Parallel Computing Using MPI & OpenMP

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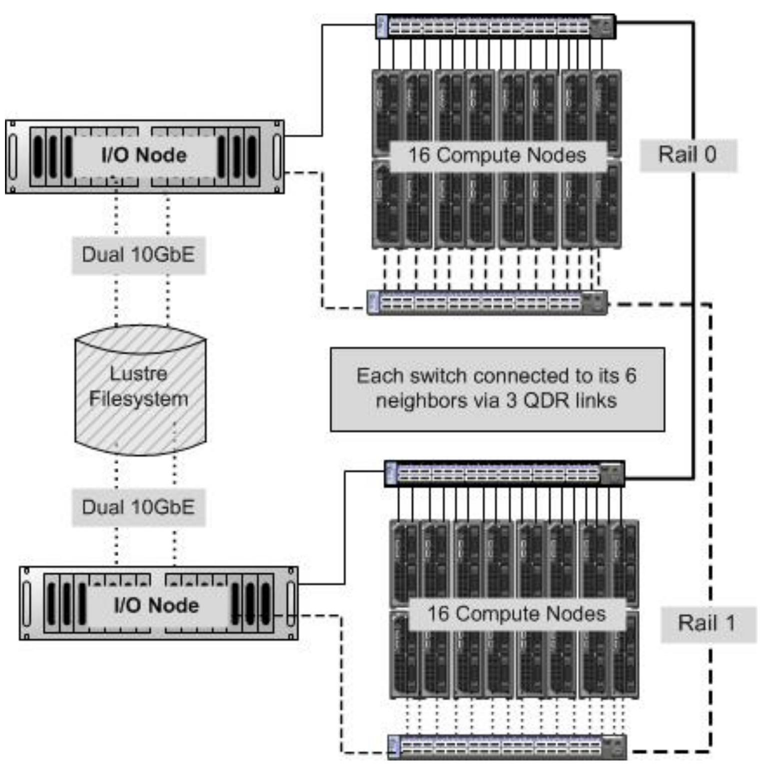
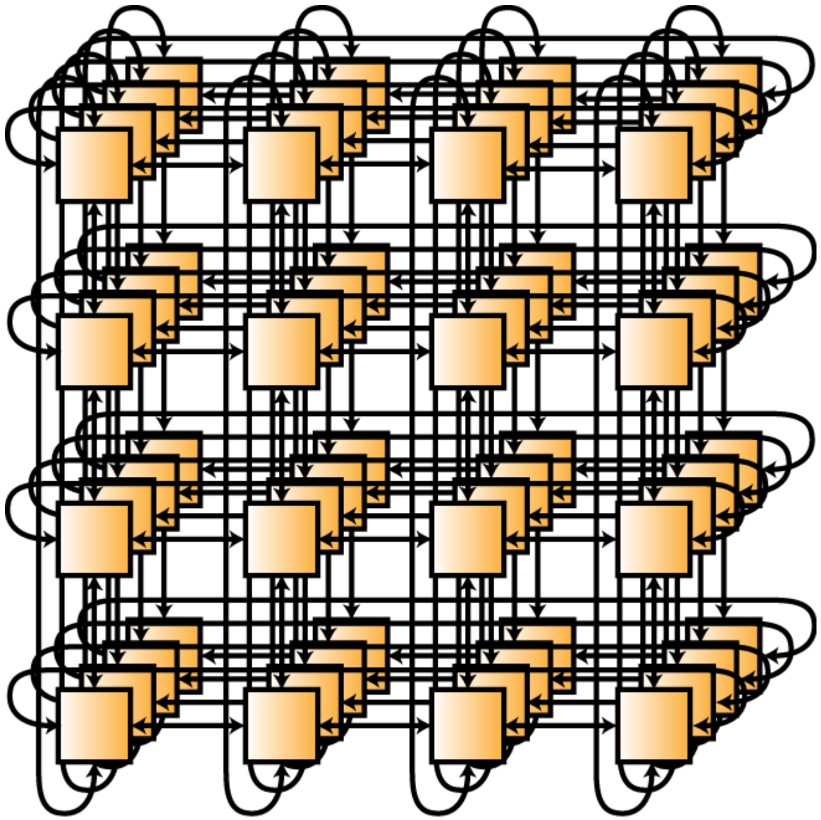
General System Architecture Overview

