



MVAPICH

MPI, PGAS and Hybrid MPI+PGAS Library



Exploiting Computation and Communication Overlap in MVAPICH2 and MVAPICH2-GDR MPI Libraries

Talk at

Overlapping Communication with Computation Symposium (April '18)

by

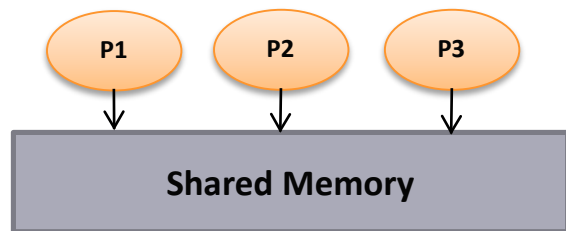
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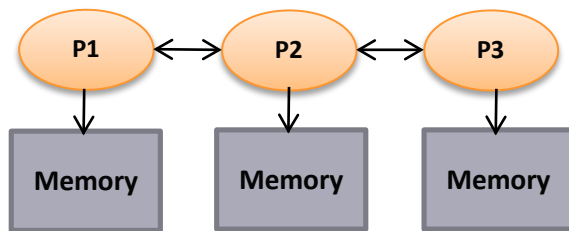
<http://www.cse.ohio-state.edu/~panda>

Parallel Programming Models Overview



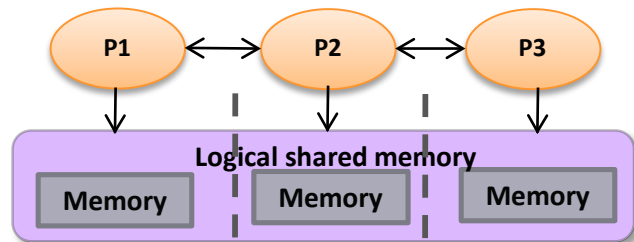
Shared Memory Model

SHMEM, DSM



Distributed Memory Model

MPI (Message Passing Interface)



Partitioned Global Address Space (PGAS)

Global Arrays, UPC, Chapel, X10, CAF, ...

- Programming models provide abstract machine models
- Models can be mapped on different types of systems
 - e.g. Distributed Shared Memory (DSM), MPI within a node, etc.
- PGAS models and Hybrid MPI+PGAS models are gradually receiving importance

Supporting Programming Models for Multi-Petaflop and Exaflop Systems: Challenges

Application Kernels/Applications

Middleware

Programming Models

MPI, PGAS (UPC, Global Arrays, OpenSHMEM), CUDA, OpenMP, OpenACC, Cilk, Hadoop (MapReduce), Spark (RDD, DAG), etc.

Communication Library or Runtime for Programming Models

Point-to-point
Communication

Collective
Communication

Energy-
Awareness

Synchronization
and Locks

I/O and
File Systems

Fault
Tolerance

Networking Technologies

(InfiniBand, 40/100GigE,
Aries, and Omni-Path)

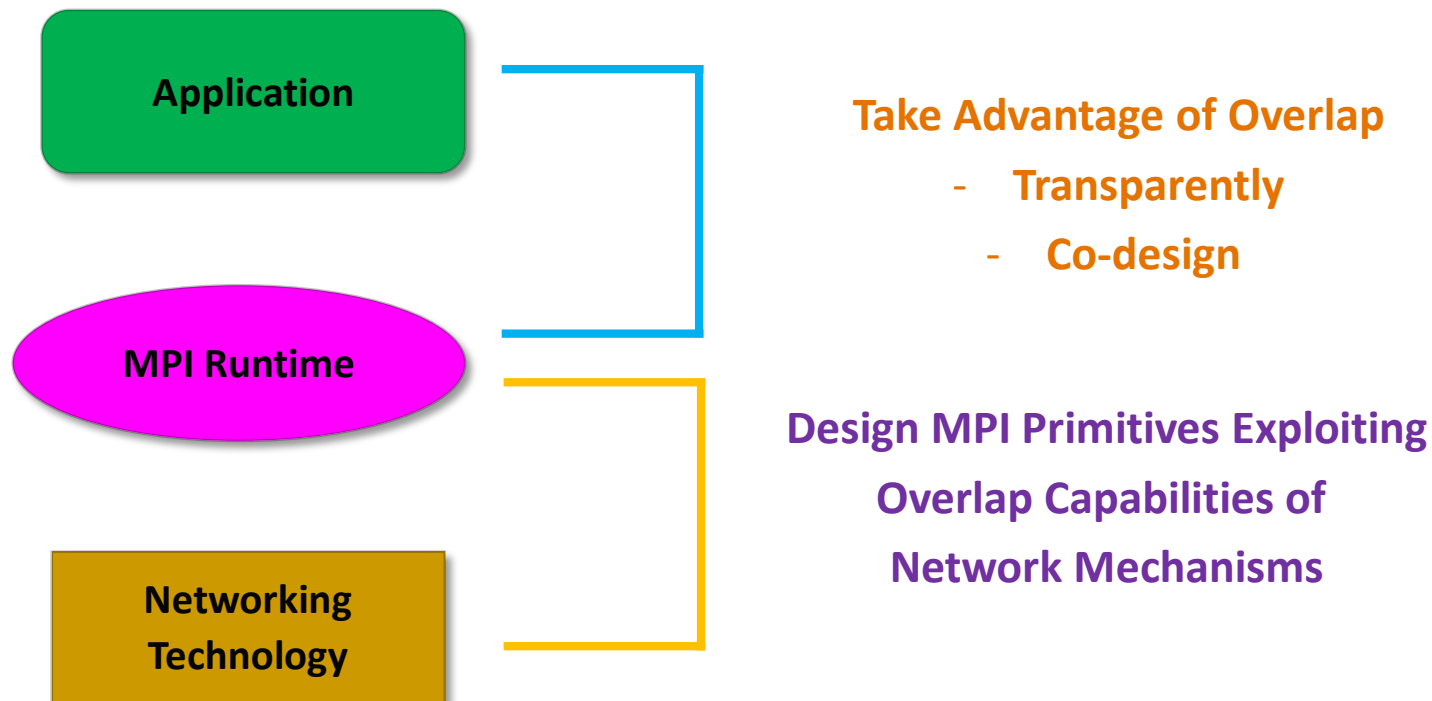
**Multi-/Many-core
Architectures**

**Accelerators
(GPU and FPGA)**

Co-Design
Opportunities
and
Challenges
across Various
Layers

Performance
Scalability
Resilience

Basic Concept of Overlapping Communication with Computation

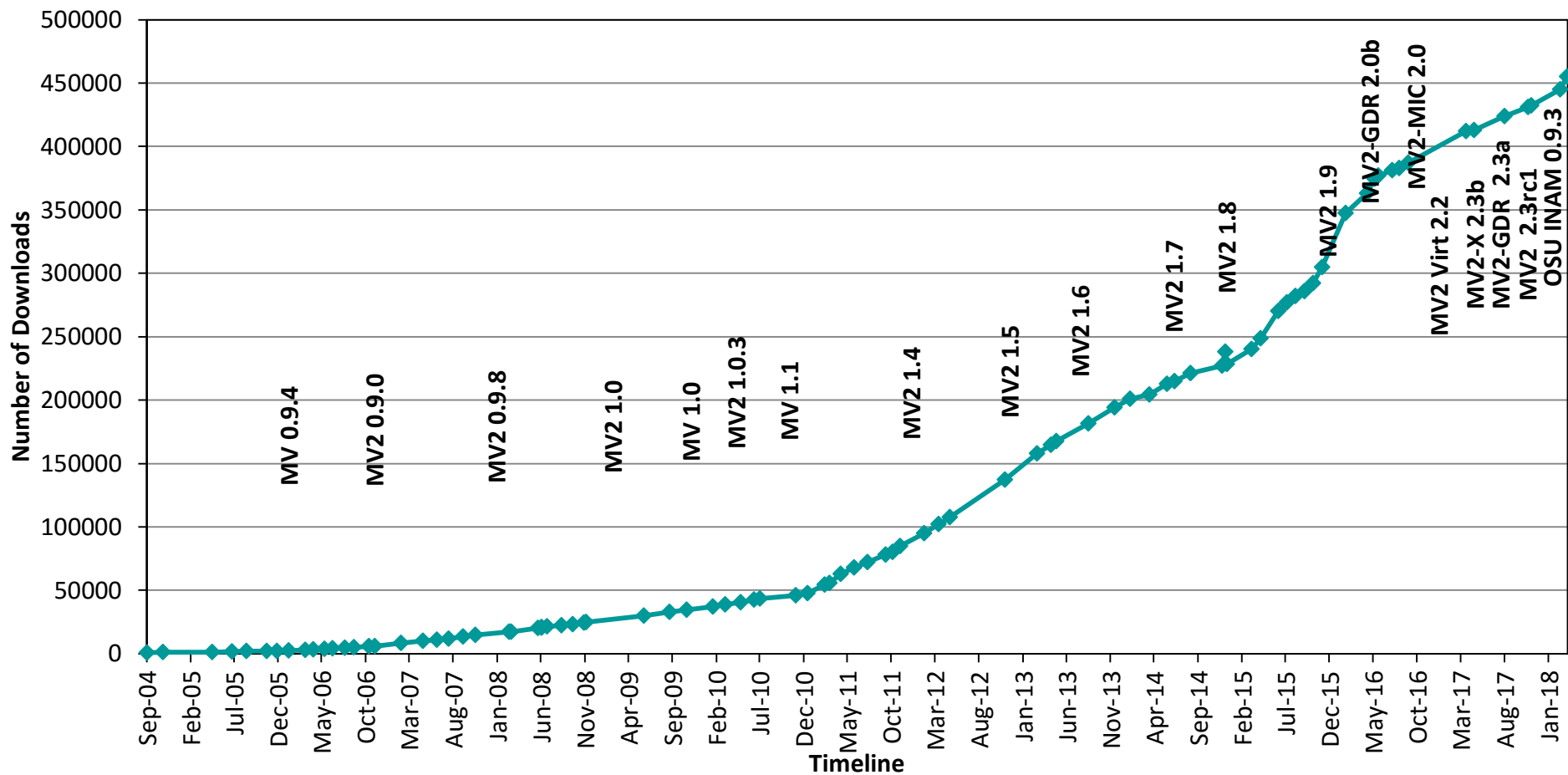


Overview of the MVAPICH2 Project

- High Performance open-source MPI Library for InfiniBand, Omni-Path, Ethernet/iWARP, and RDMA over Converged Ethernet (RoCE)
 - MVAPICH (MPI-1), MVAPICH2 (MPI-2.2 and MPI-3.1), Started in 2001, First version available in 2002
 - MVAPICH2-X (MPI + PGAS), Available since 2011
 - Support for GPGPUs (MVAPICH2-GDR) and MIC (MVAPICH2-MIC), Available since 2014
 - Support for Virtualization (MVAPICH2-Virt), Available since 2015
 - Support for Energy-Awareness (MVAPICH2-EA), Available since 2015
 - Support for InfiniBand Network Analysis and Monitoring (OSU INAM) since 2015
 - **Used by more than 2,875 organizations in 86 countries**
 - **More than 460,000 (> 0.46 million) downloads from the OSU site directly**
 - Empowering many TOP500 clusters (Nov '17 ranking)
 - **1st, 10,649,600-core (Sunway TaihuLight) at National Supercomputing Center in Wuxi, China**
 - 9th, 556,104 cores (Oakforest-PACS) in Japan
 - 12th, 368,928-core (Stampede2) at TACC
 - 17th, 241,108-core (Pleiades) at NASA
 - 48th, 76,032-core (Tsubame 2.5) at Tokyo Institute of Technology
 - Available with software stacks of many vendors and Linux Distros (RedHat and SuSE)
 - <http://mvapich.cse.ohio-state.edu>
- Empowering Top500 systems for over a decade



MVAPICH2 Release Timeline and Downloads



Architecture of MVAPICH2 Software Family

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)

Transport Protocols

RC

XRC

UD

DC

Modern Features

UMR

ODP

SR-IOV

Multi
Rail

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

Transport Mechanisms

Shared
Memory

CMA

IVSHMEM

XPMMEM*

Modern Features

MCDRAM*

NVLink*

CAPI*

* Upcoming

MVAPICH2 Software Family

High-Performance Parallel Programming Libraries

MVAPICH2	Support for InfiniBand, Omni-Path, Ethernet/iWARP, and RoCE
MVAPICH2-X	Advanced MPI features, OSU INAM, PGAS (OpenSHMEM, UPC, UPC++, and CAF), and MPI+PGAS programming models with unified communication runtime
MVAPICH2-GDR	Optimized MPI for clusters with NVIDIA GPUs
MVAPICH2-Virt	High-performance and scalable MPI for hypervisor and container based HPC cloud
MVAPICH2-EA	Energy aware and High-performance MPI
MVAPICH2-MIC	Optimized MPI for clusters with Intel KNC

Microbenchmarks

OMB	Microbenchmarks suite to evaluate MPI and PGAS (OpenSHMEM, UPC, and UPC++) libraries for CPUs and GPUs
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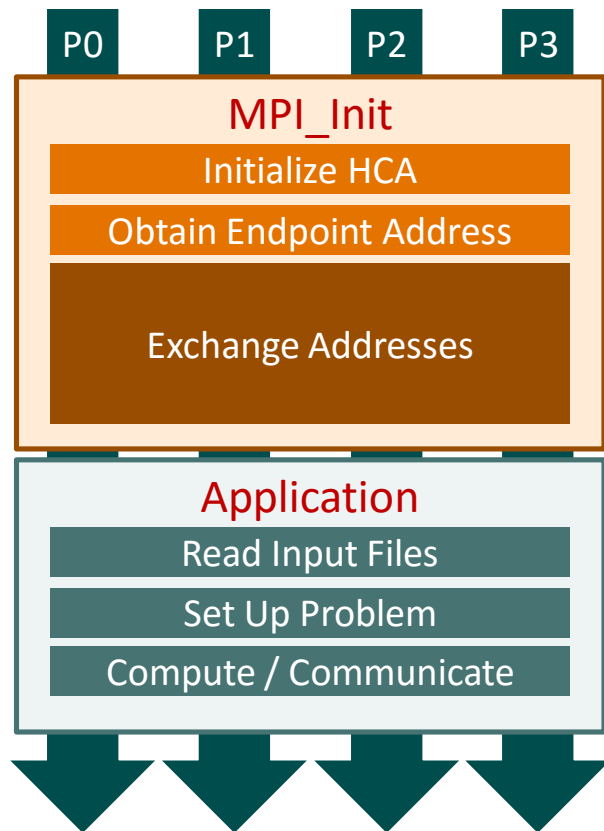
Tools

OSU INAM	Network monitoring, profiling, and analysis for clusters with MPI and scheduler integration
OEMT	Utility to measure the energy consumption of MPI applications

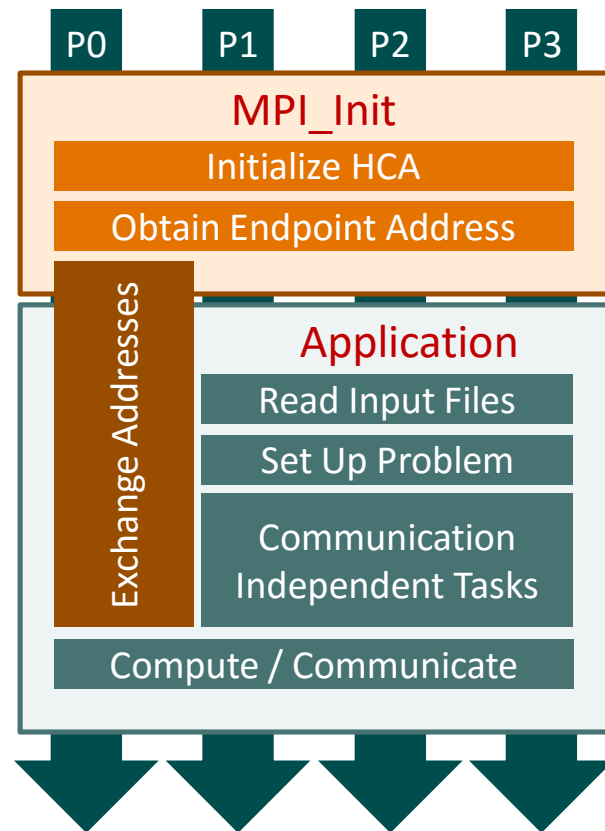
Presentation Outline

- MVAPICH2/MVAPICH2-X
 - Job Startup
 - Point-to-point Communication
 - Remote Memory Access (RMA)
 - Collective Communication
- MVAPICH2-GDR
 - Support for InfiniBand Core-Direct
 - GPU-kernel based Reduction
 - Datatype Processing
- Deep Learning Application: OSU Caffe

Overlapping Application Compute with MPI Startup

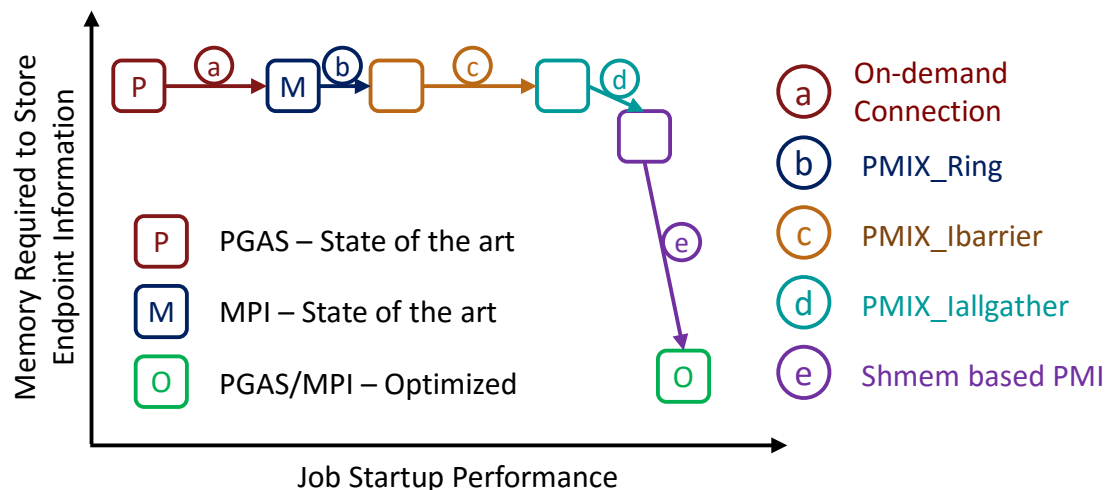


No Overlap between MPI_Init and Application Computation



MPI can continue to initialize in the background while Application starts

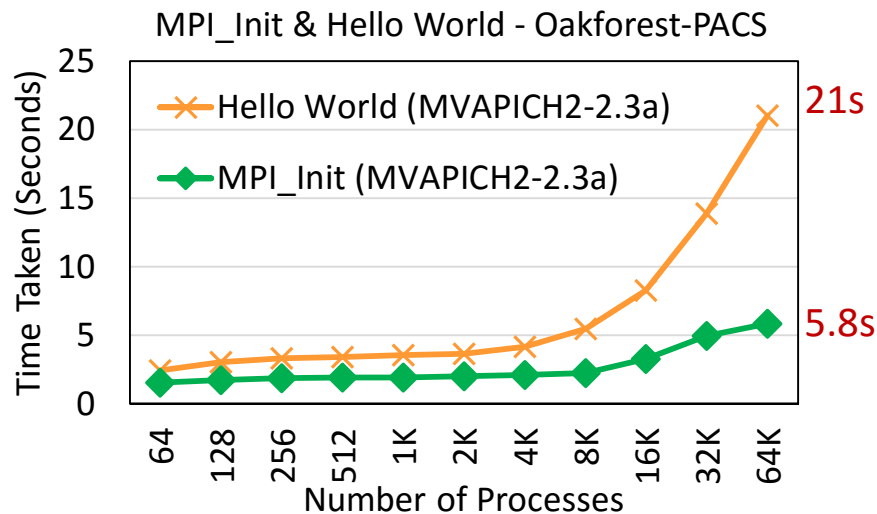
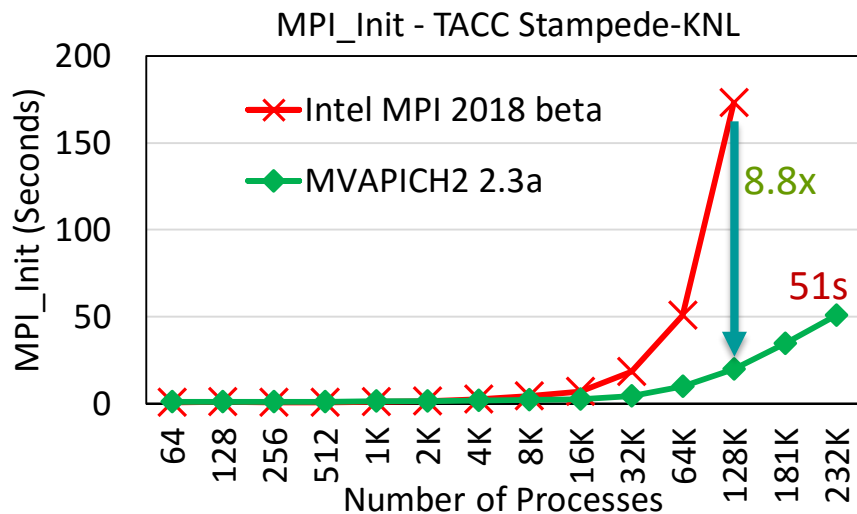
Towards High Performance and Scalable Startup at Exascale



