HPC and Data Science Summer Institute

Title: Parallel Computing Using MPI and OpenMP

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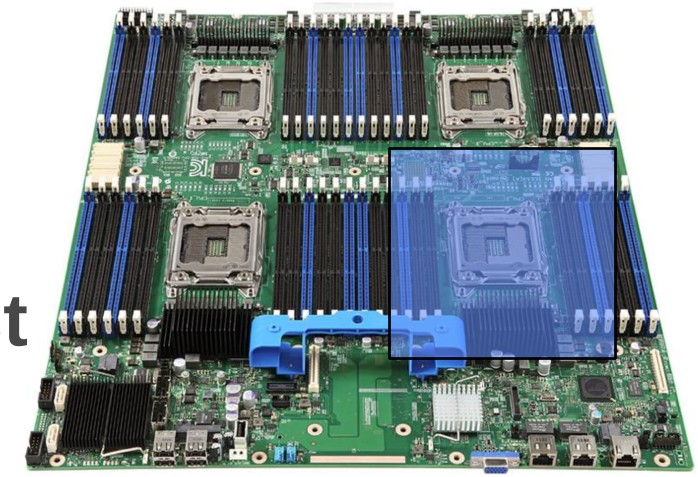
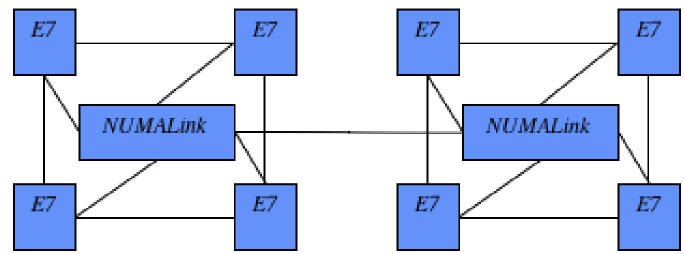
SDSC SAN DIEGO SUPERCOMPUTER CENTER

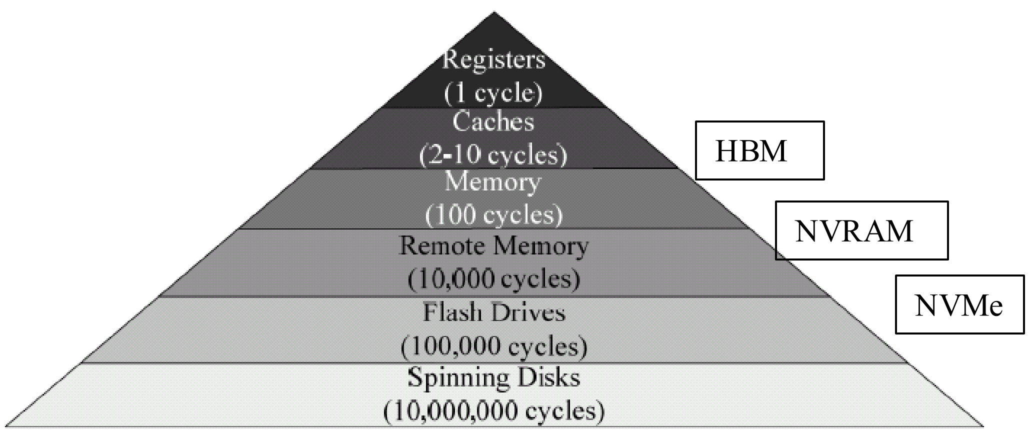
UC San Diego

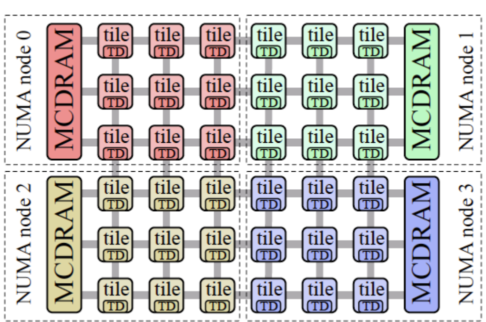
Current Supercomputer Architectures

- **Multi-socket server nodes**
  - NUMA
  - Accelerators
- **High performance interconnect**
  - e.g. InfiniBand
- ***Scalable parallel approach needed to achieve performance***



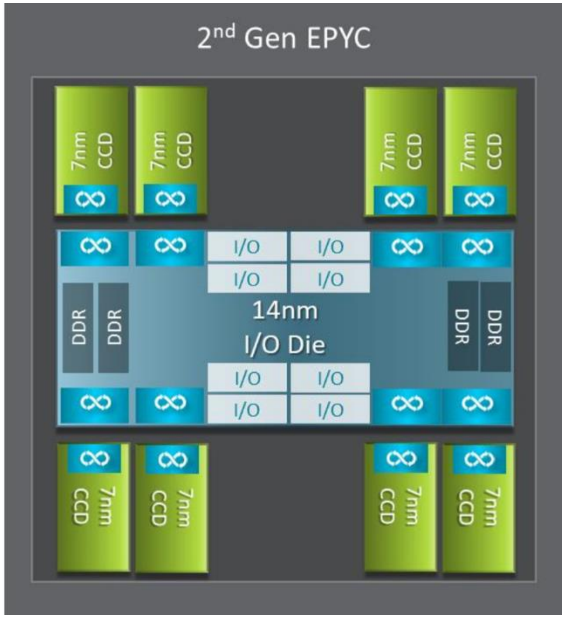






AMD EPYC 7742 Processor Architecture

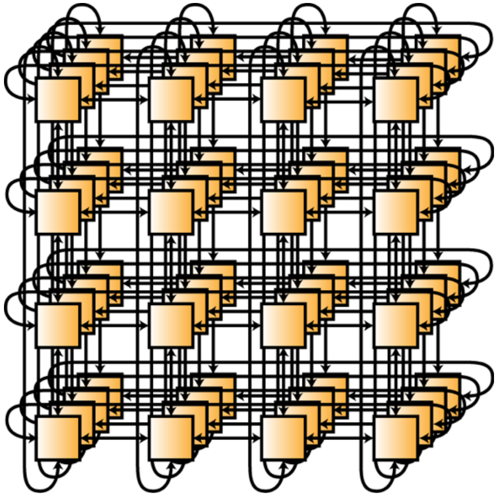
- 8 Core Complex Dies (CCDs).
- CCDs connect to memory, I/O, and each other through the I/O Die.
- 8 memory channels per socket.
- DDR4 memory at 3200MHz.
- PCI Gen4, up to 128 lanes of high speed I/O.
- Memory and I/O can be abstracted into separate quadrants each with 2 DIMM channels and 32 I/O lanes.

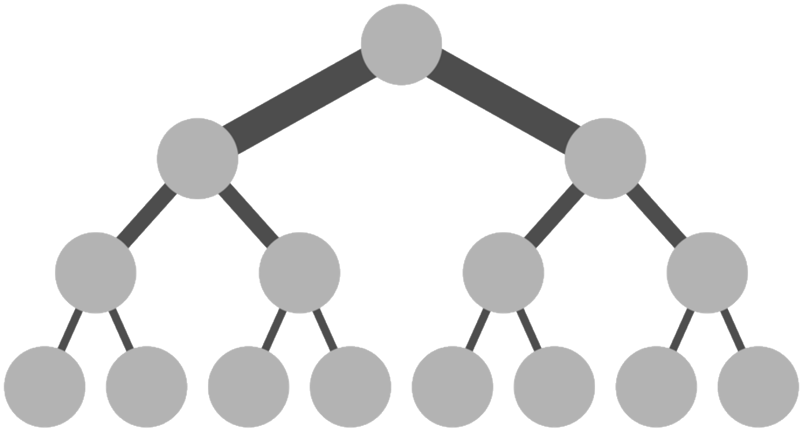


Reference: https://developer.amd.com/wp-content/resources/56827-1-0.pdf

Network Topologies

- **Mesh, Torus, Hypercube**
- **Tree based**
  - Fat-tree
  - Clos
- **Dragonfly**
- **Metrics**
  - Bandwidth
  - Diameter, Connectivity
  - Bisection bandwidth





Parallel Computing

- **Executing instructions concurrently on physical resources (not time slicing)**
  - Multiple tightly coupled resources (e.g. cores) collaboratively solving a single problem
- **Benefits**
  - Capacity
    - Memory, storage
  - Performance
    - More instructions per unit of time (FLOPS)
    - Data streaming capability
- **Cost and Complexity**
  - Coordinate tasks and resources
  - Use resources efficiently

Memory, Communication, and Execution Models

- **Shared**
  - Communication model: shared memory
- **Distributed**
  - Communication model: exchange messages
- **Execution Models**
  - Fork-Join (e.g. Thread Level Parallelism)
  - Single Program Multiple Data (SPMD)
- **Parallelism enabled by decomposing work**
  - Tasks can be executed concurrently
  - Some tasks can have dependencies

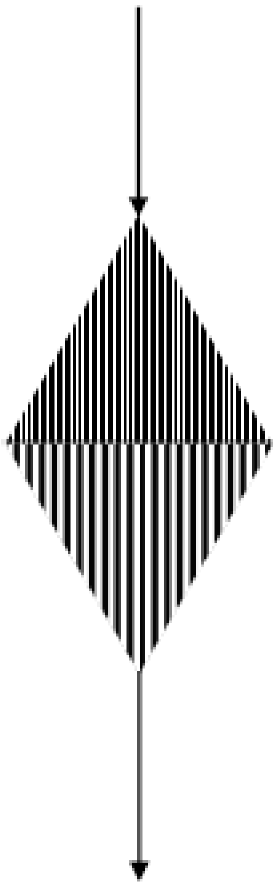
What is OpenMP?

- **High level parallelism abstraction based on thread**
  - Easy to use
  - Suitable to an incremental approach
- **A specification and evolving standard**
  - “a portable, scalable model … for developing portable parallel programs”
  - http://openmp.org
  - GNU, Intel, PGI, etc.
- **A set of**
  - Compiler directives
  - Library routines
  - Environment variables
  - Supports C/C++ and Fortran

```
#pragma omp parallel
{
  ....
}
```

OpenMP Models

- **Fork/Join Execution**
  - Process starts single threaded (master thread)
  - Forks child threads activated in parallel regions (team)
  - The team synchronizes and threads are disbanded
    - – barrier
  - Overhead is mitigated by reusing threads
  - Master thread continues execution of serial phases
- **Work decomposition**
  - Programming constructs
  - Scope and compound statements
  - Declarative in loops
  - Mapping to threads can be static or dynamic
  - Barriers and synchronization automatically inserted



Compiler Directives

- **Compiler directives is the main mechanism for introducing parallelism. Functionality enabled includes:**
  - Spawning a parallel region
  - Diving code among threads
  - Distributing loop iterations over threads
  - Serialization of parts of the code
  - Synchronization of work
- **Example:**

```
#pragma omp parallel default(shared) private(beta,pi)
```

Regions, Loops, Sections etc

#pragma omp parallel *[clause[[,]clause] ...] new-line*
structured-block
clause:
if(*scalar-expression*)
num_threads(*integer-expression*)
default(**shared** | **none**)
private(*list*)
firstprivate(*list*)
shared(*list*)
copyin(*list*)
reduction(*operator*: *list*)

#pragma omp for *[clause[[,] clause] ...] new-line for-loops*
clause:
private(*list*)
firstprivate(*list*)
lastprivate(*list*)
reduction(*operator*: *list*)
schedule(*kind[, chunk_size]*)
collapse(*n*)
ordered
nowait

#pragma omp sections *[clause[[,] clause] ...] new-line*
{
#pragma omp section
structured-block
...
}
clause:
private(*list*)
firstprivate(*list*)
lastprivate(*list*)
reduction(*operator*: *list*)
nowait

- #pragma omp single/master
- simd
- tasks

Scope of Variables

- **Clauses determine the scope of variables**
  - Default: shared (external)
  - Private
    - Also, if declared inside region
  - firstprivate
  - shared
  - lastprivate
  - reductions
  - default
  - ….
- **Avoid race conditions!**

Data Scope Attribute Clauses

- **PRIVATE – variables in the list are private to each thread.**
- **SHARED – variables in the list are shared between all threads.**
- **DEFAULT – default scope for all variables in a parallel region.**
- **FIRSTPRIVATE – variables are private and initialized according to value prior to entry into parallel or work sharing construct.**
- **LASTPRIVATE – variables are private, the value from the last iteration or section is copied to original variable object.**
- **Others – COPYIN, COPYPRIVATE**
- **REDUCTION – reduction on variables in the list**

Parallel Region Construct

```
!$OMP PARALLEL [clause ...]
          IF (scalar_logical_expression)
          PRIVATE (list)
          SHARED (list)
          DEFAULT (PRIVATE | FIRSTPRIVATE | SHARED | NONE)
          FIRSTPRIVATE (list)
          REDUCTION (operator: list)
          COPYIN (list)
          NUM_THREADS (scalar-integer-expression)

   code block
!$OMP END PARALLEL
```

Number of Threads

- **Number of threads will be determined in the following order of precedence:**
  - Evaluation of the IF clause
  - Setting of NUM_THREADS clause
  - omp_set_num_threads() library function
  - OMP_NUM_THREADS environment variable
  - Default – usually ends up being the ***number of cores on the node*** (!)

- **The last factor can accidentally lead to oversubscription of nodes in hybrid MPI/OpenMP codes.**

Work – Sharing Constructs

Directive format (C version):

```
#pragma omp for [clause ...]  newline
            schedule (type [,chunk])
            ordered
            private (list)
            firstprivate (list)
            lastprivate (list)
            shared (list)
            reduction (operator: list)
            collapse (n)
            nowait

  for_loop
```

Work-Sharing

- **Schedule:**
  - Static – Loop iterations are statically divided (chunk or as close to even as possible)
  - Dynamic – Loop iterations are divided in size chunk, and dynamically scheduled among threads. When a thread finishes one chunk it is dynamically assigned another
  - Guided – Similar to dynamic but chunk size is proportionally reduced based on work remaining.
  - Runtime – set at runtime by environment variables
  - Auto – set by compiler or runtime system.

