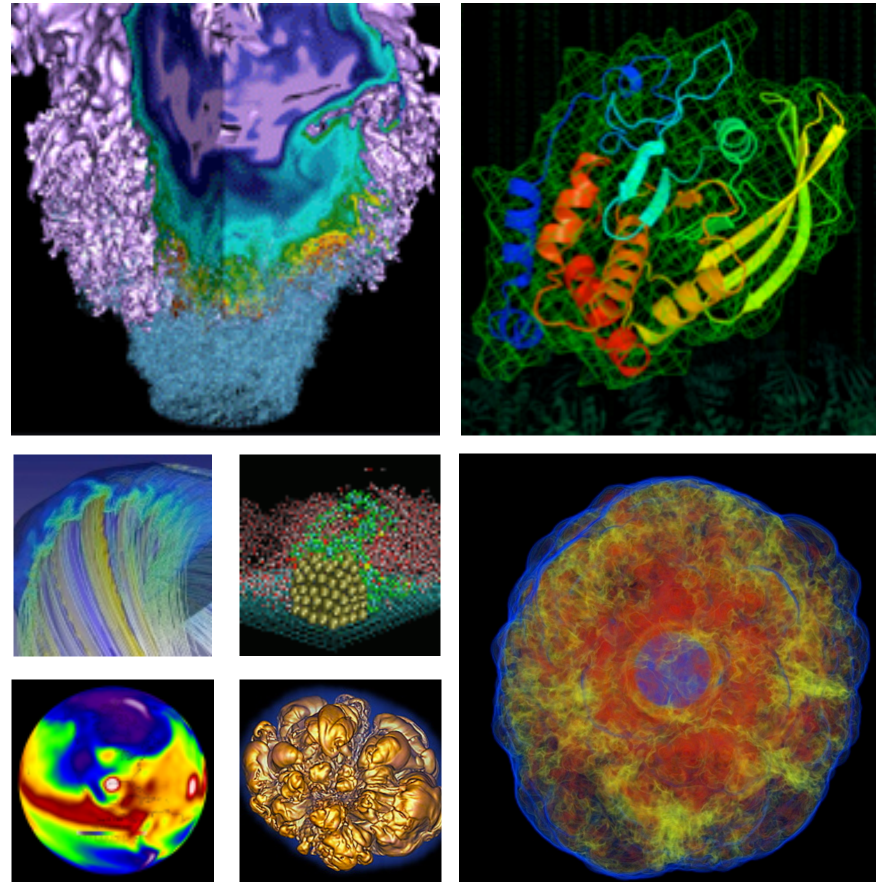
Hybrid MPI/ OpenMP Programming



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Outline

- Architecture Trend
- Brief Review of OpenMP Basics
- Benefits of Hybrid MPI/OpenMP
- Hybrid MPI/OpenMP Programming Model
- Hybrid MPI/OpenMP Issues
- Compile and Run hybrid MPI/OpenMP at NERSC

Common Architectures

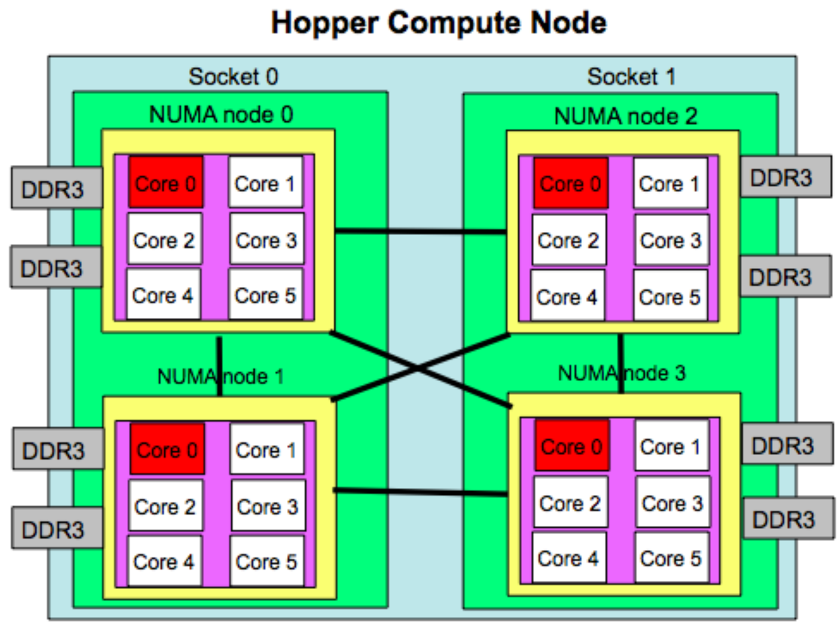
- **Shared Memory Architecture**
  - Multiple CPUs share global memory, could have local cache
  - Uniform Memory Access (UMA)
  - Typical Shared Memory Programming Model: OpenMP, Pthreads, …
- **Distributed Memory Architecture**
  - Each CPU has own memory
  - Non-Uniform Memory Access (NUMA)
  - Typical Message Passing Programming Model: MPI, …
- **Hybrid Architecture**
  - UMA within one SMP node or socket
  - NUMA across nodes or sockets
  - Typical Hybrid Programming Model: hybrid MPI/OpenMP, ...

Technology Trends

- Multi-socket nodes with rapidly increasing core counts.
- Memory per core decreases.
- Memory bandwidth per core decreases.
- Network bandwidth per core decreases.
- Deeper memory hierarchy.

Hopper Compute Nodes

- 2 twelve-core AMD 'MagnyCours' 2.1-GHz processors per node (2 sockets)
- 2 dies per socket
- 6 cores per die
- Each core has own L1 and L2 caches
- Each die (NUMA node) shares an L3 cache
- Each core has shared access to memory on all NUMA nodes
- But memory access to the remote NUMA nodes are slower



Edison and Carver Compute Nodes

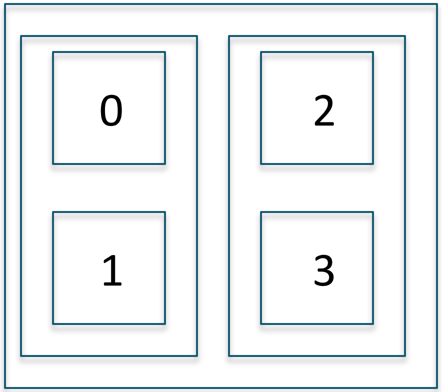
- **Edison:**
  - Each compute node consists of two 8-core Intel Sandy Bridge 2.6 GHz processors (2 sockets)
  - 16 physical cores per node.
  - 32 logical cores when Hyper Threading (HT) is used.
- **Carver:**
  - Each compute node consists of two quad-core Intel Nehalem 2.67 GHz processors (2 sockets)

