Tune for your system • GPU type, host architecture and CUDA version: impact pipelining overheads and P2P bandwidth bottlenecks</td>
</tr>
<tr>
<td><strong>MV2_USE_GPUDIRECT_RECEIVE_LIMIT</strong></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 • GPU type, HCA type and configuration</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)
MVAPICH2-GDR with CUDA-aware MPI Support

**GPU-GPU Inter-node Latency**

Latency (us)

Message Size (Bytes)

- MV2-(NO-GDR)
- MV2-GDR 2.3

- 1.85us
- 10x

**GPU-GPU Inter-node Bi-Bandwidth**

Bandwidth (MB/s)

Message Size (Bytes)

- MV2-(NO-GDR)
- MV2-GDR-2.3

- 11X

**GPU-GPU Inter-node Bandwidth**

Bandwidth (MB/s)

Message Size (Bytes)

- MV2-(NO-GDR)
- MV2-GDR-2.3

- 9X

MVAPICH2-GDR-2.3.7

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
**Application-Level Evaluation (HOOMD-blue)**

**64K Particles**

<table>
<thead>
<tr>
<th>Number of Processes</th>
<th>Average Time Steps per second (TPS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>MV2</td>
</tr>
<tr>
<td>8</td>
<td>MV2</td>
</tr>
<tr>
<td>16</td>
<td>MV2</td>
</tr>
<tr>
<td>32</td>
<td>MV2</td>
</tr>
</tbody>
</table>

**256K Particles**

<table>
<thead>
<tr>
<th>Number of Processes</th>
<th>Average Time Steps per second (TPS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>MV2</td>
</tr>
<tr>
<td>8</td>
<td>MV2</td>
</tr>
<tr>
<td>16</td>
<td>MV2</td>
</tr>
<tr>
<td>32</td>
<td>MV2</td>
</tr>
</tbody>
</table>

- **Platform:** Wilkes (Intel Ivy Bridge + NVIDIA Tesla K20c + Mellanox Connect-IB)
- **HoomDBlue Version 1.0.5**
  - GDRCOPY enabled: `MV2_USE_CUDA=1 MV2_IBA_HCA=mlx5_0 MV2_IBA_EAGER_THRESHOLD=32768 MV2_VBUF_TOTAL_SIZE=32768 MV2_USE_GPUDIRECT_LOOPBACK_LIMIT=32768 MV2_USE_GPUDIRECT_GDRCOPY=1 MV2_USE_GPUDIRECT_GDRCOPY_LIMIT=16384`
MPI Datatype support in MVAPICH2

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

At Sender:

```c
MPI_Type_vector (n_blocks, n_elements, stride, old_type, &new_type);
MPI_Type_commit(&new_type);
...
MPI_Send(s_buf, size, new_type, dest, tag, MPI_COMM_WORLD);
```

• Inside MVAPICH2
  - 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

Application-Level Evaluation (Cosmo) and Weather Forecasting in Switzerland

Wilkes GPU Cluster

CSCS GPU cluster

- 2X improvement on 32 GPUs nodes
- 30% improvement on 96 GPU nodes (8 GPUs/node)

CSCS and MeteoSwiss (Switzerland) co-design of MV2-GDR and Cosmo Application


Cosmo model: http://www2.cosmo-model.org/content/tasks/operational/meteoSwiss/
**MVAPICH2-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

**Graphs**

- **GPU-based DDTBench mimics MILC communication kernel**
  - Problem size
  - MILC
  - Speedup
  - OpenMPI 4.0.0
  - MVAPICH2-GDR 2.3.1
  - MVAPICH2-GDR-Next

- **Communication Kernel of COSMO Model**
  - Improved 3.4X
  - Improved 15X

**Platform:**
- **Nvidia DGX-2 system** (NVIDIA Volta GPUs connected with NVSwitch), CUDA 9.2
- **Cray CS-Storm** (16 NVIDIA Tesla K80 GPUs per node), CUDA 8.0

**Figure References:**
- [GitHub](https://github.com/cosunae/HaloExchangeBenchmarks)
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