- Near-constant MPI and OpenSHMEM initialization time at any process count
- 10x and 30x improvement in startup time of MPI and OpenSHMEM respectively at 16,384 processes
- Memory consumption reduced for remote endpoint information by $O(\text{processes per node})$
- 1GB Memory saved per node with 1M processes and 16 processes per node

- (a) On-demand Connection Management for OpenSHMEM and OpenSHMEM+MPI.** S. Chakraborty, H. Subramoni, J. Perkins, A. A. Awan, and D K Panda, 20th International Workshop on High-level Parallel Programming Models and Supportive Environments (HIPS '15)
- (b) PMI Extensions for Scalable MPI Startup.** S. Chakraborty, H. Subramoni, A. Moody, J. Perkins, M. Arnold, and D K Panda, Proceedings of the 21st European MPI Users' Group Meeting (EuroMPI/Asia '14)
- (c) (d) Non-blocking PMI Extensions for Fast MPI Startup.** S. Chakraborty, H. Subramoni, A. Moody, A. Venkatesh, J. Perkins, and D K Panda, 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid '15)
- (e) SHMEMPMI – Shared Memory based PMI for Improved Performance and Scalability.** S. Chakraborty, H. Subramoni, J. Perkins, and D K Panda, 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid '16)

Startup Performance on KNL + Omni-Path

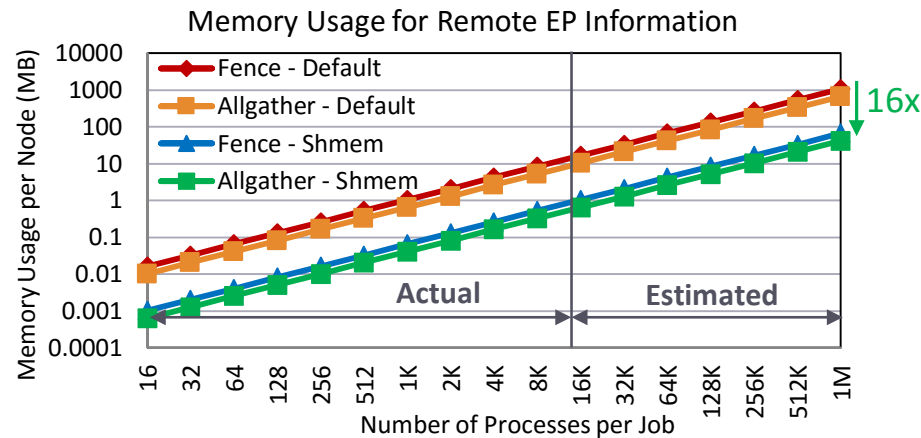
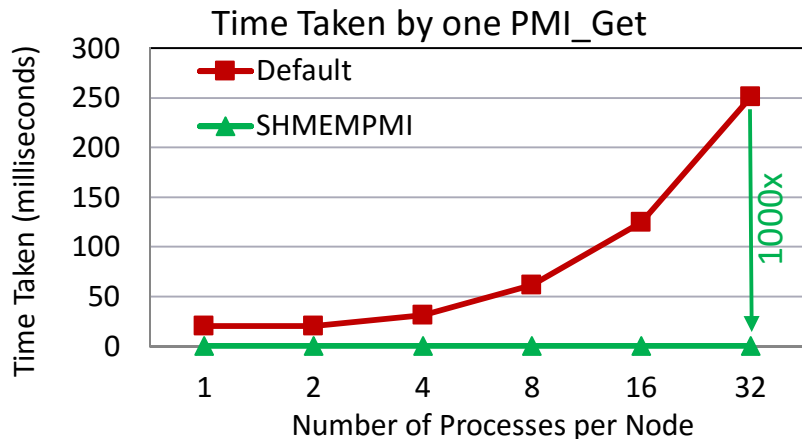


- MPI_Init takes 51 seconds on 231,956 processes on 3,624 KNL nodes (Stampede – Full scale)
- 8.8 times faster than Intel MPI at 128K processes (Courtesy: TACC)
- At 64K processes, MPI_Init and Hello World takes 5.8s and 21s respectively (Oakforest-PACS)
- All numbers reported with 64 processes per node

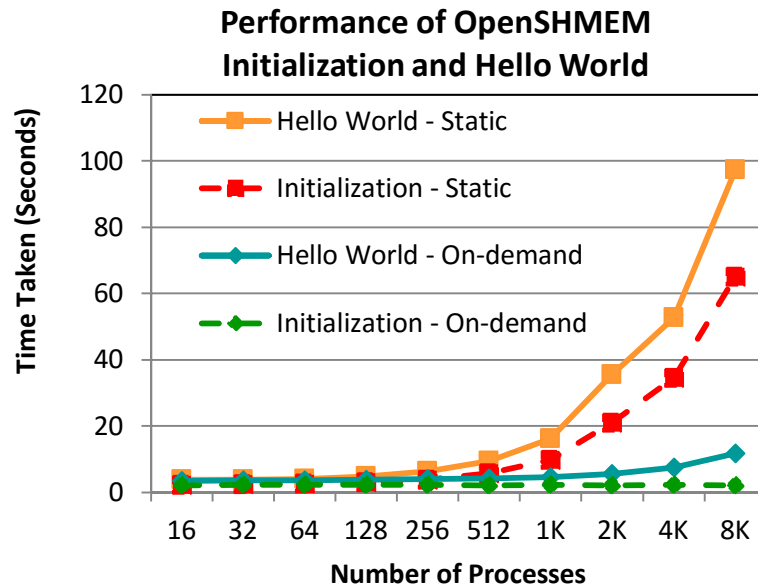
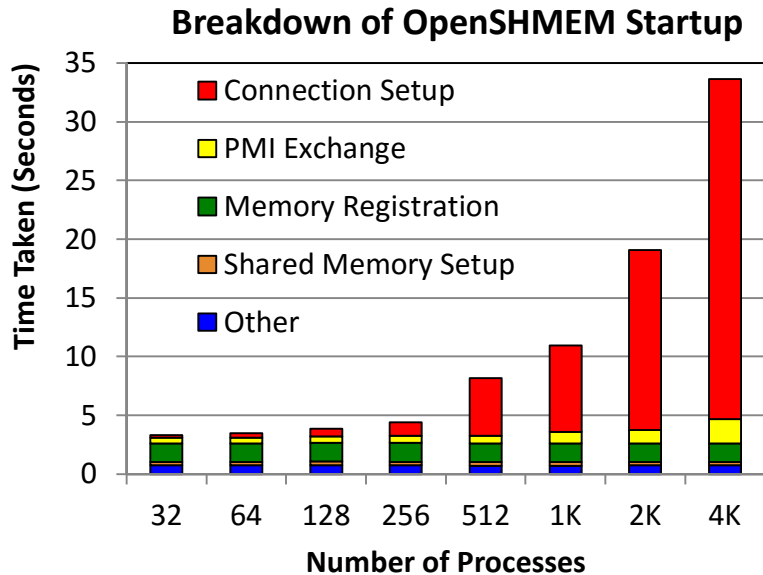
New designs available in MVAPICH2-2.3a and as patch for SLURM-15.08.8 and SLURM-16.05.1

Process Management Interface (PMI) over Shared Memory (SHMEMPMI)

- SHMEMPMI allows MPI processes to directly read remote endpoint (EP) information from the process manager through shared memory segments
- Only a single copy per node - $O(\text{processes per node})$ reduction in memory usage
- Estimated savings of 1GB per node with 1 million processes and 16 processes per node
- Up to 1,000 times faster PMI Gets compared to default design
- Available since MVAPICH2 2.2rc1 and SLURM-15.08.8



On-demand Connection Management for OpenSHMEM+MPI



- Static connection establishment wastes memory and takes a lot of time
- On-demand connection management improves OpenSHMEM initialization time by **29.6 times**
- Time taken for Hello World reduced by **8.31 times** at 8,192 processes
- **Available since MVAPICH2-X 2.1rc1**

How to Get the Best Startup Performance with MVAPICH2?

- **MV2_HOMOGENEOUS_CLUSTER=1**
- **MV2_ON_DEMAND_UD_INFO_EXCHANGE=1**

//Set for homogenous clusters

//Enable UD based address exchange

Using SLURM as launcher

- **Use PMI2**
 - `./configure --with-pm=slurm --with-pmi=pmi2`
 - `srun --mpi=pmi2 ./a.out`
- **Use PMI Extensions**
 - Patch for SLURM available at <http://mvapich.cse.ohio-state.edu/download/>
 - Patches available for SLURM 15, 16, and 17
 - PMI Extensions are automatically detected by MVAPICH2

Using mpirun_rsh as launcher

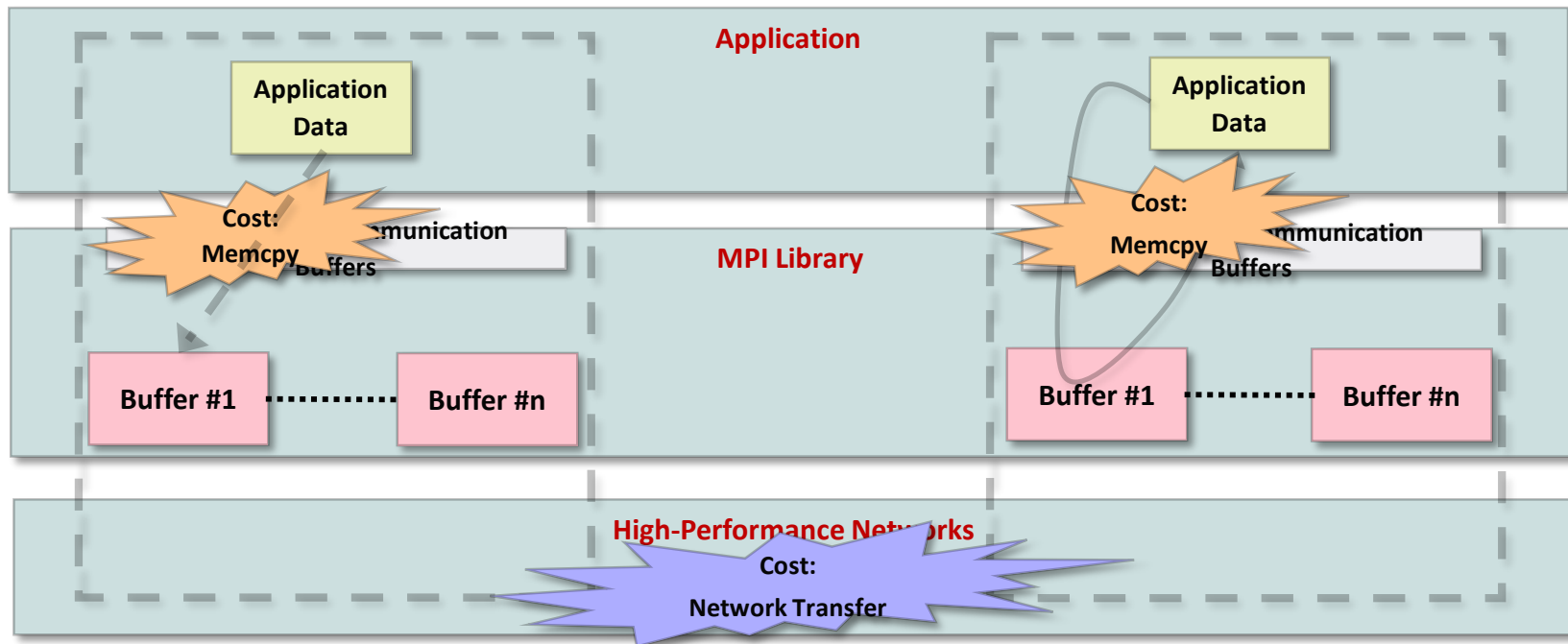
- **MV2_MT_DEGREE**
 - degree of the hierarchical tree used by mpirun_rsh
- **MV2_FASTSSH_THRESHOLD**
 - #nodes beyond which hierarchical-ssh scheme is used
- **MV2_NPROCS_THRESHOLD**
 - #nodes beyond which file-based communication is used for hierarchical-ssh

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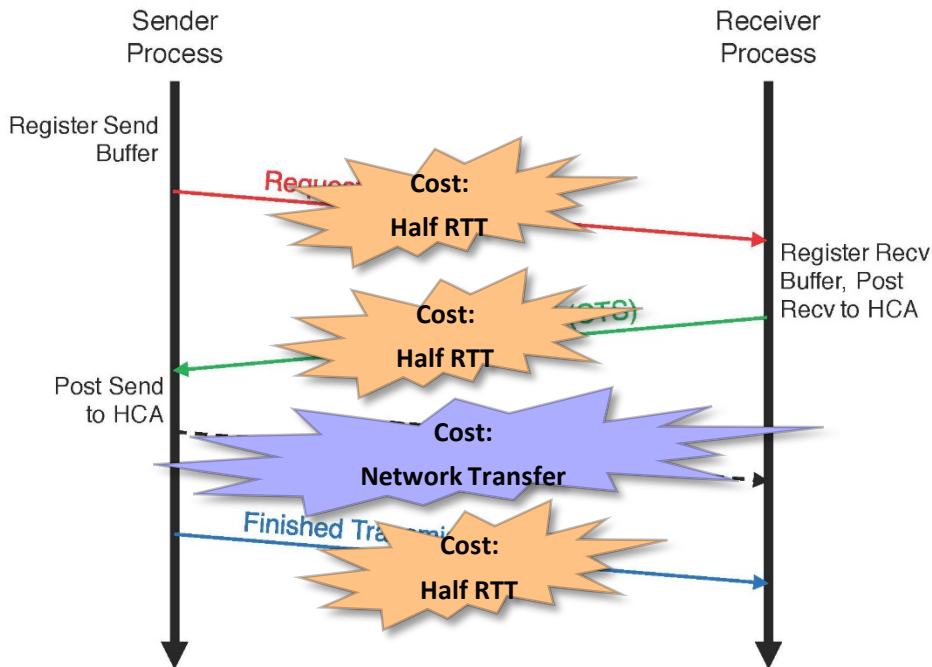
Communication Costs of Point-to-point Protocols - Eager

- Good communication performance for smaller messages
- No synchronization required between sender and receiver
- Cost of extra copies is high for large messages

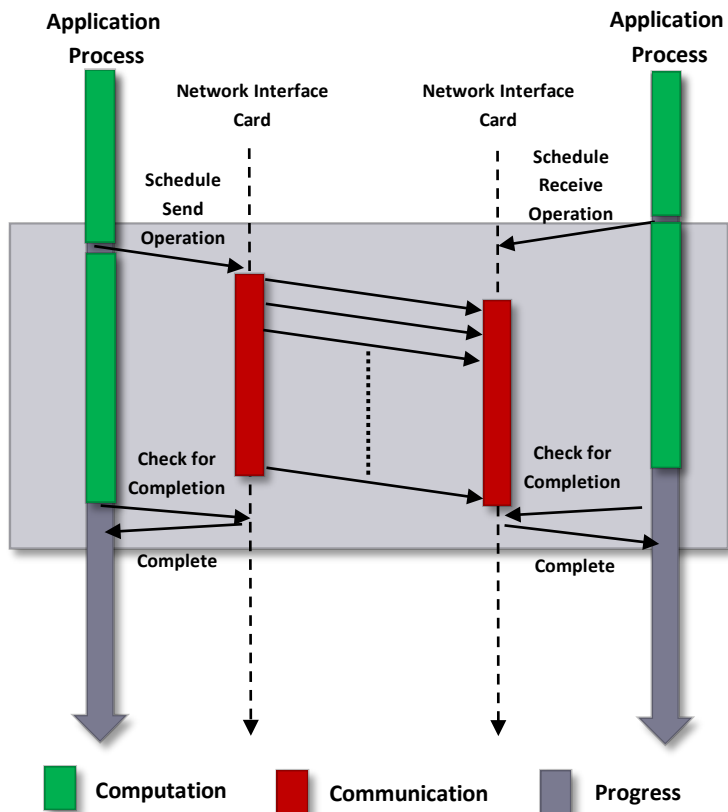


Communication Costs of Point-to-point Protocols - Rendezvous

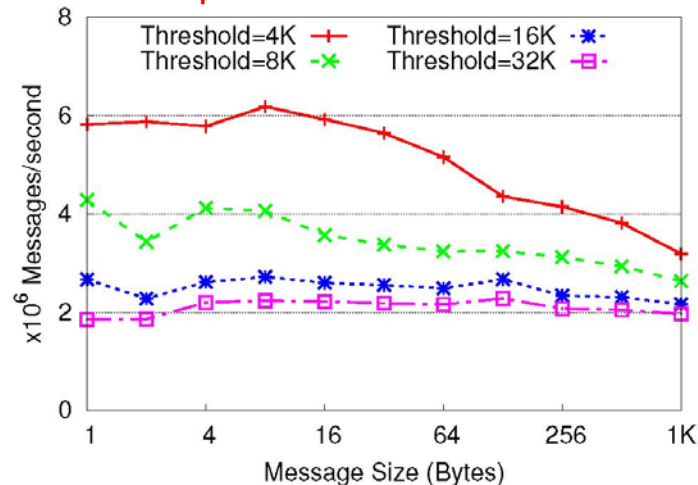
- Avoid extra copies for larger messages
- Synchronization required between sender and receiver
- Can be based on RDMA Read or RDMA Write (shown here)



Analyzing Overlap Potential of Eager Protocol

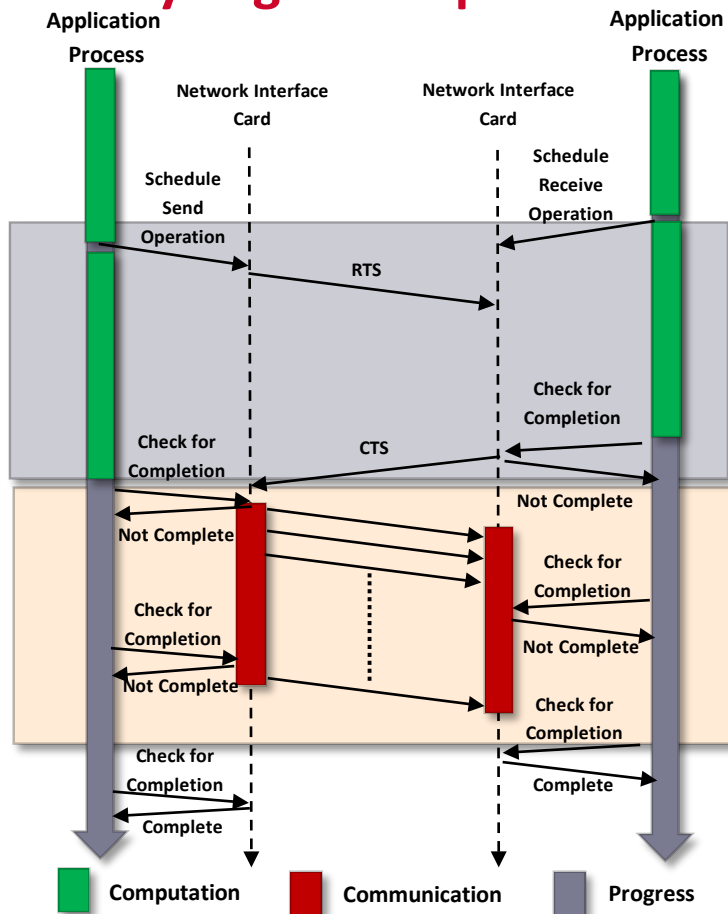


- Application processes schedule communication operation
- Network adapter progresses communication in the background
- Application process free to perform useful compute in the foreground
- **Overlap of computation and communication => Better Overall Application Performance**
- **Increased buffer requirement**
- **Poor communication performance if used for all types of communication operations**



