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MPI Programming

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Outline

- Introduction
- Basic MPI programming
- Examples
  - Finite Difference Method
  - Finite Element Method
  - LU Factorization
  - Monte Carlo Method
  - Molecular Dynamics
  - MPMD Models

Introduction

Acknowledgments

- Thanks to Professor Lasse Natvig and Associate Professor Jørn Amundsen from IDI, NTNU for allowing me to copy from their “Parallel Programming” lecture slides
- Thanks to IBM for allowing me to copy from their MPI redbook:
  - www.redbooks.ibm.com/redbooks/pdfs/sg245380.pdf

The Examples

- No exercises, but 7 working examples are explained
  - The last 6 are larger examples
- Kongull:
  - ssh -Y kongull.hpc.ntnu.no
  - cp -r /home/hrn/Kurs/mpi .
  - module load intelcomp
- Vilje:
  - ssh -Y vilje.hpc.ntnu.no
  - cp -r /home/ntnu/hrn/Kurs/mpi .
  - module load intelcomp mpt

Basic MPI Programming

MPI Programs in C

- A C program
  - Has a main() function
  - Includes stdio.h, string.h, etc.
- Need to include mpi.h header file
- Indentifiers defined by MPI start with “MPI_”
- First letter following underscore is uppercase
  - For function names and MPI-defined types
  - Helps to avoid confusion

MPI Programs in Fortran

- include 'mpif.h'
  - No argument checking! Don't use it.
- use mpi
  - Provide explicit interfaces for all MPI routines → compile time argument checking
- use mpi_f08
  - Fully Fortran 2008 compatible definition of all MPI routines
  - New syntax TYPE(*), DIMENSION(...) to define choice buffers in a standardized way

Identifying MPI Processes

- Common practice is to identify processes by non-negative integer ranks
- p processes are numbered 0, 1, 2, …, p-1
- This can be:
  - p processes distributed over p processors (“physical parallelism”)
  - p processes running time-multiplexed on a single processor (“logical parallelism”)

Example 1: Hello, World!

- Change to the directory:
```
$ cd mpi/ex1
```
- Compile the code:
```
$ make
cc -O2 mpi_hello.c -o mpi_hello
```
- Edit the job script:
```
$ vim run.job (change ACCOUNT)
```
- Run the job
```
$ qsub run.job
```

MPI Start and End

- MPI_Init()
  - Tells MPI to do all the necessary setup

```
int MPI_Init(
        int*    argc_p
        char*** argv_p);
```

Pointers to the arguments to main: argc & arv

- MPI_Finalize()
  - Tells MPI we're done, so clean up anything allocated

```
int MPI_Finalize(void);
```

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Basic Outline

```
...
#include <mpi.h>
...
int main(int argc, char* argv[]) {
  ...
  /* No MPI calls before this */
  MPI_Init(&argc, &argv);
  ...
  MPI_Finalize();
  /* No MPI calls after this */
  ...
  return 0;
}
```

Communicators

- A collection of processes that can send messages to each other
- MPI_Init() defines a communicator that consists of all the processes created when the program is started
  - MPI_COMM_WORLD

Communicators

```
int MPI_Comm_size(
      MPI_Comm    comm  /* in  */,
      int*        size  /* out */);
```

number of processes in the communicator

```
int MPI_Comm_rank(
      MPI_Comm    comm  /* in  */
      int*        rank  /* out */);
```

my rank
(the process making this call)

Communication

number of elements in
the send buffer

```
int MPI_Send(
      void*        buf           /* in */,
      int          count         /* in */,
      MPI_Datatype datatype      /* in */,
      int          dest          /* in */,
      int          tag           /* in */,
      MPI_Comm     communicator  /* in */);
```

Data Types

MPI datatype	C datatype
MPI_CHAR	signed **char**
MPI_SHORT	signed **short int**
MPI_INT	signed **int**
MPI_LONG	signed **long int**
MPI_LONG_LONG	signed **long long int**
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	
MPI_PACKED	

Communication

max. number of elements to receive

```
int MPI_Recv(
      void*         buf           /* out */,
      int           count         /* in  */,
      MPI_Datatype datatype       /* in  */,
      int           source        /* in  */,
      int           tag           /* in  */,
      MPI_Comm      communicator  /* in  */,
      MPI_Status*   status        /* out */);
```

Message Matching

- Process q calls MPI_Send()

```
MPI_Send(send_buf, send_count, send_type, dest,
         send_tag, send_comm);
```

r

- Process r calls MPI_Recv()

```
MPI_Recv(recv_buf, recv_count, recv_type, src,
         recv_tag, recv_comm, &status);
```

q

Receiving Messages

- A receiver can get a message without knowing:
  - the amount of data in the message,
  - the sender of the message
    - MPI_ANY_SOURCE
  - or the tag of the message
    - MPI_ANY_TAG

The Status Argument

- If MPI_ANY_SOURCE or MPI_ANY_TAG have been used, you can get help from MPI_Status

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

```
MPI_Status status;

status.MPI_SOURCE
status.MPI_TAG
```

How much data am I receiving?

```
int MPI_Probe(
      int           source      /* in */,
      int           tag         /* in */,
      MPI_Comm      comm        /* in */
      MPI_Status*   status      /* out */);

int MPI_Get_count(
      MPI_Status*    status     /* in  */,
      MPI_Datatype   datatype   /* in  */,
      int*           count      /* out */);
```

Issues with Send and Receive

- Exact behavior is determined by the MPI implementation
- MPI_Send() is blocking as defined in the standard, but is non-blocking up to a certain message size in most implementations
  - MPI_Ssend() might be used to force blocking untill a receive is posted
  - MPI_Bsend() can be used with a user defined send buffer - then always non-blocking
- MPI_Recv() always blocks until a matching message is received

Issues with Send and Receive

- AND, …
  - MPI programs will easily hang!
    - A receive without corresponding send
    - A send without corresponding receive
    - Or deadlock
      - Circular waiting

Non-Blocking Communication

```
int MPI_Isend(void* buffer, int count, MPI_Datatype
      datatype, int destination, int tag, MPI_Comm comm,
      MPI_Request* request);

int MPI_Irecv(void* buffer, int count, MPI_Datatype
      datatype, int source, int tag, MPI_Comm comm,
      MPI_Request* request);

int MPI_Wait(MPI_Request* request, MPI_Status* status);

int MPI_Waitall(int array_size,
      MPI_Request requests[], MPI_Status statuses[]);
```

I = Immediate

Non-Blocking Communication

- Immediate-mode MPI_Isend() and MPI_Irecv() only start the data copy operation
- MPI_Wait() and MPI_Waitall() are used to complete the operations
- Useful in complicated send-receive situations (e.g. 2D grid of processes)
- Calculations can take place between those two calls
  - Difficult to make good use of
  - Communication and calculation at the same time is more efficient

Global Reduction

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

- op determines which global reduction to perform
- Predefined reductions for the most used types, like MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, etc.
- Also possible to specify user defined reduction operations with MPI_Op_create()
- MPI_IN_PLACE specified for sendbuf at rank root, makes the receive buffer a send-and-receive buffer

Broadcast

```
int MPI_Bcast(void *buffer, int count, MPI_Datatype
      Datatype, int root, MPI_Comm comm);
```

- Broadcasts a message from the process with rank root to all other processes of the communicator

Scatter and gather

```
int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype
      sendtype, void *recvbuf, int recvcount,
      MPI_Datatype recvtype, int root, MPI_Comm comm);

int MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype
      sendtype, void *recvbuf, int recvcount,
      MPI_Datatype recvtype, int root, MPI_Comm comm);
```

- Routines to spread and collect data from or to root
- MPI_Scatter: if root sends 100 numbers to 10 processes, then sendbuf on root must be 1000 long
- MPI_Gather: if root receives 100 numbers from 10 processes, then recvbuf on root must be 1000 long

Allreduce, allgather and more

- MPI_Allreduce() and MPI_Allgather() are identical to their siblings, except that the end result is made available to all ranks
- As if the operation was followed by a broadcast
- There are also more elaborate combined all-to-all scatter-gather functions, like MPI_Alltoall(), MPI_Alltoallv() and MPI_Alltoallw()
- Use the man pages to get more information, e.g.:

```
$ man MPI_Allreduce
```