Hopper Memory Bandwidth

% qsub –I
% setenv CRAY_ROOTFS DSL
% aprun -n 1 numactl --hardware
available: 4 nodes (0-3)
node 0 cpus: 0 1 2 3 4 5
node 0 size: 8191 MB
node 0 free: 7837 MB
node 1 cpus: 6 7 8 9 10 11
node 1 size: 8192 MB
node 1 free: 7883 MB
node 2 cpus: 12 13 14 15 16 17
node 2 size: 8192 MB
node 2 free: 7803 MB
node 3 cpus: 18 19 20 21 22 23
node 3 size: 8192 MB
node 3 free: 7844 MB

32 GB per node

```
node distances:
node   0   1   2   3
  0:  10  16  16  16
  1:  16  10  16  16
  2:  16  16  10  16
  3:  16  16  16  10
```



	0	1	2	3
0	21.3	19.2	12.8	6.4
1	19.2	21.3	6.4	12.8
2	12.8	6.4	21.3	19.2
3	6.4	12.8	19.2	21.3

GB/sec

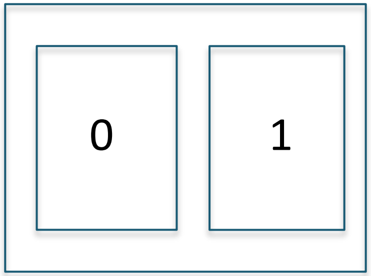
Edison Memory Bandwidth

% qsub –I
% setenv CRAY_ROOTFS DSL
% aprun -n 1 numactl –hardware
available: 2 nodes (0-1)
node 0 cpus: 0 1 2 3 4 5 6 7 16 17 18 19 20 21 22 23
node 0 size: 32744 MB
node 0 free: 31693 MB
node 1 cpus: 8 9 10 11 12 13 14 15 24 25 26 27 28 29 30 31
node 1 size: 32768 MB
node 1 free: 31335 MB

node distances:

node	0	1
0:	10	20
1:	20	10

2 NUMA domains



64 GB per node

Reports 32 cores with HT enabled

Streams Triad Numbers:
Full node: 78 GB/sec.
All cores within same NUMA node: 39 GB/sec
1 core between NUMA node 0 and 1: 9 GB/sec

What is OpenMP

- **OpenMP is an industry standard API of C/C++ and Fortran for shared memory parallel programming.**
- **OpenMP components:**
  - Compiler Directives and Clauses
    - Interpreted when OpenMP compiler option is turned on.
    - Each directive applies to the succeeding structured block.
  - Runtime Libraries
  - Environment Variables

OpenMP Programming Model

- **Fork and Join Model**
  - Master thread forks new threads at the beginning of parallel regions.
  - Multiple threads share work in parallel.
  - Threads join at the end of the parallel regions.
- **Each thread works on global shared and its own private variables.**
- **Threads synchronize implicitly by reading and writing shared variables.**

Advantages of OpenMP

- **Simple programming model**
  - Data decomposition and communication handled by compiler directives
- **Single source code for serial and parallel codes**
- **No major overwrite of the serial code**
- **Portable implementation**
- **Progressive parallelization**
  - Start from most critical or time consuming part of the code

Loop-based *vs.* SPMD

Loop-based:

```
!$OMP PARALLEL DO PRIVATE(i)
!$OMP&            SHARED(a,b,n)
      do I =1, n
         a(i) = a(i) + b(i)
    enddo
!$OMP END PARALLEL DO
```

SPMD (Single Program Multiple Data):

```
!$OMP PARALLEL DO PRIVATE(start, end, i)
!$OMP&                   SHARED(a,b)
    num_thrds = omp_get_num_threads()
    thrd_id = omp_get_thread_num()
    start = n * thrd_id/num_thrds + 1
    end = n * (thrd_num+1)/num_thrds
    do i = start, end
       a(i) = a(i) + b(i)
    enddo
!$OMP END PARALLEL DO
```

SPMD code normally gives better performance than loop-based code, but is more difficult to implement:

- **Less thread synchronization.**
- **Less cache misses.**
- **More compiler optimizations.**

OMP task and taskwait

Serial:
```
int fib (int n)
{
   int x, y;
   if (n < 2) return n;
   x = fib (n – 1);
   y = fib (n – 2);
   return x+y;
}
```

OpenMP:
```
int fib (int n) {
   int x,y;
   if (n < 2) return n;
#pragma omp task shared (x)
   x = fib (n – 1);
#pragma omp task shared (y)
   y = fib (n – 2);
#pragma omp taskwait
   return x+y;
}
```

- **Major OpenMP 3.0 addition. Flexible and powerful.**
- **The task directive defines an explicit task. Threads share work from all tasks in the task pool. The taskwait directive makes sure all child tasks created for the current task finish.**
- **Helps to improve load balance.**

OMP schedule Choices

- **Static**: Loops are divided into *#thrds* partitions.
- **Guided**: Loops are divided into progressively smaller chunks until the chunk size is 1.
- **Dynamic, *#chunk***: Loops are divided into chunks containing *#chunk* iterations.
- **Auto**: The compiler (or runtime system) decides what to use.
- **Runtime**: Use OMP_SCHEDULE environment variable to determine at run time.

OMP_STACK_SIZE

- OMP_STACK_SIZE defines the private stack space each thread has.
- Default value is implementation dependent, and is usually quite small.
- Behavior is undefined if run out of space, mostly segmentation fault.
- To change, set OMP_STACK_SIZE to n (B,K,M,G) bytes. setenv OMP_STACK_SIZE 16M

Cache Coherence and False Sharing

- ccNUMA node: cache-coherence NUMA node.
- Data from memory are accessed via cache lines.
- Multiple threads hold local copies of the same (global) data in their caches. Cache coherence ensures the local copy to be consistent with the global data.
- Main copy needs to be updated when a thread writes to local copy.
- Writes to same cache line is called false sharing or cache thrashing, since it needs to be done in serial. Use atomic or critical to avoid race condition.
- False sharing hurts parallel performance.

Thread Safety

- **In general, IO operations, general OS functionality, common library functions may not be thread safe. They should be performed by one thread only or serialized.**
- **Avoid race condition in OpenMP program.**
  - Race condition: Multiple threads are updating the same shared variable simultaneously.
  - Use “critical” directive
  - Use “atomic” directive
  - Use “reduction” directive

Why not perfect speedup with OpenMP?

