MPI for Cray XE/XK Systems & Recent Enhancements

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Topics

- Cray MPI overview
- Development focus / recent enhancements
- Overlapping computation and communication
- Memory footprint
- MPI I/O statistics
- MPI Tuning controls for Cray systems

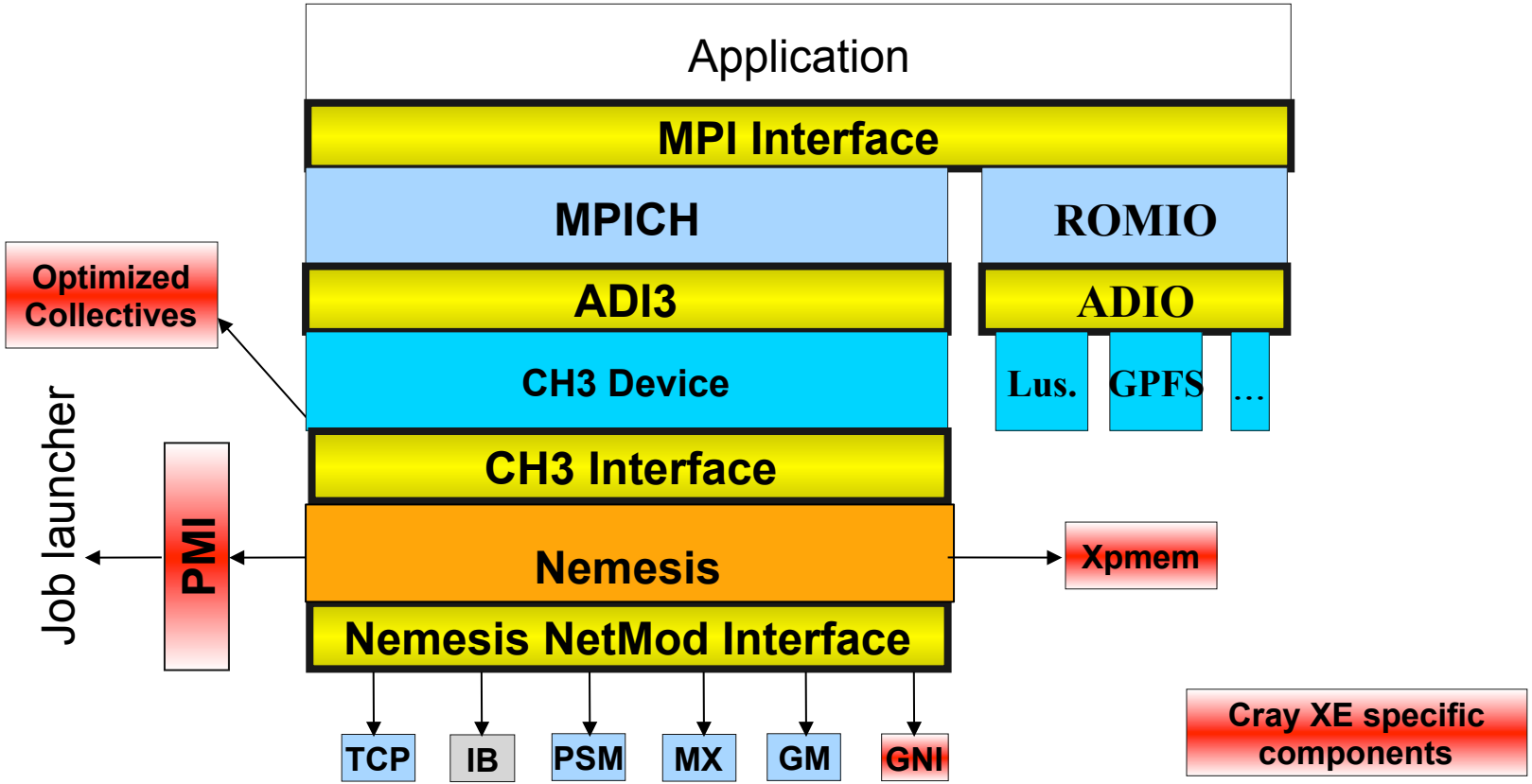
Cray MPI

- **Implementation based on MPICH3 from ANL**
  - ANL does base MPI standard support, we add new functionality, improve performance both on-node, and all ranges of scale including at very high scale
- **Full MPI-3.1 support (Dec 2015) with the exception of**
  - MPI-2 Dynamic process management (MPI_Comm_spawn)
- **MPI Forum active participant**
- **Participated in the MPICH ABI Consortium**
  - ANL MPICH, Intel MPI, IBM PE MPI and Cray MPI

Development Focus Areas

- Minimize communication latency, maximize communication bandwidth
- Improve support for asynchronous communication (communication/computation overlap)
- Architecture-specific solutions to optimize communication performance
- New tools and features to help users understand application performance bottlenecks

MPICH/Cray MPI Layout



Gemini Features Used by Cray MPI

- **FMA (Fast Memory Access)**
  - Used for small messages
  - Very low overhead ➔ good latency
- **DMA offload engine (BTE or Block Transfer Engine)**
  - Used for larger messages
  - All ranks on node share BTE resources (4 virtual channels / node)
  - Can be initiated in user mode
  - Once initiated, BTE transfers proceed without processor intervention
    - Best means to overlap communication with computation

