



The Abdus Salam  
International Centre  
for Theoretical Physics



IAEA  
International Atomic Energy Agency

# Overview on Common Strategies for Parallelization

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# Static Data Partitioning

**The simplest data decomposition schemes for dense matrices are 1-D block distribution schemes.**

row-wise distribution

|       |
|-------|
| $P_0$ |
| $P_1$ |
| $P_2$ |
| $P_3$ |
| $P_4$ |
| $P_5$ |
| $P_6$ |
| $P_7$ |

column-wise distribution

|       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|
| $P_0$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ | $P_6$ | $P_7$ |
|-------|-------|-------|-------|-------|-------|-------|-------|

# Distributed Data Vs Replicated Data

- Replicated data distribution is useful if it helps to reduce the communication among process at the cost of bounding scalability
- Distributed data is the ideal data distribution but not always applicable for all data-sets
- Usually complex application are a mix of those techniques

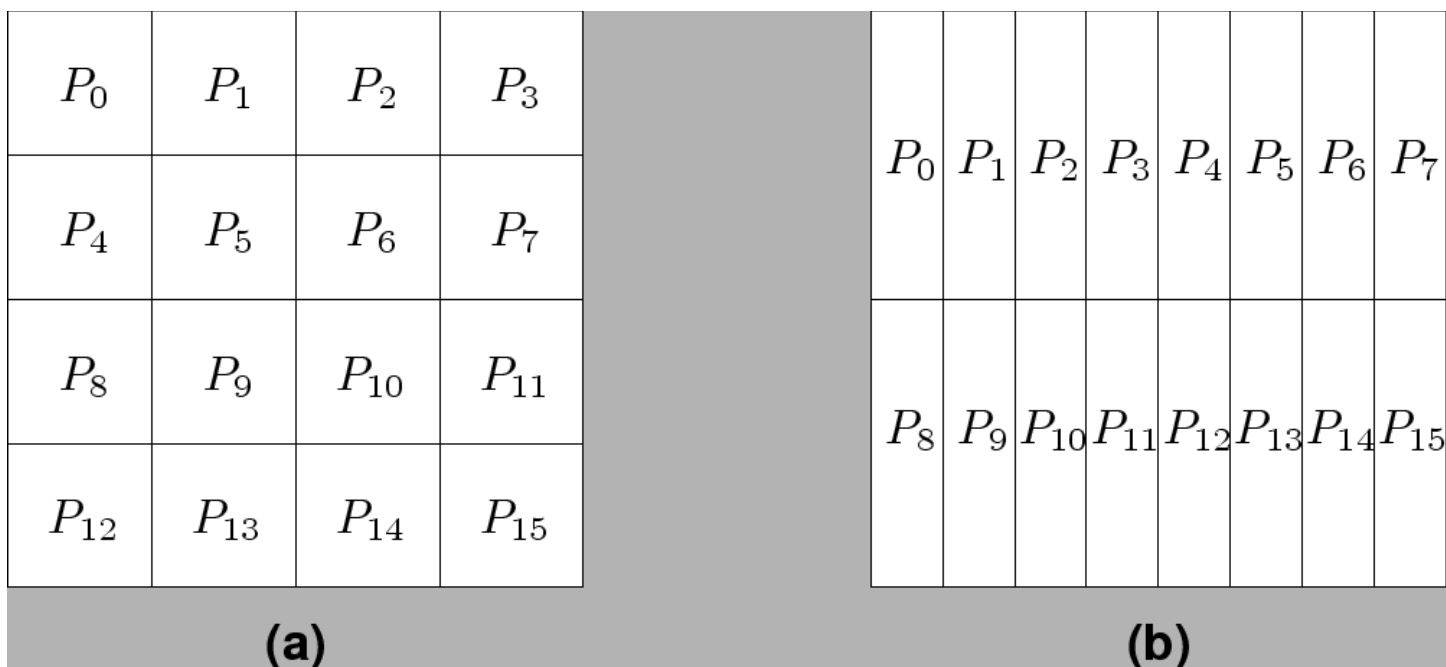
# Global Vs Local Indexes

- In sequential code you always refer to global indexes
- With distributed data you must handle the distinction between global and local indexes (and possibly implementing utilities for transparent conversion)

|            |  |   |   |   |  |   |   |   |  |   |   |   |
|------------|--|---|---|---|--|---|---|---|--|---|---|---|
| Local Idx  | <table><tr><td>1</td><td>2</td><td>3</td></tr></table> | 1 | 2 | 3 | <table><tr><td>1</td><td>2</td><td>3</td></tr></table> | 1 | 2 | 3 | <table><tr><td>1</td><td>2</td><td>3</td></tr></table> | 1 | 2 | 3 |
| 1          | 2  | 3 |   |   |  |   |   |   |  |   |   |   |
| 1          | 2  | 3 |   |   |  |   |   |   |  |   |   |   |
| 1          | 2  | 3 |   |   |  |   |   |   |  |   |   |   |
| Global Idx | <table><tr><td>1</td><td>2</td><td>3</td></tr></table> | 1 | 2 | 3 | <table><tr><td>4</td><td>5</td><td>6</td></tr></table> | 4 | 5 | 6 | <table><tr><td>7</td><td>8</td><td>9</td></tr></table> | 7 | 8 | 9 |
| 1          | 2  | 3 |   |   |  |   |   |   |  |   |   |   |
| 4          | 5  | 6 |   |   |  |   |   |   |  |   |   |   |
| 7          | 8  | 9 |   |   |  |   |   |   |  |   |   |   |

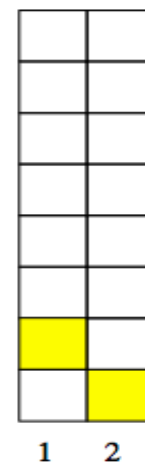
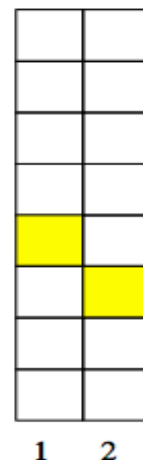
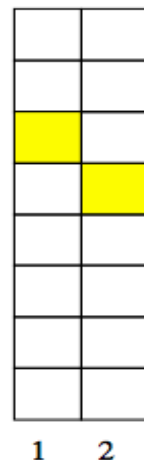
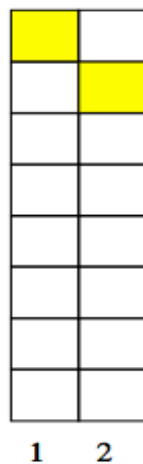
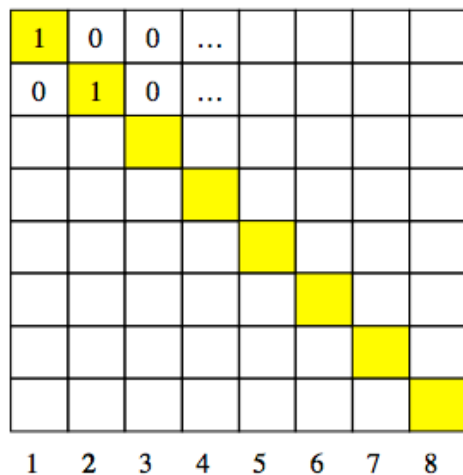
# Block Array Distribution Schemes

Block distribution schemes can be generalized to higher dimensions as well.



