Using MPI Effectively on Theta

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Acknowledgements
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Outline

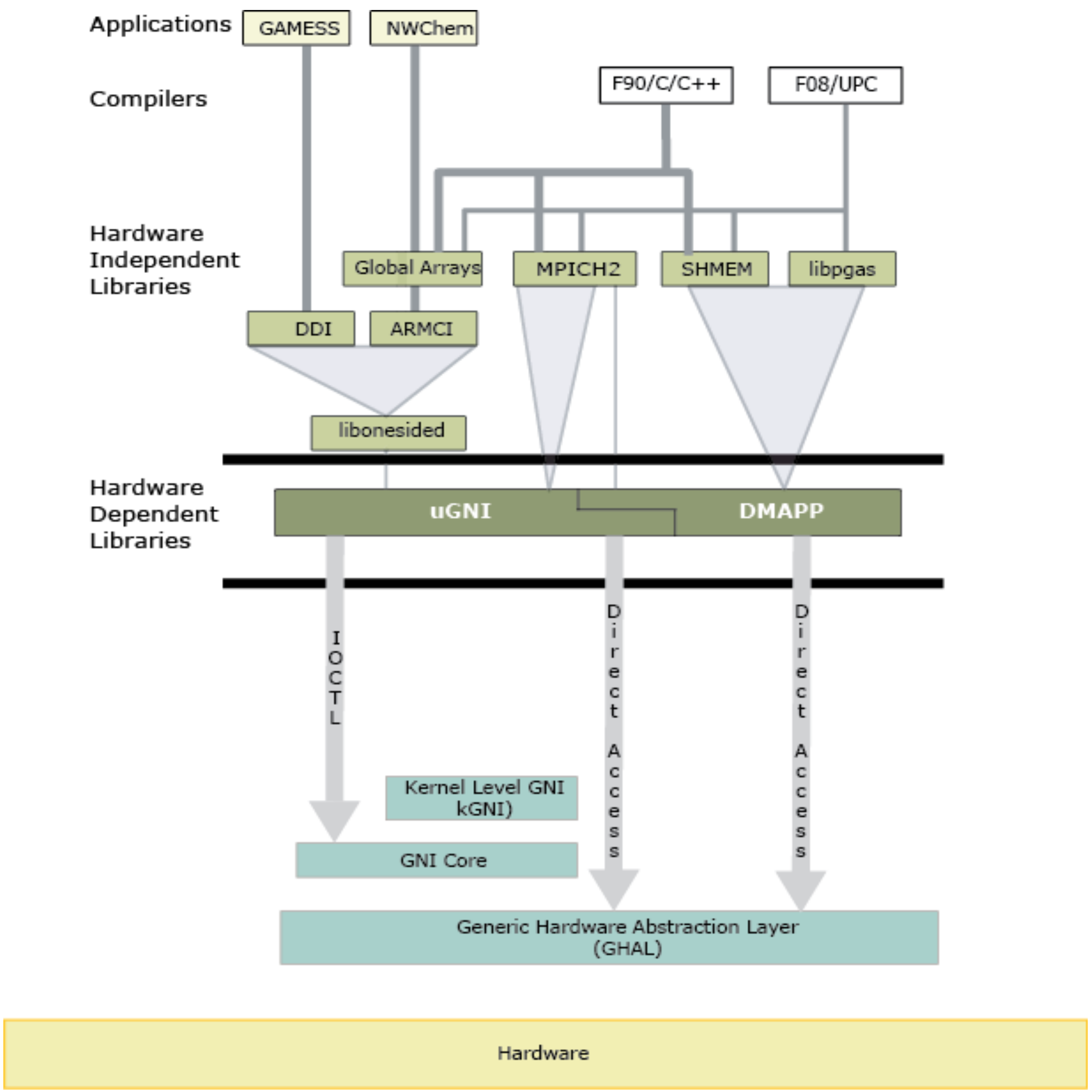
- Cray XC40 (Theta) Network Software Stack
- Introduction to MPI on Theta (Cray MPICH)
  - MPI 3.0 feature support in Cray MPICH
- MPI Tuning Parameters
  - KNL specific
  - Network specific
- Recommendations for optimizing MPI performance

