CME 213
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PARALLEL PROGRAMMING USING MESSAGE PASSING
Why MPI?

- Shared memory is a good model for a small number of processes.
- The main difficulty is ensuring a consistent view of memory as threads read and write to memory.
- This can scale to many cores but beyond ~ 100s, it does not work anymore.
- Instead, we need to switch to computer nodes connected through a network.
- In that case, the memory becomes distributed.
- Processes need to communicate explicitly. This can be done using MPI.
- MPI is the standard for distributed memory computing.
Flynn’s taxonomy

We have seen the following different types of parallelism:

**SIMD: single instruction multiple data**
- All processing units execute the same instruction at any given clock cycle.
- Each processing unit can operate on a different data element.
- This applies for example to a GPU streaming multiprocessor.
- The thread index is used to determine which data the thread operates with.

**MIMD: multiple instruction, multiple data**
- Every processor executes a different instruction stream.
- Every processor works with a different data stream.
- This applies to Pthreads for example. Threads can execute different routines.

**MPI follows this model.**
Parallel computer memory architecture

Shared memory: all cores can read and write to the same memory space
CUDA, Pthreads, OpenMP

Distributed memory:
- Cores read and write to different memory spaces
- If a core needs data in some other memory space, explicit communication is required

MPI

Network

Core 0 - Memory 0 - Core 2 - Memory 2
Core 1 - Memory 1 - Core 3 - Memory 3
Core 0 - Memory 0
Core 1 - Memory 1
Core 2 - Memory 2
Core 3 - Memory 3
Core 0 - Memory 0
Core 1 - Memory 1
Core 2 - Memory 2
Core 3 - Memory 3
MPI: message passing interface

- All processes run the same program. This is a MIMD system.
- Processes are assigned a rank.
- Based on the rank, processes perform calculations on different data.
- Processes communicate by sending and receiving messages.
- Message passing:
  - Data transfer requires cooperative operations to be performed by each process.
  - For example, a send operation must have a matching receive operation.

Communication: Sending Messages
OUR FIRST MPI PROGRAM
MPI implementations

- **MVAPICH**: mvapich.cse.ohio-state.edu
- **MPICH**: www.mpich.org
- **OpenMPI**: www.open-mpi.org

- Download your favorite implementation and install it!
- You can test MPI using a multicore computer.
- Each process runs on its own core.
MPI on Certainty

- How can you run an MPI code?
- You start a single command that spawns multiple programs running on one or multiple nodes.

.bashrc:
module load mvapich2/2.3a-intel-16

MVAPICH2 user guide

Compile with:
mpic++
How to run

Run program on 8 processors

\texttt{mpirun\_rsh -np 8 -hostfile $PBS\_NODEFILE ./mpi\_hello}

or

\texttt{mpirun -np 4 ./mpi\_hello}

Works only with less than 24 processes (MVAPICH issue on Certainty)
// Some MPI magic to get started
MPI_Init(&argc, &argv);

// How many processes are running
int numtasks;
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
// What's my rank?
int taskid;
MPI_Comm_rank(MPI_COMM_WORLD, &taskid);
// Which node am I running on?
int len;
char hostname[MPI_MAX_PROCESSOR_NAME];
MPI_Get_processor_name(hostname, &len);

printf("Hello from task %2d running on node: %s\n", taskid, hostname);

// Only one processor will do this
if(taskid == MASTER) {
    printf("MASTER process: the number of MPI tasks is: %2d\n",numtasks);
}

// Close down all MPI magic
MPI_Finalize();
Hello from task 7 running on node: gpu-205-3.local
Hello from task 6 running on node: gpu-205-3.local
Hello from task 1 running on node: gpu-205-3.local
Hello from task 4 running on node: gpu-205-3.local
Hello from task 0 running on node: gpu-205-3.local
Hello from task 5 running on node: gpu-205-3.local
MASTER process: the number of MPI tasks is: 8
Hello from task 2 running on node: gpu-205-3.local
Hello from task 3 running on node: gpu-205-3.local
The work gets distributed across multiple nodes if you need more than 24 cores.
Example

