Introduction

Background and Motivation

- Parallel computing is a part of HPC.
 - HPC also includes everything else that makes the computation fast.
 - No point parallelizing without increasing performance.
 - You might want to optimize for the architecture.
 - Sometimes overhead outweighs benefits from parallelization.
- Focusing on parallel algorithms.
 - Different version of parallel algorithms suits different architecture or models.
- Many application yo.
- People made super computers throughout the 1900s
- Super computers rely on carefully designed interconnects.
- Cloud computers are just AWS instances.
- Many aspects

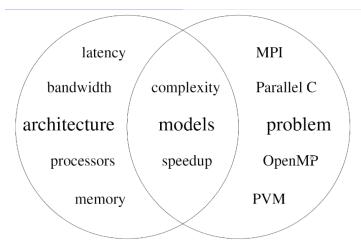


Figure: Overlapping aspects of parallel computing

Complexity

- $f(n) = O(g(n)) \Rightarrow f$ grows no faster than g
- $f(n) = \Omega(g(n)) \Rightarrow f$ grows no slower than g
- $f(n) = o(g(n)) \Rightarrow f$ grows slower than g
- $f(n) = \omega(g(n)) \Rightarrow f$ grows faster than g
- $f(n) = \Omega(g(n)) \land f(n) = O(g(n)) \Rightarrow f(n) = \Theta(g(n))$
- Strictly speaking we should really use \in instead of =
- Some common name for complexities:
 - Constant
 - Logarithmic
 - Polylog: $(\log(n))^c$
 - Linearithmic: $n \log n$
 - Quadratic: n^2
 - Polynomial or geometric
 - Exponential
 - Factorial
- Log factor are often ignored.

Model

- RAM model: random access machine
 - Common model when we talk about sequential time complexity.
- Multiplying the number of computers by a constant factor doesn't change the complexity.
 - Solution: allow p, the number of processors to increase with problem size and hence reduces the complexity.

PRAM

- Parallel Random Access Machine
- *p* number of RAM processors, each have private memory and share a large shared memory, all memory access takes the same amount of time.
- Does things synchronously, AKA in lock steps.
- PRAM pseudo code looks like regular pseudo code but there's this

 $\label{eq:continuous} \begin{tabular}{ll} \textbf{for } i \leftarrow 0 \begin{tabular}{ll} \textbf{to } n-1 \begin{tabular}{ll} \textbf{do in parallel} \\ \textbf{processor} \begin{tabular}{ll} \textbf{does thingy} \\ \end{tabular}$

Many different PRAM model

- EREW: exclusive read, exclusive write
- CREW: concurrent read, exclusive write
- CRCW: concurrent read, concurrent write
 - Concurrent write have different types
 - COMMON: Error when two processor tries to write to the same location with different value.
 - ARBITRARY: Pick a arbitrary processor if many processor writes the same time.
 - PRIORITY: Processor with lowest ID writes.
 - COMBINING: Runs a function whenever multiple processors tries to write at the same time.
 - Too powerful.
- ERCW: exclusive read, concurrent write (never used)

Power of model: expresses the set of all problems that can be solved within a certain complexity.

- A is more powerful that B if A can solve a larger set of problems within any complexities.
- A is equally powerful as B if they can solve the same set problems within any complexities.
- Partial ordering.
- COMMON, ARBITRARY, PRIORITY and COMBINING are in increasing order of power.
- Any CRCW PRIORITY PRAM can be simulated by a EREW PRAM with a complexity increase of $\mathcal{O}(\log p)$
- *Parallel Computation Thesis*: any thing can be solved with a Turing Machine with polynomially bounded space can be solved in polynomially bounded space with unlimited processors.
 - Unbounded *word sizes* are not useful, so we limit word counts to $\mathcal{O}(\log p)$
- *Nick's Class* (NC): Solvable in polylog time with ploy number of processors.
- Widely believed that $\mathbf{NP}
 eq P$

Definitions (need to remember)

