PARALLEL PROGRAMMING...

Parallel Programming: Overview

SESSION 2/3

GOAL

Programming Interface for parallel computing

MPI (Message Passing Interface)

OpenMP (Open Multi-Processing)

Programming interface for parallel computing

병렬 컴퓨팅을 위한 프로그래밍 인터페이스

Programming interface…

Remember

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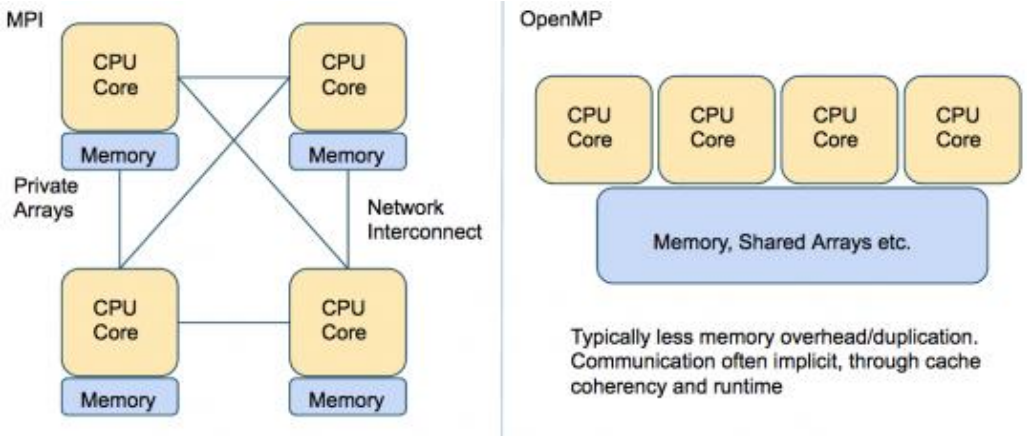

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MPI (Message Passing Interface) is a multi-process model whose mode of communication between the processes is **explicit.**

==> communication management is the responsibility of the user.

.

OpenMP (Open Multi-Processing) is a multitasking model whose mode of communication between tasks is **implicit**

==> communications is the responsibility of the compiler.

MPI (Message Passing Interface)

MPI

MPI (Message Passing Interface)

MPI is a library of subroutines (in Fortran,C, C++)

Allows the coordination of a program running as multiple processes in a distributed-memory environment.

Flexible enough to also be used in a shared-memory environment.

Can be used and compiled on a wide variety of single platforms or (homogeneous or heterogeneous) clusters of computers over a network.

The scalability of MPI is not limited by the number of processors/cores on one computation node, as opposed to shared memory parallel models.

MPI library is standardized, should work (without further changes!)
on any machine on which the MPI library is installed.

MPI: Basic Environment

MPI programs start with a function call which initializes the message passing library.

```
MPI_Init(&argc, &argv)
```

Initializes MPI environment
Must be called in every MPI program
Must be first MPI call
Can be used to pass command line arguments to all

```
MPI_Finalize()
```

Terminates MPI environment
Last MPI function call

MPI: Basic Environment

```
MPI_Comm_rank(comm, &rank)
```

Returns the rank of the calling MPI process
Within the communicator, comm
MPI_COMM_WORLD is set during Init(...)
Other communicators can be created if needed

```
MPI_Comm_size(comm, &size)
```

Returns the total number of processes
Within the communicator, comm

```
int my_rank, size;
MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
```

MPI: Point-to-Point Communication

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

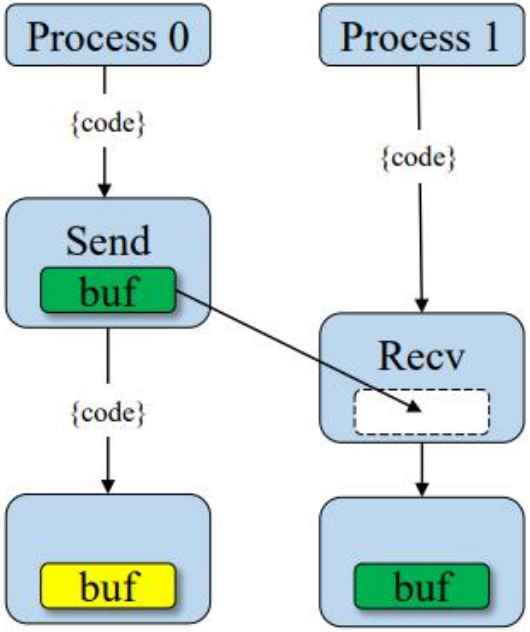
Send a message
Returns only after buffer is free for reuse
Blocking

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

Received a message
Returns only when the data is avaible
Blocking

```
MPI_SendRecv(...)
```

Two way communication
Blocking



MPI: Point-to-Point Communication

Blocking

- Only returns after completed
  - Received: data has arrived and ready to use
  - Send: safe to reuse sent buffer
- Be aware of deadlocks !!!
- Tip: use when possible

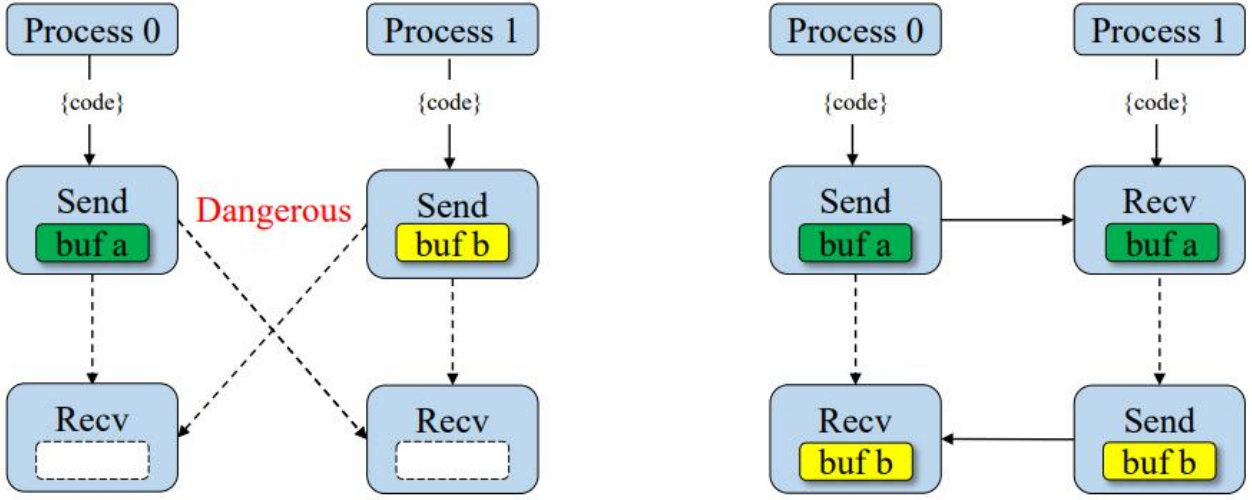
Non-Blocking

- returns immediately
  - Unsafe to modify buffers until operation is known to be complete
- Allows computation and communication to overlap
- Tip: Use only when needed