**Degree to which tasks/data can be subdivided is limit to concurrency and parallel execution!!**

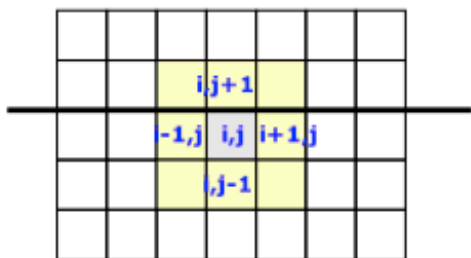
# Collaterals to Domain Decomposition /1



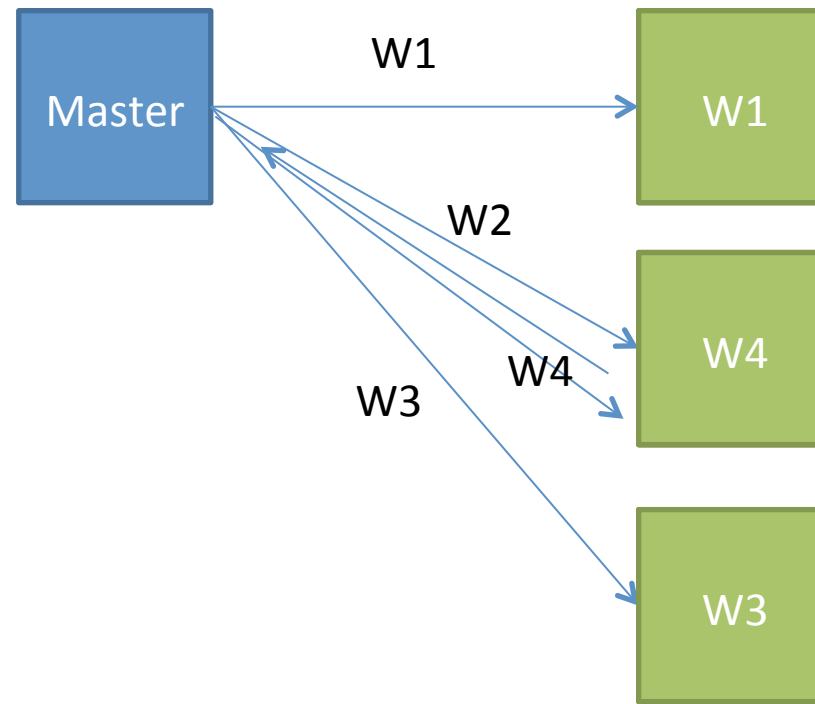
**Are all the domain's dimensions  
always multiple of the number  
of tasks/processes we are  
willing to use?**

# Collaterals to Domain Decomposition /2

sub-domain boundaries



# Master/Slave





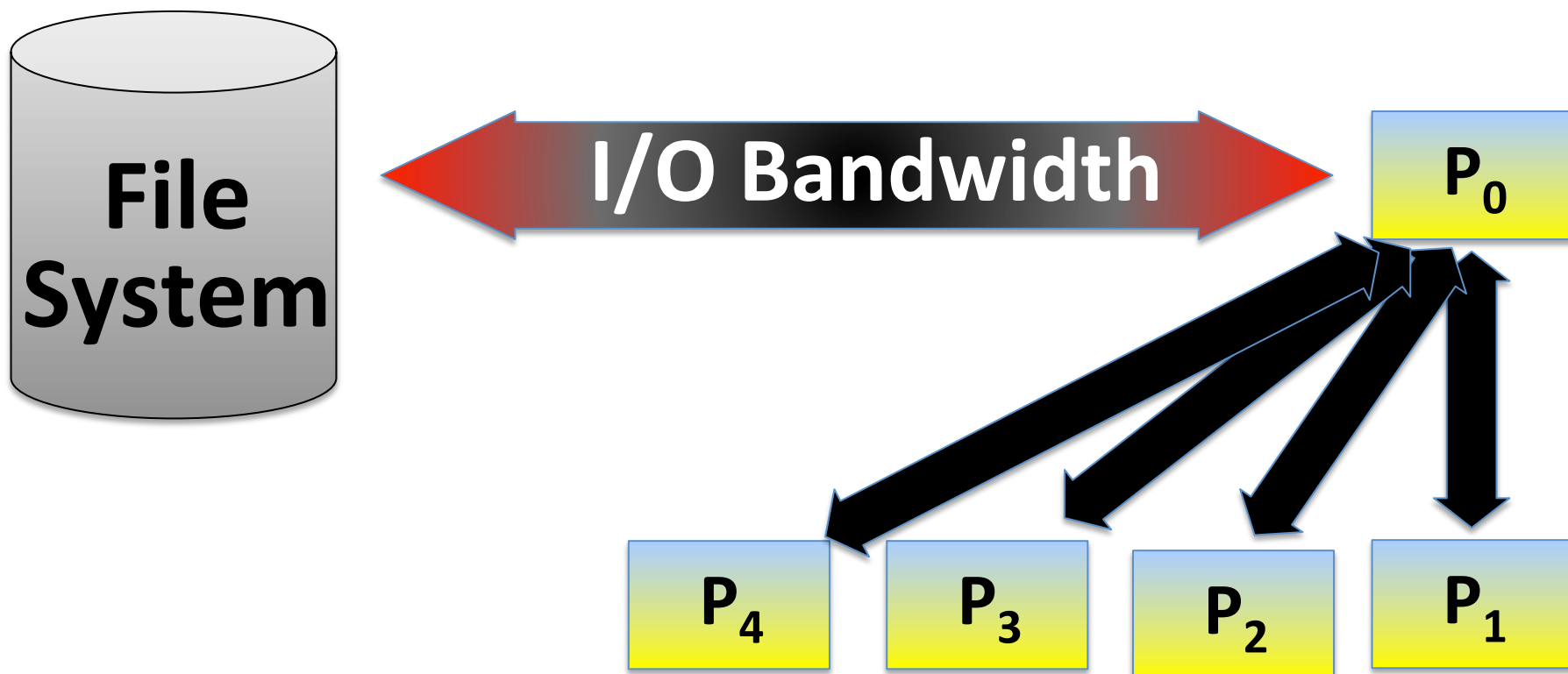
# Task Farming

- Many independent programs (tasks) running at once
  - each task can be serial or parallel
  - “independent” means they don’t communicate directly
  - Processes possibly driven by the mpirun framework