- $w(n) = t(n) \times p(n)$ where w(n) is the work / cost, t(n) is the time and p(n) is the number of processors.
 - Optimal processor allocation means: $t(n) \times p(n) = \Theta(T(n))$ where T(n) is the time taking by a sequential algorithm.
 - Equivalent to $t(n) \times p(n) = O(T(n))$ because $t(n) \times p(n) = \Omega(T(n))$ always.
 - Speedup $(n) = \frac{T(n)}{t(n)}$
 - Speedup optimal = processor optimal.
 - Optimal: processor optimal AND $t(n) = \mathcal{O}(\log^k n)$
 - Processor optimal and polylog in time.
 - Efficient: Assume $T(n) = \Omega(n) w(n) = \mathcal{O}(T(n) \log^{\alpha} n)$ AND polylog in time
 - Optimal but polylog increase in work.
- *size*: Size(n) is the total number of operations it does.
- efficiency: $\eta(n)$ speedup per processor $\eta(n) = \frac{T(n)}{w(n)} = \frac{\operatorname{Speedup}(n)}{p(n)}$
- You can decrease p and increase t by a factor of $O\left(\frac{p_1}{p_2}\right)$, w(n) doesn't increase its complexity.
 - · Can't do it the other way around.

Brent's Principle (important)

• If something can be done with size x and t time with infinite processors, then it can be done in $t + \frac{x-t}{n}$ time with p processors

Amdahl's Law

- Maximum speedup: if f is the fraction of time that can't be parallelized, then Speedup $(p) \to \frac{1}{f}$ as $p \to \infty$
 - Honestly very obvious.

Gustafson's Law

- s is fraction time of serial part, r is fraction time of parallel part, then Speedup $(p) = \Omega(p)$
 - Very obvious again...

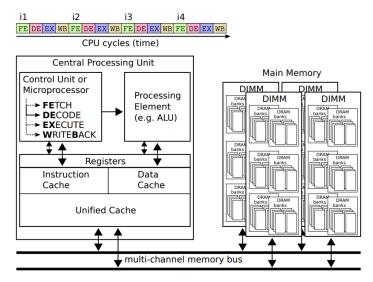
Algorithms

- sum
- · logical or
- Maximum
 - n^2 processors all compare all elements and set is max array to false if element isn't maximum.
 - Only processor with element being max write it to the returning memory address.
- Maximum n^2
 - $\mathcal{O}(\log \log n)$
 - *n* processor on *n* elements.
 - Is efficient
 - Make elements into a square, find maximum on each row recursively.
 - Find maximum of maximum of the rows using maximum.
 - $\mathcal{O}(\log \log n)$ levels of recursion, each level takes $\mathcal{O}(1)$ times
- Element Uniqueness
 - Have an array size of MAX INT.
 - Write processor ID to the array with the element.
 - Check if processor ID is indeed there, if not there's another element there.
- Replication

- $O(\log n)$
- · Replication optimal
 - $p = \frac{n}{\log(n)}$ and copy at the end.
- Broadcast
 - Just replicate
- Simulate PRIORITY with COMMON n^2
 - Minimum version of Maximum
- Simulate PRIORITY with EREW
 - All processor wants to write
 - Sort array A of tuples (address, processorID) using Cole's Merge Sort.
 - For each processor k, if A[k].address $\neq A[k-1]$.address then A[k].processorID is the smallest ID that wants to write to that address.

Architecture

• Fetch Decode Execute WriteBack



- Bus is a wire and everyone can see everything on that wire.
- Pipeline: let's do all of them at the same time for the next 4 instructions
 - Need to predict the next 4 instructions sometimes.
- Superpipeline: Do all of them for the next 8 (or more) instructions.
- Superscalar: Multiple pipeline in parallel
- Word size: 64 bits, 32 bits etc, various aspects:
 - Integer size
 - Float size
 - Instruction size
 - Address resolution (mostly bytes)
- Single instruction multiple data SIMD
 - Make word size more complicated
- Coprocessor
 - Used to means stuff directly connected to the CPU like a floating point processor.
 - Now can means FPGA or GPU.
- Multicore processor are just single core duplicated but they all have one extra single shared cache.