Cray XC Network Software Stack

DMAPP - Distributed Shared Memory Application APIs (shared memory)

uGNI - Generic Network Interface (message passing based)

uGNI and **DMAPP** provide low-level communication services to user-space software



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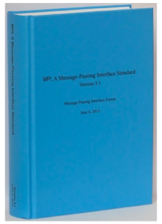
Brief Introduction to Cray MPICH

- Cray MPI compliant with MPI 3.1
  - Cray MPI uses MPICH3 distribution from Argonne
  - Merge to ANL MPICH 3.2 – latest release MPT 7.7.1

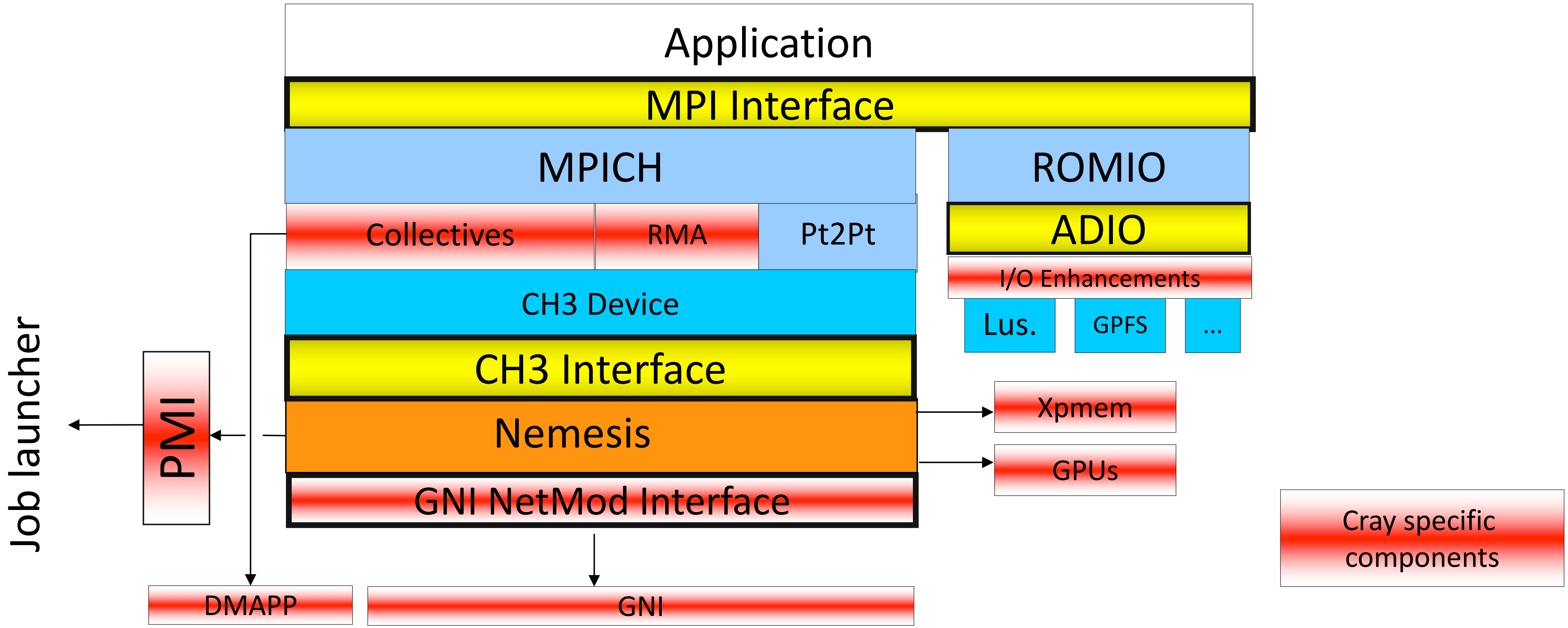


- I/O, collectives, P2P, and one-sided all optimized for XC architecture
  - SMP aware collectives
  - High performance single-copy on-node communication via xpmem (not necessary to program for shared memory)
  - HW collectives to optimize small message collectives at scale (MPI-3)
  - Non-Blocking Collectives (MPI-3)
  - Highly optimized "Thread-Hot" MPI-3 one-sided (RMA) communication (MPI-3)
  - Dynamic Process Management Support (MPI-3)
  - Optimized and Tuned MPI I/O

