Introduction to the Message Passing Interface (MPI)

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Outline

- Distributed-memory architecture: general considerations
- Programming model: Message Passing Interface (MPI)
 - Point-to-point communication
 - Blocking communication
 - Point to point network performance
 - Non-blocking communication
 - Collective communication
 - Collective communication algorithms
 - Global network performance
- Parallel program performance evaluation
 - Amdahl's law
 - Gustafson's law
- Parallel program development: case studies

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Moore's Law

Microprocessor Transistor Counts 1971-2011 & Moore's Law



Moore's Law



Illustration from Wikipedia

Evolution of top 500 supercomputers over time



Application area – performance share



Operating system family



Motivation for parallel computing

- Want to run the **same program faster**
 - Depends on the application what is considered an acceptable runtime
 - SETI@Home, Folding@Home, GIMPS: years may be acceptable
 - For **R&D** applications: days or even weeks are acceptable
 - CFD, CEM, Bioinformatics, Cheminformatics, and many more
 - **Prediction of tomorrow's weather** should take less than a day of computation time.
 - Some applications require **real-time behavior**
 - Computer games, algorithmic trading
- Want to run **bigger datasets**
- Want to reduce **financial cost** and/or **power consumption**

Distributed-memory architecture



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Message Passing Interface (MPI)

- MPI = **library specification**, not an implementation
- Most important implementations
 - Open MPI (http://www.open-mpi.org, MPI-3 standard)
 - Intel MPI (proprietary, MPI-3 standard)
- Specifies routines for (among others)
 - Point-to-point communication (between 2 processes)
 - Collective communication (> 2 processes)
 - Topology setup
 - Parallel I/O
- Bindings for C/C++ and Fortran

MPI reference works

MPI standards: <u>http://www.mpi-forum.org/docs/</u>



Using MPI Portable Parallel Programming with the Message-Passing Interfa second edition MPI: The Complete Reference (M. Snir, S. Otto, S Huss-Lederman, D. Walker, J. Dongarra) Available from <u>http://switzernet.com/people/emin-</u> gabrielyan/060708-thesis-ref/papers/Snir96.pdf

Using MPI: Portable Parallel Programming with the Message Passing Interface, 2nd ed. (W. Gropp, E. Lusk, A. Skjellum).

MPI standard

- Started in 1992 (Workshop on Standards for Message-Passing in a Distributed Memory Environment) with support from vendors, library writers and academia.
- MPI version 1.0 (May 1994)
 - Final pre-draft in 1993 (Supercomputing '93 conference)
 - Final version June 1994
- MPI version 2.0 (July 1997)
 - Support for one-sided communication
 - Support for process management
 - Support for parallel I/O
- MPI version 3.0 (September 2012)
 - Support for non-blocking collective communication
 - Fortran 2008 bindings
 - New one-sided communication routines

Hello world example in MPI

```
#include <mpi.h>
#include <iostream>
#include <cstdlib>
using namespace std;
int main(int argc, char* argv[]) {
    int rank, size;
    MPI Init( &argc, &argv );
    MPI Comm rank ( MPI COMM WORLD, &rank );
    MPI Comm size ( MPI COMM WORLD, & size );
    cout << "Hello World from process" << rank << "/" << size << endl;
    MPI Finalize();
    return EXIT SUCCESS;
```

Output **order** is random

john@doe ~]\$ mpirun -np 4 ./helloWorld
Hello World from process 2/4
Hello World from process 3/4
Hello World from process 0/4
Hello World from process 1/4

Basic MPI routines

- int MPI_Init(int *argc, char ***argv)
 - Initialization: all processes must call this prior to any other MPI routine.
 - Strips of (possible) arguments provided by "mpirun".
- int MPI_Finalize(void)
 - Cleanup: all processes must call this routine at the end of the program.
 - All pending communication should have finished before calling this.
- int MPI_Comm_size(MPI_Comm comm, int *size);
 - Returns the size of the "Communicator" associated with "comm"
 - Communicator = user defined subset of processes
 - MPI_COMM_WORLD = communicator that involves all processes
- int MPI_Comm_rank(MPI_Comm comm, int *rank);
 - Return the rank of the process in the Communicator
 - Range: [0 ... size 1]

Message Passing Interface Mechanisms



mpirun launches P independent processes across the different machines

Each process is a instance of the same program

Terminology

- **Computer program** = passive collection of instructions.
- **Process** = instance of a computer program that is being executed.
- **Multitasking** = running multiple processes on a CPU.
- Thread = smallest stream of instructions that can be managed by an OS scheduler (= light-weight process).
- Distributed-memory system = multi-processor systems where each processor has direct access (fast) to its own private memory and relies on inter-processor communication to access another processor's memory (typically slower).

Multithreading versus multiprocessing

Multi-threading

Single process Shared memory address space Protect data against simultaneous writing Limited to a single machine E.g. Pthreads, CILK, OpenMP, etc.

Message passing

Multiple processes



Separate memory address spaces



Multiple machines possible
 E.g. MPI, Unified Parallel C, PVM





Message Passing Interface (MPI)

- **MPI** mechanisms (depends on implementation)
 - Compiling an MPI program from source •
 - mpicc -O3 main.cpp -o main •

gcc -O3 main.cpp -o main -L<IncludeDir> -l<mpiLibs>

- Also mpic++ (or mpicxx), mpif77, mpif90, etc.
- Running MPI applications (manually) •
 - mpirun -np <number of program instances> <your program>
 - List of worker nodes specified in some config file.