Copy the Examples Directory

cp -r /cm/shared/examples/sdsc/si/2024/PARALLEL $HOME/

Verify:

ls $HOME/PARALLEL

```
[train106@login01 ~]$ cp -r /cm/shared/examples/sdsc/si/2023/PARALLEL $HOME/

[train106@login01 ~]$
[train106@login01 ~]$ ls $HOME/PARALLEL
COLLECTIVES  DOMAIN  MISC  OPENMP  PTOP  run_commands.txt  SIMPLE
[train106@login01 ~]$
```

Simple OpenMP Program – Compute PI

- Find the number of tasks and taskids (omp_get_num_threads, omp_get_thread_num)
- PI is calculated using an integral. The number of intervals used for the integration is fixed at 128000.
- Use OpenMP loop parallelization to divide up the compute work.
- Introduce concept of private and shared variables.
- OpenMP reduction operation used to compute the sum for the final integral.
- Today's OpenMP examples are in: **$HOME/PARALLEL/OPENMP**
- If you don't see the directory, you can copy it from:
  /cm/shared/examples/sdsc/si/2024/PARALLEL

OpenMP Program to Compute PI

```
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
int main (int argc, char *argv[])
{
int nthreads, tid;
int i, INTERVALS;
double n_1, x, pi = 0.0;

INTERVALS=128000;
/* Fork a team of threads giving them their own
     copies of variables */
#pragma omp parallel private(nthreads, tid)
  {
  /* Obtain thread number */
  tid = omp_get_thread_num();
  printf("Hello from thread = %d\n", tid);

 /* Only master thread does this */
  if (tid == 0)
    {
    nthreads = omp_get_num_threads();
    printf("Number of threads = %d\n", nthreads);
    }

  }  /* All threads join master thread and disband */

  n_1 = 1.0 / (double)INTERVALS;

/* Parallel loop with reduction for calculating PI */
#pragma omp parallel for private(i,x)
shared(n_1,INTERVALS) reduction(+:pi)
  for (i = 0; i < INTERVALS; i++)
    {
    x = n_1 * ((double)i  + 0.5);
    pi += 4.0 / (1.0 + x * x);
    }
    pi *= n_1;
    printf ("Pi = %.12lf\n", pi);
}
```

OpenMP result: 1-D Heat Equation

Compile:

module reset

module load gcc/10.2.0

gcc -fopenmp -o pi_openmp pi_openmp.c

Submit: sbatch --res=si24 pi_openmp.sb

```
[mahidhar@login02 OPENMP]$ more pi.24508633.exp-1-11.out
Resetting modules to system default. Reseting $MODULEPATH back to system default. All extra directories will be removed
from $MODULEPATH.
Hello from thread = 15
Hello from thread = 14
Hello from thread = 13
Hello from thread = 6
Hello from thread = 1
Hello from thread = 11
Hello from thread = 3
Hello from thread = 0
Hello from thread = 2
Number of threads = 16
Hello from thread = 8
Hello from thread = 4
Hello from thread = 5
Hello from thread = 10
Hello from thread = 7
Hello from thread = 9
Hello from thread = 12
Pi = 3.141592653595
```

More Work-Share Constructs

- **SECTIONS** directive – enclosed sections are divided among the threads.

- **WORKSHARE** directive – divides execution of block into units of work, each of which is executed once.

- **SINGLE** directive – Enclosed code is executed by only one thread.

Synchronization Constructs

- **MASTER** directive – Specifies region is executed only by the master thread.
- **CRITICAL** directive – Region of the code that is executed one thread at a time.
- **BARRIER** directive – synchronize all threads
- **TASKWAIT** directive – wait for all child tasks to complete
- **ATOMIC** directive – specific memory location updated atomically (not let all threads write at the same time)

Simple Application using OpenMP: 1-D Heat Equation

- $\partial T/\partial t = \alpha(\partial^2 T/\partial x^2)$; $T(0) = 0$; $T(1) = 0$; $(0 \leq x \leq 1)$
  $T(x,0)$ is know as an initial condition.

- Discretizing for numerical solution we get:
  $T^{(n+1)}_i - T^{(n)}_i = (\alpha\Delta t/\Delta x^2)(T^{(n)}_{i-1} - 2T^{(n)}_i + T^{(n)}_{i+1})$
  (*n* is the index in time and *i* is the index in space)

Fortran OpenMP Code: 1-D Heat Equation

```
PROGRAM HEATEQN
   implicit none
   integer :: iglobal, itime, nthreads
   real*8 :: xalp,delx,delt,pi
   real*8 :: T(0:100,0:10)
   integer:: id
   integer:: OMP_GET_THREAD_NUM,
     OMP_GET_NUM_THREADS

!$OMP PARALLEL SHARED(nthreads)
!$OMP MASTER
   nthreads = omp_get_num_threads()
   write (*,*) 'There are', nthreads, 'threads'
!$OMP END MASTER
!$OMP END PARALLEL
   if (nthreads.ne.3) then
     write(*,*)"Use exactly 3 threads for this case"
     stop
   endif
   delx = 0.1d0
   delt = 1d-4
   xalp = 2.0d0
```

```
************* Initial Conditions
*****************************
   pi = 4d0*datan(1d0)
   do iglobal = 0, 10
     T(0,iglobal) = dsin(pi*delx*dfloat(iglobal))
   enddo
************* Iterations
***********************************
   do itime = 1 , 3
    write(*,*)"Running Iteration Number ", itime
!$OMP PARALLEL DO PRIVATE(iglobal)
SHARED(T,xalp,delx,delt,itime)
    do iglobal = 1, 9
     T(itime,iglobal)=T(itime-1,iglobal)+
  +  xalp*delt/delx/delx*
  +  (T(itime-1,iglobal-1)-2*T(itime-1,iglobal)+T(itime-
1,iglobal+1))
    enddo
!$OMP BARRIER
   enddo
   do iglobal = 0, 10
     write(*,*)iglobal,T(3, iglobal)
   enddo
   END
```

OpenMP result: 1-D Heat Equation

Compile:

module reset

module load gcc/10.2.0

gfortran -fopenmp -ffixed-form -o heat_openmp heat_openmp.f90

Submit: sbatch --res=si24 heat_openmp.sb

```
[mahidhar@login02 OPENMP]$ more heat.24508716.exp-1-11.out
Resetting modules to system default. Reseting $MODULEPATH back to system default. All extra directories will be removed
from $MODULEPATH.
 There are           3 threads
 Running Iteration Number           1
 Running Iteration Number           2
 Running Iteration Number           3
           0   0.0000000000000000
           1  0.30720562101728494
           2  0.58433981542197655
           3  0.80427475735827125
           4  0.94548168233259799
           5  0.99413827268197230
           6  0.94548168233259799
           7  0.80427475735827125
           8  0.58433981542197666
           9  0.30720562101728505
          10   1.1588922802093023E-310
```

Run Time Library Routines

- Setting and querying number of threads
- Querying thread identifier, team size
- Setting and querying dynamic threads feature
- Querying if in parallel region and at what level
- Setting and querying nested parallelism
- Setting, initializing and terminating locks, nested locks.
- Querying wall clock time and resolution.

Environment Variables

- OMP_SCHEDULE – e.g set to “dynamic”
- OMP_NUM_THREADS
- OMP_DYNAMIC (TRUE or FALSE)
- OMP_PROC_BIND (TRUE or FALSE)
- OMP_NESTED (TRUE of FALSE)
- OMP_STACKSIZE – size of stack for created threads
- OMP_THREAD_LIMIT

General OpenMP Performance Considerations

- Avoid or minimize use of BARRIER, CRITICAL (complete serialization here!), ORDERED regions, and locks. Can use NOWAIT clause to avoid redundant barriers.

- Parallelize at a high level, i.e. maximize the work in the parallel regions to reduce parallelization overhead.

- Use appropriate loop scheduling – static has low synchronization overhead but can be unbalanced, dynamic (and guided) have higher synchronization overheads but can improve load balancing.

- Avoid false sharing (more about it in following slide)!

What is False Sharing?

- Most modern processors have a cache buffer between slow memory and high-speed registers of the CPU.
- Accessing a memory location causes a “cache line” to be copied into the cache.
- In an OpenMP code two processors may be accessing two different elements in the same cache line. On writes this will lead to “cache line” being marked invalid (because cache coherency is being maintained).
- This will lead to an increase in memory traffic even though the write is to different elements (hence the term false sharing).
- This can have a drastic performance impact if such updates are occurring frequently in a loop.

Detailed info:

https://www.youtube.com/watch?v=CMJXvTF-gJk

False Sharing Example

Code snippet:

```
double global=0.0, local[NUM_THREADS];
#pragma omp parallel num_threads(NUM_THREADS)
{
 int tid = omp_get_thread_num();
 local[tid] = 0.0;
 #pragma omp for
 for (i = 0; i < N; i++)
 local[tid] += x[i];
 #pragma omp atomic
 global += local[me];
}
```

False Sharing - Solutions

- **Three options**
  - Compiler directives to align individual variables on cache line boundaries

```
__declspec (align(64)) int thread1_global_variable;
__declspec (align(64)) int thread2_global_variable;
```

  - Pad arrays/data structures to make sure array elements begin on cache line boundary.

  - Use thread local copies of data (assuming the copy overhead is small compared to overall run time).

Homework!

- **Download matrix multiply example from LLNL site:**
  - https://hpc-tutorials.llnl.gov/openmp/code_examples/Fortran/omp_mm.f
  - Download using wget on Expanse:

```
wget https://hpc-tutorials.llnl.gov/openmp/code_examples/Fortran/omp_mm.f
```

- **Compile (gfortran -std=legacy -fopenmp omp_mm.f) and run the example. See if you can vary the environmental variables, scheduling to get better performance!**

- **This is very quick intro. Lot of ongoing developments. Detailed specifications at:**
  - https://www.openmp.org/specifications/

Message Passing Interface (MPI)

- **Low level message passing abstraction**
  - SPMD execution model + messages
  - Designed for distributed memory. Implemented on hybrid distributed memory/shared memory systems.
- **MPI: API specification**
  - Portable: de-fact standard for parallel computing, portable, system specific optimizations without changing code interface
  - http://www.mpi-forum.org
  - Several implementations - e.g MVAPICH2, Intel MPI, and OpenMPI – *all 3 are available on Expanse*
  - High performance implementations available virtually on any interconnect and system
  - Point-to-point communication, datatypes, collective operations
  - One-sided communication, Parallel file I/O, Tool support, …

Typical MPI Code Structure

MPI Include File

Variable declarations, etc

Begin Program

…

Serial code

….

MPI Initialization

Parallel Code begins

MPI Rank (process identification)

…

Parallel code based on rank

…

MPI Communications between processes

…

Parallel code based on rank

…

MPI Communications between processes

MPI Finalize (terminate)

Parallel Code ends

Serial Code

Simple MPI Program – Compute PI

- **Initialize MPI (MPI_Init function)**

- **Find the number of tasks and taskids (MPI_Comm_size, MPI_Comm_rank)**

- **PI is calculated using an integral. The number of intervals used for the integration is fixed at 128000.**

- **Computes the sums for a different sections of the intervals in each MPI task.**

- **At the end of the code, the sums from all the tasks are added together to evaluate the final integral. This is accomplished through a reduction operation (MPI_Reduce function).**

- **Simple code illustrates decomposition of problem into parallel components.**

MPI Program to Compute PI

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char *argv[])
  {
  int numprocs, rank;
  int i, iglob, INTERVALS, INTLOC;
  double n_1, x;
  double pi, piloc;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,
      &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  INTERVALS=128000;
  printf("Hello from MPI task= %d\n", rank);
  MPI_Barrier(MPI_COMM_WORLD);
  if (rank == 0)
    {
printf("Number of MPI tasks = %d\n", numprocs);
   }

 INTLOC=INTERVALS/numprocs;
 piloc=0.0;
 n_1=1.0/(double)INTERVALS;
 for (i = 0; i < INTLOC; i++)
   {
   iglob = INTLOC*rank+i;
   x = n_1 * ((double)iglob  - 0.5);
   piloc += 4.0 / (1.0 + x * x);
   }

MPI_Reduce(&piloc,&pi,1,MPI_DOUBLE,MPI_SUM,0,
MPI_COMM_WORLD);
 if (rank == 0)
   {
   pi *= n_1;
   printf ("Pi = %.12lf\n", pi);
   }

 MPI_Finalize();
 }
```

PI Code : MPI Environment Functions

MPI_Init(&argc, &argv);

Initializes MPI, *must* be called (only once) in every MPI program before any MPI functions.

MPI_Comm_size(MPI_COMM_WORLD, &numprocs);

Returns the total number of tasks in the communicator. MPI uses communicators to define which collections of processes can communicate with each other. The default MPI_COMM_WORLD includes all the processes. User defined communicators are an option.

MPI_Comm_rank(MPI_COMM_WORLD, &rank);

Returns the rank (ID) of the calling MPI process within the communicator.

MPI_Finalize();

Ends the MPI execution environment. No MPI calls after this.!

The other routines in the code are collectives and we will discuss them later in the talk.

Compiling and Running PI Example

cd $HOME/PARALLEL/SIMPLE

Modules: module reset; module load gcc/10.2.0 mvapich2/2.3.7

Compile: mpicc -o pi_mpi.exe pi_mpi.c

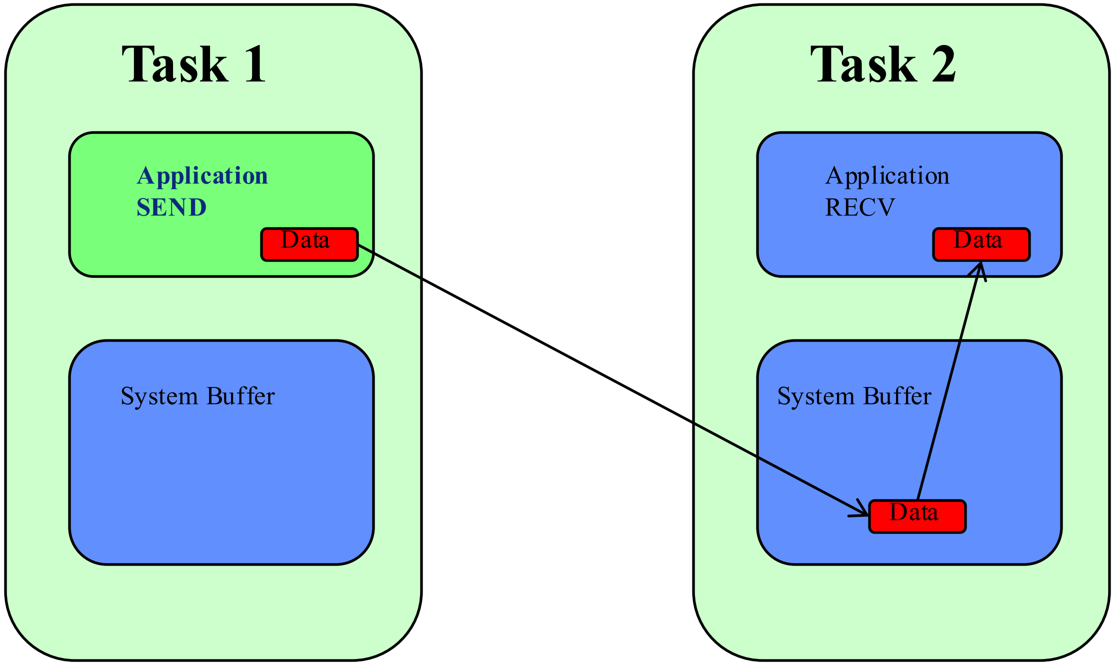
Submit Job: sbatch --res=si24 pi_mpi.sb