- Classification of parallel architectures
 - SISD regular single core.
 - SIMD regular modern single core.
 - MIMD regular multicore.
 - MISD doesn't exist.
- · SIMD vs MIMD
 - Effectively SIMD vs non-SIMD
 - Most processor have multicore and SIMD on each core.
 - So a balance between the two.
 - SIMD cores are larger so less of them fit on a die.
 - SIMD is faster at vector operations.
 - SIMD is not useful all the time so sometimes the SIMD part sit idle.
 - SIMD is harder to program.
- Shared memory: All memory can be accessed by all processors.
 - All memory access truly equal time: symmetric multi-processor.
 - Only can have so many cores when the bus is only so fast.
 - Making more buses doesn't help cause space also slows things down.
 - Sometimes can be done with switching interconnect network.
 - Some processor access some memory faster.
 - More complex network.
 - Distributed shared memory: each processor have its own memory but interconnect network exist so you can read other people's memory.
 - non-uniform memory access NUMA
 - Static interconnect network: each node connect to some neighbors.
 - *degree*: just like degree in graphs.
 - diameter: just like in graphs.
 - $cost = degree \times diameter$
- Distributed memory: Each processor have its own memory. Each process live on one processor.
- Blade contains Processor / Package / Socket which contains Core which contains ALU.
- Implicit vs explicit: explicit \rightarrow decision made by programmer
 - Parallelism: Can I write a sequential algorithm.
 - Decomposition: Can I pretend threads processes doesn't exist.
 - Mapping: Can I pretend all cores are the same.
 - Communication.
- Single Program Multiple Data: one exe
- Multiple Program Multiple Data: multiple exe

Other HPC considerations

- Cache friendliness
- Processor-specific code
- Compiler optimization.
 - Compiler from CPU maker are usually better.
 - So Intel compiler is better than both clang and gcc.

Memory interleaving

• Memory module takes a while to recharge, so we interleave a page on different memory module.

Automatic Vectorization

- Sometimes compilers automatically insert SIMD instructions in place of loops.
 - Depends on the availabilities of a lot of things, including the OS.
- Manual SIMD:

```
multiply_and_add(const float* a, const float* b, const float* c, float* d) {
   for(int i=0; i < 8; i++) {
      d[i] = a[i] * b[i];
      d[i] = d[i] + c[i];
   }
}
--m256 multiply_and_add(--m256 a, --m256 b, --m256 c) {
   return _mm256_fmadd_ps(a, b, c);
}</pre>
```

• AVX have to be aligned: i.e. 256 bits SIMD have to be 256 bits aligned - address is multiple of 256 bits.

Multithreading

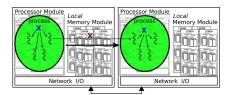
- Synchronization is more expensive if threads are on cores further away.
 - It's expensive in general.
- Instruction reordering: thread continues with other instructions while it waits on earlier instructions.
- Speculative execution: don't wait on instructions, just go for it and if it fails then unroll.
- Some programming patterns are more friendly to NUMA.

Message passing considerations

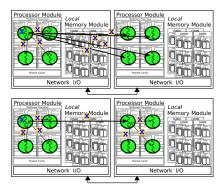
- Multi processing have to pass messages around because processes don't share address space.
- Hard to predict performance.

Wants good communication patterns

• For multithread multiprocess:



• For single thread multiprocess:



OpenMP

• Abstracts single process, multithreaded program execution on a single machine.

- Abstracts: Multi-socket, multi-core, threads, thread synchronization, memory hierarchy, SIMD, NUMA.
- Everything OMP does are hints.
- *internal control variable*: ICV: OMP_NUM_THREADS, OMP_THREAD_LIMIT, OMP_PLACES, OMP_MAX_ACTIVE_LEVELS.
- Can also be set with functions in #include "omp.h"

Execution Model

- There's an implicit parallel region on the outside.
- There's by default an implicit barrier at the end of each parallel region.
 - no-wait removes the implicit barrier
- If a parallel region is encountered, then the threads split and a new team is created.
- A lot of parallel region nested can create a lot of thread very quickly.
 - Can limit nesting by OMP_MAX_ACTIVE_LEVELS.

Memories: global, stack, heap

• Threads have their own stack but share global and heap.

Directives

- The #pragma omp thingy.
- Allows specifying parallelism and still allow the base language to be the same.
 - Theoretically, simply remove the directives and program will just run like a sequential program.
- Syntax:

```
#pragma omp <directive name> [[,]<clause> [[,]<clause> [...]]]
<statement / block>
```

- Multiple directives can be applied to one following block
- Some directives are *stand alone*, they don't have structured block following them.