---

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

• MPC
  - Installation (Built-in with MVAPICH2-GDR)
  - Runtime parameters
    MV2_USE_CUDA=1 MV2_USE_COMPRESSION=1 MV2_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"
    MV2_USE_CUDA=1 MV2_USE_COMPRESSION=1 MV2_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>MV2_USE_COMPRESSION</td>
<td>0</td>
<td>Enable compression</td>
</tr>
<tr>
<td>MV2_COMPRESSION_ALGORITHM</td>
<td>1</td>
<td>1: Use MPC compression 2: Use ZFP compression</td>
</tr>
<tr>
<td>MV2_COMPRESSION_THRESHOLD</td>
<td>524288</td>
<td>Threshold of using compression for inter-node pt2pt GPU communication</td>
</tr>
<tr>
<td>MV2_COMPRESSION_THRESHOLD_INTRA</td>
<td>524288</td>
<td>Threshold of using compression for intra-node pt2pt GPU communication</td>
</tr>
<tr>
<td>MV2_COMPRESSION_DIMENSION</td>
<td>Depends on compression library</td>
<td>Dimensionality of input data [1, 31]: For MPC compression 1: For ZFP compression</td>
</tr>
<tr>
<td>MV2_COMPRESSION_ZFP_RATE</td>
<td>8</td>
<td>Compressed bits/value [1, 32]: For ZFP compression only</td>
</tr>
</tbody>
</table>
“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

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

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MUG’22
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Collectives Performance on DGX2-A100 – Small 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)
Collectives Performance on DGX2-A100 – Large Message

- **Allgather (4 nodes, 8 ppn, 32 GPUs)**
  - MVAPICH2-GDR 2.3.7
  - NCCL

- **Bcast (4 nodes, 8 ppn, 32 GPUs)**
  - MVAPICH2-GDR 2.3.7
  - NCCL

- **Reduce (4 nodes, 8 ppn, 32 GPUs)**
  - MVAPICH2-GDR 2.3.7
  - NCCL

- **Allreduce (4 nodes, 8 ppn, 32 GPUs)**
  - MVAPICH2-GDR 2.3.7
  - NCCL
Highly Efficient Optimized Alltoall(v) Communication

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

**ROCm-aware MVAPICH2-GDR - Support for AMD GPUs**

**Intra-Node Point-to-Point Latency**

- **Allreduce** - 64 GPUs (8 nodes, 8 GPUs Per Node)
  - MVAPICH2-GDR 2.3.6 vs OpenMPI 4.1.1 + UCX 1.11.0
  - MVAPICH2-GDR 2.3.6: 1.75 us
  - OpenMPI 4.1.1 + UCX 1.11.0: 3.99 us

**Inter-Node Point-to-Point Latency**

- **Bcast** - 64 GPUs (8 nodes, 8 GPUs Per Node)
  - MVAPICH2-GDR 2.3.6 vs OpenMPI 4.1.1 + UCX 1.11.0
  - MVAPICH2-GDR 2.3.6: 16.27 us
  - OpenMPI 4.1.1 + UCX 1.11.0: 2645.23 us

Corona Cluster @ LLNL - ROCm-4.3.0 (mi50 AMD GPUs)

Available with MVAPICH2-GDR 2.3.5+ & OMB v5.7+

MVAPICH2-GDR on Slingshot-10 - GPU

Point-to-Point – Intra-Node

Latency:

Bandwidth:

Point-to-Point – Inter-Node

Latency:

Bandwidth:

MPI_Bcast (4 Nodes, 64PPN)

MPI_Allreduce (4 Nodes, 64PPN)

AMD Epyc Rome CPUs and AMD MI100 GPUs
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.
Amber: Impact of Tuning Eager Threshold

- Tuning the Eager threshold has a significant impact on application performance by avoiding the synchronization of rendezvous protocol and thus yielding better communication computation overlap
- 19% improvement in overall execution time at 256 processes
- Library Version: MVAPICH2 2.2
- MVAPICH Flags used
  - MV2_IBA_EAGER_THRESHOLD=131072
  - MV2_VBUF_TOTAL_SIZE=131072
- Input files used
  - Small: MDIN
  - Large: PMTOP

Data Submitted by: Dong Ju Choi @ UCSD
MiniAMR: Impact of Tuning Eager Threshold

- Tuning the Eager threshold has a significant impact on application performance by avoiding the synchronization of rendezvous protocol and thus yielding better communication computation overlap
- 8% percent reduction in total communication time
- Library Version: MVAPICH2 2.2
- MVAPICH Flags used
  - MV2_IBA_EAGER_THRESHOLD=32768
  - MV2_VBUF_TOTAL_SIZE=32768

Data Submitted by Karen Tomko @ OSC and Dong Ju Choi @ UCSD
SMG2000: Impact of Tuning Transport Protocol

- UD-based transport protocol selection benefits the SMG2000 application
- 22% and 6% on 1,024 and 4,096 cores, respectively
- Library Version: MVAPICH2 2.1
- MVAPICH Flags used
  - MV2_USE_ONLY_UD=1
- System Details
  - Stampede@ TACC
  - Sandybridge architecture with dual 8-cores nodes and ConnectX-3 FDR network

Data Submitted by Jerome Vienne @ TACC
UD-based transport protocol selection benefits the SMG2000 application

- 15% and 27% improvement is seen for 768 and 1,024 processes respectively

- Library Version: MVAPICH2 2.2
- MVAPICH Flags used
  - MV2_USE_ONLY_UD=1
- Input File
  - YuEtAl2012
- System Details
  - Comet@SDSC
  - Haswell nodes with dual 12-cores socket per node and Mellanox FDR (56 Gbps) network.