```
[mahidhar@login02 SIMPLE]$ more pi_mpi.24508779.exp-1-11.out
Resetting modules to system default. Reseting $MODULEPATH back to system default. All extra directories will be removed
from $MODULEPATH.
Hello from MPI task= 13
Hello from MPI task= 14
Hello from MPI task= 15
Hello from MPI task= 12
Hello from MPI task= 3
Hello from MPI task= 1
Hello from MPI task= 2
Hello from MPI task= 4
Hello from MPI task= 5
Hello from MPI task= 6
Hello from MPI task= 7
Hello from MPI task= 8
Hello from MPI task= 9
Hello from MPI task= 10
Hello from MPI task= 11
Hello from MPI task= 0
Number of MPI tasks = 16
Pi = 3.141592653590
```

Point to Point Communication

- Passing data between two, and only two different MPI tasks.
- Typically one task performs a send operation and the other task performs a matching receive.
- MPI Send operations have choices with different synchronization (when does a send complete) and different buffering (where the data resides till it is received) modes.
- Any type of send routine can be paired with any type of receive routine.
- MPI also provides routines to probe status of messages, and "wait" routines.

Buffers



- Buffer space is used for data in transit – whether its waiting for a receive to be ready or if there are multiple sends arriving at the same receiving tasks.
- Typically a system buffer area managed by the MPI library (opaque to the user) is used. Can exist on both sending & receiving side.
- MPI also provides for user managed send buffer.

Blocking MPI Send, Receive Routines

- Blocking send call will return once it is safe for the application buffer (send data) to be reused.

- This can happen as soon as the data is copied into the system (MPI) buffer on receiving process.

- Synchronous if there is confirmation of safe send, and asynchronous otherwise.

- Blocking receive returns once the data is in the application buffer (receive data) and can by used by the application.

Blocking Send, Recv Example (Code Snippet)

```
if(myid == 0) {
      for(i = 0; i < 10; i++) {
         s_buf[i] = i*4.0;
      }
      MPI_Send(s_buf, size, MPI_FLOAT, 1, tag, MPI_COMM_WORLD);
   }
   else if(myid == 1) {
      MPI_Recv(r_buf, size, MPI_FLOAT, 0, tag, MPI_COMM_WORLD,
&reqstat);
      for (i = 0; i < 10; i++ ){
        printf("r_buf[%d] = %f\n", i, r_buf[i] );
      }
   }
```

Break

Blocking Send, Recv Example

Location:$HOME/PARALLEL/PTOP

Compile: **mpicc -o blocking.exe blocking.c**

Submit Job: **sbatch --res=si24 blocking.sb**

Output:

```
r_buf[0] = 0.000000
r_buf[1] = 4.000000
r_buf[2] = 8.000000
r_buf[3] = 12.000000
r_buf[4] = 16.000000
r_buf[5] = 20.000000
r_buf[6] = 24.000000
r_buf[7] = 28.000000
r_buf[8] = 32.000000
r_buf[9] = 36.000000
```

Deadlocking MPI Tasks

- Take care to sequence blocking send/recvs. Easy to deadlock processes waiting on each other with circular dependencies.
- Can also occur with control errors and unexpected symantics
- For example, take the following code snippet:

```
if(myid == 0) {
      MPI_Ssend(s_buf, size, MPI_FLOAT, 1, tag1, MPI_COMM_WORLD);
      MPI_Recv(r_buf, size, MPI_FLOAT, 1, tag2, MPI_COMM_WORLD, &reqstat);
  }
  else if(myid == 1) {
      MPI_Ssend(s_buf, size, MPI_FLOAT, 0, tag2, MPI_COMM_WORLD);
      MPI_Recv(r_buf, size, MPI_FLOAT, 0, tag1, MPI_COMM_WORLD, &reqstat);
      for (i = 0; i < 10; i++ ){
        printf("r_buf[%d] = %f\n", i, r_buf[i] );
      }
```

- The MPI_Ssend on both tasks will not complete till the MPI_Recv is posted (which will never happen given the order).

Deadlock Example

- **Location: $HOME/PARALLEL/PTOP**
- **Compile: mpicc -o deadlock.exe deadlock.c**
- **Submit Job: sbatch --res=si24 deadlock.sb**
- **It should technically finish in less than a second since the data transferred is a few bytes. However, the code deadlocks and hits the wallclock limit (1 minute in the script).**

```
[mahidhar@login02 PTOP]$ more deadlock.24508842.exp-1-11.out
Resetting modules to system default. Reseting $MODULEPATH back to system default. All extra directories will be removed
from $MODULEPATH.
srun: Job step aborted: Waiting up to 32 seconds for job step to finish.
slurmstepd: error: *** STEP 24508842.0 ON exp-1-11 CANCELLED AT 2023-08-10T11:44:38 DUE TO TIME LIMIT ***
slurmstepd: error: *** JOB 24508842 ON exp-1-11 CANCELLED AT 2023-08-10T11:44:38 DUE TO TIME LIMIT ***
[mahidhar@login02 PTOP]$
```

Deadlock Example – Simple Fix

- Change the order on one of processes!
- For example, take the following code snippet:

```
 if(myid == 0) {
     MPI_Ssend(s_buf, size, MPI_FLOAT, 1, tag1, MPI_COMM_WORLD);
     MPI_Recv(r_buf, size, MPI_FLOAT, 1, tag2, MPI_COMM_WORLD, &reqstat);
   }
   else if(myid == 1) {
     MPI_Recv(r_buf, size, MPI_FLOAT, 0, tag1, MPI_COMM_WORLD, &reqstat);
     MPI_Ssend(s_buf, size, MPI_FLOAT, 0, tag2, MPI_COMM_WORLD);
     for (i = 0; i < 10; i++ ){
       printf("r_buf[%d] = %f\n", i, r_buf[i] );
     }
```

- Now the MPI_Ssend on task 0 will complete since the corresponding MPI_Recv is posted first on task 1. (qsub deadlock-fix1.cmd)
- We will look at **Non-Blocking** options next.

Deadlock Example (Fix 1)

- **Location: $HOME/PARALLEL/PTOP**
- **Compile: mpicc -o deadlock-fix1.exe deadlock-fix1.c**
- **Submit Job: sbatch --res=si24 deadlock-fix1.sb**
- **Fix works!**

```
$ more deadlock-fix1.out
r_buf[0] = 0.000000
r_buf[1] = 4.000000
r_buf[2] = 8.000000
r_buf[3] = 12.000000
r_buf[4] = 16.000000
r_buf[5] = 20.000000
r_buf[6] = 24.000000
r_buf[7] = 28.000000
r_buf[8] = 32.000000
r_buf[9] = 36.000000
```

Non-Blocking MPI Send, Receive Routines

- Non-Blocking MPI Send, Receive routines return before there is any confirmation of receives or completion of the actual message copying operation.
- The routines simply put in the request to perform the operation.
- MPI wait routines can be used to check status and block till the operation is complete and it is safe to modify/use the information in the application buffer.
- This non-blocking approaches allows computations (that don't depend on this data in transit) to continue while the communication operations are in progress. This allows for hiding the communication time with useful work and hence improves parallel efficiency.

Non-Blocking Send, Recv Example

- **Example uses MPI_Isend, MPI_Irecv, MPI_Wait**
- **Code snippet:**

```
if(myid == source){
        s_buf=1024;
        MPI_Isend(&s_buf,count,MPI_INT,destination,tag,MPI_COMM_WORLD,&request);
    }
    if(myid == destination {
        MPI_Irecv(&r_buf,count,MPI_INT,source,tag,MPI_COMM_WORLD,&request);
    }
    MPI_Wait(&request,&status);
```

- **Compile & Run:**

mpicc -o nonblocking.exe nonblocking.c

sbatch --res=si24 nonblocking.sb

Sample output:

processor 0 sent 1024

processor 1 got 1024

Deadlock Example – Non-Blocking Option

- Change the order on one of processes!
- For example, take the following code snippet:

```
if(myid == 0) {
    MPI_Isend(s_buf, size, MPI_FLOAT, 1, tag1, MPI_COMM_WORLD, &request);
    MPI_Recv(r_buf, size, MPI_FLOAT, 1, tag2, MPI_COMM_WORLD, &reqstat);
 }
 else if(myid == 1) {
    MPI_Ssend(s_buf, size, MPI_FLOAT, 0, tag2, MPI_COMM_WORLD);
    MPI_Recv(r_buf, size, MPI_FLOAT, 0, tag1, MPI_COMM_WORLD, &reqstat);
    for (i = 0; i < 10; i++ ){
      printf("r_buf[%d] = %f\n", i, r_buf[i] );
    }
```

- Now the MPI_Ssend on task 0 will complete since the corresponding MPI_Recv is posted first on task 1. (qsub deadlock-fix1.cmd)
- We will look at **Non-Blocking** options next.

Deadlock Example (Fix 2)

- **Location: $HOME/PARALLEL/PTOP**
- **Compile: mpicc -o deadlock-fix2-nb.exe deadlock-fix2-nb.c**
- **Submit Job: sbatch --res=si24 deadlock-fix2-nb.sb**
- **Fix works!**

```
$ more deadlock-fix2-nb.out
r_buf[0] = 0.000000
r_buf[1] = 4.000000
r_buf[2] = 8.000000
r_buf[3] = 12.000000
r_buf[4] = 16.000000
r_buf[5] = 20.000000
r_buf[6] = 24.000000
r_buf[7] = 28.000000
r_buf[8] = 32.000000
r_buf[9] = 36.000000
```

Collective MPI Routines

- Synchronization Routines: All processes in group/communicator wait till they get synchronized.
- Data Movement: Send/Receive data from all processes. E.g. Broadcast, Scatter, Gather, AlltoAll.
- Collective Computation (reductions): Perform reduction operations (min, max, add, multiply, etc.) on data obtained from all processes.
- Collective Computation and Data Movement combined (Hybrid).

Examples for Collectives

- **Location**

  $HOME/PARALLEL/COLLECTIVES

- **Switch compilers**

  module reset; module load intel/19.1.3.304; module load openmpi/4.1.3

Synchronization Example

- **Our simple PI program had a synchronization example.**
- **Code Snippet:**

```
printf("Hello from MPI task= %d\n", rank);
MPI_Barrier(MPI_COMM_WORLD);
if (rank == 0)
  {
  printf("Number of MPI tasks = %d\n", numprocs);
  }
```

- **All tasks will wait till they are synchronized at this point.**

Broadcast Example

- **Code Snippet** (**All collectives examples in $HOME/PARALLEL/COLLECTIVES**)**:**
  - if(myid .eq. source)then
  - do i=1,count
  - buffer(i)=i
  - enddo
  - endif
  - **Call MPI_Bcast(buffer, count, MPI_INTEGER,source,&**
  - **MPI_COMM_WORLD,ierr)**
- **Compile:**
  - **mpif90 -o bcast.exe bcast.f90**
- **Run:**
  - **sbatch --res=si24 bcast.sb**
- **Output:**

```
processor    1  got    1    2    3    4
processor    0  got    1    2    3    4
processor    2  got    1    2    3    4
processor    3  got    1    2    3    4
```

Reduction Example

- **Code Snippet:**

```
myidp1 = myid+1
call MPI_Reduce(myidp1,ifactorial,1,MPI_INTEGER,MPI_PROD,root,MPI_COMM_WORLD,ierr)
if (myid.eq.root) then
    write(*,*)numprocs,"! = ",ifactorial
endif
```

- **Compile:**

```
mpif90 -o factorial.exe factorial.f90
```

- **Run:**

```
sbatch --res=si24 factorial.sb
```

- **Output:**

```
8 ! =        40320
```

MPI_Allreduce example

- **Code Snippet:**

```
imaxloc=IRAND(myid)
call MPI_ALLREDUCE(imaxloc,imax,1,MPI_INTEGER,MPI_MAX,MPI_COMM_WORLD,
mpi_err)
if (imax.eq.imaxloc) then
    write(*,*)"Max=",imax,"on task",myid
endif
```

- **Compile:**