- Example code:
  - `mpi_hello.c`  `mpi_pi_send.c`
- `mpi_pi_send`: calculates $\pi$ by throwing darts, i.e., one draws two uniform random numbers $(x,y)$ in the $(0,1)$ interval and calculates how many, on average, fall inside the 2D unit circle. From this average, $\pi$ can be estimated.
- We will see later on how to do this better using collective communications.
for(int i = 0; i < ROUND; i++) {
    double my_pi = DartBoard(DARTS);
    if(taskid != MASTER) {
        int tag = i;
        int rc = MPI_Send(&my_pi, 1, MPI_DOUBLE,
                        MASTER, tag, MPI_COMM_WORLD);
    } else {
        int tag = i;
        double pisum = 0;
        for(int n = 1; n < numtasks; n++) {
            double pirecv;
            MPI_Status status;
            int rc = MPI_Recv(&pirecv, 1, MPI_DOUBLE, MPI_ANY_SOURCE,
                               tag, MPI_COMM_WORLD, &status);
            pisum += pirecv;
        }
        double pi = (pisum + my_pi)/numtasks;
        printf("    pi for this round = %10.8f\n", pi);
        avepi = ((avepi * i) + pi)/(i + 1);
        printf("    After %8d throws, average value of pi = %10.8f\n",
               (DARTS * (i + 1) * numtasks), avepi);
    }
}
MPI task 7 has started on gpu-205-2.local [total number of processors 8]
MPI task 6 has started on gpu-205-2.local [total number of processors 8]
MPI task 0 has started on gpu-205-2.local [total number of processors 8]
MPI task 3 has started on gpu-205-2.local [total number of processors 8]
MPI task 4 has started on gpu-205-2.local [total number of processors 8]
MPI task 5 has started on gpu-205-2.local [total number of processors 8]
MPI task 1 has started on gpu-205-2.local [total number of processors 8]
MPI task 2 has started on gpu-205-2.local [total number of processors 8]

After 40000000 throws, average value of pi = 3.14189700
After 80000000 throws, average value of pi = 3.14156450
After 120000000 throws, average value of pi = 3.14163733
After 160000000 throws, average value of pi = 3.14153375
After 200000000 throws, average value of pi = 3.14150340
After 240000000 throws, average value of pi = 3.14158200
After 280000000 throws, average value of pi = 3.14155329
After 320000000 throws, average value of pi = 3.14160950
After 360000000 throws, average value of pi = 3.14149211
After 400000000 throws, average value of pi = 3.14149820

Exact value of pi: 3.1415926535897
mpi_pi_send

- 4 identical programs are running.
- Depending on taskid, cores do different things.
- A send/recv pair is used to exchange data.
- Messages can arrive in any order.
- The use of a tag ensures that master will wait for all messages corresponding to a given round before printing the approximation.
Send

```c
int MPI_Send(void *smessage, int count,
               MPI_Datatype datatype, int dest,
               int tag,
               MPI_Comm comm)
```

- **smessage** buffer which contains the data elements to be sent
- **count** number of elements to be sent
- **datatype** data type of entries
- **dest** rank of the target process
- **tag** message tag which can be used by the receiver to distinguish between different messages from the same sender
- **comm** communicator used for the communication (more on this later)
Recv

int MPI_Recv(void *rmessage, int count,
              MPI_Datatype datatype, int source,
              int tag, MPI_Comm comm,
              MPI_Status *status)

- Same as before.
- New argument: `status` data structure that contains information about the message that was received.
## MPI data types

<table>
<thead>
<tr>
<th>MPI data type</th>
<th>C data type</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_CHAR</td>
<td>signed char</td>
</tr>
<tr>
<td>MPI_SHORT</td>
<td>signed short int</td>
</tr>
<tr>
<td>MPI_INT</td>
<td>signed int</td>
</tr>
<tr>
<td>MPI_LONG</td>
<td>signed long int</td>
</tr>
<tr>
<td>MPI_LONGLONG_INT</td>
<td>long long int</td>
</tr>
<tr>
<td>MPI_UNSIGNED_CHAR</td>
<td>unsigned char</td>
</tr>
<tr>
<td>MPI_UNSIGNED_SHORT</td>
<td>unsigned short int</td>
</tr>
<tr>
<td>MPI_UNSIGNED</td>
<td>unsigned int</td>
</tr>
<tr>
<td>MPI_UNSIGNED_LONG</td>
<td>unsigned long int</td>
</tr>
<tr>
<td>MPI_UNSIGNED_LONG_LONG_LONG</td>
<td>unsigned long long long int</td>
</tr>
<tr>
<td>MPI_FLOAT</td>
<td>float</td>
</tr>
<tr>
<td>MPI_DOUBLE</td>
<td>double</td>
</tr>
<tr>
<td>MPI_LONG_DOUBLE</td>
<td>long double</td>
</tr>
<tr>
<td>MPI_WCHAR</td>
<td>wide char</td>
</tr>
<tr>
<td>MPI_PACKED</td>
<td>special data type for packing</td>
</tr>
<tr>
<td>MPI_BYTE</td>
<td>single byte value</td>
</tr>
</tbody>
</table>
How does it work?

