Introduction to Parallel Programming with MPI

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Why Parallel Computing?

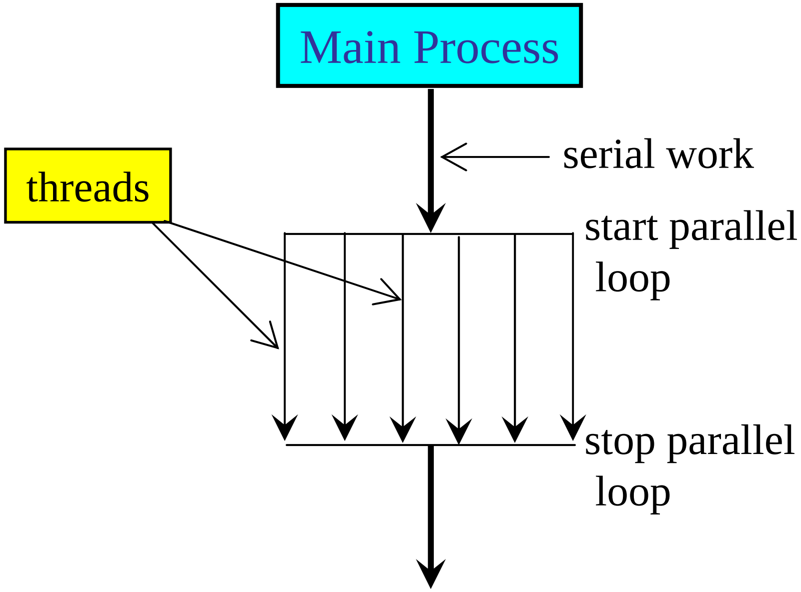
- Want to speed up a calculation.
- Solution:
  - Split the work between several processors.
- How?
  - It depends on the type of parallel computer
    - Shared memory (usually thread-based)
    - Distributed memory (process-based)
  - MPI works on all of them!

Shared memory parallelism

- Program runs inside a single process
- Several “execution threads” are created within that process and work is split between them.
- The threads run on different processors.
- All threads have access to the shared data through shared memory access.
- Must be careful not the have threads overwrite each other’s data.

Shared memory programming

- Easy to do loop-level parallelism.
- Compiler-based automatic parallelization
  - Easy but not always efficient
  - Better to do it yourself with OpenMP
- Coarse-grain parallelism can be difficult



Distributed memory parallelism

- Process-based programming.
- Each process has its own memory space that cannot be accessed by the other processes.
- The work is split between several processes.
- For efficiency, each processor runs a single process.
- Communication between the processes must be explicit, e.g. Message Passing

How to split the work between processors?

- Most widely used method for grid-based calculations:
  - **DOMAIN DECOMPOSITION**
- Split particles in particle-in-cell (PIC) or molecular dynamics codes.
- Split arrays in PDE solvers
- etc…
- Keep it LOCAL

What is MPI?

- MPI stands for Message Passing Interface.
- It is a message-passing specification, a standard, for the vendors to implement.
- In practice, MPI is a set of functions (C) and subroutines (Fortran) used for exchanging data between processes.
- An MPI library exists on most, if not all, parallel computing platforms so it is highly portable.

How much do I need to know?

- MPI is small (6 functions)
  - Many parallel programs can be written with just 6 basic functions.
- MPI is large (125 functions)
  - MPI's extensive functionality requires many functions
  - Number of functions not necessarily a measure of complexity
- MPI is just right
  - One can access flexibility when it is required.
  - One need not master all parts of MPI to use it.

How MPI works

- Launch the parallel calculation with:

```
mpirun –np #proc a.out
mpiexec –n #proc a.out
```

- Copies of the same program run on each processor within its own process (private address space).
- Each processor works on a subset of the problem.
- Exchange data when needed
  - Can be exchanged through the network interconnect
  - Or through the shared memory on SMP machines (Bus?)
- Easy to do coarse grain parallelism = scalable

Good MPI web sites

- http://www.llnl.gov/computing/tutorials/mpi/
- http://www.nersc.gov/nusers/help/tutorials/mpi/intro/
- http://www-unix.mcs.anl.gov/mpi/tutorial/gropp/talk.html
- http://www-unix.mcs.anl.gov/mpi/tutorial/

- MPI on Linux clusters:
  - MPICH (http://www-unix.mcs.anl.gov/mpi/mpich/)
  - Open MPI (http://www.open-mpi.org/)