MPI: Deadlock

Blocking calls can **results in deadlock**

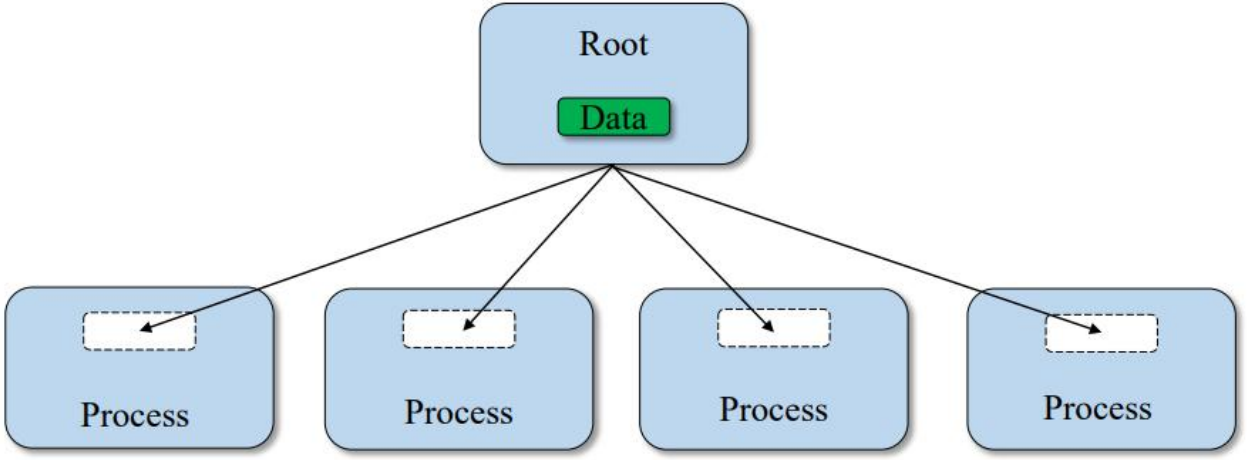
One process is waiting for message that will never arrive
Only option is to abort the interrupt/kill the code (CTRL-c)
Might not always deadlock - depends on size of system buffer



MPI: Coolective Communication (BCast)

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

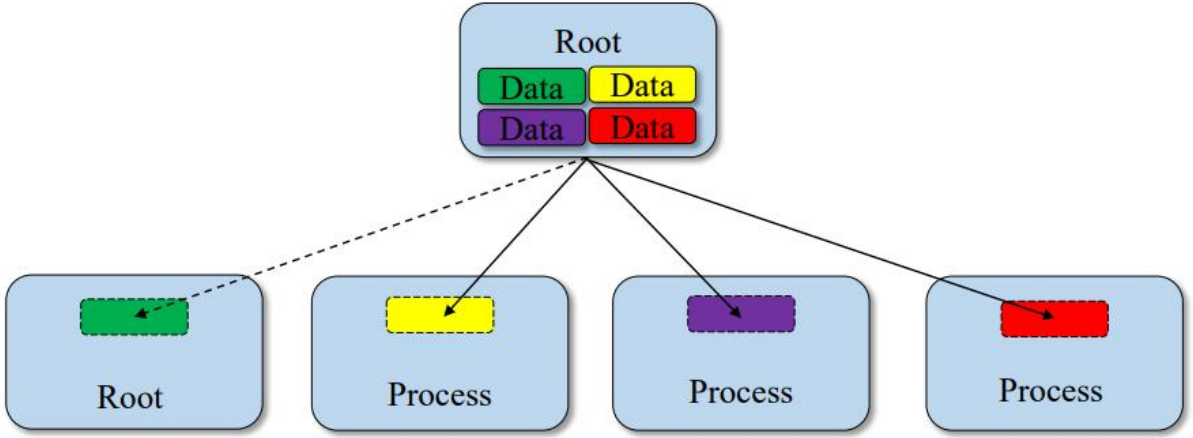
Broadcast a message from the root process to all other processes.
Useful when reading in input parameters from file.



MPI: Collective Communication (Scatter)

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

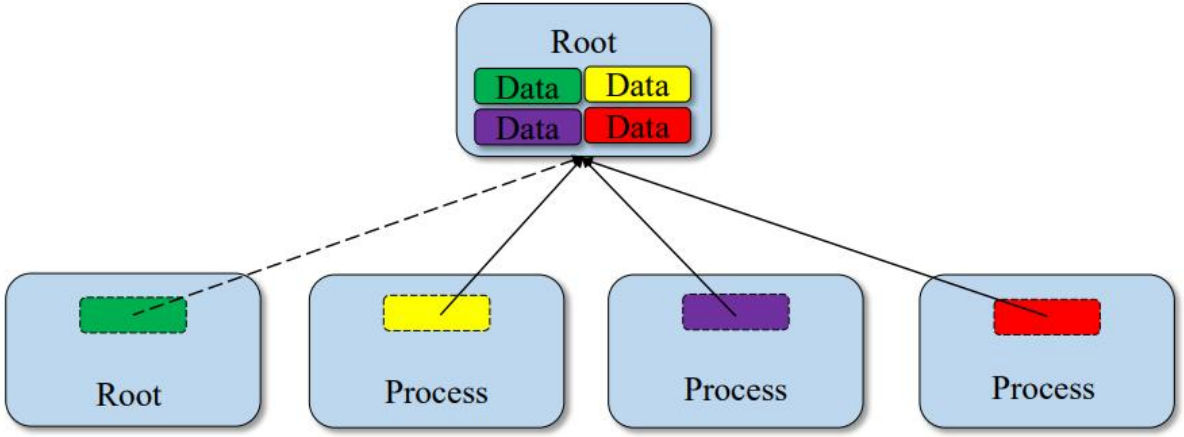
Sends individual messages from the root process to all other processes.



MPI: Collective Communication (Gather)

```
MPI_Gather(&sendbuf, sendcnt, sendtype, &recvbuf,
           recvcnt, recvtype, root, comm)
```

Opposite of **Scatter.**



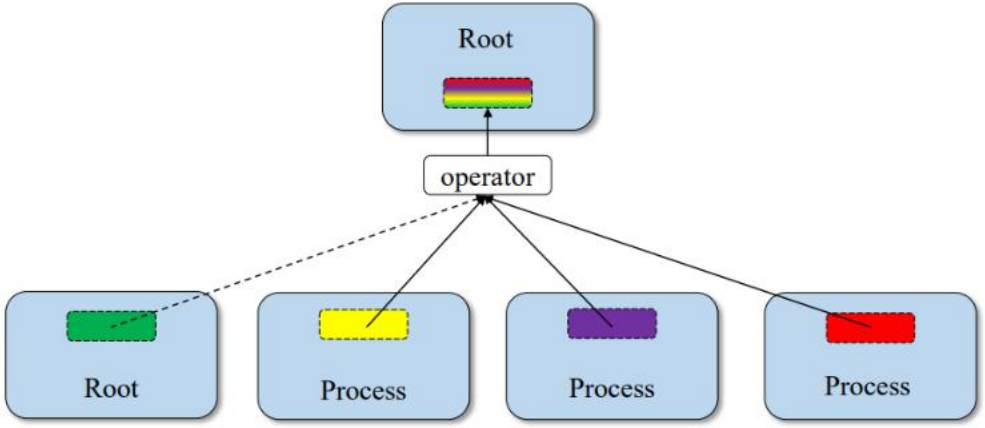
MPI: Collective Communication (Reduce)

```
MPI_Reduce(&sendbuf, &recvbuf, count, datatype,
           mpi_operation, root, comm)
```

Applies **reduction** operation on data from **all processes**.

Puts results on root process.