- Each **Send** must be matched with a corresponding **Recv**.
- **Order**: messages are delivered in the order in which they have been sent.
- If a sender sends two messages of the same type one after another to the same receiver, the MPI runtime system ensures that the first message sent is always received first.
COLLECTIVE COMMUNICATIONS
Point-to-point vs collective

• What we have discussed so far is point-to-point communication, that is one process communicates with another process.

• All communications can be ultimately broken down into this type of exchanges.

• Nevertheless, let’s say that we have a group of processes that need to exchange data. For example we want to do a reduction.

• This is called a collective communication, i.e., multiple processes need to communicate.

• In that case, for best performance, we need to orchestrate the communication. Simply having each process send its data to the master node is inefficient.
There is an optimal routing algorithm to bring all the goods to the same place while minimizing mileage and gas.
Network and highways

- Think of a computer network as a network of highways.
- Each highway has a number of lanes and a maximum traffic it can support. This is the bandwidth.
- If all the cars in the bay area decide to take US 101 at the same time, you get a huge traffic jam.
- Computer network is the same. You cannot have too many messages traveling across the same wire of the network. There is a maximum bandwidth that each wire in the network can support.
- Depending on the network topology, there is an optimal algorithm to route the messages in order to minimize the total wall clock time of the collective communication.
- There are three key issues:
  - These communication algorithms can be complicated.
  - They depend on the network topology.
  - There are relatively few collective communication patterns that get reused over and over again.
Collective communications

- MPI provides a library of collective communications.
- It covers 99% of the use cases.
- For the rest, we still have point-to-point.
- All these operations are blocking.
Single broadcast

The simplest communication: one process sends a piece of data to all other processes.

```
int MPI_Bcast(void *message, int count,
              MPI_Datatype type, int root,
              MPI_Comm comm)
```

```
P_1 : [x]  P_1 : [x]
P_2 : [  ]  P_2 : [x]
    broadcast

P_p : [  ]  P_p : [x]
```
Single accumulation

- Each process provides a block of data with the same type and size.
- When performing the operation, a reduction operation is applied element by element to the data blocks provided by the processes.
- The resulting accumulated data block is collected at a specific root process.

```c
int MPI_Reduce(void *sendbuf, void *recvbuf,
                int count, MPI_Datatype type, MPI_Op op,
                int root, MPI_Comm comm)
```

\[
P_1 : x_1 \\
P_2 : x_2 \\
\vdots \\
P_p : x_p
\]

\[
P_1 : x_1 + x_2 + \cdots + x_p \\
P_2 : x_2 \\
\vdots \\
P_p : x_p
\]
<table>
<thead>
<tr>
<th>Representation</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_MAX</td>
<td>Maximum</td>
</tr>
<tr>
<td>MPI_MIN</td>
<td>Minimum</td>
</tr>
<tr>
<td>MPI_SUM</td>
<td>Sum</td>
</tr>
<tr>
<td>MPI_PROD</td>
<td>Product</td>
</tr>
<tr>
<td>MPI_LAND</td>
<td>Logical and</td>
</tr>
<tr>
<td>MPI_BAND</td>
<td>Bit-wise and</td>
</tr>
<tr>
<td>MPI_LOR</td>
<td>Logical or</td>
</tr>
<tr>
<td>MPI_BOR</td>
<td>Bit-wise or</td>
</tr>
<tr>
<td>MPI_LXOR</td>
<td>Logical exclusive or</td>
</tr>
<tr>
<td>MPI_BXOR</td>
<td>Bit-wise exclusive or</td>
</tr>
<tr>
<td>MPI_MAXLOC</td>
<td>Maximum value and corresponding index</td>
</tr>
<tr>
<td>MPI_MINLOC</td>
<td>Minimum value and corresponding index</td>
</tr>
</tbody>
</table>
Code example

mpi_prime.C

- Computing prime numbers in parallel.
- We want to compute the total number of primes smaller than \( N \) and the largest prime smaller than \( N \).
for(int n=mystart; n<=LIMIT; n+=stride) {
    if(IsPrime(n)) {
        pc++; // found a prime
        foundone = n; // last prime that we have found
    }
}