Using MPI on the Ugent HPC cluster

- Load appropriate module first, e.g. •
 - module load intel/2017a
- Compiling an MPI program from source
- C { mpigcc (uses the GNU "gcc" C compiler) mpiicc (uses the Intel "icc" C compiler)
- C++ { mpigxx (uses the GNU "g++" C++ compiler)
 mpiicpc (uses the Intel "icpc" C++ compiler)

 - Submit job using a jobscript (see further)

mpicc / mpic++ defaults to gcc

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Basic MPI point-to-point communication



I received Hello World from process 3 with size 12 and tag 123

Message Passing Interface Mechanisms



mpirun launches P independent processes across the different machines

Each process is a instance of the same program

Blocking send and receive

- **buf**: pointer to the message to send
- count: number of items to send
- datatype: datatype of each item
 - number of bytes sent: count * sizeof(datatype)
- **dest**: rank of destination process
- tag: value to identify the message [0 ... at least (32 767)]
- comm: communicator specification (e.g. MPI_COMM_WORLD)

- **buf:** pointer to the buffer to store received data
- count: upper bound (!) of the number of items to receive
- datatype: datatype of each item
- source: rank of source process (or MPI_ANY_SOURCE)
- tag: value to identify the message (or MPI_ANY_TAG)
- **comm**: communicator specification (e.g. MPI_COMM_WORLD)
- status: structure that contains { MPI_SOURCE, MPI_TAG, MPI_ERROR }

Sending and receiving

Two-sided communication:

- Both the sender and receiver are involved in data transfer As opposed to one-sided communication
- Posted send must match receive

When do MPI_Send and MPI_recv match ?

- 1. Rank of *receiver* process
- 2. Rank of *sending* process
- 3. *Tag*
 - custom value to distinguish messages from same sender
- 4. Communicator

Rationale for Communicators

- Used to create subsets of processes
- Transparent use of tags
 - modules can be written in isolation
 - communication within module through own Communicator
 - communication between modules through shared Communicator

MPI Datatypes

MPI_Datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long in
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	no conversion, bitpattern transferred as is
MPI_PACKED	grouped messages

Querying for information

• MPI_Status

• Stores information about the MPI_Recv operation

```
typedef struct MPI_Status {
    int MPI_SOURCE;
    int MPI_TAG;
    int MPI_ERROR;
}
```

- Does not contain the size of the received message
- int MPI_Get_count (MPI_Status *status, MPI_Datatype datatype, int *count)
 - returns the number of data items received in the count variable
 - not directly accessible from status variable

Blocking send and receive



- a) sender comes first,
 idling at sender (no
 buffering of message)
- b) sending/receiving at about the same time, idling minimized
- c) receiver comes first, idling at receiver

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Deadlocks



If MPI_Send is blocking (handshake protocol), this program will deadlock

- If 'eager' protocol is used, it may run
- Depends on message size

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Network cost modeling

- Various choices of **interconnection network**
 - Gigabit Ethernet: cheap, but far too slow for HPC applications
 - Infiniband /Myrinet: high speed interconnect
- Simple performance model for point-to-point communication

 $T_{comm} = \alpha + \beta * n$

- α = latency
- $B = 1/\beta$ = saturation (asymptotic) bandwidth (bytes/s)
- n = number of bytes to transmit
- Effective bandwidth B_{eff}:

$$B_{eff} = \frac{n}{\alpha + \beta * n} = \frac{n}{\alpha + \frac{n}{B}}$$

The case of Gengar (UGent cluster)

Bandwidth and latency



Measure effective bandwidth: ringtest

Idea: send a single message of size N in a circle



- Increase the message N size exponentially
 - 1 byte, 2 bytes, 4 bytes, ... 1024 bytes, 2048 bytes, 4096 bytes
- Benchmark the results (measure wall clock time T), ...
 - Bandwidth = N * P / T

Hands-on: ringtest in MPI

```
void sendRing( char *buffer, int length ) {
    /* send message in a ring here */
int main( int argc, char * argv[] )
    . . .
    char *buffer = (char*) calloc ( 1048576, sizeof(char) );
    int msqLen = 8;
    for (int i = 0; i < 18; i++, msqLen *= 2) {
        double startTime = MPI Wtime();
        sendRing( buffer, msqLen );
        double stopTime = MPI Wtime();
        double elapsedSec = stopTime - startTime;
        if (rank == 0)
           printf( "Bandwidth for size %d is : %f\", ...);
```

Jobscript example

mpijob.sh job script example:

```
#!/bin/sh
#
#
PBS -o output.file
#PBS -e error.file
#PBS -1 nodes=2:ppn=all
#PBS -1 walltime=00:02:00
#PBS -m n
cd $VSC_SCRATCH/<yourdirectory>
module load intel/2017a
module load scripts
mympirun ./program name> program arguments>
```

qsub mpijob.sh qstat / qdel / etc remains the same

Hands-on: ringtest in MPI (solution)

```
void sendRing( char *buffer, int msgLen )
   int myRank, numProc;
   MPI Comm rank ( MPI COMM WORLD, & myRank );
   MPI Comm size ( MPI COMM WORLD, &numProc );
   MPI Status status;
   int prevR = (myRank - 1 + numProc) % numProc;
   int nextR = (myRank + 1 ) % numProc;
   if (myRank == 0) { // send first, then receive
       MPI Send ( buffer, msgLen, MPI CHAR, nextR, 0, MPI COMM WORLD);
       MPI Recv ( buffer, msgLen, MPI CHAR, prevR, 0, MPI COMM WORLD,
                 &status );
   } else {
                           // receive first, then send
       MPI Recv ( buffer, msqLen, MPI CHAR, prevR, 0, MPI COMM WORLD,
                 &status );
       MPI Send ( buffer, msgLen, MPI CHAR, nextR, 0, MPI COMM WORLD);
   }
```
Basic MPI routines