Operator
MPI_SUM
MPI_MAX
MPI_MIN
MPI_PROD



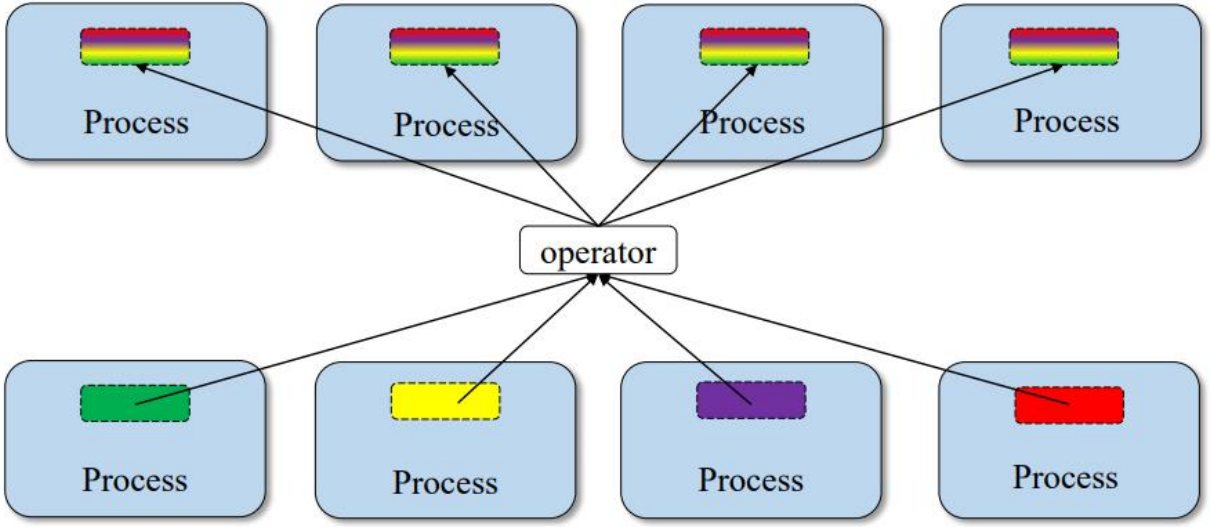
MPI: Collective Communication (Allreduce)

```
MPI_Allreduce(&sendbuf, &recvbuf, count,
              datatype, mpi_operation, comm)
```

Operator
MPI_SUM
MPI_MAX
MPI_MIN
MPI_PROD

Applies **reduction** operation on data **from all processes**.

Store results on all processes.



MPI: Collective Communication (Barrier)

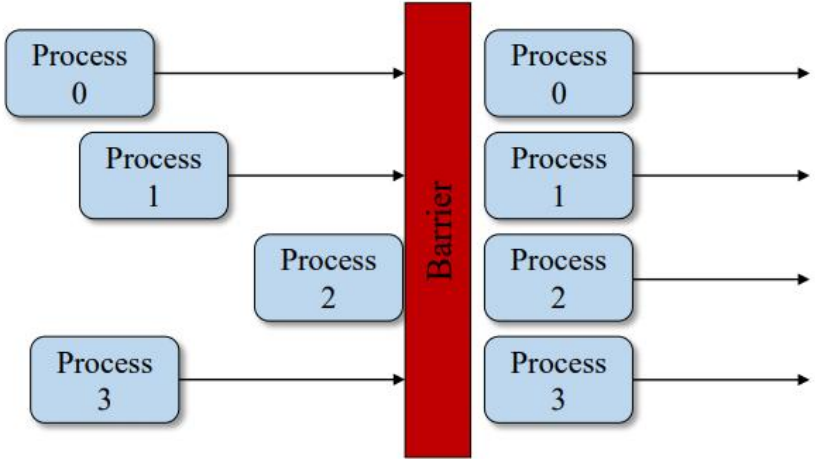
```
MPI_Barrier(comm)
```

Process synchronization (blocking).

All processes forced to wait for each other.

Use only where necessary.

Will reduce parallelism.



MPI: keywords

1 environment
- MPI Init: Initialization of the MPI environment
- MPI Comm rank: Rank of the process
- MPI Comm size: Number of processes
- MPI Finalize: Deactivation of the MPI environment
- MPI Abort: Stopping of an MPI program
- MPI Wtime: Time taking

2 Point-to-point communications
- MPI Send: Send message
- MPI Isend: Non-blocking message sending
- MPI Recv: Message received
- MPI Irecv: Non-blocking message reception
- MPI Sendrecv and MPI Sendrecv replace: Sending and receiving messages
- MPI Wait: Waiting for the end of a non-blocking communication
- MPI Wait all: Wait for the end of all non-blocking communications

3 Collective communications
- MPI Bcast: General broadcast
- MPI Scatter: Selective spread
- MPI Gather and MPI Allgather: Collecting
- MPI Alltoall: Collection and distribution
- MPI Reduce and MPI Allreduce: Reduction
- MPI Barrier: Global synchronization

4 Derived Types
- MPI Contiguous type: Contiguous types
- MPI Type vector and MPI Type create hvector: Types with a constanding
- MPI Type indexed: Variable pitch types
- MPI Type create subarray: Sub-array types
- MPI Type create struct: H and erogenous types
- MPI Type commit: Type commit
- MPI Type get extent: Recover the extent
- MPI Type create resized: Change of scope
- MPI Type size: Size of a type
- MPI Type free: Release of a type

MPI: Keywords

5 Communicator
• MPI Comm split: Partitioning of a communicator
• MPI Dims create: Distribution of processes
• MPI Cart create: Creation of a Cart´esian topology
• MPI Cart rank: Rank of a process in the Cart´esian topology
• MPI Cart coordinates: Coordinates of a process in the Cart´esian topology
• MPI Cart shift: Rank of the neighbors in the Cart´esian topology
• MPI Comm free: Release of a communicator

6 MPI-IO
• MPI File open: Opening a file
• MPI File set view: Changing the view
• MPI File close: Closing a file

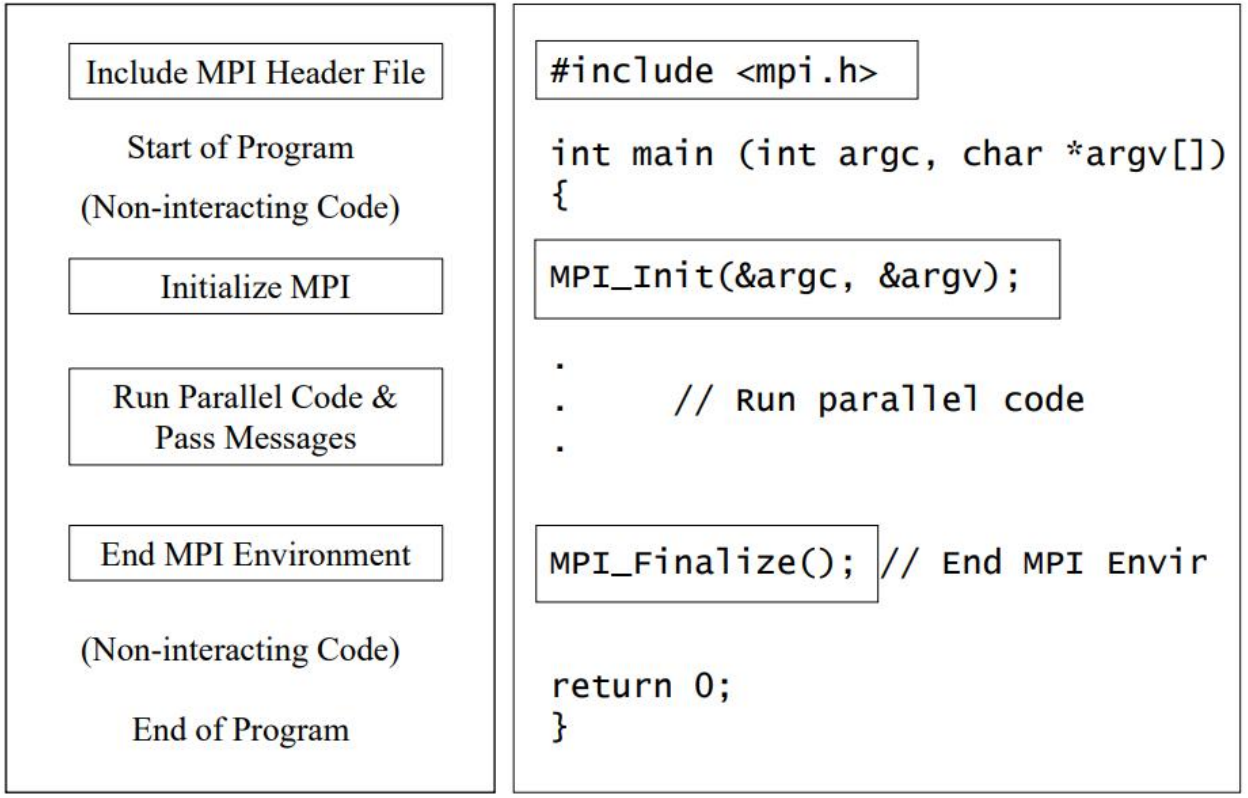
6.1 Explicit addresses
• MPI File read at: Reading
• MPI File read at all: Collective reading
• MPI File write at: Writing