```
mpif90 -o allreduce.exe allreduce.f90
```

- **Run:**

```
sbatch --res=si24 allreduce.sb
```

- **Output:**

```
Max=     337897 on task          7
```

Data Types

C Data Types		FORTRAN Data Types
MPI_CHAR MPI_WCHAR MPI_SHORT MPI_INT MPI_LONG MPI_LONG_LONG_INT MPI_LONG_LONG MPI_SIGNED_CHAR MPI_UNSIGNED_CHAR MPI_UNSIGNED_SHORT MPI_UNSIGNED_LONG MPI_UNSIGNED MPI_FLOAT MPI_DOUBLE MPI_LONG_DOUBLE MPI_C_COMPLEX MPI_C_FLOAT_COMPLEX	MPI_C_DOUBLE_COMPLEX MPI_C_LONG_DOUBLE_COMPLEX MPI_C_BOOL MPI_LOGICAL MPI_C_LONG_DOUBLE_COMPLEX MPI_INT8_T MPI_INT16_T MPI_INT32_T MPI_INT64_T MPI_UINT8_T MPI_UINT16_T MPI_UINT32_T MPI_UINT64_T MPI_BYTE MPI_PACKED	MPI_CHARACTER MPI_INTEGER MPI_INTEGER1 MPI_INTEGER2 MPI_INTEGER4 MPI_REAL MPI_REAL2 MPI_REAL4 MPI_REAL8 MPI_DOUBLE_PRECISION MPI_COMPLEX MPI_DOUBLE_COMPLEX MPI_LOGICAL MPI_BYTE MPI_PACKED

MPI Reduction Operations

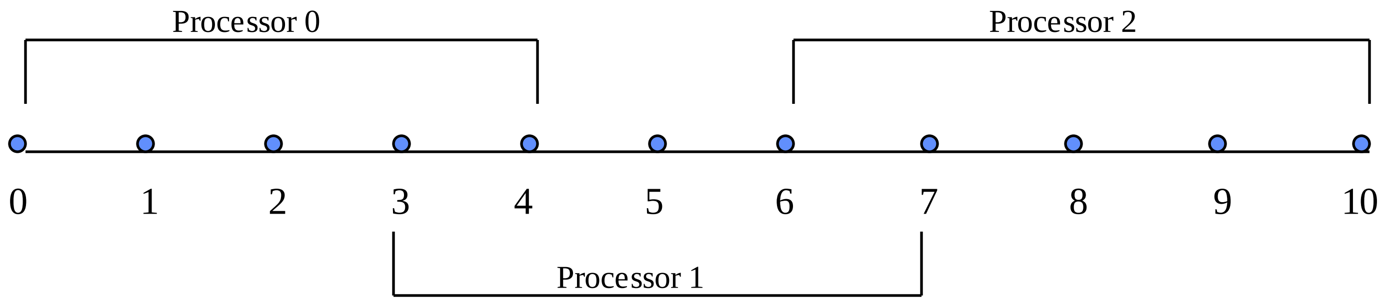
NAME	OPERATION
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical AND
MPI_BAND	Bit-wise AND
MPI_LOR	Logical OR
MPI_BOR	Bit-wise OR
MPI_LXOR	Logical XOR
MPI_BXOR	Bit-wise XOR
MPI_MAXLOC	Maximum value and location
MPI_MINLOC	Minimum value and location

Decomposition and Mapping

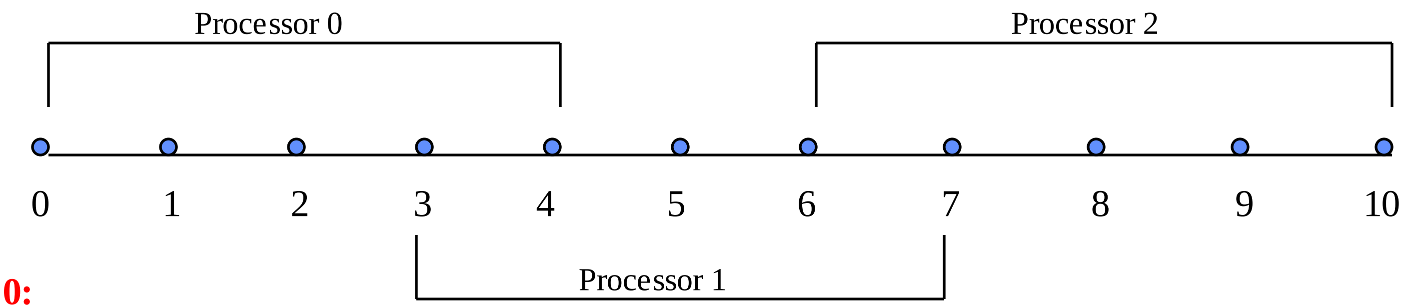
- **Data and work decomposition**
  - Map partitioned domain to processes
- **Mapping**
  - Processes/ranks topology
  - System/Domain/Data
- **How to share data?**
  - Exchange messages and replicate data
- **Load imbalance**
  - What if the system is not regular?
  - Is work proportional to size of partitions?

Simple Application using MPI: 1-D Heat Equation

- $\partial T/\partial t = \alpha(\partial^2 T/\partial x^2)$; $T(0) = 0$; $T(1) = 0$; $(0 \leq x \leq 1)$
  $T(x,0)$ is know as an initial condition.
- Discretizing for numerical solution we get:
  $T^{(n+1)}_i - T^{(n)}_i = (\alpha\Delta t/\Delta x^2)(T^{(n)}_{i-1} - 2T^{(n)}_i + T^{(n)}_{i+1})$
  (*n* is the index in time and *i* is the index in space)
- In this example we solve the problem using 11 points and we distribute this problem over exactly 3 processors (for easy demo) shown graphically below:



Simple Application using MPI: 1-D Heat Equation



Processor 0:

Local Data Index : ilocal = 0 , 1, 2, 3, 4

Global Data Index: iglobal = 0, 1, 2, 3, 4

Solve the equation at (1,2,3)

Data Exchange: Get 4 from processor 1; Send 3 to processor 1

Processor 1:

Local Data Index : ilocal = 0, 1, 2, 3, 4

Global Data Index : iglobal = 3, 4, 5, 6, 7

Solve the equation at (4,5,6)

Data Exchange: Get 3 from processor 0; Get 7 from processor 2; Send 4 to processor 0; Send 6 to processor 2

Processor 2:

Local Data Index : ilocal = 0, 1, 2, 3, 4

Global Data Index : iglobal = 6, 7, 8, 9, 10

Solve the equation at (7,8,9)

Data Exchange: Get 6 from processor 1; Send 7 to processor 1

FORTRAN MPI CODE: 1-D Heat Equation

```
 PROGRAM HEATEQN
   implicit none
   include "mpif.h"
   integer :: iglobal, ilocal, itime
   integer :: ierr, nnodes, my_id
   integer :: dest, from, status(MPI_STATUS_SIZE),tag
   integer :: msg_size
   real*8 :: xalp,delx,delt,pi
   real*8 :: T(0:100,0:5), TG(0:10)
   CHARACTER(20) :: FILEN

   delx = 0.1d0
   delt = 1d-4
   xalp = 2.0d0

   call MPI_INIT(ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD,
nnodes, ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD,
my_id, ierr)

   if (nnodes.ne.3) then
     if (my_id.eq.0) then
      print *, "This test needs exactly 3 tasks"
     endif
```

```
 print *, "Process ", my_id, "of", nnodes ,"has started"
!************* Initial Conditions
********************************
     pi = 4d0*datan(1d0)
     do ilocal = 0, 4
      iglobal = 3*my_id+ilocal
      T(0,ilocal) = dsin(pi*delx*dfloat(iglobal))
     enddo
     write(*,*)"Processor", my_id, "has finished setting
    + initial conditions"
!************* Iterations
***************************************
     do itime = 1 , 3
      if (my_id.eq.0) then
        write(*,*)"Running Iteration Number ", itime
      endif
      do ilocal = 1, 3
        T(itime,ilocal)=T(itime-1,ilocal)+
    +   xalp*delt/delx/delx*
    +   (T(itime-1,ilocal-1)-2*T(itime-1,ilocal)+T(itime-
1,ilocal+1))
      enddo
      if (my_id.eq.0) then
        write(*,*)"Sending and receiving overlap points"
        dest = 1
```

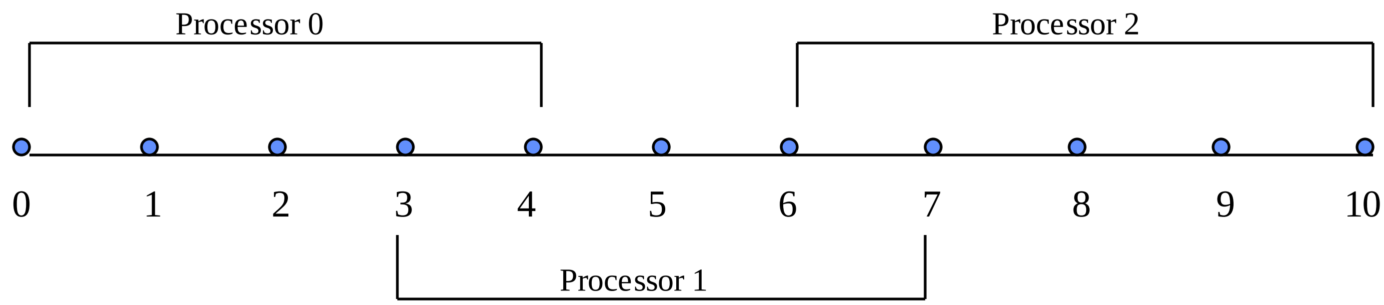
Fortran MPI Code: 1-D Heat Equation (Contd.)

```
 msg_size = 1
     call
MPI_SEND(T(itime,3),msg_size,MPI_DOUBLE_PRECISION,dest,
   +              tag,MPI_COMM_WORLD,ierr)
     endif
     if (my_id.eq.1) then
       from = 0
       dest = 2
       msg_size = 1
       call
MPI_SEND(T(itime,3),msg_size,MPI_DOUBLE_PRECISION,dest,
   +              tag,MPI_COMM_WORLD,ierr)
       call
MPI_RECV(T(itime,0),msg_size,MPI_DOUBLE_PRECISION,from
,
   +              tag,MPI_COMM_WORLD,status,ierr)
     endif
     if (my_id.eq.2) then
       from = 1
       dest = 1
       msg_size = 1
       call
MPI_SEND(T(itime,1),msg_size,MPI_DOUBLE_PRECISION,dest,
   +              tag,MPI_COMM_WORLD,ierr)
       call
MPI_RECV(T(itime,0),msg_size,MPI_DOUBLE_PRECISION,from
,
   +              tag,MPI_COMM_WORLD,status,ierr)
     endif
     if (my_id.eq.1) then
       from = 2
        dest = 0
       msg_size = 1
       call MPI_RECV(T(itime,4),msg_size,MPI_DOUBLE_PRECISION,from,
   +              tag,MPI_COMM_WORLD,status,ierr)
       call MPI_SEND(T(itime,1),msg_size,MPI_DOUBLE_PRECISION,dest,
   +              tag,MPI_COMM_WORLD,ierr)
     endif
     if (my_id.eq.0) then
       from = 1
       msg_size = 1
       call MPI_RECV(T(itime,4),msg_size,MPI_DOUBLE_PRECISION,from,
   +              tag,MPI_COMM_WORLD,status,ierr)
     endif
    enddo

    if (my_id.eq.0) then
      write(*,*)"SOLUTION SENT TO FILE AFTER 3 TIMESTEPS:"
    endif
    FILEN = 'data'//char(my_id+48)//'.dat'
    open (5, file=FILEN)
    write(5,*)"Processor ",my_id
    do ilocal = 0 , 4
     iglobal = 3*my_id + ilocal
     write(5,*)"ilocal=",ilocal,";iglobal=",iglobal,";T=",T(3,ilocal)
    enddo
    close(5)
    call MPI_FINALIZE(ierr)

    END
```

Simple Application using MPI: 1-D Heat Equation



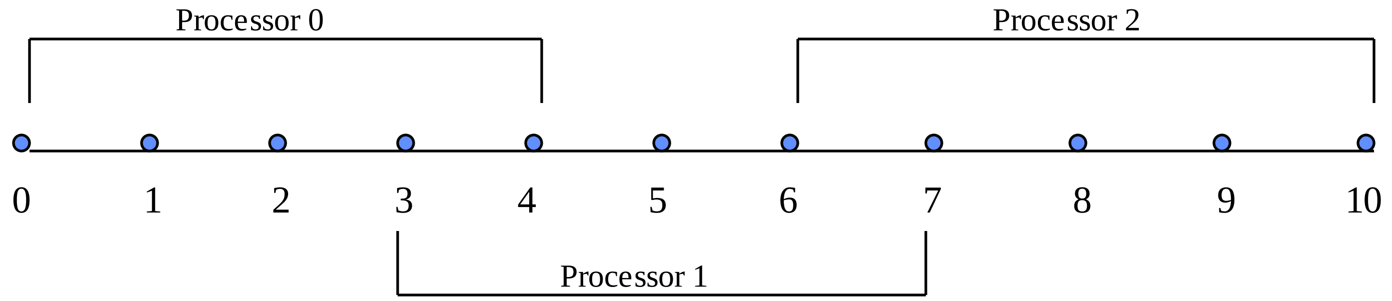
- Compilation

```
module reset
module load gcc/10.2.0 mvapich2/2.3.7
mpif90 -ffixed-form heat_mpi.f90 -o heat_mpi.exe
```

- Run Job:

```
sbatch --res=si24 heat_mpi.sb
```

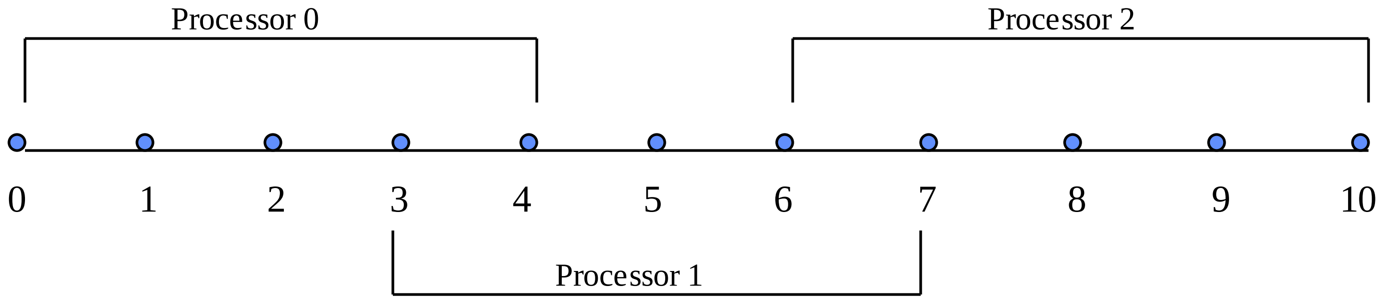
Simple Application using MPI: 1-D Heat Equation



OUTPUT FROM SAMPLE PROGRAM

Process 0 of 3 has started
Processor 0 has finished setting initial conditions
Process 1 of 3 has started
Processor 1 has finished setting initial conditions
Process 2 of 3 has started
Processor 2 has finished setting initial conditions
Running Iteration Number 1
Sending and receiving overlap points
Running Iteration Number 2
Sending and receiving overlap points
Running Iteration Number 3
Sending and receiving overlap points
SOLUTION SENT TO FILE AFTER 3 TIMESTEPS:

Simple Application using MPI: 1-D Heat Equation




```
% more data0.dat
 Processor  0
 ilocal= 0 ;iglobal= 0 ;T= 0.000000000000000000E+00
 ilocal= 1 ;iglobal= 1 ;T= 0.307205621017284991
 ilocal= 2 ;iglobal= 2 ;T= 0.584339815421976549
 ilocal= 3 ;iglobal= 3 ;T= 0.804274757358271253
 ilocal= 4 ;iglobal= 4 ;T= 0.945481682332597884
```

```
% more data2.dat
 Processor  2
 ilocal= 0 ;iglobal= 6 ;T= 0.945481682332597995
 ilocal= 1 ;iglobal= 7 ;T= 0.804274757358271253
 ilocal= 2 ;iglobal= 8 ;T= 0.584339815421976660
 ilocal= 3 ;iglobal= 9 ;T= 0.307205621017285102
 ilocal= 4 ;iglobal= 10 ;T= 0.000000000000000000E+00
```

```
% more data1.dat
 Processor  1
 ilocal= 0 ;iglobal= 3 ;T= 0.804274757358271253
 ilocal= 1 ;iglobal= 4 ;T= 0.945481682332597884
 ilocal= 2 ;iglobal= 5 ;T= 0.994138272681972301
 ilocal= 3 ;iglobal= 6 ;T= 0.945481682332597995
 ilocal= 4 ;iglobal= 7 ;T= 0.804274757358271253
```

Performance Considerations

- **Overlap communication with computation**
  - Use non-blocking primitives
  - Hide communication cost
  - Split-phase programming
- **Minimize surface-to-volume ratio**
  - Ghost cell exchange
- **Avoid communication**
  - Even at the cost of some more computation
  - Example: double size of ghost cell and communicate every other time step
  - Communication avoiding algorithms

Asynchronous Communication

- **Overlap communication w/ computation**
  - High performance interconnects can offload communication tasks from CPU to adapter
- **Condition**
  - No data dependencies on transfer
- **Split-phase programming**

BSP loop	BSP loop
compute	compute some
communicate	initiate communication
	complete computation
	complete communication

MPI – Profiling, Tracing Tools

- Several options available. On Expanse we have mpiP and TAU installed.
- Useful when you are trying to isolate performance issues.
- Tools can give you info on how much time is being spent in communication. The levels of detail vary with each tool.
- In general identify scaling bottlenecks and try to overlap communication with computation where possible.

mpiP example

- **Location: $HOME/PARALLEL/MISC**
- **Modules:**

  module reset; module load gcc/10.2.0 mvapich2/2.3.7 mpip/3.5
- **Compile (compile_profile.readme.txt):**

  mpif90 -ffixed-form -g -o heat_mpi_profile.exe heat_mpi.f90 -L$MPIPHOME/lib -lmpiP
- **Executable already exists. Just submit**

  sbatch --res=si24 heat_mpi_profile.sb
- **Once the job runs you get a .mpiP file.**

mpiP output