Jacobi OpenMP	Execution Time (sec)	Speedup
1 thread	121	1
2 threads	63	1.92
4 threads	36	3.36

- **Why not perfect speedup?**
  - Serial code sections not parallelized
  - Thread creation and synchronization overhead
  - Memory bandwidth
  - Memory access with cache coherence
  - Load balancing
  - Not enough work for each thread

MPI *vs.* OpenMP

- Pure MPI Pro:
  - Portable to distributed and shared memory machines.
  - Scales beyond one node
  - No data placement problem
- Pure MPI Con:
  - Difficult to develop and debug
  - High latency, low bandwidth
  - Explicit communication
  - Large granularity
  - Difficult load balancing
- Pure OpenMP Pro:
  - Easy to implement parallelism
  - Low latency, high bandwidth
  - Implicit Communication
  - Coarse and fine granularity
  - Dynamic load balancing
- Pure OpenMP Con:
  - Only on shared memory machines
  - Scale within one node
  - Possible data placement problem
  - No specific thread order

Why Hybrid MPI/OpenMP

- Hybrid MPI/OpenMP paradigm is the software trend for clusters of SMP architectures.
- Elegant in concept and architecture: using MPI across nodes and OpenMP within nodes. Good usage of shared memory system resource (memory, latency, and bandwidth).
- Avoids the extra communication overhead with MPI within node. Reduce memory footprint.
- OpenMP adds fine granularity (larger message sizes) and allows increased and/or dynamic load balancing.
- Some problems have two-level parallelism naturally.
- Some problems could only use restricted number of MPI tasks.
- Possible better scalability than both pure MPI and pure OpenMP.

Hybrid MPI/OpenMP Reduces Memory Usage

- **Smaller number of MPI processes. Save the memory needed for the executables and process stack copies.**
- **Save memory for MPI buffers due to smaller number of MPI tasks.**
- **Fewer messages, larger message sizes, and smaller MPI all-to-all communication sizes improve performance.**
- **Larger domain for each MPI process, so fewer ghost cells**
  - e.g. Combine four 10x10 domains to one 20x20. Assume 2 ghost layers.
  - Total grid size: Original: 4x14x14=784, new: 24x24=576.

A Pseudo Hybrid Code

```
Program hybrid
 call MPI_INIT (ierr)
 call MPI_COMM_RANK (…)
 call MPI_COMM_SIZE (…)
  …  some computation and MPI communication
  call OMP_SET_NUM_THREADS(4)
 !$OMP PARALLEL DO PRIVATE(i)
 !$OMP&                    SHARED(n)
    do i=1,n
        … computation
    enddo
  !$OMP END PARALLEL DO
  …  some computation and MPI communication
 call MPI_FINALIZE (ierr)
 end
```

MPI_INIT_Thread Choices

- **MPI_INIT_THREAD (required, provided, ierr)**
  – IN: required, desired level of thread support (integer).
  – OUT: provided, provided level of thread support (integer).
  – Returned provided maybe less than required.
- **Thread support levels:**
  – MPI_THREAD_SINGLE: Only one thread will execute.
  – MPI_THREAD_FUNNELED: Process may be multi-threaded, but only master thread will make MPI calls (all MPI calls are ''funneled'' to master thread)
  – MPI_THREAD_SERIALIZED: Process may be multi-threaded, multiple threads may make MPI calls, but only one at a time: MPI calls are not made concurrently from two distinct threads (all MPI calls are ''serialized'').
  – MPI_THREAD_MULTIPLE: Multiple threads may call MPI, with no restrictions.

Thread Support Levels

environment variable MPICH_MAX_THREAD_SAFETY	Hopper/Edison	Carver
not set	MPI_THREAD_SINGLE	MPI_THREAD_SINGLE
single	MPI_THREAD_SINGLE	MPI_THREAD_SINGLE
funneled	MPI_THREAD_FUNNELED	MPI_THREAD_SINGLE
serialized	MPI_THREAD_SERIALIZED	MPI_THREAD_SINGLE
multiple	MPI_THREAD_MULTIPLE	MPI_THREAD_SINGLE

MPI Calls Inside OMP MASTER

- **MPI_THREAD_FUNNELED is required.**
- **OMP_BARRIER is needed since there is no synchronization with OMP_MASTER.**
- **It implies all other threads are sleeping!**

```
!$OMP BARRIER
!$OMP MASTER
    call MPI_xxx(...)
!$OMP END MASTER
!$OMP BARRIER
```

MPI Calls Inside OMP SINGLE

- **MPI_THREAD_SERIALIZED is required.**
- **OMP_BARRIER is needed since OMP_SINGLE only guarantees synchronization at the end.**
- **It also implies all other threads are sleeping!**

```
!$OMP BARRIER
!$OMP SINGLE
    call MPI_xxx(...)
!$OMP END SINGLE
```

THREAD FUNNELED/SERIALIZED *vs.* Pure MPI

- **FUNNELED/SERIALIZED:**
  - All other threads are sleeping while single thread communicating.
  - Only one thread communicating maybe not able to saturate the inter-node bandwidth.
- **Pure MPI:**
  - Every CPU communicating may over saturate the inter-node bandwidth.
- **Overlap communication with computation!**

Overlap COMM and COMP

- Need at least MPI_THREAD_FUNNELED.
- Many "easy" hybrid programs only need MPI_THREAD_FUNNELED
- While master or single thread is making MPI calls, other threads are computing
- Must be able to separate codes that can run before or after halo info is received. Very hard
- Lose compiler optimizations.

```
!$OMP PARALLEL
    if (my_thread_rank < 1) then
        call MPI_xxx(…)
    else
        do some computation
    endif
!$OMP END PARALLEL
```

Thread Affinity

- **Thread affinity: forces each process or thread to run on a specific subset of processors, to take advantage of local process state.**
- **OpenMP 3.1 introduces the OMP_PROC_BIND env variable**
- **On Hopper/Edison, there is aprun command option “-cc”:**
  - **-cc cpu (default)**: Each PE’s thread is constrained to the CPU closest to the PE.
  - **-cc numa_node**: Each PE’s thread is constrained to the same NUMA node CPUs.
  - **-cc none**: Each thread is not binded to a specific CPU.
- **On Carver, “mpirun” has options:**
  - **bind-to-socket**: bind processes to processor sockets
  - **bind-to-core**: bind processes to cores.
  - **bind-to-none (default)**: do not bind processes.

Memory Affinity

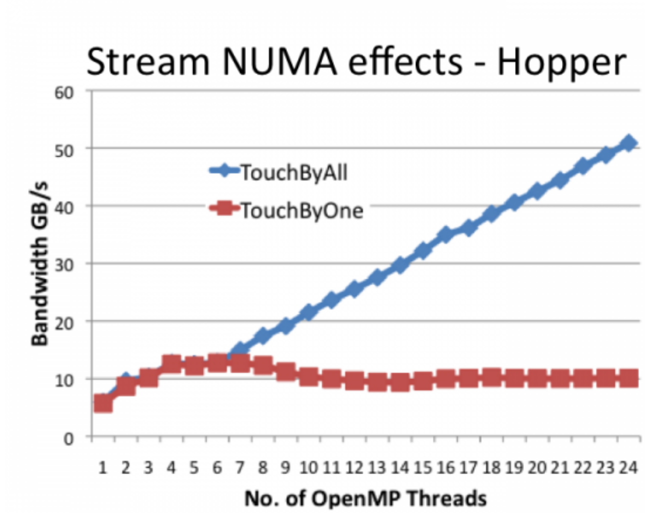
- **Memory affinity: allocate memory as close as possible to the core on which the task that requested the memory is running.**
- **Hopper/Edison: "aprun" option: "-ss"**
  - Specifies strict memory containment per NUMA node. A process can only access memory local to its assigned NUMA node.
  - Only makes sense if the thread affinity is accomplished with "–cc cpu" (default) or "–cc numa_node" first.
- **No memory affinity option for Carver.**