6.2 Individual pointers
• MPI File read: Reading
• MPI File read all: collective reading
• MPI File write: Writing
• MPI File write all: collective writing
• MPI File seek: Pointer positioning

6.3 Shared pointers
• MPI File read shared: Read
• MPI File read ordered: Collective reading
• MPI File seek shared: Pointer positioning

7.0 Symbolic constants
• MPI COMM WORLD, MPI SUCCESS
• MPI STATUS IGNORE, MPI PROC NULL
• MPI INTEGER, MPI REAL, MPI DOUBLE PRECISION
• MPI ORDER FORTRAN, MPI ORDER C
• MPI MODE CREATE,MPI MODE RONLY,MPI MODE WRONLY

MPI: Program Basics



MPI: Example

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


int main (int argc, char *argv[]) {

  int rank, size;

  MPI_Init (&argc, &argv);  //initialize MPI library

  MPI_Comm_size(MPI_COMM_WORLD, &size); //get number of processes
  MPI_Comm_rank(MPI_COMM_WORLD, &rank); //get my process id

  //do something
  printf ("Hello World from rank %d\n", rank);
  if (rank == 0) printf("MPI World size = %d processes\n", size);

  MPI_Finalize(); //MPI cleanup

  return 0;
}
```

- 4 processes

```
Hello World from rank 3
Hello World from rank 0
MPI World size = 4 processes
Hello World from rank 2
Hello World from rank 1
```

- Code ran on each process independently
- MPI Processes have *private* variables
- Processes can be on completely different machines

MPI: Example Broadcast

```
#include<iostream>
#include<mpi.h>
using namespace std;
int main (int argc, char *argv[])
{
        int numprocs,myid,namelen;
        char processor_name[MPI_MAX_PROCESSOR_NAME];
        MPI_Init(&argc,&argv);
        MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
        MPI_Comm_rank(MPI_COMM_WORLD,&myid);
        MPI_Get_processor_name(processor_name,&namelen);

        double reel=(double) myid;
        cout<<"Before " <<myid<<" of "<<numprocs<<" on "<<processor_name<<" integervalue "<<reel<<endl;

        MPI_Bcast(&reel,1, MPI_DOUBLE,3,MPI_COMM_WORLD);
        MPI_Barrier( MPI_COMM_WORLD);

        cout<<"After " <<myid<<" of "<<numprocs<<" on "<<processor_name<<" integervalue "<<reel<<endl;

        MPI_Finalize();
        exit(0);
        }
```

Broadcast a message from the root process to all other processes.
Useful when reading in input parameters from file.

MPI: Example Point-to-Point communication

```
#include<iostream>
#include<mpi.h>
using namespace std;
int main (int argc, char *argv[])
{
        int numprocs,myid;
        MPI_Init(&argc,&argv);

        MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
        MPI_Comm_rank(MPI_COMM_WORLD,&myid);

        MPI_Status status;
        int small=myid;
        cout<<"Before " <<myid<<" of "<<,numprocs<<" small = "<<small,<<endl;

        If (myid==0) { MPI_Send(&small,1,MPI_INT,3,10,MPI_COMM_WORLD); }

        If (myid==3) { MPI_Recv(&small,1,MPI_INT,0,10,MPI_COMM_WORLD,&status) }

        MPI_Barrier( MPI_COMM_WORLD);

        cout<<"After " <<myid<<" of "<<numprocs<<" small = "<<small<<endl;

        MPI_Finalize();
        }
```

MPI: Example Reduction

```
...
#include<mpi.h>
using namespace std;
double f( double a ) {return (4.0 / (1.0 + a*a));}
int main (int argc, char *argv[])
{
        int myid, numprocs;
        MPI_Init(&argc,&argv);
        MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
        MPI_Comm_rank(MPI_COMM_WORLD,&myid);
        int n = 1000000000;
        double pi,sum=0.0;
        double startwtime = 0.0;
        if (myid == 0) { startwtime = MPI_Wtime(); }
        MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
        for (int i = myid + 1; i <= n; i += numprocs) { sum += f((i-0.5)/(double) n); }
        sum/= (double) n;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        if (myid == 0)
        {
          cout<<"pi is approximately equal "<<setprecision(16) << pi <<" Error is"<<fabs(pi - M_PI)<<endl;
          cout<<"Wall clock time = "<<MPI_Wtime()-startwtime<<endl;
        }
        MPI_Finalize();
        Exit(0);
        }
```

GOAL : The following code computes the π number by using a numerical evaluation of an integral by a rectangle method.

Each virtual core computes a part of the loop and a reduction instruction is performed

COMPILING an MPI Program

- **Compiling a program** for MPI is almost just like compiling a regular C or C++ program
  - The C compiler is **mpicc** and the **C++** compiler is **mpic++**.
    - For example, to compile **MyProg.c** you would use a command like
      - **mpicc** - O2 -o **MyProg MyProg . c**

OpenMP (Open Multi-Processing)

OpenMP (Open Multi-Processing)

OpenMP is a programming interface for parallel computing on shared memory architecture.

The OpenMP API consists of

- compiler directives (for insertion ***into sequential*** Fortran/C/C++$code)
- a few library routines
- some environment variables

Advantages:

- User-friendly
- Incremental parallelization of a serial code
- Possible to have a single source code for both serial and parallelized versions

Disadvantages:

- Relatively limited user control
- Most suitable for parallelizing loops (data parallelism)
- Performance?

OpenMP (Open Multi-Processing)

OpenMP is a programming interface for parallel computing on shared memory architecture.

- **It allows you to manage:**

  - the creation of light processes
  - the sharing of work between these lightweight processes
  - synchronizations (explicit or implicit) between all light processes
  - the status of the variables (private or shared).

OpenMP (Open Multi-Processing)

- **Shared memory model**
  - Threads communicate by accessing shared variables

    - **The sharing is defined syntactically**
      - Any variable that is seen by two or more threads is shared
      - Any variable that is seen by one thread only is private

        - **Race conditions possible**
          - Use synchronization to protect from conflicts
          - Change how data is stored to minimize the synchronization

OpenMP (Open Multi-Processing)

- **Multicore CPUs are everywhere:**
  - Servers with over 100 cores today and more
  - Even smartphone CPUs have 8 cores

- **Multithreading, natural programming model**
  - All processors share the same memory
  - Threads in a process see same address space
  - Many shared-memory algorithms developed

- **Multithreading is hard**
  - Lots of expertise necessary
  - Deadlocks and race conditions
  - Non-deterministic behavior makes it hard to debug

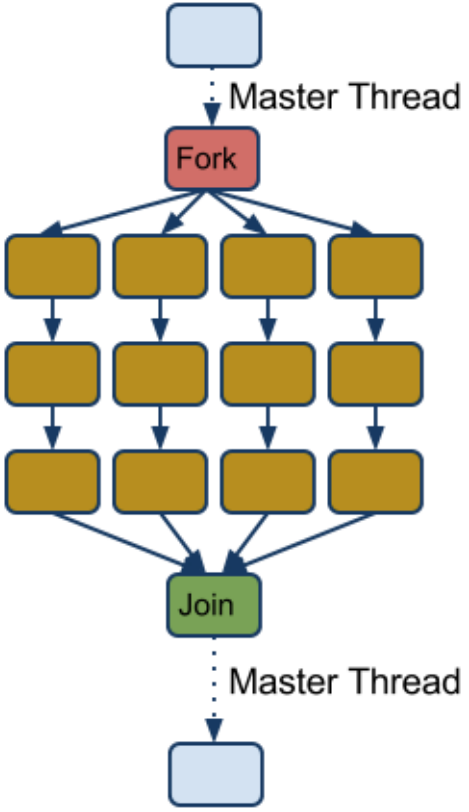
OpenMP: Process and thread: whatis the difference ?

- You need an existing process to create a thread.
- Each process has at least one thread of execution.
- A process has its own virtual memory space that cannot be accessed by other processes running on the same or on a different processor.
- All threads created by a process share the virtual address space of that process. They read and write to the same address space in memory. They also share the same process and user ids, file descriptors, and signal handlers. However, they have their own program counter value and stack pointer, and can run independently on several processors.

OpenMP: Terminology and behavior

- **OpenMP Team** = Master + Worker

- **Parallel Region** is a block of code executed by all threads simultaneously (has implicit barrier)
  - The master thread always has thread id 0
  - Parallel regions can be nested
  - If clause can be used to guard the parallel region



OpenMP: General Code Structure