Data Submitted by Mahidhar Tatineni @ SDSC
HPCG: Impact of Collective Tuning for MPI+OpenMP Programming Model

- Partial subscription nature of hybrid MPI+OpenMP programming requires a new level of collective tuning
  - For PPN=2 (Processes Per Node), the tuned version of MPI_Reduce shows 51% improvement on 2,048 cores
- 24% improvement on 512 cores
  - 8 OpenMP threads per MPI processes
- Library Version: MVAPICH2 2.1
- MVAPICH Flags used
  - The tuning parameters for hybrid MPI+OpenMP programming models is on by default from MVAPICH2-2.1 onward
- System Details
  - Stampede@ TACC
  - Sandybridge architecture with dual 8-cores nodes and ConnectX-3 FDR network

Data Submitted by Jerome Vienne and Carlos Rosales-Fernandez @ TACC
HOOMD-blue: Impact of GPUDirect RDMA Based Tuning

- HOOMD-blue is a Molecular Dynamics simulation using a custom force field.
- GPUDirect specific features selection and tuning significantly benefit the HOOMD-blue application. We observe a factor of 2X improvement on 32 GPU nodes, with both 64K and 256K particles.

- Library Version: MVAPICH2-GDR 2.2
- MVAPICH-GDR Flags used
  - MV2_USE_CUDA=1
  - MV2_USE_GPUDIRECT=1
  - MV2_GPUDIRECT_GDRCOPY=1

- System Details
  - Wilkes@Cambridge
  - 128 Ivybridge nodes, each node is a dual 6-cores socket with Mellanox FDR

Data Submitted by Khaled Hamidouche @ OSU
MVAPICH2-J 2.3.7

- Released on 08/12/2022
- Provides Java bindings to the MVAPICH2 family of libraries
- Support for communication of basic Java datatypes and Java new I/O (NIO) package direct ByteBuffers
- Support for blocking and non-blocking point-point communication protocols
- Support for blocking collective and strided collective communication protocols
- Support for Dynamic Process Management (DPM) functionality
- Support for all high-speed interconnects that MVAPICH2 supports including InfiniBand, Internet Wide-area RDMA Protocol (iWARP), RDMA over Converged Ethernet (RoCE), Intel's Performance Scaled Messaging (PSM), Omni-Path, etc.

More details in the talk “Benchmarking Parallel Python and Java Applications using OMB and MVAPICH2” by Aamir Shafi and Nawras Alnaasan, The Ohio State University
OMB 6.0

- Released on 08/19/2022
- Support for Java pt2pt benchmarks
- Support for Java collective benchmarks
- Support for Python pt2pt benchmarks
- Support for Python collective benchmarks

More details in the talk “Benchmarking Parallel Python and Java Applications using OMB and MVAPICH2” by Aamir Shafi and Nawras Alnaasan, The Ohio State University
MVAPICH2 – Future Roadmap and Plans for Exascale

- Initial support for the CH4 channel
  - Late 2022
- Making CH4 channel default
  - Early 2023
- 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*
  - CAPI*
  - Bluefield2*
- 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 MVAPICH2 Releases
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- A. H. Tu (Ph.D.)
- H. Ahn (Ph.D.)

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- 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 (M.S.)
- S. Dandapanthula (M.S.)
- V. Dhanraj (M.S.)
- C.-H. Chu (Ph.D.)
- T. Gangadhara (M.S.)
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- W. Jiang (M.S.)
- J. Jose (Ph.D.)
- M. Kedia (M.S.)
- S. Kini (M.S.)
- M. Koop (Ph.D.)
- K. Kulkarni (M.S.)
- R. Kumar (M.S.)
- S. Krishnamoorthy (M.S.)
- K. Kandalla (Ph.D.)
- M. Li (Ph.D.)

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- M. S. Ghazimeersaeed
- H.-W. Jin
- E. Mancini
- A. Ruhela

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- T. Chen
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- R. Vaidya (Ph.D.)
- J. Yao (Ph.D.)
- M. Han (M.S.)
- A. Gupta (M.S.)
- P. Lai (M.S.)
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- A. Mamidala (Ph.D.)
- G. Marsh (M.S.)
- V. Meshram (M.S.)
- A. Moody (M.S.)
- S. Naravula (Ph.D.)
- R. Noronha (Ph.D.)
- X. Ouyang (Ph.D.)
- J. Wu (Ph.D.)
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The High-Performance MPI/PGAS Project
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/