```
@ mpiP
@ Command : /home/mahidhar/PARALLEL/MISC/./heat_mpi_profile.exe
@ Version                  : 3.4.1
@ MPIP Build date          : Feb 26 2021, 06:50:01
@ Start time               : 2021 08 04 22:18:31
@ Stop time                : 2021 08 04 22:18:31
@ Timer Used               : PMPI_Wtime
@ MPIP env var             : [null]
@ Collector Rank           : 0
@ Collector PID            : 74358
@ Final Output Dir         : .
@ Report generation        : Single collector task
@ MPI Task Assignment      : 0 exp-1-01
@ MPI Task Assignment      : 1 exp-1-01
@ MPI Task Assignment      : 2 exp-1-01

---------------------------------------------------------------------------
@--- MPI Time (seconds) ---------------------------------------------------
---------------------------------------------------------------------------
Task    AppTime    MPITime     MPI%
   0     0.0241   0.000554     2.30
   1     0.0242   0.000716     2.96
   2     0.0242   0.000657     2.72
```

mpiP Output

```
  *    0.0724     0.00193     2.66
---------------------------------------------------------------------------
@--- Callsites: 8 ---------------------------------------------------------
---------------------------------------------------------------------------
 ID Lev File/Address        Line Parent_Funct             MPI_Call
  1   0 0x408ac2                 [unknown]                Recv
  2   0 0x4087db                 [unknown]                Send
  3   0 0x40897b                 [unknown]                Recv
  4   0 0x408924                 [unknown]                Send
  5   0 0x408a50                 [unknown]                Send
  6   0 0x408855                 [unknown]                Send
  7   0 0x4089f9                 [unknown]                Recv
  8   0 0x4088ac                 [unknown]                Recv
---------------------------------------------------------------------------
@--- Aggregate Time (top twenty, descending, milliseconds) ----------------
---------------------------------------------------------------------------
Call                 Site       Time    App%    MPI%     COV
Recv                    8      0.611    0.84   31.73    0.00
Recv                    3      0.583    0.81   30.25    0.00
Recv                    1      0.492    0.68   25.55    0.00
Send                    6      0.082    0.11    4.25    0.00
Send                    4     0.0739    0.10    3.84    0.00
Send                    2     0.0615    0.08    3.19    0.00
```

mpiP output

```
Send                      5      0.0174     0.02     0.91     0.00
Recv                      7     0.00552     0.01     0.29     0.00
---------------------------------------------------------------------------
@--- Aggregate Sent Message Size (top twenty, descending, bytes) ----------
---------------------------------------------------------------------------
Call                 Site       Count      Total       Avrg  Sent%
Send                    2           3         24          8  25.00
Send                    4           3         24          8  25.00
Send                    5           3         24          8  25.00
Send                    6           3         24          8  25.00

---------------------------------------------------------------------------
@--- Callsite Time statistics (all, milliseconds): 8 ---------------------
---------------------------------------------------------------------------
Name              Site Rank  Count      Max     Mean      Min   App%   MPI%
Recv                 1    0      3    0.487    0.164  0.00253   2.05  88.90
Recv                 1    *      3    0.487    0.164  0.00253   0.68  25.55

Recv                 3    2      3    0.539    0.194   0.0113   2.41  88.75
Recv                 3    *      3    0.539    0.194   0.0113   0.81  30.25

Recv                 7    1      3  0.00317  0.00184  0.00115   0.02   0.77
Recv                 7    *      3  0.00317  0.00184  0.00115   0.01   0.29
```

More Complex routines

- Derived Data Types
- User defined reduction functions
- Groups/communicator management
- Parallel I/O
- One Sided Communication Routines (RDMA)
- MPI-3 Standard has over 400 routines(!).

Homework!

- **Change directory to $HOME/PARALLEL/MISC**

- **Code “sample.f” has two bugs.**

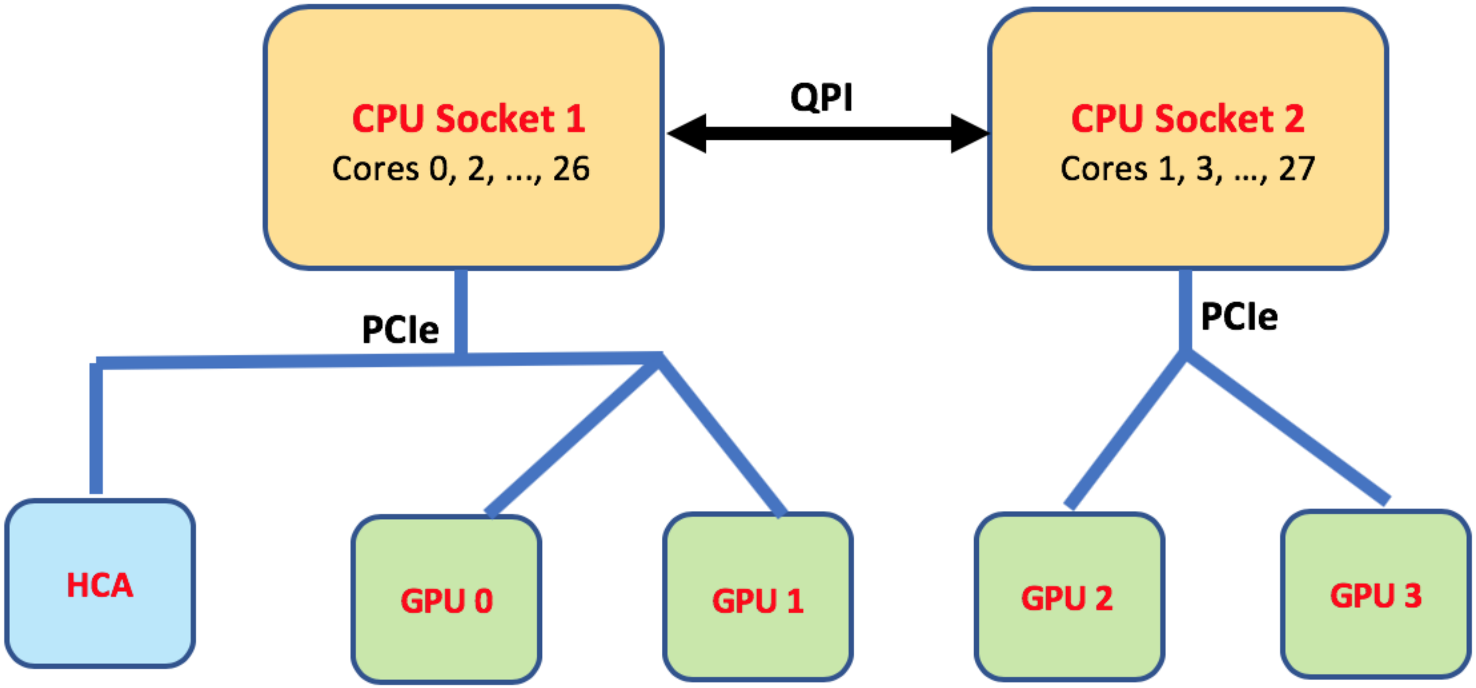
- **Compile:**

  module reset
  module load cpu/0.15.4
  module load intel mvapich2
  mpif90 -o sample.exe sample.f

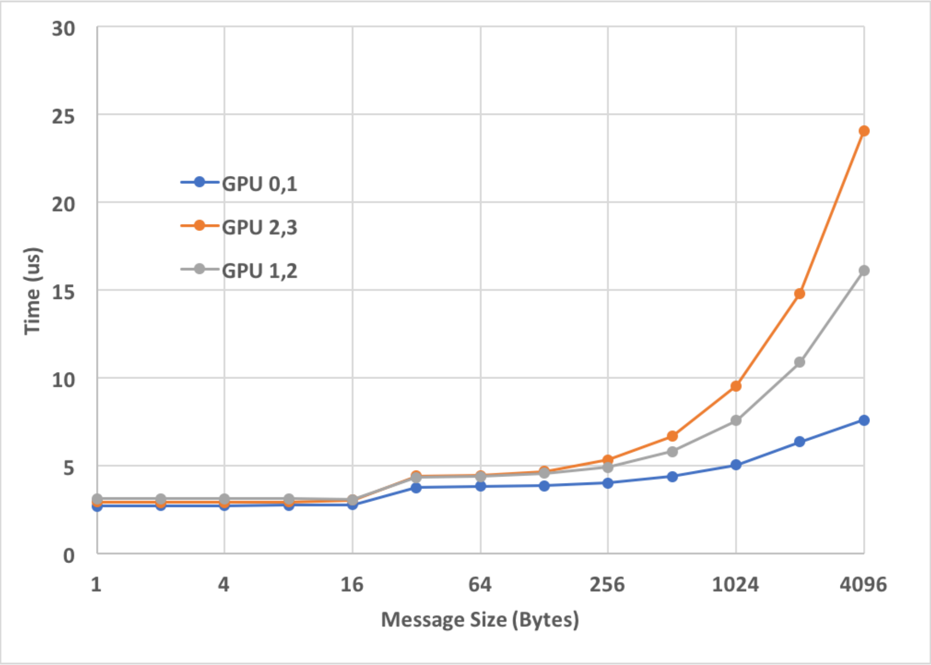
  Run: sbatch --res=si24 sample.sb
  See if you can identify the two bugs!

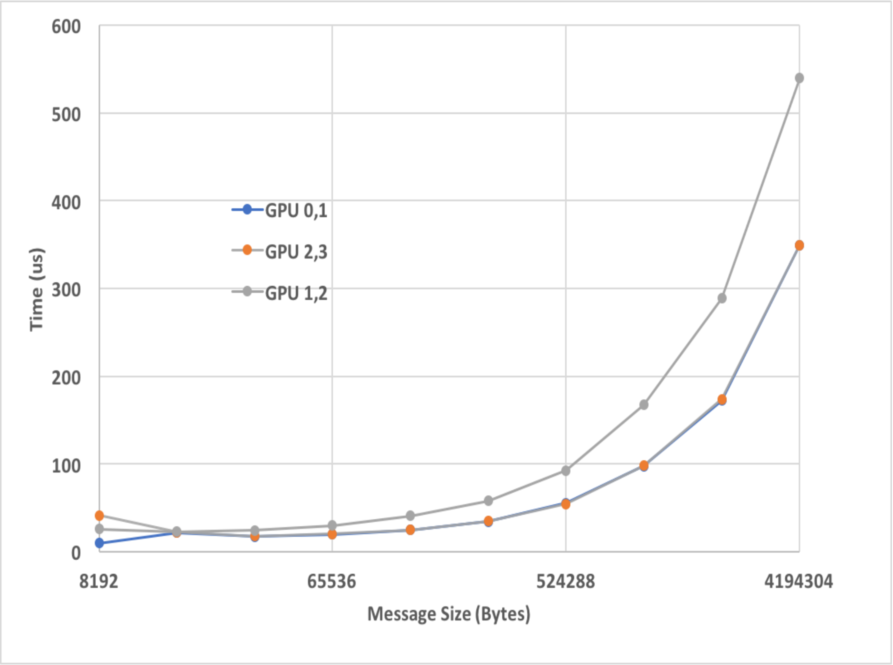
MVAPICH2-GDR

Example node layout



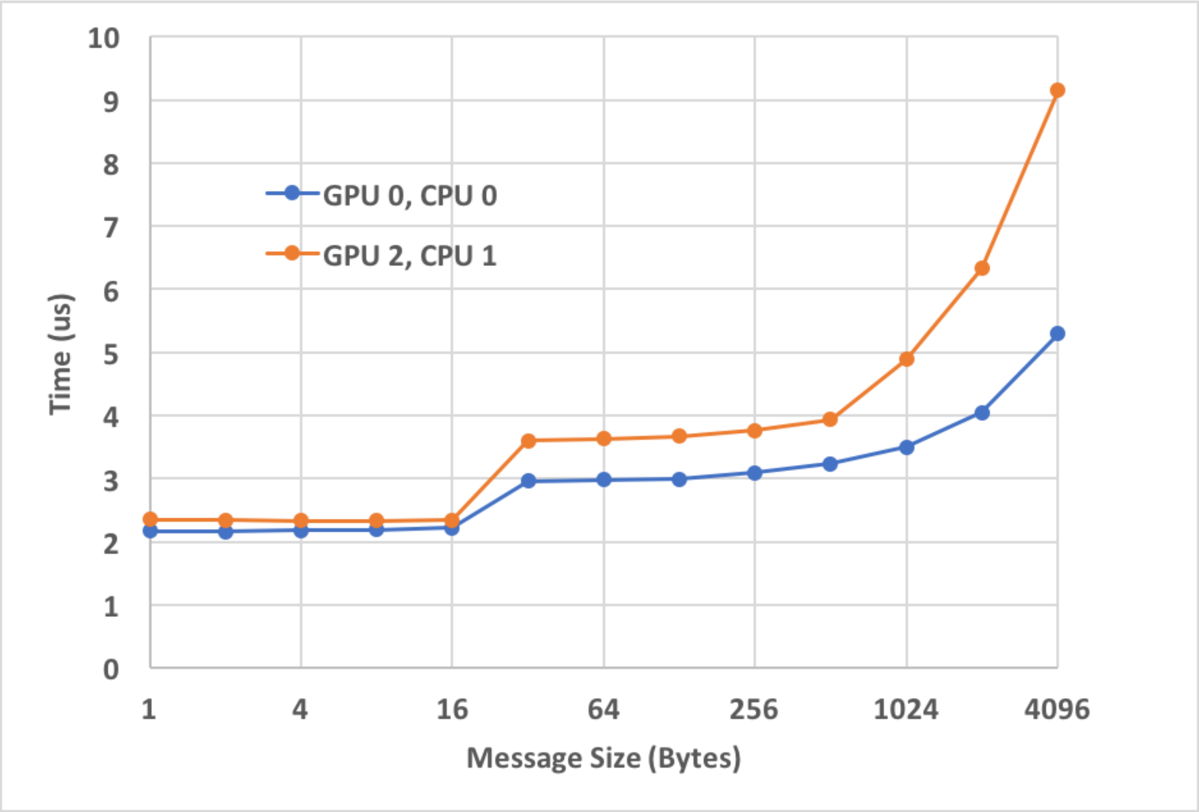
OSU Latency (osu_latency) Benchmark Intra-node, Comet nodes





- Latency between GPU 0 , GPU 1: 2.73 µs
- Latency between GPU 2 , GPU 3: 2.95 µs
- Latency between GPU 1 , GPU 2: 3.13 µs

OSU Latency (osu_latency) Benchmark
Inter-node, Comet nodes



- Latency between GPU 0 , process bound to CPU 0 on both nodes: 2.17 µs
- Latency between GPU 2 , process bound to CPU 1 on both nodes: 2.35 µs

Expanse GPU Node Architecture

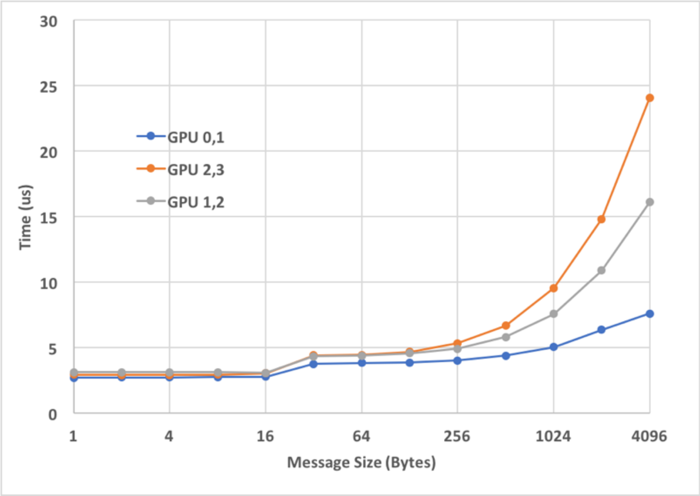
- **4 V100 32GB SMX2 GPUs**
- **384 GB RAM, 1.6 TB PCIe NVMe**
- **2 Intel Xeon 6248 CPUs**
- **Topology:**

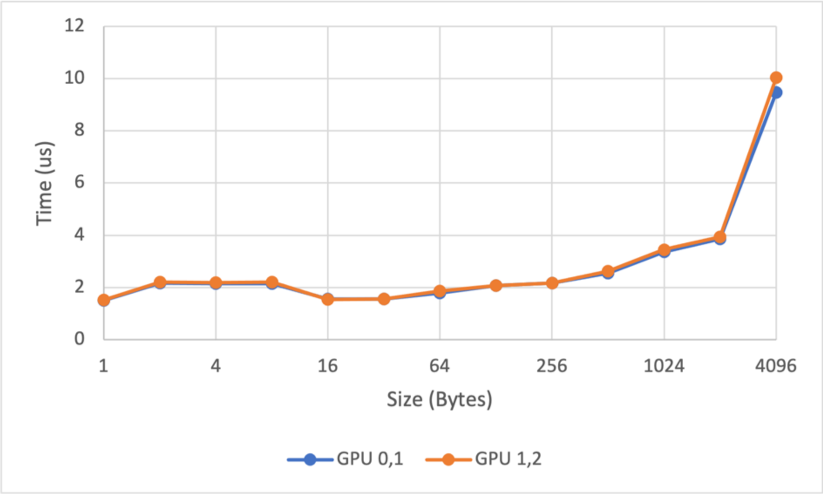
```
        GPU0    GPU1    GPU2    GPU3    mlx5_0  CPU Affinity
GPU0     X      NV2     NV2     NV2     SYS     0-0,4-4,8-8,12-12,16-16,20-20,24-24,28-28,32-32,36-36
GPU1    NV2      X      NV2     NV2     SYS     0-0,4-4,8-8,12-12,16-16,20-20,24-24,28-28,32-32,36-36
GPU2    NV2     NV2      X      NV2     SYS     1-1,5-5,9-9,13-13,17-17,21-21,25-25,29-29,33-33,37-37
GPU3    NV2     NV2     NV2      X      SYS     1-1,5-5,9-9,13-13,17-17,21-21,25-25,29-29,33-33,37-37
mlx5_0  SYS     SYS     SYS     SYS      X