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Examples

Writing Larger MPI Programs

- Question:
  - Now that we can write “Hello World!” MPI programs, then what do we need in order to write larger MPI programs for scientific projects?
- Answer:
  - Parallel algorithms
  - Data must be distributed to all proceses so that they all are kept busy during the entire execution of MPI programs

Data Distribution

- The majority of time is usually spent in DO/FOR loops
- Multiple data distribution methods:
  - Block distribution
    - Column wise
    - Row wise
    - In both dimensions
  - Cyclic distribution
  - Master-worker
- 6 examples

2. Finite Difference Method

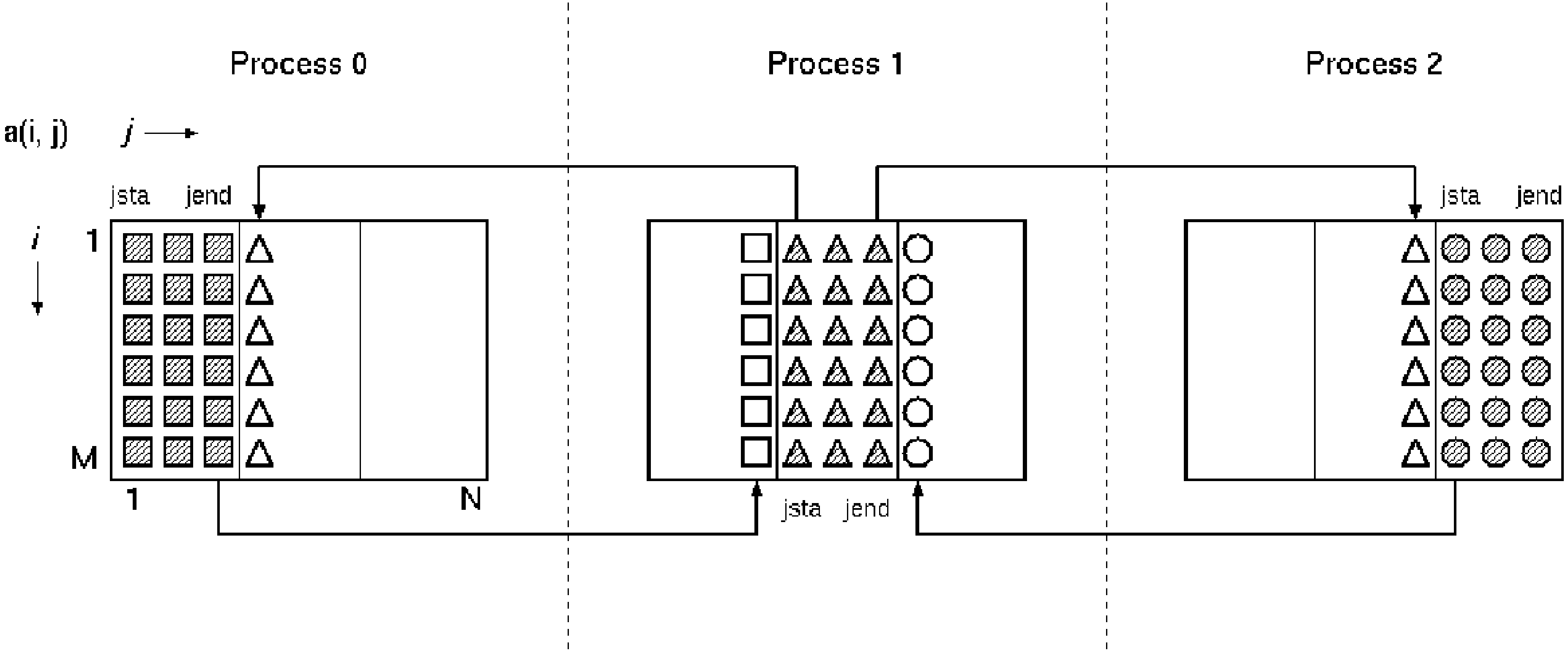
- Wikipedia:

  "Numerical methods for solving differential equations by approximating them with difference equations"
- Only a skeleton 2D FDM program is shown here
- Coefficients and the enclosing loop are omitted
- Data dependencies exist in both dimensions

The Sequential Algorithm

```
PROGRAM main
IMPLICIT REAL*8 (a-h,o-z)
PARAMETER (m=6, n=9)
DIMENSION a(m,n), b(m,n)
DO j=1, n
  DO i=1, m
    a(i,j) = i + 10.0 * j
  ENDDO
ENDDO
DO j=2, n-1
  DO i=2, m-1
    b(i,j) = a(i-1,j) + a(i,j-1) + a(i,j+1) + a(i+1,j)
  ENDDO
ENDDO
END
```

Column-Wise Block Distribution



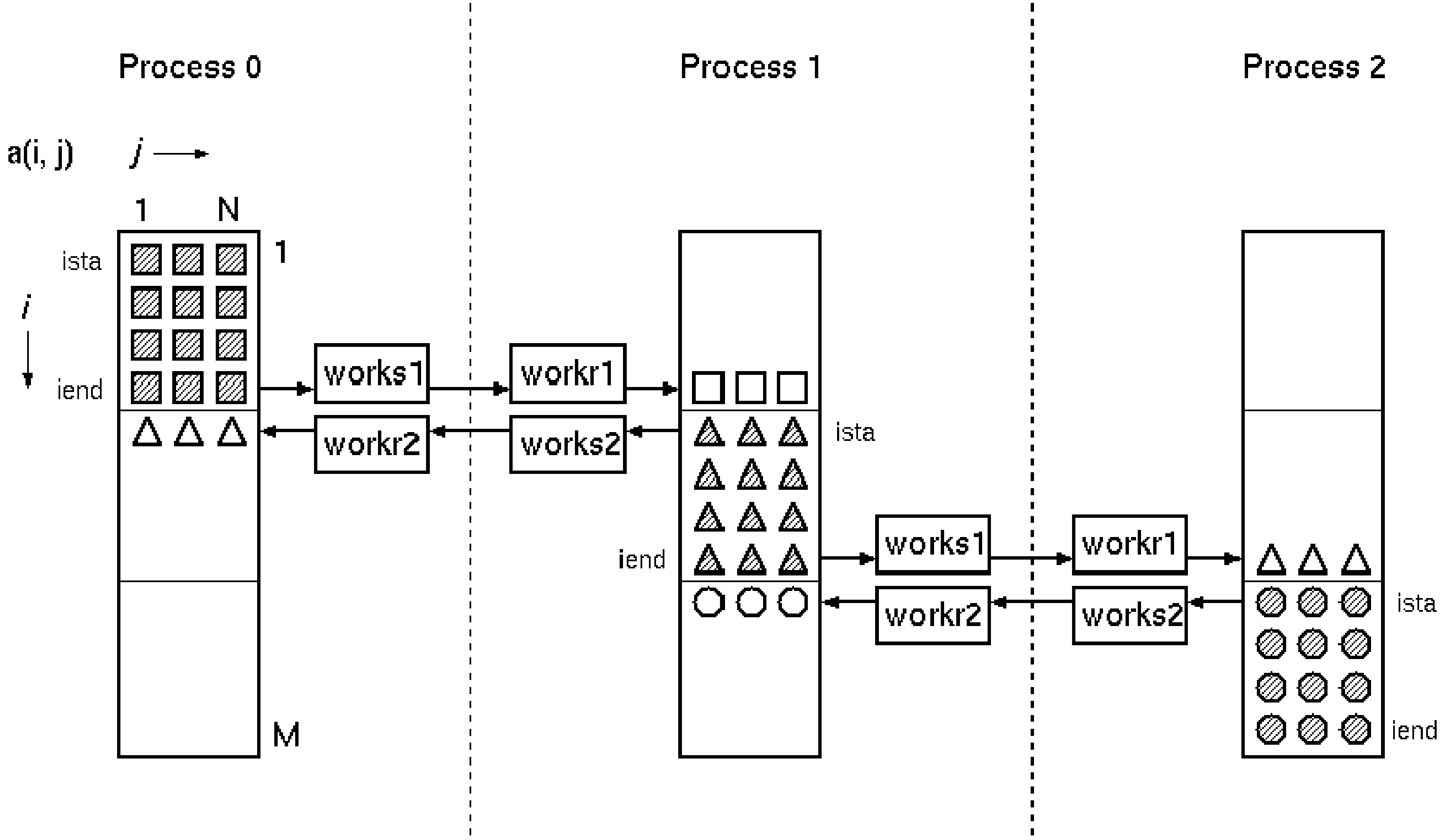
Column-Wise Block Distribution

- We must distribute a 2D matrix onto the processes
- Fortran stores arrays in column-major order
- Boundary elements between processes are contiguous in memory
- There are no problems with using MPI_SEND and MPI_RECV