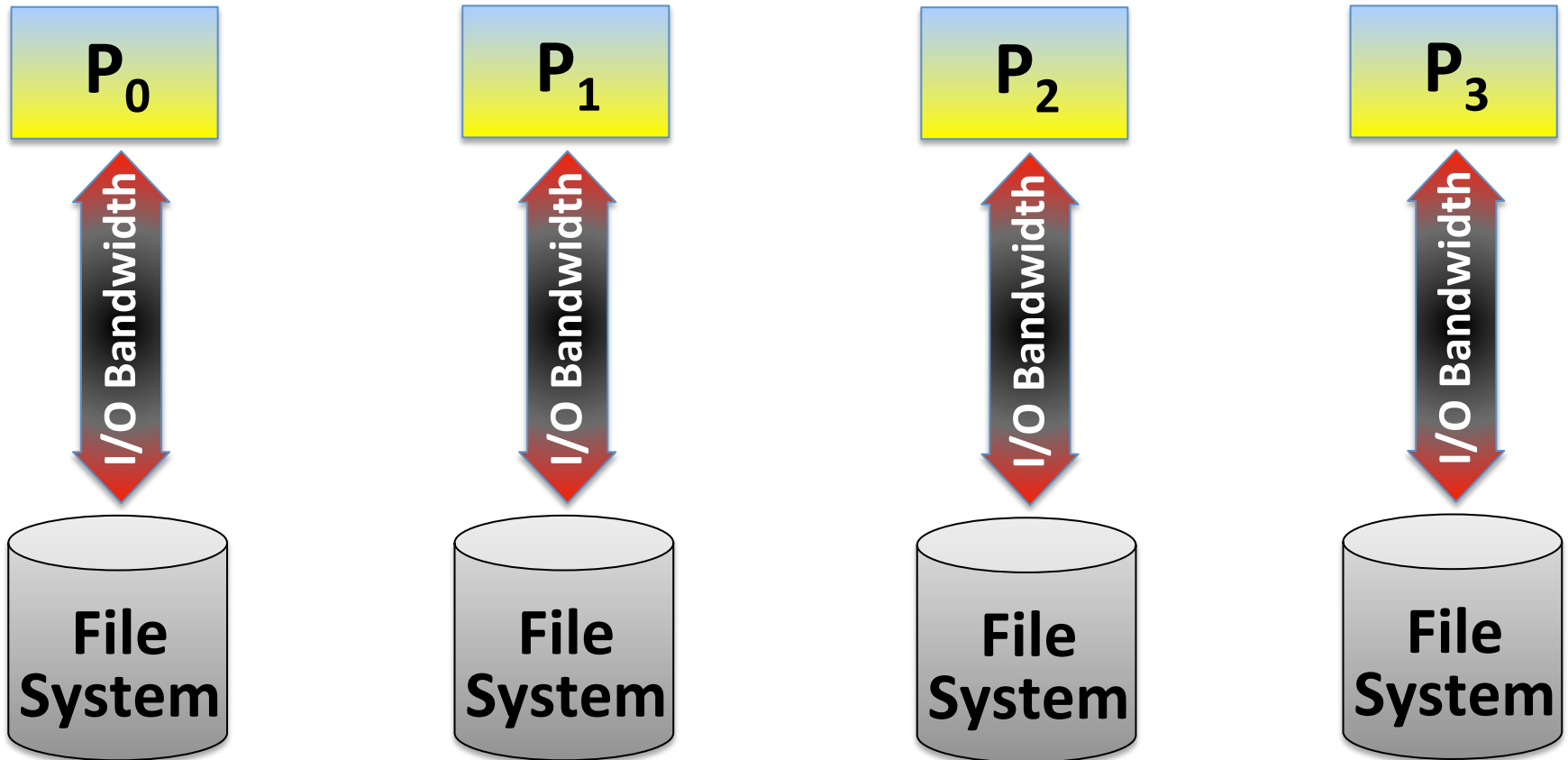
```
[igirotto@localhost]$ more my_shell_wrapper.sh
#!/bin/bash
#example for the OpenMPI implementation
./prog.x --input input_${OMPI_COMM_WORLD_RANK}.dat

[igirotto@localhost]$ mpirun -np 400 ./my_shell_wrapper.sh
```