“First Touch” Memory

- **Memory affinity is not decided by the memory allocation, but by the initialization. This is called “first touch” policy.**
- **Hard to do “perfect touch” for real applications.**
- **On Hopper: NERSC recommends do not use more than 6 threads per node to avoid NUMA effect.**

```
#pragma omp parallel for
for (j=0; j<VectorSize; j++) {
a[j] = 1.0; b[j] = 2.0; c[j] = 0.0;}

#pragma omp parallel for
for (j=0; j<VectorSize; j++) {
a[j]=b[j]+d*c[j];}
```



Courtesy Hongzhang Shan

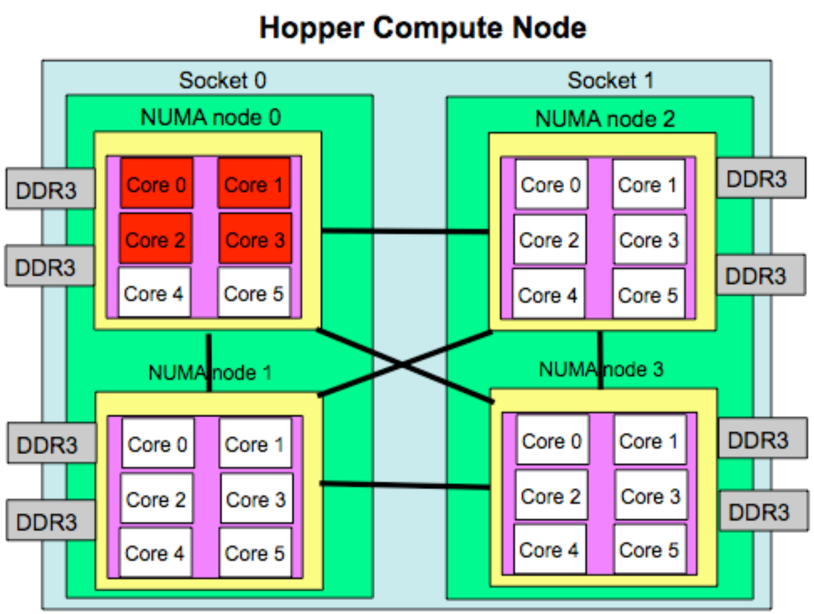
More aprun Options

Option	Descriptions
-n	Number of MPI tasks.
-N	(Optional) Number of MPI tasks per Node.
-d	(Optional) Depth, or number of threads, per MPI task. Required in addition to **OMP_NUM_THREADS** for OpenMP.
-S	(Optional) Number of MPI tasks per NUMA node.
-sn	(Optional) Number of NUMA nodes to use per node
-ss	(Optional) Demands strict memory containment per NUMA node. The default is the opposite - to allow remote NUMA node memory access. Use this for most OpenMP codes.
-cc	(Optional) Controls how tasks are bound to cores and NUMA nodes. Options are: -cc cpu (default), -cc numa_node, and –cc none.

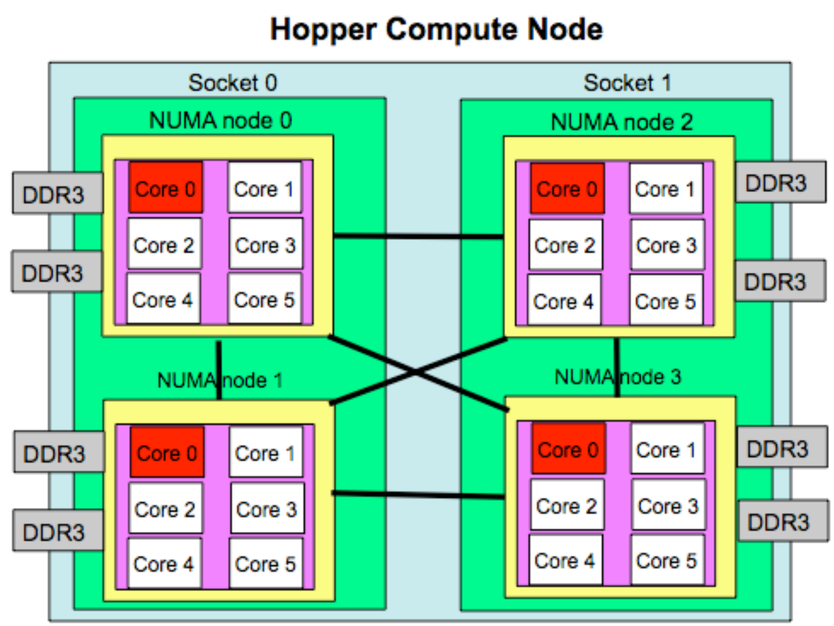
aprun "-S" option

- The "-S" option is especially important for hybrid MPI/ OpenMP applications, since we would like to spread the MPI tasks onto different NUMA nodes.

aprun –n 4 –d 6…



aprun –n 4 –S 1 –d 6 …



Hopper aprun Command Example

- **#PBS -l mppwidth=72 (so 3 nodes!)**
- **1 MPI task per NUMA node with 6 threads**
  - setenv OMP_NUM_THREADS 6
  - aprun –n 12 –N 4 –S 1 -d 6 -ss ./a.out
- **2 MPI tasks per NUMA node with 3 threads**
  - setenv OMP_NUM_THREADS 3
  - aprun –n 24 –N 8 –S 2 -d 3 –ss ./a.out

Hopper Core Affinity

- "xthi.c": a hybrid MPI/OpenMP code that reports process and thread affinity.
- Source code can be found at (page 95-96): http://docs.cray.com/books/S-2496-4101/S-2496-4101.pdf

```
% aprun -n 4 ./xthi
Hello from rank 0, thread 0, on nid01085. (core affinity = 0)
Hello from rank 1, thread 0, on nid01085. (core affinity = 1)
Hello from rank 3, thread 0, on nid01085. (core affinity = 3)
Hello from rank 2, thread 0, on nid01085. (core affinity = 2)

% aprun -n 4 -S 1  ./xthi
Hello from rank 3, thread 0, on nid01085. (core affinity = 18)
Hello from rank 0, thread 0, on nid01085. (core affinity = 0)
Hello from rank 2, thread 0, on nid01085. (core affinity = 12)
Hello from rank 1, thread 0, on nid01085. (core affinity = 6)
```