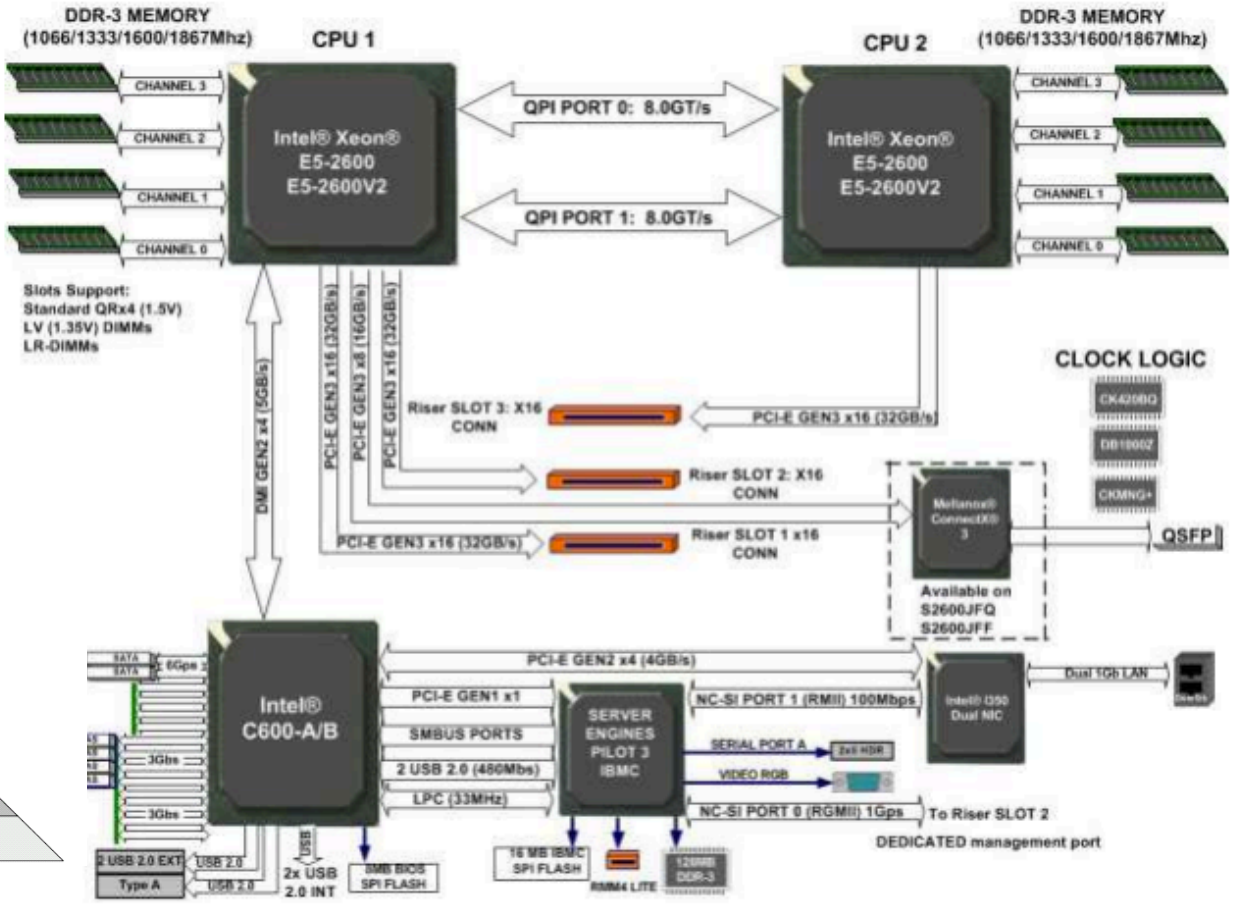
- Today's supercomputers are massively parallel with thousands of nodes interconnected with a fast low latency network.
- The nodes typically feature multiple processors, each of which has multiple cores. Gordon system level architecture shown below:

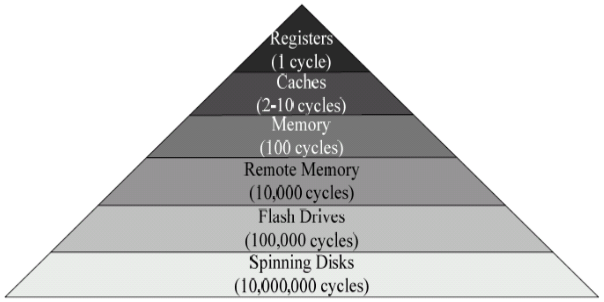




Typical Node Architecture

- Typical compute node features a multi-socket (processor) architecture. Each processor has multiple cores.
- Memory hierarchy – multiple levels of cache, main memory, disk.





Registers (1 cycle)
Caches (2-10 cycles)
Memory (100 cycles)
Remote Memory (10,000 cycles)
Flash Drives (100,000 cycles)
Spinning Disks (10,000,000 cycles)

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Parallel Computing

- Bulk of the speed up on modern supercomputers comes from scaling up the number of processing units available => programmers need to parallelize their codes to see this benefit.
- Parallelism needed both at the node level (given the availability of multiple cores), and at the system level (to utilize all the available nodes).
- In addition to the performance benefit, parallel approach is needed to make large/complex simulations feasible – often times the memory and storage resource on a single node are not sufficient to handle large problems.
- Lot of real world problems are inherently parallel and conducive to using massively parallel resources.

Classification

- **Single Instruction, Single Data [Serial codes]**
- **Single Instruction, Multiple Data**
  - Processors run the same instructions, each operates on different data
  - Technically, Hadoop MapReduce fits this mode
  - GPUs
- **Multiple Instruction, Single Data**
  - Multiple instructions acting on single data stream. E.g. Different analysis on same set of data.
- **Multiple Instruction, Multiple Data**
  - Every processor may execute different instructions
  - Every processor may work on different parts of data
  - Execution can be synchronous or asynchronous, deterministic or non-deterministic

Message Passing Interface (MPI)

- MPI is a standard; Several implementations available. On Comet and Gordon we use MVAPICH2 and OpenMPI.
- Originally designed for distributed memory architectures.
- Present implementations work on hybrid distributed memory/shared memory systems.
- Implementations adapted/developed for handling most network interconnects and protocols – for example InifiniBand, and Ethernet (TCP).
- MPI standard allows for easy portability, standard functionality, and implementations can optimize functions to exploit native hardware. User does not need to be aware of the hardware level optimizations.