# Parallel I/O



# Parallel I/O



# Parallel I/O

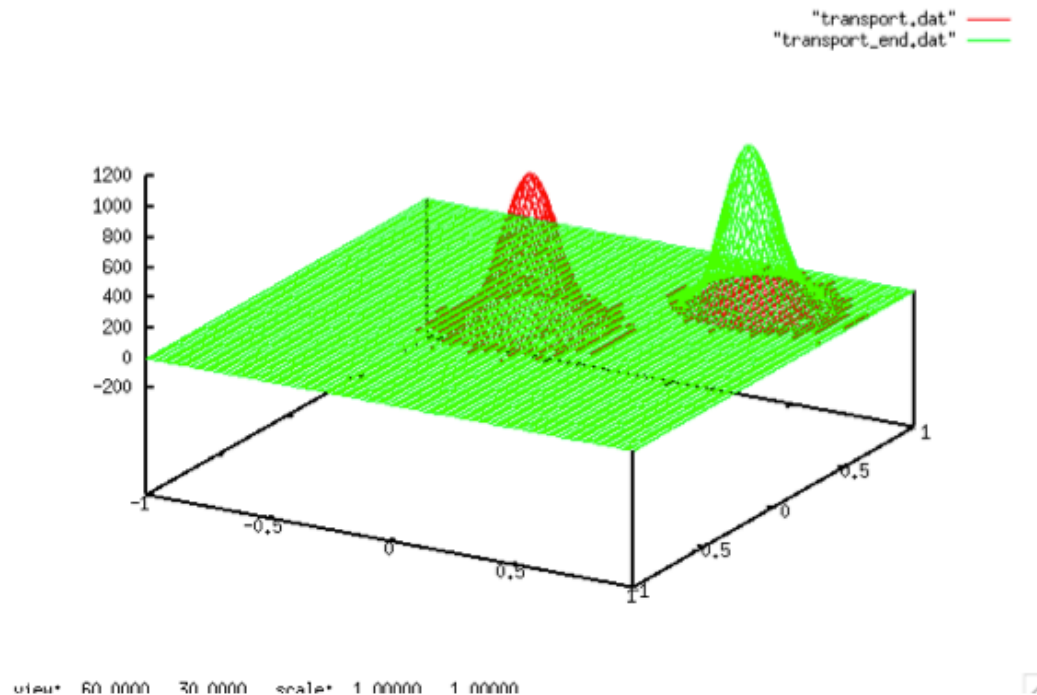


**MPI I/O & Parallel I/O Libraries (Hdf5, Netcdf, etc...)**

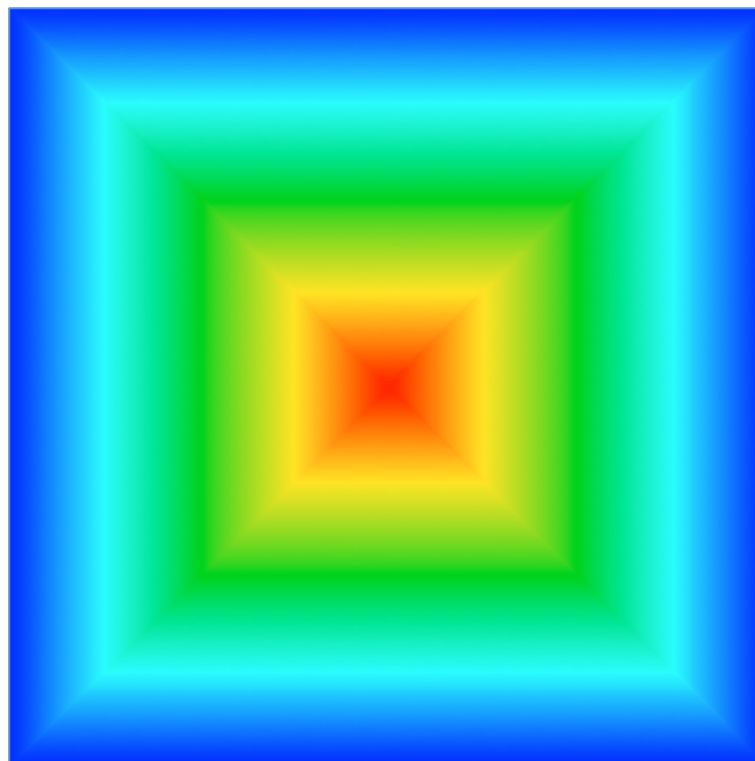
## Parallel File System



# The Transport Code - Parallel Version



$P_0$



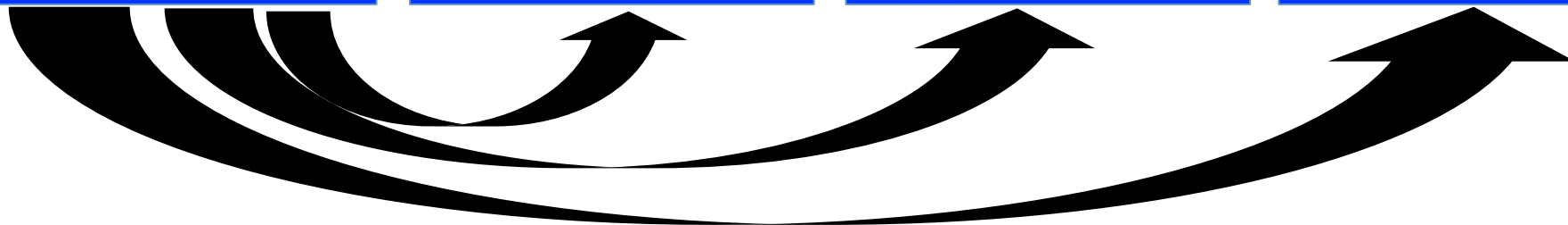
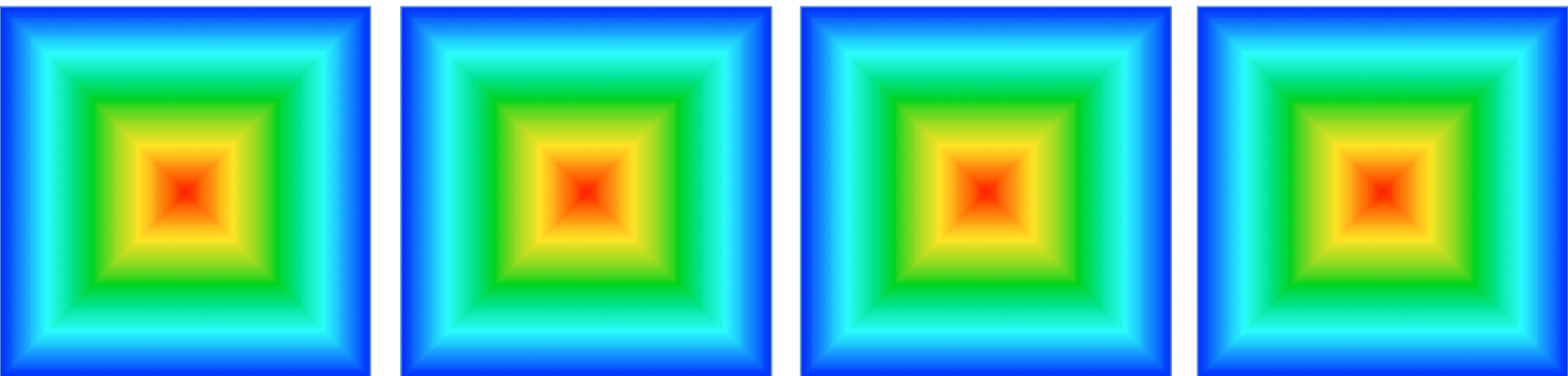
call `MPI_BCAST( ... )`

$P_0$  (root)