Legend:

  X    = Self
  SYS  = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI)
  NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
  PHB  = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
  PXB  = Connection traversing multiple PCIe bridges (without traversing the PCIe Host Bridge)
  PIX  = Connection traversing at most a single PCIe bridge
  NV#  = Connection traversing a bonded set of # NVLinks
```

OSU Latency (osu_latency) Benchmark
Intra-node, P100 nodes on Comet, V100 nodes on Expanse

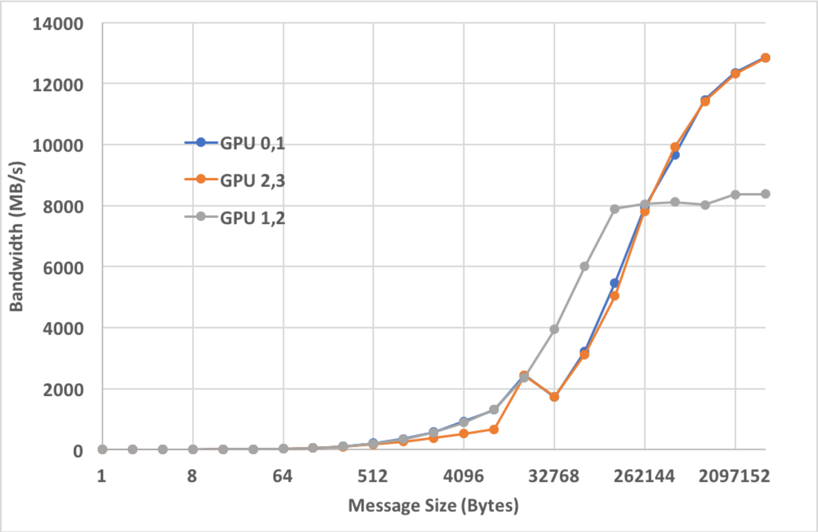


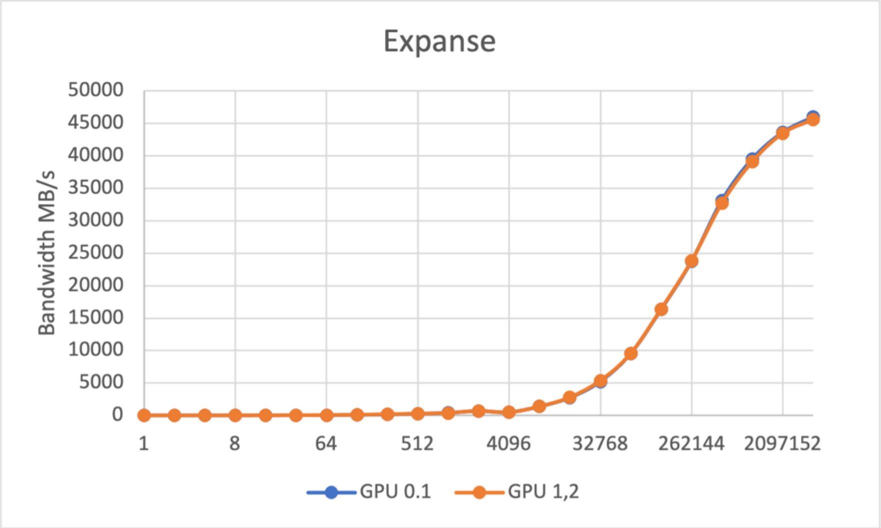


- COMET - P100 nodes
- Latency between GPU 0 , GPU 1: 2.73 µs
- Latency between GPU 2 , GPU 3: 2.95 µs
- Latency between GPU 1 , GPU 2: 3.13 µs

- Expanse - V100 nodes
- Latency between GPU 0 , GPU 1: 1.51 µs
- Latency between GPU 1 , GPU 2: 1.53 µs
- MVAPICH2 GDR 2.3.6, GCC 8.3.1

OSU Bandwidth (osu_bw) Benchmark
Intra-node, P100 nodes on Comet, V100 nodes on Expanse





- MVAPICH2 GDR 2.3.6, GCC 8.3.1

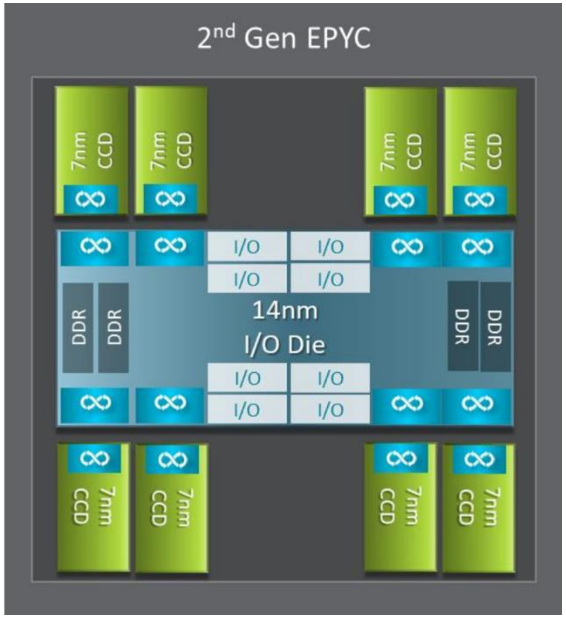
Hybrid MPI/OpenMP Jobs and SLURM Usage on Expanse

Ref: ibrun scripts developed by Manu Shantharam at SDSC

module load sdsc
(puts ibrun in your path)

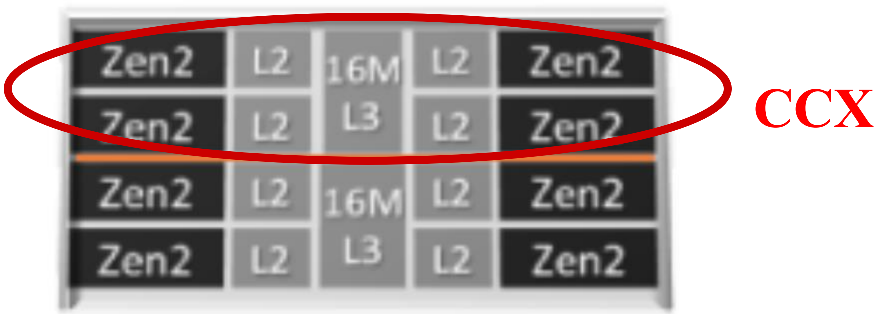
AMD EPYC 7742 Processor Architecture

- 8 Core Complex Dies (CCDs).
- CCDs connect to memory, I/O, and each other through the I/O Die.
- 8 memory channels per socket.
- DDR4 memory at 3200MHz.
- PCI Gen4, up to 128 lanes of high speed I/O.
- Memory and I/O can be abstracted into separate quadrants each with 2 DIMM channels and 32 I/O lanes.



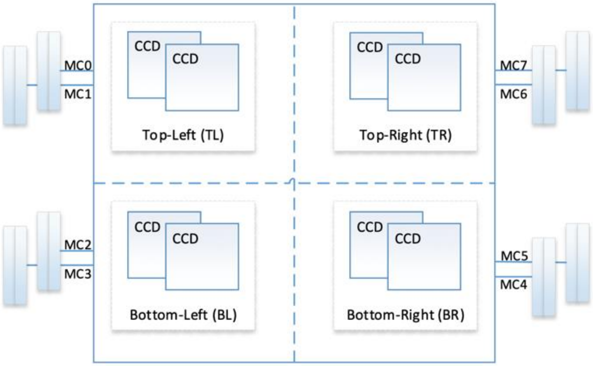
AMD EPYC 7742 Processor: Core Complex Die (CCD)

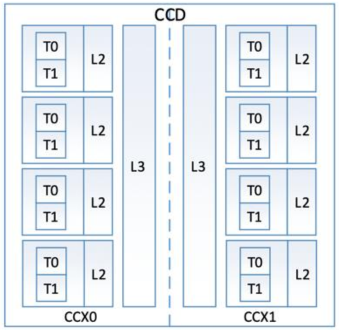
- 2 Core Complexes (CCXs) per CCD
- 4 Zen2 cores in each CCX shared a 16M L3 cache. Total of 16 x 16 = 256MB L3 cache.
- Each core includes a private 512KB L2 cache.



AMD EPYC 7742 Processor : NUMA Nodes Per Socket

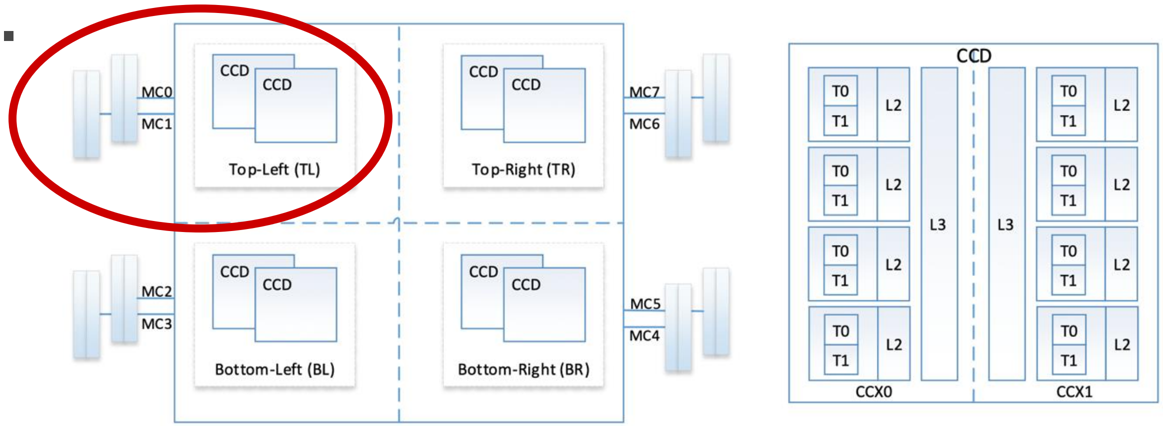
- The four logical quadrants allow the processor to be partitioned into different NUMA domains. Options set in BIOS.
- Domains are designated as NUMA per socket (NPS).
- NPS4: Four NUMA domains per socket is the typical HPC configuration.





NPS4 Configuration

- The processor is partitioned into four NUMA domains.
- Each logical quadrant is a NUMA domain.
- Memory is interleaved across the two memory channels
- PCIe devices will be local to one of four NUMA domains (the IO die that has the PCIe root for the device)
- *This is the typical HPC configuration* as workload is NUMA aware, ranks and memory can be pinned to cores and NUMA nodes.



AMD EPYC: Optimization/Usage Guidelines

- **Processor is x86_64**
  - Supports AVX2 instruction set
  - Multiple separate L3 caches - 16 on 64-core CPUs. Thread migration affects cache locality
- **Make sure the threads stay close to their cache**
  - Pinning can make a big impact on performance
  - Need to use at least 2 cores on CCD to maximize cache
- **Typically, hybrid approach works better**
  - One MPI rank/L3 cache and then OpenMP threads on each core

Using MPI options

- **All MPI implementations have affinity options.**

- **Example OpenMPI run command:**

  mpirun -np 32 --mca pml ucx --mca osc ucx --map-by l3cache xhpl

- **Example Intel MPI setup:**

  export OMP_NUM_THREADS=16

  mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./hello_hybrid

- **Can also combine with application pinning options. For example, for NAMD:**

  mpirun -np 8 --map-by ppr:4:node namd2 +setcpuaffinity +ppn 31 +commap 0,32,64,96 +pemap 1-31,33-63,65-95,97-127 stmv.namd

ibrun and affinity options

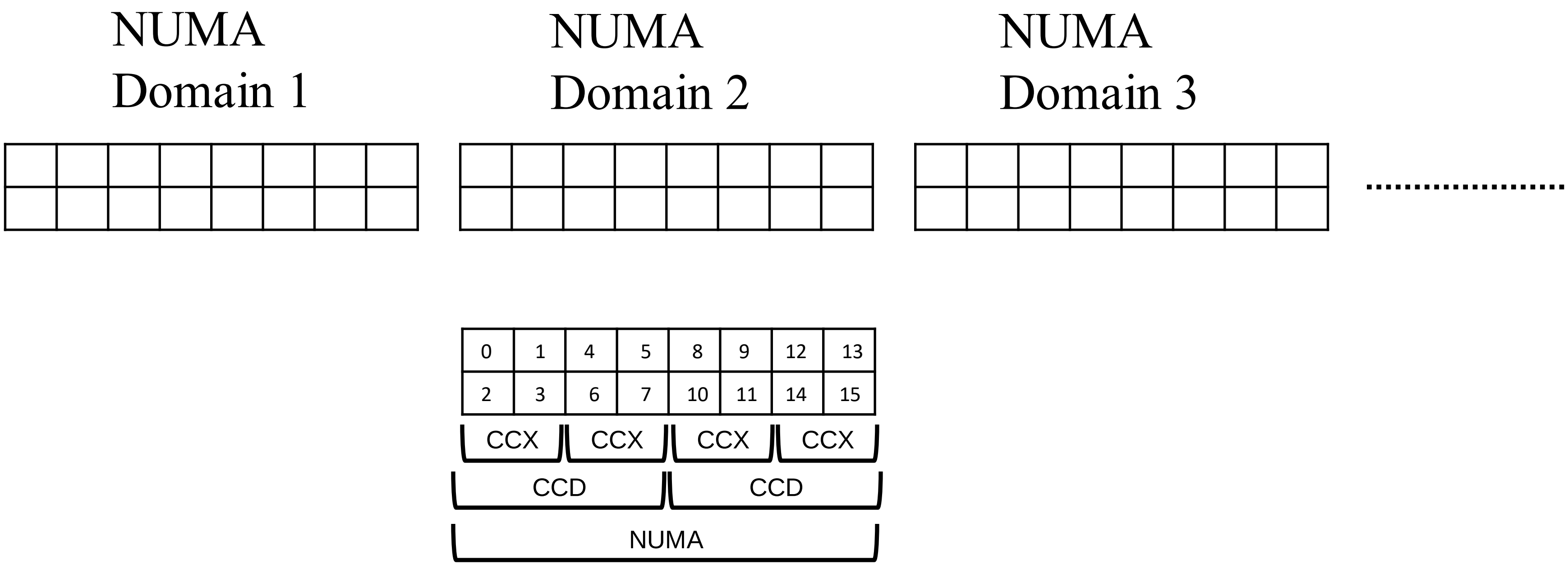
- **Basic usage**
  - ibrun ./executable <executable_opions>

- **With affinity**
  - ibrun affinity <hints> ./executable <executable_opions>

- **Affinity options**
  - **scatter**: scatters the ranks across all numa domains in a cyclic manner
  - **scatter-ccd**: scatters the ranks across all AMD CCD domains in a cyclic manner
  - **scatter-ccx**: scatters the ranks across all AMD CCX domains in a cyclic manner
  - **scatter blk <blk_size>**: scatters the ranks across all numa domains in a cyclic manner, but with 'blk_size' (1-16) consecutive ranks packed into a single numa domain
  - **scatter-ccd blk <blk_size>**: scatters the ranks across AMD CCD domains in a cyclic manner, but with 'blk_size' (1-8) consecutive ranks packed into a single CCD domain
  - **scatter-ccx blk <blk_size>**: scatters the ranks across AMD CCX domains in a cyclic manner, but with 'blk_size' (1-4) consecutive ranks packed into a single CCX domain