Asynchronous Progress Engine

- Used to improve communication/computation overlap
- Used for non-blocking pt2pt and collective MPI calls
- Each MPI rank starts a “helper thread” during MPI_Init
- Helper threads progress the MPI state engine for both Send and Recv while application is computing
- Only effective if used with core specialization to reserve a core/node for the helper threads or using the Intel hyper-threads
- Must set the following to enable Asynchronous Progress Threads:
  - export MPICH_NEMESIS_ASYNC_PROGRESS=(SC or MC)
  - export MPICH_MAX_THREAD_SAFETY=multiple
- 10% or more performance improvements with some apps

Fine-Grained Multi-threading for MPI

- Optimized support for programs that perform MPI operations within threaded regions
- Only MPI point-to-point operations optimized at this time
- Default MPI library uses a global lock
  - A single global_mutex is used for all MPI calls
- Separate MT MPI library uses per-object (fine-grained) locks
  - The global_mutex is still used, but critical sections are much smaller
  - Additional small locks have also been added
- Must link with a separate version of Cray MPI library
  - Use the compiler driver option: -craympich-mt
- To use:
  - `> cc -craympich-mt -o mpi_mt_test.x  mpi_mt_test.c`
  - `> export MPICH_MAX_THREAD_SAFETY=multiple`

Cray MPI-3 Non-blocking Collectives

- Allows overlap with computation during collective operations
- All MPI collectives have MPI_I<name> versions (i.e. MPI_Ibcast)
- MPI Asynchronous Progress Engine Feature is needed to give the best overlap
- To enable, use the following environment variables
  - MPICH_NEMESIS_ASYNC_PROGRESS=(SC or MC)
    (setting to 1 is the same as setting it to SC on Gemini, MC on Aries)
  - MPICH_MAX_THREAD_SAFETY=multiple
- Best to run using:
  - Core-specialization (aprun –r) on Gemini, or if no hyperthreads available.
  - Unused Intel hyperthread cores (aprun –j) on Aries

Minimized MPI Memory Footprint

- **Implemented a Dynamic Virtual Channel (VC) Feature**
  - Internal VC structures only allocated when one rank makes direct contact with another rank
  - Prior MPT versions allocated VCs statically for all ranks in job during MPI_Init
  - Enabled by default starting with MPT 7.2.3
- **Implemented special optimizations for MPI_Alltoall and MPI_Alltoallv that don't require use of VC structures**
- **Significantly reduces MPI footprint for many HPC apps (nearest neighbor communication plus global collectives)**

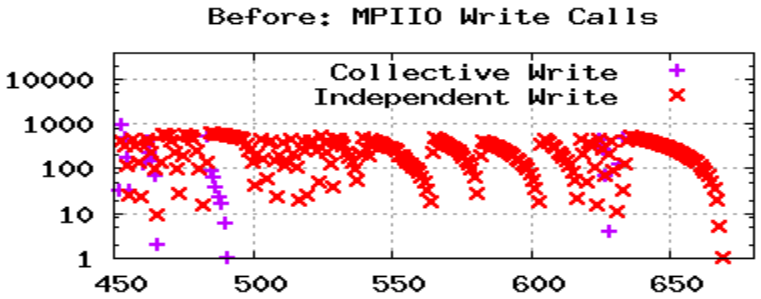
MPI I/O File Access Pattern Statistics

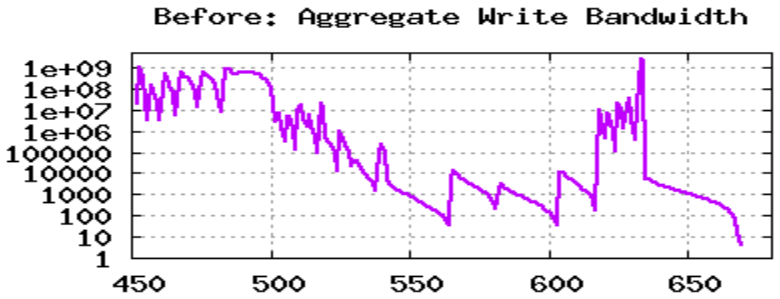
- When setting MPICH_MPIIO_STATS=1, a summary of file write and read access patterns are written by rank 0 to stderr
- When setting MPICH_MPIIO_STATS=2, a set of data files (one per rank) are written which can be summarized with the supplied cray_mpiio_summary script
- The "Optimizing MPI I/O" white paper describes how to interpret the data and makes suggestions on how to improve your application.
  - Available on docs.cray.com under Knowledge Base

