Cray MPI for KNL

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XC Topology and Aries

- I will not be covering details of the XC topology and Aries interconnect

- Please refer to the following document or feel free to talk with me at any time the rest of the workshop

http://www.cray.com/sites/default/files/resources/CrayXCNetwork.pdf

Agenda

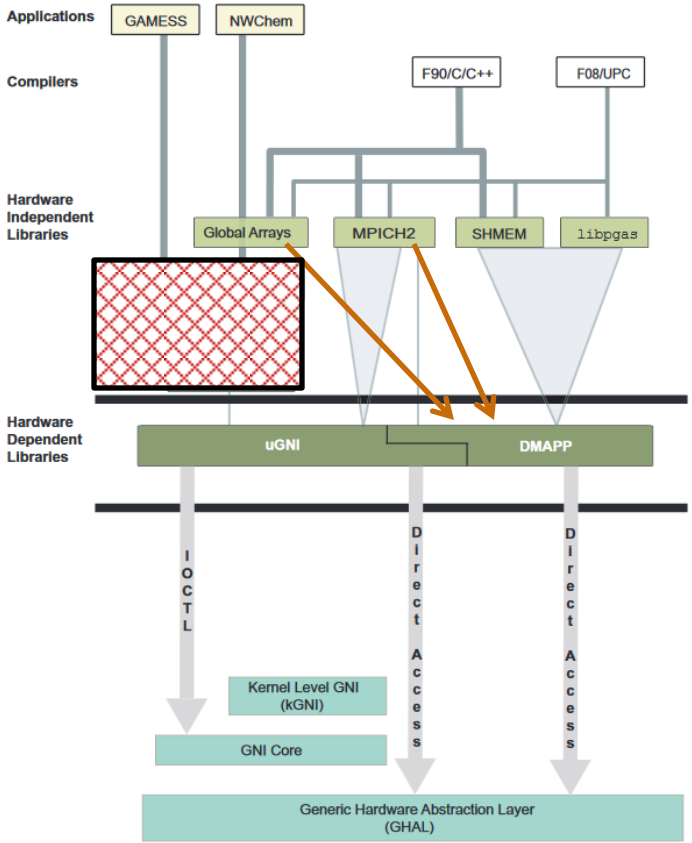
- **Brief Introduction to Cray MPICH**
- **Specific KNL optimizations including MCDRAM**
- **Optimizations for Hybrid (MPI/OpenMP) applications**
  - Application study of astrophysics code Wombat
- **Q&A (feel free to ask questions along the way)**

Introduction to Cray MPICH

Brief Introduction to Cray MPICH

- **Cray MPI compliant with MPI 3.1**
  - Merge to ANL MPICH 3.2rc1 – in MPT 7.3.0 (Dec 2015)
- **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)
- **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

Figure 1. GNI and DMAPP Software Layers



Cray MPI Resources

- **Primary user resource for tuning and feature documentation is the manpage**
  - man intro_mpi

  OR
  - man MPI
- **Standard function documentation available as well**
  - E.g., man mpi_isend

Key Environment Variables for XC

- **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 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
    - export MPICH_RANK_REORDER_METHOD=3

Key Environment Variables for XC

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

Key Environment Variables for XC

- **MPICH_USE_DMAPP_COLL / MPICH_RMA_OVER_DMAPP**
  - 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
    - 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

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

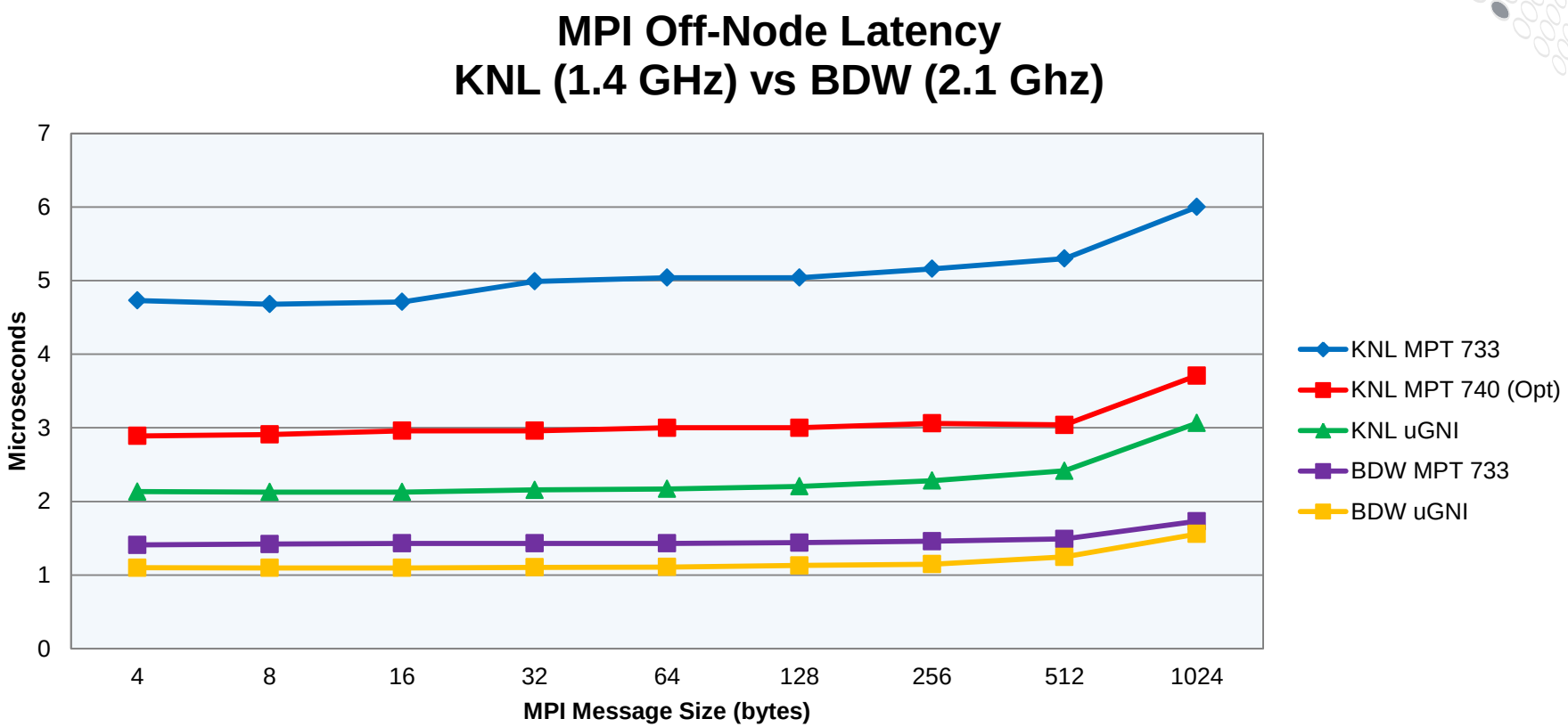
- **Specific Collective Algorithm Tuning**
  - Different algorithms may be used for different message sizes in collectives (e.g.)
    - Algorithm A might be used for Alltoall for messages < 1K.
    - Algorithm B might be used for messages >= 1K.
  - To optimize a collective, you can modify the cutoff points when different algorithms are used. This may improve performance.
  - 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

KNL Optimizations

Latency studies on KNL with Cray MPI

- **MPI is typically all scalar code**
  - Lots of branches
  - Lots of small functions and function calls using pointers
  - With smaller Branch Target Buffer (BTB) KNL does not handle this type of scalar code as well as the Xeon processor (even when adjusting to the slower CPU frequency)
- **Optimizing the “critical path”**
  - More inlining of small functions
  - Using higher compiler optimization
  - Hand-optimizations (avoid taking branches in critical path)
  - Disable FMA sharing when not needed
  - Provide a KNL-optimized memcpy