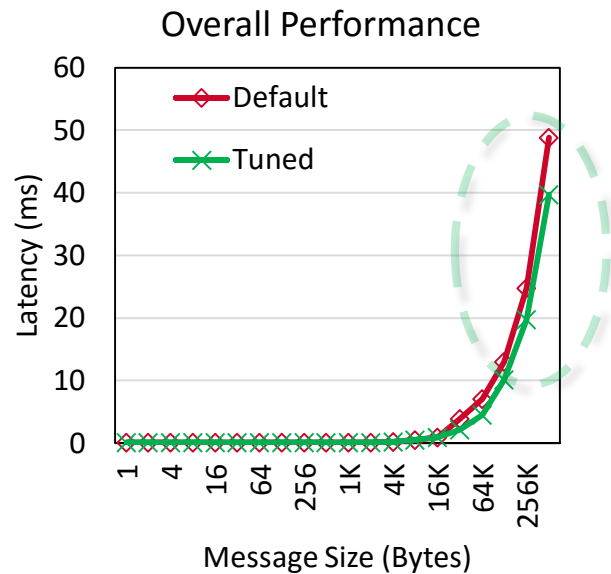
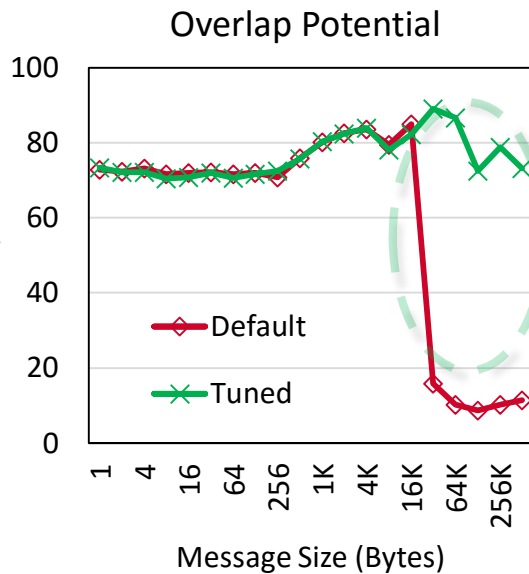
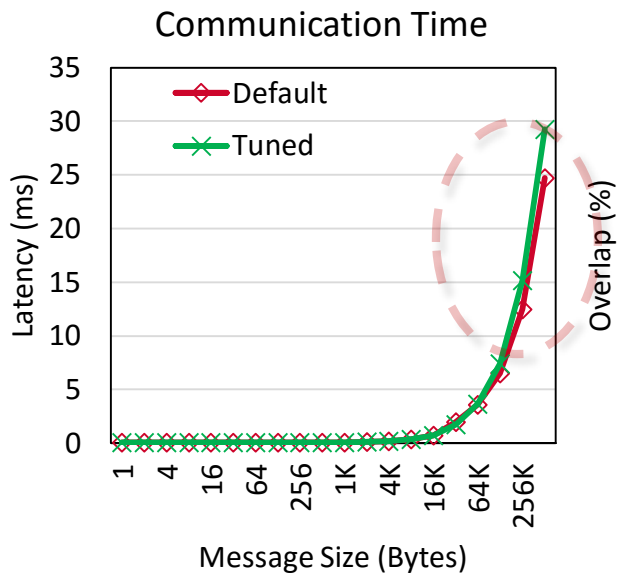
Impact of changing Eager Threshold on performance of multi-pair message-rate benchmark with 32 processes on Stampede

Analyzing Overlap Potential of Rendezvous Protocol



- Application processes schedule communication operation
- Application process free to perform useful compute in the foreground
- Little communication progress in the background
- All communication takes place at final synchronization
- **Reduced buffer requirement**
- **Good communication performance if used for large message sizes and operations where communication library is progressed frequently**
- **Poor overlap of computation and communication => Poor Overall Application Performance**

Impact of Tuning Rendezvous Threshold on 3D-Stencil



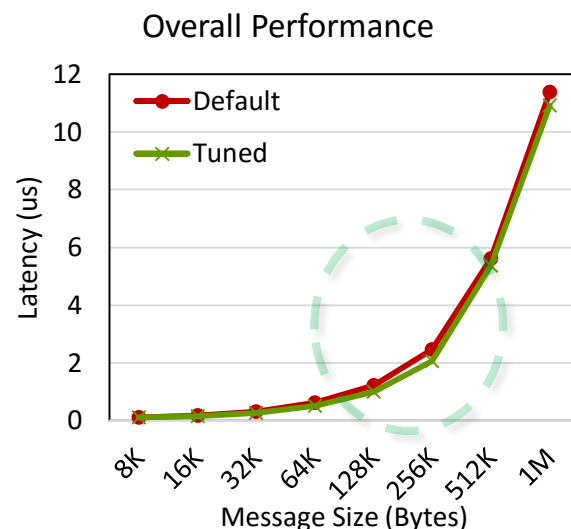
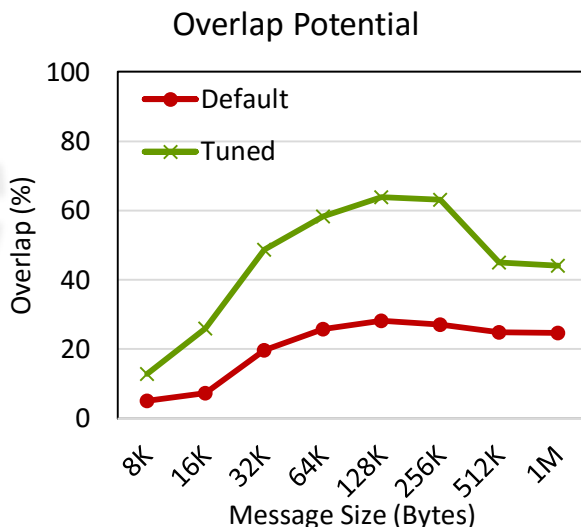
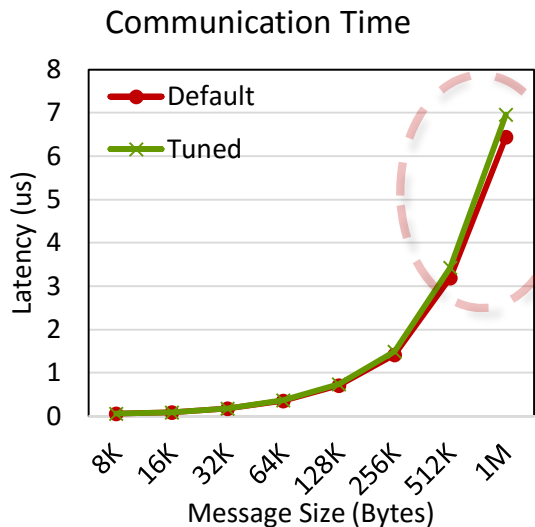
- Increased eager threshold from 16KB to 512KB
- Very small degradation in raw communication performance
- Significant improvement in overlap of computation and communication
- ~18% Improvement in overall performance

MV2_IBA_EAGER_THRESHOLD=512K
MV2_SMP_EAGERSIZE=512K

(Applicable to both InfiniBand and
Omni-Path)

8192 Processes, SandyBridge + FDR

Impact of Tuning Rendezvous Protocol on 3D-Stencil



- RDMA Read based protocol (RGET) used instead of RDMA Write
- Very minor penalty in raw performance
- Offers more overlap due to less synchronization overhead
- Up to 15% improvement in overall execution time

MV2_RNDV_PROTOCOL=RGET

(Applicable to InfiniBand)

64 Processes, Broadwell + EDR

Dynamic and Adaptive MPI Point-to-point Communication Protocols

- Different communication protocols have different trade-offs
 - Need to consider performance, overlap, memory requirement
 - Manual tuning is difficult and time-consuming
- Can the MPI library select the best protocol at runtime?
 - Use different protocols and thresholds between different pair of processes
 - Deliver good performance and minimize resource consumption
 - Dynamically adapt to the application's communication requirements at runtime

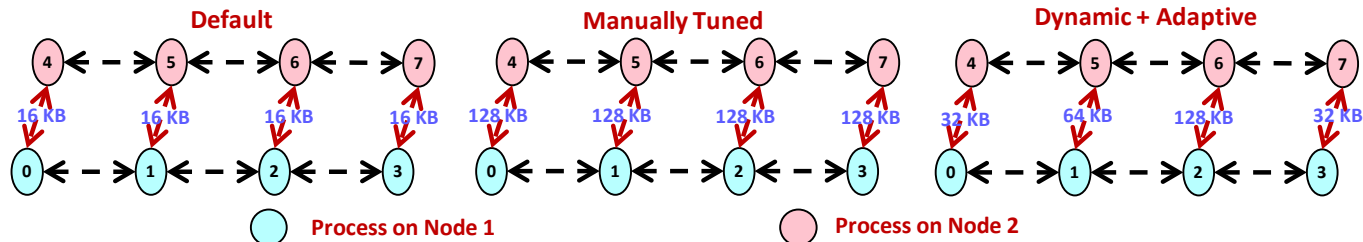
Default	Poor overlap; Low memory requirement	Low Performance; High Productivity
Manually Tuned	Good overlap; High memory requirement	High Performance; Low Productivity
Dynamic + Adaptive	Good overlap; Optimal memory requirement	High Performance; High Productivity

Dynamic and Adaptive MPI Point-to-point Communication Protocols (cont.)

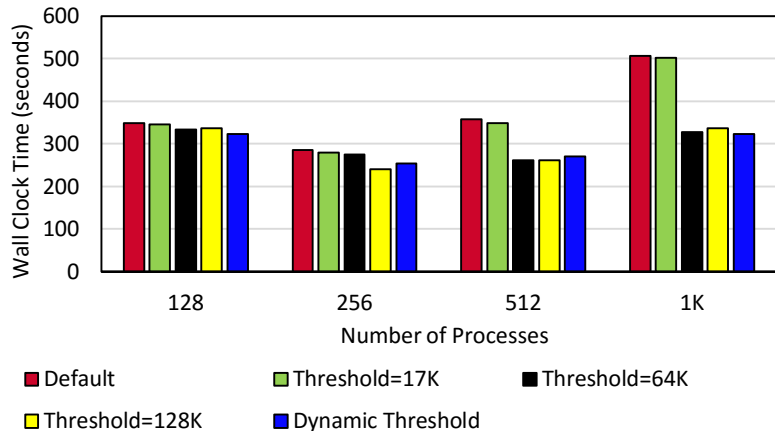
Desired Eager Threshold

Process Pair	Eager Threshold (KB)
0 - 4	32
1 - 5	64
2 - 6	128
3 - 7	32

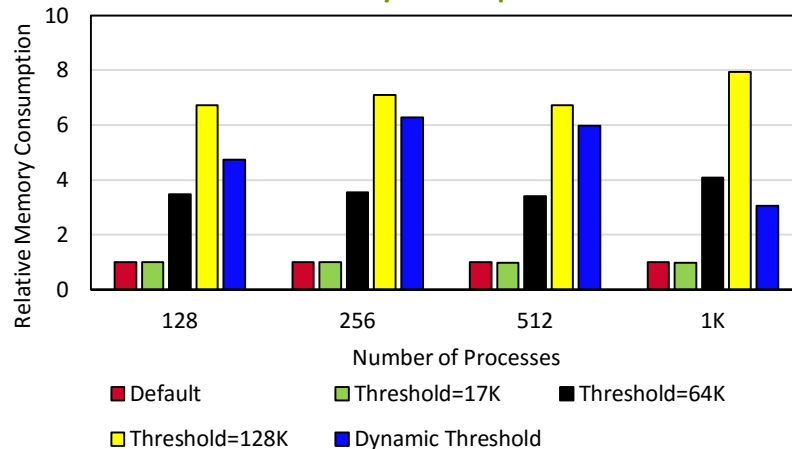
Eager Threshold for Example Communication Pattern with Different Designs



Execution Time of Amber



Relative Memory Consumption of Amber



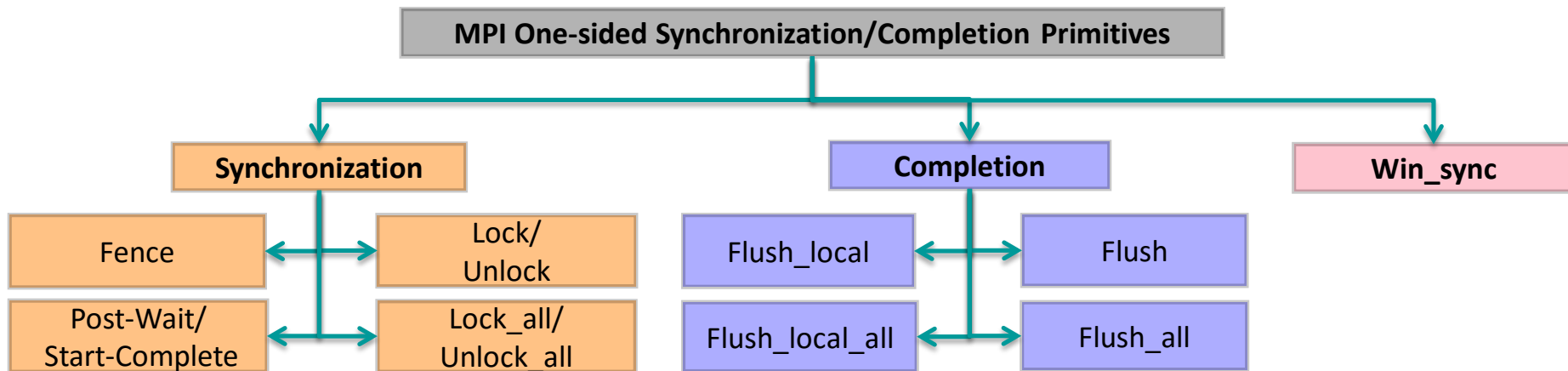
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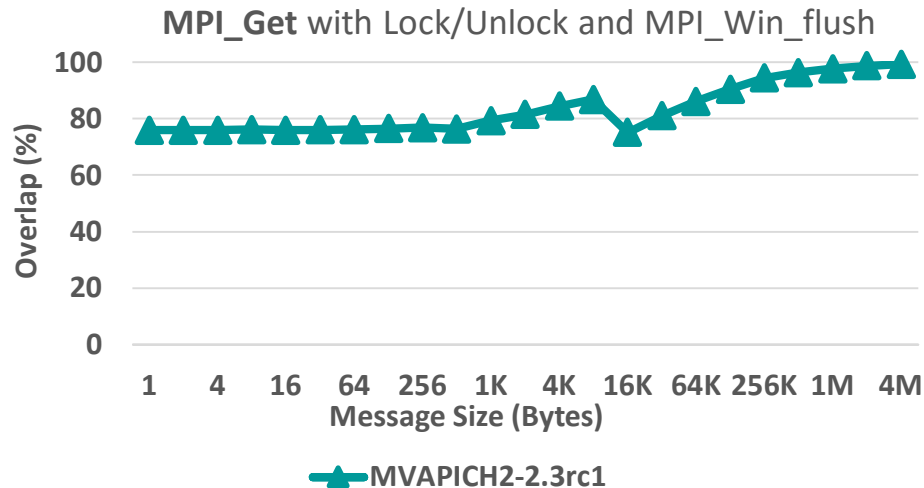
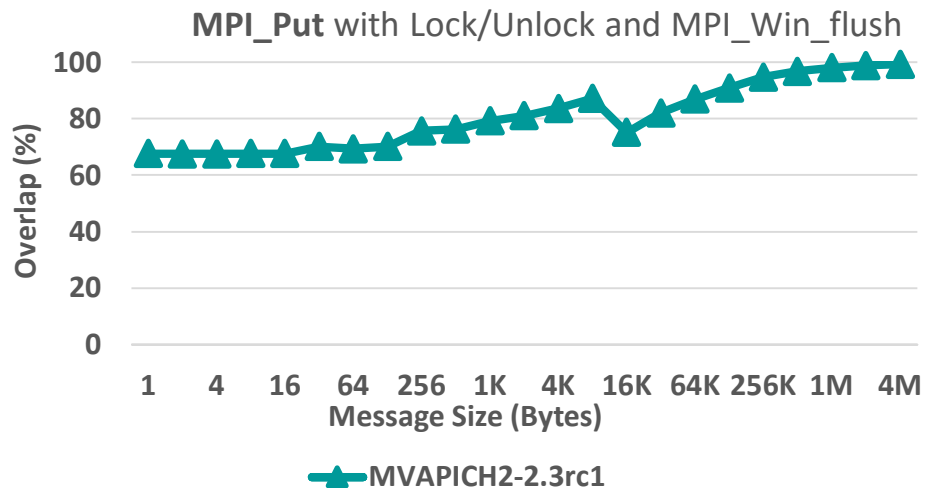
MPI-3 RMA: Communication and synchronization Primitives

- Non-blocking one-sided communication routines
 - Put, Get (Rput, Rget)
 - Accumulate, Get_accumulate
 - Atomics
- Flexible synchronization operations to control initiation and completion

**MVAPICH2 supports all
RMA communication with
Best performance and overlap**



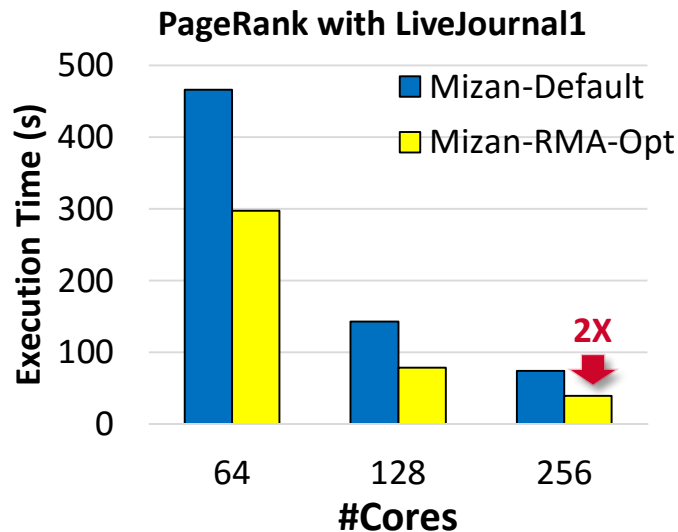
Overlap between Computation and RMA Operations



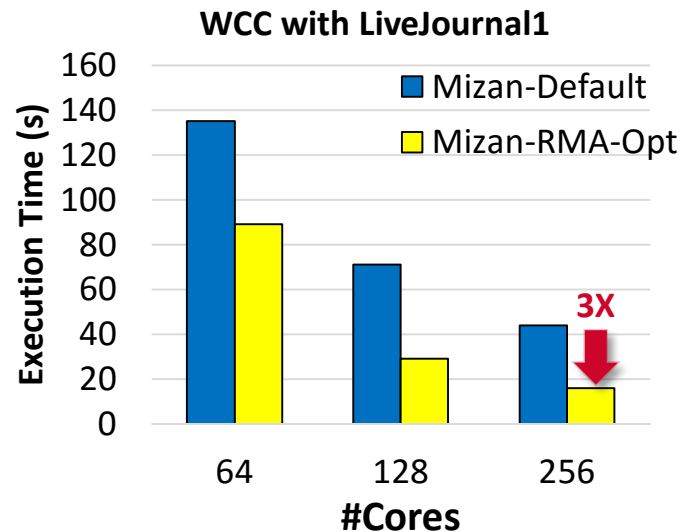
- **67-99%** overlap between **MPI_Put** and computation
- **75-99%** overlap between **MPI_Get** and computation

MVAPICH2-2.3rc1
Intel Haswell (E5-2687W @ 3.10 GHz) node - 20 cores
Mellanox Connect-X4 EDR HCA
Mellanox OFED 4.3

