Cray MPI for KNL

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XC Topology and Aries

- Not covering details of the XC topology and Aries interconnect today

- Please refer to the following document or feel free to ask questions at any time the rest of the workshop

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

Agenda

- **Introduction to Cray MPICH**
- **KNL/MCDRAM optimizations**
- **Optimizations for Hybrid MPI+OpenMP applications**
  - Hybrid MPI+OpenMP application study

Introduction to Cray MPICH

Brief Introduction to Cray MPICH

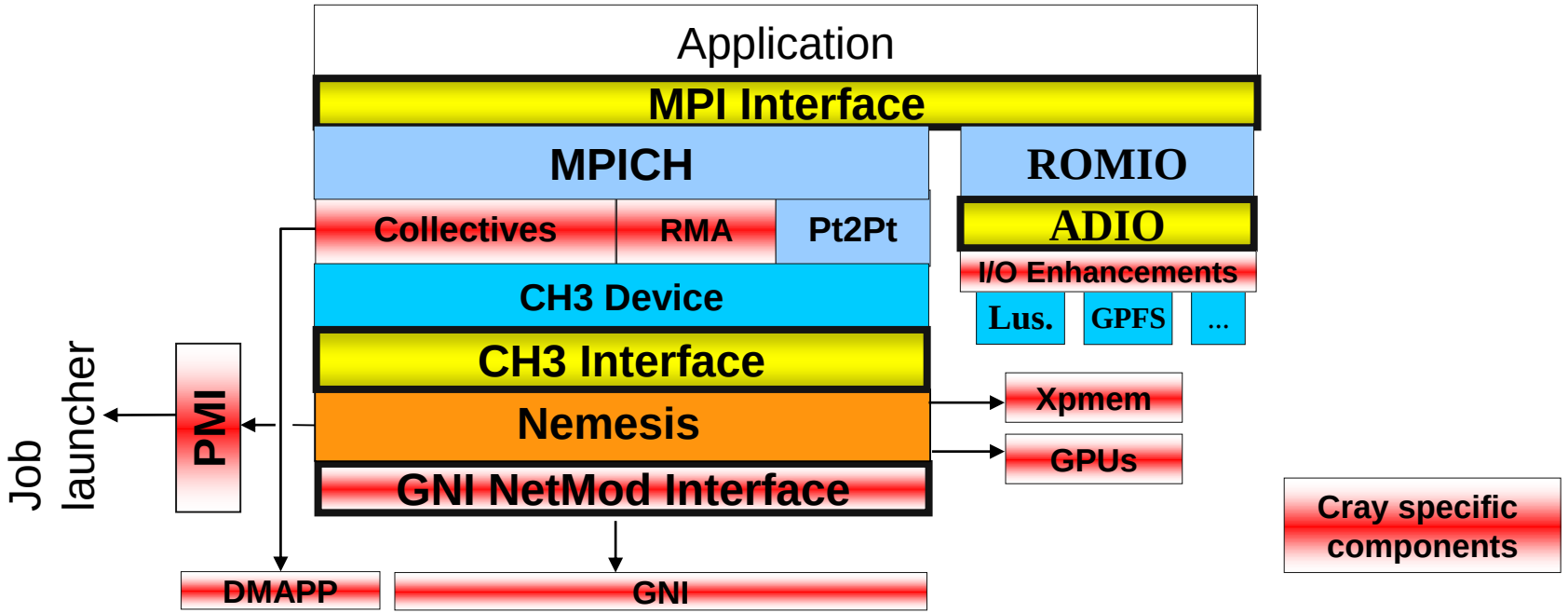
- **Cray MPI compliant with MPI 3.1**
  - Merge to ANL MPICH 3.2 – latest release MPT 7.7.0 (Dec 2017)
- **I/O, collectives, P2P, and one-sided all optimized for XC architecture**
  - SMP aware collectives
  - High performance single-copy on-node communication via xpmem (not necessary to program for 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

