Using Hybrid MPI/OpenMP, UPC, and CAF at NERSC

Yun (Helen) He and Woo-Sun Yang

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BERKELEY LAB Lawrence Berkeley National Laboratory

Outline

- Architecture Trend
- Benefits of Hybrid MPI/OpenMP
- Hybrid MPI/OpenMP Programming Model
- Hybrid MPI/OpenMP Issues
- Compile and Run hybrid MPI/OpenMP
- Using UPC and CAF on Hopper

Common Architectures

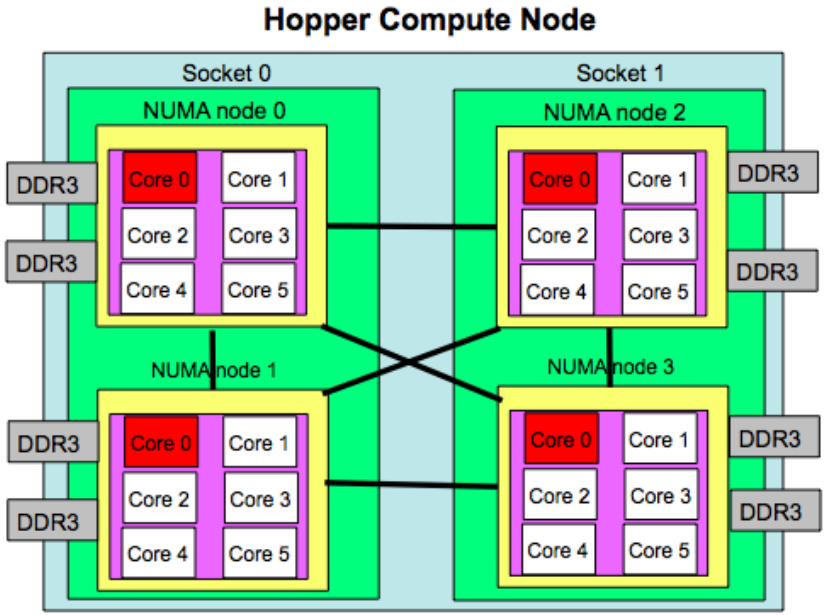
- Shared Memory Architecture
  - Multiple CPUs share global memory, could have local cache
  - Uniform Memory Access (UMA)
  - Typical Shared Memory Programming Model: OpenMP, Pthreads, …
- Distributed Memory Architecture
  - Each CPU has own memory
  - Non-Uniform Memory Access (NUMA)
  - Typical Message Passing Programming Model: MPI, …
- Hybrid Architecture
  - UMA within one SMP node
  - NUMA across nodes
  - 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 and Carver 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
- 32 GB per node (some 64GB), 1.33 GB/core (some 2.66GB/core)
- Each core has shared access to memory on all NUMA nodes
- But memory access to the remote NUMA nodes are slower



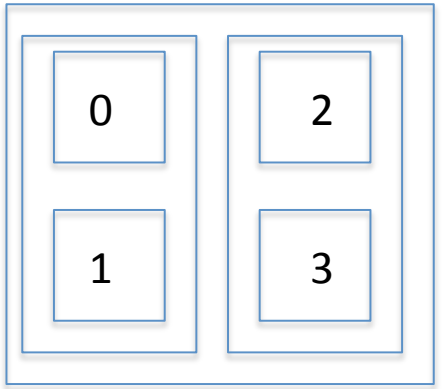
Carver: each compute node consists of 2 quad-core Intel Nehalem 2.67 GHz processors (2 sockets)

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
```

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

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.

A Simple OpenMP Program

```
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
int main () {
    int tid, nthreads;
#pragma omp parallel private(tid)
   {
    tid = omp_get_thread_num();
    printf("Hello World from thread %d\n", tid);
#pragma omp barrier
     if ( tid == 0 ) {
        nthreads = omp_get_num_threads();
        printf("Total threads= %d\n",nthreads);
     }
  }
}
```

Sample Compile and Run:

```
% pgf90 –mp test.f90
% setenv OMP_NUM_THREADS 4
% ./a.out
```

```
Program main
use omp_lib       (or: include "omp_lib.h")
integer :: id, nthreads
!$OMP PARALLEL PRIVATE(id)
    id = omp_get_thread_num()
    write (*,*) "Hello World from thread", id
!$OMP BARRIER
    if ( id == 0 ) then
        nthreads = omp_get_num_threads()
        write (*,*) "Total threads=",nthreads
     end if
!$OMP END PARALLEL
End program
```

Sample Output: (no specific order)

```
Hello World from thread        0
Hello World from thread        2
Hello World from thread        3
Hello World from thread        1
Total threads=       4
```

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

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

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

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

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

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.

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 1 ghost layer.
  - Total grid size: Original: 4x12x12=576, new: 42x42=484.

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 main thread will make MPI calls (all MPI calls are ''funneled'' to main 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	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.
- Current OpenMP 3.0 has no specification for thread affinity.
  - OpenMP 3.1 introduces the OMP_PROC_BIND environment variable (not available on Hopper and Carver yet)

- On Hopper, 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

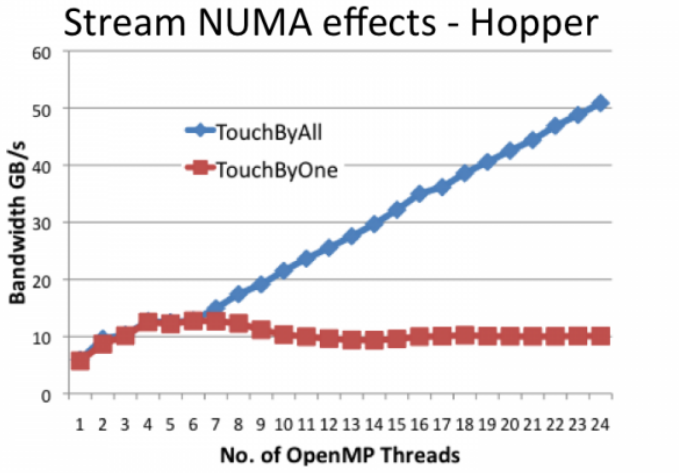
- Memory affinity: allocation memory as close as possible to the core on which the task that requested the memory is running
- Hopper "aprun" option: "**-ss**"