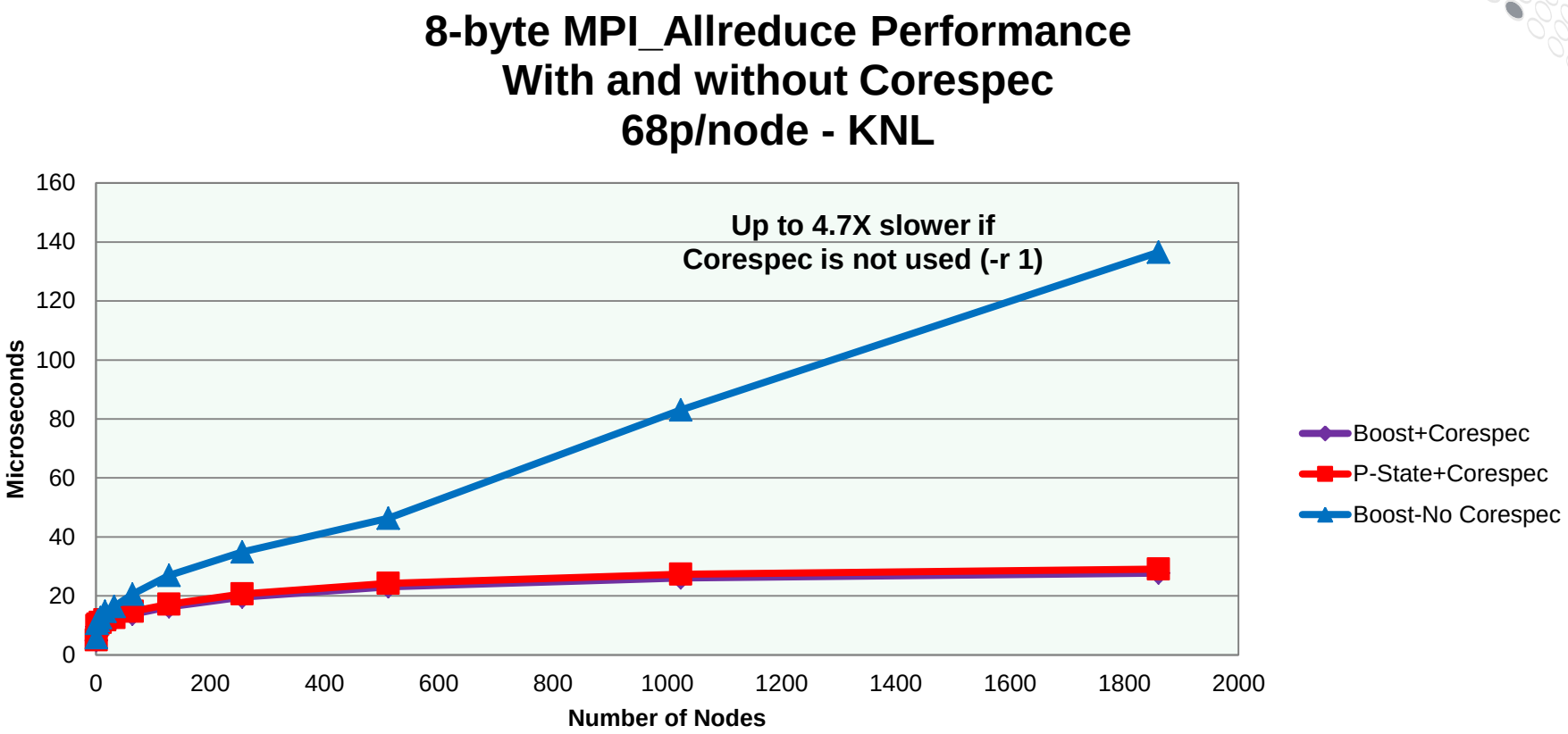
MPI Off-node Latency on KNL



OS Noise Plays a Role – How Big?

- **Studied performance with and without corespec (-r 1)**
- **MPI Latency: Collectives 1P / node**
  - Results show 5.5X slower when not using corespec
- **MPI Latency: Collectives 2-68 P / node**
  - Results show 4.7X slower when not using corespec

With and Without Corespec



Cray MPI support for MCDRAM on KNL

- **Cray MPI will offer 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
- **Preliminary release will expose feature via 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)
- **Follow-on release will offer Info Key Support for MPI_Alloc_mem and MPI_Win_allocate**
  - Allows user to specify characteristics via Info keys for each call

Cray MPI support for MCDRAM on KNL

- MPI_Alloc_mem: not restricted to be used only for communication buffers, or MPI's internal buffers. Can also be used to allocate application's data buffers
- Cray MPI does not register the memory returned by Alloc_mem
- Cray MPI also does not "touch" memory allocated via Alloc_mem()
  NUMA Affinity resolved when the memory pages are first touched by the process/threads.
  (Not ideal from a NUMA perspective to have the master thread alone touch the entire buffer right after allocation)
- MPI_Alloc_mem returns page-aligned memory for all page sizes

Cray MPI support for MCDRAM on KNL Typical use cases

- **When the entire data set fits within MCDRAM, on a Quad/Flat system:**

  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

- **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 MPI support for MCDRAM on KNL: Typical Use cases (Dataset size > 16GB)

- **Quad/Flat mode, without numactl options:**
  - malloc(), memalign() will use DDR first
  - Can access MCDRAM via hbw_* or compiler directives.
  - craype-hugepages module honored *only* on DDR
  - hbw_malloc will return memory backed by basepages
  - Memkind can be used to get 2M hugepages on MCDRAM (but not larger)

- **Users need to identify critical buffers and use MPI_Alloc_mem() to allocate hugepages with larger page sizes, and set affinity to MCDRAM**

- **Use following env. vars:**

  MPICH_ALLOC_MEM_AFFINITY=M (or MCDRAM)

  MPICH_ALLOC_MEM_PG_SZ = 16M (16M hugepages)

  MPICH_ALLOC_MEM_POLICY = P (or Preferred)

Cray MPI support for MCDRAM on KNL: Typical Use cases (Datset size > 16GB)

- **Quad/Flat mode, with numactl --membind=1**
  - Malloc(),memalign() will use MCDRAM
  - Hugepage allocations via the craype-hugepages module now possible on MCDRAM
  - But, MCDRAM space is limited. Scaling issues

- **Users can identify buffers *not* critical to application performance and use MPI_Alloc_mem() to set affinity to DDR**

- **Use following env. vars:**

  MPICH_ALLOC_MEM_AFFINITY=D (or DDR)

  MPICH_ALLOC_MEM_PG_SZ = <as needed, defaults to 4KB base pages>

  MPICH_ALLOC_MEM_POLICY = P (or Preferred)

Using MPI_Alloc_mem/MPI_Free_mem with a 3DFFT Kernel (Fortran)

```
..
lenr    = nx * ny * mynz
lenc    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
lenm    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
rc_grid = FFTW_ALLOC_REAL(lenr * nvars)
cc_grid = FFTW_ALLOC_COMPLEX(lenc * nvars)
mc_grid = FFTW_ALLOC_COMPLEX(lenm)

CALL C_F_POINTER(rc_grid, rgrid,
                        (/nx, ny, mynz, nvars/))
CALL C_F_POINTER(cc_grid, cgrid,
                        (/lenc, INT(nvars, C_SIZE_T)/))
CALL C_F_POINTER(mc_grid, mgrid, (/lenm/))

..
```

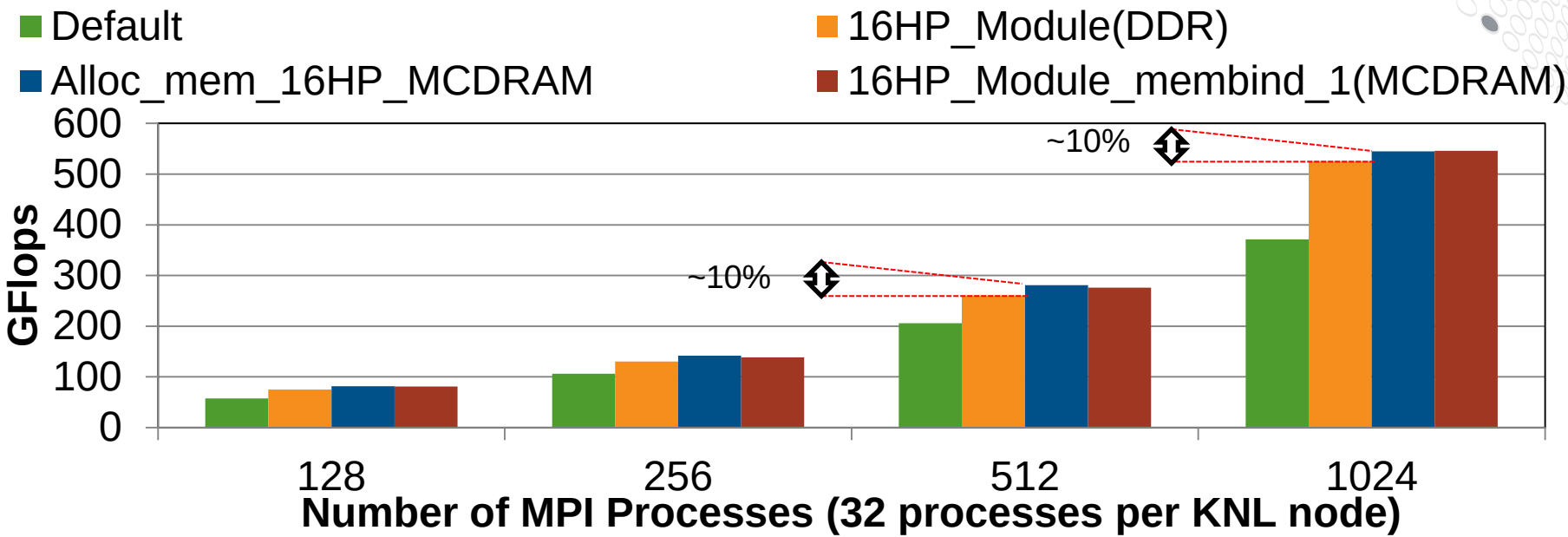
```
lenr    = nx * ny * mynz
lenc    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
lenm    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
info    = MPI_INFO_NULL
CALL MPI_ALLOC_MEM(lenr * nvars * 8_8, info,
                                rc_grid, ierr)
CALL MPI_ALLOC_MEM(lenc * nvars * 16_8, info,
                                cc_grid, ierr)
CALL MPI_ALLOC_MEM(lenm * 16_8, info,
                                mc_grid, ierr)

CALL C_F_POINTER(rc_grid, rgrid,
                        (/nx, ny, mynz, nvars/))
CALL C_F_POINTER(cc_grid, cgrid,
                        (/lenc, INT(nvars, C_SIZE_T)/))
CALL C_F_POINTER(mc_grid, mgrid, (/lenm/))
..
```