Example 2

ex2/fdm1.f90

Row-Wise Block Distribution



Row-Wise Block Distribution

- Fortran stores arrays in column-major order
- Boundary elements between processes are not contiguous in memory
- Boundary elements can be copied by:
  - Using derived data types
  - Writing code for packing data, sending/receiving it, and then unpacking it

Example 2

ex2/fdm2.f90

Block Distribution in Both Dim. (1)

- The amount of data transferred might be minimized
  - Depends upon the matrix size and the number of processes
- A process grid itable is prepared for looking up processes quickly

Block Distribution in Both Dim. (1)

a(i, j) $j \rightarrow$

$i \downarrow$

	1								N
1	0	0	0	1	1	1	2	2	2
	0	0	0	1	1	1	2	2	2
	0	0	0	1	1	1	2	2	2
	0	0	0	1	1	1	2	2	2
	3	3	3	4	4	4	5	5	5
	3	3	3	4	4	4	5	5	5
	3	3	3	4	4	4	5	5	5
	3	3	3	4	4	4	5	5	5
	6	6	6	7	7	7	8	8	8
	6	6	6	7	7	7	8	8	8
	6	6	6	7	7	7	8	8	8
M	6	6	6	7	7	7	8	8	8

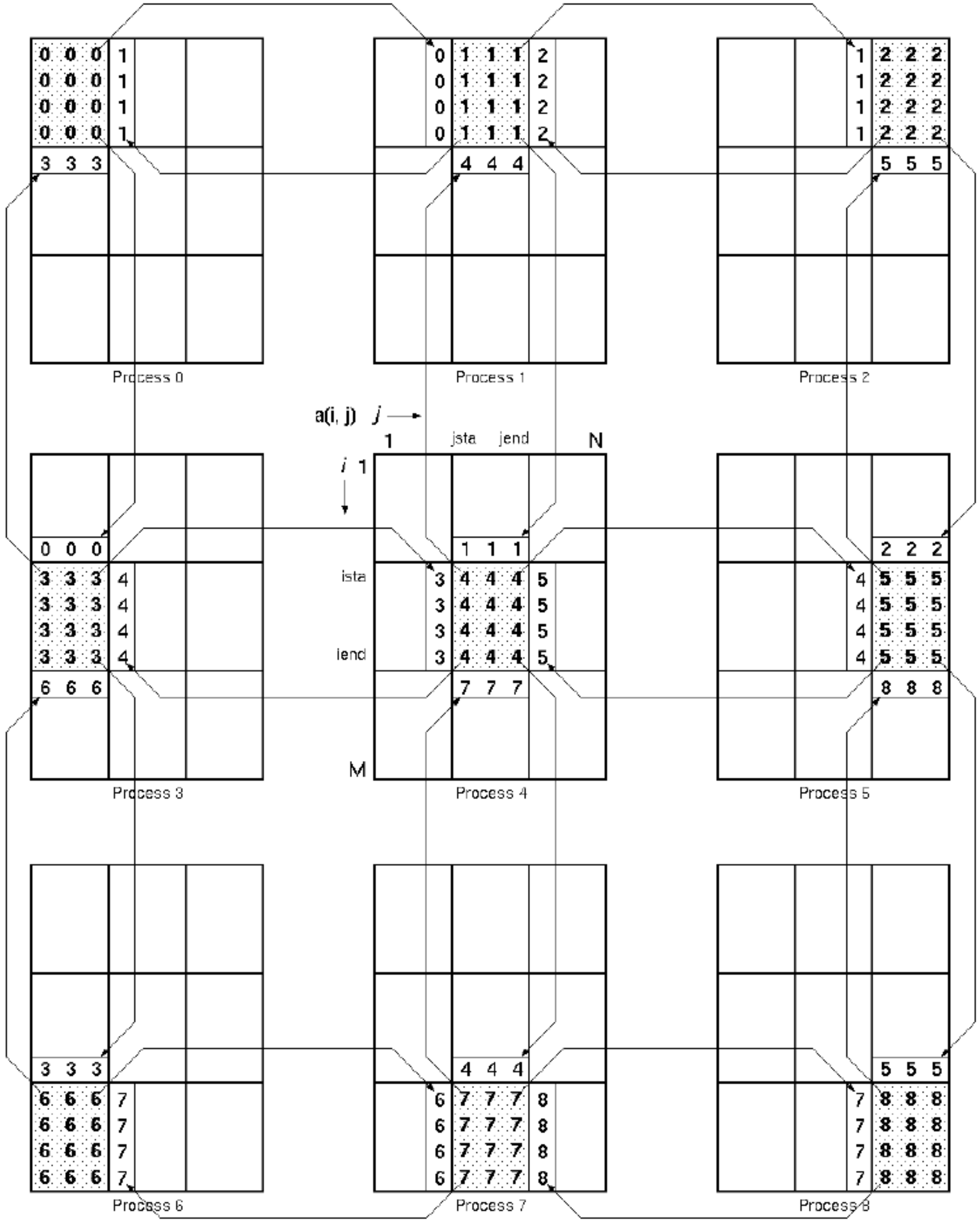
(a) The distribution of a()

itable(i, j) $j \rightarrow$

$i \downarrow$

	−1	0	1	2	3
−1	null	null	null	null	null
0	null	0	1	2	null
1	null	3	4	5	null
2	null	6	7	8	null
3	null	null	null	null	null

(b) The process grid



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Example 2

ex2/fdm3.f90

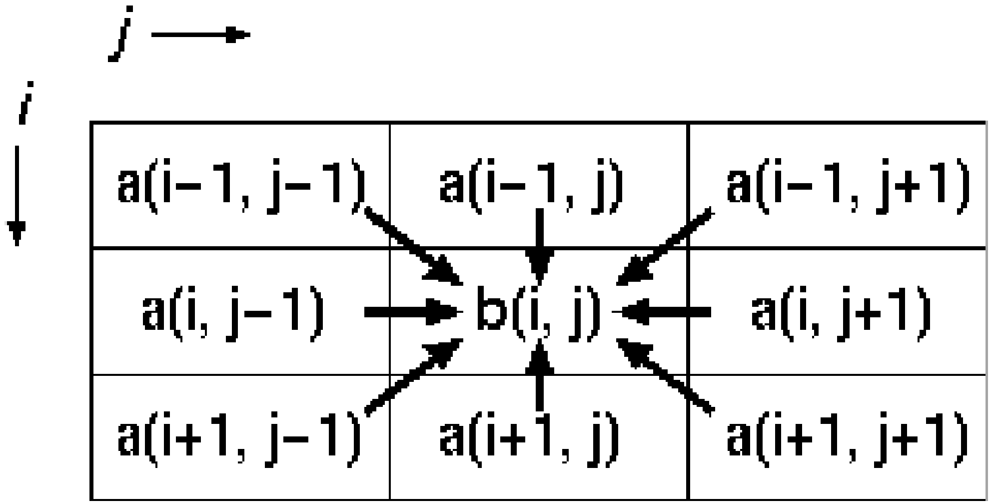
Block Distribution in Both Dim. (2)