  - Specifies strict memory containment per NUMA node. A process can only access memory local to its assigned NUMA node.
  - Only makes sense 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. 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

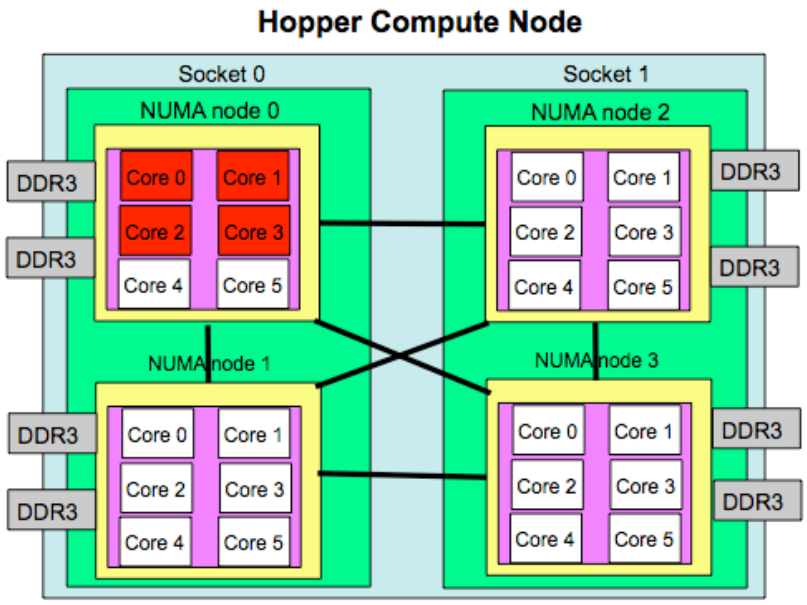
More aprun Options

Option	Descriptions
-n	Number of MPI tasks.
-N	(Optional) Number of tasks per Hopper Node. Default is 24.
-d	(Optional) Depth, or number of threads, per MPI task. Use this very important option *in addition to* ***OMP_NUM_THREADS*** for OpenMP. Values can be 1-24. The default is 1. For OpenMP, values of 2-6 are recommended.
-S	(Optional) Number of tasks per NUMA node. Values can be 1-6; default 6
-sn	(Optional) Number of NUMA nodes to use per Hopper node. Values can be 1-4; default 4
-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. The recommend setting for most codes is -cc cpu which restricts each task to run on a specific core.

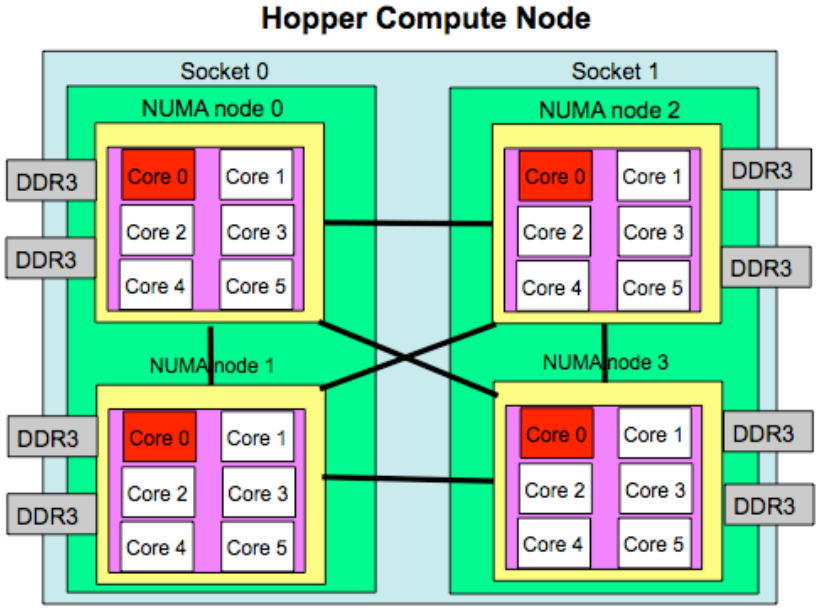
aprun "-S" option

- 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 …



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 92-93): http://docs.cray.com/books/S-2496-4002/S-2496-4002.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: ftn, cc, C++
  - Carver: mpif90, mpicc, mpiCC
- Need to use the programming environment for each compiler
- Portland Group Compilers
  - Add compiler option "-mp"
  - For example: **% ftn –mp mycode.f90** (Hopper)

    % mpif90 –mp mycode.f90 (Carver)
  - Supports OpenMP 3.0 from pgi/8.0

Compile Hybrid MPI/OpenMP (2)

- Pathscale Compilers (Hopper only)
  - **% module swap PrgEnv-pgi PrgEnv-pathscale**
  - Add compiler option "-mp"
  - For example: **% ftn –mp mycode.f90**
- GNU Compilers