- Highly tunable through environment variables
  - Defaults should generally be best, but some cases benefit from fine tuning

- Integrated within the Cray Programming Environment
  - Compiler drivers manage compile flags and linking automatically
  - Profiling through Cray Perftools

Cray MPI Software Stack (CH3 device)



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MPI-3 Nonblocking Collectives

- Enables **overlap of communication/computation** similar to nonblocking (send/recv) communication
- Non-blocking variants of all collectives: MPI_Ibcast (<bcast args>, MPI_Request *req);
- Semantics
  - Function returns no matter what
  - Usual completion calls (wait, test)
  - Out-of-order completion
- Semantic advantages
  - Enables asynchronous progression (software pipelining)
  - Decouple data transfer and synchronization (Noise Resiliency)
  - Allow overlapping communicators
  - Multiple outstanding operations at any time

```
MPI_Comm comm;
int array1[100], array2[100];
int root=0;
MPI_Request req;
...
MPI_Ibcast(array1, 100, MPI_INT,
root, comm, &req);
compute(array2, 100);
MPI_Wait(&req, MPI_STATUS_IGNORE);
```

MPI-3 Nonblocking Collectives Support

- Cray MPT includes many optimizations for MPI-3 nonblocking Collectives
- *Not on by default.* User must set the following env. Variables:

  export MPICH_NEMESIS_ASYNC_PROGRESS=[SC|MC|<u>ML</u>] (network interface DMA engine enables asynchronous progress)

  export MPICH_MAX_THREAD_SAFETY=multiple

- Special optimizations for Small message MPI_Iallreduce, based on Aries HW Collective Engine:

  Users must link against DMAPP

  -Wl, --whole-archive, -ldmapp, --no-whole-archive (static linking)

  -ldmapp (dynamic linking)

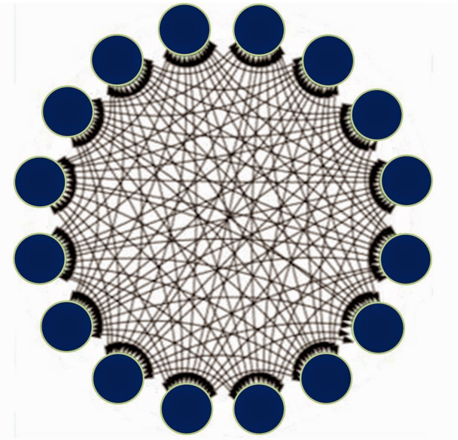
  export MPICH_NEMESIS_ASYNC_PROGRESS =[SC|MC|<u>ML</u>]

  export MPICH_MAX_THREAD_SAFETY=multiple

  export MPICH_USE_DMAPP_COLL=1

Topology Mapping and Neighborhood Collectives

- Topology mapping
  - Minimize communication costs through interconnect topology aware *task mapping*
  - Could ***potentially*** help reduce congestion
  - Node placement for the job could be a factor (no explicit control available to request a specific placement)
- *Application communication pattern*
  - MPI process topologies expose this in a portable way
  - Network topology agnostic
- *Rank reordering*
  - Can override the default mapping scheme
  - The default policy for **aprun** launcher is SMP-style placement
  - To display the MPI rank placement information, set **MPICH_RANK_REORDER_DISPLAY**.



Rank Reordering

- MPICH_RANK_REORDER_METHOD
  - Vary rank placement to optimize communication (Maximize on-node communication between MPI ranks)
  - Use CrayPat with “-g mpi” to produce a specific **MPICH_RANK_ORDER** file to maximize intra-node communication
  - Or, use perf_tools **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
    - This approach is physical system topology agnostic