Structure of an MPI program

```
Program mpi_code
  ! Load MPI definitions
    use mpi (or include mpif.h)

  ! Initialize MPI
    call MPI_Init(ierr)
  ! Get the number of processes
    call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  ! Get my process number (rank)
    call MPI_Comm_rank(MPI_COMM_WORLD,myrank,ierr)

    Do work and make message passing calls…

  ! Finalize
    call MPI_Finalize(ierr)

end program mpi_code
```

Fortran 90 Style!…

Structure of an MPI program

```
#include "mpi.h"
int main( int argc, char *argv[] )
{
  int nproc, myrank;
  /* Initialize MPI */
    MPI_Init(&argc,&argv);
  /* Get the number of processes */
    MPI_Comm_size(MPI_COMM_WORLD,&nproc);
  /* Get my process number (rank) */
    MPI_Comm_rank(MPI_COMM_WORLD,&myrank);

    Do work and make message passing calls…

  /* Finalize */
    call MPI_Finalize();
 return 0;
}
```

C
Style!…

Compilation

- mpich provides scripts that take care of the include directories and linking libraries
  - mpicc
  - mpiCC
  - mpif77
  - mpif90
- Otherwise, must link with the right MPI library

Makefile

- Always a good idea to have a Makefile

```
%cat Makefile
CC=mpicc
CFLAGS=-O

% : %.c
      $(CC) $(CFLAGS) $< -o $@
```

mpirun and mpiexec

- Both are used for starting an MPI job
- If you don’t have a batch system, use mpirun

```
_  mpirun -np #proc -machinefile mfile a.out >& out < in &

   %cat mfile
    machine1.princeton.edu
    machine2.princeton.edu
    machine3.princeton.edu
    machine4.princeton.edu
```

- PBS usually takes care of arguments to mpiexec

Batch System: PBS primer

- Submit a job script: qsub script
- Check status of jobs: qstat –a   (for all jobs)
- Stop a job: qdel job_id

```
###  --- PBS SCRIPT  ---
#PBS –l nodes=4:ppn=2,walltime=02:00:00
#PBS –q dque
#PBS –V
#PBS –N job_name
#PBS –m abe
cd $PBS_O_WORKDIR
mpiexec –np 8 a.out
```

Basic MPI calls to exchange data

Point to point: **2 processes at a time**

```
MPI_Send(buf,count,datatype,dest,tag,comm,ierr)

MPI_Recv(buf,count,datatype,source,tag,comm,status,ierr)
```

```
MPI_Sendrecv(sendbuf,sendcount,sendtype,dest,sendtag,
    recvbuf,recvcount,recvtype,source,recvtag,comm,status,ierr)
```

where types are: **MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION,
MPI_COMPLEX, MPI_CHARACTER, MPI_LOGICAL, etc…**

Predefined Communicator: **MPI_COMM_WORLD**

Collective MPI calls

Collective calls: **All processes participate**

One process sends to everybody:

```
MPI_Bcast(buffer,count,datatype,root,comm,ierr)
```

All processes send to “root” process and the operation “op” is applied

```
MPI_Reduce(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

where **op** = **MPI_SUM, MPI_MAX, MPI_MIN, MPI_PROD, etc…**

You can create your own reduction operation with **MPI_Op_create()**

All processes send to everybody and apply the operation “op”(equivalent to an MPI_Reduce followed by an MPI_Bcast)

```
MPI_Allreduce(sendbuf,recvbuf,count,datatype,op,comm,ierr)
```

Synchronize all processes

```
MPI_Barrier(comm,ierr)
```

More MPI collective calls

All processes send a different piece of data to one single "root" process which gathers everything (messages ordered by index)

```
MPI_Gather(sendbuf,sendcnt,sendtype,recvbuf,recvcount,
            recvtype,root,comm,ierr)
```

All processes gather everybody else's pieces of data

```
MPI_Allgather(sendbuf,sendcount,sendtype,recvbuf,recvcount,
               recvtype,comm,info)
```

One "root" process send a different piece of the data to each one of the other processes

```
MPI_Scatter(sendbuf,sendcnt,sendtype,recvbuf,recvcnt,
            recvtype,root,comm,ierr)
```

Each process performs a scatter operation, sending a distinct message to all the processes in the group in order by index.

```
MPI_Alltoall(sendbuf,sendcount,sendtype,recvbuf,recvcnt,
              recvtype,comm,ierr)
```