Using MPI_Alloc_mem/MPI_Free_mem with a 3DFFT Kernel (Fortran)

```
CALL FFTW_FREE(rc_grid)
CALL FFTW_FREE(cc_grid)
CALL FFTW_FREE(mc_grid)
```

```
CALL MPI_FREE_MEM(rgrid, ierr)
CALL MPI_FREE_MEM(cgrid, ierr)
CALL MPI_FREE_MEM(mgrid, ierr)
```

MCDRAM Experiments with a 3DFFT Kernel



3DFFT Weak scaling (Data Grid: 1024, 1024, 1024)

MPI_Alloc_mem with hugepages offers same performance as using membind=1

Hugepages on MCDRAM performs better than DDR with the same hugepage size

Using MPI_Alloc_mem can help cases where the entire data set does not fit within MCDRAM

Cray MPI support for MCDRAM on KNL: On-going effort

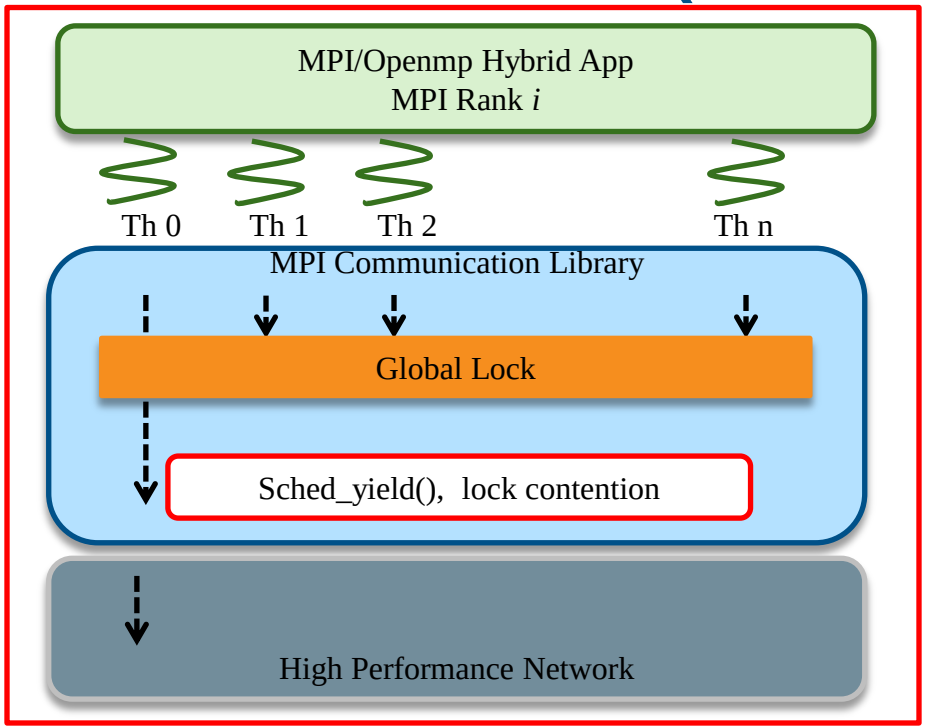
- Info key support for MPI_Alloc_mem and MPI_Win_allocate()
- Env. vars affect the entire job, info keys can offer fine-grained controls for each memory allocation
- Info keys can be used to allocate 64M Hugepages on MCDRAM for one buffer, and 64M Hugepages on DDR for a different buffer in the same job.
- Env. vars are still respected if info keys are not set
- Portable across MPI implementations. Possible to maintain info key names and format consistent between Cray MPI and Intel's MPI implementations. A different MPI impl. could choose to silently ignore the proposed info keys

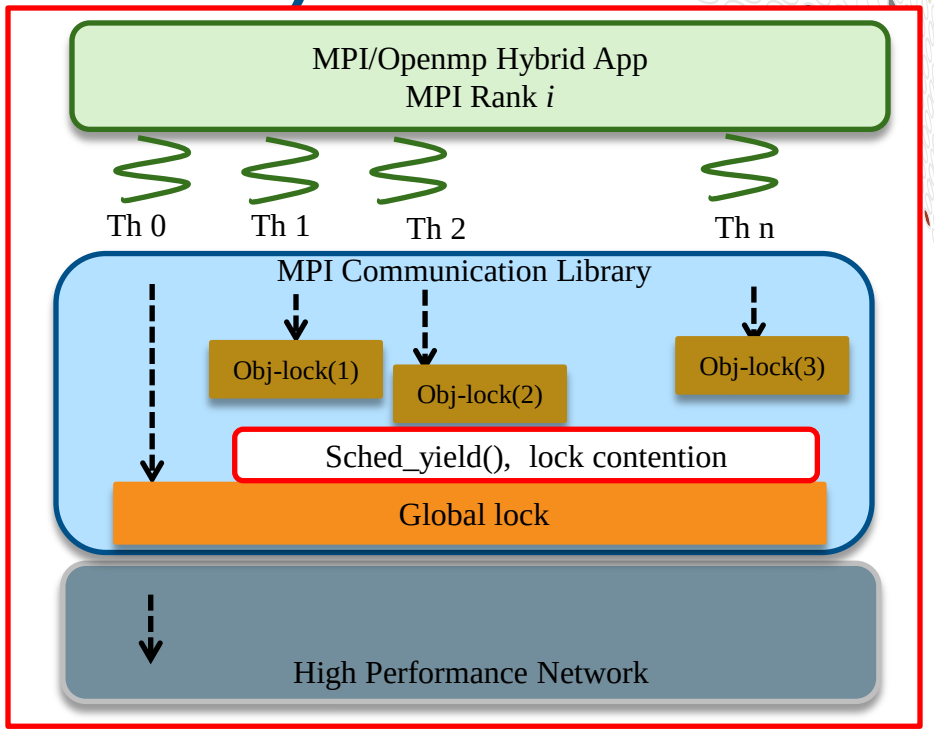
Multi-threaded MPI Support and Optimizations

CORAL NRE MS13 Milestones

Schedule	Deliverables
December 2015	**MS1:** Design Document for the Thread-Scalable MPI NRE.
Q3 2016	**MS2: Demonstrate the benefits of an optimized Cray MPICH implementation on the Theta System with Intel KNL and Aries interconnect.**
Q2 2017	**MS3:** Implement a thread-scalable prototype of Cray MPICH with the CH4 interface and the uGNI-based OFI provider layer. Demonstrate the functional characteristics of this implementation.
Q4 2017	**MS4:** Implement a thread-scalable prototype of ANL MPICH with the CH4 interface and the STL2-based OFI provider layer. This prototype is intended for an experimental system with Intel KNH and Intel STL2.
Q4 2018	**MS5:** Finalize and deliver the Thread-Scalable MPI implementation and source for the Aurora System.

Multi-Threaded MPI (State-Of-The-Art)