Graph Processing Framework with Optimized MPI RMA

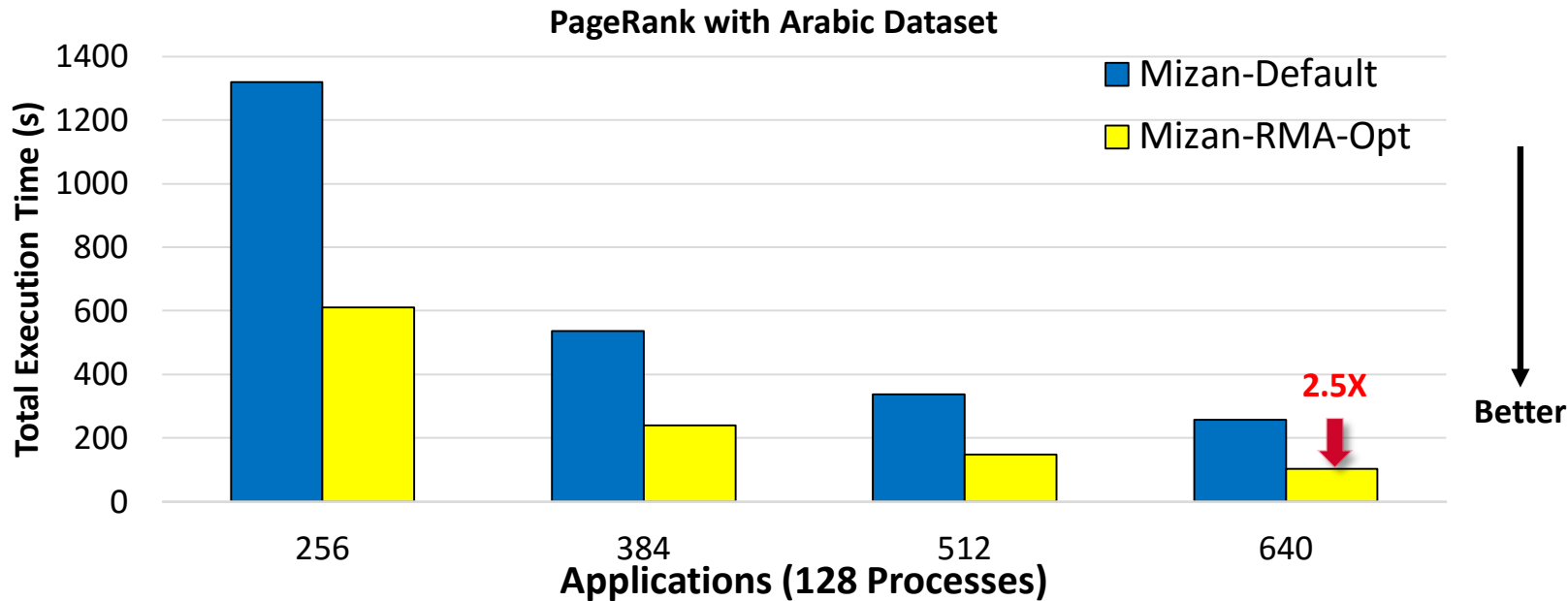


↓
Better



- Proposed design performs better than default implementation
- For Weakly Connected Components (WCC) on 256 cores, proposed design could reduce the total execution time by **2X** compared with the default scheme

Graph Processing Framework with Optimized MPI RMA



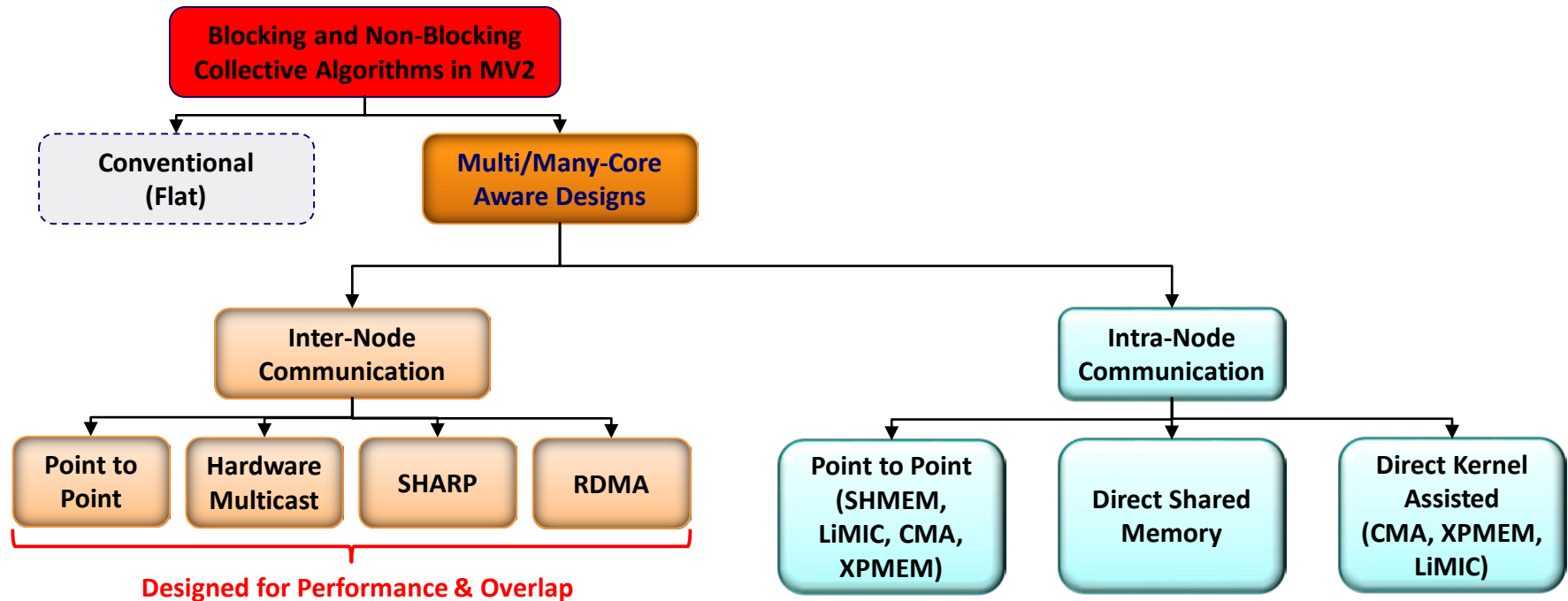
- Proposed design shows good strong scaling
- Proposed design scales better than default implementation

M. Li, X. Lu, K. Hamidouche, J. Zhang and D. K. Panda, "Mizan-RMA: Accelerating Mizan Graph Processing Framework with MPI RMA," IEEE HiPC, 2016

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Collective Communication in MVAPICH2



Run-time flags:

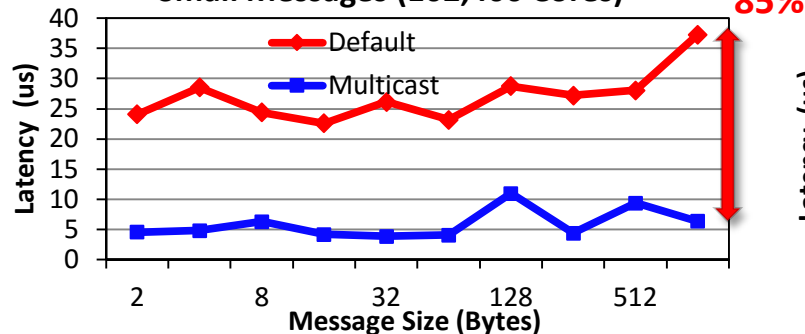
All shared-memory based collectives : MV2_USE_SHMEM_COLL (Default: ON)

Hardware Mcast-based collectives : MV2_USE_MCAST (Default : OFF)

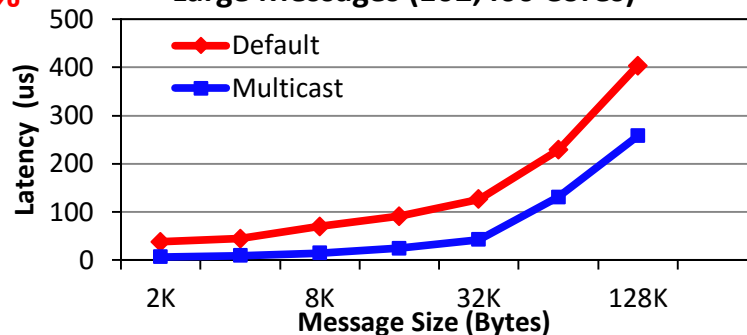
CMA-based collectives : MV2_USE_CMA_COLL (Default : ON)

Hardware Multicast-aware MPI_Bcast on TACC Stampede

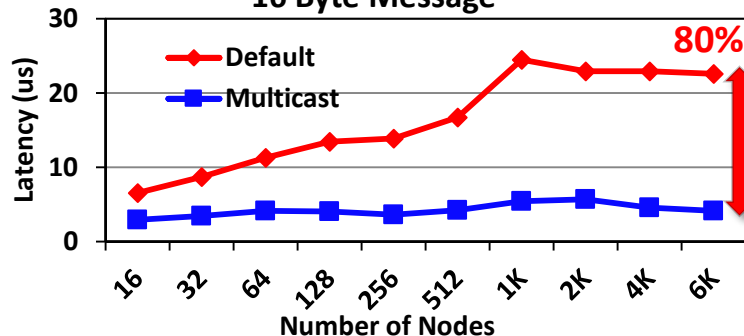
Small Messages (102,400 Cores)



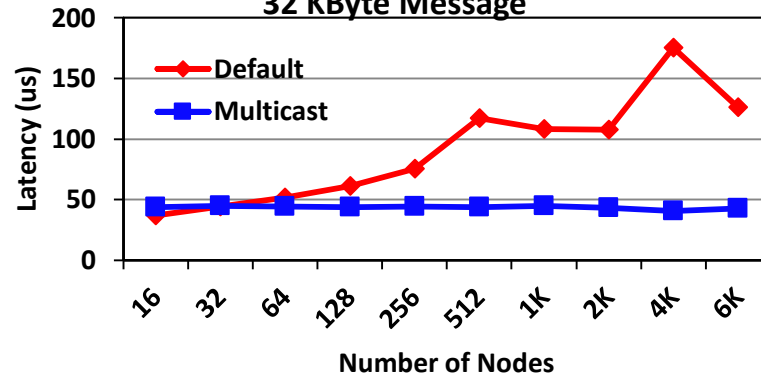
Large Messages (102,400 Cores)



16 Byte Message

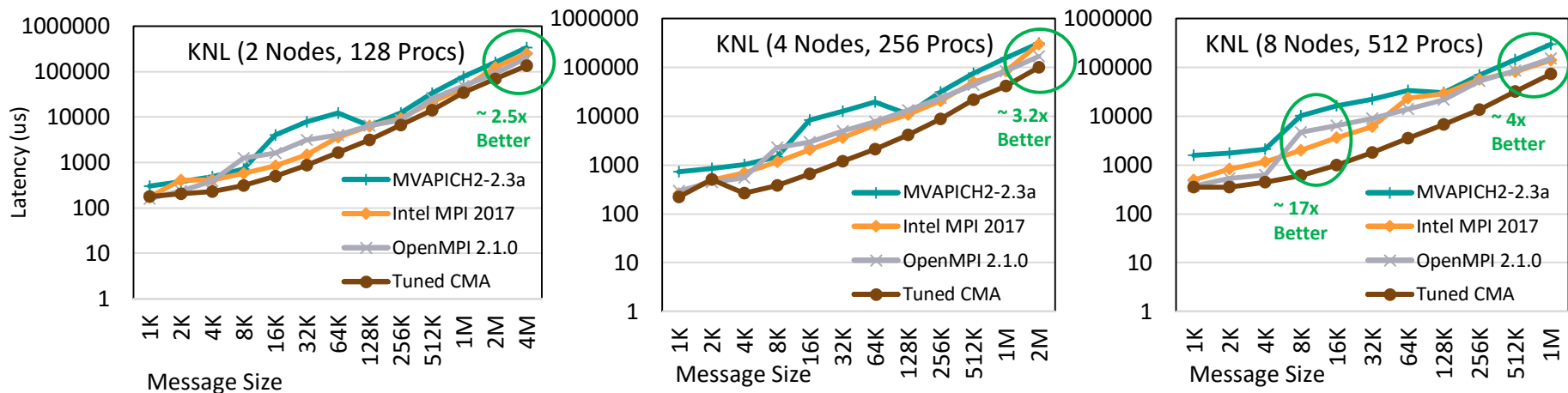


32 KByte Message



- MCAST-based designs improve latency of MPI_Bcast by up to **85%**
- Use MV2_USE_MCAST=1 to enable MCAST-based designs

Optimized CMA-based Collectives for Large Messages



Performance of MPI_Gather on KNL nodes (64PPN)

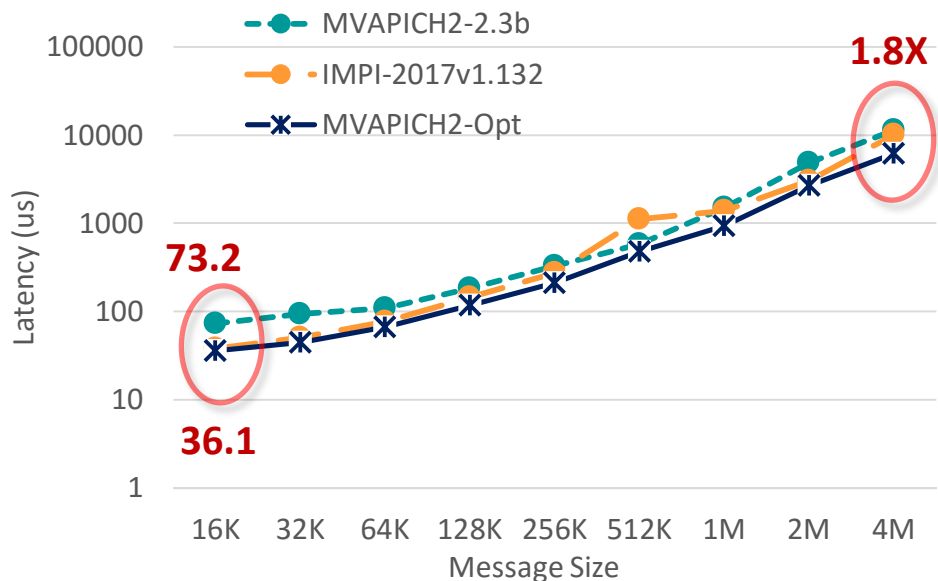
- Significant improvement over existing implementation for Scatter/Gather with 1MB messages (up to 4x on KNL, 2x on Broadwell, 14x on OpenPower)
- New two-level algorithms for better scalability
- Improved performance for other collectives (Bcast, Allgather, and Alltoall)

S. Chakraborty, H. Subramoni, and D. K. Panda, Contention Aware Kernel-Assisted MPI Collectives for Multi/Many-core Systems, *IEEE Cluster '17*, *BEST Paper Finalist*

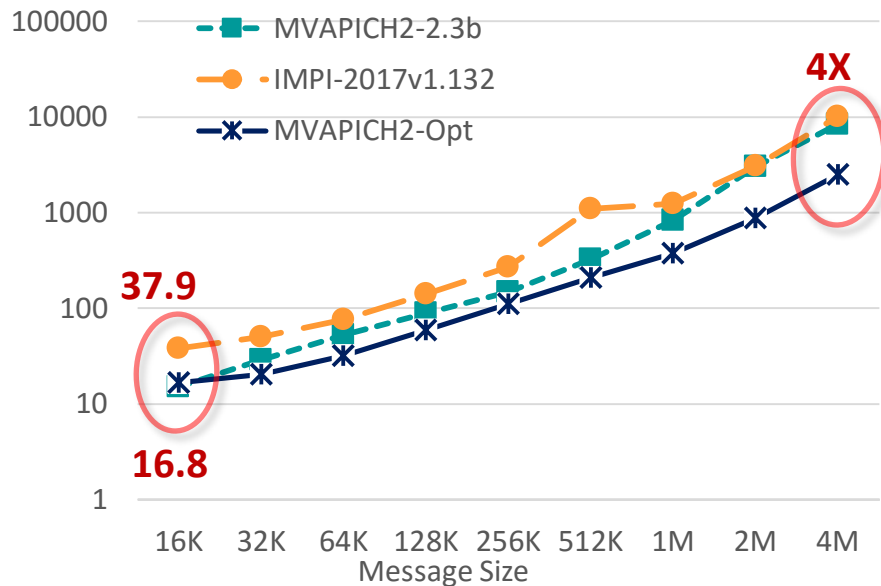
Available in MVAPICH2-X 2.3b

Shared Address Space (XPMEM)-based Collectives Design

OSU_Allreduce (Broadwell 256 procs)



OSU_Reduce (Broadwell 256 procs)



- “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

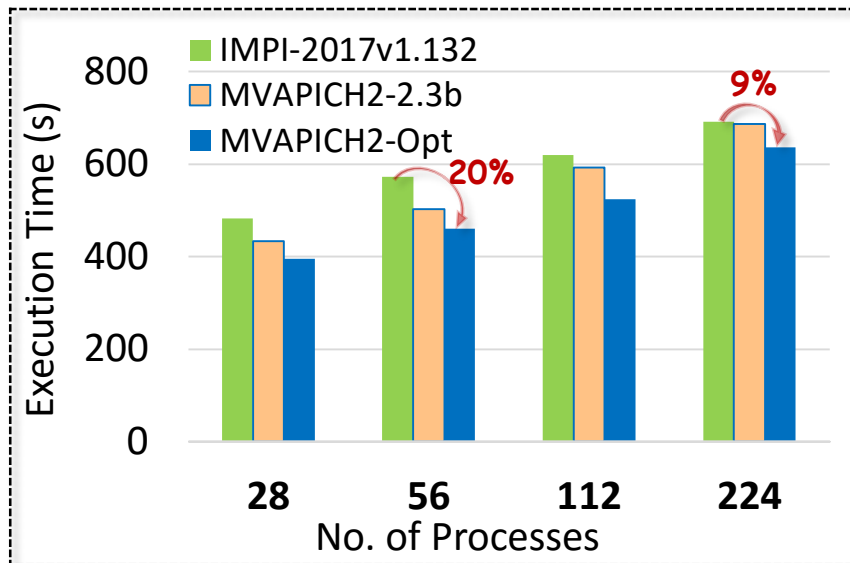
J. Hashmi, S. Chakraborty, M. Bayatpour, H. Subramoni, and D. Panda, *Designing Efficient Shared Address Space Reduction Collectives for Multi-/Many-cores*, International Parallel & Distributed Processing Symposium (IPDPS '18), May 2018.