Carver Core Affinity

2 nodes, 2 MPI tasks per node, OMP_NUM_THREADS=4

```
% mpirun -np 4 -bysocket -bind-to-socket ./xthi

Hello from rank 1, thread 0, on c0803. (core affinity = 4-7)
Hello from rank 1, thread 3, on c0803. (core affinity = 4-7)
Hello from rank 1, thread 1, on c0803. (core affinity = 4-7)
Hello from rank 1, thread 2, on c0803. (core affinity = 4-7)
Hello from rank 3, thread 1, on c0540. (core affinity = 4-7)
Hello from rank 3, thread 3, on c0540. (core affinity = 4-7)
Hello from rank 3, thread 0, on c0540. (core affinity = 4-7)
Hello from rank 3, thread 2, on c0540. (core affinity = 4-7)
Hello from rank 0, thread 0, on c0803. (core affinity = 0-3)
Hello from rank 0, thread 2, on c0803. (core affinity = 0-3)
Hello from rank 2, thread 0, on c0540. (core affinity = 0-3)
Hello from rank 2, thread 1, on c0540. (core affinity = 0-3)
Hello from rank 0, thread 1, on c0803. (core affinity = 0-3)
Hello from rank 0, thread 3, on c0803. (core affinity = 0-3)
Hello from rank 2, thread 2, on c0540. (core affinity = 0-3)
```

```
% mpirun -np 4 -bynode ./xthi

Hello from rank 1, thread 0, on c0540. (core affinity = 0-7)
Hello from rank 1, thread 1, on c0540. (core affinity = 0-7)
Hello from rank 1, thread 2, on c0540. (core affinity = 0-7)
Hello from rank 1, thread 3, on c0540. (core affinity = 0-7)
Hello from rank 0, thread 0, on c0803. (core affinity = 0-7)
Hello from rank 2, thread 0, on c0803. (core affinity = 0-7)
Hello from rank 2, thread 2, on c0803. (core affinity = 0-7)
Hello from rank 2, thread 1, on c0803. (core affinity = 0-7)
Hello from rank 0, thread 2, on c0803. (core affinity = 0-7)
Hello from rank 0, thread 3, on c0803. (core affinity = 0-7)
Hello from rank 2, thread 3, on c0803. (core affinity = 0-7)
Hello from rank 0, thread 1, on c0803. (core affinity = 0-7)
Hello from rank 3, thread 2, on c0540. (core affinity = 0-7)
Hello from rank 3, thread 1, on c0540. (core affinity = 0-7)
Hello from rank 3, thread 3, on c0540. (core affinity = 0-7)
Hello from rank 3, thread 0, on c0540. (core affinity = 0-7)
```

Compile Hybrid MPI/OpenMP

- **Always use the compiler wrappers:**
  - Hopper/Edison: ftn, cc, C++
  - Carver: mpif90, mpicc, mpiCC
- **Need to use the programming environment for each compiler**
- **Portland Group Compilers (Hopper/Carver)**
  - Add compiler option "-mp"
  - For example: **% ftn –mp mycode.f90** (Hopper)
    % mpif90 –mp mycode.f90 (Carver)
  - Fully support OpenMP 3.0 from pgi/8.0.
  - Plan to fully support OpenMP 3.1 in early 2013.
  - Partial OpenMP 3.1 support in between.

Compile Hybrid MPI/OpenMP (2)

- **Cray Compilers (Hopper/Edison)**
  - Hopper: **% module swap PrgEnv-pgi PrgEnv-cray**
    Edison: **% module swap PrgEnv-intel PrgEnv-cray**
  - No additional compiler option needed.
    - Use "–h noomp" to disable OpenMP
  - For example: **% ftn mycode.f90**
  - Fully support OpenMP 3.1 from cce/8.1.0 (released 9/20/2012).
- **Intel Compilers**
  - Hopper: **% module swap PrgEnv-pgi PrgEnv-intel**
    Edison: **no need to swap PrgEnv**
    Carver: **% module unload pgi openmpi**
    % module load intel openmpi-intel
  - Add compiler option "-openmp"
  - For example: **% ftn –openmp mycode.f90** (Hopper/Edison)
    % mpif90 –openmp mycode.f90 (Carver)
  - Fully support OpenMP 3.1 from intel/12.1 (released 9/5/2011).

Compile Hybrid MPI/OpenMP (3)

- **GNU Compilers**
  - Hopper: **% module swap PrgEnv-pgi PrgEnv-gnu**
    Edison: **% module swap PrgEnv-intel PrgEnv-gnu**
    Carver: **% module unload pgi openmpi**
    % module load gcc openmpi-gcc
  - Add compiler option "-fopenmp"
  - For example: **% ftn –fopenmp mycode.f90** (Hopper/Edison)
    % mpif90 –fopenmp mycode.f90 (Carver)
  - Fully support OpenMP 3.1 from gcc/4.7.0 (released 3/22/2012).
- **Pathscale Compilers (Hopper only)**
  - **% module swap PrgEnv-pgi PrgEnv-pathscale**
  - Add compiler option "-mp"
  - For example: **% ftn –mp mycode.f90**
  - Fully support OpenMP 2.5

Run Hybrid MPI/OpenMP on Hopper

- **Each Hopper node has 4 NUMA nodes, each with 6 UMA cores.**
- **Recommend to use max 6 OpenMP threads per node, and MPI across NUMA nodes. (although up to 24 OpenMP threads per Hopper node possible).**
- **Interactive batch jobs:**

  2 Hopper nodes, 8 MPI tasks, 6 OpenMP threads per MPI task:
  - **% qsub –I –V –q interactive –lmppwidth=48**
  - **wait for a new shell**
  - **% cd $PBS_O_WORKDIR**
  - **% setenv OMP_NUM_THREADS 6**
  - **% setenv PSC_OMP_AFFINITY FALSE (note: for Pathscale only)**
  - **% aprun –n 8 –N 4 –S 1 –ss –d 6 ./mycode.exe**
    (for Intel: add "–cc numa_node" in the aprun line).

Run Hybrid MPI/OpenMP on Hopper (2)

Sample batch script:
(pure OpenMP example,
Using 24 OpenMP threads)

```
#PBS -q debug
#PBS -l mppwidth=24
#PBS -l walltime=00:10:00
#PBS -j eo
#PBS –V
cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 24

#uncomment this line for pathscale
#setenv PSC_OMP_AFFINITY FALSE

# add "-cc numa_node" for Intel
aprun –n 1 -N 1 –d 24 ./mycode.exe
```

- **Run batch jobs:**
  - Prepare a batch script first
  - % qsub myscript
- **Hybrid MPI/OpenMP**
  - 1 Hopper node, 4 MPI tasks, 6 OpenMP threads per MPI task:
    - % aprun –n 4 –N 4 –S 1 –ss –d 6 ./mycode.exe
  - 2 Hopper nodes, 8 MPI tasks, 6 threads per MPI task:
    - #PBS -l mppwidth=48
      - 24 cores/node *2 nodes
    - % aprun –n 8 –N 4 –S 1 –ss –d 6 ./mycode.exe

Special Considerations for Pathscale and Intel Compilers on Hopper

- **For Pathscale compilers, need to set environment variable PSC_OMP_AFFINITY to FALSE at the run time.**
  - This is to turn off the Pathscale internal control of cpu affinity.
- **For Intel compilers, need to use "-cc numa_node" or "-cc none" instead of the default "-cc cpu" option for aprun.**
  - This is due to Intel starts an extra thread with OpenMP.