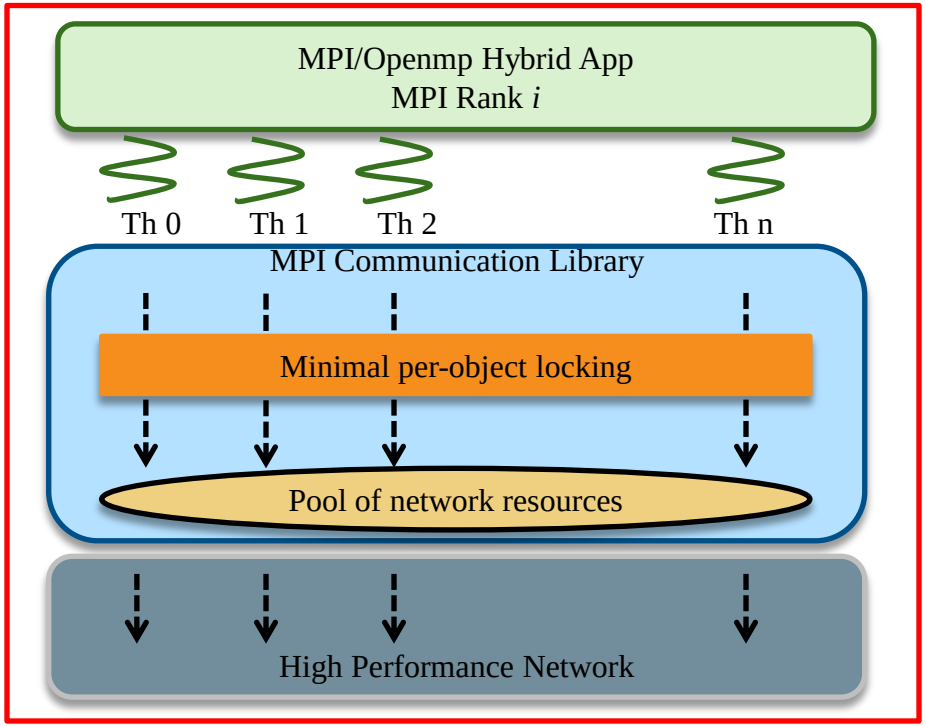




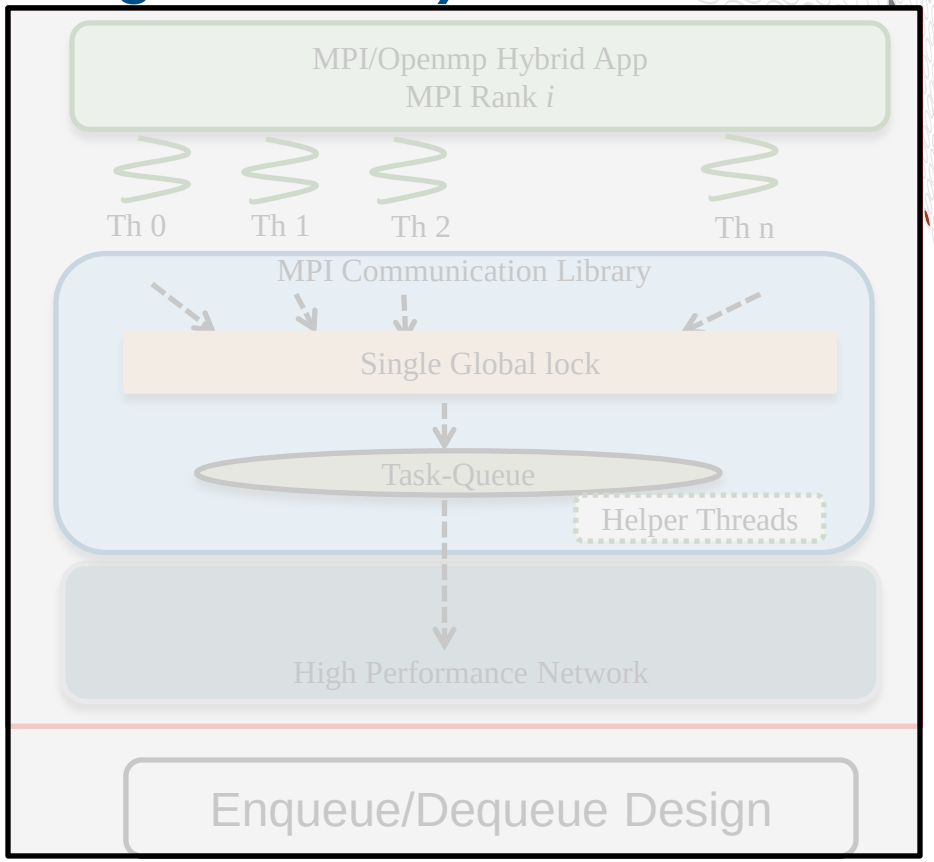
Global lock
(default in Cray MPI)

Per-Object Locks
(Alt. impl. in CrayMPI, "–craympich-mt" link time flag)

Optimized Multi-Threaded MPI (Design Choices)

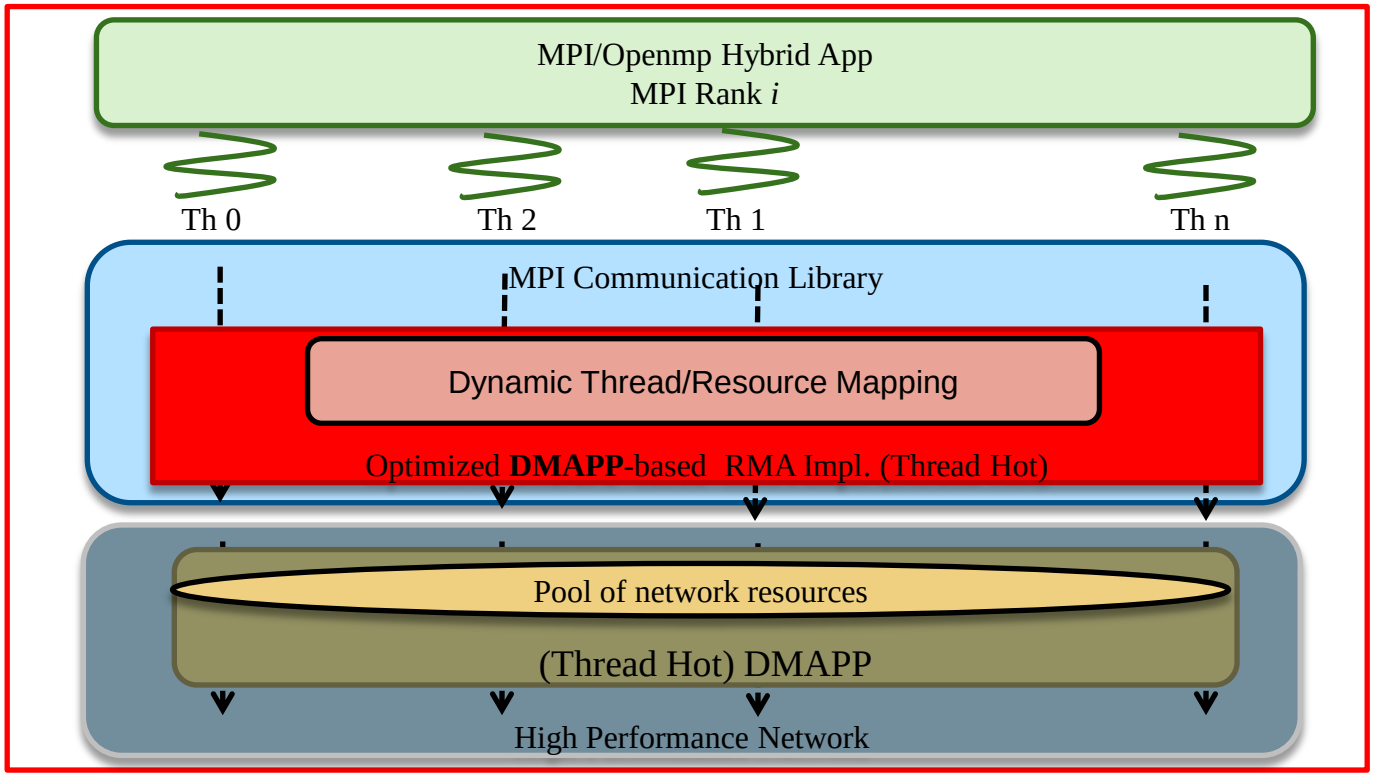


Proposed Thread-Hot Design



Enqueue/Dequeue Design

Thread Hot Communication in Cray MPI



Thread Hot Communication in Cray MPI

- Design Objectives
  - Contention Free progress and completion
  - High bandwidth and high message rate
  - Independent progress – thread(s) flush outstanding traffic, other threads make uninterrupted progress
  - Dynamic mapping between threads and network resources
  - Locks needed only if the number of threads exceed the number of network resources
- MPI-3 RMA
  - Epoch calls (Win_complete, Win_fence) are thread-safe, but not intended to be thread hot
  - All other RMA calls (including request-based operations) are thread hot
  - Multiple threads doing Passive Synchronization operations likely to perform best:
- MPI Pt2pt
  - MPI_Send/MPI_Recv, MPI_Isend/MPI_Irecv, MPI_Wait/MPI_Waitall will be thread hot.
  - Supports use cases where multiple threads issue Isend/Irecv ops, but master thread alone does Waitall
- MPI_Alltoall
  - Multiple threads can issue, progress and complete Alltoall operations concurrently. Each thread has a separate MPI_Comm handle.
  - The Allgather exchange (mem address, hndls) is protected by the big lock (room for optimization)

Multi-threading Optimizations in Cray MPI

- **Easy way to hit the ground running on a KNL – MPI only mode**
  - Works quite well in our experience
  - Scaling to more than 2-8 threads most likely requires a different application design approach
- **“Bottom-Up” OpenMP development approach is very common**
  - Most likely will not offer best performance and scaling
- **“Top-Down” SPMD model is more appealing for KNL**
  - Increases the scope of code executed by OpenMP, allows for better load balancing and overall compute scaling on KNL
    - Allows multiple threads to call MPI concurrently.
    - In this model, performance is limited by the level of support offered by MPI for multi-threaded communication
    - MPI implementations must offer “Thread-Hot” communication capabilities to improve communication performance for highly threaded use cases on KNL