Synchronization

- thread team is a group of threads.
- barrier will block threads in a team that reach it early.
- flush will enforce consistency between different thread's view of memory.
- critical ensures a critical region where only one thread can be in it at a time.
- atomic is faster than critical but only for simple operations.
- simd make use of SIMD instructions.
- *places*: specify how processing units on the architecture are partitioned.
- Thread encounters a parallel directive -> split itself into the number of threads.
- #pragma omp parallel
 - create some number of threads and do its thing.
 - clauses:
 - num threads(int) overrides ICV, limited by OMP THREAD LIMIT
 - private(list of variables) each thread will have own memory allocated to private variable.
 - Default for variables on stack.
 - shared(list of variables) all thread share the same variables, same piece of memory.
 - OpenMP will add locks.
 - threadprivate(list of variables) variable stay with the thread if all threadprivate directives are identical.
 - Can combine with for, loop, sections and workshare.

- #pragma omp for
 - clauses:
 - schedule([modifier[, modifier]:]kind[, chunk_size])
 - · kind:
 - static: divided into chunk_size (default $\frac{iterations}{num \ threads}$) and distributed round-robin over the threads
 - dynamic: chunks of chunk size (default 1) distributed to threads as they complete them.
 - guided: like dynamic but varying chunk_size, large chunks at the start and small chunks at the end.
 - auto: default.
 - runtime: determined by sched-var ICV.
 - · modifier:
 - monotonic: chunks are given in increasing logical iteration
 - nonmonotonic: default, allows work stealing: I finished early, I will now take your work.
 - simd: try to make the loop into SIMD constructs.
 - collapse(n): n nested loops are combined into one large logical loop.
 - ordered[(n)]: There are operations in the loop that must be executed in their logical order.
 - reduction([reduction-modifier,] reduction-modifier:list): a list of variable that will be used in a reduction operation.
 - Allowed operations: +, -, *, &, ^, &&, ||, max, min
 - Example: #pragma omp parallel for reduction(+:x), x is the result, + is the operation.
 - x starts as a private variable initialized to the identity value.
 - global x will be assigned to the sum of all xs at the end.
- #pragma omp loop
 - Work for any loop, not just for.
 - Main diff to for is bind
- #pragma omp sections
 - Have #pragma omp section inside.
 - Each #pragma omp section gets executed by one thread.
 - clauses:
 - private(list of variables): each thread will have its own version of the variable.
 - firstprivate(list of variables): same as private but memory is initialized to the global version.
 - lastprivate(list of variables): copy the private variables to the global version for the "lexically last" private variables.
 - A variable can be firstprivate and lastprivate at the same time.
- #pragma omp single
 - Only do it in a single thread in the team, used inside #pragma omp parallel
 - private(list of variables): each thread will have its own version of the variable.
 - firstprivate(list of variables): same as private but memory is initialized to the global version.
- #pragma omp workshare
 - Here's a bunch of independent statements / blocks, figure out how to parallelize it.
- #pragma omp atomic
 - critical for read, write, update (x += 1), compare (if (expr < x) x = expr;).
- #pragma omp critical [(name) [[,] hint(hint-expression)]]
 - clauses
 - (name): two critical region with the same name can't happen at the same time.
 - All no name critical region are treated as having the same name.

- hint(hint-expression):
 - omp_sync_hint_uncontended
 - omp_sync_hint_contended
 - omp_sync_hint_speculative: try to speculate.
 - omp_sync_hint_nonspeculative: don't try to speculate.
- #pragma omp ordered
 - Inside loops so that they're executed in their logical order.
- #pragma omp barrier
 - Explicit barrier.
- #pragma omp flush
 - Sync cache.
 - Be aware of code reordering.
- #pragma omp task
 - The *Task Model*: specify work without allocating work to threads.
 - Task is a unit of work.
 - Task have dependencies such as completion of other tasks.
 - Task may generate other tasks.
 - Uses many same clauses such as private, shared and firstprivate.
 - Task can have data affinity.
 - clauses:
 - depend([depend-modifier,] dependence-type:locator-list).
 - priority(int): hint of order of execution.
 - affinity([aff-modifier :] locator-list)
- #pragma omp taskloop
 - clauses:
 - num_tasks([strict:]num-tasks): specify the number of tasks that will be generated.
 - grainsize([strict:]grainsize): how many iteration per task.
- #pragma omp taskwait
 - · Wait for all current child tasks to finish