```
#include <omp.h>

main ()
{
      int var1, var2, var3;
      //serial code

      //start of a parallel region
      #pragma omp parallel private(var1, var2) shared(var3)
      {...}

      //more serial code
      {...}

      //another parallel region
      #pragma omp parallel
      {…}
      }
```

OpenMP: Constructs

Parallel region

Thread creates team, and becomes master (id 0)
All threads run code after
Barrier at end of parallel section

```
#pragma omp parallel [clause ...]
                     if (scalar_expression)
                     private (list)
                     shared (list)
                     default (shared | none)
                     firstprivate (list)
                     lastprivate (list)
                     reduction (operator: list)
                     num_threads (integer)

   structured_block                                  (not a complete list)
```

OpenMP: Parallel Clauses

```
#pragma omp parallel if (scalar_expression)
```

Only execute in parallel.
Otherwise serial.

```
#pragma omp parallel private (list)
```

Data local to thread.
Value are not guaranted to be defined on exit (even if defined before)
No storage associated with original object
Use firstprivate and/or lastprivate clause to override

```
#pragma omp parallel firstprivate (list)
```

Variables in list are private.
Initialized with the value the variable had before entering the construct.

```
#pragma omp parallel for lastprivate (list)
```

Only in for loops
Variables in list are private.
The thread that executes the sequentially last iteration updates the value of the variables in the list.

OpenMP: Parallel Clauses

```
#pragma omp shared (list)
```

Data is accessible by all threads in team.
All threads access same address space.

Improperly scoped variables are big source of OMP bugs
- Shared when should be private
- Race condition

```
#pragma omp default (shared | none)
```

Tip: Safest is to use default (none) and declare by hand.

OpenMP Barrier

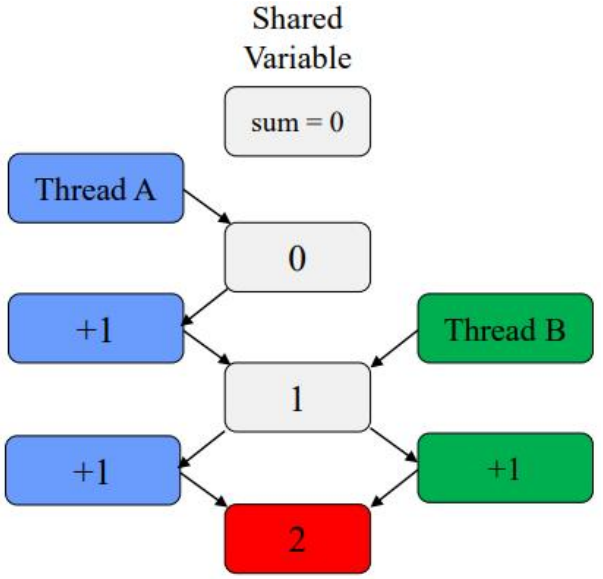
- When a thread reaches a barrier it only continues after all the threads in the same thread team have reached it
- Each barrier must be encountered by all threads in a team, or none at all
- The sequence of work-sharing regions and barrier regions encountered must be same for all threads in team
- Implicit barrier at the end of: do, parallel, single, workshare

OpenMP: Caution Race Condition

When multiple threads simultaneously read/write
Multiple OMP solutions

- Reduction
- Atomic
- Critical

```
#pragma omp parallel for private(i) shared(sum)
  for (i=0; i<N; i++) {
    sum += i;
  }
```



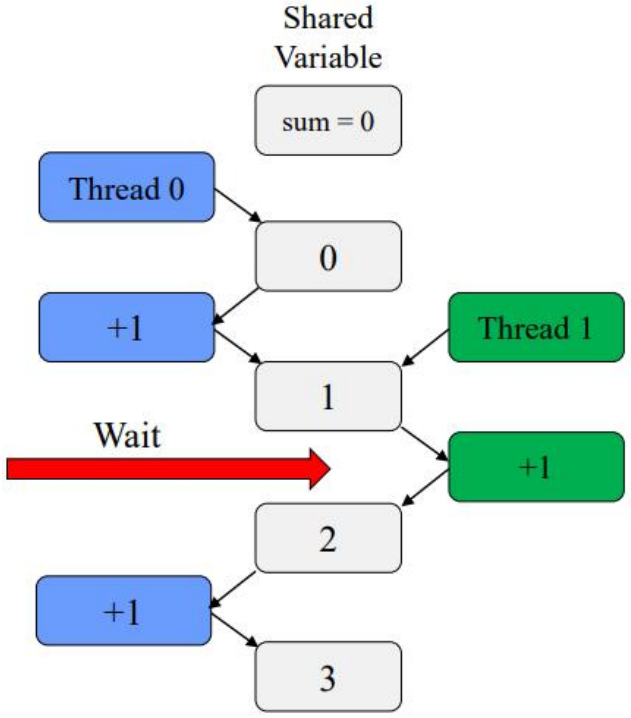
Should be 3!

OpenMP: Critical Section

One solution: use critical
Only one tread at a time can execute a critical section

```
#pragma omp critical
   {
     sum += i;
   }
```

Downside ?
SLOOOOWWW
Overhead and serialization

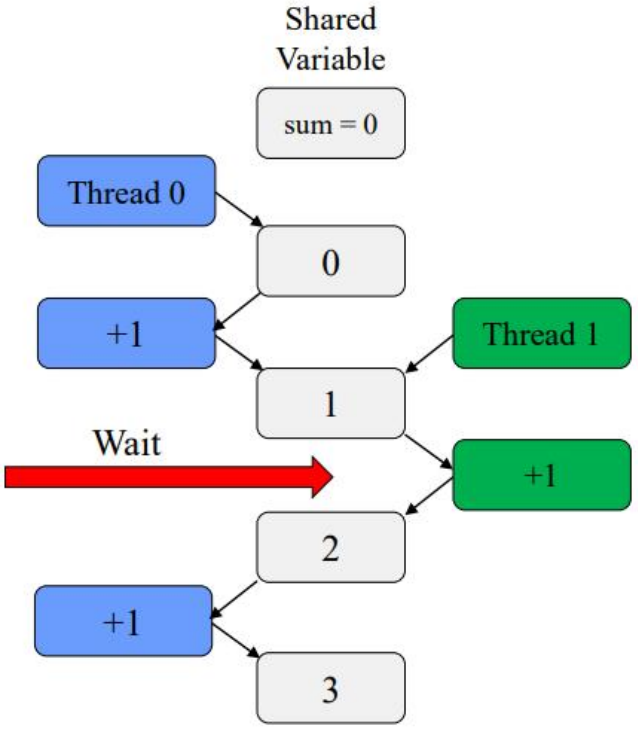


OpenMP: Atomic

Atomics like "mini" critical
Only one line
Certain limitations

```
#pragma omp atomic
    sum += i;
```

Hardware controlled
Less overhead the critical



OpenMP: Reduction

```
#pragma omp reduction (operator:variable)
```

Avoids race condition
Reduce variable must be shared
Makes variable private, then performs operator at end of loop
operator cannot be overloaded (c++)
One of: +,*,-,/ (and &,^,|,&&,||)
OpenMP 3.1: added min and max for c/c++

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

int main() {

  int i;
  const int N = 1000;
  int sum = 0;

#pragma omp parallel for private(i) reduction(+: sum)
  for (i=0; i<N; i++) {
    sum += i;
  }

  printf("reduction sum=%d (expected %d)\n", sum, ((N-1)*N)/2);
```

OpenMP: Scheduling omp for

How does a loop get split up ?