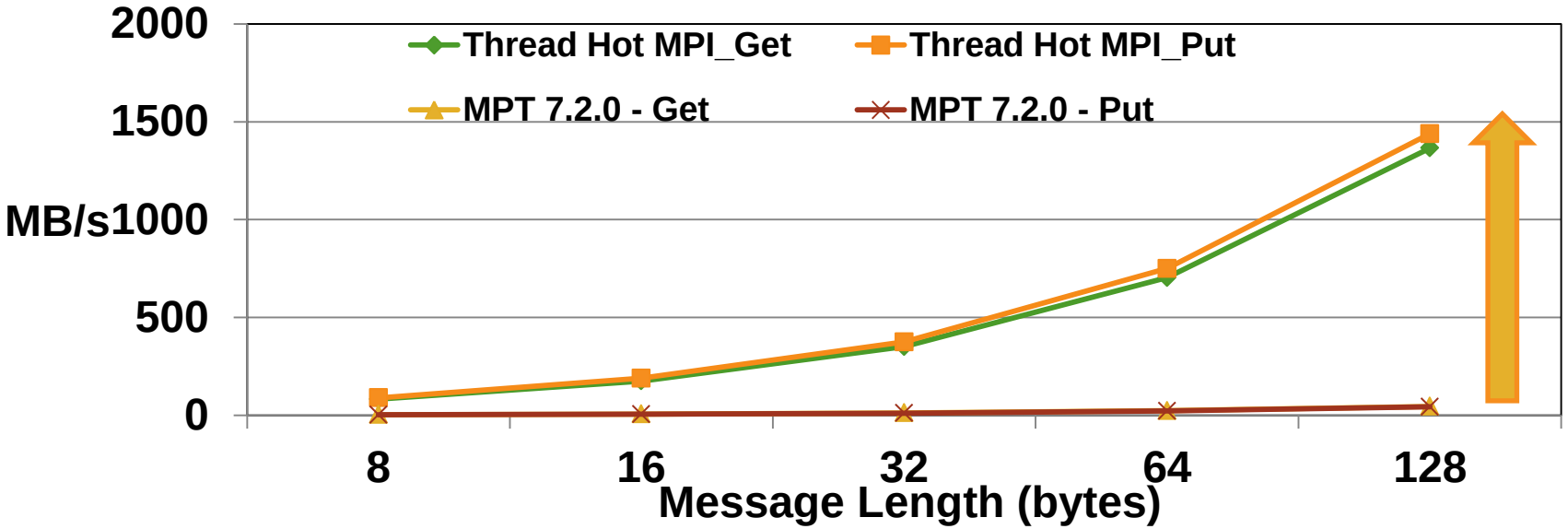
Experimental Setup

- Cray XC systems with Intel Haswell and Broadwell
- *Modified* OSU Micro Benchmarks (OMB) to study multi-threaded MPI Communication performance
  - RMA: osu_put_latency.c, osu_get_latency.c
    osu_put_bw.c, osu_get_bw.c

- Enabling the RMA over DMAPP optimization:
  - Link against DMAPP:
    If the code uses static linking:
    -Wl,--whole-archive,-ldmapp,--no-whole-archive
    If the code uses dynamic linking:
    -ldmapp
  - Set MPICH_RMA_OVER_DMAPP env. variable to 1 (export MPICH_RMA_OVER_DMAPP=1)

MPI-3 RMA Communication Bandwidth

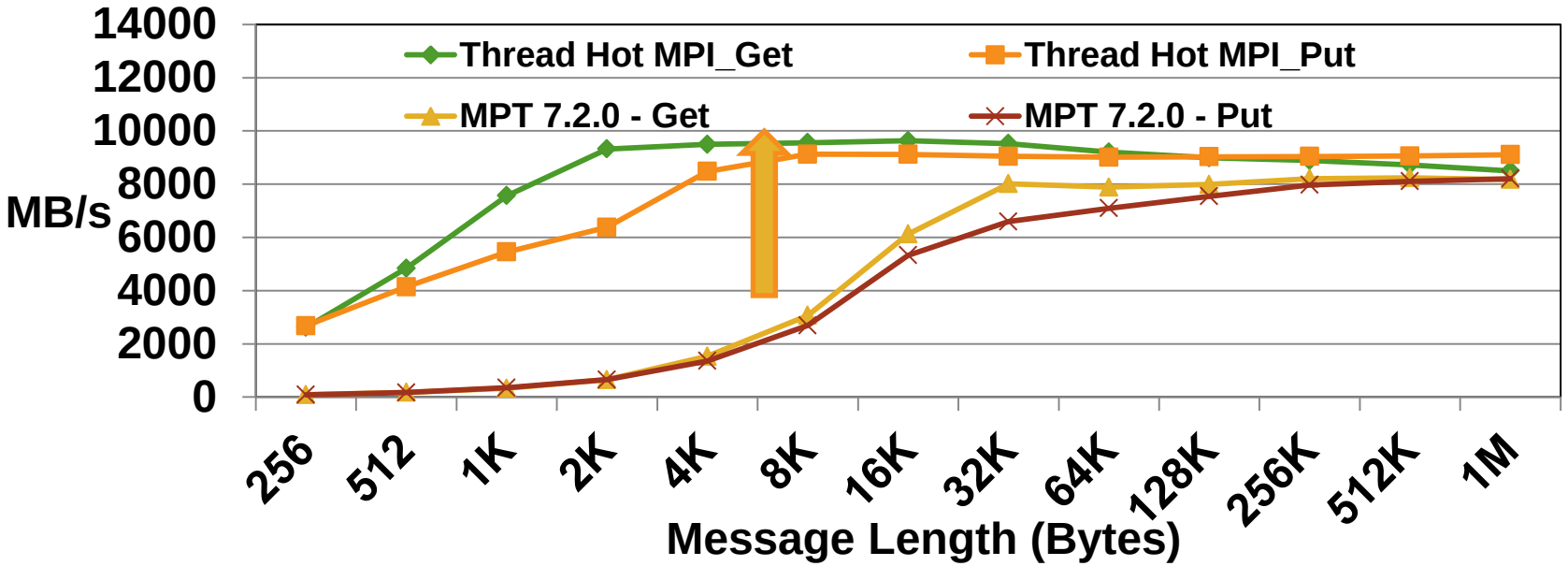
1 MPI process per node, 32 threads, Haswell, small messages



- **Thread Hot Cray MPI significantly outperforms the default (global-lock) implementation with the multi-threaded RMA benchmark for small payloads**

MPI-3 RMA Communication Bandwidth

1 MPI process per node, 32 threads, Haswell, large messages



- **Thread Hot Cray MPI outperforms the default (global-lock) implementation with the multi-threaded RMA benchmark by about 4X for small and medium sized payloads**

Wombat Project Hybrid Application Study

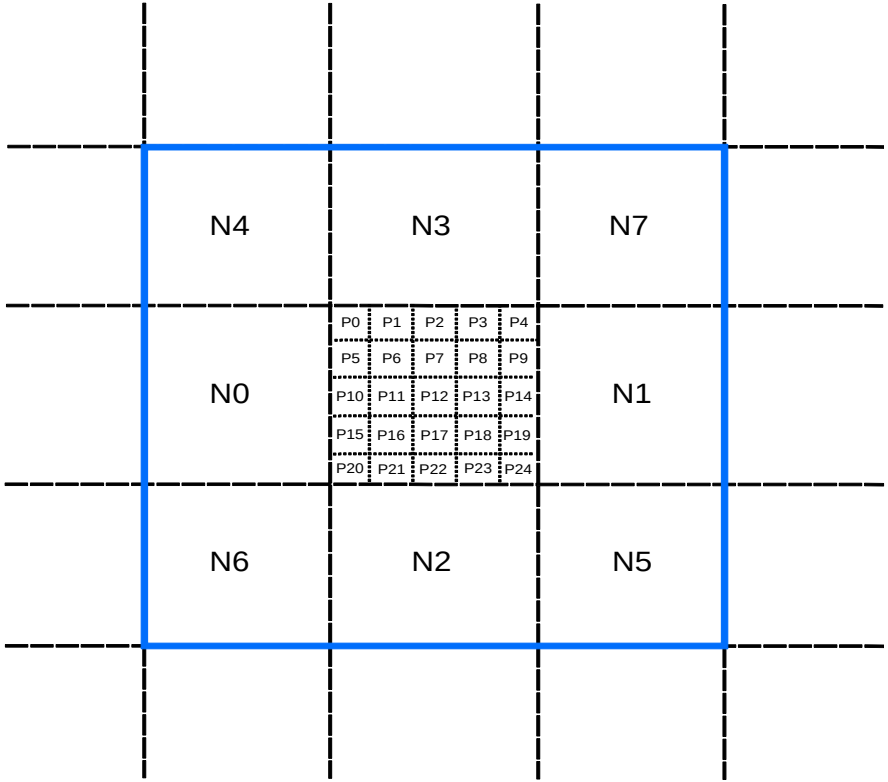
- **Wombat is being developed through a collaboration between Cray Programming Environments and the University of Minnesota Institute for Astrophysics**
  - Peter Mendygral (Cray) is lead developer
  - Tom Jones (UofM) supervises graduate students contributing to the code and drives scientific goals
  - Other contributors/users: Dongsu Ryu (UNIST), Julius Donnert (INAF)
- **Scientific goal is to study turbulence in astrophysical fluids over cosmological scales**
  - MHD + dark matter
- **Application goal is to develop a code capable of achieving the science goals on the latest HPC architectures**

Primary Development Concerns

- **Two main issues drove the design of Wombat and explain why other codes have not been sufficient for the science**
  - Scaling to extreme core count required to get to resolutions needed for MHD turbulence
  - Load balancing for SMR/AMR and dark matter particles
- **The approach to these problems in Wombat was**
  - Make communication matter as little as possible
  - Wide OpenMP on a node to soften impacts of load imbalances (and hardware imbalances) as much as possible before communicating work between ranks
  - Data structures that reduce AMR/SMR complexity and avoid significant global communication for refined patch tracking
  - Do it all in Fortran as that's what works best for me
    - Wombat uses object oriented features from Fortran 2003 and 2008

Domain Decomposition

- Domain decomposition is represented in the data classes and structures
- “Domain” is an array of “Patches” managed by a MPI rank
- “Patch” is a self-contained, self-describing piece of the world grid at some fixed logical location



Domains and Patch

- **Domains manage bookkeeping for an array of Patches**
  - Track a Patch's neighbors
  - Manage allocating/deallocating a Patch's internal grid arrays as needed
  - Multiple Domains are used on a rank for accepting Patches from neighbors