Timing routines in MPI

- double MPI_Wtime(void)
 - returns the time in seconds relative to "some time" in the past
 - "some time" in the past is fixed during process
- double MPI_Wtick(void)
 - Returns the resolution of MPI_Wtime() in seconds
 - e.g. 10^{-3} = millisecond resolution

Bandwidth on Gengar (Ugent cluster)



Benchmark results

Comparison of CPU load

top - Tasks: Cpu(s) Mem: Swap:	11:39:38 (187 tota : 99.0%us 16440052k 31357404k	וף 10 ן, , ג'ון, 0 total total	da Ss	ys, 18: wnning, y, % 0.(168400 5630	:25, , 17 0%ni 08k 0 72k 0	l us 7 slee , 0.0 used, used,	ser epi 0%i 14 30	r, loa ing, id, 0 1756044 0794332	ad ave 0 sto .0%wa, 4k fre 2k fre	erage: 0.02, 0.35, 0.32 opped, 1 zombie, 0.0%hi, 0.0%si 0.0%st ee, 227224k'buffers ee, 172864k cached	1111
PID 15879	USER vsc400	PR N 20	I 0	VIRT 65668	RES 20m	SHR 3460	S R	%CPU 100.0	%MEM 0.1	TIME+ COMMAND 0:03.23 ringtest	
15882 15883	vsc400	20 18	0 0	128m 128m	52m 20m	3460 3456	R	100.0	0.3	0:03.29 ringtest 0:03 22 ringtest	
15884	vsc400	18	0	65672	20m	3464	R	100.0	0.1	0:03.22 ringtest	
15885	vsc400	19	0	128m	52m	3460	R	100.0	0.3	0:03.28 ringtest	
15886	vsc400	20	0	192m	84m	3488	R	100.0	0.5	0:03.23 ringtest	
15880	vsc400	20	0	191m	52m	3460	R	99.7	0.3	0:03.21 ringtest	
15881	vsc400	20	0	128m	52m	3460	R	99.3	0.3	0:03.22 ringtest	

Infiniband

Gigabit Ethernet	top - 11:33:13 up 10 days, 18:19, 1 user, load average: 1.24, 0.30, 0.22 Tasks: 188 total, 10, running, 177 sleeping, 0 stopped, 1 zombie, Cpu(s): 19.8%us, 78.3%sy, 0.0%ni, 0.0%id, 0.0%wa, 0.0%hi, 1.8%si, 0.0%st Mem: 16440052k total, 1470984k used, 14969068k free, 227092K buffers Swap: 31357404k total, 563096k used, 30794308k free, 168428k cached										
	PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU ?	%MEM	TIME+ COMMAND
	14866	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.02 ringtest
	14867	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.05 ringtest
	14868	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.05 ringtest
	14869	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.05 ringtest
	14870	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.01 ringtest
	14871	vsc400	25	0	89028	18m	1892	R	100.0	0.1	0:10.05 ringtest
	14872	vsc400	25	0	89028	34m	17m	R	99.7	0.2	0:10.00 ringtest
	14865	vsc400	25	0	89028	18m	1892	S	99.3	0.1	0:09.89 ringtest

Exchanging messages in MPI

int MPI_Sendrecv(void *sendbuf, int sendcount, MPI_Datatype
 sendtype, int dest, int sendtag, void *recvbuf,
 int recvcount, MPI_Datatype recvtype, int source,
 int recvtag, MPI_Comm comm, MPI_Status *status)

- sendbuf: pointer to the message to send
- **sendcount**: number of elements to transmit
- sendtype: datatype of the items to send
- **dest:** rank of destination process
- sendtag: identifier for the message
- **recvbuf:** pointer to the buffer to store the message (**disjoint** with sendbuf)
- recvcount: upper bound (!) to the number of elements to receive
- **recvtype:** datatype of the items to receive
- source: rank of the source process (or MPI_ANY_SOURCE)
- recvtag: value to identify the message (or MPI_ANY_TAG)
- **comm**: communicator specification (e.g. MPI_COMM_WORLD)
- **status**: structure that contains { MPI_SOURCE, MPI_TAG, MPI_ERROR }
- sendbuf: pointer to the buffer to send

int MPI_Sendrecv_replace(...)

• Buffer is replace by received data

Basic MPI routines

Sendrecv example



- Compatibility between Sendrecv and 'normal' send and recv
- Sendrecv can help to prevent deadlocks

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Non-blocking communication

Idea:

- Do something useful while waiting for communications to finish
- Try to overlap communications and computations

How?