Will be available in future

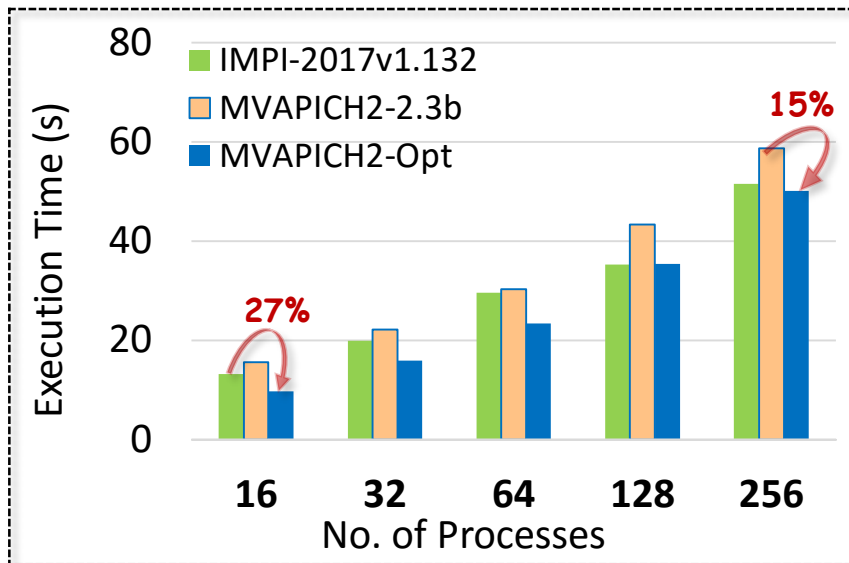
Application-Level Benefits of XPMEM-Based Collectives

CNTK AlexNet Training

(Broadwell, B.S=default, iteration=50, ppn=28)

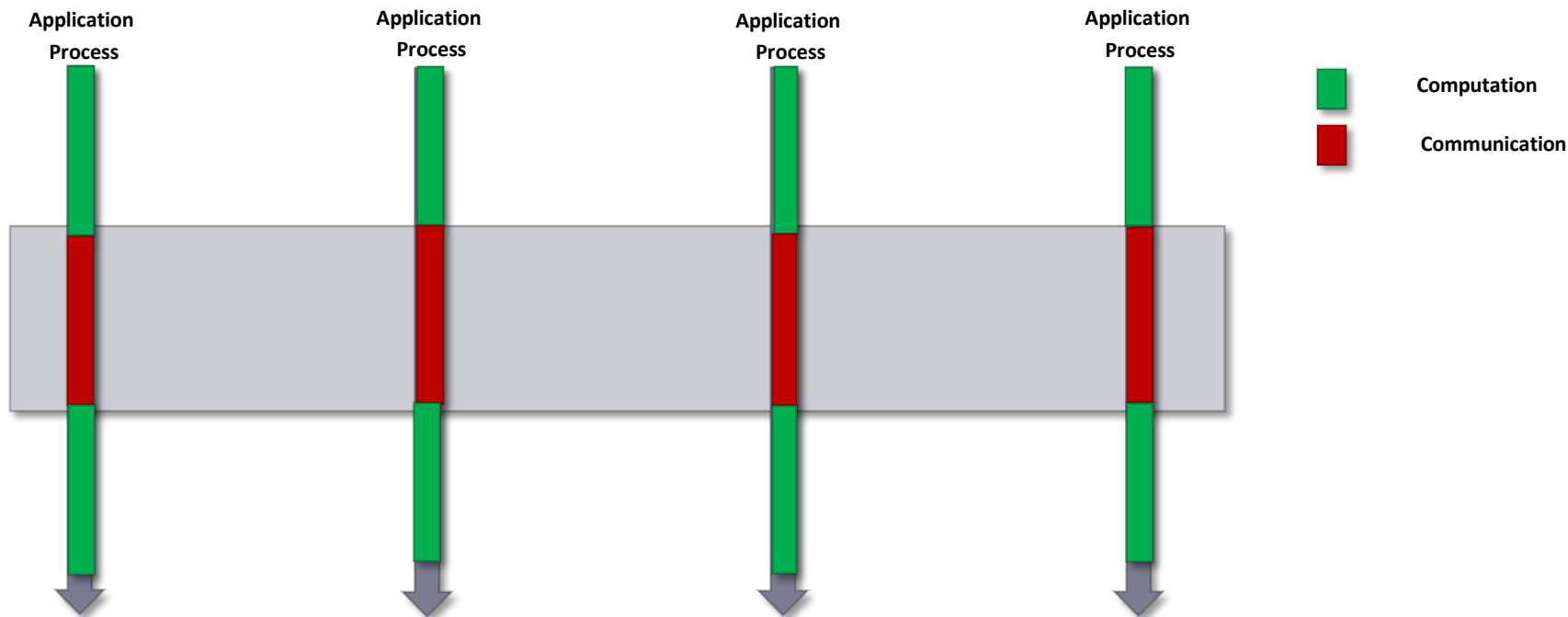


MiniAMR (Broadwell, ppn=16)



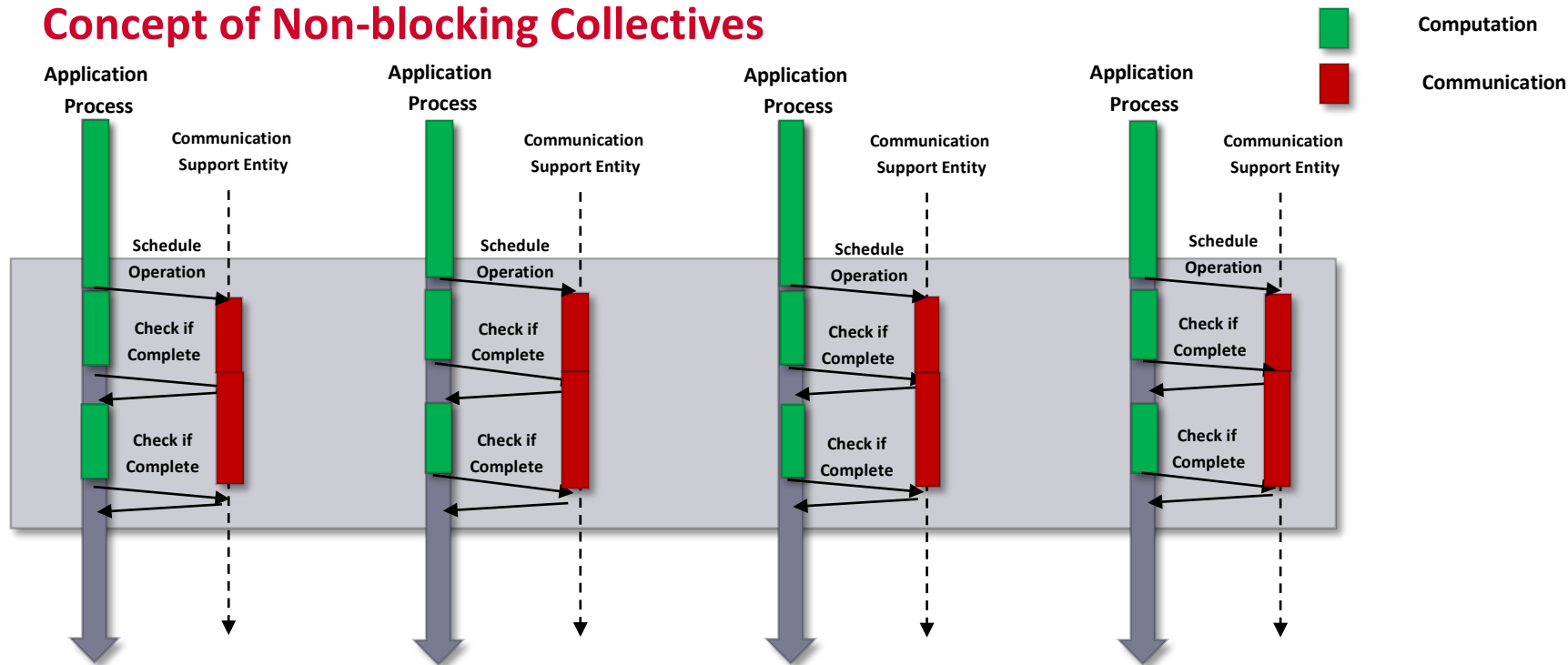
- Up to **20%** benefits over IMPI for CNTK DNN training using AllReduce
- Up to **27%** benefits over IMPI and up to **15%** improvement over MVAPICH2 for MiniAMR application kernel

Problems with Blocking Collective Operations



- Communication time cannot be used for compute
 - No overlap of computation and communication
 - Inefficient

Concept of Non-blocking Collectives



- Application processes schedule collective operation
- Check periodically if operation is complete
- **Overlap of computation and communication => Better Performance**
- *Catch: Who will progress communication*

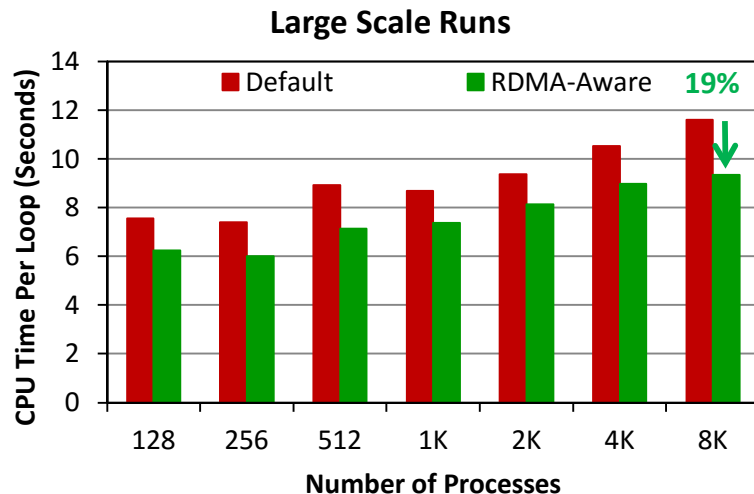
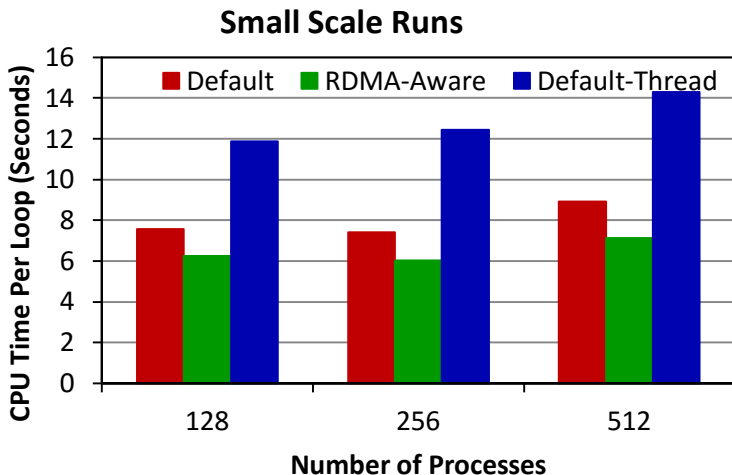
Non-blocking Collective (NBC) Operations

- Enables overlap of computation with communication
- Non-blocking calls do not match blocking collective calls
 - MPI may use different algorithms for blocking and non-blocking collectives
 - Blocking collectives: Optimized for latency
 - Non-blocking collectives: Optimized for overlap
- A process calling a NBC operation
 - Schedules collective operation and immediately returns
 - Executes application computation code
 - Waits for the end of the collective
- The communication progress by
 - Application code through MPI_Test
 - Network adapter (HCA) with hardware support
 - Dedicated processes / thread in MPI library
- There is a non-blocking equivalent for each blocking operation
 - Has an “l” in the name
 - MPI_Bcast -> MPI_Ibcast; MPI_Reduce -> MPI_Ireduce

How do I write applications with NBC?

```
void main()
{
    MPI_Init()
    ....
    MPI_lalltoall(...)
    Computation that does not depend on result of Alltoall
    MPI_Test(for lalltoall) /* Check if complete (non-blocking) */
    Computation that does not depend on result of Alltoall
    MPI_Wait(for lalltoall) /* Wait till complete (Blocking) */
    ...
    MPI_Finalize()
}
```

P3DFFT Performance with Non-Blocking Alltoall using RDMA Primitives



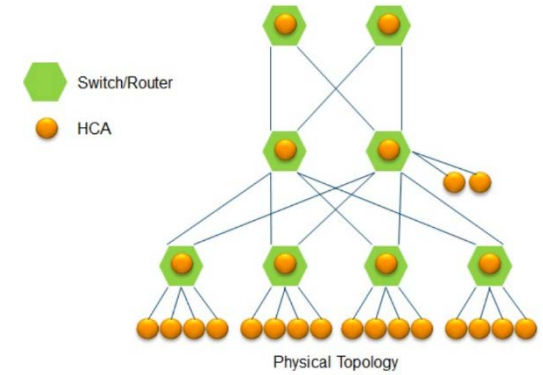
- Weak scaling experiments; problem size increases with job size
- RDMA-Aware delivers 19% improvement over Default @ 8,192 procs
- Default-Thread exhibits worst performance
 - Possibly because threads steal CPU cycles from P3DFFT
 - Do not consider for large scale experiments

Will be available in future

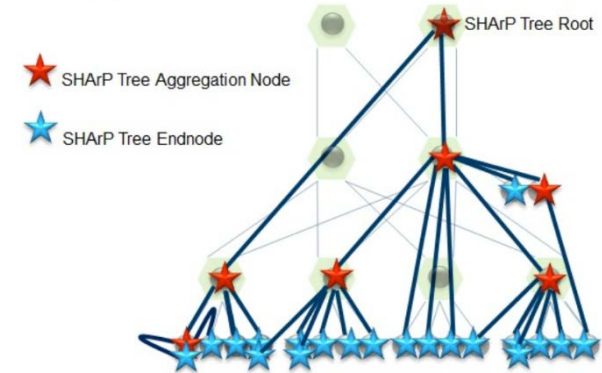
Designing Non-Blocking Personalized Collectives with Near Perfect Overlap for RDMA-Enabled Clusters, H. Subramoni ,
A. Awan , K. Hamidouche , D. Pekurovsky , A. Venkatesh , S. Chakraborty , K. Tomko , and D. K. Panda, ISC '15, Jul 2015

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 *



Physical Network Topology*

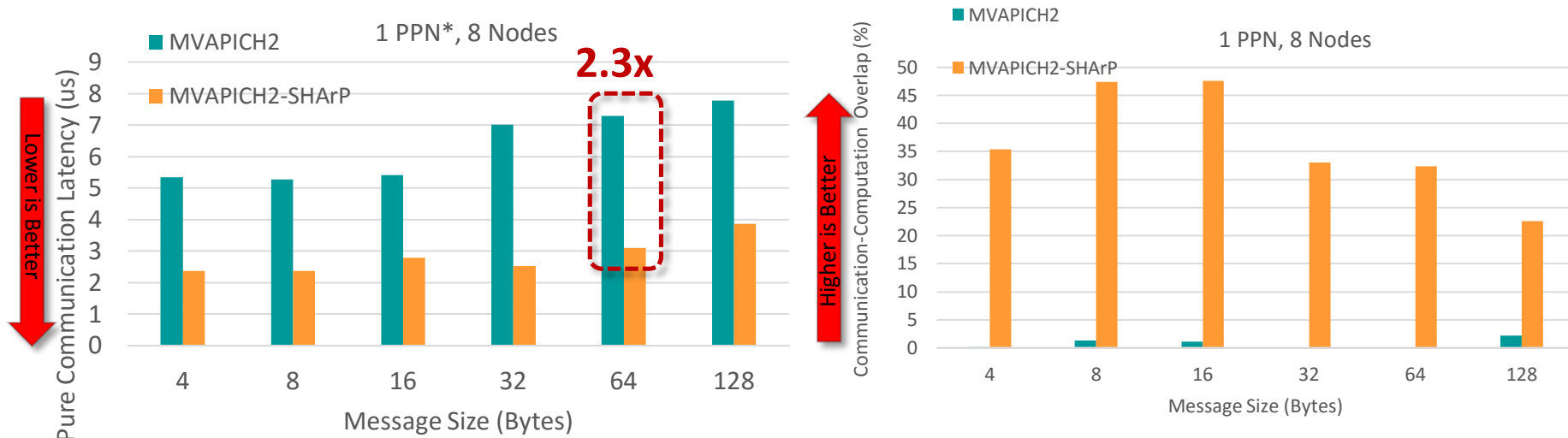


Logical SHArP Tree*

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

Evaluation of SHArP based Non Blocking Allreduce

MPI_allreduce Benchmark



- Complete offload of Allreduce collective operation to Switch helps to have much higher overlap of communication and computation

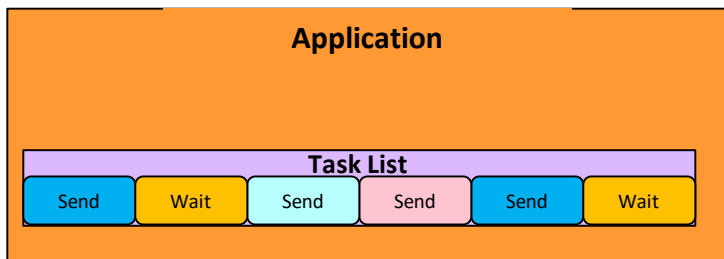
Available since MVAPICH2 2.3a

*PPN: Processes Per Node

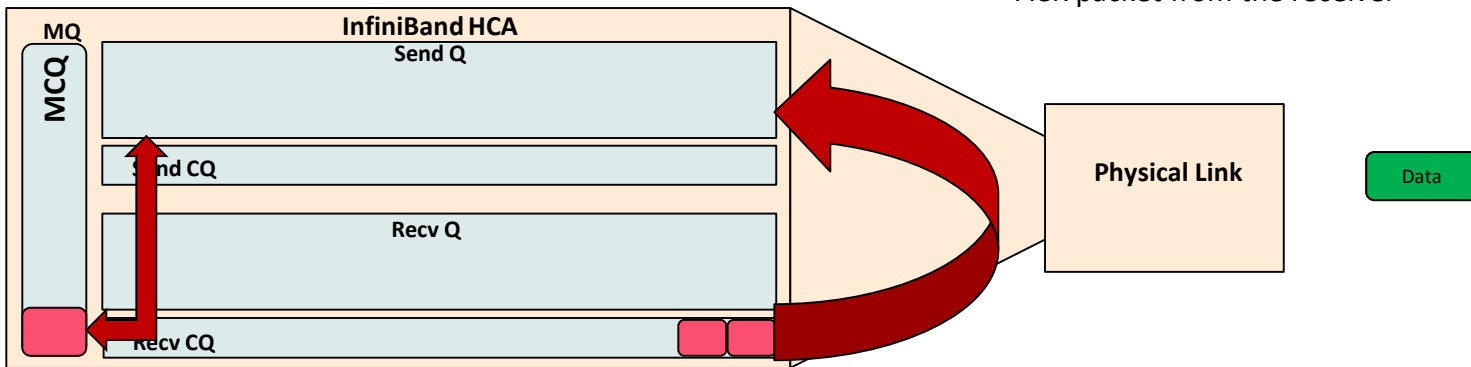
Collective Offload in ConnectX-2, ConnectX-3, Connect-IB and ConnectX-4, ConnectX-5

- Mellanox's ConnectX-2, ConnectX-3, ConnectIB, ConnectX-4, and ConnectX-5 adapters feature "task-list" offload interface
 - Extension to existing InfiniBand APIs
- Collective communication with 'blocking' feature is usually a scaling bottleneck
 - Matches with the need for non-blocking collective in MPI
- Accordingly MPI software stacks need to be re-designed to leverage offload in a comprehensive manner
- Can applications be modified to take advantage of non-blocking collectives and what will be the benefits?