// Total number of primes found by all processes: MPI_SUM
MPI_Reduce(&pc, &pcsum, 1, MPI_INT, MPI_SUM, MASTER, MPI_COMM_WORLD);

// The largest prime that was found by all processes: MPI_MAX
MPI_Reduce(&foundone, &maxprime, 1, MPI_INT, MPI_MAX, MASTER, MPI_COMM_WORLD);
## Scalability

<table>
<thead>
<tr>
<th>Processors</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 processor</td>
<td>3.56 s</td>
</tr>
<tr>
<td>2 processors</td>
<td>1.81 s</td>
</tr>
<tr>
<td>4 processors</td>
<td>0.93 s</td>
</tr>
<tr>
<td>24 processors</td>
<td>0.46 s</td>
</tr>
<tr>
<td>36 processors</td>
<td>0.30 s</td>
</tr>
<tr>
<td>48 processors</td>
<td>0.26 s</td>
</tr>
</tbody>
</table>

Multiple nodes are used
Gather/Scatter

\[ P_1 : x_1 \quad P_1 : x_1 \parallel x_2 \parallel \cdots \parallel x_p \]
\[ P_2 : x_2 \quad P_2 : x_2 \]
\[ \vdots \quad \text{gather} \quad \vdots \]
\[ P_p : x_p \quad P_p : x_p \]

\[ \text{MPI\_Gather()} \]

\[ P_1 : x_1 \parallel x_2 \parallel \cdots \parallel x_p \]
\[ P_2 : - \quad P_2 : x_2 \]
\[ \vdots \quad \text{scatter} \quad \vdots \]
\[ P_p : - \quad P_p : x_p \]

\[ \text{MPI\_Scatter()} \]
MPI and your final project

Layer 0  Layer 1  Layer 2

Input x1 →

Input x2 →

Input x3 →

Input x4 →
Parallelizing over input images

- Split your set of input images.
- Assign each subset to an MPI process.
- MPI process needs to:
  - **Compute the feed-forward**
  - This means: a sequence of **GEMM** followed by **sigmoid/softmax** functions.
  - **Compute the back-propagation**: derivative of error with respect to each NN coefficient. More GEMMs.
MPI_Scatter

Two options:

1. Each MPI process reads from file its own subset of images.

2. Rank 0 process reads data from file. `MPI_Scatter()` used to send data from rank 0 to all other MPI ranks.
Multi-broadcast/multi-accumulation

\[
P_1 : \begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_p \end{array} \quad P_1 : \begin{array}{c} x_1 \parallel x_2 \parallel \cdots \parallel x_p \end{array} \\
P_2 : \begin{array}{c} x_1 \parallel x_2 \parallel \cdots \parallel x_p \end{array} \quad P_2 : \begin{array}{c} x_1 \parallel x_2 \parallel \cdots \parallel x_p \end{array} \\
P_p : \begin{array}{c} x_p \end{array} \quad P_p : \begin{array}{c} x_1 \parallel x_2 \parallel \cdots \parallel x_p \end{array}
\]

\text{MPI\_Allgather()}

\[
P_1 : \begin{array}{c} x_{11} \parallel x_{12} \parallel \cdots \parallel x_{1p} \end{array} \quad P_1 : \begin{array}{c} x_{11} + x_{21} + \cdots + x_{p1} \end{array} \\
P_2 : \begin{array}{c} x_{21} \parallel x_{22} \parallel \cdots \parallel x_{2p} \end{array} \quad P_2 : \begin{array}{c} x_{12} + x_{22} + \cdots + x_{p2} \end{array} \\
P_p : \begin{array}{c} x_{p1} \parallel x_{p2} \parallel \cdots \parallel x_{pp} \end{array} \quad P_p : \begin{array}{c} x_{1p} + x_{2p} + \cdots + x_{pp} \end{array}
\]

\text{MPI provides a restricted version: MPI\_Allreduce(), which is a reduction followed by a broadcast.}
Project: back-propagation and gradient of error

- The error is of the form:

\[
J(W, b; x, y) = \frac{1}{N} \sum_{i=1}^{N} CE^{(i)}(y, \hat{y}) + 0.5 \lambda \|p\|^2
\]

- A simple **sum** over all images!
- Hence, each \( \Delta W \) is simply a **sum over each image subset**.
- MPI communication required: each process has a partial \( \Delta W \).
- Add them up and broadcast the result.
- This is an **MPI_Allreduce()** operation.
Code example

```cpp
proc_min_value.C
mpirun_rsh -np 4 -hostfile $PBS_NODEFILE ./proc_min_value
```

Calculates the minimum value across all processes and the rank of the process that holds the minimum.

