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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
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

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

```bash
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 >>
● 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
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
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
Thank You