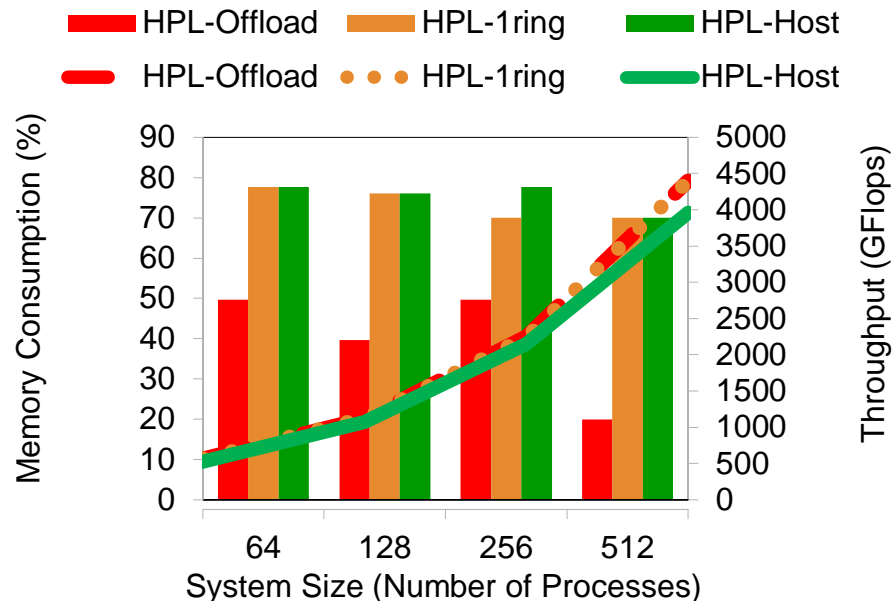
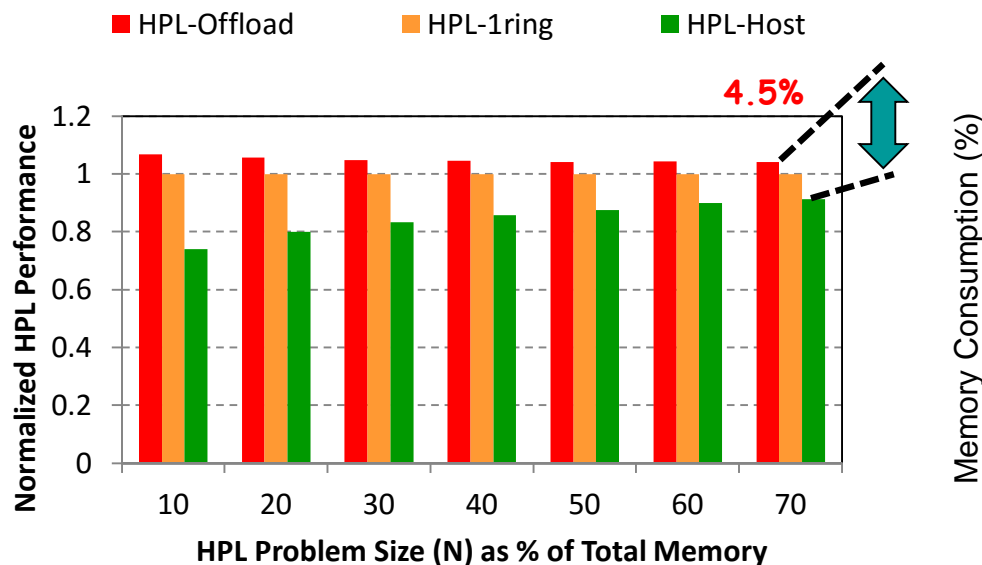
Collective Offload Support in ConnectX InfiniBand Adapter (Recv followed by Multi-Send)



- Sender creates a task-list consisting of only send and wait WQEs
 - One send WQE is created for each registered receiver and is appended to the rear of a singly linked task-list
 - A wait WQE is added to make the ConnectX-2 HCA wait for ACK packet from the receiver



Co-designing HPL with Core-Direct and Performance Benefits



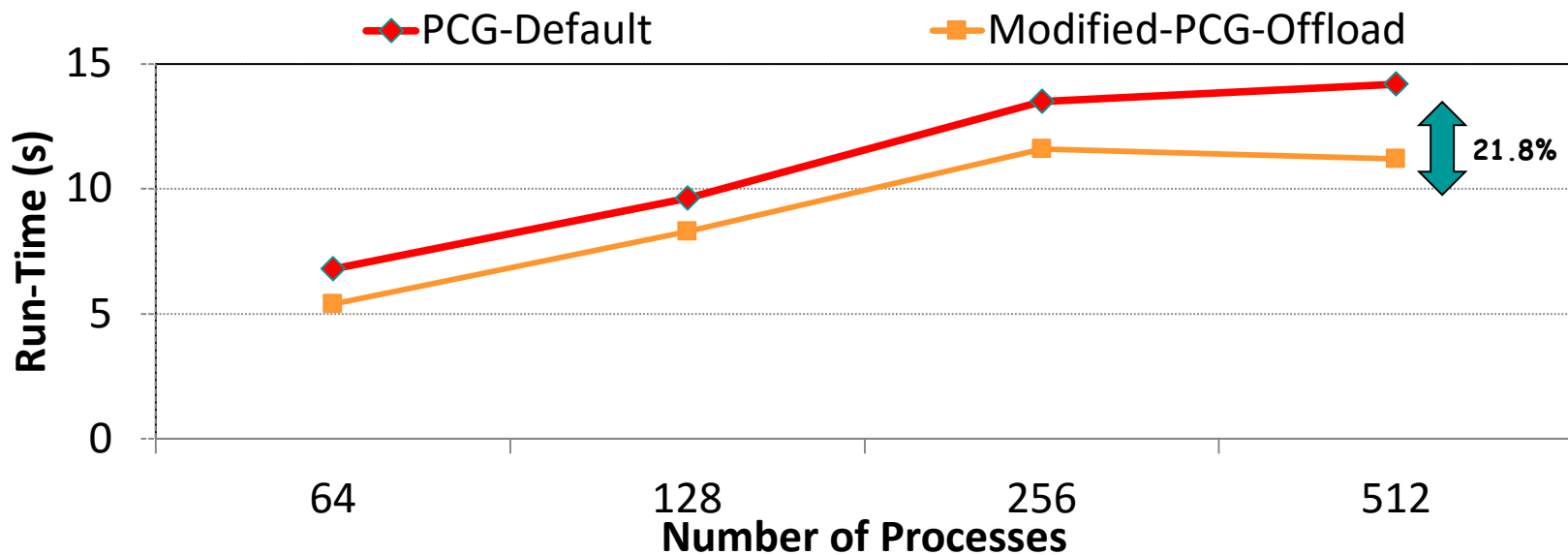
HPL Performance Comparison with 512 Processes

HPL-Offload consistently offers higher throughput than HPL-1ring and HPL-Host. Improves peak throughput by up to 4.5 % for large problem sizes

HPL-Offload surpasses the peak throughput of HPL-1ring with significantly smaller problem sizes and run-times!

K. Kandalla, H. Subramoni, J. Vienne, S. Pai Raikar, K. Tomko, S. Sur, and D K Panda,
Designing Non-blocking Broadcast with Collective Offload on InfiniBand Clusters: A Case Study with HPL, (HOTI 2011)

Pre-conditioned Conjugate Gradient (PCG) Solver Performance with Non-Blocking Allreduce based on CX-2 Collective Offload



64,000 unknowns per process.

Modified PCG with Offload-Allreduce performs **21%** better than default PCG

K. Kandalla, U. Yang, J. Keasler, T. Kolev, A. Moody, H. Subramoni, K. Tomko, J. Vienne and D. K. Panda, Designing Non-blocking Allreduce with Collective Offload on InfiniBand Clusters: A Case Study with Conjugate Gradient Solvers, IPDPS '12, May 2012.

Presentation Outline

- MVAPICH2/MVAPICH2-X
 - Job Startup
 - Point-to-point Communication
 - Remote Memory Access (RMA)
 - Collective Communication
- **MVAPICH2-GDR**
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 - GPU-kernel based Reduction
 - Datatype Processing
- Deep Learning Application: OSU Caffe

GPU-Aware (CUDA-Aware) MPI Library: MVAPICH2-GPU

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

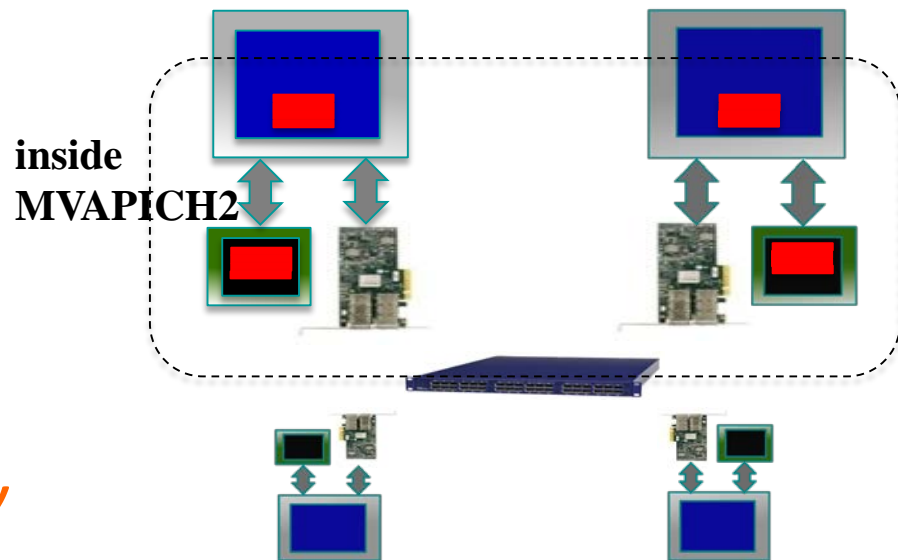
At Sender:

```
MPI_Send(s_devbuf, size, ...);
```

At Receiver:

```
MPI_Recv(r_devbuf, size, ...);
```

High Performance and High Productivity

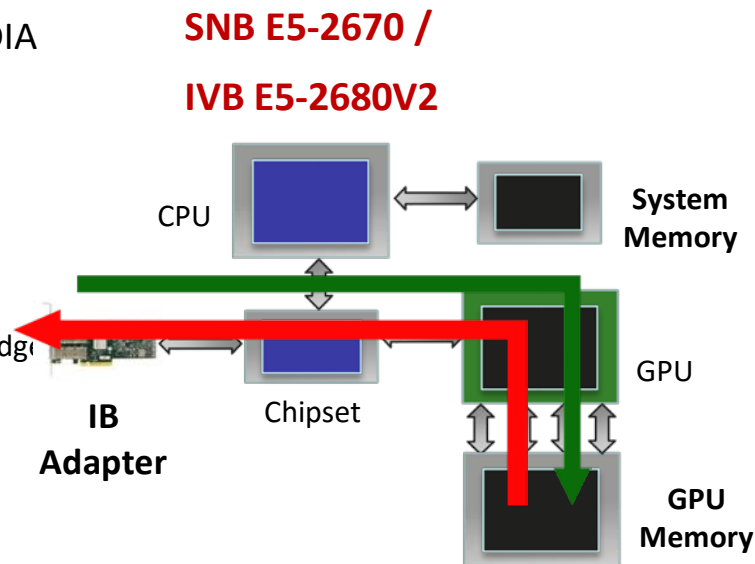


CUDA-Aware MPI: MVAPICH2-GDR 1.8-2.3 Releases

- Support for MPI communication from NVIDIA GPU device memory
- 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

GPU-Direct RDMA (GDR) with CUDA

- OFED with support for GPUDirect RDMA is developed by NVIDIA and Mellanox
- OSU has a design of MVAPICH2 using GPUDirect RDMA
 - Hybrid design using GPU-Direct RDMA
 - GPUDirect RDMA and Host-based pipelining
 - Alleviates P2P bandwidth bottlenecks on SandyBridge and IvyBridge
 - Similar bottlenecks on Haswell
 - Support for communication using multi-rail
 - Support for Mellanox Connect-IB and ConnectX VPI adapters
 - Support for RoCE with Mellanox ConnectX VPI adapters



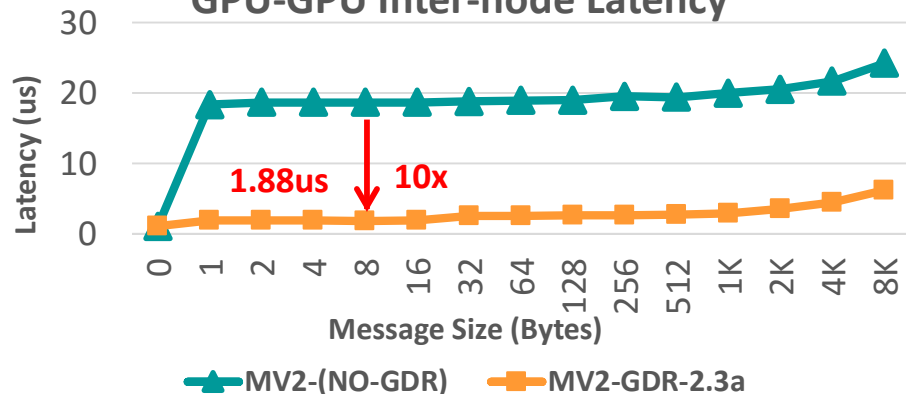
SNB E5-2670

IVB E5-2680V2

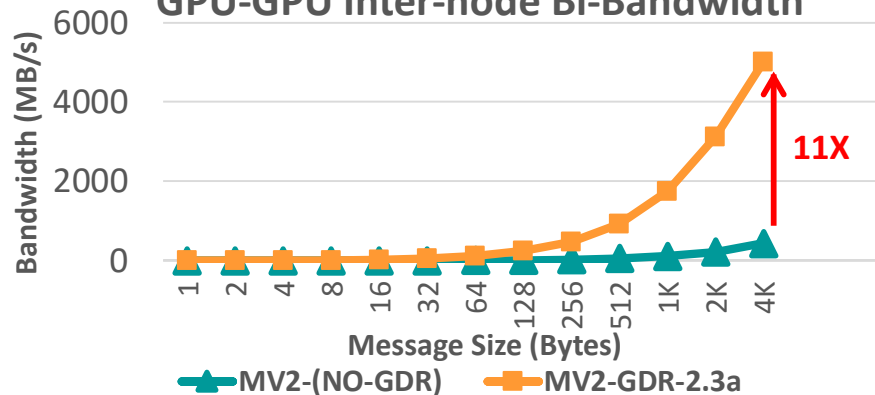
	Intra-socket	Inter-sockets	Intra-socket	Inter-sockets
P2P read	<1.0 GBs	<300 MBs	3.5 GBs	<300 MBs
P2P write	5.2 GBs	<300 MBs	6.4 GBs	<300 MBs

Optimized MVAPICH2-GDR Design

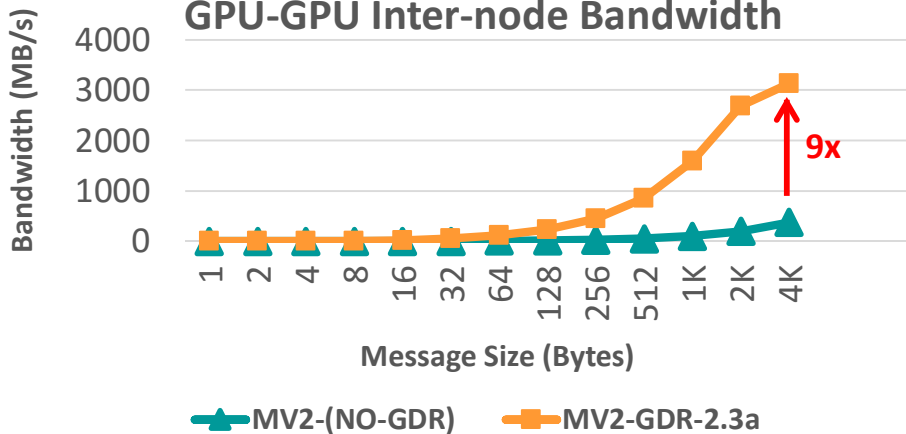
GPU-GPU Inter-node Latency



GPU-GPU Inter-node Bi-Bandwidth

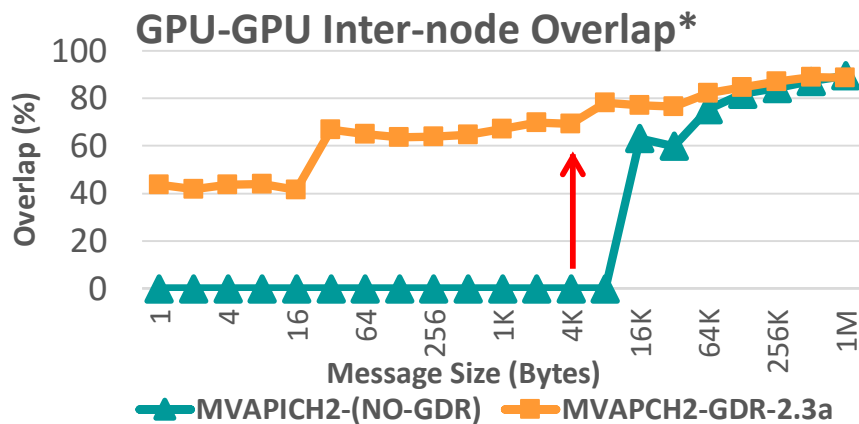
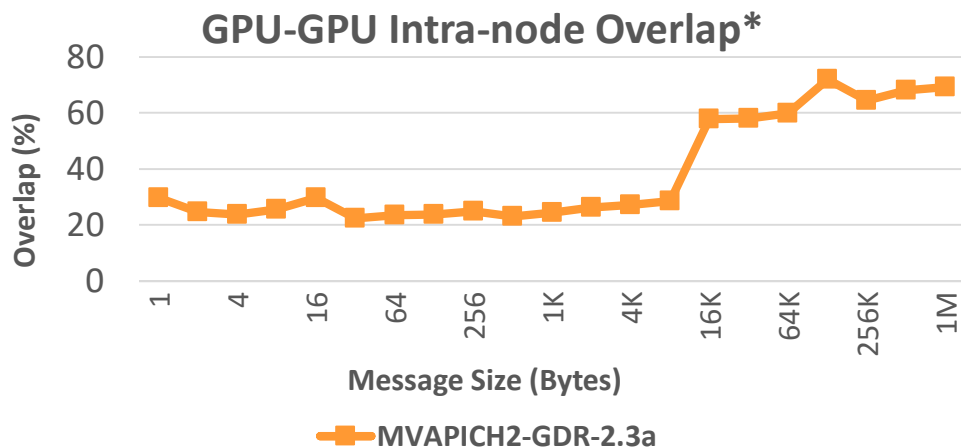


GPU-GPU Inter-node Bandwidth



MVAPICH2-GDR-2.3a
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

Overlap with Optimized MVAPICH2-GDR Design



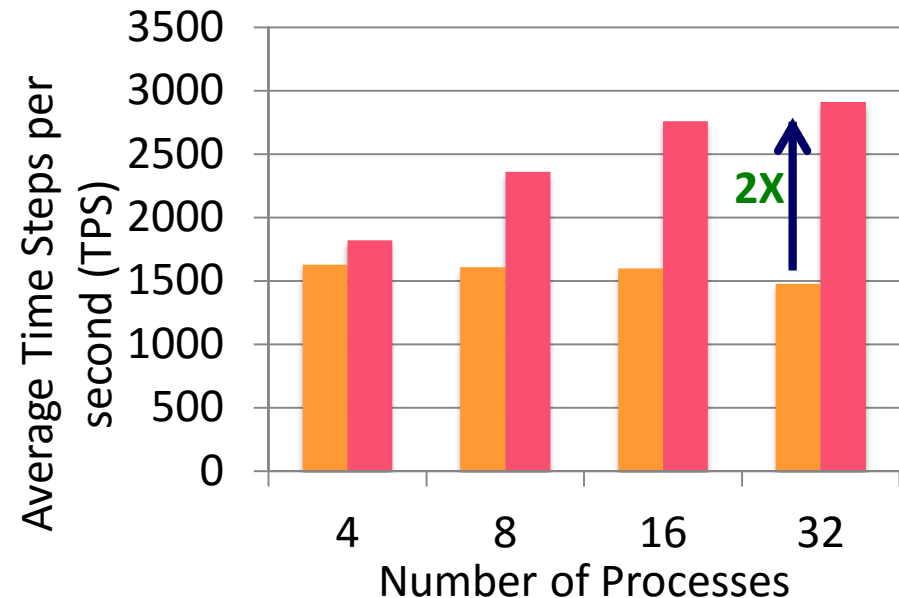
- Up to **69%** overlap* for intra-node GPU-GPU communication
- With GDR, up to **78%** overlap* for inter-node small and medium message transfers
- With intelligent pipeline, up to **88%** overlap* for inter-node large message transfers

*Overlap between GPU-to-GPU communication and CPU computation

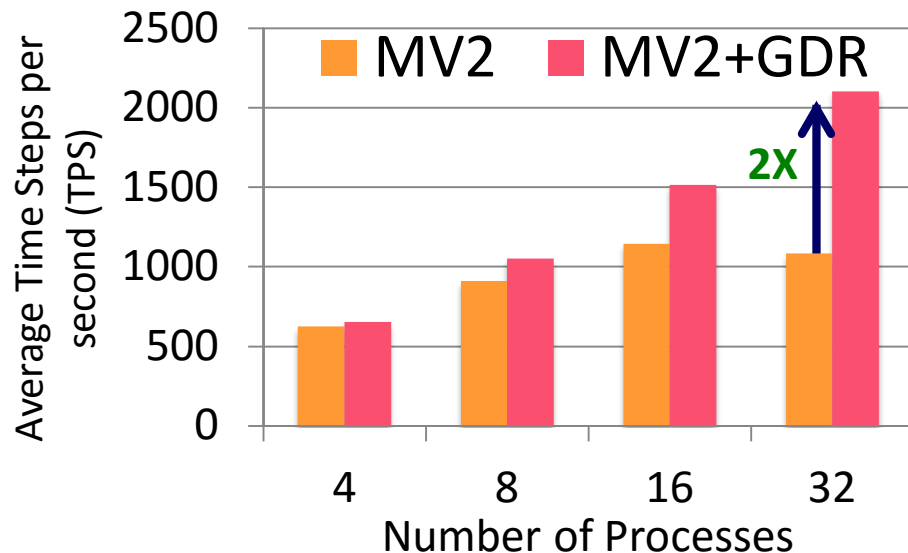
MVAPICH2-GDR-2.3a
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Mellanox Connect-X4 EDR HCA
CUDA 9.0
Mellanox OFED 4.0 with GPU-Direct-RDMA