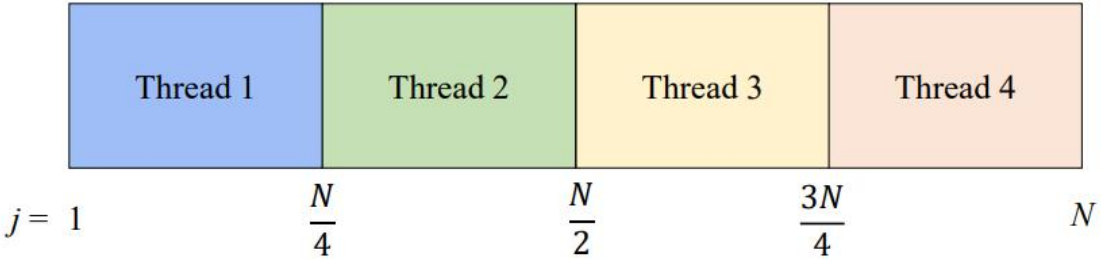
In MPI, we have to do it manually

If you do not tell what to do, the compiler decides

Usually compiler chooses "static" - chunks of N/p

```
#pragma omp parallel for default(shared) private(j)
  for (j=0; j<N; j++) {
        ... // some work here
}
```

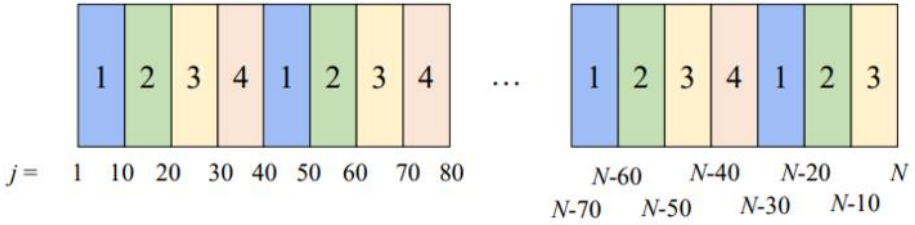
Unspecified schedule



OpenMP: Static Scheduling

You can tell the compiler what size chunks to take.

```
#pragma omp parallel for default(shared) private(j) schedule(static,10)
  for (j=0; j<N; j++) {
        ... // some work here
}
```

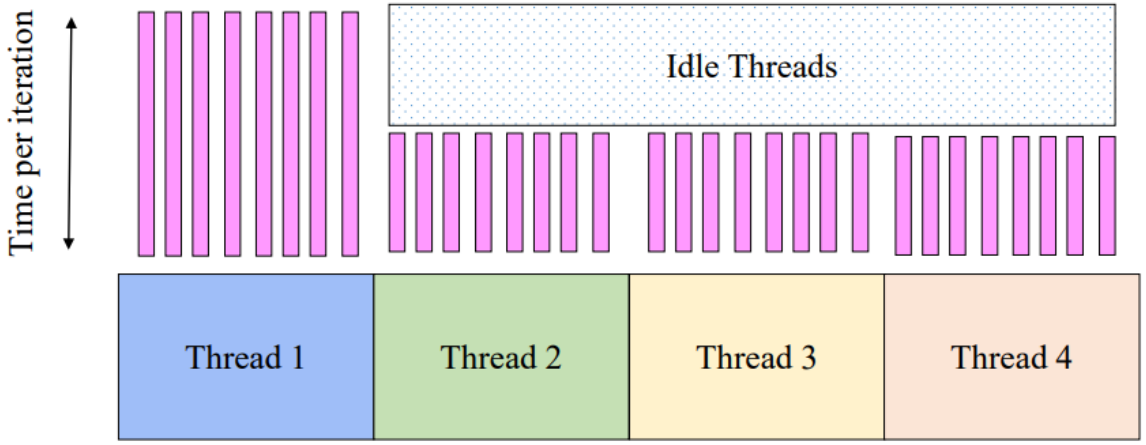


Keeps assigning chunks until done.
Chunk size that is not a multiple of the loop will results in thread with uneven numbers.

OpenMP: Problem with Static Scheduling

What happens if loop iterations do not take the same amount of time ?

Load imbalance



OpenMP: Dynamic Scheduling

Chunks are assigned on the fly, as threads become available
When a thread finishes on chunk, it is assigned another

```
#pragma omp parallel for default(shared) private(j) schedule(dynamic,10)
  for (j=0; j<N; j++) {
        ... // some work here
}
```

Caveat: higher overhead than static!

OpenMP: For Scheduling Recap

```
#pragma omp parallel for schedule(type [,size])
```

Scheduling types

Static

- Chunks of specified size assigned round-robin

Dynamic

- Chunks of specified size are assigned when thread finishes previous chunk

Guided

- Like dynamic, but chunks are exponentially decreasing
- Chunk will not be smaller than specified size

Runtime

- Type and chunk determined at runtime via environment variables

OpenMP: API

- API for library calls that perform useful functions
- Must include "omp:h"
- Will not compile without OpenMP compiler support

```
#include <omp.h>  //<-- necessary header file for OpenMP API
#include <stdio.h>

int main(int argc, char *argv[]){

  printf("OpenMP running with %d threads\n", omp_get_max_threads());

#pragma omp parallel
  {
    //Code here will be executed by all threads
    printf("Hello World from thread %d\n", omp_get_thread_num());
  }

  return 0;
}
```

OpenMP: API

```
void omp_set_num_threads(int num_threads)
```

Sets number of treads used in next parallel section
Overrides OMP_NUM_THREADS environment variable
Positive integer

```
int omp_get_max_threads()
```

Returns max possible (generally set by OMP_NUM_THREADS)

```
int omp_get_num_threads()
```

Returns number of threads currently in team

```
int omp_get_thread_num()
```

Returns thread id of calling thread
Between 0 and omp_get_num_threads-1

```
double omp_get_wtime()
```

Returns number of seconds since some point
Use inpais time=(t2-t1)

OpenMP: Example Fibonacci

```
int fib ( int n )
{
  int x,y;
  if ( n < 2 ) return n;
  #pragma omp task shared(x,n)
  x = fib(n-1);

  #pragma omp task shared(y,n)
  y = fib(n-2);

#pragma omp taskwait
return x+y;
}
```

```
int main()
{
#pragma omp parallel
  #pragma omp single nowait
  result = comp_fib_numbers(10);
return EXIT_SUCCESS;
}
```

OpenMP: Example Quicksort

```
void quick_sort (int p, int r, float *data)
{
  if (p < r) {
    int q = partition (p, r, data);
    #pragma omp task
    quick_sort (p, q-1, data, low_limit);
    #pragma omp task
    quick_sort (q+1, r, data, low_limit);}
  }
}
```