export MPICH_RANK_REORDER_METHOD=3

Rank Reordering

- MPICH_RANK_REORDER_METHOD (cont.)
  - A topology and placement aware reordering method is also available
  - Optimizes rank ordering for Cartesian decompositions using the layout of nodes in the job
  - To use:
    - **export MPICH_RANK_REORDER_METHOD=4**
    - **export MPICH_RANK_REORDER_OPTS="–ndims=3 –dims=16,16,8"**

```
MPI Grid Detection:
There appears to be point-to-point MPI communication in a 96 X 8 grid pattern. The 52% of the total execution time
spent in MPI functions might be reduced with a rank order that maximizes communication between ranks on the same node.
The effect of several rank orders is estimated below.

A file named MPICH_RANK_ORDER.Grid was generated along with this report and contains usage instructions and the Custom
rank order from the following table.

          Rank      On-Node   On-Node   MPICH_RANK_REORDER_METHOD
          Order     Bytes/PE  Bytes/PE%
                    of Total
                    Bytes/PE

          Custom     2.385e+09 95.55%   3
          SMP        1.880e+09 75.30%   1
          Fold       1.373e+06 0.06%    2
          RoundRobin 0.000e+00 0.00%    0
```

Profiling with CrayPat

- Application built with "pat_build –g mpi"
- Pat_report generates the CrayPat report

- Note the MPI call times, calls
- Load imbalance across the ranks

```
Table 1:  Profile by Function Group and Function

  Time% |        Time | Imb. Time |   Imb. |          Calls | Group
        |             |           |  Time% |                |  Function
        |             |           |        |                |   PE=HIDE

 100.0% | 667.935156 |        -- |     -- | 49,955,946.2 | Total
|-----------------------------------------------------------------------------
|  40.0% | 267.180169 |        -- |     -- | 49,798,359.2 | MPI
||----------------------------------------------------------------------------
||  24.0% | 160.400193 | 28.907525 |  15.3% |  2,606,756.0 | MPI_Wait
||   6.4% |  42.897564 |  0.526996 |   1.2% |    157,477.0 | MPI_Allreduce
||   4.8% |  31.749303 |  3.923541 |  11.0% | 42,853,974.0 | MPI_Comm_rank
||   3.5% |  23.303805 |  1.774076 |   7.1% |  1,303,378.0 | MPI_Isend
||   1.1% |   7.658009 |  0.637044 |   7.7% |  1,303,378.0 | MPI_Irecv
||============================================================================
|  39.1% | 260.882504 |        -- |     -- |          2.0 | USER
||----------------------------------------------------------------------------
||  39.1% | 260.882424 | 17.270557 |   6.2% |          1.0 | main
||============================================================================
|  20.9% | 139.872482 |        -- |     -- |    157,585.0 | MPI_SYNC
||----------------------------------------------------------------------------
||  20.4% | 136.485384 | 36.223589 |  26.5% |    157,477.0 | MPI_Allreduce(sync)
|=============================================================================
```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Profiling with CrayPat

- MPI message sizes are reported

```
=================================================================
  Total
-----------------------------------------------------------------
  MPI Msg Bytes%                                100.0%
  MPI Msg Bytes                       18,052,938,280.0
  MPI Msg Count                            1,460,959.0 msgs
  MsgSz <16 Count                            157,529.0 msgs
  16<= MsgSz <256 Count                           65.0 msgs
  256<= MsgSz <4KiB Count                      2,815.0 msgs
  4KiB<= MsgSz <64KiB Count                1,300,511.0 msgs
  64KiB<= MsgSz <1MiB Count                       39.0 msgs
=================================================================
  MPI_Isend
-----------------------------------------------------------------
  MPI Msg Bytes%                                100.0%
  MPI Msg Bytes                       18,051,670,432.0
  MPI Msg Count                            1,303,378.0 msgs
  MsgSz <16 Count                                 16.0 msgs
  16<= MsgSz <256 Count                            0.0 msgs
  256<= MsgSz <4KiB Count                      2,812.0 msgs
  4KiB<= MsgSz <64KiB Count                1,300,511.0 msgs
  64KiB<= MsgSz <1MiB Count                       39.0 msgs
=================================================================
```

MPI Topology Functions

- Convenience functions (MPI-1)
  - Create a graph and query it, nothing else
  - Useful especially for Cartesian topologies
  - Query neighbors in n-dimensional space
  - Graph topology: each rank specifies full graph
- Scalable Graph topology (MPI-2.2)
  - Graph topology: each rank specifies its neighbors or arbitrary subset of the graph
- Neighborhood collectives (MPI-3.0)
  - Adding communication functions defined on graph topologies (neighborhood of distance one)