  - Hopper: **% module swap PrgEnv-pgi PrgEnv-gnu**
  - Carver: **% module unload pgi openmpi**
    % module load gcc openmpi-gcc
  - Add compiler option "-fopenmp"
  - For example: **% ftn –fopenmp mycode.f90** (Hopper)
    % mpif90 –fopenmp mycode.f90 (Carver)
  - Supports OpenMP 3.0 from gcc/4.4

Compile Hybrid MPI/OpenMP (3)

- Cray Compilers (Hopper only)
  - **% module swap PrgEnv-pgi PrgEnv-cray**
  - No additional compiler option needed
  - For example: **% ftn mycode.f90**
  - Supports OpenMP 3.0
- Intel Compilers
  - Hopper: **% module swap PrgEnv-pgi PrgEnv-intel**

    Carver: **% module unload pgi openmpi**

    % module load intel openmpi-intel
  - Add compiler option "-openmp"
  - For example: **% ftn –openmp mycode.f90** (Hopper)

    % mpif90 –openmp mycode.f90 (Carver)
  - Supports OpenMP 3.0 from intel/11.0

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:

  1 Hopper node, 4 MPI tasks, 6 OpenMP threads per MPI task:
  - **% qsub –I –V –q interactive –lmppwidth=24**
  - **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 4 –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 6 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 6

#uncomment this line for pathscale
#setenv PSC_OMP_AFFINITY FALSE

aprun –n 1 -N 1 –d 6 ./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 none" or "-cc numa_node" 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 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)

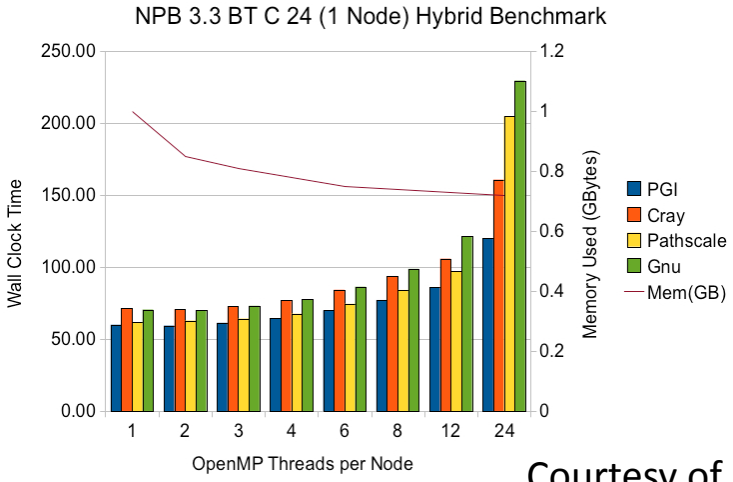
Sample batch script:
(2 Carver nodes, 4 MPI tasks,
2 MPI tasks per node,
4 OpenMP threads per MPI task)

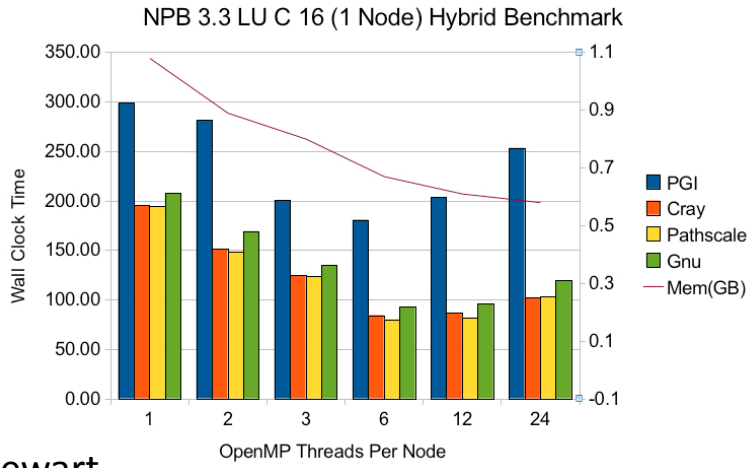
```
#PBS -q debug
#PBS -l nodes=2:ppn=2
#PBS –l pvmem=10GB
#PBS -l walltime=00:10:00
#PBS -j eo