• Replace blocking communication by non-blocking variants

MPI_Send(...) > MPI_Isend(..., MPI_Request *request)
MPI_Recv(...) > MPI_Irecv(..., status, MPI_Request *request)

- I = intermediate functions
- MPI_Isend and MPI_Irecv routines return immediately
- Need polling routines to verify progress
 - request handle is used to identify communications
 - status field moved to polling routines (see further)

Non-blocking communications

Asynchronous progress

- = ability to progress communications while performing calculations
- Depends on hardware
 - Gigabit Ethernet = very limited
 - Infiniband = much more possibilities
- Depends on MPI implementation
 - Multithreaded implementations of MPI (e.g. Open MPI)
 - Daemon for asynchronous progress (e.g. LAM MPI)
- Depends on protocol
 - Eager protocol
 - Handshake protocol
- Still the subject of ongoing research

Non-blocking sending and receiving



 network interface supports overlapping computations and communications

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no such support

Non-blocking communications

Polling / waiting routines

int MPI_Wait(MPI_Request *request, MPI_Status *status)
 request: handle to identify communication
 status: status information (cfr. 'normal' MPI_Recv)
int MPI_Test(MPI_Request *request, int *flag, MPI_Status *status)
 Returns immediately. Sets flag = true if communication has completed

Waits for exactly one communication to complete If more than one communication has completed, it picks a random one index returns the index of completed communication

Returns immediately. Sets flag = true if at least one communication completed If more than one communication has completed, it picks a random one index returns the index of completed communication If flag = false, index returns MPI_UNDEFINED

Example: client-server code

```
if ( rank != 0 ) { // client code
   while ( true ) { // generate requests and send to the server
       generate request( data, &size );
       MPI Send ( data, size, MPI CHAR, 0, tag, MPI COMM WORLD );
} else {
                      // server code (rank == 0)
   MPI Request *reqList = new MPI Request[nProc];
   for ( int i = 0; i < nProc - 1; i++ )</pre>
       MPI Irecv( buffer[i].data, MAX LEN, MPI CHAR, i+1, tag,
                 MPI COMM WORLD, &reqList[i] );
   while ( true ) { // main consumer loop
       MPI Status status;
       int reqIndex, recvSize;
       MPI Waitany( nProc-1, reqList, &reqIndex, &status );
       MPI Get count ( &status, MPI CHAR, &recvSize );
       do service( buffer[reqIndex].data, recvSize );
       MPI Irecv ( buffer [reqIndex].data, MAX LEN, MPI CHAR,
                  status.MPI SOURCE, tag, MPI COMM WORLD,
                  &reqList[reqIndex] );
```

Non-blocking communications

Polling / waiting routines (cont'd)

Waits for **all** communications to complete

Returns immediately. Sets **flag** = **true** if all communications have completed

Waits for **at least one** communications to complete **outcount** contains the number of communications that have completed Completed requests are set to **MPI_REQUEST_NULL**

Same as Waitsome, but returns immediately.

flag field no longer needed, returns **outcount = 0** if no completed communications

Example: improved client-server code

```
if ( rank != 0 ) { // same client code
} else {
                   // server code (rank == 0)
   MPI Request *reqList = new MPI Request[nProc-1];
   MPI Status *status = new MPI Status[nProc-1];
   int *reqIndex = new MPI Request[nProc];
   for ( int i = 0; i < nProc - 1; i++ )
       MPI Irecv( buffer[i].data, MAX LEN, MPI CHAR, i+1, tag,
                  MPI COMM WORLD, &reqList[i] );
   while ( true ) { // main consumer loop
       int numMsq;
       MPI Waitsome ( nProc-1, reqList, &numMsg, reqIndex, status );
       for ( int i = 0; i < numMsg; i++ ) {</pre>
           MPI Get count ( &status[i], MPI CHAR, &recvSize );
           do service( buffer[regIndex[i]].data, recvSize);
           MPI Irecv( buffer[reqIndex[i]].data, MAX SIZE, MPI CHAR,
                      status[i].MPI SOURCE, tag, MPI COMM WORLD,
                      &reqList[reqIndex[i]] );
```

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Barrier synchronization

MPI_Barrier(MPI_Comm comm)

This function does not return until all processes in comm have called it.



Broadcast





Broadcast example



john@doe ~]\$ mpirun -np 4 ./broadcast
Process 1 has Hello World stored in the buffer.
Process 0 has Hello World stored in the buffer.
Process 3 has Hello World stored in the buffer.
Process 2 has Hello World stored in the buffer.

Broadcast algorithm

- Linear algorithm, subsequent sending of n bytes from root process to P-1 other processes takes (α + β n) (P- 1) time.
- **Binary tree algorithm** takes only $(\alpha + \beta n) \lceil \log_2 P \rceil$ time.



process rank

Scatter

MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendType, void *recvbuf, int recvcount, MPI_Datatype recvType, int root, MPI_Comm comm) MPI_Scatter partitions a sendbuf at the root process into P equal parts of size sendcount and sends each process in comm (including root) a portion in rank order.



Scatter example



Scatter algorithm

- Linear algorithm, subsequent sending of n bytes from root process to P-1 other processes takes (α + β n) (P- 1) time.
- Binary algorithm takes only $\alpha \lceil \log_2 P \rceil + \beta n(P-1)$ time (reduced number of communication rounds!)