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

Location of today's examples: /home/diag/opt/SI2015/PARALLEL

Copy: cp –r /home/diag/opt/SI2015/PARALLEL $HOME/

cd $HOME/PARALLEL/SIMPLE

Compile: `mpicc -o pi_mpi.exe pi_mpi.c`

Submit Job: `qsub pi_mpi.cmd`

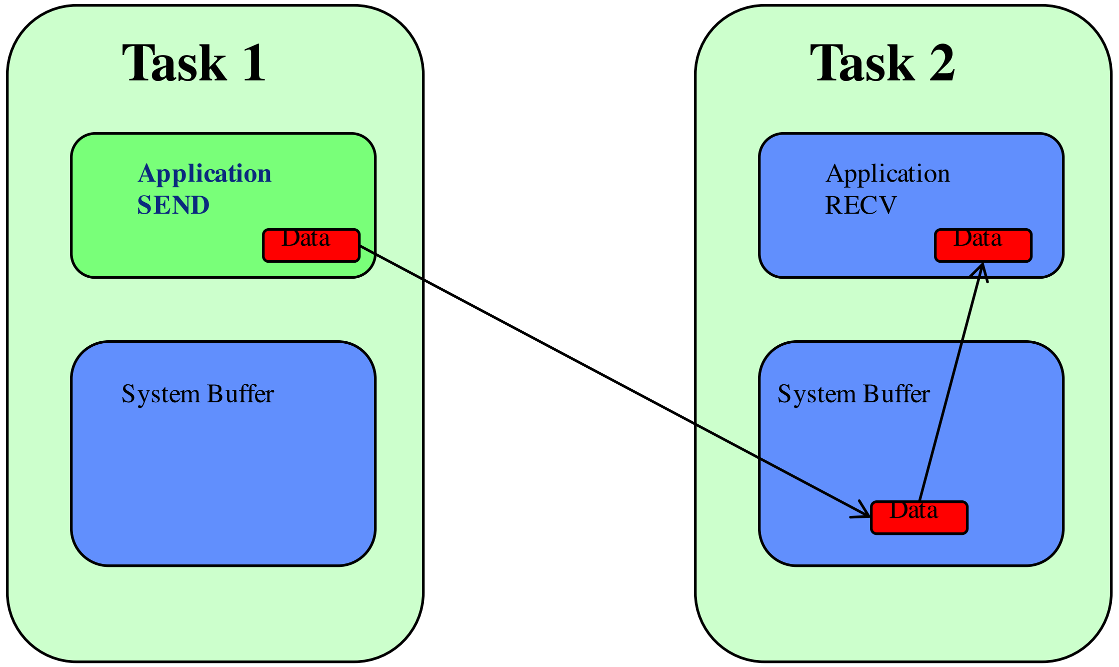
Output:

```
        Hello from MPI task= 12
        Hello from MPI task= 14
        Hello from MPI task= 8
        Hello from MPI task= 3
        Hello from MPI task= 2
        Hello from MPI task= 4
        Hello from MPI task= 13
        Hello from MPI task= 9
        Hello from MPI task= 5
        Hello from MPI task= 1
        Hello from MPI task= 11
        Hello from MPI task= 10
        Hello from MPI task= 15
        Hello from MPI task= 7
        Hello from MPI task= 6
        Hello from MPI task= 0
        Number of MPI tasks = 16
        Pi = 3.141594606714
```

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] );
      }
   }
```

Blocking Send, Recv Example

Location:$HOME/PARALLEL/PTOP

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

Submit Job: `qsub blocking.cmd`

Output: `more blocking.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
```

Deadlocking MPI Tasks

- Take care to sequence blocking send/recvs. Easy to deadlock processes waiting on each other.
- 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: `qsub deadlock.cmd`
- 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 (2 minutes in the script). Error info:

```
[gcn-9-73.sdsc.edu:mpirun_rsh][signal_processor] Caught signal 15, killing job
[gcn-9-73.sdsc.edu:mpirun_rsh][signal_processor] Caught signal 15, killing job
=>> PBS: job killed: walltime 131 exceeded limit 120
```

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: qsub deadlock-fix1.cmd**
- **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
qsub nonblocking.cmd
more nonblocking.out
        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: qsub deadlock-fix2-nb.cmd**
- **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).**

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:**
  - **qsub bcast.cmd**
- **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:**

```
qsub factorial.cmd
```