Run Hybrid MPI/OpenMP on Edison

- **Each Edison node has 2 NUMA nodes, each with 8 UMA cores (or 16 UMA logical cores with HT).**
- **Recommend to use max 8 OpenMP threads per node (max 16 threads with HT), and MPI across NUMA nodes.**
- **Interactive batch jobs:**

  2 Edison nodes, 4 MPI tasks, 8 OpenMP threads per MPI task:

  - **% qsub –I –V –q interactive –lmppwidth=32**
  - **wait for a new shell**
  - **% cd $PBS_O_WORKDIR**
  - **% setenv OMP_NUM_THREADS 8**
  - **% aprun –n 4 –N 2 –S 1 –ss –d 8 ./mycode.exe**

    (for Intel: add "setenv KMP_AFFINITY compact" before the aprun line, also add "–cc numa_node" in the aprun line).

Run Hybrid MPI/OpenMP on Edison (2)

Sample batch script:
(pure OpenMP example,
Using 16 OpenMP threads)

```
#PBS -q debug
#PBS -l mppwidth=16
#PBS -l walltime=00:10:00
#PBS -j eo
#PBS –V
cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 16

# uncomment this line for Intel
#setenv KMP_AFFINITY scatter

# need to add "-cc none" for Intel
aprun –n 1 -N 1 –d 16 ./mycode.exe
```

Sample batch script:
(hybrid MPI/OpenMP example,
Using 8 OpenMP threads per task)

```
#PBS -q debug
#PBS -l mppwidth=32
#PBS -l walltime=00:10:00
#PBS -j eo
#PBS –V
cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 8

# uncomment this line for Intel
#setenv KMP_AFFINITY compact

# need to add "-cc numa_node" for Intel
aprun –n 4 –N 2 –S 1 -ss –d 8 ./mycode.exe
```

Run Hybrid MPI/OpenMP on Edison with HT (3)

Sample batch script:
(pure OpenMP example with HT,
Using 32 OpenMP threads)

```
#PBS -q debug
#PBS -l mppwidth=32
#PBS –l mppnppn=32
#PBS -l walltime=00:10:00
#PBS -j eo
#PBS –V
cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 32

# uncomment this line for Intel
#setenv KMP_AFFINITY scatter

# need to add "-cc none" for Intel
aprun –n 1 -N 1 –j 2 –d 32 ./
mycode.exe
```

Sample batch script:
(hybrid MPI/OpenMP example with HT,
Using 16 OpenMP threads per task)

```
#PBS -q debug
#PBS -l mppwidth=64
#PBS –l mppnppn=32
#PBS -l walltime=00:10:00
#PBS -j eo
#PBS –V
cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 16

# uncomment this line for Intel
#setenv KMP_AFFINITY compact

# need to add "-cc numa_node" for Intel
aprun –n 4 –N 2 –S 1 –j 2 -ss –d 16 ./
mycode.exe
```

Special Considerations for Intel Compilers on Edison

- **For Intel compilers, need to use "-cc numa_node" or "-cc none" instead of the default "-cc cpu" option for aprun. Also set a run time env KMP_AFFINITY to compact or scatter.**
  - This is due to the conflict of the internal Intel thread affinity and the aprun thread affinity.
- **when OMP_NUM_THREADS <= 8 (or <= 16 with HT)**
  - setenv KMP_AFFINITY compact
  - add "-cc numa_node" in the aprun line
- **when OMP_NUM_THREADS > 8 (or > 16 with HT)**
  - setenv KMP_AFFINITY scatter
  - add "-cc none" in the aprun line

Run Hybrid MPI/OpenMP on Carver

- **Each Carver node has 8 cores, 2 sockets with 4 cores each.**
- **Use max 8 OpenMP threads per node.**
- **Interactive batch jobs:**
  - Pure OpenMP example, using 8 OpenMP threads:
  - % qsub –I –V –q interactive –lnodes=1:ppn=1,pvmem=20GB
  - wait for a new shell
  - % cd $PBS_O_WORKDIR
  - setenv OMP_NUM_THREADS 8
  - % mpirun –np 1 ./mycode.exe
- **Change nodes:ppn, pvmem and mpirun –np options for hybrid MPI/OpenMP jobs.**

Run Hybrid MPI/OpenMP on Carver (2)

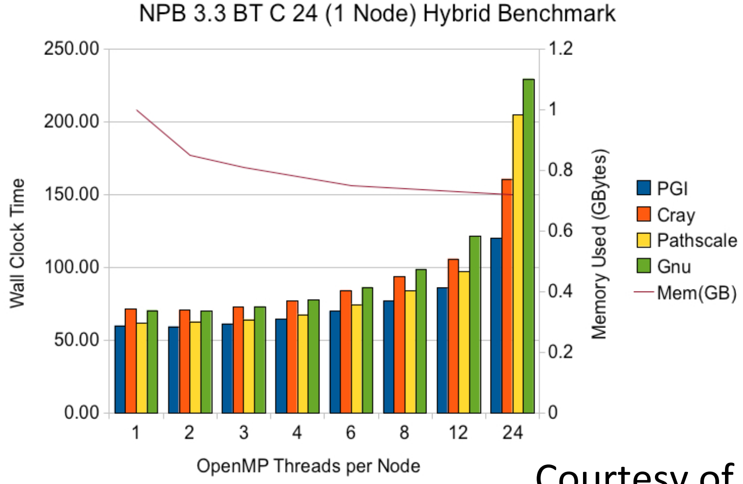
Sample batch script:
(2 Carver nodes, 4 MPI tasks,
2 MPI tasks per node,
4 OpenMP threads per MPI task)