Scatter (vector variant)



Gather

MPI Gather (void *sendbuf, int sendcount, MPI Datatype sendType, void *recvbuf, int recvcount, MPI Datatype recvType, int root, MPI Comm comm) MPI Gather gathers equal partitions of size recvcount from each of the P processes in comm (including root) and stores them in recybuf at the root process in rank order. Gather is the receive buffer (only matters at **root** process) opposite of Scatter sendcount elements root = p_1 d_0 d_0 \mathbf{p}_0 d **p**₁ MPI Gather **p**₂ recvcount elements **p**₃ e send buffer **p**₄ process rank process rank

A vector variant, MPI_Gatherv, exists, a similar generalization as MPI_Scatterv

Gather example



```
john@doe ~]$ mpirun -np 4 ./gather
Receive buffer at root process:
0 1 2 3
```

Gather algorithm

- Linear algorithm, subsequent sending of n bytes from P-1 processes to root takes $(\alpha + \beta n)$ (P- 1) time.
- Binary algorithm takes only $\alpha \lceil \log_2 P \rceil + \beta n(P-1)$ time (reduced number of communication rounds!)



AllGather



Allgather algorithm

- **P** calls to gather takes $P[\alpha \lceil \log_2 P \rceil + \beta n(P-1)]$ time (using the best gather algorithm)
- Gather followed by broadcast takes $2\alpha \lceil \log_2 P \rceil + \beta n(P \lceil \log_2 P \rceil + P-1)$ time.
- **"Butterfly" algorithm** takes only $\alpha \log_2 P + \beta n(P-1)$ time (in case P is a power of two)



All to all communication





A vector variant, MPI_Alltoallv, exists, allowing for different sizes for each process

Reduce



♦ = operation, like sum, product, maximum, etc.

Reduce operations

Available reduce operations (associative and commutative) User defined operations are also possible

MPI_MAX	maximum
MPI_MIN	minimum
MPI_SUM	sum
MPI_PROD	product
MPI_LAND	logical AND
MPI_BAND	bitwise AND
MPI_LOR	logical OR
MPI_BOR	bitwise OR
MPI_LXOR	logical exclusive OR
MPI_BXOR	bitwise exclusive OR
MPI_MAXLOC	maximum and its location
MPI_MINLOC	maximum and its location

Allreduce operation



Scan operation



Hands-on

Matrix-vector multiplication

Master : Coordinates the work of others Slave : does a bit of work

Task : compute A . b

continue

- A : double precision (m x n) matrix
- **b** : double precision (n x 1) column matrix

Master algorithm

```
1. Broadcast b to each slave
2. Send 1 row of A to each slave
3. while ( not all m results received ) {
    Receive result from any slave s
    if ( not all m rows sent )
        Send new row to slave s
    else
        Send termination message to s
    }
```

Slave algorithm

- 1. Broadcast b (in fact receive b)
- 2. do {

Receive message m
if(m != termination)
 compute result
 send result to master
} while(m != termination)

3. slave terminates

Matrix-vector multiplication

```
int main( int argc, char** argv ) {
    int rows = 100, cols = 100; // dimensions of a
    double **a;
    double *b, *c;
    int master = 0;
                               // rank of master
    int myid;
                                   // rank of this process
    int numprocs;
                                   // number of processes
    // allocate memory for a, b and c
    a = (double**)malloc(rows * sizeof(double*));
    for( int i = 0; i < rows; i++ )</pre>
        a[i]=(double*)malloc(cols * sizeof(double));
    b = (double*)malloc(cols * sizeof(double));
    c = (double*)malloc(rows * sizeof(double));
    MPI Init( &argc, &argv );
    MPI Comm rank ( MPI COMM WORLD, &myid );
    MPI Comm size ( MPI COMM WORLD, & numprocs );
    if( myid == master )
        // execute master code
    else
        // execute slave code
    MPI Finalize();
```

Matrix vector multiplication

```
// initialize a and b
for(int j=0;j<cols;j++) {b[j]=1.0; for(int i=0;i<rows;i++) a[i][j]=i;}</pre>
// broadcast b to each slave
MPI Bcast( b, cols, MPI DOUBLE PRECISION, master, MPI COMM WORLD );
// send row of a to each slave, tag = row number
int numsent = 0;
for( int i = 0; (i < numprocs-1) && (i < rows); i++ ) {</pre>
     MPI Send(a[i], cols, MPI DOUBLE PRECISION, i+1, i, MPI COMM WORLD);
     numsent++;
for( int i = 0; i < rows; i++ ) {</pre>
    MPI Status status; double ans; int sender;
    MPI Recv( &ans, 1, MPI DOUBLE PRECISION, MPI ANY SOURCE,
              MPI ANY TAG, MPI COMM WORLD, &status );
    c[status.MPI TAG] = ans;
    sender = status.MPI SOURCE;
    if ( numsent < rows ) { // send more work if any
        MPI Send( a[numsent], cols, MPI DOUBLE PRECISION,
                  sender, numsent, MPI COMM WORLD );
        numsent++;
    } else // send termination message
        MPI Send ( MPI BOTTOM, 0, MPI DOUBLE PRECISION, sender,
                  rows, MPI COMM WORLD );
```