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

Hybrid MPI/OpenMP NPB





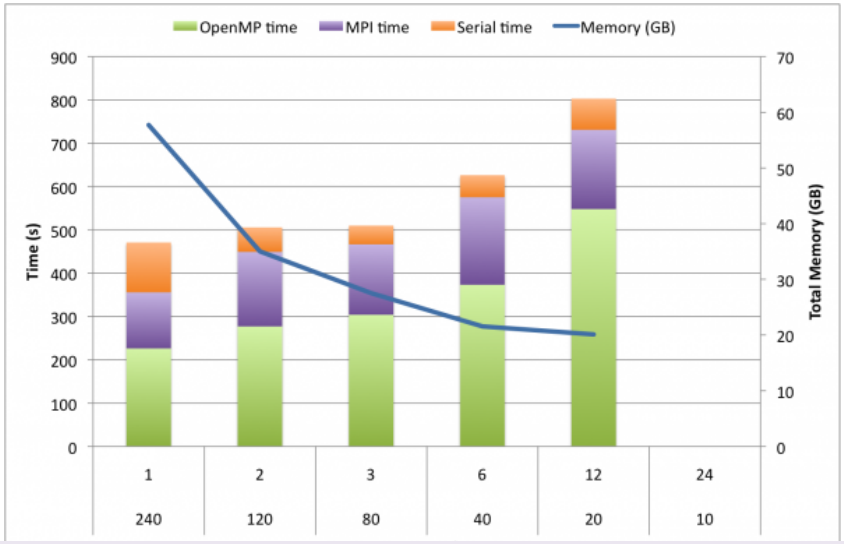
Courtesy of Mike Stewart

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

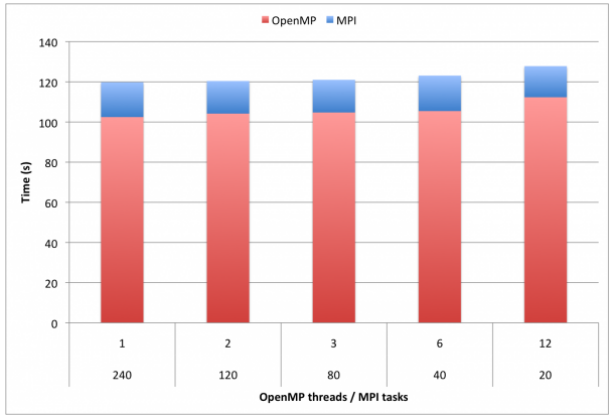
- **Reduced memory footprint with increased OpenMP threads.**
- **Hybrid MPI/OpenMP can be faster or comparable to pure MPI.**
- **Try different compilers.**
- **Sweet spot: BT: 1-3 threads; LU: 6 threads.**