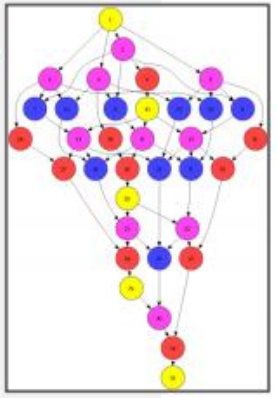
```
void par_quick_sort (int n, float *data)
{
  #pragma omp parallel
  {
    #pragma omp single nowait
    quick_sort (0, n, data);
  }
```

OpenMP: Example Cholesky Factorization

```c
#include <stdio.h>

int main(int argc, char* argv[])
{
  printf("Hello world! -main\n");
#pragma omp parallel
  {
    printf(".. worker reporting for duty.\n");
  }
  printf("Over and out! -main\n");
}
```

```
> gcc -fopenmp omp_hello.c -o omp
> OMP_NUM_THREADS=3 ./omp
Hello world! -main
.. worker reporting for duty.
.. worker reporting for duty.
.. worker reporting for duty.
Over and out! -main
```

```c
void cholesky(int ts, int nt, double* a[nt][nt]) {
  for (int k = 0; k < nt; k++) {
    // Diagonal Block factorization
    #pragma omp task depend(inout: a[k][k])
    potrf(a[k][k], ts, ts);

    // Triangular systems
    for (int i = k + 1; i < nt; i++) {
      #pragma omp task depend(in: a[k][k])
                       depend(inout: a[k][i])
      trsm(a[k][k], a[k][i], ts, ts);
    }

    // Update trailing matrix
    for (int i = k + 1; i < nt; i++) {
      for (int j = k + 1; j < i; j++) {
        #pragma omp task depend(inout: a[j][i])
                         depend(in: a[k][i], a[k][j])
        dgemm(a[k][i], a[k][j], a[j][i], ts, ts);
      }
      #pragma omp task depend(inout: a[i][i])
                       depend(in: a[k][i])
      syrk(a[k][i], a[i][i], ts, ts);
    }
  }
}
```

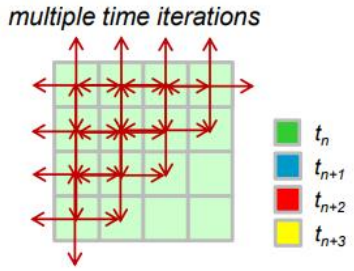


OpenMP 4.0

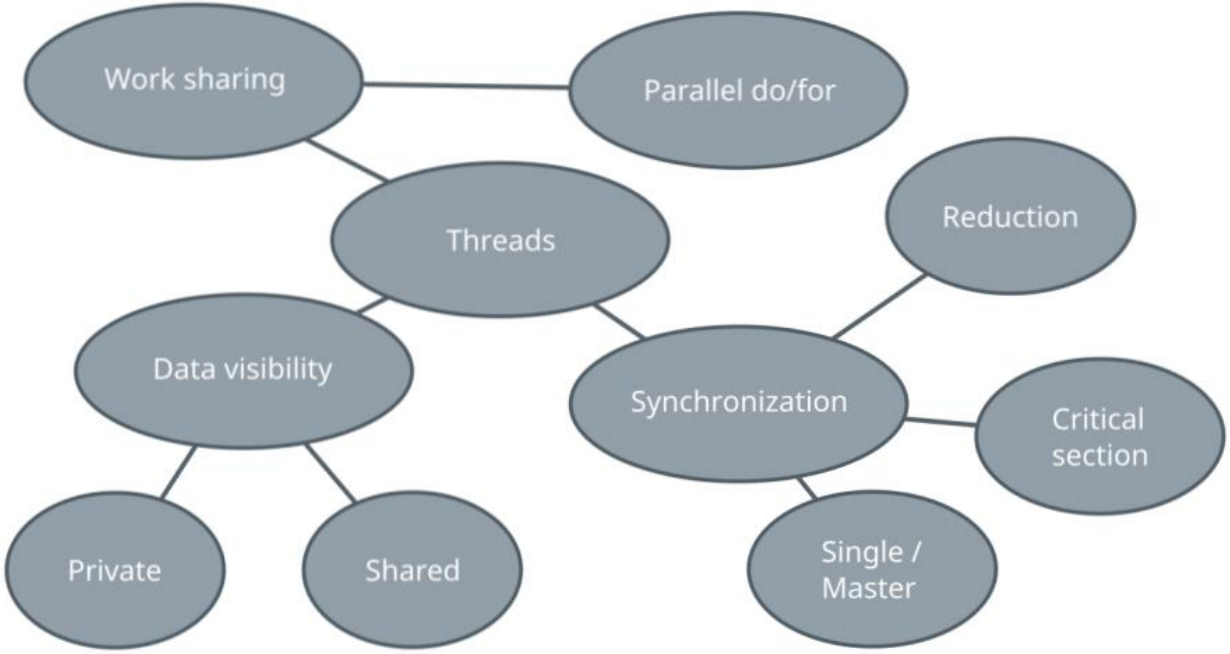
OpenMP: Example Gauss-Seidel

```
void gauss_seidel(int tsteps, int size, int TS, int (*p)[size]) {
  int NB = size / TS;

  #pragma omp parallel
  #pragma omp single
  for (int t = 0; t < tsteps; ++t)
    for (int ii=1; ii < size-1; ii+=TS)
      for (int jj=1; jj < size-1; jj+=TS) {
        #pragma omp task depend(inout: p[ii:TS][jj:TS])
            depend(in: p[ii-TS:TS][jj:TS], p[ii+TS:TS][jj:TS],
                       p[ii:TS][jj-TS:TS], p[ii:TS][jj:TS])
        {
          for (int i=ii; i<(1+ii)*TS; ++i)
            for (int j=jj; j<(1+jj)*TS; ++j)
              p[i][j] = 0.25 * (p[i][j-1] * p[i][j+1] *
                                p[i-1][j] * p[i+1][j]);
        }
      }
}
```

Gauss-Seidel Method is used to solve the linear system Equations. It is a method of iteration for solving n linear equation Ax=b with the unknown variables.



OpenMP: Summary



OpenMP: Summary Overview

OpenMP language extensions

parallel control structures	work sharing	data environment	synchronization	runtime functions, env. variables

governs flow of control in the program
 	
`parallel` directive
	distributes work among threads
	
	`do/parallel do` and `section` directives
		scopes variables
		
		`shared` and `private` clauses
			coordinates thread execution
			
			`critical` and `atomic` directives
			`barrier` directive
				runtime environment
				
				`omp_set_num_threads()`
				`omp_get_thread_num()`
				`OMP_NUM_THREADS`
				`OMP_SCHEDULE`

OpenMP: Performance Tips

- Avoid serialization!
- Avoid using `#pragma omp parallel for` before each loop
  - Can have significant overhead
    - Thread creation and scheduling is NOT free!!
  - Try for broader parallelism
    - One `#pragma omp parallel`, multiple `#pragma omp for`
  - Always try to parallelize the outer most loop
- Use reduction whenever possible
- Minimize I/O
- Minimize `critical`
  - Use `atomic` instead of `critical` where possible

Hybrid OpenMP-MPI

Hybrid MPI and OpenMP

Hybrid application programs using **MPI + OpenMP** are now common place on large HPC systems.

There are basically two main motivations:

1. Reduced memory footprint, both in the application and in the MPI library (eg communication buffers).
2. Improved performance, especially at high core counts where pure MPI scalability runs out.