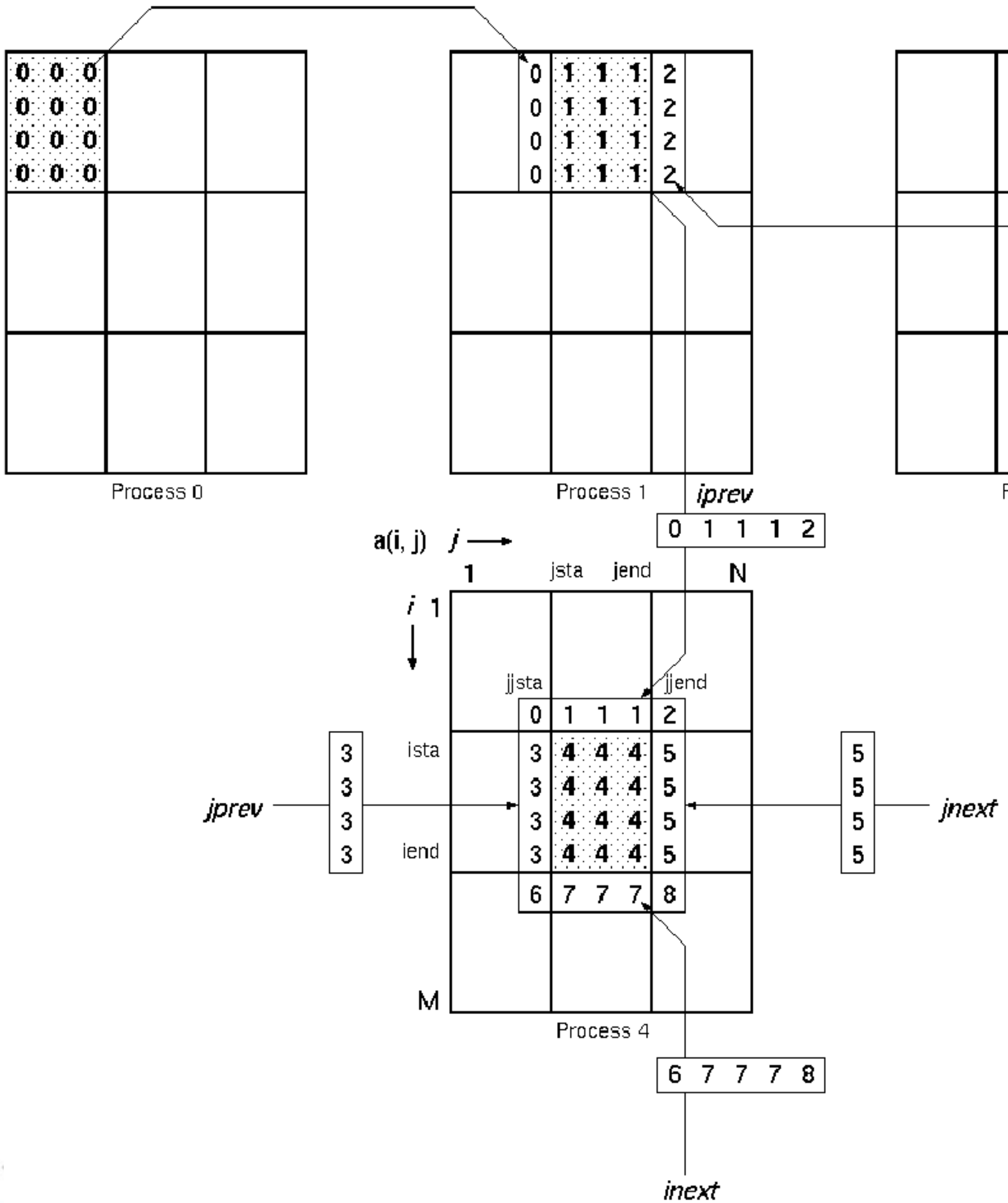
- The corner elements are now included
- The data dependencies are therefore more complex

The Sequential Algorithm

```
PROGRAM main
IMPLICIT REAL*8 (a-h,o-z)
PARAMETER (m=12, n=9)
DIMENSION a(m,n), b(m,n)
DO j=1, n
  DO i=1, m
    a(i,j) = i + 10.0 * j
  ENDDO
ENDDO
DO j=2, n-1
  DO i=2, m-1
    b(i,j) = a(i-1,j) + a(i,j-1) + a(i,j+1) + a(i+1,j) + &
             a(i-1,j-1) + a(i+1,j-1) + a(i-1,j+1) +a(i+1,j+1)
  ENDDO
ENDDO
END
```

The Data Dependency





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Example 2

ex2/fdm4.f90

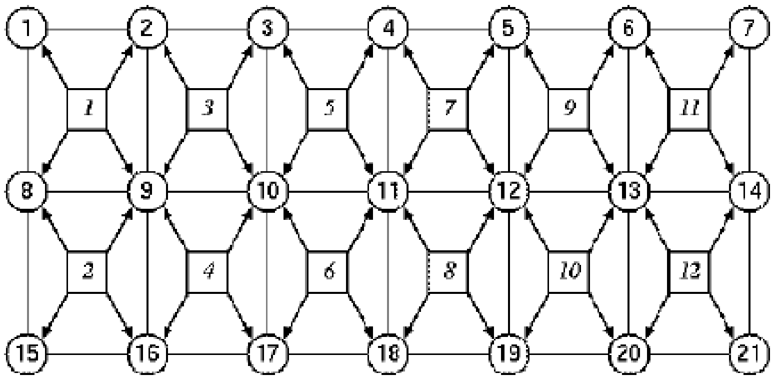
3. Finite Element Method

- Wikipedia:

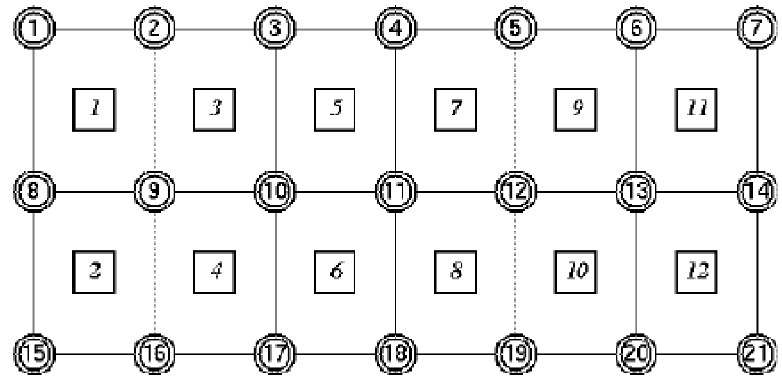
  “Numerical technique for finding approximate solutions to boundary value problems for partial differential equations”