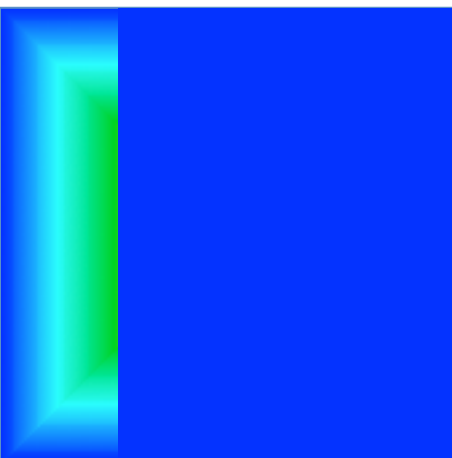
$P_1$

$P_2$

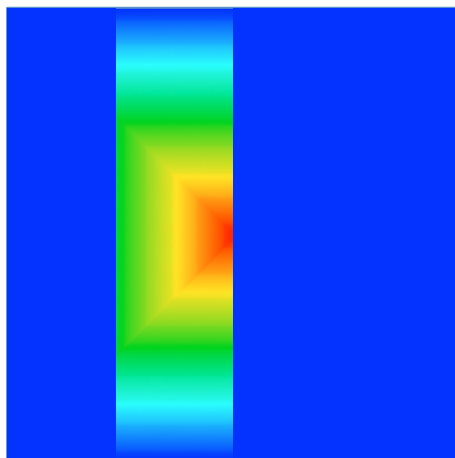
$P_3$



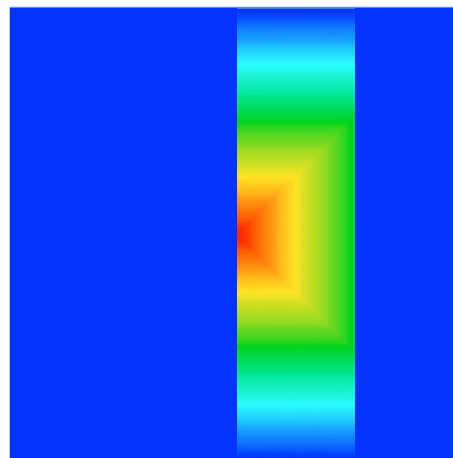
$P_0$



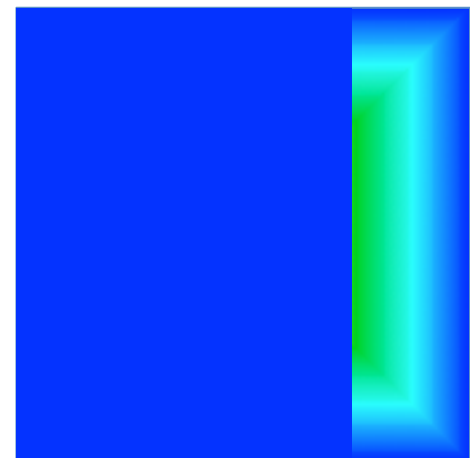
$P_1$



$P_2$



$P_3$



**call evolve( dtfact )**



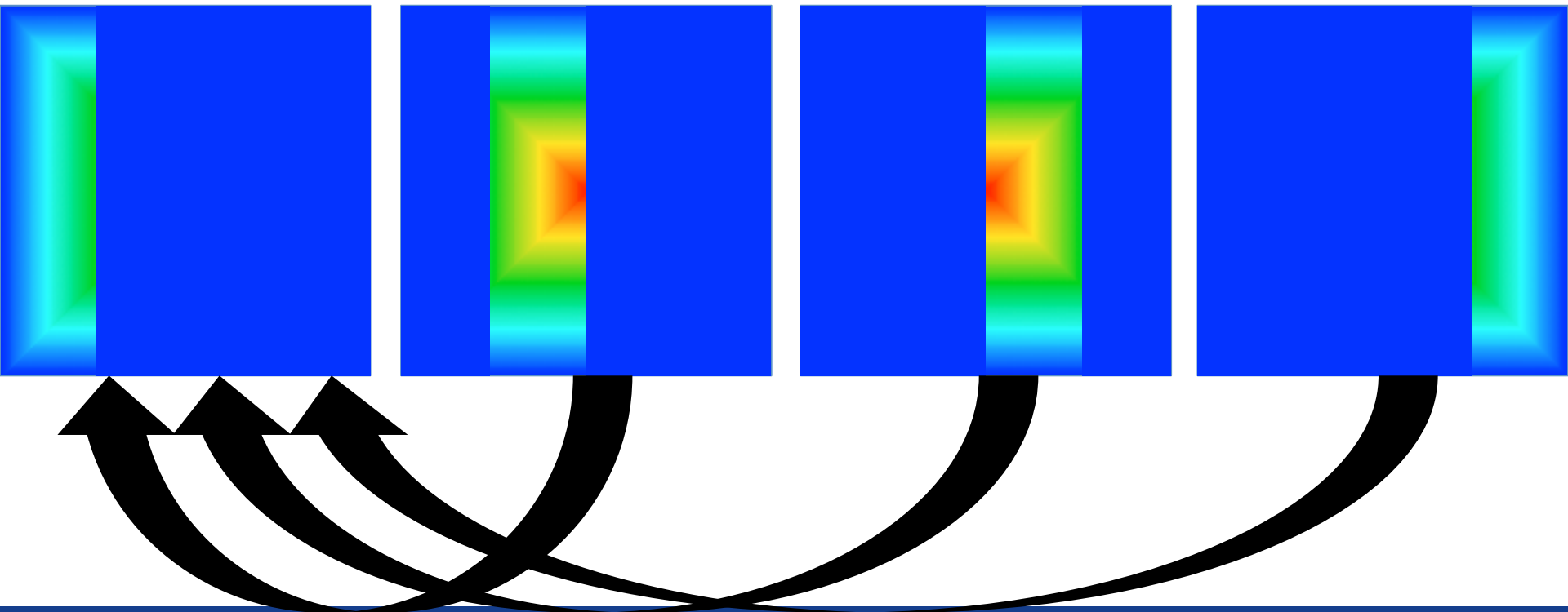
call `MPI_REDUCE( ..., MPI_SUM, ... )`

$P_0$  (root)