- **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:**

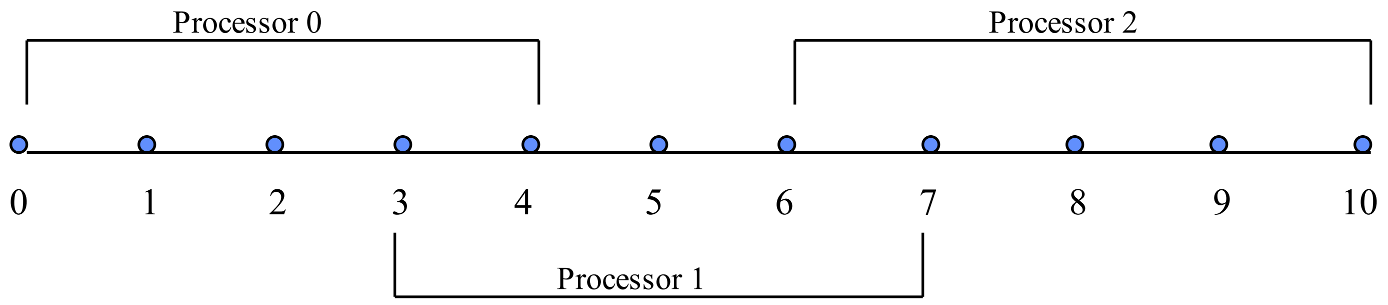
```
qsub allreduce.cmd
```

- **Output:**

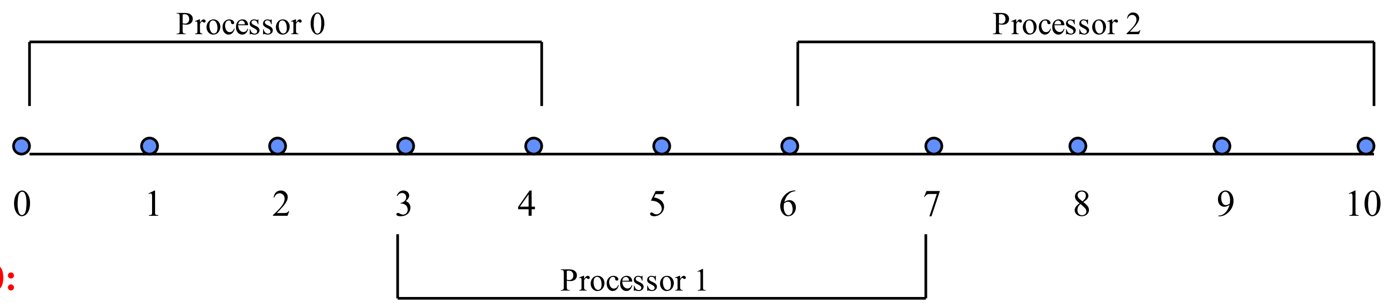
```
Max=      337897 on task           7
```

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
```

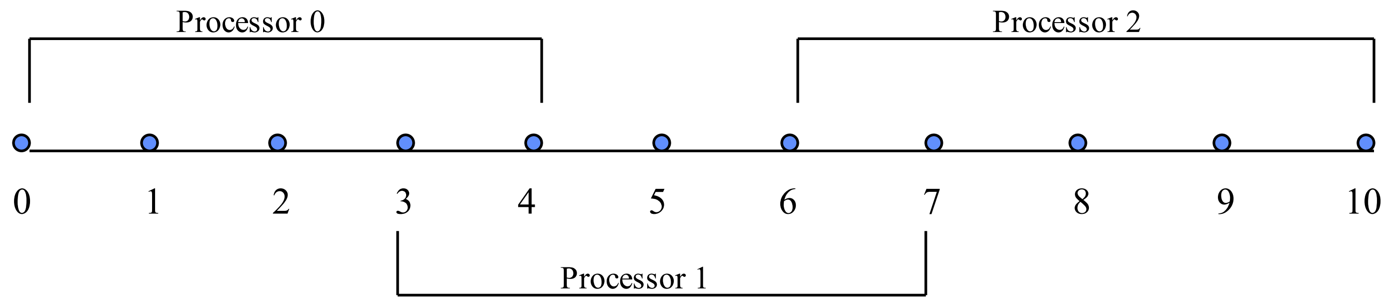
Fortran MPI Code: 1-D Heat Equation (Contd.)