- A more complete example that produces a result

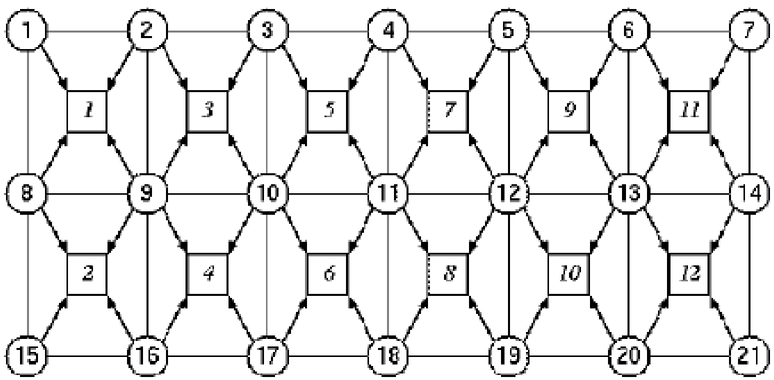
Finite Element Method



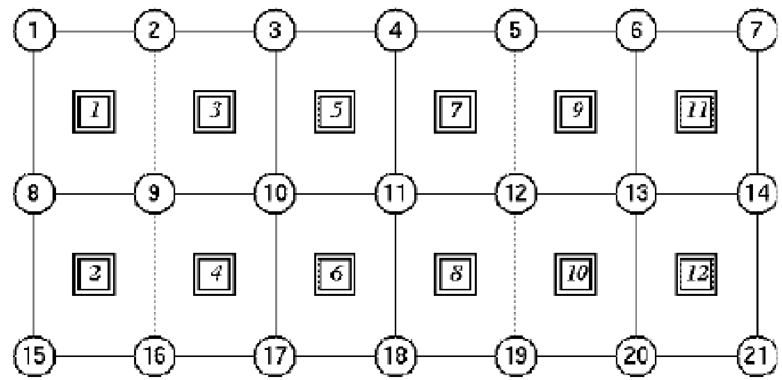
(a) Elements -> Nodes



(b) Update Nodes



(c) Nodes -> Elements



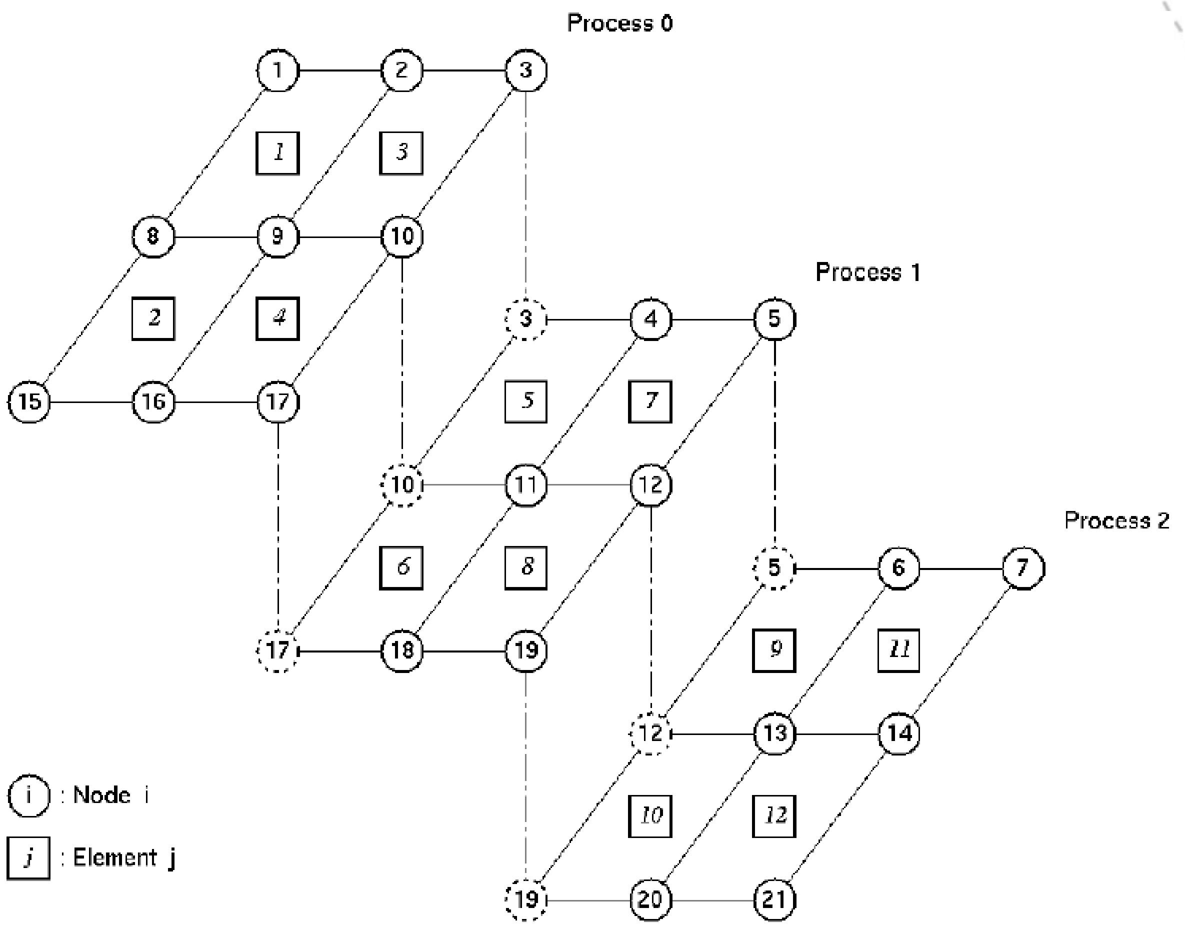
(d) Update Elements

The Sequential Algorithm

```
PARAMETER(iemax=12, inmax=21)
REAL*8 ve(iemax), vn(inmax)
INTEGER index(4,iemax)
...
DO ie=1, iemax
  ve(ie) = ie * 10.0
ENDDO
DO in=1, inmax
  vn(in) = in * 100.0
ENDDO
DO itime=1, 10
  DO ie=1, iemax
    DO j=1, 4
      vn(index(j,ie)) =
vn(index(j,ie)) + ve(ie)
    ENDDO
  ENDDO
```

```
  DO in = 1, inmax
    vn(in) = vn(in) * 0.25
  ENDDO
  DO ie = 1, iemax
    DO j = 1, 4
      ve(ie) = ve(ie) + vn(index(j,ie))
    ENDDO
  ENDDO
  DO ie = 1, iemax
    ve(ie) = ve(ie) * 0.25
  ENDDO
ENDDO
PRINT *,'Result',vn,ve
```

Distributing the Data



Differences from IBM version

- 2D enumeration (row, column) is used instead of 1D enumeration
- The amount of memory allocated by each process is minimized
- A node column is sent to the right
- An element column is sent to the left

Example 3

ex3/main.f90 and ex3/grid.f90

4. LU Factorization

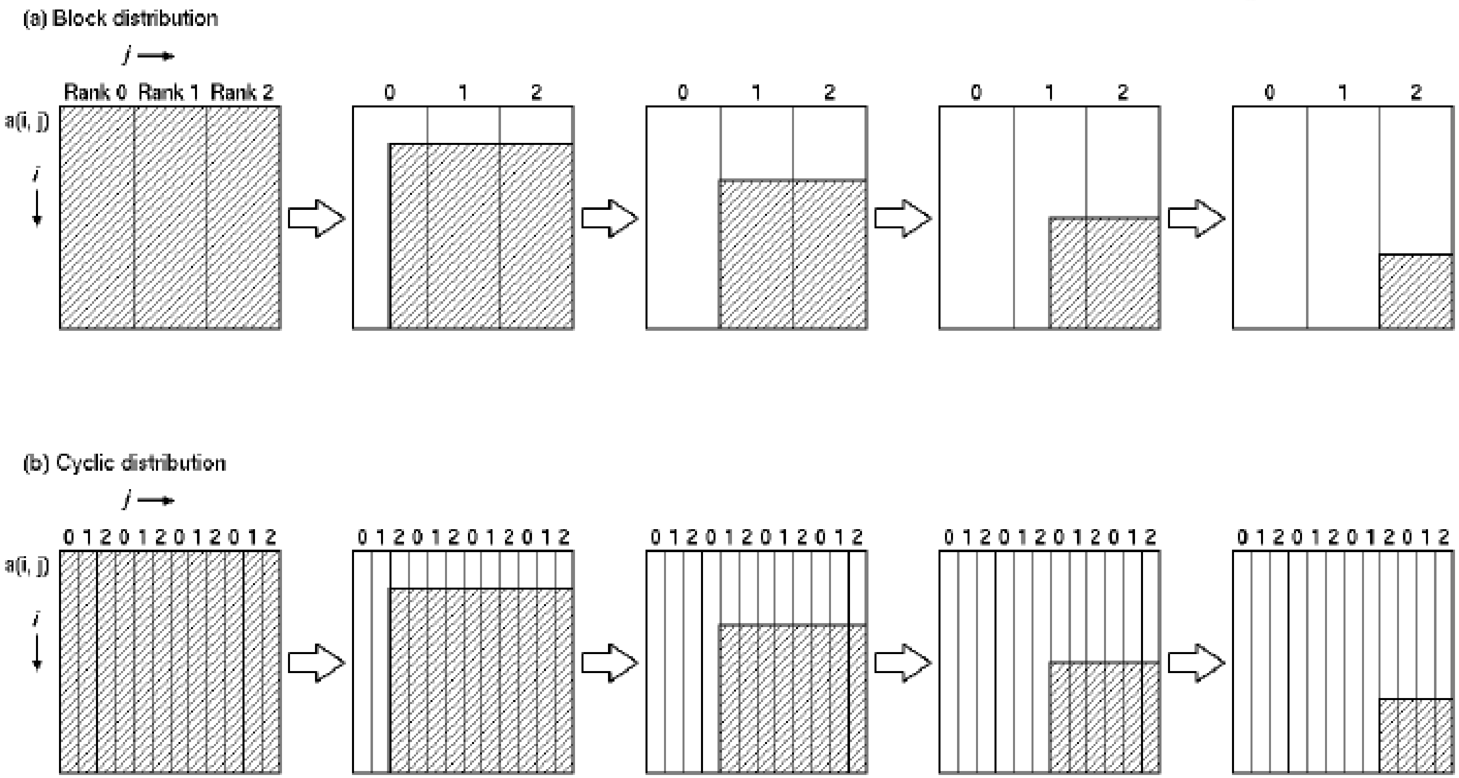
- Wikipedia:
  - “Factors a matrix as the product of a lower triangular matrix and an upper triangular matrix”
  - Used for solving square systems of linear equations: $Ax = b$
- ScaLAPACK and Intel's MKL library have optimized subroutines for this (outside the scope of this course)
- Pivoting and loop-unrolling is not considered