MPI Dynamic Process Management

- **All DPM functionality (except spawn) supported as of MPT 7.7.0**
- **Spawn support coming in Q2 2018**
- **New MPIX function to make MPI_Comm_spawn simpler**
  - MPIX_Comm_rankpool converts an MPI communicator into a pool of compute resources for spawning new MPI jobs
  - Generally called from a separate MPI job
  - Rank pool “name” parameter used to specify pool when spawning new MPI job, i.e., MPI_Info_set(info, “rankpool”, “name_of_pool”)
  - A “timeout” parameter determines the lifetime of the rank pool

Cray MPI Software Stack (CH3 device)

Gemini/Aries



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

- **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"

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 and large data footprint
  - 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 and 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
- **For thread multiple support**
  - export MPICH_MAX_THREAD_SAFETY=multiple
- **See the MPI man page for further details**

KNL Optimizations

MCDRAM on KNL

- **KNL nodes in cache mode are a good starting point for many applications**
  - No extra work for user
  - Typically good performance
- **KNL nodes in flat mode is attractive when**
  - Can benefit from extra memory of DDR+MCDRAM
  - Observing performance variability related to MCDRAM direct map cache
- **Effective use of flat mode requires users understand more about what memory in their application matters and how it is being used**
  - All performance critical memory should reside in MCDRAM if possible

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

- **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 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

- **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)

- **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 (Dataset size > 16GB)

- **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. Memory 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)

  Add internal MPI mailbox and SHM collectives buffer affinity variable

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/))

..
```

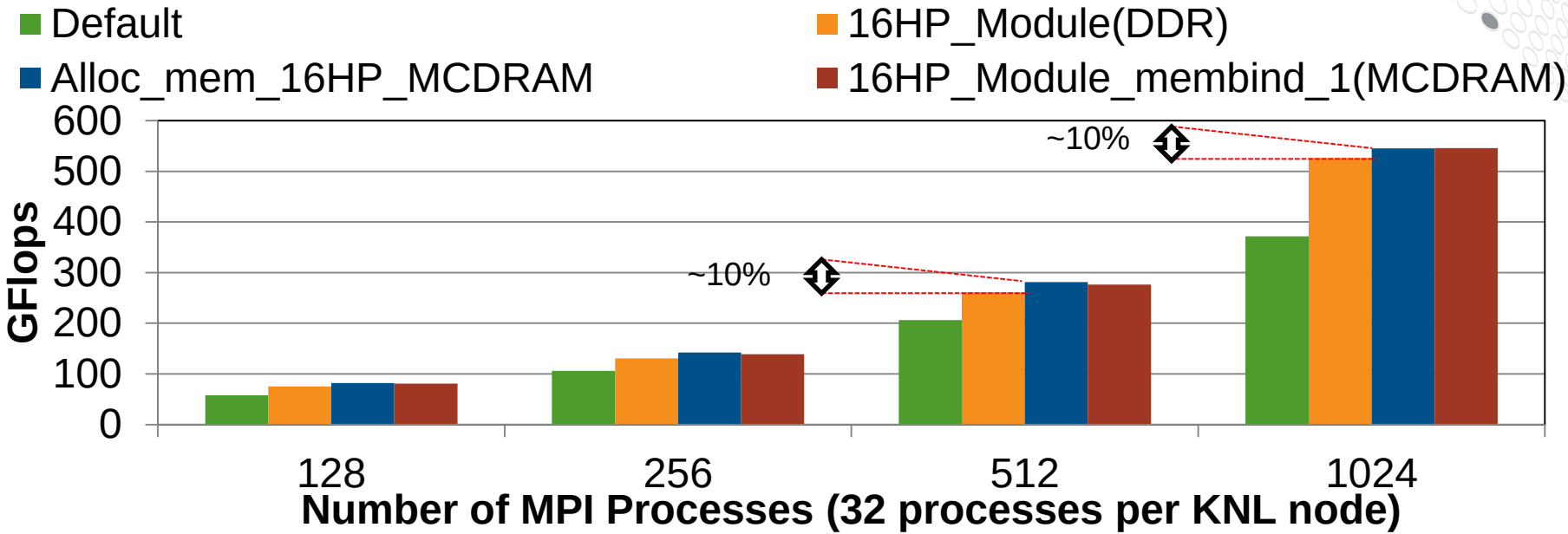
```
lenr    = nx * ny * mynz
lenc    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
lenm    = MAX((nxd2p1 * ny * mynz),
                (nxd2p1 * nz * myny))
info    = MPI_INFO_NULL
CALL MPI_ALLOC_MEM(lenr * nvars * 8_8, info,
                                rc_grid, ierr)
CALL MPI_ALLOC_MEM(lenc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