- **Patches are**
  - Of some uniform fixed size (for a given Domain refinement level)
  - Fixed in a location that is known for all times by all ranks

- **Patches provide**
  - An atomic unit of work
  - Units to thread across
  - Unit to transfer for load balancing
  - A level of cache blocking

High-level OpenMP

Option A – "bottom up"

```
! Keep OpenMP within a "compute" loop

DO WHILE (t .LT. tend)

   DO patch = 1, npatches

      CALL update_patch()

      …CALL MPI…

   END DO

END DO

SUBROUTINE update_patch()

   !$OMP PARALLEL DO
   DO i = 1, nx
   …do work…
   END DO

END SUBROUTINE
```

Option B – "SPMD"

```
! Move OpenMP near the top of the call stack

!#OMP PARALLEL
DO WHILE (t .LT. tend)

   !#OMP DO
   DO patch = 1, npatches

      CALL update_patch()

      …CALL MPI…

   END DO

END DO
```

High-level OpenMP

- **Benefits of high-level SPMD OpenMP**
  - Application more closely mimics completely independent processes
    - Less likely to be in the same portion of code at the same time
    - Bandwidth competition may decrease
    - Amdahl's law
  - Threads are less coupled => infrequent thread synchronization
  - Much less likely to have issues with memory conflicts between threads
  - Simpler to implement when done right
    - Large reduction in the amount of OpenMP directives
    - Very little variable scoping needed as most everything is shared => reduced memory footprint
  - Easier to make use of all cores on node (e.g., 68) that can be hard to use for domain decomposition reasons
  - Effective way to manage natural hardware induced imbalance and algorithmic load imbalance

High-level OpenMP

- **Challenges for high-level SPMD OpenMP**
  - Requires full understanding of data dependencies and potential for race conditions
  - For best performance requires revisiting approach to MPI
    - Goal should be to remove any thread synchronization you can
    - Serializing MPI will limit the benefit and scalability of SPMD
  - In my experience, it is easier to implement SPMD in a data centric model
    - Present work as independent units
    - Let threads work on that set in any order with a non-static schedule
  - MPI work should be treated the same as data if possible
    - Independent units of communication to be worked on in any order with non-static schedule

Wombat Driver and Parallel Region

Setup and object constructors

Thread parallel region

Array allocation and initialization

Time step loop

DomainSolver%solve(mhd)
DomainSolver%solve(ct)
DomainSolver%solve(passive)
DomainSolver%solve(particle kick+drift)
FMGSolver%solve(all levels)
DomainSolver%solve(particle kick)

I/O data dump(s)

Update time step

Array cleanup

Object destructors

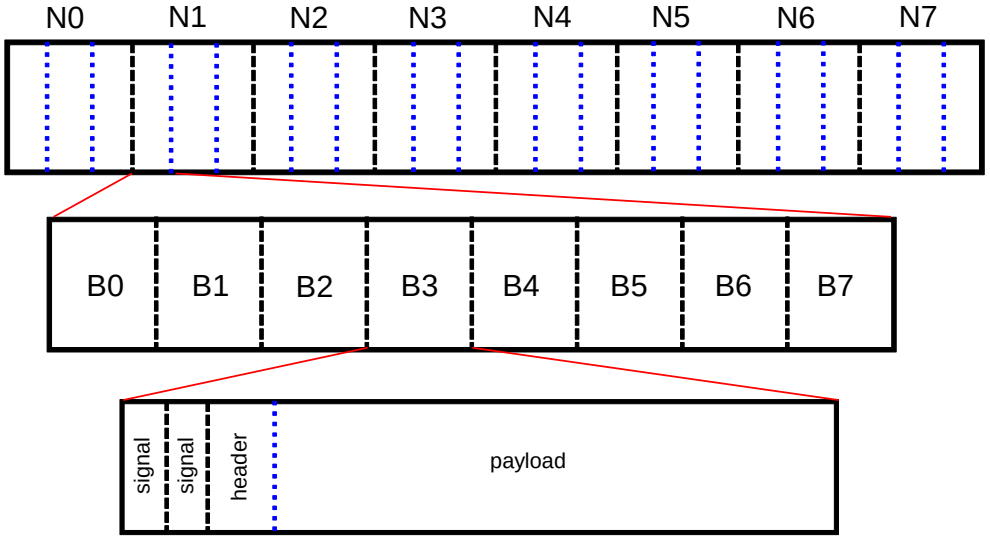
Simulation complete

Communication Concerns

- **If a rank is made much wider with threads, serialization around MPI will limit thread scaling and overall performance**
  - Nearly all MPI libraries implement thread safety with a global lock
  - Cray (and other vendors) is addressing this issue
- **Wide OpenMP also means more communication to process per rank**
  - Every Patch now has its own smaller boundaries to communicate
  - Starts tipping the behavior towards the message rate limit
- **Slower serial performance of KNL => maybe look for the lightest weight MPI layer available**
  - MPI-RMA over DMAPP on Cray systems is a thin software layer that achieves similar performance to SHMEM

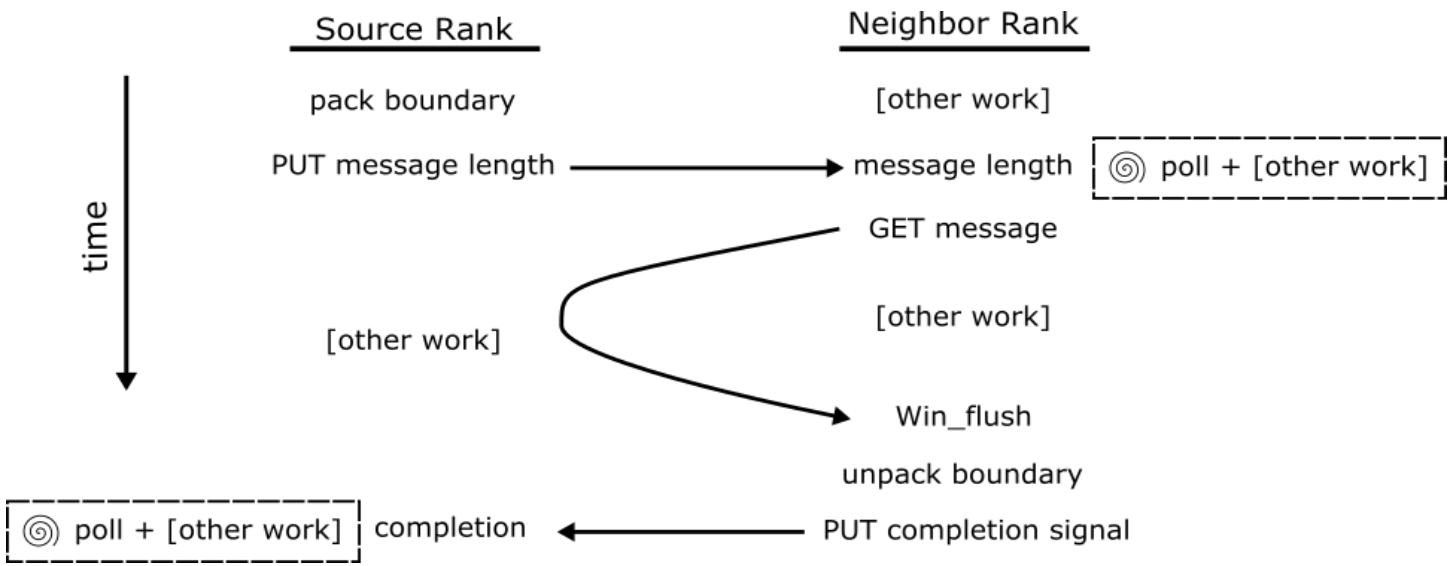
Single RMA Window Buffer

- Single buffer used for (almost) all communication
- Messages can be processed concurrently if MPI allows it
- Design is similar to mailboxes within MPI
  - Can process an arbitrary amount of communication



RMA Boundary Communication Cycle

- **Single passive RMA window used for the duration of the application**
  - No explicit synchronization between ranks
  - RMA semantics make computation/communication overlap simpler to achieve
- **All "solvers" in Wombat utilize a generalized class that implements the communication/computation cycle below**