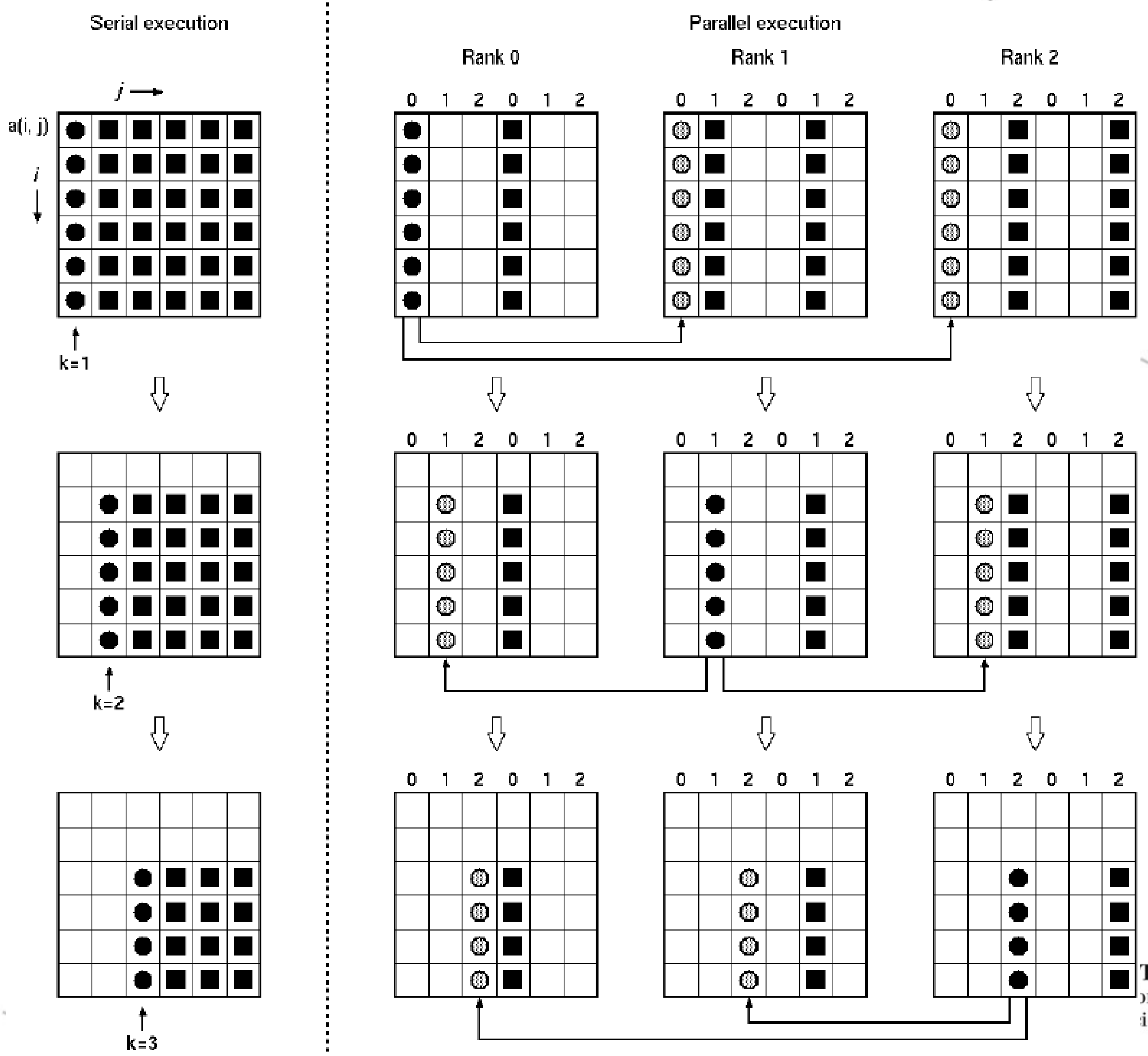
The Sequential Algorithm

```
PROGRAM main
PARAMETER (n = ...)
REAL a(n,n), b(n)
...
! LU factorization
DO k = 1, n-1
  DO i = k+1, n
    a(i,k) = a(i,k) / a(k,k)
  ENDDO
  DO j = k+1, n
    DO i = k+1, n
      a(i,j) = a(i,j)-a(i,k)*a(k,j)
    ENDDO
  ENDDO
ENDDO
```

```
! Forward elimination
DO i = 2, n
  DO j = 1, i - 1
    b(i) = b(i) - a(i,j)*b(j)
  ENDDO
ENDDO
! Backward substitution
DO i = n, 1, -1
  DO j = i + 1, n
    b(i) = b(i) - a(i,j)*b(j)
  ENDDO
  b(i) = b(i) / a(i,i)
ENDDO
...
END
```

Cyclic Data Distributing




Serial execution
Parallel execution
Rank 0
Rank 1
Rank 2
j
a(i, j)
i
k=1
k=2
k=3
0 1 2 0 1 2