Neighborhood Collectives

- New functions MPI_Neighbor_allgather, MPI_Neighbor_alltoall, and their variants define collective operations among a process and its neighbors
  - Allgather: One item to all neighbors
  - Alltoall: Personalized item to each neighbor
- Neighborhood collectives add communication functions to process topologies
  - Neighbors are defined by an MPI Cartesian or graph virtual process topology that must be previously set
- There functions are useful, for example, in stencil computations that require nearest-neighbor Exchanges
- Enables "Build your own collective" functionality in MPI
  - Neighborhood collectives are a simplified version – data types for communication patterns
- They also represent sparse all-to-many communication concisely, which is essential when running on many thousands of processes
  - Do not require passing long vector arguments as in MPI_Alltoallv

Hugepages to Optimize MPI

- Use HUGEPAGES
  - While this is not an MPI env variable, 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
  - Most important for applications calling `MPI_Alltoall[v]` or performing point to point operations with a similarly well connected pattern and large data footprint

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

Key Environment Variables for XC

- Use `MPICH_USE_DMAPP_COLL` for hardware supported collectives
  - Most of MPI's optimizations are enabled by default, but not the DMAPP-optimized features, because…
  - Using DMAPP may have some disadvantages
    - May reduce resources MPICH has available (share with DMAPP)
    - Requires more memory (DMAPP internals)
    - DMAPP does not handle transient network errors
  - These are highly-optimized algorithms which may result in significant performance gains, but user has to request them
  - Supported DMAPP-optimized functions:
    - `MPI_Allreduce` (4-8 bytes)
    - `MPI_Bcast` (4 or 8 bytes)
    - `MPI_Barrier`
  - To use (link with libdmapp):
    - Collective use: **export MPICH_USE_DMAPP_COLL=1**

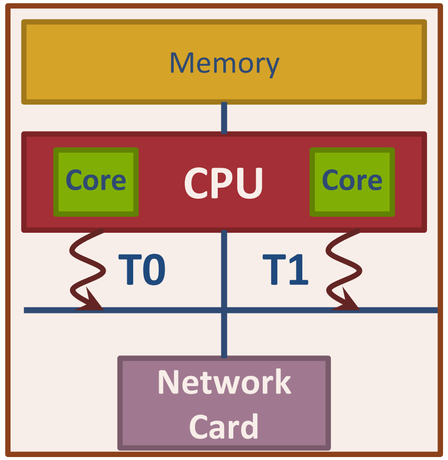
Key Environment Variables for XC

- MPICH GNI environment variables
  - To optimize inter-node traffic using the Aries interconnect, the following are the most significant env variables to play with (*avoid significant deviations from the default if possible*):
  - `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: 4MB)
  - `MPICH_GNI_RDMA_THRESHOLD`
    - Controls threshold for switching to BTE from FMA (Default: 1K bytes)
- See the MPI man page for further details

Key Environment Variables for XC

- 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. A few important ones are:
    - `MPICH_ALLGATHER_VSHORT_MSG`
    - `MPICH_ALLGATHERV_VSHORT_MSG`
    - `MPICH_GATHERV_SHORT_MSG`
    - `MPICH_SCATTERV_SHORT_MSG`
    - `MPICH_GNI_A2A_BLK_SIZE`
    - `MPICH_GNI_A2A_BTE_THRESHOLD`
- See the MPI man page for further details

MPI+X Hybrid Programming Optimizations



MPI + Threads

- MPI Thread Multiple Support for
  - Point to point operations & Collectives (optimized global lock)
  - MPI-RMA (thread hot)
- All supported in default library
  (Non-default Fine-Grained Multi-Threading library is no longer needed)
- Users must set the following env. variable: **export MPICH_MAX_THREAD_SAFETY=multiple**
- Global lock optimization ON by default (N/A for MPI-RMA)
  - **export MPICH_OPT_THREAD_SYNC=0** falls back to pthread_mutex()
- "Thread hot" optimizations for MPI-3 RMA:
  - Contention free progress and completion
  - High bandwidth and high message rate
  - Independent progress – thread(s) flush outstanding traffic, other threads make uninterrupted progress
  - Locks needed (within the MPI library) only if the number of threads exceed the number of network resources
  - Dynamic mapping between threads and network resources
    - Helps mitigate load imbalance and skew between threads