Thread Hot MPI-RMA

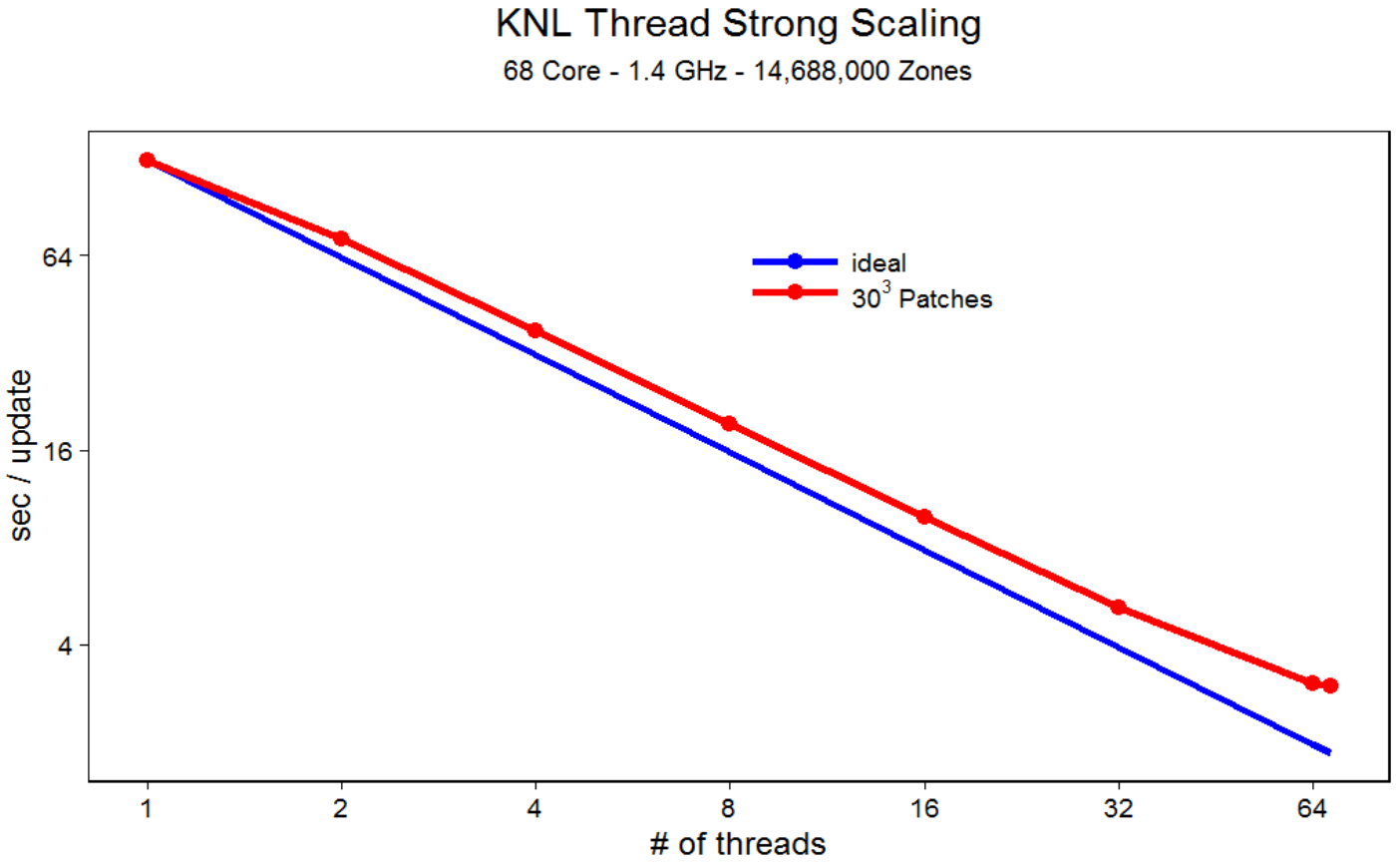
- **Future release of Cray MPICH will include new performance feature that allows for efficient message completion in a threaded region**
  - Can call completion routines (e.g., MPI_WIN_FLUSH) in a threaded region (not required)
  - Threads collaboratively complete messages from all threads
  - Removes the need for any additional thread barriers after MPI_PUT/MPI_GET/etc in threaded region

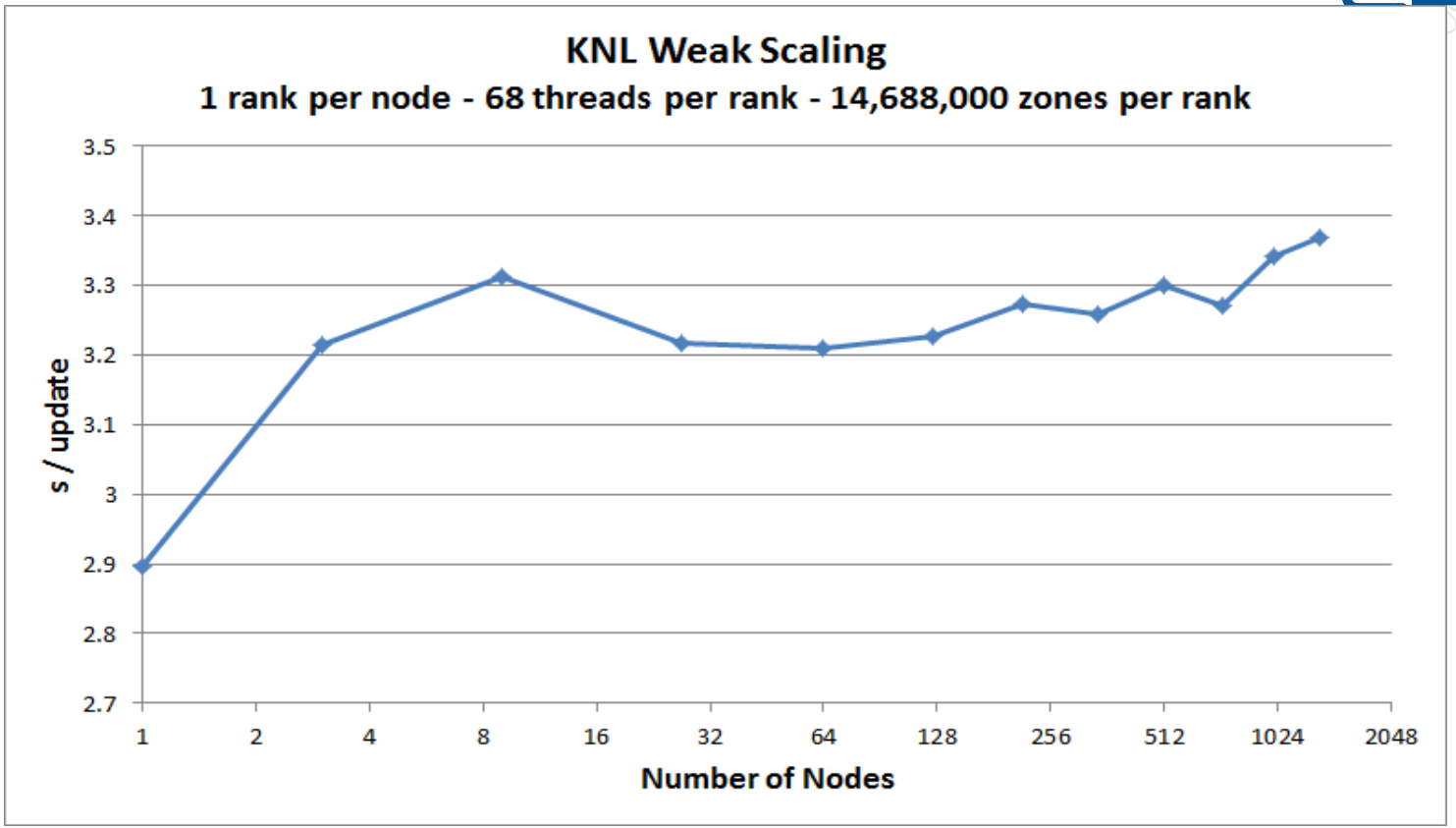
```
!$OMP DO
DO n = 1, n_neighbors

CALL MPI_PUT(…)

END DO
!$OMP END DO

!$OMP MASTER
CALL  MPI_WIN_FLUSH_ALL()
!$OMP BARRIER
```

```
!$OMP DO
DO n = 1, n_neighbors

CALL MPI_PUT(…)

END DO
!$OMP END DO NOWAIT

CALL  MPI_WIN_FLUSH_ALL()
```

Wombat Benchmarking Notes

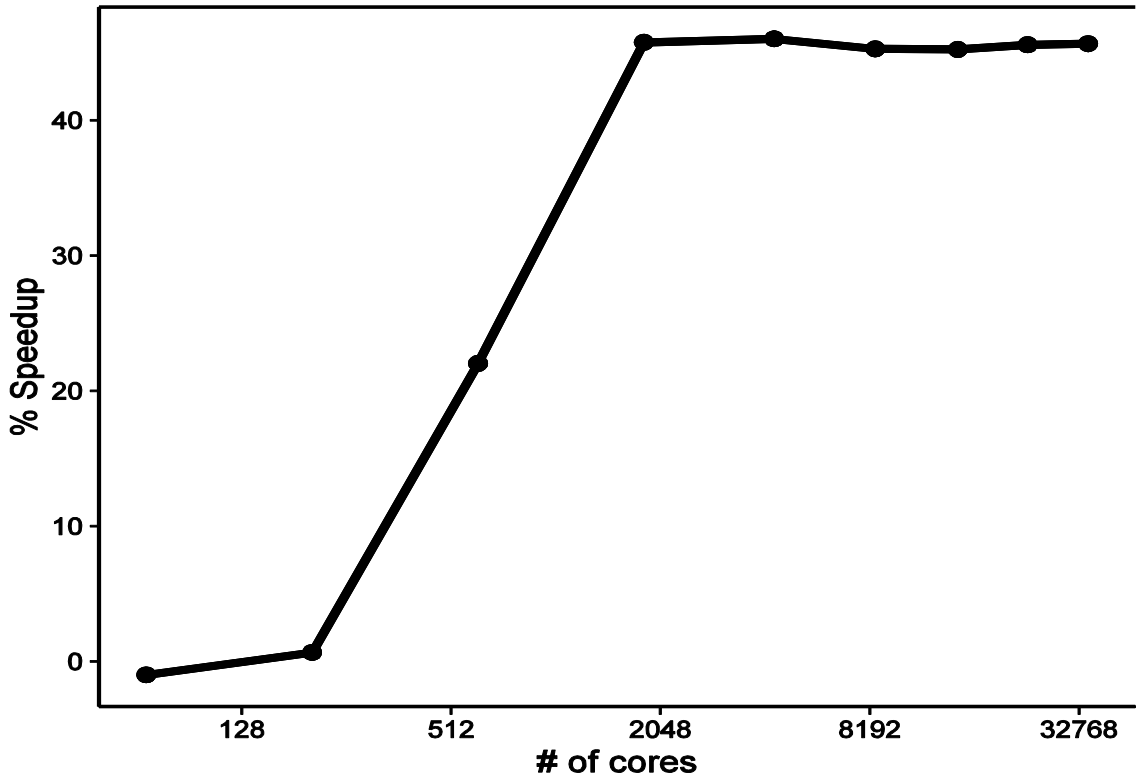
- **Only MHD was enabled on fixed grid**
- **In all cases 2 MB hugepages were used**
  - module load craype-hugepages2MB
  - Loaded at link and run time
  - Link with dmapp (statically)
    -Wl,--whole-archive,-ldmapp,--no-whole-archive
- **The following environment variables were set**
  - export MPICH_MAX_THREAD_SAFETY=multiple
  - export MPICH_RMA_OVER_DMAPP=1
- **CCE was always used**
  - Needed for vectorization in eigenvector/flux calculation
- **KNL was configured with MCDRAM as cache**