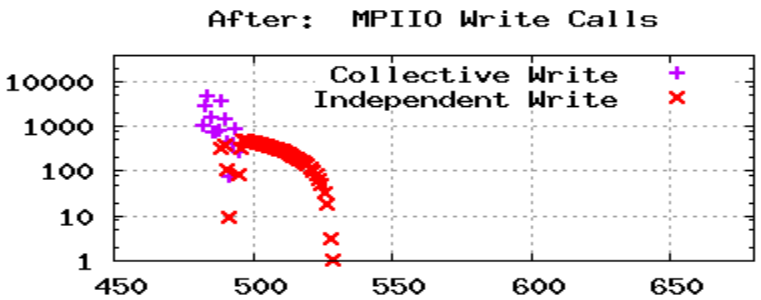
MPI I/O File Access Pattern Statistics (2)

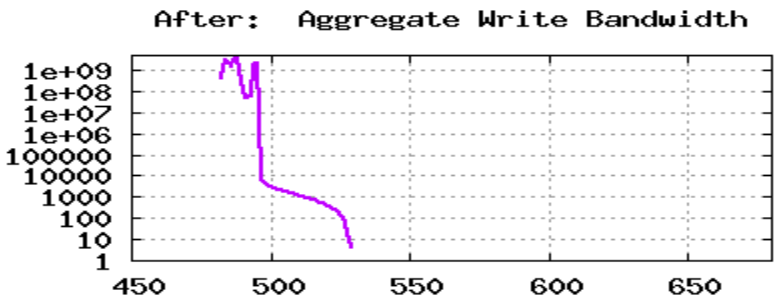
Timeline of MPI-I/O statistics. Many different variables tracked

```
export MPICH_MPIIO_STATS=2
```









MPI Tuning Controls for Cray Systems with Gemini

MPICH_RANK_REORDER_METHOD

- Vary your rank placement to optimize communication
- Can be a quick, low-hassle way to improve performance
- Use CrayPat to produce a specific MPICH_RANK_ORDER file to maximize intra-node communication
- Or, use perftools grid_order command with your application's grid dimensions to layout MPI ranks in alignment with data grid
- To use:
  - name your custom rank order file: MPICH_RANK_ORDER
  - export MPICH_RANK_REORDER_METHOD=3

Use HUGEPAGES

Linking and running with hugepages can offer a significant performance improvement for many MPI communication sequences, including MPI collectives and basic MPI_Send/MPI_Recv calls.

- **To use HUGEPAGES:**
  - **`module load craype-hugepages8M`** (many sizes supported)
  - *<< compile your app >>*
  - **`module load craype-hugepages8M`**
  - *<< run your app >>*

MPICH_USE_DMAPP_COLL / MPICH_RMA_OVER_DMAPP

- **Enables highly optimized algorithms which may result in significant performance gains**
- **Not enabled by default to avoid disadvantages**
  - May reduce resources MPICH has available (share with DMAPP)
  - DMAPP does not handle transient network errors
- **Supported DMAPP-optimized functions:**
  - MPI_Allreduce
  - MPI_Bcast
  - MPI_Barrier
  - MPI_Put / MPI_Get / MPI_Accumulate
- **To use (link with libdmapp):**
  - Collective use: export MPICH_USE_DMAPP_COLL=1
  - RMA one-sided use: export MPICH_RMA_OVER_DMAPP=1

Tune Inter-node Traffic on Gemini

- **Most significant env variables to play with:**
  - **MPICH_GNI_MAX_VSHORT_MSG_SIZE**
    - Controls max message size for E0 mailbox path (Default: varies)
  - **MPICH_GNI_MAX_EAGER_MSG_SIZE**
    - Controls max message size for E1 Eager Path (Default: 8K bytes)
  - **MPICH_GNI_NUM_BUFS**
    - Controls number of 32KB internal buffers for E1 path (Default: 64)
  - **MPICH_GNI_NDREG_MAXSIZE**
    - Controls max message size for R0 Rendezvous Path (Default: 512K bytes)
  - **MPICH_GNI_RDMA_THRESHOLD**
    - Controls threshold for switching to BTE from FMA (Default: 1K bytes)
  - See the MPI man page for further details

MPICH_NEMESIS_ASYNC_PROGRESS

- **Maximize overlap of communication with computation**
- **Enable asynchronous progress engine**
  - Launches additional thread per MPI process to help progress communication in the background
- **Consider trying this if all of these apply to your application:**
  - App uses non-blocking MPI communication (MPI_Isend/MPI_Irecv or non-blocking collectives) with medium-large messages
  - There is computation work between MPI communication sequences
  - Hyperthreads are available on each node (not in use by your application)
- **To use:**
  - export MPICH_MAX_THREAD_SAFETY=multiple
  - export MPICH_NEMESIS_ASYNC_PROGRESS=SC
  - Use aprun –r1 option

Specific Collective Algorithm Tuning

- **Different algorithms may be used for different message sizes in collectives (e.g.)**
  - Algorithm A might be used for Alltoall for messages < 1K.
  - Algorithm B might be used for messages >= 1K.
- **To optimize a collective, you can modify the cutoff points when different algorithms are used. This may improve performance.**
- **MPICH_ALLTOALL_SHORT_MSG**
- **MPICH_ALLGATHER_VSHORT_MSG**
- **MPICH_ALLGATHERV_VSHORT_MSG**
- **MPICH_GATHERV_SHORT_MSG**
- **MPICH_SCATTERV_SHORT_MSG**
- **See the MPI man page for further details**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