Hybrid MPI and OpenMP

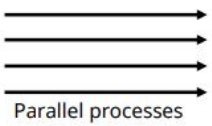
Parallel programming models

Parallel execution is based on threads or processes (or both) which run at the same time on different CPU cores

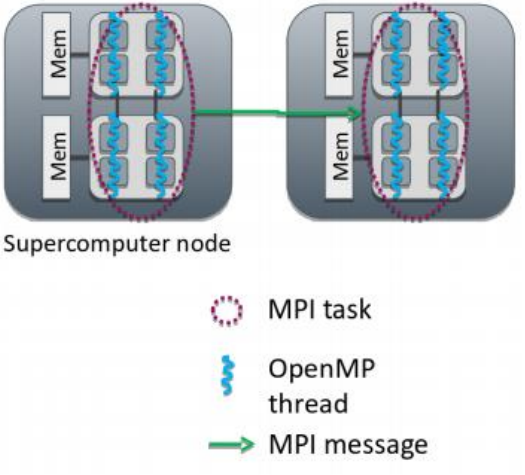
Processes
- Interaction is based on exchanging messages between processes
- MPI (Message passing interface)

Threads
- Interaction is based on shared memory, i.e. each thread can access directly other threads data
- OpenMP

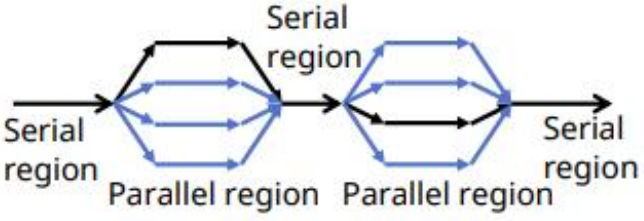
Hybrid MPI and OpenMP



1: MPI: Processes
- Independent execution units
- Have their own memory space
- MPI launches N processes at application startup
- Works over multiple nodes



2: OpenMP: Threads
- Threads share memory space
- Threads are created and destroyed (parallel regions)
- Limited to a single node



3: Hybrid programming: Launch threads (OpenMP) within processes (MPI)

- Shared memory programming inside a node, message passing between nodes
- Optimum MPI task per node ratio depends on the application and should always be experimented.

Hybrid Programming

In hybrid programming each process can have **multiple threads executing simultaneously**
All threads within a process share all MPI objects Communicators, requests, etc.

MPI defines 4 levels of thread safety:

- **MPI_THREAD_SINGLE** : One thread exists in program
- **MPI_THREAD_FUNNELED** : Multithreaded but only the master thread can make MPI calls Master is one that calls MPI_Init_thread()
- **MPI_THREAD_SERIALIZED:** Multithreaded, but only one thread can make MPI calls at a time
- **MPI_THREAD_MULTIPLE:** Multithreaded and any thread can make MPI calls at any time. Use MPI_Init_thread instead of MPI_Init if more than single thread

Hybrid Programming

Potential advantages of the hybrid approach

- Fewer MPI processes for a given amount of cores
  - Improved load balance
  - All-to-all communication bottlenecks alleviated
- Decreased memory consumption if an implementation uses replicated data
- Additional parallelization levels may be available
- Possibility for dedicating threads for different tasks
  - e.g. dedicated communication thread or parallel I/O
- Dynamic parallelization patterns often easier to implement with OpenMP

Disadvantages of hybridization

- Increased overhead from thread creation/destruction
- More complicated programming
  - Code readability and maintainability issues
- Thread support in MPI and other libraries needs to be considered

Hybrid Programming: Example

```c
#include <mpi.h>
#include <omp.h>

int main(int argc, char *argv[]) {
    int my_id, omp_rank;
    int provided, required=MPI_THREAD_FUNNELED;

    MPI_Init_thread(&argc, &argv, required,
                    &provided);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_id);
#pragma omp parallel private(omp_rank)
{
    omp_rank = omp_get_thread_num();
    printf("I'm thread %d in process %d\n",
           omp_rank, my_id);
}
    MPI_Finalize();
}
```

```
$ mpicc -fopenmp hybrid-hello.c -o hybrid-hello
$ srun  --ntasks=2 --cpus-per-task=4
  ./hybrid-hello

I'm thread 0 in process 0
I'm thread 0 in process 1
I'm thread 2 in process 1
I'm thread 3 in process 1
I'm thread 1 in process 1
I'm thread 3 in process 0
I'm thread 1 in process 0
I'm thread 2 in process 0
```

Hybrid Programming Example

- **Numerical integration**

$$\int_0^1 \frac{4}{1+x^2}\,dx = \pi$$

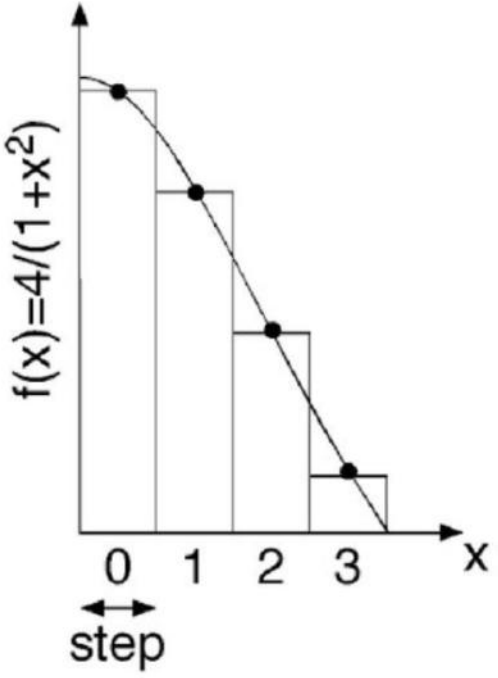
- **Discretization:**

$\Delta = 1/N$: `step = 1/NBIN`

$x_i = (i+0.5)\Delta$ $(i = 0,\ldots,N-1)$

$$\sum_{i=0}^{N-1} \frac{4}{1+x_i^2}\Delta \cong \pi$$

```
#include <stdio.h>
#define NBIN 100000
void main() {
  int i; double step,x,sum=0.0,pi;
  step = 1.0/NBIN;
  for (i=0; i<NBIN; i++) {
    x = (i+0.5)*step;
    sum += 4.0/(1.0+x*x);}
  pi = sum*step;
  printf("PI = %f\n",pi);
}
```




```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>              /* MPI header file */
#include <omp.h>              /* OpenMP header file */
#define NUM_STEPS 100000000
#define MAX_THREADS 4

int main(int argc, char *argv[]) {
   int nprocs, myid;
   int tid, nthreads, nbin;
   double start_time, end_time;
   double pi, Psum=0.0, sum[MAX_THREADS]={0.0};
   double step = 1.0/(double) NUM_STEPS;

   /* initialize for MPI */
  MPI_Init(&argc, &argv);       /* starts MPI */
   /* get number of processes */
   MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
   /* get this process's number (ranges from 0 to nprocs - 1) */
   MPI_Comm_rank(MPI_COMM_WORLD, &myid);

  nbin= NUM_STEPS/nprocs;
```

Hybrid Programming Example

```
#pragma omp parallel private(tid)
{
      int i;
      double x;
      nthreads=omp_get_num_threads();
      tid=omp_get_thread_num();
      for (i=nbin*myid+tid; i < nbin*(myid+1); i+= nthreads) { /* changed*/
         x = (i+0.5)*step;
         sum[tid] += 4.0/(1.0+x*x);
      }
}
 for(tid=0; tid<nthreads; tid++)   /*sum by each mpi process*/
      Psum += sum[tid]*step;

MPI_Reduce(&Psum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);/* added */

   if (myid == 0) {
      printf("parallel program results with %d processes:\n", nprocs);
      printf("pi = %g  (%17.15f)\n",pi, pi);
   }
   MPI_Finalize();

   return 0;
}
```

Results

- MPI

  MPI uses 8 processes:
  pi = 3.14159 (3.141592653589828)

- OpenMP

  OpenMP uses 8 threads:
  pi = 3.14159 (3.141592653589882)

- Hybrid

  mpi process 0 uses 4 threads
  mpi process 1 uses 4 threads
  mpi process 1 sum is 1.287 (1.287002217586605)
  mpi process 0 sum is 1.85459 (1.854590436003132)
  Total MPI processes are 2
  pi = 3.14159 (3.141592653589738)

Thank you for your attention !