Multi-threaded MPI Support and Optimizations

MPI Thread Multiple Support in Cray MPI

- **Thread multiple support for**
  - point to point operations (optimized global lock)
  - Collectives (optimized global lock)
  - MPI-RMA (thread hot)
- **All supported in default library**
- **export MPICH_MAX_THREAD_SAFETY=multiple**
- **Global lock optimization on by default (N/A for MPI-RMA)**
  - 50% better 8B latency than pthread_mutex() (OSU latency_mt, 32 threads per node, Broadwell)
  - export MPICH_OPT_THREAD_SYNC=0 falls back to pthread_mutex()

MPI-RMA Thread Hot Communication in Cray MPI

- "Thread hot" means high performance thread multiple support
- 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

Multi-threading Approaches with 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**
  - Likely will not offer best performance and thread 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
  - Leads to multiple threads calling 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

MPI+OpenMP Models

“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
```

“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
  - Less likely to have issues with memory conflicts between threads
  - Potentially simpler to implement
    - 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 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
  - Best performance requires new approach to MPI
    - Goal should be to remove any thread synchronization you can
    - Serializing MPI will limit the benefit and scalability of SPMD
  - SPMD is 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 compute if possible
    - Independent units of communication to be worked on in any order with non-static schedule

Wombat Project Hybrid Application Study

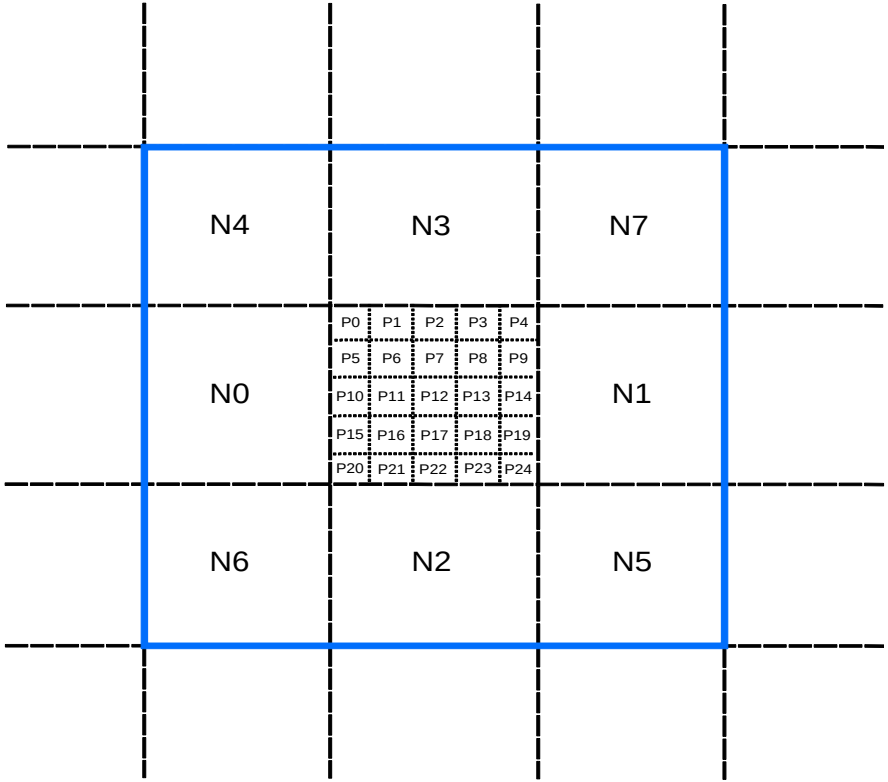
- **Wombat is being developed through a collaboration between Cray Programming Environments and the University of Minnesota Institute for Astrophysics**
  - Peter Mendygral (Cray) is lead developer
  - Tom Jones (UofM) supervises graduate students contributing to the code and drives scientific goals
  - 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

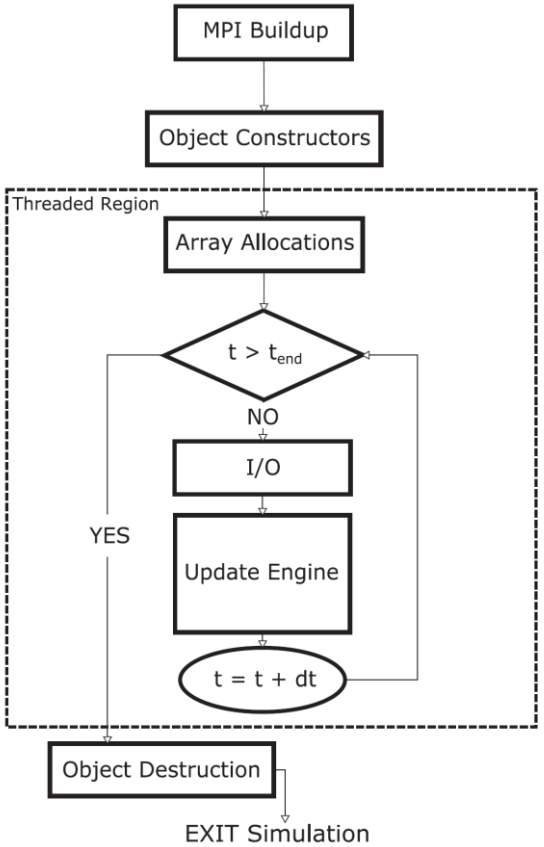
- **Two main issues drove the design of Wombat and explain why other codes have not been sufficient for the science**
  - Scaling to extreme core count required to get to resolutions needed for MHD turbulence
  - Load balancing for SMR/AMR and dark matter particles
- **The approach to these problems in Wombat was**
  - Design to hid communication behind computation as much 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

Domain Decomposition

- Domain decomposition is represented in the Fortran 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



Wombat Driver and Parallel Region

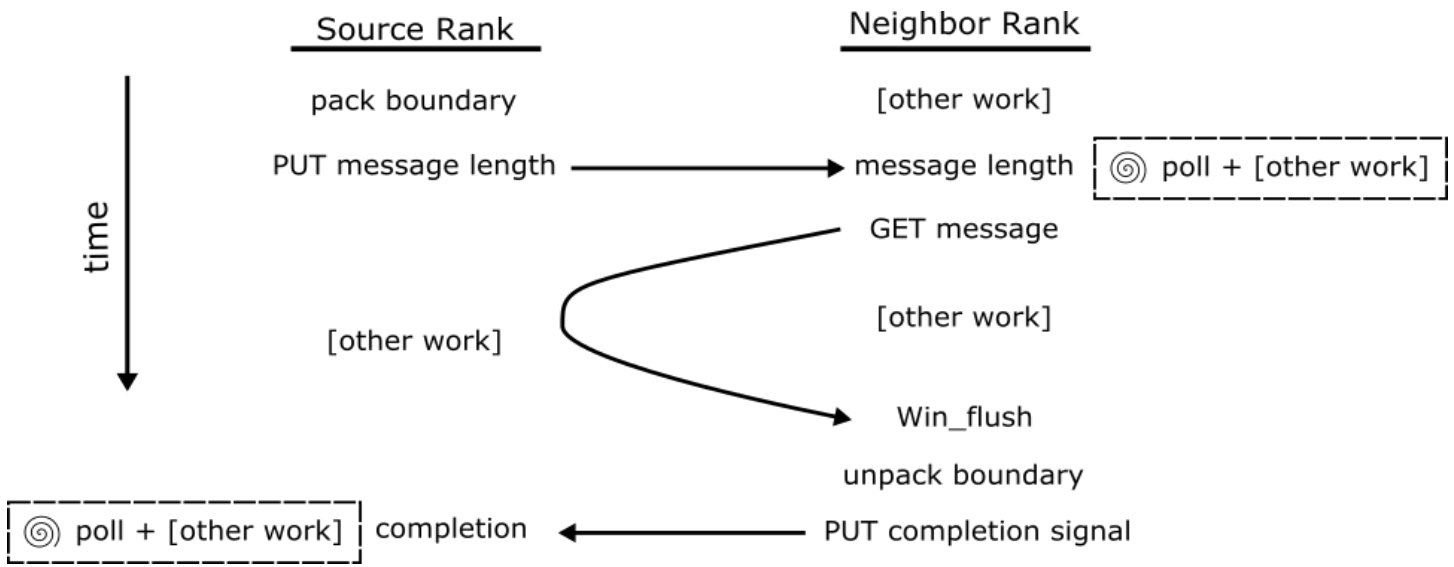


Communication Considerations for Wide Threading

- **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) 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 on Cray systems is a thin software layer that achieves similar performance to SHMEM

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**



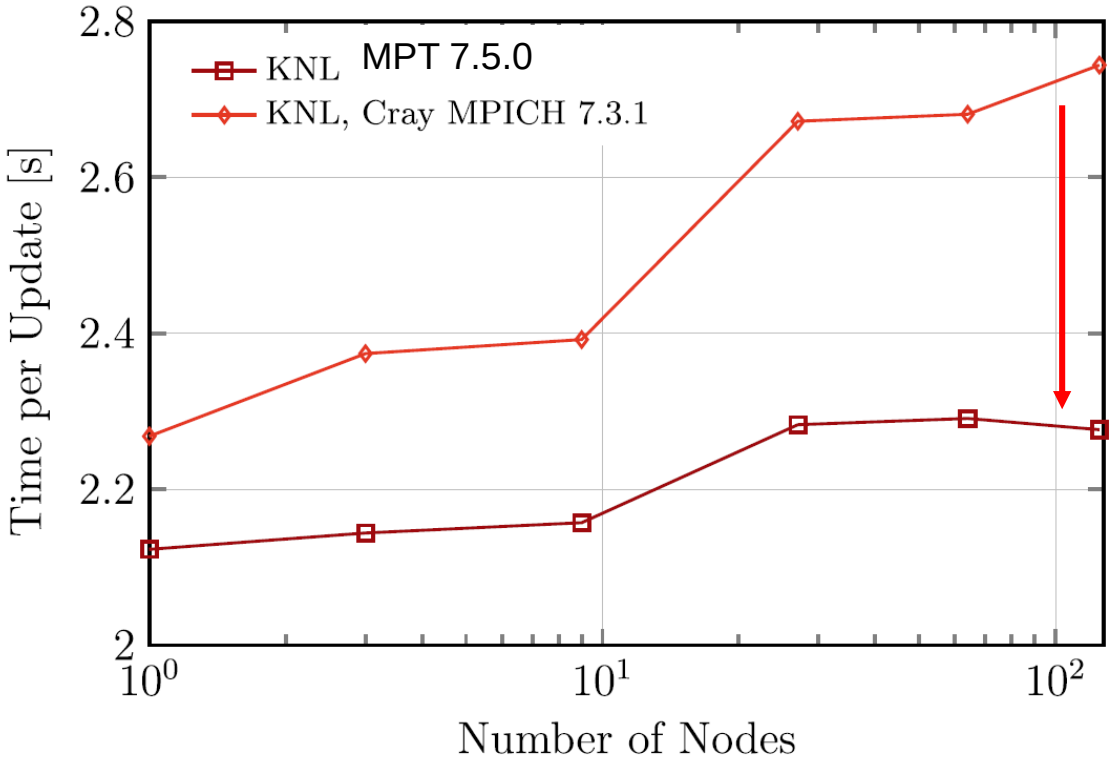
Thread Hot MPI-RMA Synchronization

- **Cray MPICH 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 issued 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
```

