Parallel Computing Using MPI

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Current Supercomputer Architectures

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

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

Classification - Flynn's Taxonomy

- **Single Instruction, Single Data (SISD)**
  - Serial codes
- **Single Instruction, Multiple Data (SIMD)**
  - Processors run the same instructions, each operates on different data
  - Technically, Hadoop MapReduce fit this mode
  - GPUs
- **Multiple Instruction, Single Data (MISD)**
  - Multiple instructions acting on single data stream e.g. different analysis on same set of data.
- **Multiple Instruction, Multiple Data (MIMD)**
  - 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
  - Since 2006, all top 10 and most of TOP500 systems are MIMD

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

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
  - 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

Examples

- **Copy the following directory on Expanse to your home directory:**

```
cp -r /cm/shared/examples/sdsc/classes/hpctraining2022/PARALLEL  $HOME
```

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();
  }
```

Message Passing Interface (MPI)

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 mvapich2

Compile: mpicc -o pi_mpi.exe pi_mpi.c

Submit Job: sbatch pi_mpi.sb

Sample 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: sbatch 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 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).
- Error info:

srun: Job step aborted: Waiting up to 32 seconds for job step to finish.

slurmstepd: error: *** STEP 4918983.0 ON exp-1-01 CANCELLED AT 2021-08-04T21:46:24 DUE TO TIME LIMIT ***

slurmstepd: error: *** JOB 4918983 ON exp-1-01 CANCELLED AT 2021-08-04T21:46:24 DUE TO TIME LIMIT ***

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 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 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 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).

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.**

MPI Collectives

broadcast

scatter

gather

reduction

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 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  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 allreduce.sb

- **Output:**

  Max= 337897 on task 7

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

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 mvapich2
mpif90 -ffixed-form -o heat_mpi.exe  heat_mpi.f90
```

- Run Job:

```
sbatch 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
```

2D Matrix on 4 Tasks by Columns

2D Matrix on 2 Processors using submatrices

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}$$

Task 0

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \end{pmatrix}$$

Task 1

$$\begin{pmatrix} a_{13} & a_{14} \\ a_{23} & a_{24} \\ a_{33} & a_{34} \\ a_{43} & a_{44} \end{pmatrix}$$

2D Checkerboard Decomposition

- Use 2D cartesian mapping for processors
- Use 2D cartesian mapping of the data
- Allocate space on each MPI task for subarrays of A, B, and C.
- Distribute A, B, C subarrays
- Calculate local data for C
- Exchange A, B data as needed.

$$C = A\,B$$

Distributed subarrays of A

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**

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 openmpi mpip
- Compile (compile_profile.readme.txt):

  mpif90 -ffixed-form -g -o heat_mpi_profile.exe heat_mpi.f90 -L$MPIPHOME/lib -lmpiP -L/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-10.2.0/libunwind-1.4.0-2jrfg2ur46us6d3yaz44xs5c3k3bi4lx/lib -lunwind
- Executable already exists. Just submit 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(!).

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.

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

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.

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

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.

https://developer.amd.com/wp-content/resources/56338_1.00_pub.pdf

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.

https://developer.amd.com/wp-content/resources/56338_1.00_pub.pdf

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 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 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 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 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 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 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
```

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!

Exercise

- Use MPI to do the Matrix-Vector Multiplication for a Hilbert matrix. Analytic result available for verification.
- Show parallel speedup and efficiency up to 64 cores

A Hilbert matrix is a square matrix with elements that are unit fractions given by

$$H_{ij} = \frac{1}{i+j-1}$$

For example, the Hilbert matrix of dimension 4 is

$$\mathbf{H} = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$

If $\mathbf{H}$ is a Hilbert matrix of dimension $n = 122880$ and $\mathbf{x} = [1 \cdots 1]^T$ is an all-ones vector of the same dimension, compute the resultant vector $\mathbf{y} = \mathbf{H}\mathbf{x}$.

Check your result by computing the sum of the elements of $\mathbf{y}$. For $\mathbf{H}$ and $\mathbf{x}$ of dimension n, the sum of the elements of $\mathbf{y}$ is given analytically by

$$\sum_{i=1}^{n} y_i = n + \sum_{j=1}^{n-1} \frac{n-j}{n+j}.$$

Extra credit: Optimize your code and recompute for both $n = 122880$ and $n = 1048576$. Plot the parallel speedup and efficiency of your code.

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.llnl.gov/tuts/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/