Hybrid MPI/OpenMP fvCAM

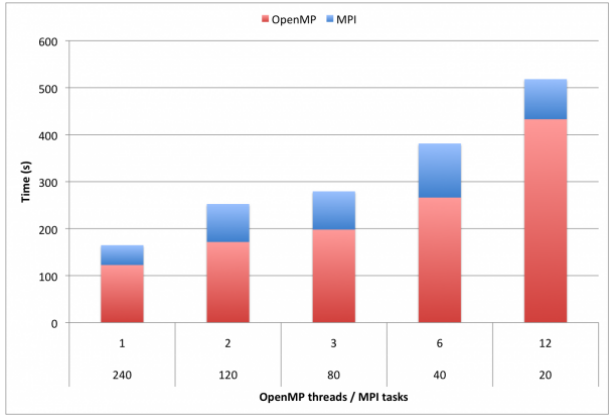
Total



"Physics" Component



"Dynamics" Component

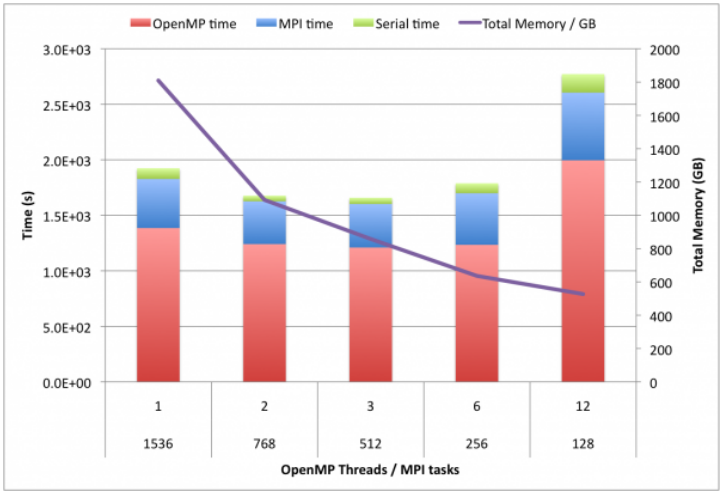


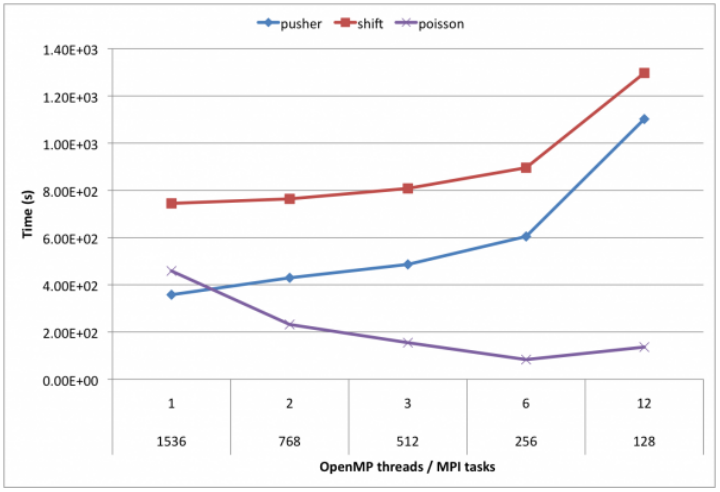
Community Atmospheric Model:

- **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"

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.
- Could use MPI inside parallel region with thread-safe MPI.

Why Mixed OpenMP/MPI Code is Sometimes Slower?

- OpenMP has less scalability due to implicit parallelism while MPI allows multi-dimensional blocking.
- 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. Less MPI tasks may not saturate inter-node bandwidth.
- Adjust 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.
- 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
############################
```

PGAS Languages

- Partitioned Global Address Space (PGAS):
  - Any process/thread/image can read/write any memory
  - UPC (C), CAF (Fortran), Titanium (Java),
  - Chapel (Cray), X10 (IBM), Fortress (Sun)
- PGAS languages attempts to combine the benefits of distributed memory and shared memory languages.
  - SPMD like parallelism (work sharing similar to MPI): good performance
    - UPC, CAF, Titanium
  - Global address space (data access similar to OpenMP, but with locality control): simple programming
- Good for latency hiding and memory bandwidth optimization.

UPC

- UPC (Unified Parallel C) is an extension of C.
- Each process is called a thread in UPC.
- Each thread has its local data, and can access shared data
- Total number of threads and thread index intrinsic:
  - #include <upc.h>
  - numprocs = THREADS;
  - myrank = MYTHREAD;
- Synchronization: upc_barrier
- Work sharing: upc_forall
- Pointers, collectives, …

Example Codes

- To obtain example codes and sample batch scripts:
  - % module load training
  - % cd $EXAMPLES/NUG2012
  - check sample codes in subdirectories:
    - hybrid, UPC, CAF, parallel_jacobi

Compile and Run UPC on Hopper (1)

hello_upc.c:

```
#include <upc.h>
#include <stdio.h>
int main(int argc, char** argv)
{
  if (MYTHREAD == 0) printf("hello world\n");
  printf("I am thread number %d of %d threads\n",
MYTHREAD, THREADS);
  return 0;
}
```

hello_upc.pbs:

```
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=10:00
#PBS –j oe

cd $PBS_O_WORKDIR

module swap PrgEnv-pgi PrgEnv-cray
cc –h upc -o hello_upc hello_upc.c

aprun -n 48 ./hello_upc
```

Cray compiler has the support for UPC:

```
% module swap PrgEnv-pgi PrgEnv-cray
% cc –h upc –o hello_upc hello_upc.c
% qsub hello_upc.c
```

Sample Output: (no specific order)

```
hello world
I am thread number 5 of 24 threads
I am thread number 7 of 24 threads
I am thread number 14 of 24 threads
I am thread number 21 of 24 threads
…
```

Compile and Run UPC on Hopper (2)

data_upc.c:

```
#include <upc.h>
#include <stdio.h>
shared int data[THREADS];
int main(int argc, char** argv)
{
  int i;
  if (MYTHREAD == 0) {
    for (i = 0; i < THREADS; i++)
      data[i] = i+1000;
    }
  upc_barrier;
  …
  printf("data on thread %d is %d\n", MYTHREAD,
data[MYTHREAD]);
}
```

Berkeley "bupc" module supports UPC in other compilers too (use PGI as example):