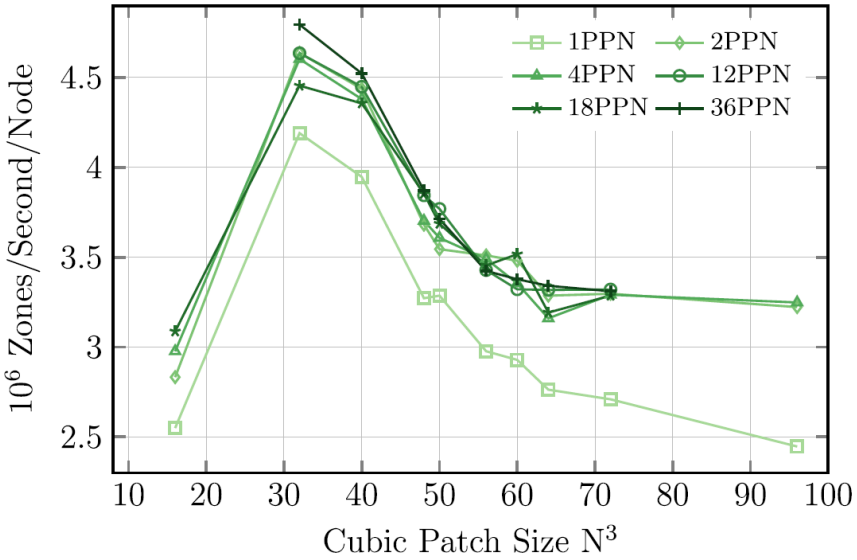
```
!$OMP DO
DO n = 1, n_neighbors

CALL MPI_PUT(…)

END DO
!$OMP END DO NOWAIT

CALL  MPI_WIN_FLUSH_ALL()
!$OMP BARRIER
```