```
 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



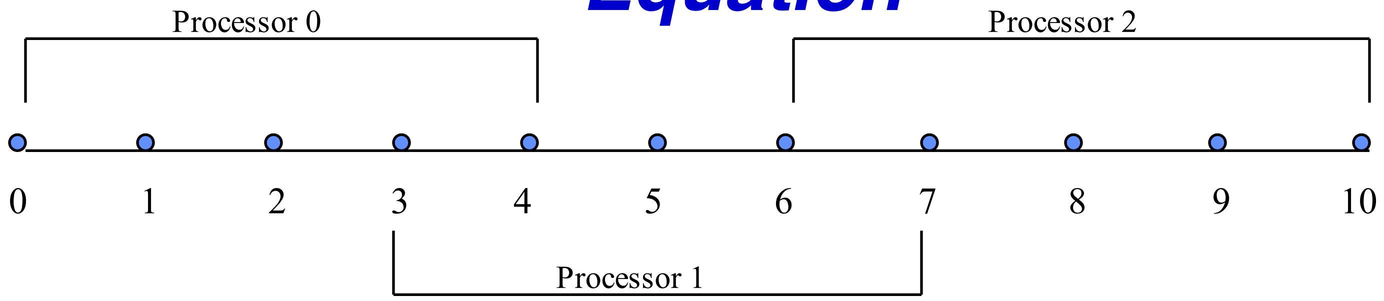
- Compilation

Fortran: mpif90 –nofree –o heat_mpi.exe heat_mpi.f90

- Run Job:

qsub heat_mpi.cmd

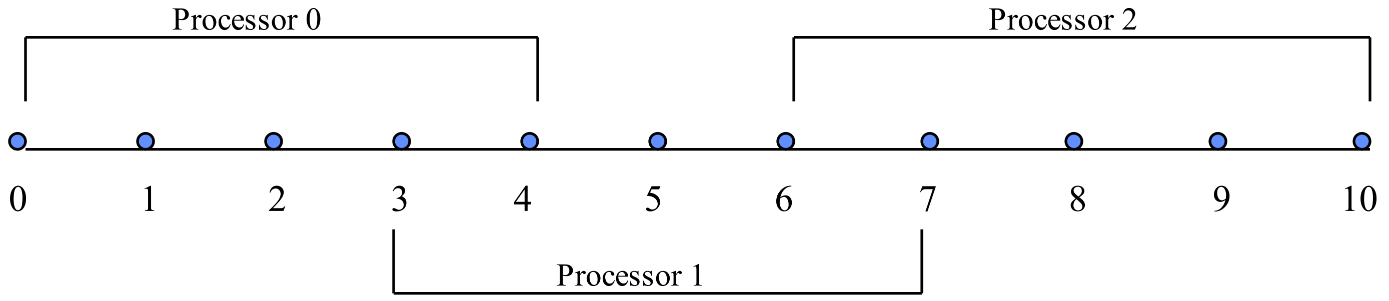
Simple Application using MPI: 1-D Heat Equation



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
```

MPI – Profiling, Tracing Tools

- Several options available. On Gordon we have mpiP, TAU, and IPM 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**

- **Compile:**

  ```
  mpif90 -nofree -g -o heat_mpi_profile.exe heat_mpi.f90 -L/home/diag/opt/mpiP/v3.4.1/lib  -lmpiP -L/opt/gnu/lib  -lbfd  -lz -liberty
  ```

- **Executable already exists. Just submit heat_mpi_profile.cmd.**

- **Once the job runs you get a .mpiP file.**

mpiP output

```
@ mpiP
@ Command : ./heat_mpi_profile.exe
@ Version                   : 3.4.1
@ MPIP Build date           : Aug  3 2014, 19:18:28
@ Start time                : 2014 08 06 08:50:44
@ Stop time                 : 2014 08 06 08:50:44
@ Timer Used                : PMPI_Wtime
@ MPIP env var              : [null]
@ Collector Rank            : 0
@ Collector PID             : 53941
@ Final Output Dir          : .
@ Report generation         : Single collector task
@ MPI Task Assignment       : 0 gcn-13-35.sdsc.edu
@ MPI Task Assignment       : 1 gcn-13-35.sdsc.edu
@ MPI Task Assignment       : 2 gcn-13-35.sdsc.edu
```

mpiP Output