This may be important if you need that process to send more data to the other processes (e.g., a broadcast).

Example that illustrates:
- **MPI_Allreduce** reduction + broadcast.
- **MPI_MINLOC** takes the minimum value + value attached to the minimum (in this example the rank of the process).
- **MPI_Barrier** processes wait until all processes have reached that point. (This is only moderately useful in practice.)
```c
int localres[2];
int globalres[2];

// Compute the minimum of localarr and store the result in localres[0]
localres[0] = localarr[0];
for(int i=1; i<locn; i++)
    if(localarr[i] < localres[0]) {
        localres[0] = localarr[i];
    }

// The second entry is the rank of this process.
localres[1] = rank;
MPI_Allreduce(localres, globalres, 1, MPI_2INT, MPI_MINLOC, MPI_COMM_WORLD);
```
<table>
<thead>
<tr>
<th>Rank</th>
<th>Has values:</th>
<th>8071</th>
<th>1347</th>
<th>839</th>
<th>2390</th>
<th>5379</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rank</td>
<td>1</td>
<td>8542</td>
<td>1166</td>
<td>3510</td>
<td>7451</td>
<td>2227</td>
</tr>
<tr>
<td>Rank</td>
<td>2</td>
<td>4341</td>
<td>4158</td>
<td>6383</td>
<td>1559</td>
<td>1566</td>
</tr>
<tr>
<td>Rank</td>
<td>3</td>
<td>2437</td>
<td>1848</td>
<td>4815</td>
<td>1564</td>
<td>2616</td>
</tr>
</tbody>
</table>

Rank 0 has the lowest value of 839

Rank 0 has received the value: 839
Rank 1 has received the value: 839
Rank 3 has received the value: 839
Rank 2 has received the value: 839
Total exchange

\[
\begin{align*}
P_1 & : \begin{array}{c|c|c|c}
  x_{11} \parallel x_{12} & \cdots & \parallel x_{1p} \\
  x_{21} & x_{22} & \cdots & x_{2p} \\
  \vdots & \vdots & \ddots & \vdots \\
  x_{p1} & x_{p2} & \cdots & x_{pp}
\end{array} \\
\end{align*}
\]

\[
\begin{align*}
P_2 & : \begin{array}{c|c|c|c}
  x_{11} & x_{21} & \cdots & x_{p1} \\
  x_{12} & x_{22} & \cdots & x_{p2} \\
  \vdots & \vdots & \ddots & \vdots \\
  x_{1p} & x_{2p} & \cdots & x_{pp}
\end{array} \\
\end{align*}
\]

\[\text{total exchange}\]  

\[
\begin{align*}
P_1 & : \begin{array}{c|c|c|c}
  x_{11} \parallel x_{12} & \cdots & \parallel x_{1p} \\
  x_{21} & x_{22} & \cdots & x_{2p} \\
  \vdots & \vdots & \ddots & \vdots \\
  x_{p1} & x_{p2} & \cdots & x_{pp}
\end{array} \\
\end{align*}
\]

\[
\begin{align*}
P_2 & : \begin{array}{c|c|c|c}
  x_{11} & x_{21} & \cdots & x_{p1} \\
  x_{12} & x_{22} & \cdots & x_{p2} \\
  \vdots & \vdots & \ddots & \vdots \\
  x_{1p} & x_{2p} & \cdots & x_{pp}
\end{array} \\
\end{align*}
\]

\[\text{MPI\_Alltoall()}
\]

Similar to a matrix transpose!
CONCEPTUAL RELATIONS BETWEEN COLLECTIVE COMMUNICATIONS
Duality

- Some communication operations are dual of each other.
- Communication operations are **dual** if one can be obtained by reversing the direction and the sequence of communication of the other.

Left: single-broadcast operation using a spanning tree.
Right: single-accumulation that uses the same communication tree.
Relation between collective communication operations

Important to understand performance and if you are interested in how these collective communication operations can be implemented.

Specialization, e.g., multi-broadcast is the same as total exchange if the p data blocks of a process are the same.