Thread Hot MPI-RMA Speedup

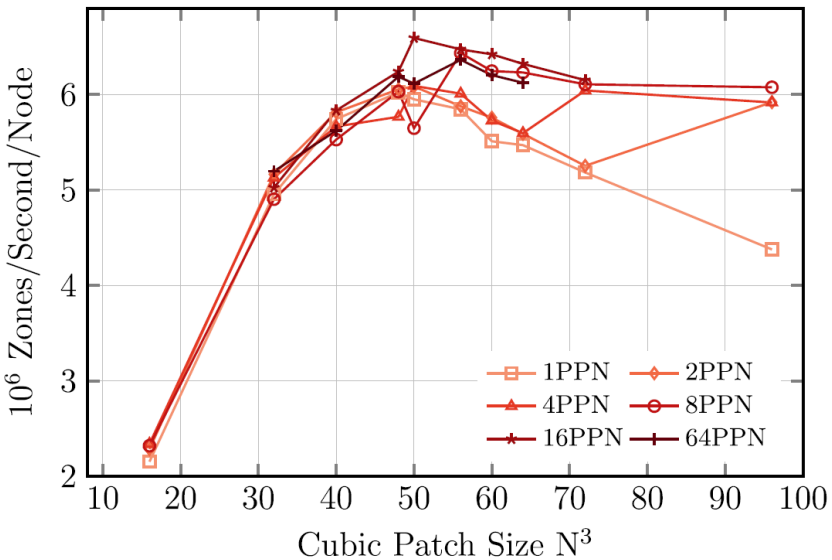


~20% walltime speedup

Dual Socket Broadwell - 36 cores



KNL - 64 cores



- **Measure performance at 27 nodes varying patch size and thread/MPI rank**
- **Fixed grid calculation should not theoretically favor threads or ranks**
  - 9 threads/rank on BDW (nearly optimal performance, good memory footprint)
  - 8 threads/rank on KNL for same reasons
- **~33% higher throughput on KNL over dual socket BDW**

Summary and Recommendations

- Enhancements in Cray MPI to enable users best utilize the MCDRAM technology in flat mode on KNL
- Cray MPI offers Thread-Hot capabilities on Intel Xeon and Intel KNL architectures
- Reviewed design and performance study 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
- Using hugepages on MCDRAM can improve large message communication performance
- Thread multiple support in MPI is a key tool on KNL for hybrid applications
- Use asynchronous communication to 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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Questions?
Thank You!