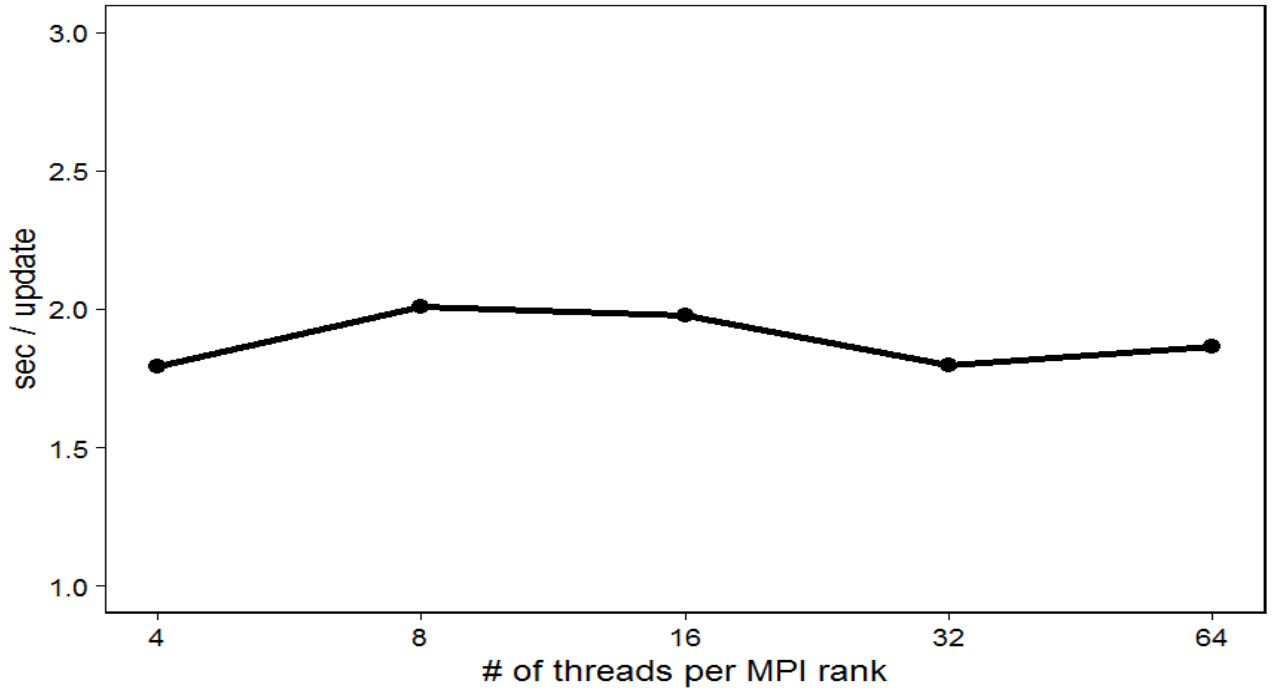




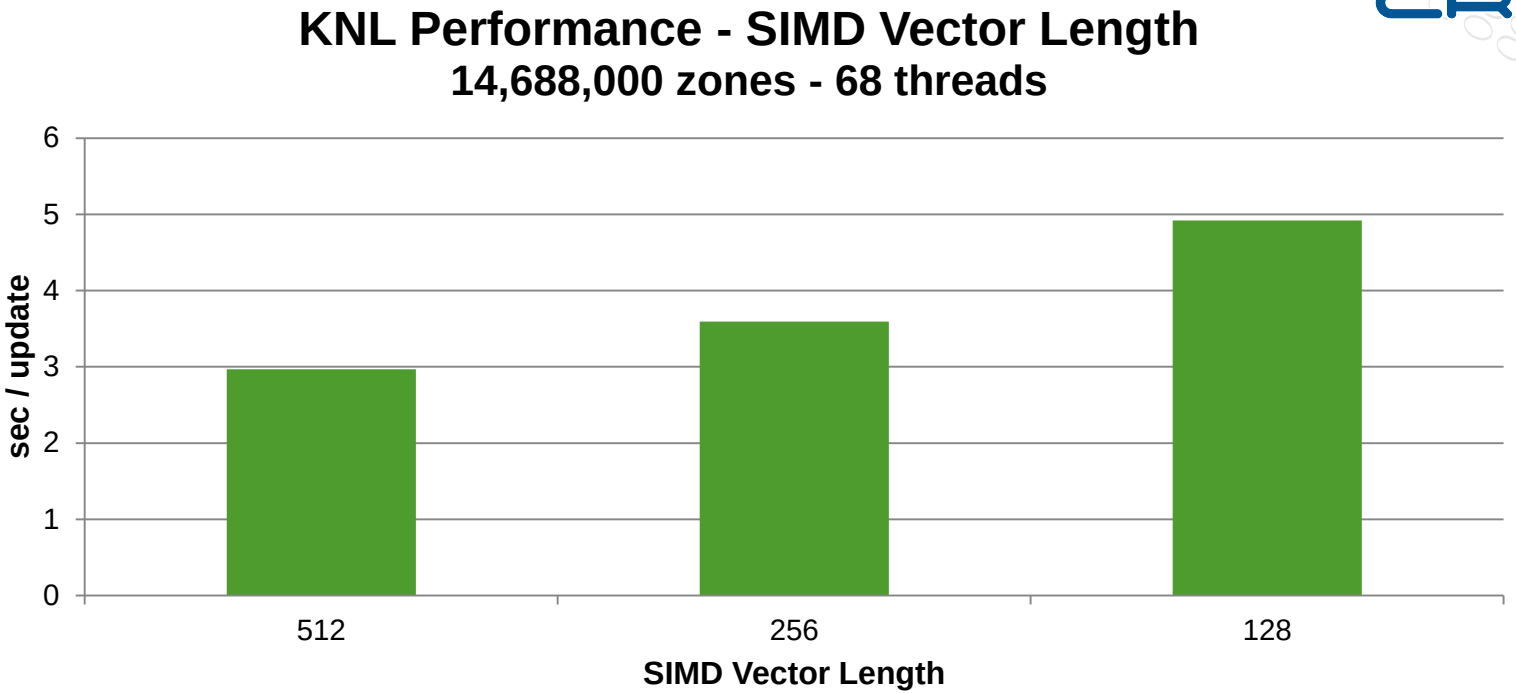
Thread-Hot / Global Lock MPI-RMA Speedup on KNL

1 Rank per Node - 68 threads per rank - 14,688,000 Zones per Rank





- Less than 5% difference between full ranks and full threads
- Ideal for application like Wombat for fixed grid is 0%



- Vector length very important
- Significant effort went into making solver loops (compute and copy) vectorize

Summary and Recommendations

- Optimizations in Cray MPI to improve pt2pt and collective latency on KNL
- Enhancements in Cray MPI to enable users best utilize the MCDRAM technology on KNL
- New solutions in Cray MPI to offer Thread-Hot capabilities on Intel Xeon and Intel KNL architectures
- Design and development details of Wombat, a high performance astrophysics application that relies on multi-threaded MPI-3 RMA implementation in Cray MPI

- MPI-only works quite well on KNL
  - Threading can be helpful, but unless SPMD with “thread-hot” MPI is used scaling to more than 2-8 threads not recommended
- Necessary to use –r1 to reduce performance variability
- Using hugepages on MCDRAM can improve large message communication performance
- Multi-threaded MPI will be a key tool on KNL for hybrid applications
- Asynchronous communication can hide/overlap communication overheads on KNL
- Collectives implemented with user pt2pt is strongly discouraged
  - Especially for alltoall, bcast, and gather
  - Very unlikely pt2pt will perform better
  - If they do, please file a bug with Cray

Q&A