Application-Level Evaluation (HOOMD-blue)

64K Particles



256K Particles



- 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

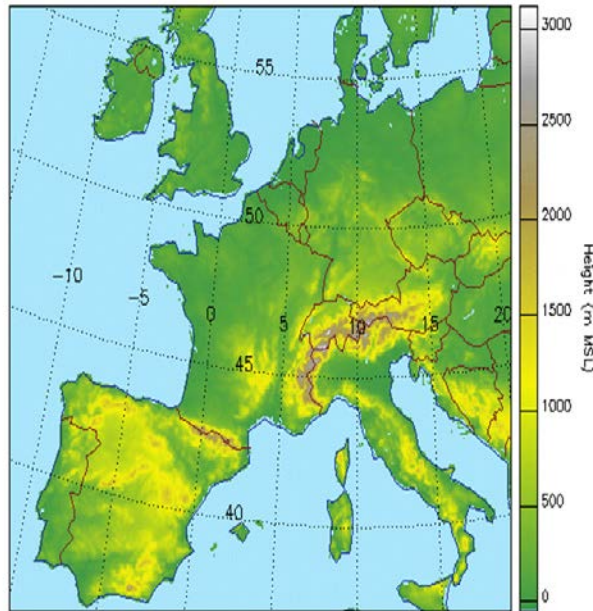
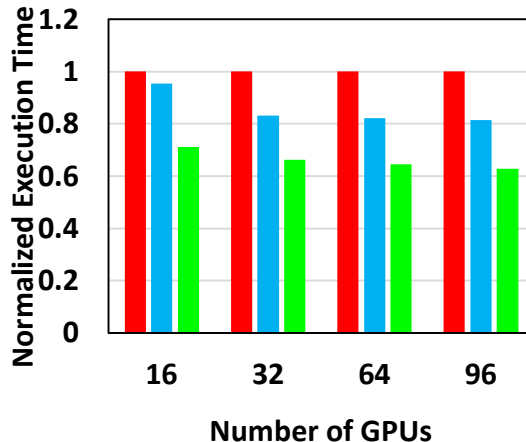
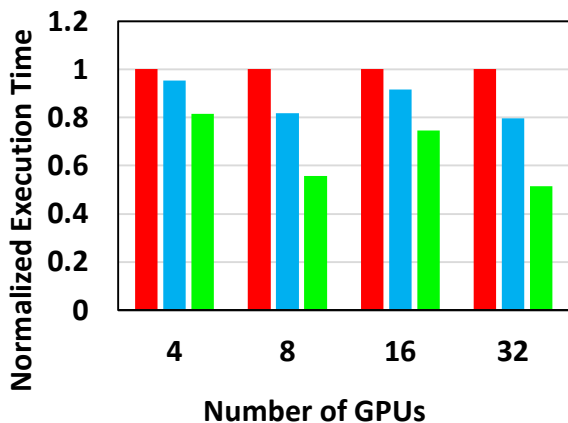
Application-Level Evaluation (Cosmo) and Weather Forecasting in Switzerland

Wilkes GPU Cluster

CSCS GPU cluster

■ Default ■ Callback-based ■ Event-based

■ Default ■ Callback-based ■ Event-based



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

Cosmo model: <http://www2.cosmo-model.org/content/tasks/operational/meteoSwiss/>

On-going collaboration with CSCS and MeteoSwiss (Switzerland) in co-designing MV2-GDR and Cosmo Application

C. Chu, K. Hamidouche, A. Venkatesh, D. Banerjee, H. Subramoni, and D. K. Panda, Exploiting Maximal Overlap for Non-Contiguous Data Movement Processing on Modern GPU-enabled Systems, IPDPS'16

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 - Support for InfiniBand CORE-Direct
 - GPU-kernel based Reduction
 - Datatype Processing
- OSU Caffé

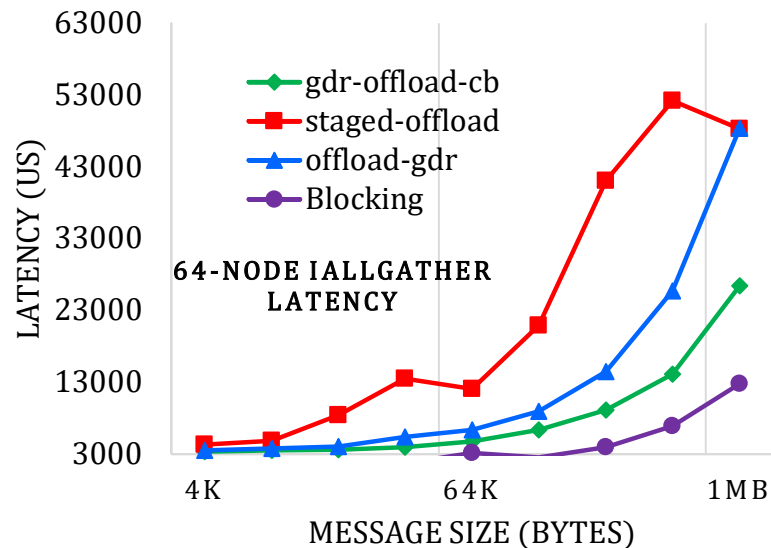
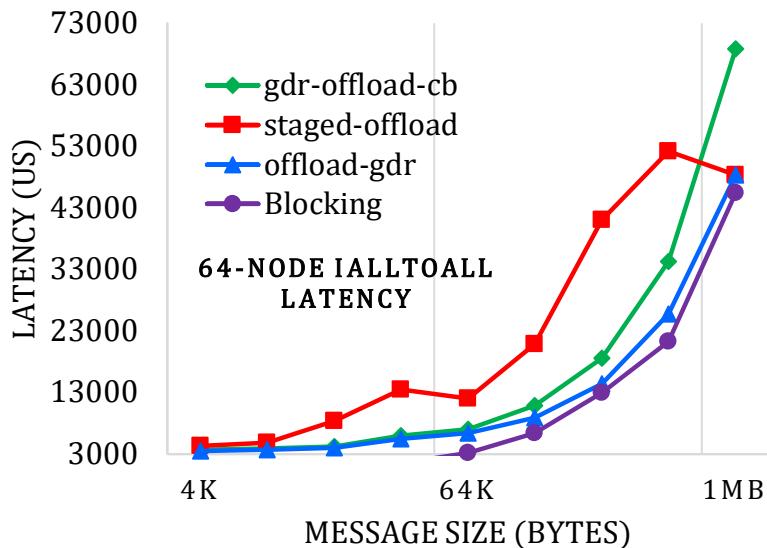
Motivation: Exploiting CORE-Direct and GPUDirect RDMA

- Applications use GPU/CPU resources for computation and MPI for communication directly from GPU buffers
- MPI collectives common in GPU applications. E.g.: Alltoall for FFTs
- Collectives are time consuming with scale so MPI-3.0 introduced NBCs
- Non-blocking communication operations from GPU buffers can
 - Allow CPU to overlap GPU-based communication with CPU compute
 - Ease GPU kernels redundancy in waiting for non-dependent communication
 - Allow power efficient execution from CPU perspective
- Rich set of GPU and network primitives available for NBC designs but architectural limitations must be addressed

Overview of Core-Direct + GPUDirect Designs

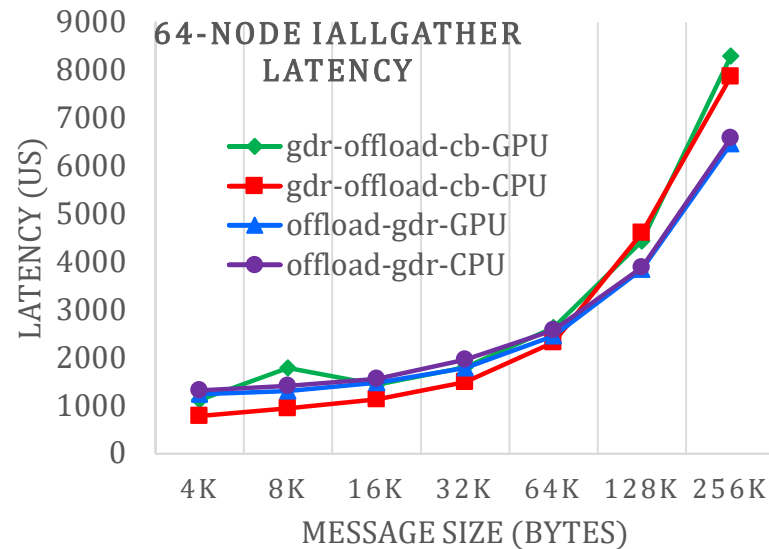
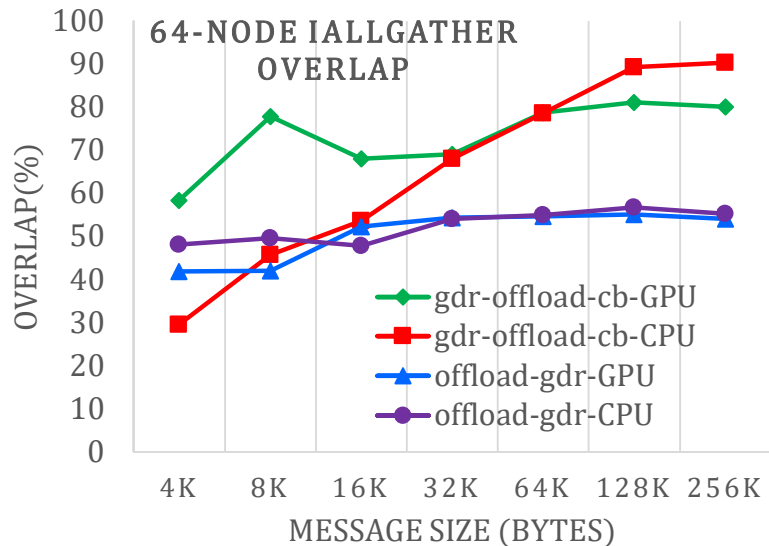
- Realized through mapping of MPICH schedule abstraction
 - Schedule composed of sched_send, sched_barrier, sched_recv, sched_start etc
 - Mapped to Core-Direct primitives with collective-specific GPU↔Host done additionally
- Multiple designs explored
 - Naïve Design: Host-assisted GPU NBC (Scatter)
 - Offload-Staged: Host-assisted GPU NBC + Core-Direct
 - Offload-GDR: (GDR + Core-Direct)-based NBC
 - Offload-Callback: (Core-Direct, GDR, CUDA)-based NBC

Latency Comparison with Blocking Collectives



- Use of GDR and CUDA callback mechanisms improve latency (comparable for alltoall)
- Latency high for the case of alltoall even though callback designed to avoid staging latency

Effect of Compute Location on Overlap/Latency



- New schemes are able to exploit overlap well

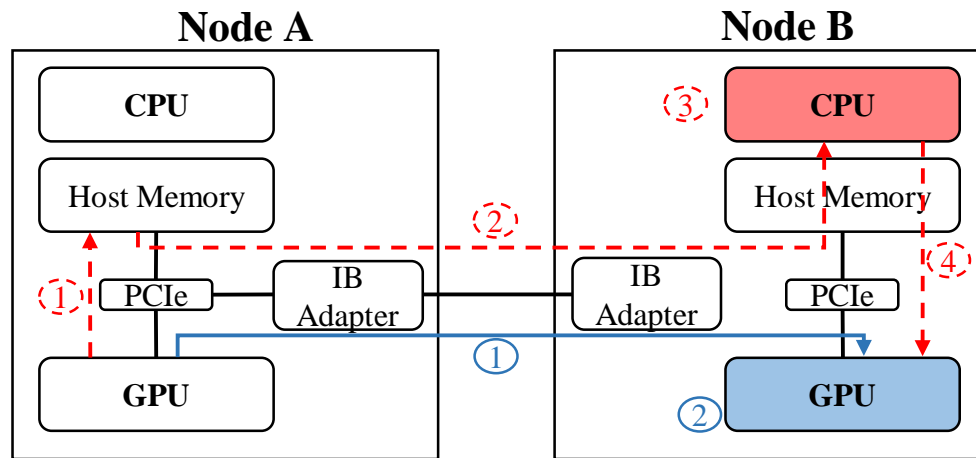
Available in MVAPICH2-GDR 2.3a

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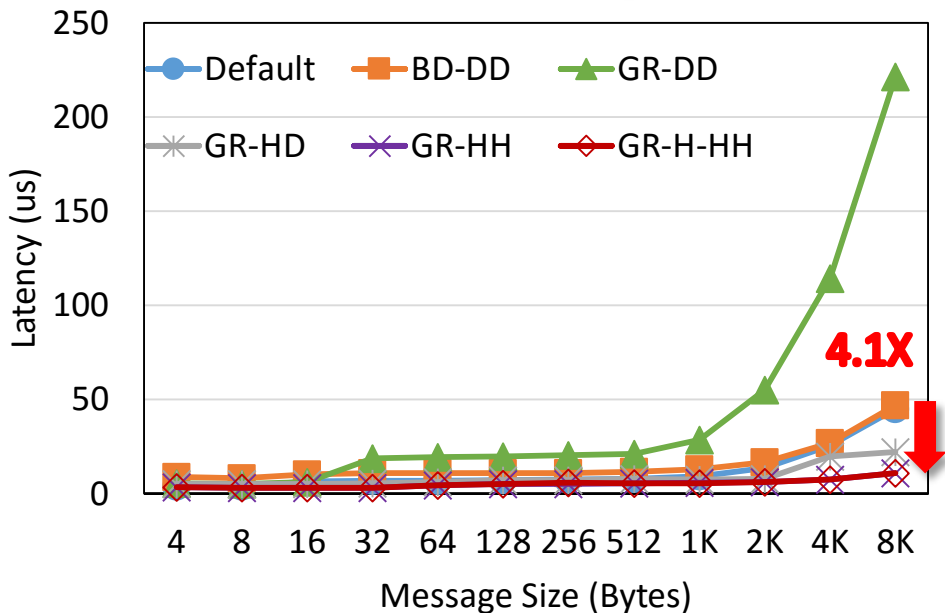
GPU-kernel based Reduction

- Scientific parallel applications spend a considerable amount of time in GPU-based collective communication operations
 - E.g. Deep learning frameworks such as TensorFlow and Caffe
- Optimized computation-intensive collectives in MVAPICH2-GDR
 - MPI_Reduce and MPI_Allreduce
 - Exploring the best combinations
 - Computation on
 - CPU or GPU
 - Communication through
 - Host or GPU memory

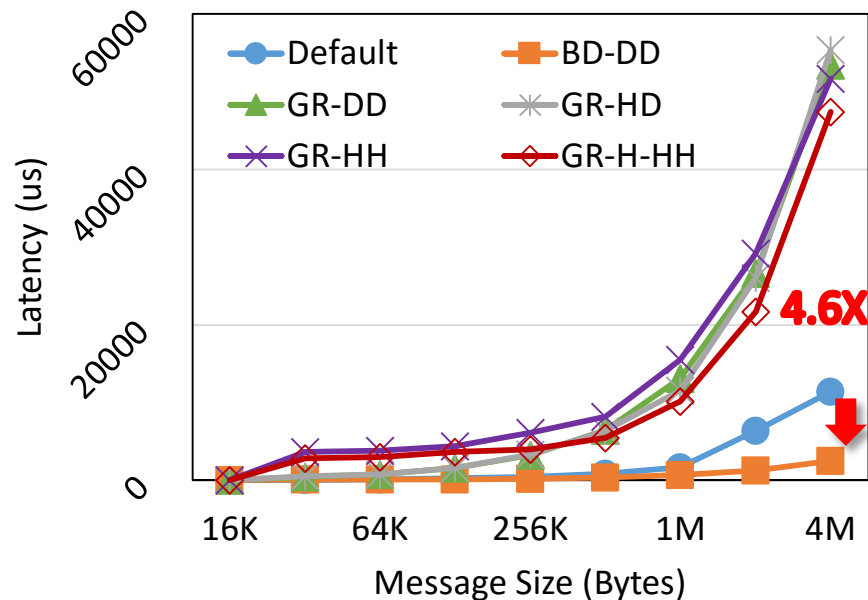


Evaluation - MPI_Reduce @ CSCS (96 GPUs)

Gather-first approaches*
win for small messages



K-nomial GPU-based approach* win for large messages



*Ching-Hsiang Chu, Khaled Hamidouche, Akshay Venkatesh, Ammar Ahmad Awan, and Dhabaleswar K. Panda, "CUDA Kernel based Collective Reduction Operations on Large-scale GPU Clusters," IEEE/ACM CCGrid'16.

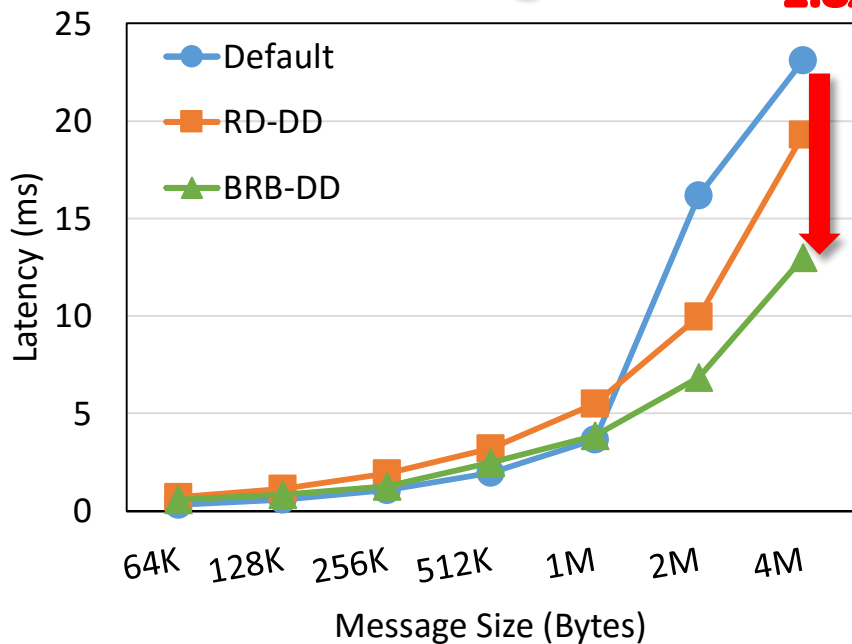
Evaluation - MPI_Allreduce

Available in MVAPICH2-GDR 2.3a

Good Scalability

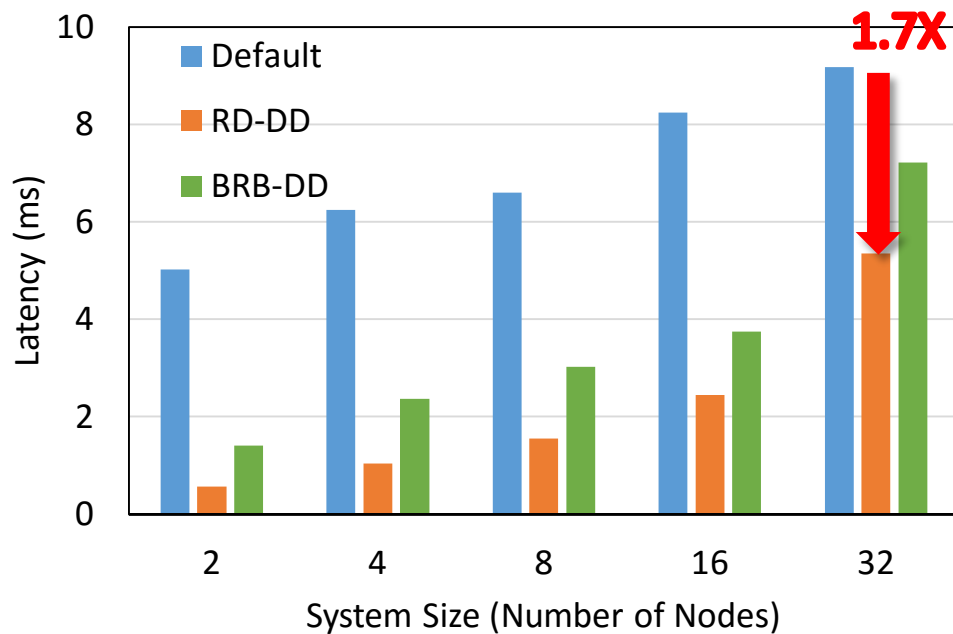
96 GPUs @ CSCS

1.8X



32 GPU Nodes @ Wilkes

1.7X



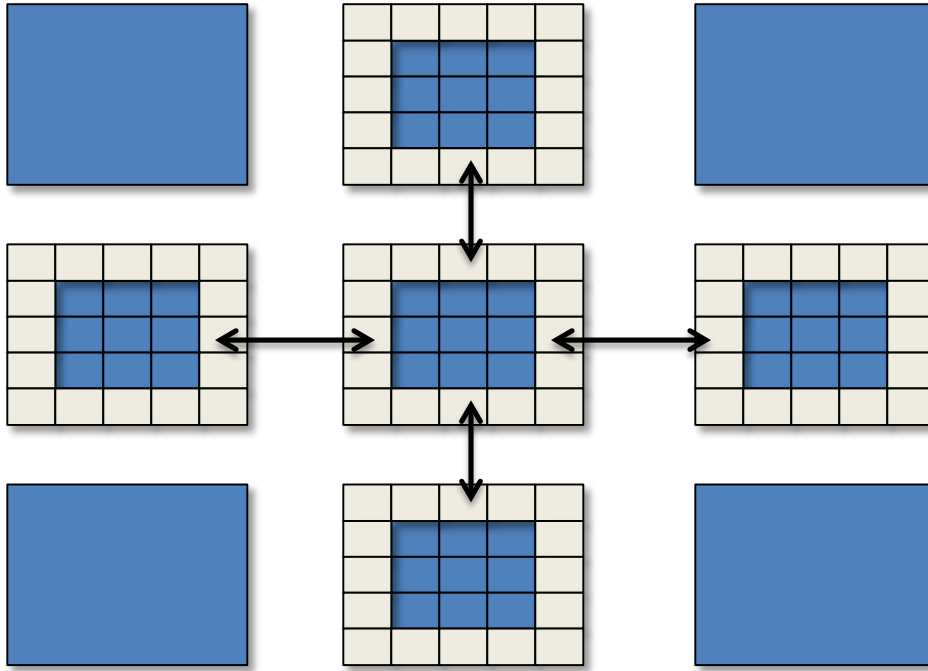
Ching-Hsiang Chu, Khaled Hamidouche, Akshay Venkatesh, Ammar Ahmad Awan, and Dhabaleswar K. Panda, "CUDA Kernel based Collective Reduction Operations on Large-scale GPU Clusters," IEEE/ACM CCGrid'16.