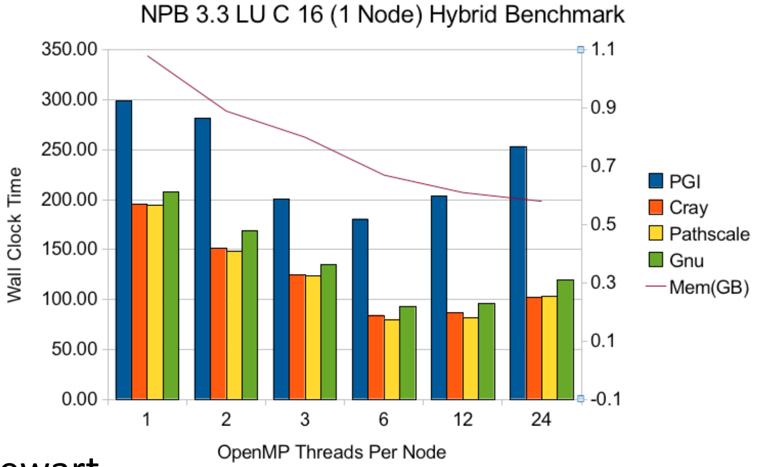
```
#PBS -q debug
#PBS -l nodes=2:ppn=2
#PBS –l pvmem=10GB
#PBS -l walltime=00:10:00
#PBS -j eo

cd $PBS_O_WORKDIR
setenv OMP_NUM_THREADS 4
mpirun –np 4 –bysocket –bind-
to-core ./mycode.exe
```

- **Run batch jobs:**
  - Prepare a batch script first
  - % qsub myscript
- **Hybrid MPI/OpenMP**
  - 2 Carver nodes, 1 MPI task per node, 8 OpenMP threads per MPI task:
    - #PBS -l nodes=2:ppn=1
    - #PBS -l pvmem=20GB
    - setenv OMP_NUM_THREADS 8
    - % mpirun –np 2 ./mycode.exe
- **Notice the setting for pvmem**
  - Default is 20GB per MPI process per node.
  - Set to 10GB for 2 MPI tasks per node
  - Set to 5 GB for 4 MPI tasks per node

Hopper: Hybrid MPI/OpenMP NPB





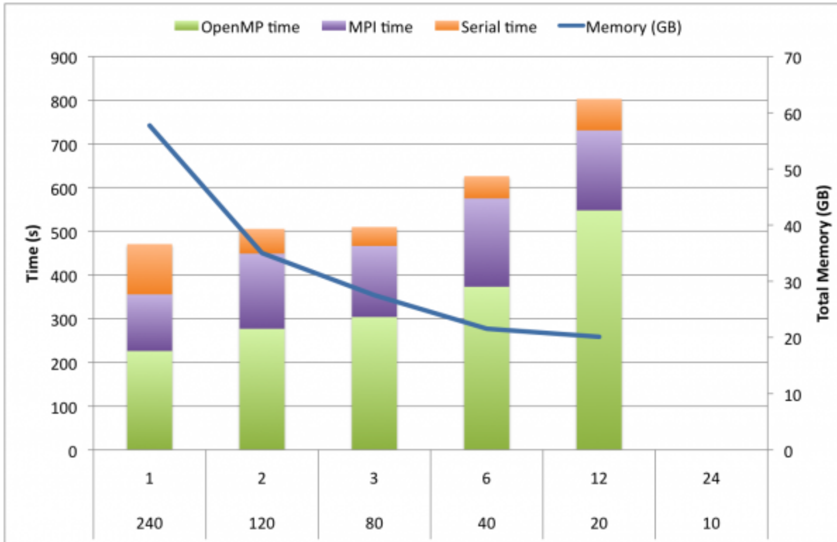
Courtesy of Mike Stewart

On a single node, hybrid MPI/OpenMP NAS Parallel Benchmarks:

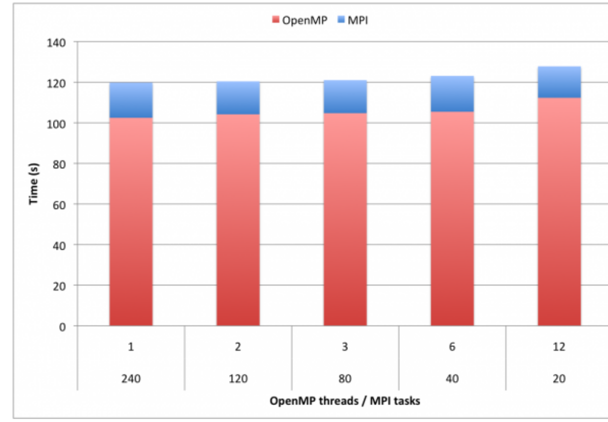
- **Reduced memory footprint with increased OpenMP threads.**
- **Hybrid MPI/OpenMP can be faster or comparable to pure MPI.**
- **Try different compilers.**
- **Sweet spot: BT: 1-3 threads; LU: 6 threads.**

Hopper: Hybrid MPI/OpenMP fvCAM

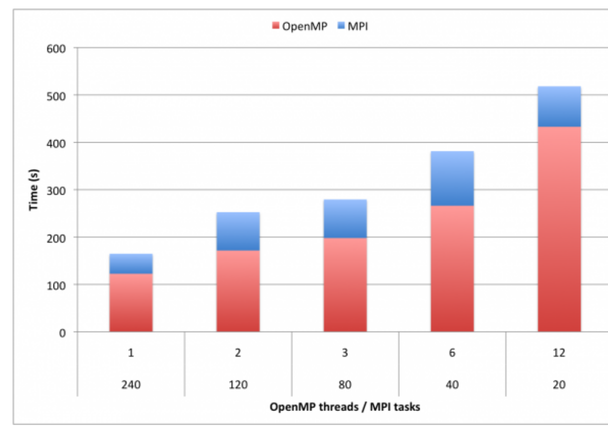
Total



"Physics" Component



"Dynamics" Component

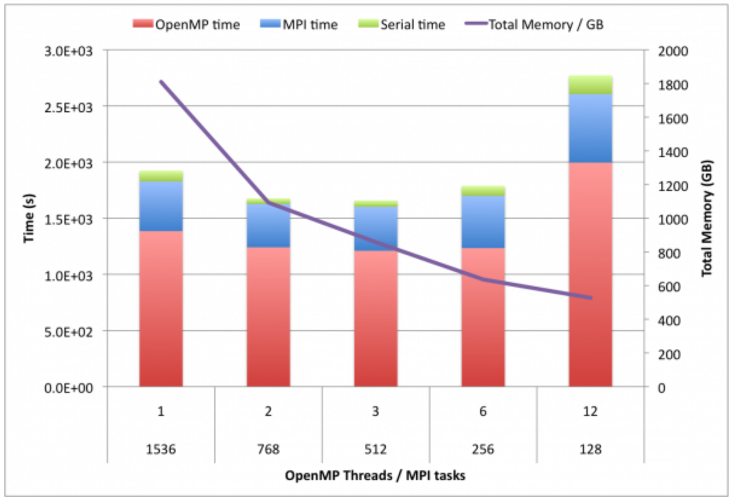


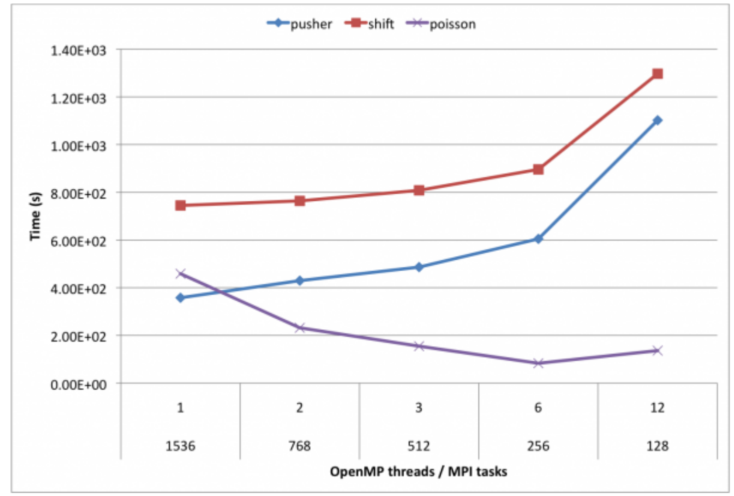
Community Atmospheric Model:

- **Memory reduces to 50% with 3 threads but only 6% performance drop.**
- **OpenMP time starts to grow from 6 threads.**
- **Load imbalance in "Dynamics" OpenMP**

Courtesy of Nick Wright, et. al, NERSC/Cray Center of Excellence"

Hopper: Hybrid MPI/OpenMP GTC





3d Gyrokinetic Toroidal Code:

- **Memory reduces to 50% with 3 threads, also 15% better performance**
- **NUMA effects seen with 12 threads**
- **Mixed results in different kernels**

Courtesy of Nick Wright, et. al, NERSC/Cray Center of Excellence

Hybrid Parallelization Strategies

- From sequential code, decompose with MPI first, then add OpenMP.
- From OpenMP code, treat as serial code.
- From MPI code, add OpenMP.
- Simplest and least error-prone way is to use MPI outside parallel region, and allow only master thread to communicate between MPI tasks. MPI_THREAD_FUNNELED is usually the best choice.
- Could use MPI inside parallel region with thread-safe MPI.
- Avoid MPI_THREAD_MULTIPLE if you can. It slows down performance due to the usage of global locks for thread safety.

Why Mixed OpenMP/MPI Code is Sometimes Slower?

- **All threads are idle except one while MPI communication.**
  - Need overlap comp and comm for better performance.
  - Critical Section for shared variables.
- **Thread creation overhead**
- **Cache coherence, false sharing.**
- **Data placement, NUMA effects.**
- **Natural one level parallelism problems.**
- **Pure OpenMP code performs worse than pure MPI within node.**
- **Lack of optimized OpenMP compilers/libraries.**

Debug and Tune Hybrid Codes

- Debugger tools: DDT, Totalview, gdb, Valgrind.
- Profiling: IPM, CrayPat, TAU.
- Decide which loop to parallelize. Better to parallelize outer loop. Decide whether Loop permutation, fusion or exchange is needed. Use NOWAIT clause if possible.
- Choose between loop-based or SPMD.
- Use different OpenMP task scheduling options.
- Experiment with different combinations of MPI tasks and number of threads per MPI task. Fewer MPI tasks may not saturate inter-node bandwidth.
- Adjust MPI and OpenMP runtime environment variables.
- Aggressively investigate different thread initialization options and the possibility of overlapping communication with computation.
- Try OpenMP TASK.
- Leave some cores idle on purpose: memory capacity or bandwidth capacity.
- Try different compilers.

OpenMP Profiling with IPM

- **IPM is a light weight profiling tool. OpenMP profiling currently works with PGI and Cray compilers on Hopper. Will be available on Edison soon with Intel and Cray compilers .**
- **PGI compiler:**
  - **% module load ipm-openmp/pgi**
  - **% ftn –mp=trace test_omp.f $IPM**
  - **% cc –mp=trace test_omp.c $IPM**
- **Cray compiler:**
  - **% module swap PrgEnv-pgi PrgEnv-cray**
  - **% module load ipm-openmp/cray**
  - **% ftn -h omp_trace test_omp.f $IPM**
  - **% cc -h omp_trace test_omp.c $IPM**
- **Run the code as usual on the compute nodes.**
- **OMP_PARALLEL: Total time spent in OMP regions.**
- **OMP_IDLE: total time from each thread waiting for others. This shows load imbalance.**

```
##IPM2v0.xx##############################################
# command   : ./jacobi_mpiomp
# start     : Thu Feb 02 10:04:21 2012   host      : nid01840
# stop      : Thu Feb 02 10:04:22 2012   wallclock : 0.77
# mpi_tasks : 4 on 1 nodes               %comm     : 12.50
# omp_thrds : 6                          %omp      : 85.05
# mem [GB]  : 0.03                       gflop/sec : 1.52
#
#           :     [total]     <avg>      min       max
# wallclock :      3.09       0.77       0.77      0.77
# MPI       :      0.39       0.10       0.01      0.13
# OMP       :      2.63       0.66       0.64      0.71
# OMP idle  :      0.10       0.03       0.01      0.07
# %wall     :
#   MPI     :                12.50       1.02     16.38
#   OMP     :                85.05      82.60     92.30
# #calls    :
#   MPI     :     14056       3514       3514      3514
# mem [GB]  :      0.03       0.01       0.01      0.01
#
#                     [time]      [count]     <%wall>
# @OMP_PARALLEL         2.63        9010        85.05
# @OMP_IDLE             0.62       54060        19.91
# MPI_Allreduce         0.22        2000         7.14
# MPI_Bcast             0.12          16         3.84
# MPI_Sendrecv          0.05        4000         1.49
# MPI_Comm_size         0.00        4016         0.02
# MPI_Comm_rank         0.00        4016         0.01
# MPI_Init              0.00           4         0.00
# MPI_Finalize          0.00           4         0.00
###############################
```

Conclusions

- Flat MPI is still the dominant parallel programming model today. But it is time to consider adding thread parallelism to MPI.
- Hybrid MPI/OpenMP is suited for the multi-core architecture trend.
- Whether hybrid MPI/OpenMP performs better than MPI depends on whether the communication advantage outcomes the thread overhead, etc. or not.
- A great benefit for using hybrid MPI/OpenMP is the reduced memory footprint per node.

Further References

- **Sample Codes and Scripts**
  - **module load training/2013**
  - **cd $EXAMPLES/NUG/hybrid**
- **MPI: http://www.mcs.anl.gov/research/projects/mpi/**
- **OpenMP: http://openmp.org**
- **Using Hybrid/OpenMP on NERSC Cray Systems:**
  http://www.nersc.gov/nusers/systems/XT/openmp.php
- **Using OpenMP Effectively:**
  http://www.nersc.gov/users/computational-systems/hopper/performance-and-optimization/using-openmp-effectively-on-hopper/
- **NERSC Hopper, Edison, and Carver web pages:**
  https://www.nersc.gov/users/computational-systems/hopper
  https://www.nersc.gov/users/computational-systems/edison
  https://www.nersc.gov/users/computational-systems/carver

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