Matrix-vector multiplication

```
// broadcast b to each slave (receive here)
MPI Bcast( b, cols, MPI DOUBLE PRECISION, master, MPI COMM WORLD );
// send row of a to each slave, tag = row number
if( myid <= rows ) {</pre>
    double* buffer=(double*)malloc(cols*sizeof(double));
    while (true) {
        MPI Status status;
        MPI Recv( buffer, cols, MPI DOUBLE PRECISION, master,
                  MPI ANY TAG, MPI COMM WORLD, & status );
        if ( status.MPI TAG != rows ) { // not a termination message
            double ans = 0.0;
            for(int i=0; i < cols; i++)</pre>
                ans += buffer[i]*b[i];
            MPI Send ( & ans, 1, MPI DOUBLE PRECISION, master,
                       status.MPI TAG, MPI COMM WORLD );
        } else
            break;
 // more processes than rows => no work for some nodes
```
Outline

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Network cost modeling

- Simple performance model for multiple communications
 - Bisection bandwidth: sum of the bandwidths of the (average number of) links to cut to partition the network in two halves.
 - **Diameter**: maximum number of hops to connect any two devices



Bus topology

Bus = communication channel that is **shared** by all connected devices

- No more than two devices can communicate at any given time
- Hardware controls which devices have access
- High risk of **contention** when multiple devices try to access the bus simultaneously. Bus is a "**blocking**" interconnect.



Bus network properties

- Bisection bandwidth = point-to-point bandwidth (independent of # devices)
- Diameter = 1 (single hop)

Crossbar switch



Static routing in crossbar switch



Input – output pairings

Input	Output		
i ₁	0 ₂		
i ₂	0 ₄		
i ₃	0 ₁		
i ₄	0 ₃		
state A	state B		

Switches at crossing of input/output should be in state B. Other switches should be in state A. Path selection is fixed = static routing

Crossbar switch for distributed memory systems



- Crossbar implementation of a switch with P = 4 machines.
 - Fully non-blocking
 - Expensive: P² switches and O(P²) wires



- Built in **three stages**, using crossbar switches as components.
- Every output of an input stage switch is connected a different middle stage switch.
- Every input can be connected to every output, using any one of the middle stage switches.
- All input / output pairs can communicate simultaneously (non-blocking)
- Requires far less wiring than conventional CB switches.

output stage



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- Requires far less wiring than conventional CB switches.
- Adaptive routing may be necessary: can not find a connection for E !

output stage



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- **Every input** can be connected to every output, using any one of the middle stage switches.
- All input / output pairs can communicate simultaneously (non-blocking)
- Requires far less wiring than conventional CB switches.
- Adaptive routing may be necessary: reroute an existing path



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- Every output of an input stage switch is connected a different middle stage switch.
- Every input can be connected to every output, using any one of the middle stage switches.
- All input / output pairs can communicate simultaneously (non-blocking)
- Requires far less wiring than conventional CB switches.
- Adaptive routing may be necessary: E can now be connected

Switch examples

Infiniband switch (24 ports)





Gigabit Ethernet switch (24 ports)







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Basic performance terminology

- **Runtime** ("How long does it take to run my program")
 - In practice, only wall clock time matters
 - Depends on the number of parallel processes P
 - T_P = runtime using P processes
- **Speedup** ("How much faster does my program run in parallel")
 - $S_{P} = T_{1} / T_{P}$
 - In the ideal case, S_P = P
 - Super linear speedup are usually due to cache effects
- **Parallel efficiency** ("How well is the parallel infrastructure used")
 - $\eta_{P} = S_{P} / P$ ($0 \le \eta_{P} \le 1$)
 - In the ideal case, $\eta_P = 1 = 100\%$
 - Depends on the application what is considered acceptable efficiency

Strong scaling: Amdahl's law

- Strong Scaling = increasing the number of parallel processes for a fixed-size problem
- Simple model: partition sequential runtime T₁ in a parallelizable fraction (1-s) and inherently sequential fraction (s).



Strong scaling: Amdahl's law

• Consequently,
$$S_P = \frac{T_1}{T_P} = \frac{T_1}{sT_1 + \frac{(1-s)T_1}{P}} = \frac{1}{s + \frac{1-s}{P}}$$
 (Amdahl's law)

- Speedup is **bounded** $S_{\infty} = \frac{1}{s}$
 - e.g. s = 1%, S_∞ = 100
 - e.g. s = 5%, S_∞ = 20
- Sources of sequential fraction sT₁
 - Process startup overhead
 - Inherently sequential portions of the code
 - Dependencies between subtasks
 - Communication overhead
 - Function calling overhead
 - Load misbalance

Amdahl's law



Amdahl's law



Amdahl's law



Weak scaling: Gustafson's law

- Weak scaling: increasing both the number of parallel processes P and the problem size N.
- Simple model: assume that the sequential part is constant, and that the parallelizable part is proportional to N.

• $T_1(N) = T_1(1)[s + (1-s)N]$ ($0 \le s \le 1$)



Gustafson's law

 Solve increasingly larger problems using a proportionally higher number of processes (N = P).