```
% module load bupc
% upcc –o data_upc data_upc.c
% qsub data_upc.pbs
```

data_bupc.pbs:

```
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=10:00

cd $PBS_O_WORKDIR

module load bupc
upcc -o data_bupc data_upc.c

upcrun -n 48 ./data_bupc
```

Sample Output: (no specific order)

```
data on thread 1 is 1001
data on thread 4 is 1004
data on thread 0 is 1000
data on thread 2 is 1002
data on thread 22 is 1022
…
```

Coarray Fortran

- New feature in Fortran 2008 standard.
- Variables are declared as coarrays.
- Each process is called an image.
- Coarrays are accessible by remote images using array subscripts in square brackets
  - A(:) = B(:)[image]
- Total number of images and image index intrinsic:
  - numimages = num_images()
  - myimage = this_image()
- Synchronization: sync all, sync images

Compile and Run CAF on Hopper

data_caf.f90:

```
program data_caf
implicit none
integer :: data(10)[*], i
if (THIS_IMAGE() == 1) then
  do i = 1, NUM_IMAGES()
  data(:)[i]=i+1000
  enddo
endif
sync all
…
write (*,*) 'data on image', THIS_IMAGE(), 'is', data
end program data_caf
```

Only Cray compiler has the support for CAF:

```
% module swap PrgEnv-pgi PrgEnv-cray
% ftn –h caf –o data_caf data_caf.f90
% qsub data_caf.pbs
```

data_caf.pbs:

```
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=10:00

cd $PBS_O_WORKDIR

module swap PrgEnv-pgi PrgEnv-cray
ftn -h caf -o data_caf data_caf.f90

aprun -n 48 ./data_caf
```

Sample Output: (no specific order)

```
data on image 2 is 10*1002
data on image 4 is 10*1004
data on image 7 is 10*1007
data on image 14 is 10*1014
data on image 5 is 10*1005
…
```

PGAS Additional Considerations

- UPC and CAF only supported on Hopper, not on Carver.
- Recommend to link with –lhugetlbfs to map the static data section and private heap onto huge pages.
- For UPC, using PrgEnv-cray is recommended over bupc for general users, due to its simplicity.
- Use the "-e m" compile option for CAF if the Fortran 90 module files are needed.
- Coarrays in CAF are stored on the symmetric heap. The default value for the env XT_SYMMETRIC_HEAP_SIZE is 32M. This value needs to be increased for larger problems.

MPI + PGAS? PGAS + OpenMP?

- Can have hybrid MPI with CAF or UPC.
  - MPI, CAF, and UPC sections can not be interleaved due to the same lower level libraries being used.
- Can also mix CAF with OpenMP.
- $EXAMPLES/parallel_jacobi directory has various versions of the parallel Jacobi solver:
  - serial, pure MPI, pure OpenMP
  - pure UPC, pure CAF
  - hybrid MPI/OpenMP, hybrid CAF/OpenMP

Conclusions

- Flat MPI is still the dominant parallel programming model today.
- Hybrid MPI/OpenMP is suited for the multi-core architecture trend. Hopper is an example.
- 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.
- NERSC recommends to use 2 to 6 OpenMP threads per node on Hopper.
- New emerging programming models are being explored: UPC, CAF. Mixing these with MPI or OpenMP is also possible.

Further References

- MPI: http://www.mcs.anl.gov/research/projects/mpi/
- OpenMP: http://openmp.org
- Using Hybrid/OpenMP on NERSC Cray XT: 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 PGAS Language Codes (UPC, CoArray Fortran) on Hopper: https://www.nersc.gov/users/computational-systems/hopper/programming/PGAS/
- NERSC Hopper and Carver web pages: https://www.nersc.gov/users/computational-systems/hopper https://www.nersc.gov/users/computational-systems/carver
- CAF: http://www.co-array.org
- UPC: http://upc.gwu.edu