$P_1$

$P_2$

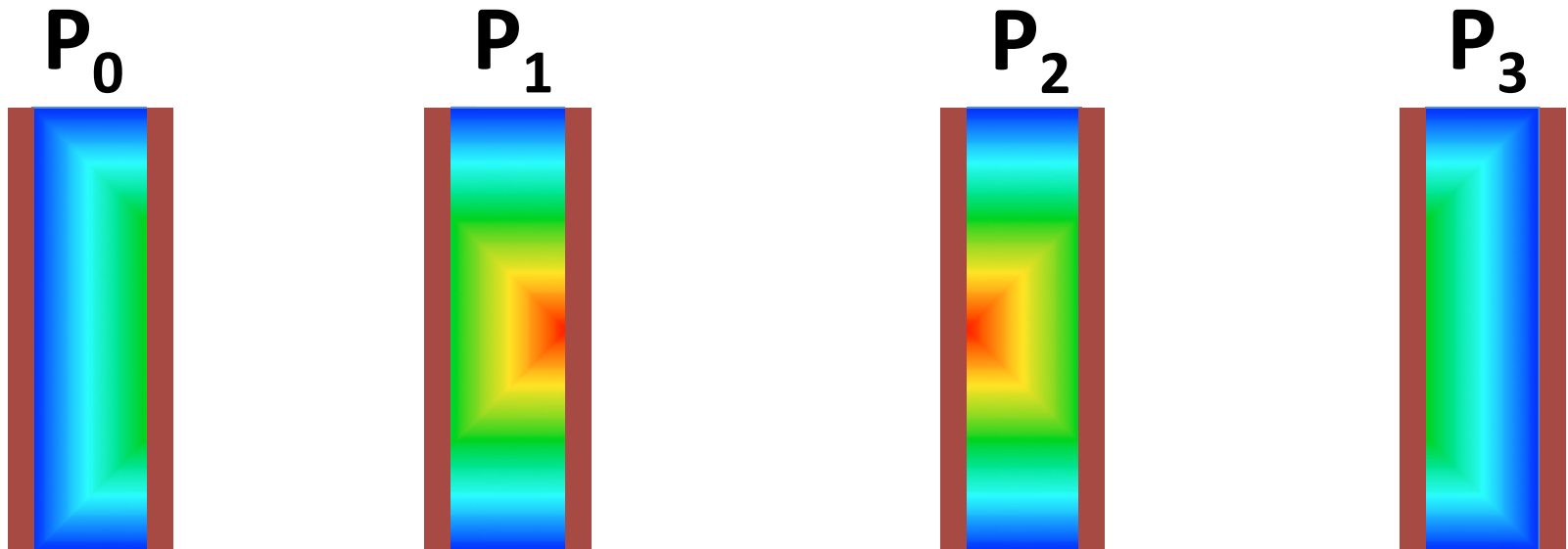
$P_3$



# The Transport Code - Parallel Version

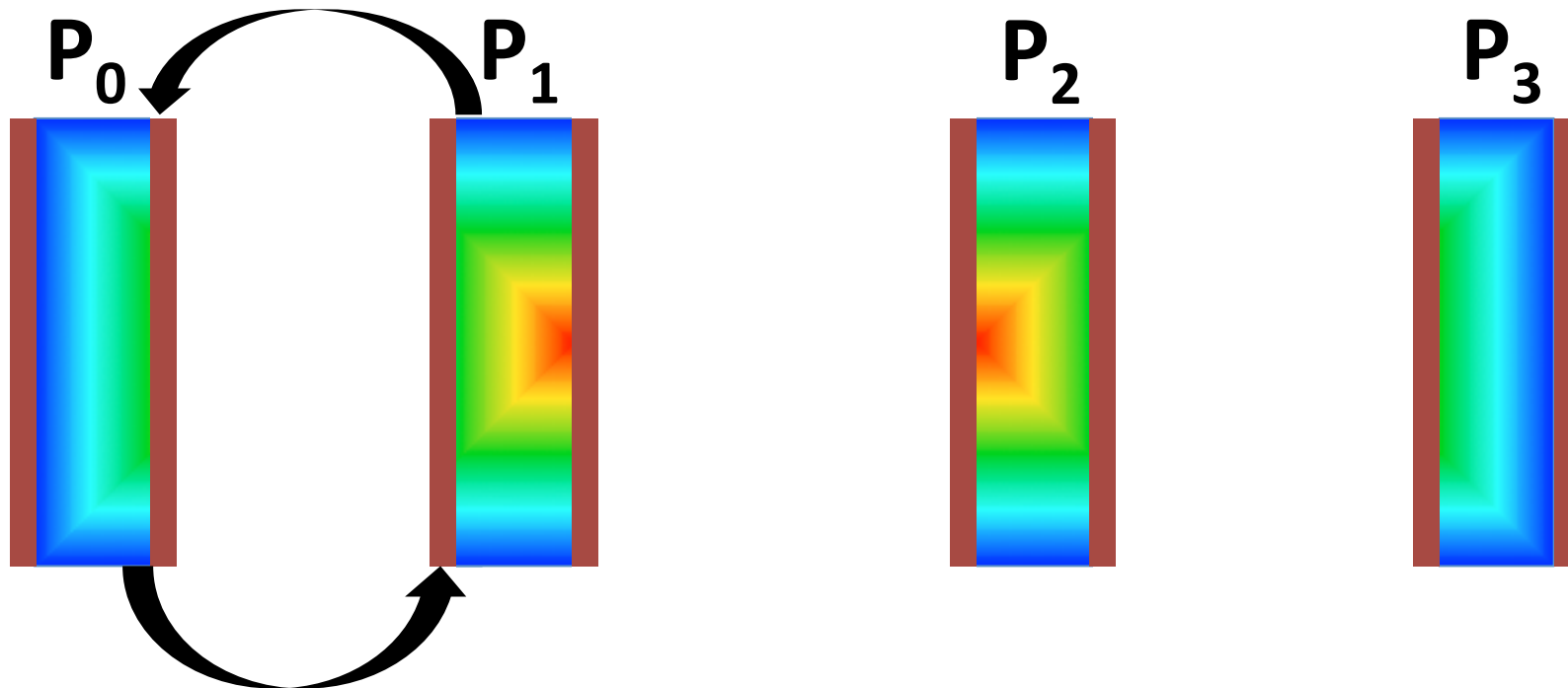
- Replicated data
- Compute domain (and workload) distribution among processes
- Master-slaves:  $P_0$  drives all processes
- Large amount of data communication
  - at each step  $P_0$  distribute data to all processes and collect the contribution of each process
- Problem size scaling limited in memory capacity

# The Transport Code - Parallel Version



**call evolve( dtfact )**

# Data exchange among processes





PROGRAM send\_recv

```
INCLUDE 'mpif.h'
```

```
INTEGER :: ierr, myid, nproc, status(MPI_STATUS_SIZE)
```

```
REAL A(2)
```

```
CALL MPI_INIT(ierr)
```

```
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
```

```
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
```

```
IF( myid .EQ. 0 ) THEN
```

```
    A(1) = 3.0
```

```
    A(2) = 5.0
```

```
    CALL MPI_SEND(A, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
```

```
ELSE IF( myid .EQ. 1 ) THEN
```

```
    CALL MPI_RECV(A, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
```

```
    WRITE(6,*) myid,': a(1)=',a(1),' a(2)=',a(2)
```

```
END IF
```

```
CALL MPI_FINALIZE(ierr)
```

END



PROGRAM error\_lock

```
INCLUDE 'mpif.h'
INTEGER :: ierr, myid, nproc, status(MPI_STATUS_SIZE)
REAL :: A(2), B(2)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
IF( myid .EQ. 0 ) THEN
    a(1) = 2.0
    a(2) = 4.0
    CALL MPI_SEND(a, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
    CALL MPI_RECV(b, 2, MPI_REAL, 1, 11, MPI_COMM_WORLD, status, ierr)
ELSE IF( myid .EQ. 1 ) THEN
    a(1) = 3.0
    a(2) = 5.0
    CALL MPI_SEND(a, 2, MPI_REAL, 0, 11, MPI_COMM_WORLD, ierr)
    CALL MPI_RECV(b, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
END IF
WRITE(6,*) myid, ': a(1)=', a(1), ' a(2)=', a(2)
CALL MPI_FINALIZE(ierr)
```