Example 4

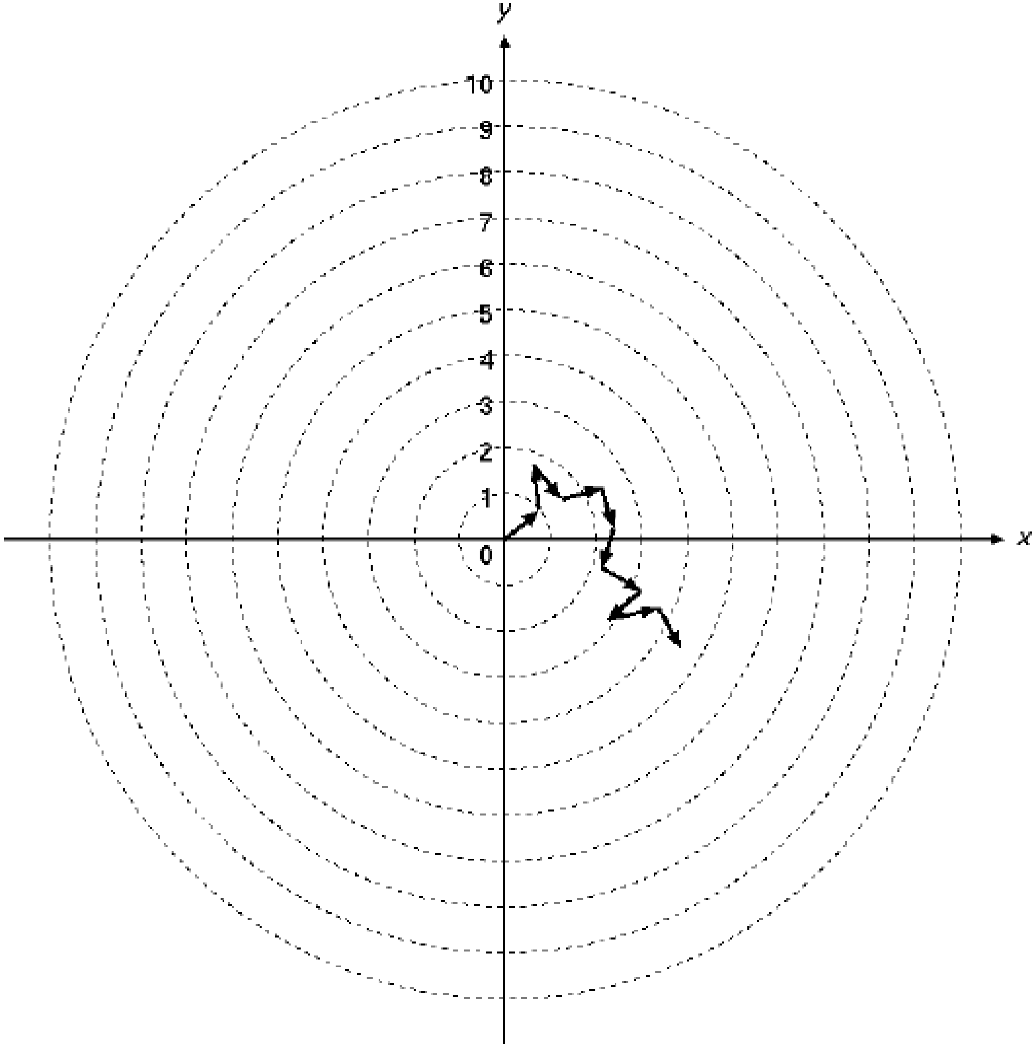
ex4/lu.f90

5. The Monte Carlo Method

- Wikipedia:

  “A broad class of computational algorithms that rely on repeated random sampling to obtain numerical results”
- A random walk in 2D
- 100,000 particles
- 10 steps

A Sample Trajectory



The Sequential Algorithm

```
PROGRAM main
PARAMETER (n=100000)
INTEGER itotal(0:9)
REAL seed
pi = 3.1415926
DO i = 0, 9
  itotal(i) = 0
ENDDO
seed = 0.5
CALL srand(seed)
```

```
DO i = 1, n
  x = 0.0
  y = 0.0
  DO istep = 1, 10
    angle = 2.0 * pi * rand()
    x = x + cos(angle)
    y = y + sin(angle)
  ENDDO
  itemp = sqrt(x**2 + y**2)
  itotal(itemp) = itotal(itemp) + 1
ENDDO
PRINT *,'total =',itotal
END
```

Example 5

ex5/mc.f90

6. Molecular Dynamics

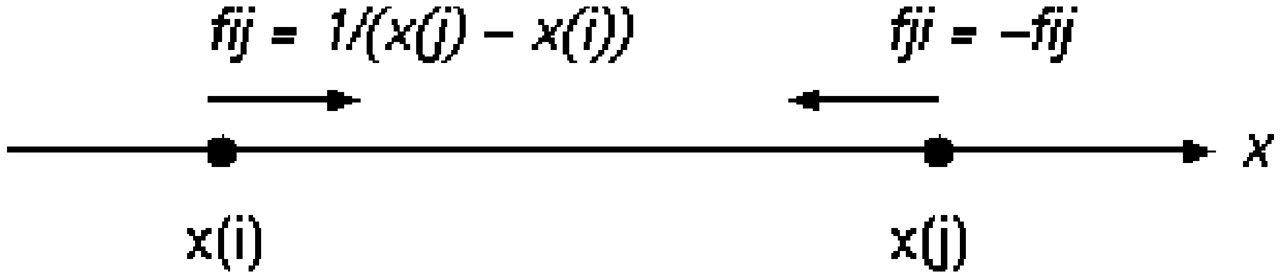
- Wikipedia:

  "a computer simulation of physical movements of atoms and molecules"
- N particles interact in 1 dimension
- The force on particle i from particle j is given by

  $f_{ij} = 1/(x_j - x_i)$
- The law of action and reaction applies:

  $f_{ij} = -f_{ji}$

Forces in 1D



Forces Acting on 7 Particles

f(1) =		+f12	+f13	+f14	+f15	+f16	+f17
f(2) =	−f12		+f23	+f24	+f25	+f26	+f27
f(3) =	−f13	−f23		+f34	+f35	+f36	+f37
f(4) =	−f14	−f24	−f34		+f45	+f46	+f47
f(5) =	−f15	−f25	−f35	−f45		+f56	+f57
f(6) =	−f16	−f26	−f36	−f46	−f56		+f67
f(7) =	−f17	−f27	−f37	−f47	−f57	−f67	

The Sequential Algorithm

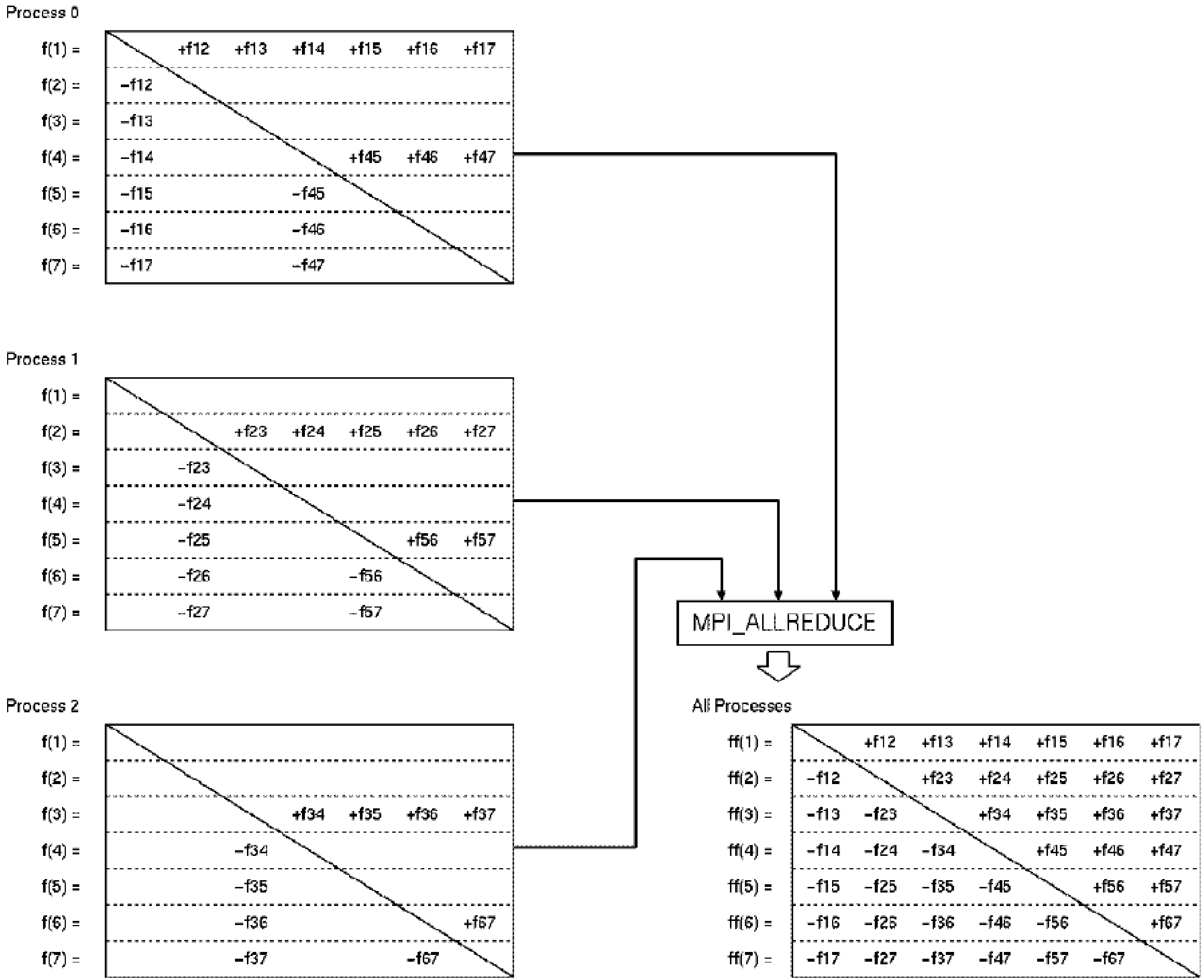
```
PARAMETER (n = ...)
REAL f(n), x(n)
...
DO itime = 1, 100
  DO i = 1, n
    f(i) = 0.0
  ENDDO
  DO i = 1, n-1
    DO j = i+1, n
      fij = 1.0 / (x(j)-x(i))
      f(i) = f(i) + fij
      f(j) = f(j) - fij
    ENDDO
  ENDDO
  DO i = 1, n
    x(i) = x(i) + f(i)
  ENDDO
ENDDO
```