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Non-contiguous Data Exchange

Halo data exchange



- Multi-dimensional data
 - Row based organization
 - Contiguous on one dimension
 - Non-contiguous on other dimensions
- Halo data exchange
 - Duplicate the boundary
 - Exchange the boundary in each iteration

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:

```
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

H. Wang, S. Potluri, D. Bureddy, C. Rosales and D. K. Panda, GPU-aware MPI on RDMA-Enabled Clusters: Design, Implementation and Evaluation, IEEE Transactions on Parallel and Distributed Systems, Vol. 25, No. 10, pp. 2595-2605, Oct 2014.

MPI Datatype Processing (Computation Optimization)

- Comprehensive support
 - Targeted kernels for regular datatypes - vector, subarray, indexed_block
 - Generic kernels for all other irregular datatypes
- Separate non-blocking stream for kernels launched by MPI library
 - Avoids stream conflicts with application kernels
- Flexible set of parameters for users to tune kernels
 - Vector
 - MV2_CUDA_KERNEL_VECTOR_TIDBLK_SIZE
 - MV2_CUDA_KERNEL_VECTOR_YSIZE
 - Subarray
 - MV2_CUDA_KERNEL_SUBARR_TIDBLK_SIZE
 - MV2_CUDA_KERNEL_SUBARR_XDIM
 - MV2_CUDA_KERNEL_SUBARR_YDIM
 - MV2_CUDA_KERNEL_SUBARR_ZDIM
 - Indexed_block
 - MV2_CUDA_KERNEL_IDXBLK_XDIM

MPI Datatype Processing (Communication Optimization)

Common Scenario

```
MPI_Isend(Buf1, ..., req1);
```

```
MPI_Isend(Buf2, ..., req2);
```

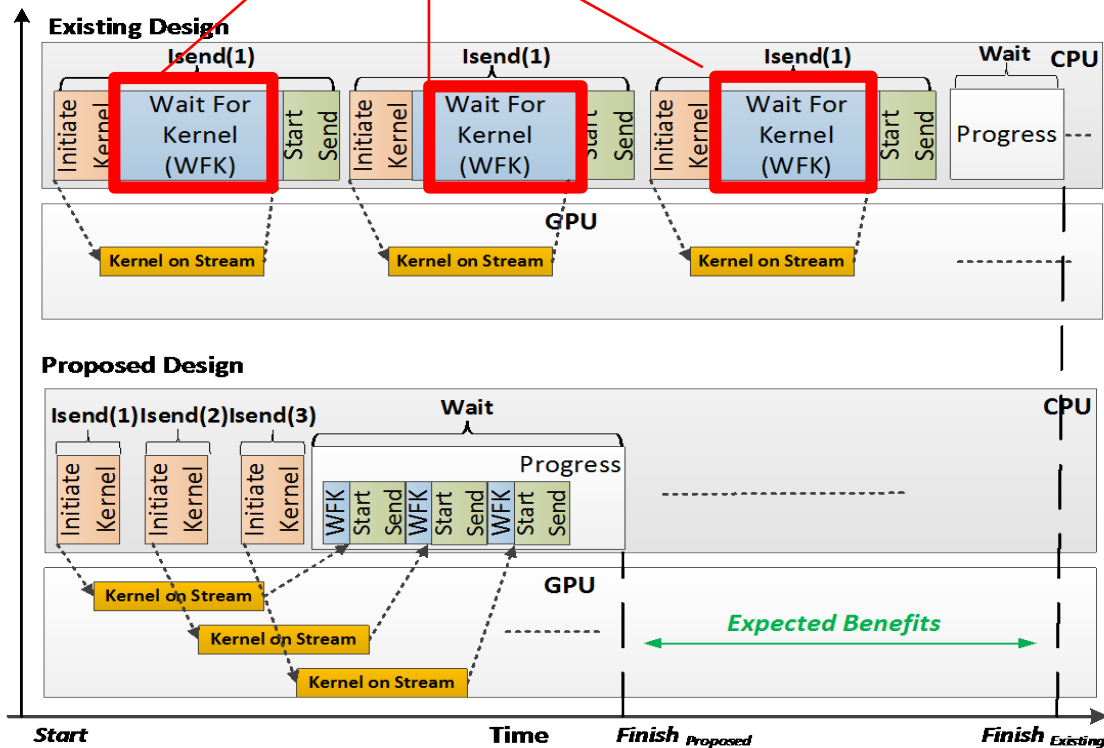
⋮

Application work on the
CPU/GPU

```
MPI_Waitall(requests, ...)
```

*Buf1, Buf2...contain non-contiguous MPI Datatype

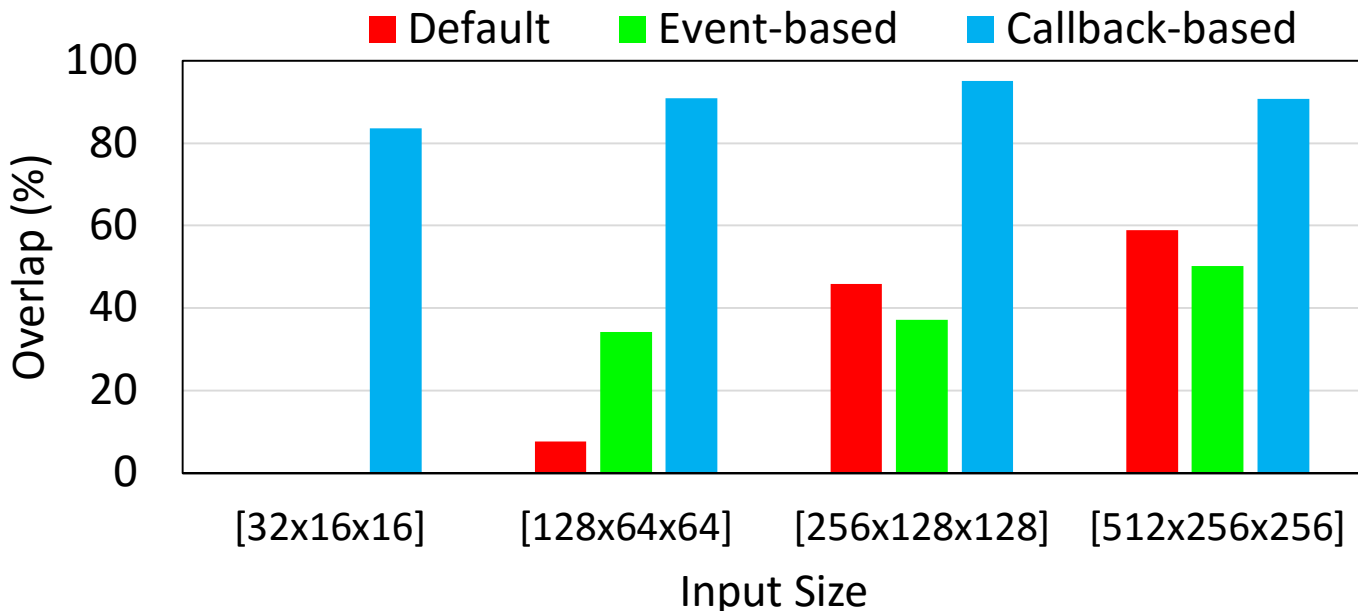
Waste of computing resources on CPU and GPU



MPI Datatype Processing (Communication Optimization)

Available in MVAPICH2-GDR 2.3a

- **Modified ‘CUDA-Aware’ DDTBench for *NAS_MG_y***
 - Up to **90% overlap** between datatype processing and other computation

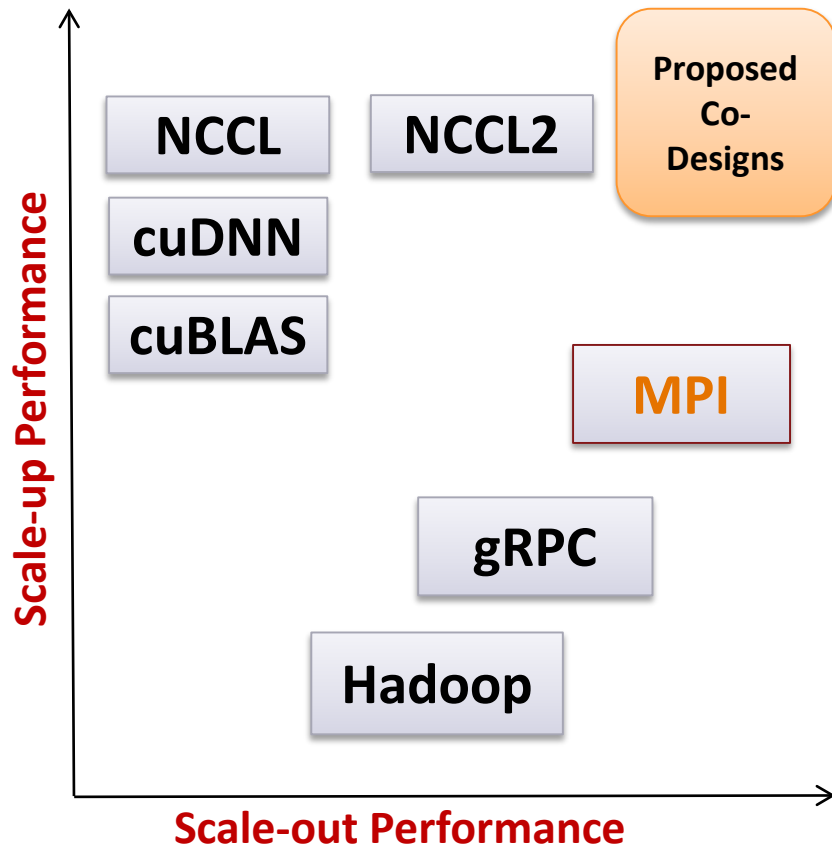


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- MVAPICH2/MVAPICH2-X
 - Job Startup
 - Point-to-point Communication
 - Remote Memory Access (RMA)
 - Collective Communication
- MVAPICH2-GDR
 - Support for InfiniBand CORE-Direct
 - GPU-kernel based Reduction
 - Datatype Processing
- Deep Learning Application: OSU Caffe

Deep Learning: New Challenges for MPI Runtimes

- Deep Learning frameworks are a different game altogether
 - Unusually large message sizes (order of megabytes)
 - Most communication based on GPU buffers
- Existing State-of-the-art
 - cuDNN, cuBLAS, NCCL --> **scale-up** performance
 - NCCL2, CUDA-Aware MPI --> **scale-out** performance
 - For small and medium message sizes only!
- Proposed: Can we **co-design** the MPI runtime (**MVAPICH2-GDR**) and the DL framework (**Caffe**) to achieve both?
 - Efficient **Overlap** of Computation and Communication
 - Efficient **Large-Message** Communication (Reductions)
 - What **application co-designs** are needed to exploit **communication-runtime co-designs**?



A. A. Awan, K. Hamidouche, J. M. Hashmi, and D. K. Panda, S-Caffe: Co-designing MPI Runtimes and Caffe for Scalable Deep Learning on Modern GPU Clusters. In *Proceedings of the 22nd ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP '17)*

OSU-Caffe: Proposed Co-Design Overview

- To address the limitations of Caffe and existing MPI runtimes, we propose the **OSU-Caffe (S-Caffe)** framework
- At the application (DL framework) level
 - Develop a fine-grain workflow – i.e. layer-wise communication instead of communicating the entire model
- At the runtime (MPI) level
 - Develop support to perform reduction of very-large GPU buffers
 - Perform reduction using GPU kernels

OSU-Caffe is available from the HiDL project page
(<http://hidl.cse.ohio-state.edu>)

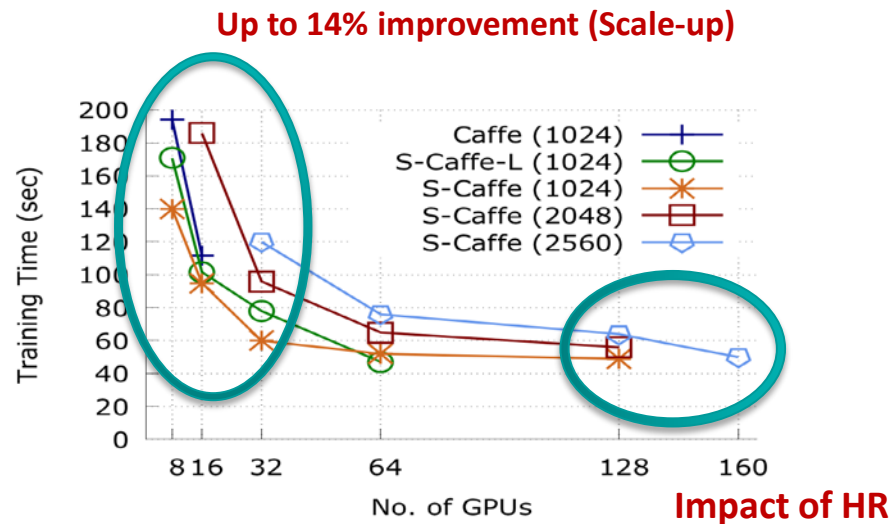
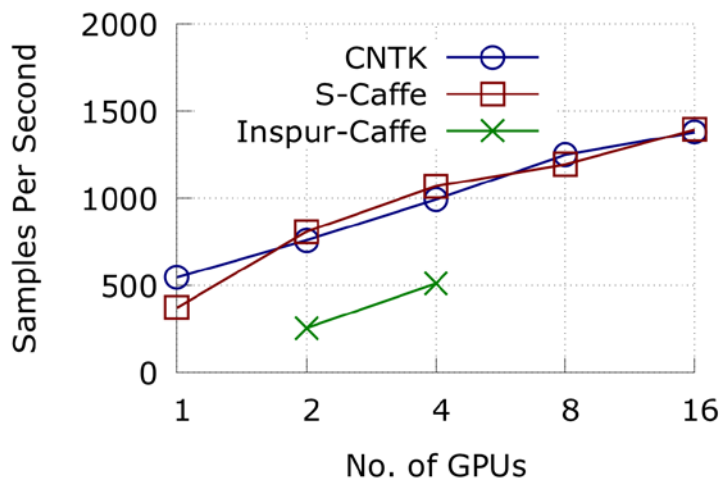
Optimized Data Propagation and Gradient Aggregation using NBC Designs

- Exploit Non-Blocking Collective (NBC) operations in MPI-3
 - Divide communication into fine-grain steps
 - Overlap computation of layer “i” with communication of layer “i+1”
 - **MPI_Ibcast** to post all communication in advance
 - Wait in an on-demand fashion
 - Allow for runtime selection of data propagation design
 - Based on message (DL model) size, number of GPUs, and number of nodes
- Co-design gradient aggregation at application level
 - **Helper thread** based approach to realize a **non-blocking MPI_Reduce**

S-Caffe vs. Inspur-Caffe and Microsoft CNTK

- AlexNet: Notoriously hard to scale-out on multiple nodes due to comm. overhead!
- Large number of parameters ~ 64 Million (comm. buffer size = 256 MB)

- GoogLeNet is a popular DNN
- 13 million parameters (comm. buffer size = ~50 MB)



S-Caffe delivers better or comparable performance with other multi-node capable DL frameworks

Concluding Remarks

- Exploiting overlap between computation and communication is significant in HPC
- Presented some of the approaches and results along these directions taken by the MVAPICH2 and MVAPICH2-GDR Libraries
- Allows applications to take advantage of the overlap capabilities
- As exascale systems are getting more complicated in their architectures, solutions exploiting overlap capabilities will be important

Additional Presentation and Tutorials

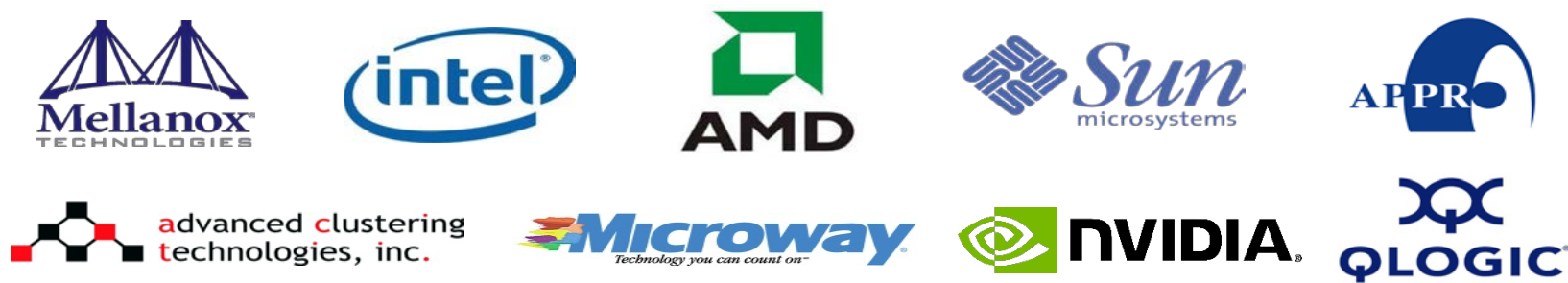
- Tutorial: **How to Boost the Performance of Your MPI and PGAS Applications with MVAPICH2 Libraries**
 - 04/05/18, 9:00 am-12:00 noon
- Tutorial: **High Performance Distributed Deep Learning: A Beginner's Guide**
 - 04/05/18, 1:00pm-4:00 pm

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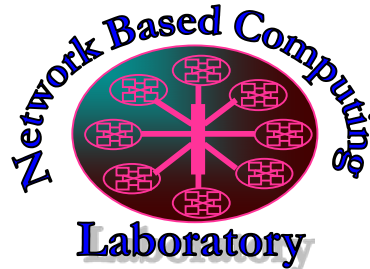
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Thank You!

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Network-Based Computing Laboratory

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



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/>