END

PROGRAM error\_lock

```

INCLUDE 'mpif.h'
INTEGER :: ierr, myid, nproc, status(MPI_STATUS_SIZE)
REAL :: A(2), B(2)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
IF( myid .EQ. 0 ) THEN
    a(1) = 2.0
    a(2) = 4.0
    CALL MPI_SEND(a, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
    CALL MPI_RECV(b, 2, MPI_REAL, 1, 11, MPI_COMM_WORLD, status, ierr)
ELSE IF( myid .EQ. 1 ) THEN
    a(1) = 3.0
    a(2) = 5.0
    CALL MPI_SEND(a, 2, MPI_REAL, 0, 11, MPI_COMM_WORLD, ierr)
    CALL MPI_RECV(b, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
END IF
WRITE(6,*) myid, ': a(1)=', a(1), ' a(2)=', a(2)
CALL MPI_FINALIZE(ierr)

```



**Deadlock!!**

END



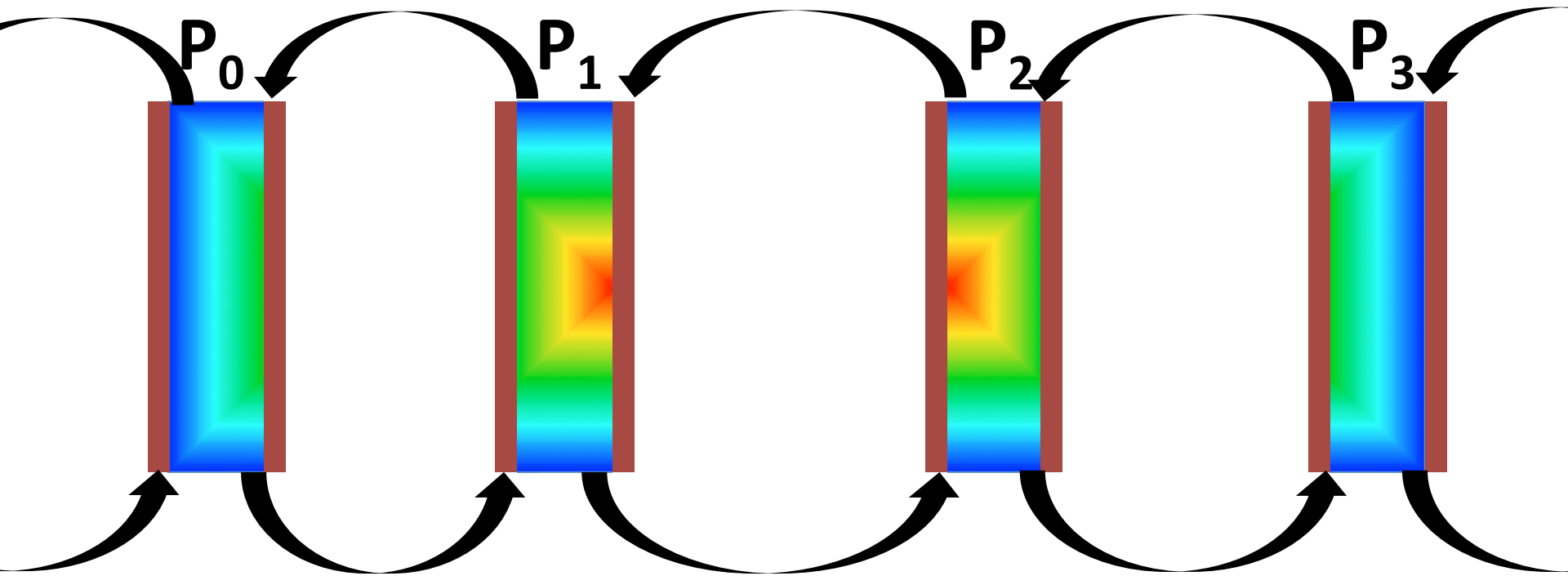
PROGRAM error\_lock

```
INCLUDE 'mpif.h'
INTEGER :: ierr, myid, nproc, status(MPI_STATUS_SIZE)
REAL :: A(2), B(2)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
IF( myid .EQ. 0 ) THEN
    a(1) = 2.0
    a(2) = 4.0
    CALL MPI_RECV(b, 2, MPI_REAL, 1, 11, MPI_COMM_WORLD, status, ierr)
    CALL MPI_SEND(a, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
ELSE IF( myid .EQ. 1 ) THEN
    a(1) = 3.0
    a(2) = 5.0
    CALL MPI_SEND(a, 2, MPI_REAL, 0, 11, MPI_COMM_WORLD, ierr)
    CALL MPI_RECV(b, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
END IF
WRITE(6,*) myid, ': a(1)=', a(1), ' a(2)=', a(2)
CALL MPI_FINALIZE(ierr)
```

END



$$\text{proc\_down} = \text{mod}(\text{proc\_me} - 1 + \text{nprocs}, \text{nprocs})$$



$$\text{proc\_up} = \text{mod}(\text{proc\_me} + 1, \text{nprocs})$$



# STANDARD NO-BLOCKING SEND - RECV

- Basic point-2-point communication routines in MPI.

**MPI\_ISEND(buf, count, type, dest, tag, comm, req, ierr)**

**MPI\_IRecv(buf, count, type, source, tag, comm, req, ierr)**

**Buf** array of MPI type **type**.

**Count** (INTEGER) number of element of **buf** to be sent

**Type** (INTEGER) MPI type of **buf**

**Dest** (INTEGER) rank of the destination process / **Source** (INTEGER) rank of the source process

**Tag** (INTEGER) number identifying the message

**Comm** (INTEGER) communicator of the sender and receiver

**Req** (INTEGER) output, identifier of the communications handle

**Ierr** (INTEGER) error code

# STANDARD NO-BLOCKING WAIT

- A call to this subroutine cause the code to wait until the communication pointed by req is complete
- Handler for no-blocking communication