Therefore, $T_P(N) = T_1(1)[s + \frac{(1-s)N}{P}]$ and hence $T_P(P) = T_1(1)$ Speedup $S_P(P) = s + (1-s)P = P - s(P-1)$ (Gustafson's law)

Gustafson's law



Gustafson's law



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Case study: parallel matrix multiplication

- Matrix-matrix multiplication: $C = \alpha^* A^* B + \beta^* C$ (BLAS xgemm)
 - Assume C = m x n; A = m x k; B = k x n matrix.
 - α , β = scalars; assume α = β = 1 in what follows, i.e. C = C + A*B
- Initially, matrix elements are distributed among P processes
 - Assume same scheme for each matrix A, B and C
- Each process computes values for C that are local to that process
 - Required data from A and B that is not local needs to be communicated
 - Performance modeling assuming the α , β , γ model
 - $\circ \alpha$ = latency
 - \circ β = per element transfer time
 - \circ γ = time for single floating point computation

- Two dimensional partitioning
 - Partition matrices in 2D in an r x c mesh (P = r*c)
 - X(I, J) refers to block (I, J) of matrix X (X = {A, B, C})
 - Process p_n is also denoted by p_{i,j} (n = i*c + j) and holds X(I,J)



- Second approach: two dimensional partitioning (SUMMA)
 - Process p_{i,i} needs to compute C(I, J):

$$C(I, J) = C(I, J) + \sum_{i=0}^{k-1} A(I, i) * B(i, J)$$

index i refers to a single column of A or single row of B

do this in parallel

 $\forall I = 0 \dots r$

 $\forall J = 0 \dots c$



- Second approach: two dimensional partitioning
 - SUMMA algorithm (all I and J in parallel)

```
for i = 0 to k-1
    broadcast A(I, i) within process row
    broadcast B(i, J) within process column
    C(I,J) += A(I, i) * B(i, J)
endfor
```

Cost for inner loop (executed k times):

 \circ log₂c (α + β(m/r)) + log₂r (α + β(n/c)) + 2mnγ/P

- Total $T_P = 2kmn\gamma/P + k\alpha(log_2c + log_2r) + k\beta((m/r)log_2c) + (n/c)log_2r)$
- For n = m = k and r = c = sqrt(P) we find:
 Parallel efficiency η_P = 1 / (1 + (α/γ)(Plog₂P)/(2n²) + (β/γ)∨P logP/n) Isoefficiency when n grows as √P (constant memory per node!)

Even more efficient: use "blocking" algorithm



- SUMMA algorithm is implemented in **PBLAS = Parallel BLAS**
- Algorithm can be extended to block-cyclic layout (see further)

Case study: parallel Gaussian Elimination

ScalaPACK SOFTWARE HIERARCHY



Case Study 2: Parallel Sorting



Case study: parallel sorting algorithm

- **Sequential** sorting of n keys (1st Bachelor)
 - Bubblesort: O(n²)
 - Mergesort: O(n log n), even in worst-case
 - Quicksort: O(n log n) expected, O(n²) worst-case, fast in practice
- **Parallel** sorting of n keys, using P processes
 - Initially, each process holds n/p keys (unsorted)
 - Eventually, each process holds n/p keys (sorted)
 - Keys per process are sorted
 - If q < r, each key assigned to process q is less than or equal to every key assigned to process r (sort keys in rank order)

Case study: parallel sorting algorithm

Bubblesort algorithm: O(n²)

Example:	$52481 \rightarrow$	2451 <mark>8</mark>	after iteration 1
	\rightarrow	2 4 1 <mark>5 8</mark>	after iteration 2
	\rightarrow	2 1 4 5 8	after iteration 3
	\rightarrow	1 2 4 5 8	after iteration 4
Bubblesort

- Result of current step (a[i] > a[i+1]) depends on previous step
 - Value of a[i] is determined by previous step
 - Algorithm is "inherently serial"
 - Not much point in trying to parallelize this algorithm
- Odd-even transposition sort
 - Decouple algorithm in two phases: even and odd
 - Even phase: compare-swap on following elements: (a[0], a[1]), (a[2], a[3]), (a[4], a[5]), ...
 - Odd phase: compare-swap operations on following elements: (a[1], a[2]), (a[3], a[4]), (a[5], a[6]), ...

Even-odd transposition sort algorithm: O(n²)

```
void Even odd sort(int *a, int n) {
    for (int phase = 0; phase < n; phase++)</pre>
        if (phase % 2 == 0) { // even phase
            for (int i = 0; i < n-1; i += 2)
                 if (a[i] > a[i+1]) { ]
                     temp = a[i];
                     a[i] = a[i+1]
                                         "Compare-swap" operation
                     a[i+1] = temp;
        } else {
                              // odd phase
            for (int i = 1; i < n-1; i += 2)
                 if (a[i] > a[i+1]) {
                     temp = a[i];
                     a[i] = a[i+1]
                                         "Compare-swap" operation
                     a[i+1] = temp;
                 }
```

Even-odd transposition sort algorithm: O(n²)

Example:
$$52481 \rightarrow 25481$$
 even phase
 $\rightarrow 24518$ odd phase
 $\rightarrow 24158$ even phase
 $\rightarrow 21458$ odd phase
 $\rightarrow 12458$ even phase

Parallelism within each even or odd phase is now obvious: Compare-swap between (a[i], a[i+1]) independent from (a[i+2], a[i+3])



Communicate value with neighbor

- Right process (highest rank) keeps largest value
- Left process (lowest rank) keeps smallest value

Image reproduced from P. Pacheco

Parallel algorithm

- Now, assume n/P >> 1 (as is typically the case)
- Example: P = 4; n = 16



Theorem: Parallel odd-even transposition sort algorithm will sort the input list after P (= number of processes) phases.