Places

- OMP_PLACES: list of power units by their identifiers
 - {0,1,2,3}, {4,5,6,7}: specify two places each with 4 processing units.
 - use hwloc-ls to find processing unit number.
 - threads(8): 8 places on 8 hardware threads
 - cores(4): 4 places on 4 cores.
 - ll_caches(2): 2 places on 2 set of cores where all the cores in a set shares their last level cache.
 - numa_domains(2): 2 places on 2 set of cores whose closes memory is the same or similar distance.
 - sockets(2): 2 places on two sockets
 - OMP_PLACES partition power units into places. Which can then be referred to by proc_bind(type) clause in parallel directives.
- proc_bind(type): overrides OMP_PROC_BIND, only in parallel directives.
 - primary: All threads created in the team are in the same place.
 - close: Threads are allocated to places in a round-robin fashion first thread in place i, second thread in place i+1, third thread in place i+2
 - spread: Place thread in a way so that the distance between the power unit ID are as far as possible.

Memory

- Sending memory to other numa domains cost cache as well because the send operation needs to be done by a CPU which means cache.
- OpenMP memory classification:
 - omp_default_mem_space: DRAM
 - omp_large_cap_mem_space: SSD
 - omp const mem space: optimized for read only
 - omp high bw mem space: high bandwidth
 - omp_low_lat_mem_space: low latency.
- Memory allocator have traits:
 - sync_hint: expected concurrency contended (default), uncontended, serialized, private
 - alignment: default byte.
 - access: which thread can access the memory, all (default), cgroup, pteam, thread
 - pool_size: total amount of memory the allocator can allocate.
 - fallback: on error return null or exit, default is first try standard allocator and return null if fail.
 - partition: environment (default), nearest, blocked, interleaved. How is the allocated memory partitioned over the allocator's storage resource.

Prefix Sum

- Doesn't have to be sum, can also be any other associative operations (like prod, min, max).
- The only way to reduce depth is to increase size (hopefully only slightly).

Upper/Lower parallel prefix algorithm

- Divide array into two parts and compute their prefix sum.
- Add the sum of the first part to the second part.
- $\Theta(\log n)$ time complexity
- $\Theta(n \log n)$ work
- $\Theta(n \log n)$ size
- Half of the processors are idle all time except first iteration. (can probably be easily fixed)

Odd/Even parallel prefix algorithm

- Divide array into odd and even indices parts.
- Add odd indices to even indices.
- Compute prefix of even part recursively.
 - Now the even part contains the correct prefix.
- Compute the odd part in one parallel step.
- Same complexity as Upper/Lower, but 2 times slower.

Ladner and Fischer's parallel prefix algorithm.

- Optimal possible time.
- Split array into two parts and use odd even for the first part, upper lower for the second part.
 - Odd even for the first part is beneficial because the last element is available one step earlier.

Pointer jumping

• All processor replace next with next next, so you start going in 2^n steps for each iteration.

Sorting

- Merge sort parallelized is O(n) because last merge is sequential.
- Quick sort parallelized is O(n) because the first split is sequential.

Parallel merge

- $\mathcal{O}\left(\frac{n}{p} + \log p\right)$ or $\mathcal{O}(\log n)$ where p = n
- Two sorted list, assume all value are below n where n is the length of the resulting array.
- Count unique value for both of them.
- Write the sum of count for both array to result array with index X.
- Now the count is sorted.
- Compact the result array.
- Use prefix sum to space the resulting array evenly so that there are count -1 null element after even element.
- Use distribution to fill out the rest of the array.

Compaction

- Move all non null element to the first part of the array.
- Use prefix sum to count the index of each empty element.
- Move each non empty element to its index.

Unique Counts

- Sorted array to (value, count) element.
- Find all places where the adjacent values are different.
- Use prefix sum to find their index.
- · Reverse engineer their count with old indices.

Distribution

- Array with some null value, fill with the closest non null value to the left.
- Best complexity is achieved with simple broadcast.
- 1. Use prefix sum and unique count to figure out how many empty element are after each non empty one.
- 2. Do sequential distribute with each processor.
- 3. For the processors where their first element is null:
 - 1. Still need to fill
 - 2. Use info obtained previously at the very first step to calculate how long does this null sequence last.
 - 3. All processor involved in the null sequence, broadcast!

Rank sort

- Count the number of element smaller and number of element bigger, and just write this element to the array.
- Use n^2 processors. Can count the index in $\mathcal{O}(\log n)$ time.
- With a combine PRAM, it can be done in $\mathcal{O}(1)$ time.

Rank Merge

• Much simpler than Parallel merge, just use binary search to find the ranks.