Cray MPI support for MCDRAM on KNL

- Cray MPI offers allocation + hugepage support for MCDRAM on KNL
  - Must use: MPI_Alloc_mem() or MPI_Win_Allocate()
  - Dependencies: memkind, NUMA libraries and dynamic linking.
    module load cray-memkind

- Feature controlled with env variables
  - Users select: Affinity, Policy and PageSize
  - `MPICH_ALLOC_MEM_AFFINITY =  DDR or MCDRAM`
    - DDR = allocate memory on DDR (default)
    - MCDRAM = allocate memory on MDCRAM
  - `MPICH_ALLOC_MEM_POLICY  =  M/ P/ I`
    - M = Mandatory: fatal error if allocation fails
    - P = Preferred: fall back to using DDR memory (default)
    - I = Interleaved: Set memory affinity to interleave across MCDRAM NUMA nodes (For SNC* cases)
  - `MPICH_ALLOC_MEM_PG_SZ`
    - 4K, 2M, 4M, 8M, 16M, 32M, 64M, 128M, 256M, 512M (default 4K)

Cray MPI support for MCDRAM on KNL (use cases)

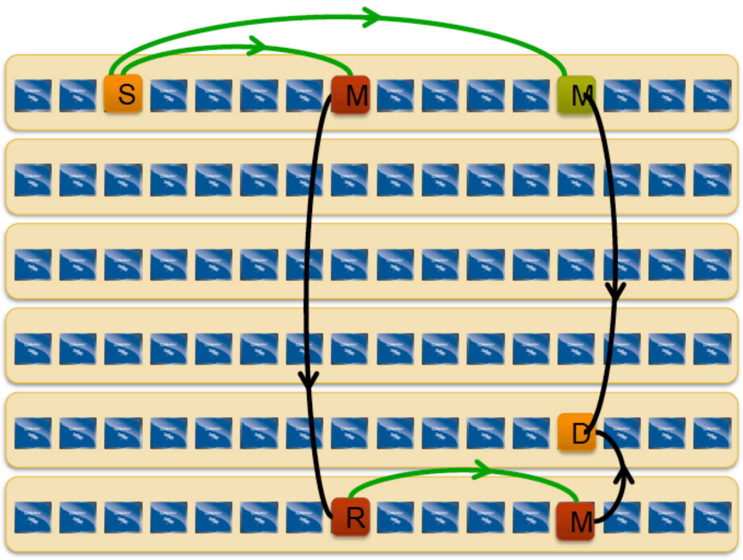
- When the entire data set fits within MCDRAM, on KNL nodes in flat mode:

```
aprun –Nx –ny numactl –membind=1 ./a.out
```

  - Easiest way to utilize hugepages on MCDRAM
  - craype-hugepage module is honored.
  - Allocations (malloc, memalign) on MCDRAM will be backed by hugepages
  - However, all memory allocated on MCDRAM (including MPI's internal memory)
  - Memory available per node limited to % of MCDRAM configured as FLAT memory
- MPICH_INTERNAL_MEM_AFFINITY=DDR
  - forces shared-memory and mail-box memory(internal memory regions allocated by the MPI library) to DDR
- Alternate solutions needed to utilize hugepage memory on MCDRAM, when the data set per node exceeds 16G
  - Necessary to identify performance critical buffers
  - Replace memory allocation calls with MPI_Alloc_mem() or MPI_Win_allocate()
  - Use Cray MPI env. vars to control page size, memory policy and memory affinity for allocations

Cray XC Routing

- Aries provides three basic routing modes
  - Deterministic (minimal)
  - Hashed deterministic (minimal, non-minimal), hash on “address”
  - Adaptive
    - 0 – No bias (default)
    - 1 – Increasing bias towards minimal (as packet travels)
      - Used for MPI all-to-all
    - 2 – Straight minimal bias (non-increasing)
    - 3 – Strong minimal bias (non-increasing)
- Non-adaptive modes are more susceptible to congestion unless the traffic is very uniform and well-behaved
- `MPICH_GNI_ROUTING_MODE` environment variable
  - Set to one of ADAPTIVE_[0123], MIN_HASH, NMIN_HASH, IN_ORDER
  - `MPICH_GNI_A2A_ROUTING_MODE` also available