Parallel even-odd transposition sort pseudocode

```
sort local keys
for (int phase = 0; phase < P; phase++) {
    neighbor = computeNeighbor(phase, myRank);
    if (I'm not idle) { // first and/or last process may be idle
        send all my keys to neighbor
        receive all keys from neighbor
        if (myRank < neighbor)
            keep smaller keys
        else
            keep larger keys
    }
}</pre>
```

Implementation of computeNeighbor (MPI)

```
int computeNeighbor(int phase, int myRank) {
    int neighbor;
    if (phase % 2 == 0) {
        if (myRank % 2 == 0)
             neighbor = myRank + 1;
        else
             neighbor = myRank - 1;
    } else {
        if (myRank % 2 == 0)
             neighbor = myRank - 1;
        else
             neighbor = myRank + 1;
    }
    if (neighbor == -1 || neighbor == P-1)
        neighbor = MPI PROC NULL;
    return neigbor;
                            When used as destination or source rank in MPI Send
}
                            or MPI_Recv, no communication takes place
```

Implementation of data exchange in MPI

- Be careful of deadlocks
- In both even and odd phases, communication always takes place between a process with even, and a process with odd rank



```
MPI Sendrecv(...)
```

Algorithm reproduced from P. Pacheco

Parallel odd-even transposition sort algorithm analysis

- Initial sorting: O(n/P log(n/P)) time
 - Use an efficient sequential sorting algorithm, e.g. quicksort or mergesort
- **Per phase**: $2(\alpha + n/P \beta) + \gamma n/P$
- Total runtime $T_P(n) = O(n/P \log(n/P) + 2(\alpha P + n\beta) + \gamma n$ = 1/P O(n log n) + O(n)
- Linear speedup when P is small and n is large
- However, bad asymptotic behaviour
 - When n and P increase proportionally, runtime per process is O(n)
 - What we really want: O(log n)
 - Difficult! (but possible!)

- Sorting networks (= graphical depiction of sorting algorithms)
 - Number of horizontal "wires" (= elements to sort)
 - Connected by vertical "comparators" (= compare and swap)



Example (4 elements to sort)





Same bubblesort algorithm (parallel)



Sequential runtime = number of comparators = "size of the sorting network" = n * (n - 1) / 2

Parallel runtime (assume P == n processes) = "depth of sorting network" = 2n - 3

Definition: **depth of a sorting network** (= parallel runtime)

- Zero at the inputs or each wire
- For a comparator with inputs with depth d₁ and d₂, the depth of its outputs is 1 + max(d₁, d₂)
- Depth of the sorting network = maximum depth of each output



• Sorting network of **odd-even transposition sort**



- Parallel runtime = "depth of sorting network" = n
- ... or P (we assume n == P)

• Can we do better?

- Sequential sorting algorithms are **O(n log n)**
- Ideally, P and n can scale proportionally: P = O(n)
- That means that we want to sort n numbers in O(log n) time
 - This is possible (!), however, big constant pre-factor
- We will describe an algorithm that can sort n numbers in O(log² n) parallel time (using P = O(n) processes)
 - This algorithm has **best performance in practice**
 - ... unless n becomes huge (n > 2^{2000})
 - Nobody wants to sort that many numbers

• **Theorem**: If a sorting network with n inputs sorts all 2ⁿ binary strings of length n correctly, then it sorts all sequences correctly (proof: see references).



We will design an algorithm that can sort binary sequences in O(log₂²n) time

- **Step 1:** create a sorting network that sorts bitonic sequences
- **Definition**: A **bitonic sequence** is a sequence which is first increasing and then decreasing, or can be circularly shifted to become so.
 - (1, 2, 3, 3.14, 5, 4, 3, 2, 1) is bitonic
 - (4, 5, 4, 3, 2, 1, 1, 2, 3) is bitonic
 - (1, 2, 1, 2) is not bitonic
- Over zeros and ones, a bitonic sequence is of the form
 - $0^{i}1^{j}0^{k}$ or $1^{i}0^{j}1^{k}$ (with e.g. $0^{i} = 0000...0 = i$ consecutive zeros)
 - i, j or k can be zero

- Now, let's create a sorting network that sorts a **bitonic sequence**
- A half-cleaner network connects line i with line i + n/2



- If the input is a binary bitonic sequence then for the output
 - Elements in the top half are smaller than the corresponding elements in the bottom half, i.e. halves are relatively sorted.
 - One of the halves of the output consists of only zeros or ones (i.e. is "clean"), the other half is bitonic.

• Example of a half-cleaner network

input = bitonic sequence



 Therefore, a bitonic sorter[n] (i.e. network that sorts a bitonic sequence of length n) is obtained as



A bitonic sorter sorts a bitonic sequence of length n = 2^k using

- size = nk/2 = n/2 log₂n comparators (= sequential time)
- depth = k = log₂n (= parallel time)

- Step 2: Build a network merger[n] that merges two sorted sequences of length n/2 so that the output is sorted
 - Flip second sequence and concatenate first and flipped second
 - Concatenated sequence is bitonic, sort using step 1



- **Step 3**: Build a **sorter[n]** network that sorts arbitrary sequences
 - Do this recursively from merger[n] building blocks
 - Depth: D(1) = 0 and D(n) = D(n/2) + log₂n = O(log₂²n)





- Further reading of bitonic networks:
 - http://valis.cs.uiuc.edu/~sariel/teach/2004/b/ webpage/lec/14_sortnet_notes.pdf
- In case **n is not a power of two**:
 - http://www.iti.fh-flensburg.de/lang/algorithmen/ sortieren/bitonic/oddn.htm