NOTE: valid blk_sizes depend on the **cpus-per-task a**nd the **domain type** (numa, CCD, CCX). 'blk’ is optional and is set to '1' by default

Guide for Layout Diagrams
(for upcoming slides)



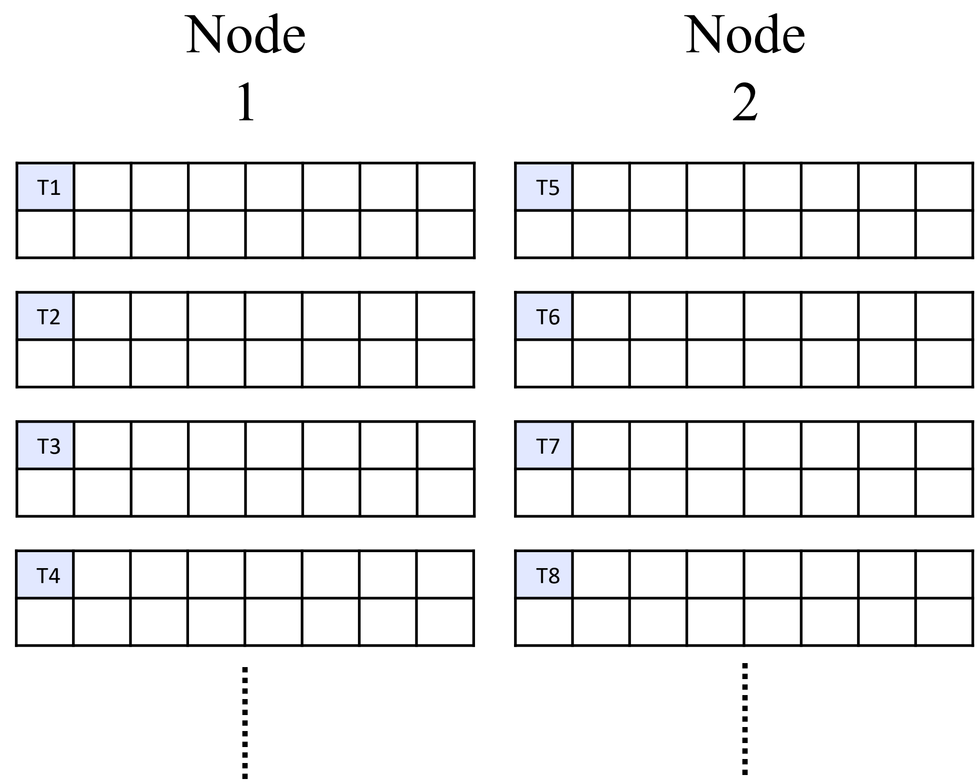
Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=4
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load cpu/0.15.4
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun ./hy-gcc-openmpi.exe

(same as srun –n 8 ./hy-gcc-openmpi.exe)

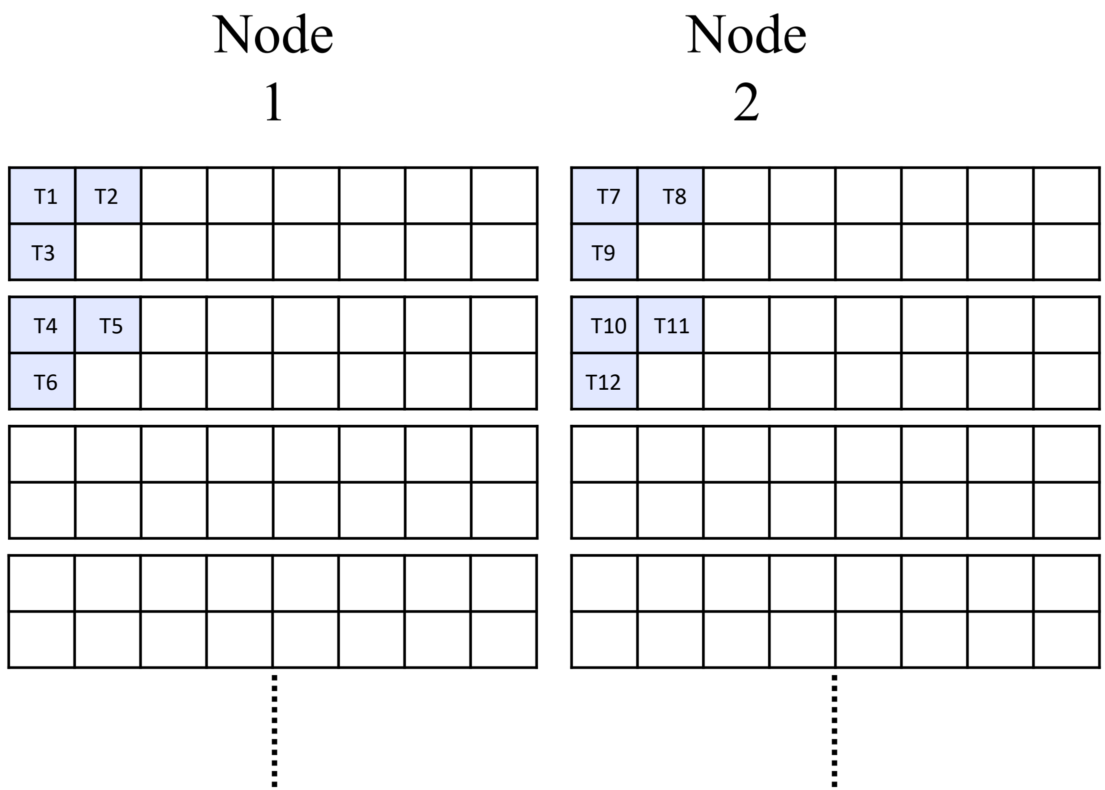


Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load cpu/0.15.4
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun affinity scatter blk 3 ./hy-gcc-openmpi.exe

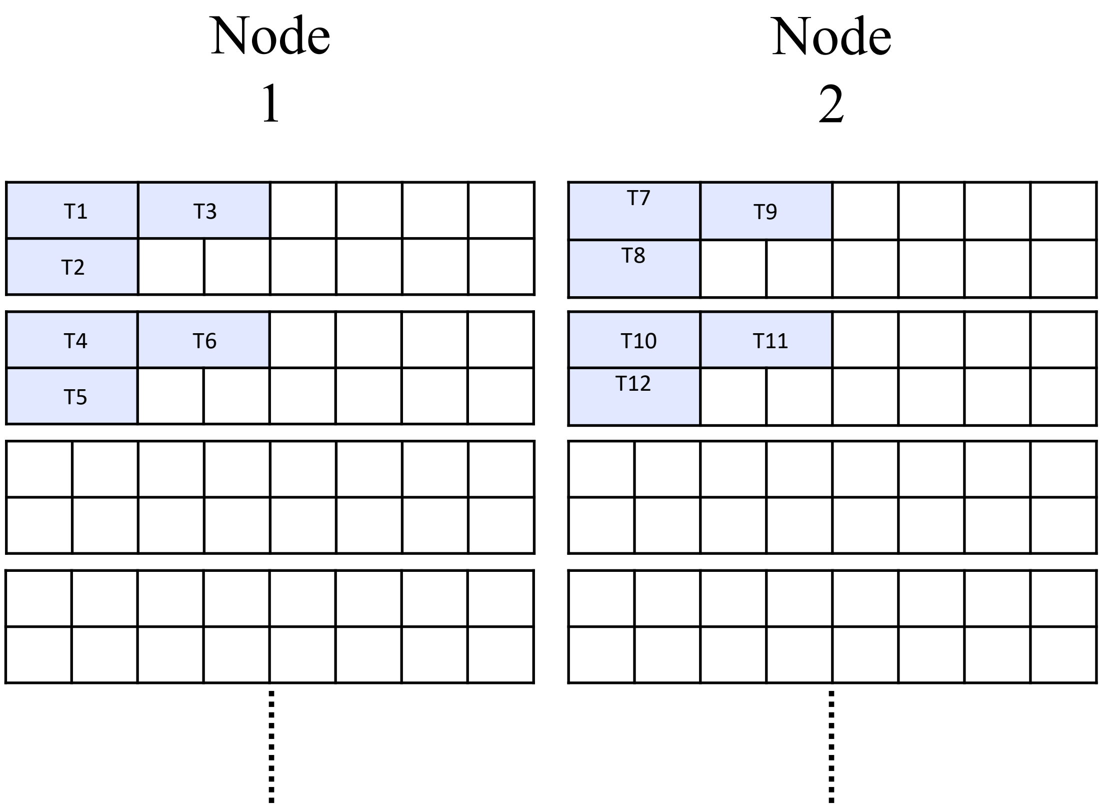


Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=2
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load cpu/0.15.4
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun affinity scatter blk 3 ./hy-gcc-openmpi.exe

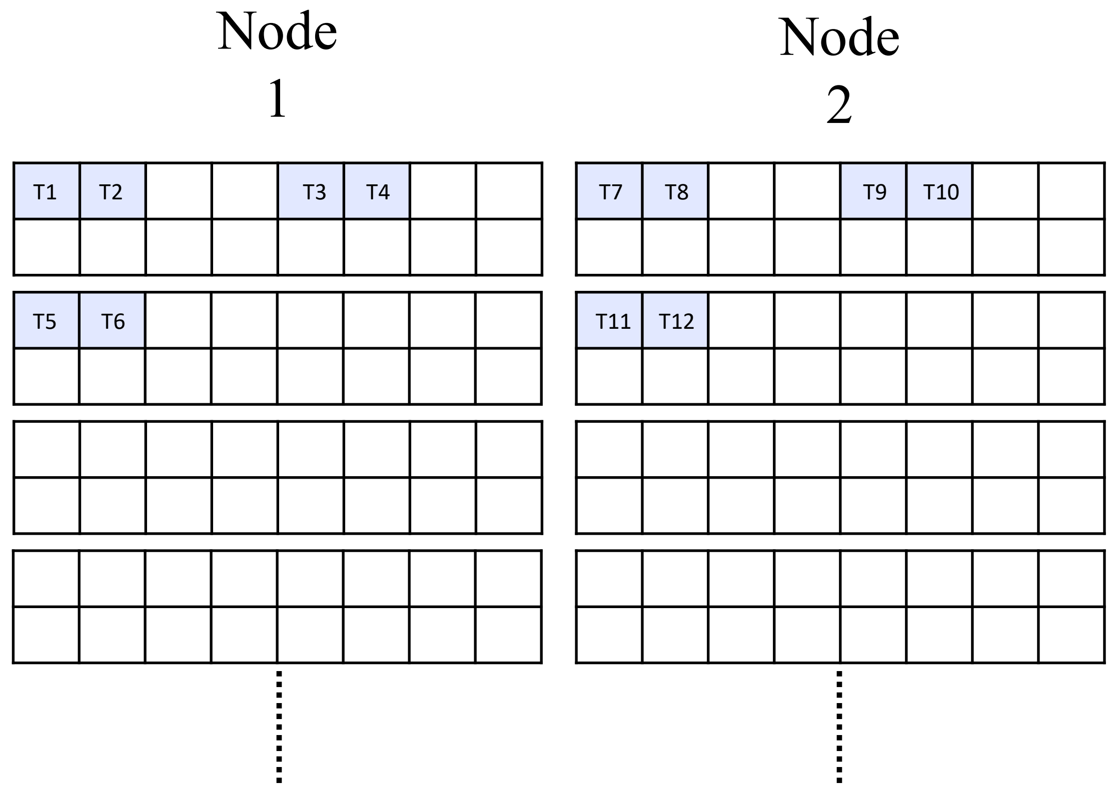


Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load cpu/0.15.4
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun affinity scatter-ccd blk 2 ./hy-gcc-openmpi.exe

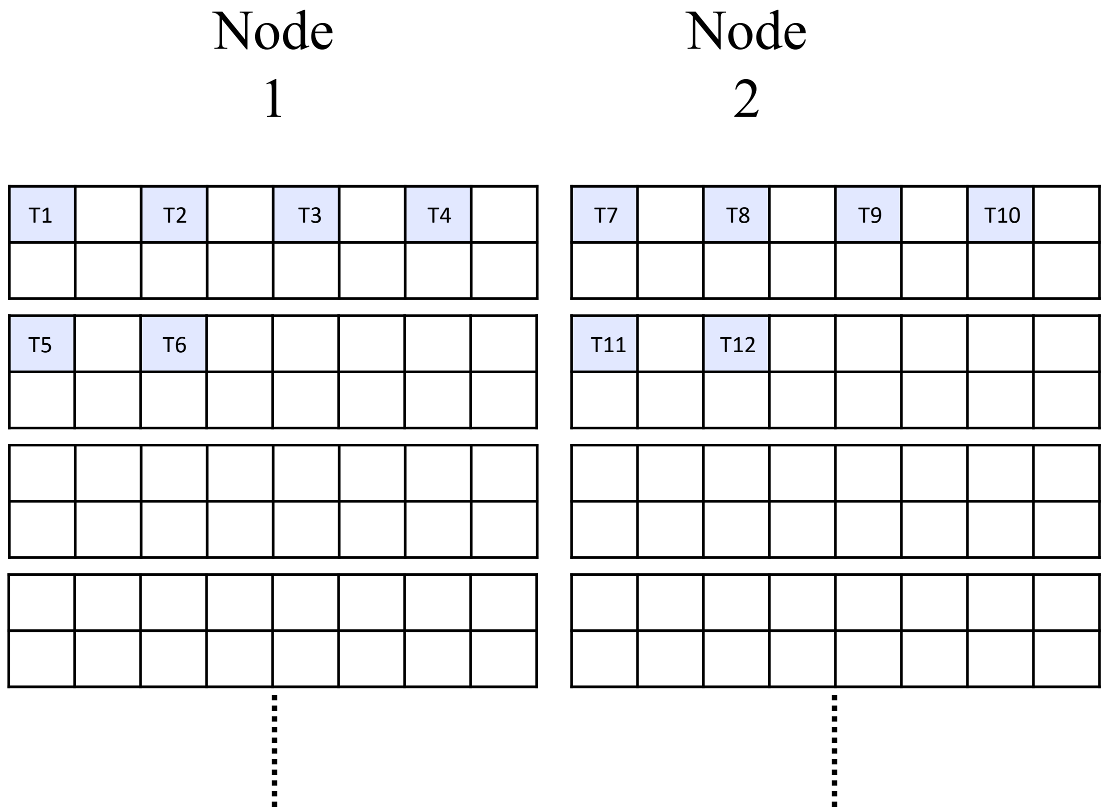


Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load cpu/0.15.4
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun affinity scatter-ccx ./hy-gcc-openmpi.exe



Snapshot of task layout with wrong layout

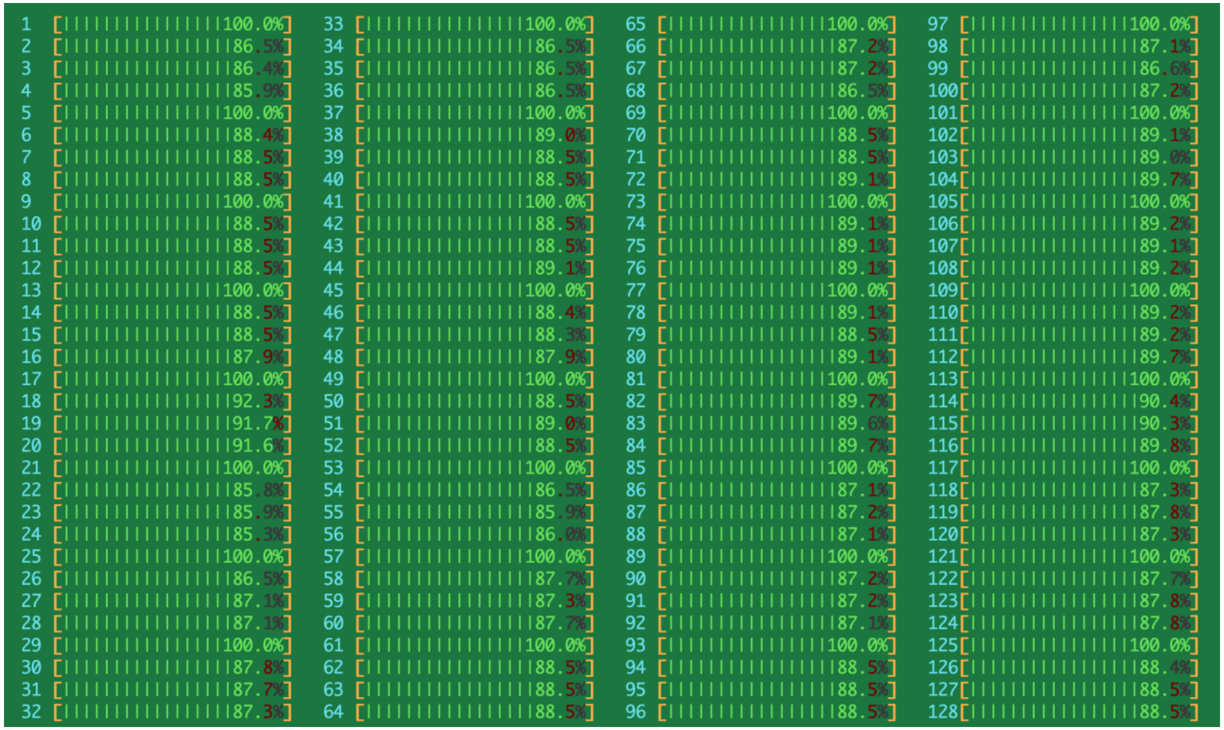
```
  1[||||||||||||||100.0%]  33[||||||||||||||100.0%]  65[||||||||||||||100.0%]  97[||||||||||||||100.0%]
  2[||||||||||||||100.0%]  34[||||||||||||||100.0%]  66[||||||||||||||100.0%]  98[||||||||||||||100.0%]
  3[||||||||||||||100.0%]  35[||||||||||||||100.0%]  67[||||||||||||||100.0%]  99[||||||||||||||100.0%]
  4[||||||||||||||100.0%]  36[||||||||||||||100.0%]  68[||||||||||||||100.0%] 100[||||||||||||||100.0%]
  5[|              3.2%]  37[               0.0%]  69[               0.0%] 101[               0.0%]
  6[               0.0%]  38[               0.0%]  70[               0.0%] 102[               0.0%]
  7[               0.0%]  39[               0.0%]  71[               0.0%] 103[               0.0%]
  8[               0.0%]  40[               0.0%]  72[               0.0%] 104[               0.0%]
  9[               0.0%]  41[               0.0%]  73[               0.0%] 105[               0.0%]
 10[               0.0%]  42[               0.0%]  74[               0.0%] 106[               0.0%]
 11[               0.0%]  43[               0.0%]  75[               0.0%] 107[               0.0%]
 12[               0.0%]  44[               0.0%]  76[               0.0%] 108[               0.0%]
 13[               0.0%]  45[               0.0%]  77[               0.0%] 109[               0.0%]
 14[               0.0%]  46[               0.0%]  78[               0.0%] 110[               0.0%]
 15[               0.0%]  47[               0.0%]  79[               0.0%] 111[               0.0%]
 16[               0.0%]  48[               0.0%]  80[               0.0%] 112[               0.0%]
 17[||||||||||||||100.0%]  49[||||||||||||||100.0%]  81[||||||||||||||100.0%] 113[||||||||||||||100.0%]
 18[||||||||||||||100.0%]  50[||||||||||||||100.0%]  82[||||||||||||||100.0%] 114[||||||||||||||100.0%]
 19[||||||||||||||100.0%]  51[||||||||||||||100.0%]  83[||||||||||||||100.0%] 115[||||||||||||||100.0%]
 20[||||||||||||||100.0%]  52[||||||||||||||100.0%]  84[||||||||||||||100.0%] 116[||||||||||||||100.0%]
 21[               0.0%]  53[               0.0%]  85[               0.0%] 117[               0.0%]
 22[               0.0%]  54[               0.0%]  86[               0.0%] 118[               0.0%]
 23[               0.0%]  55[               0.0%]  87[               0.0%] 119[               0.0%]
 24[               0.0%]  56[               0.0%]  88[               0.0%] 120[               0.0%]
 25[               0.0%]  57[               0.0%]  89[               0.0%] 121[               0.0%]
 26[               0.0%]  58[               0.0%]  90[               0.0%] 122[               0.0%]
 27[               0.0%]  59[               0.0%]  91[               0.0%] 123[               0.0%]
 28[               0.0%]  60[               0.0%]  92[               0.0%] 124[               0.0%]
 29[               0.0%]  61[               0.0%]  93[               0.0%] 125[               0.0%]
 30[               0.0%]  62[               0.0%]  94[               0.0%] 126[               0.0%]
 31[               0.0%]  63[               0.0%]  95[               0.0%] 127[|              1.3%]
```