```
---------------------------------------------------------------
@--- MPI Time (seconds) ------------------------------------------
---------------------------------------------------------------
Task    AppTime    MPITime     MPI%
   0     0.0702    0.00513     7.30
   1     0.0728    0.00516     7.09
   2     0.0732    0.00519     7.08
   *     0.216     0.0155     7.16
---------------------------------------------------------------
@--- Callsites: 1 -----------------------------------------------
---------------------------------------------------------------
 ID Lev File/Address        Line Parent_Funct          MPI_Call
  1   0 0x40dbf4                 main                  Send
---------------------------------------------------------------
@--- Aggregate Time (top twenty, descending, milliseconds) -------------
---------------------------------------------------------------
Call              Site      Time    App%    MPI%     COV
Send                 1       15.2   7.04   98.34    0.00
Recv                 1      0.257   0.12    1.66    0.23
```

mpiP output

```
---------------------------------------------------------------------------
@--- Aggregate Sent Message Size (top twenty, descending, bytes) ----------
---------------------------------------------------------------------------
Call             Site     Count     Total      Avrg  Sent%
Send                1        12        96         8 100.00
---------------------------------------------------------------------------
@--- Callsite Time statistics (all, milliseconds): 6 ---------------------
---------------------------------------------------------------------------
Name             Site Rank  Count      Max     Mean      Min   App%   MPI%
Recv                1    0      3    0.052   0.0233    0.008   0.10   1.37
Recv                1    1      6    0.026   0.0132    0.004   0.11   1.53
Recv                1    2      3    0.057    0.036     0.02   0.15   2.08
Send                1    0      3     5.05     1.69    0.004   7.20  98.63
Send                1    1      6     5.06    0.847    0.003   6.98  98.47
Send                1    2      3     5.07     1.69    0.004   6.93  97.92
Send                1    *     24     5.07    0.645    0.003   7.16 100.00
---------------------------------------------------------------------------
@--- Callsite Message Sent statistics (all, sent bytes) -------------------
---------------------------------------------------------------------------
Name             Site Rank   Count       Max      Mean       Min       Sum
Send                1    0       3         8         8         8        24
Send                1    1       6         8         8         8        48
Send                1    2       3         8         8         8        24
Send                1    *      12         8         8         8        96
---------------------------------------------------------------------------
@--- End of Report --------------------------------------------------------
---------------------------------------------------------------------------
```

Data Types

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

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

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:**

  ```
  mpif90 -o sample.exe sample.f
  ```

  Run: qsub sample.cmd

  See if you can identify the two bugs!

What is OpenMP?

- An API to direct multi-threaded, shared memory parallelism. Provides a Standard for a variety of shared memory architectures.
- Components – Compiler Directives, Runtime Library Routines, Environment Variables
- Can achieve parallelism with very few simple directives.
- C/C++ and Fortran support.
- Easy to use, can be incrementally implemented, at both coarse and fine grain levels.

Fork-Join Model

- OpenMP uses the fork-join model of execution.
- Programs start with a single process (master thread).
- Master thread forks parallel threads.
- Once the parallel work is done the threads synchronize and terminate leaving the master thread (JOIN).
- This can be repeated arbitrary number of times.
- No explicit parallel I/O options. Can be programmed.

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)
```

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.

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.

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);
}
```

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)

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

```
$ export OMP_NUM_THREADS=3
$ ./a.out
 There are           3 threads
 Running Iteration Number          1
 Running Iteration Number          2
 Running Iteration Number          3
           0 0.000000000000000E+000
           1  0.307205621017285
           2  0.584339815421976
           3  0.804274757358271
           4  0.945481682332598
           5  0.994138272681972
           6  0.945481682332598
           7  0.804274757358271
           8  0.584339815421977
           9  0.307205621017285
          10 0.000000000000000E+000
```

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**

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.**

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 += 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://computing.llnl.gov/tutorials/openMP/samples/Fortran/omp_mm.f

  (wget https://computing.llnl.gov/tutorials/openMP/samples/Fortran/omp_mm.f on Gordon)

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

References

- **Excellent tutorials from LLNL:**
  - https://computing.llnl.gov/tutorials/mpi/
  - https://computing.llnl.gov/tutorials/openMP/

- **MPI for Python:**
  - http://mpi4py.scipy.org/docs/usrman/tutorial.html

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