Two Parallelisation Methods

- Most of the time is spent in the calculation loop:

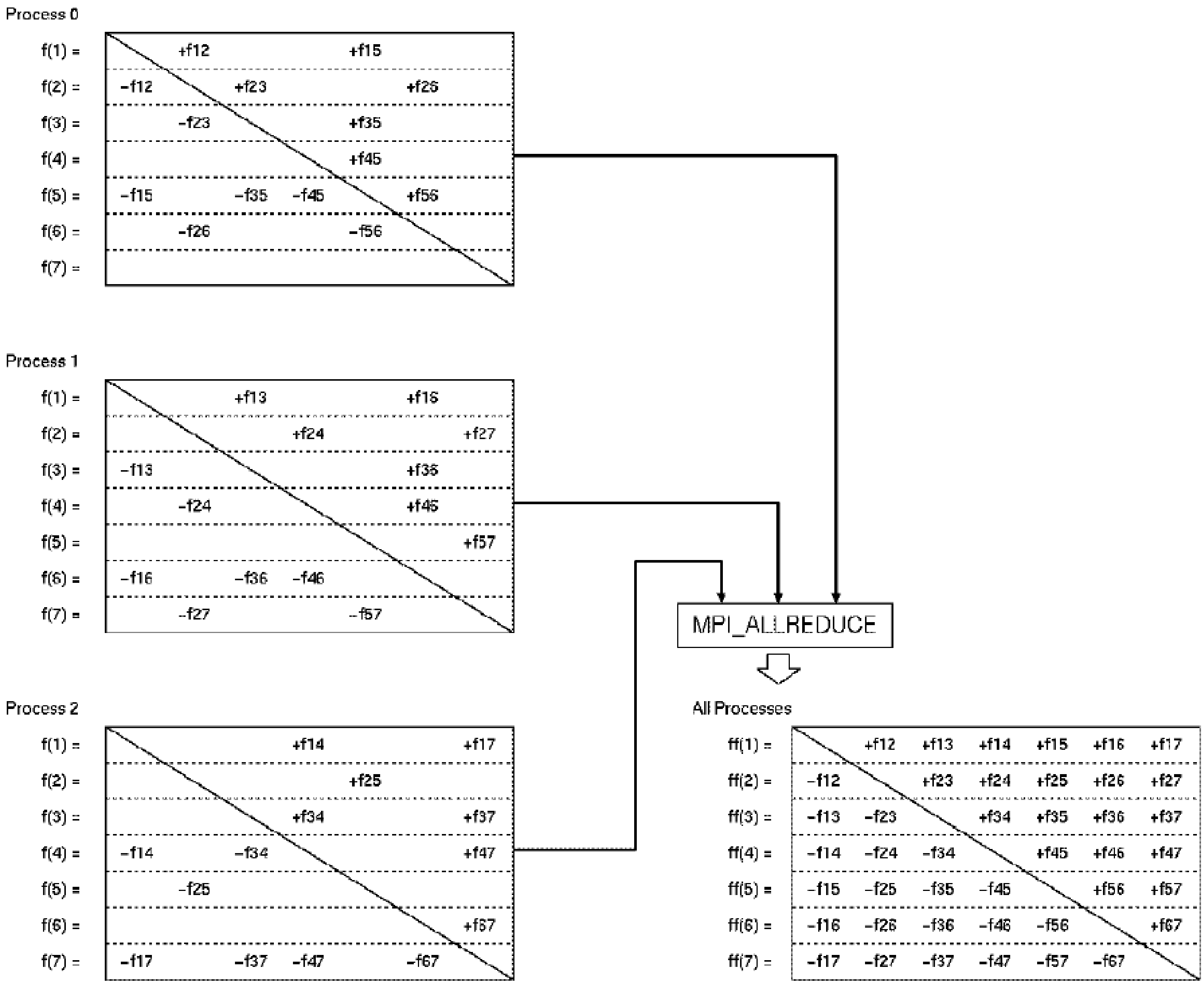
```
DO i = 1, n-1
  DO j = i+1, n
    fij = 1.0/(x(j) - x(i))
    f(i) = f(i) + fij
    f(j) = f(j) - fij
  ENDDO
ENDDO
```

- Two parallelization methods:
  – Cyclic distribution of the outer loop
  – Cyclic distribution of the inner loop


Process 0
f(1) = +f12 +f13 +f14 +f15 +f16 +f17
f(2) = −f12
f(3) = −f13
f(4) = −f14 +f45 +f46 +f47
f(5) = −f15 −f45
f(6) = −f16 −f46
f(7) = −f17 −f47
Process 1
f(1) =
f(2) = +f23 +f24 +f25 +f26 +f27
f(3) = −f23
f(4) = −f24
f(5) = −f25 +f56 +f57
f(6) = −f26 −f56
f(7) = −f27 −f57
Process 2
f(1) =
f(2) =
f(3) = +f34 +f35 +f36 +f37
f(4) = −f34
f(5) = −f35
f(6) = −f36 +f67
f(7) = −f37 −f67
MPI_ALLREDUCE
All Processes
ff(1) = +f12 +f13 +f14 +f15 +f16 +f17
ff(2) = −f12 +f23 +f24 +f25 +f26 +f27
ff(3) = −f13 −f23 +f34 +f35 +f36 +f37
ff(4) = −f14 −f24 −f34 +f45 +f46 +f47
ff(5) = −f15 −f25 −f35 −f45 +f56 +f57
ff(6) = −f16 −f26 −f36 −f46 −f56 +f67
ff(7) = −f17 −f27 −f37 −f47 −f57 −f67

Example 6

ex6/md1.f90



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Example 6

ex6/md2.f90

7. MPMD Models

- Wikipedia:

  “Multiple Program, Multiple Data: multiple autonomous processors simultaneously operating at least 2 independent programs”

- Different programs run in parallel and communicate with each other

An example

Process 0

```
PROGRAM fluid
INCLUDE 'mpif.h'
...
CALL MPI_INIT
CALL MPI_COMM_SIZE
CALL MPI_COMM_RANK
...
DO itime = 1, n

    Computation of
    Fluid Dynamics

   CALL MPI_SEND
   CALL MPI_RECV
ENDDO
...
END
```

Process 1

```
PROGRAM struct
INCLUDE 'mpif.h'
...
CALL MPI_INIT
CALL MPI_COMM_SIZE
CALL MPI_COMM_RANK
...
DO itime = 1, n

    Computation of
    Structural Analysis

   CALL MPI_RECV
   CALL MPI_SEND
ENDDO
...
END
```

Master/Worker Programs

- The master coordinates the execution of all the other processes
- The master has a list of jobs that must be processed
- Suitable if:
  - The processing time varies greatly from job to job
  - Neither block nor cyclic distribution gives a good load balancing
  - A heterogeneous environment where the performance of the machines is not uniform

Example 7

ex7/master.f90 and ex7/worker.f90

More Information

- All examples are based on:
  - www.redbooks.ibm.com/redbooks/pdfs/sg245380.pdf
- Our Web-site:
  - http://www.hpc.ntnu.no/
- Send an e-mail to:
  - support-ntnu@notur.no
  - support-kongull@hpc.ntnu.no