```
3296452 xhpl          mahidhar    3205092 R 75.4 00:00:59  19
3296452 xhpl          mahidhar    3205092 S  9.3 00:00:06  19
3296452 xhpl          mahidhar    3205092 S  9.3 00:00:06  19
3296452 xhpl          mahidhar    3205092 S  9.3 00:00:06  19
3296453 xhpl          mahidhar    3205092 R 75.7 00:00:59  35
3296453 xhpl          mahidhar    3205092 S  9.2 00:00:06  35
3296453 xhpl          mahidhar    3205092 S  9.2 00:00:06  35
3296453 xhpl          mahidhar    3205092 S  9.2 00:00:05  35
3296454 xhpl          mahidhar    3205092 R 75.5 00:00:59  51
```

Snapshot of task layout with scatter-ccx option

#SBATCH --nodes=1
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=4

ibrun affinity scatter-ccx $XHPL



Snapshot of task layout with scatter-ccx option

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=4

ibrun affinity scatter-ccx $XHPL
```

```
82667 xhpl            mahidhar    2526976 R 98.4 00:02:10   0
82667 xhpl            mahidhar    2526976 S  0.0 00:00:00   0
82667 xhpl            mahidhar    2526976 S  0.8 00:00:01   0
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   1
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   2
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   3
82668 xhpl            mahidhar    2527544 R 98.4 00:02:09  40
82668 xhpl            mahidhar    2527544 S  0.0 00:00:00  40
82668 xhpl            mahidhar    2527544 S  0.9 00:00:01  40
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  41
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  42
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  43
82669 xhpl            mahidhar    2527532 R 98.3 00:02:09   4
82669 xhpl            mahidhar    2527532 S  0.0 00:00:00   4
82669 xhpl            mahidhar    2527532 S  0.7 00:00:00   4
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   5
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   6
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   7
```

slurm-aff-prod script for MPI/Pthreads codes

- The slurm-aff-prod script is used to bind Pthreads after MPI job launch.
- Can be used by wrapping binary based on name.

```
#!/bin/bash
#SBATCH -p shared
#SBATCH -N 1
#SBATCH --ntasks-per-node=10
#SBATCH --cpus-per-task=4
#SBATCH --mem=77G
#SBATCH -t 00:10:00
#SBATCH -J A76BE.GTRGAMMA.mpi10pt4NautoMRExfa
#SBATCH -o A76BE.GTRGAMMA.mpi10pt4NautoMRExfa.%j.%N.out
#SBATCH -e A76BE.GTRGAMMA.mpi10pt4NautoMRExfa.%j.%N.err
#SBATCH -A use300

export NP=$SLURM_TASKS_PER_NODE
export THREADS=$SLURM_CPUS_PER_TASK

rm RAx*

export AFFINITY_INFO=0
export AFFINITY_DEBUG=0

srun --mpi=pmi2 -n $NP ./raxmlHPC-HYBRID_8.2.12_expanse -s ./A76BE.txt -n A76BE.GTRGAMMA.mpi10pt4NautoMRExfa -m GTRGAMMA -N a
utoMRE -p 12345 -x 12345 -f a
```

```
#!/bin/sh

# This is for running on EXPANSE

#source $HOME/.bashrc

module reset
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
module load raxml/8.2.12
module load slurm

EXE='raxmlHPC-HYBRID-AVX'
slurm-aff-prod-test $EXE &

echo "running:"
echo " $EXE -T ${THREADS} $*"

$EXE -T ${THREADS} $*
```

Summary of Binding Options on Expanse

- AMD Processor on Expanse has 4 NUMA domains with 16 cores each.
- 8 Core Complex Dies (CCDs) per processor, with 2 Core Complexes (CCXs) per CCD. Four cores in a CCX share L3 cache.
- For hybrid MPI/OpenMP and MPI/Pthreads codes it is important to lay out tasks correctly and binding is important for performance.
- **ibrun, affinity, and slurm-aff-prod** scripts available to make it easier to lay out and bind tasks.
- Tools are being updated so feedback is encouraged!

MPI and OpenMP References

- **Excellent tutorials from LLNL:**
  - https://hpc-tutorials.llnl.gov/mpi/
  - https://hpc.llnl.gov/sites/default/files/DavidCronkSlides.pdf
  - https://hpc-tutorials.llnl.gov/openmp

- **MPI for Python:**
  - https://mpi4py.readthedocs.io/en/stable/

- **OpenMPI User Guide:**
  - https://www.open-mpi.org/doc/current/

- **MVAPICH2 User Guide:**
  - http://mvapich.cse.ohio-state.edu/userguide/