Cray XC group:
Minimal routing - *2 hops*
Non-minimal routing – *4 hops*

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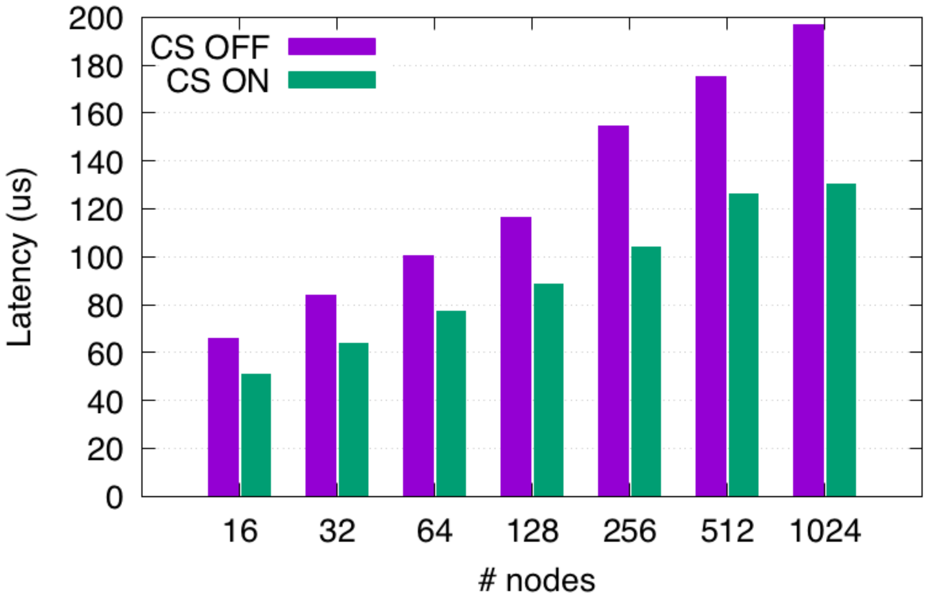
Core Specialization

- Offloads some kernel and MPI work to unused Hyper-Thread(s)
- Good for large jobs and latency sensitive MPI collectives
- Highest numbered unused thread on node is chosen
  - Usually the highest numbered HT on the highest numbered physical core
- Examples
  - `aprun -r 1 ...`
  - `aprun -r N ...   # use several extra threads`
- Cannot oversubscribe, OS will catch
  - `Illegal: aprun -r1 -n 256 -N 256 -j 4 a.out`
  - `Legal: aprun -r1 -n 255 -N 255 -j 4 a.out`
  - `Legal: aprun –r8 –n 248 –N 248 –j 4 a.out`

8-Byte Allreduce on Theta
64 processes per node
(run in production – other jobs are running)



Summary

- Optimizations were done in Cray MPI to improve pt2pt and collective latency on KNL
- Further tuning is possible through the environment variables
- Topology & routing based optimizations, huge-page and hybrid programming optimizations could be explored
- MPI 3.0 nonblocking and neighborhood collectives are optimized
- Necessary to use -r1 (core spec) to reduce performance variability due to OS noise

References:

- Cray XC series Network: *https://www.cray.com/sites/default/files/resources/CrayXCNetwork.pdf*
- MPI 3.1 Standard: *https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf*
- Cray MPI for KNL: *https://www.alcf.anl.gov/files/Chunduri_MPI_Theta.pdf (May 18 workshop - slightly basic version than this talk)*
- MPI benchmarking on Theta: *https://cug.org/proceedings/cug2018_proceedings/includes/files/pap131s2-file1.pdf*
- Advanced MPI Programming Tutorial at SC17, November 2017 (https://www.mcs.anl.gov/~thakur/sc17-mpi-tutorial/)
- *Low-overhead MPI profiling tool (Autoperf): https://www.alcf.anl.gov/user-guides/automatic-performance-collection-autoperf*
- *Run-to-run Variability: https://dl.acm.org/citation.cfm?id=3126908.3126926*