Bitonic MergeSort

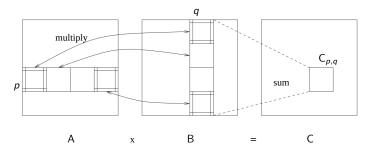
- Bitonic is a sequence is two monotonic sequences but one up and one down.
- · You can find the pivot and turn this into a regular merge.
- Alternatively:
 - compare and maybe swap each two pair of element in two part of the array (none of them reversed.)
 - You end up getting two bitonic array.
 - · Keep doing this and you sort it.

• Same time complexity.

You can use bitonic sort to do bitonic merge sort, by keep constructing bitonic lists and merging them with bitonic sort.

Matrix Multiplication

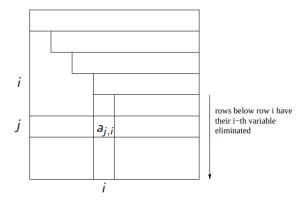
- Matrix multiplication doesn't have dependencies between them, so easy to parallelize with less than n^2 processors.
- Pretty trivial to parallelize in ideal conditions, so we will focus on practical side of matrix multiplication.
- For huge matrices, we can divide them into smaller one, multiply the smaller ones, and then sum the smaller ones.



• You can divide the matrices into 4 parts recursively, until the matrix is small enough to fit into the cache.

Gaussian elimination

- Common for matrix to be sparse, aka mostly zero.
- Gaussian elimination is for dense matrix.
- Solving system of linear equation by getting rid of variables one by one by rewriting them in terms of other variables.

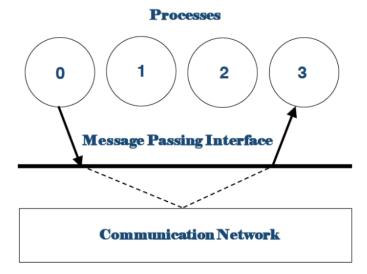


- If a coefficient of a variables is close to zero, then we run into numerical problems.
 - We can swap this row with the rows below to fix this. This is called *partial pivoting*
 - Partial because the columns aren't being swapped.
 - Can be done in $\mathcal{O}(\log_2 n)$
 - We will ignore partial pivoting to simplify our problem. (make it more theoretical)
- The eliminate step can be parallelized. Resulting in time complexity of $\mathcal{O}(n^2)$ with p=n
 - We can more better utilize processor if there are less than n processor by using *cyclic-striped* partitioning.

processor 1
processor 2
processor 3
processor 1
processor 2
processor 3
processor 1
processor 2

MPI

• Pass messages between processes.



- Provide consistent interface to have portable code on different architectures.
- Can be sync or async
 - sync: returns after message being read by receiver process.
 - async: returns asap and have some other thread or the kernel do the sending.
- MPI is a language.

Communicator

- Communicators: a set of processes.
 - \bullet MPI_COMM_WORLD: all processes.
- Rank: 0 based index of your processes given a communicator.
- Size: size of the communicator.

Functions

- int MPI_Init(int *argc, char ***argv): first MPI call, initialize the MPI execution environment, takes away the MPI arguments by modifying argc and argv.
- int MPI_Finalize(): last MPI call.
- int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)

- int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)
 - For send and receive to succeed, rank must be valid, communicator must be same, tags must be same (or say idk what tag), message datatype must be compatible.
- int MPI_Bcast(void *buf, int count, MPI_Datatype, int root, MPI_Comm comm)
- int MPI_Scatter(void *buf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI Datatype recvtype, int root, MPI Comm comm)
 - One node send different data to other nodes.
- int MPI_Gather(void *buf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
 - Opposite of scatter.
- int MPI_Allgather(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)
- int MPI_Alltoall(void * sendbuf, int sendcount, MPI_Datatype sendtype, void * recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)
- int MPI_Alltoallv(void * sendbuf, int * sendcounts, int * sdispls, MPI_Datatype sendtype, void * recvbuf, int * recvcounts, int * rdispls, MPI_Datatype recvtype, MPI Comm comm)
- int MPI_Reduce(void * sendbuf, void * recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)
 - MPI_Op can be: MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, MPI_LAND, MPI_BAND, MPI_LOR, MPI_BOR, MPI_LXOR, MPI_BXOR.
- int MPI Barrier(MPI Comm comm)
 - Mostly used to share OS resource are not controlled by MPI.