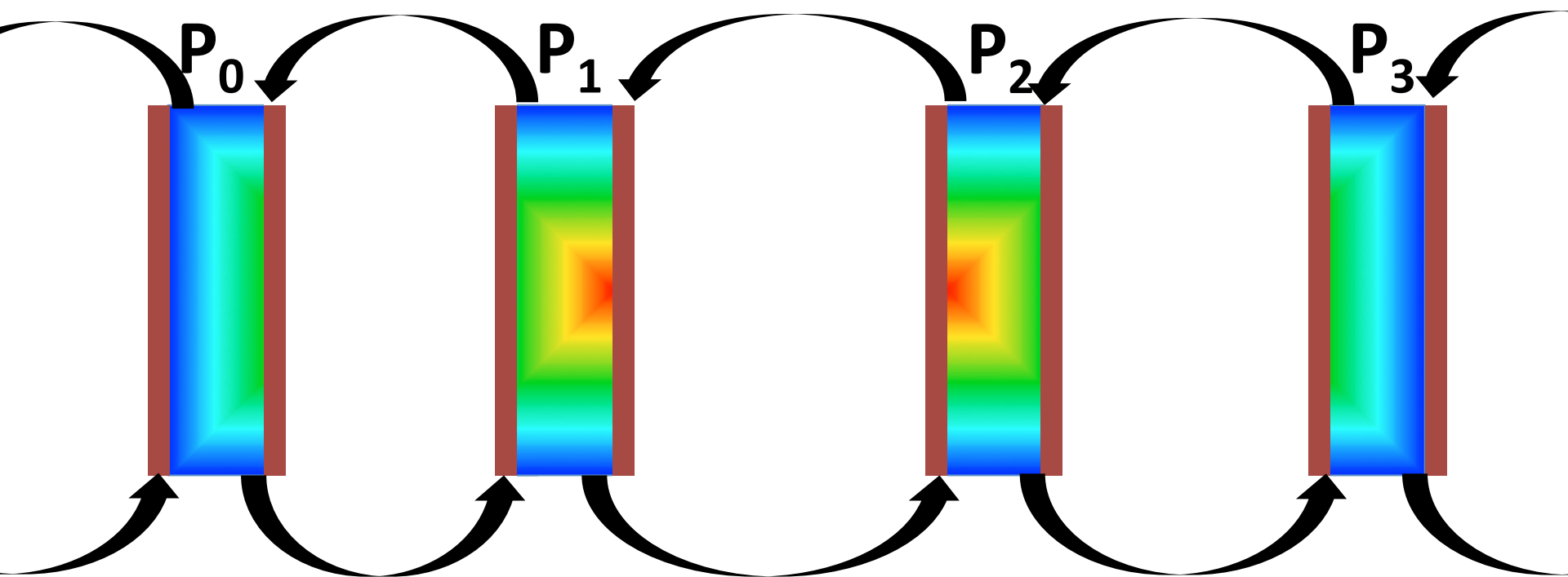
## **MPI\_WAIT(req, status, ierr)**

**Req** (INTEGER) output, identifier of the communications handle

**Status** (INTEGER) array of size **MPI\_STATUS\_SIZE** containing communication status information

**ierr** (INTEGER) error code

# The Transport Code - Parallel Version





# The Transport Code - Parallel Version

- Distributed Data
- Global and Local Indexes
- Ghost Cells Exchange Between Processes
  - Compute Neighbor Processes
- Serialized Output on Process 0 (provided)

# SendRecv

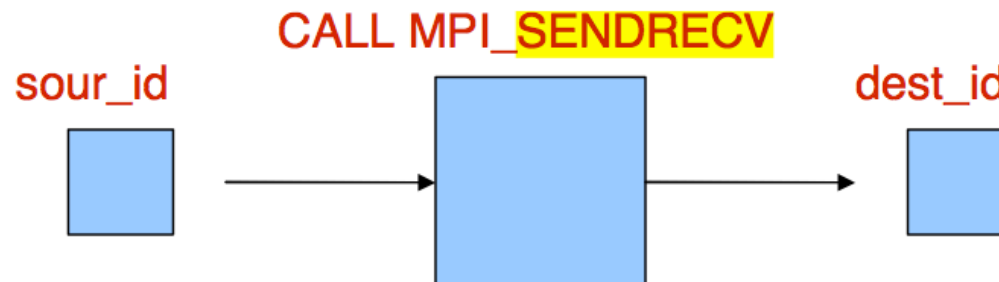
The easiest way to send and receive data without warring about deadlocks

## Sender side

Fortran:

```
CALL MPI_SENDRECV(sndbuf, snd_size, snd_type, dest_id, tag,  
rcvbuf, rcv_size, rcv_type, sour_id, tag, comm, status, ierr)
```

## Receiver side





```
PROGRAM send_recv
INCLUDE 'mpif.h'
INTEGER ierr, myid, nproc
INTEGER status(MPI_STATUS_SIZE)
REAL A(2), B(2)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
IF( myid .EQ. 0 ) THEN
    a(1) = 2.0
    a(2) = 4.0
    CALL MPI_SENDRECV(a, 2, MPI_REAL, 1, 10, b, 2, MPI_REAL, 1, 11, MPI_COMM_WORLD, status, ierr)
ELSE IF( myid .EQ. 1 ) THEN
    a(1) = 3.0
    a(2) = 5.0
    CALL MPI_SENDRECV(a, 2, MPI_REAL, 0, 11, b, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
END IF
WRITE(6,*) myid, ': b(1)=', b(1), ' b(2)=', b(2)
CALL MPI_FINALIZE(ierr)
END
```



# Communication Cycle

**! right to left !**

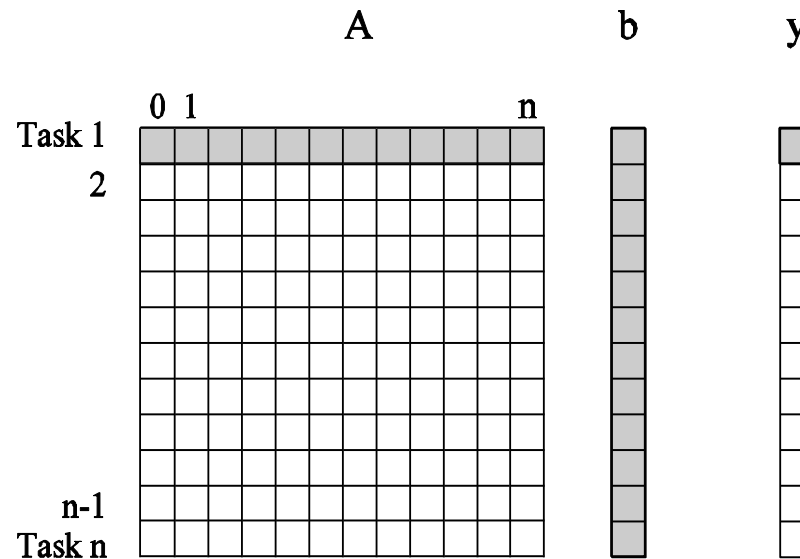
```
call MPI_SENDRECV(snd_buffer, ibuf, MPI_REAL, right, 1, &  
    rcv_buffer, ibuf, MPI_REAL, left , 1, &  
    comm_cart, istatus, ierr)
```

**! left to right !**

```
call MPI_SENDRECV (snd_buffer, ibuf, MPI_REAL, left, 1, &  
    rcv_buffer, ibuf, MPI_REAL, right , 1, &  
    comm_cart, istatus, ierr)
```



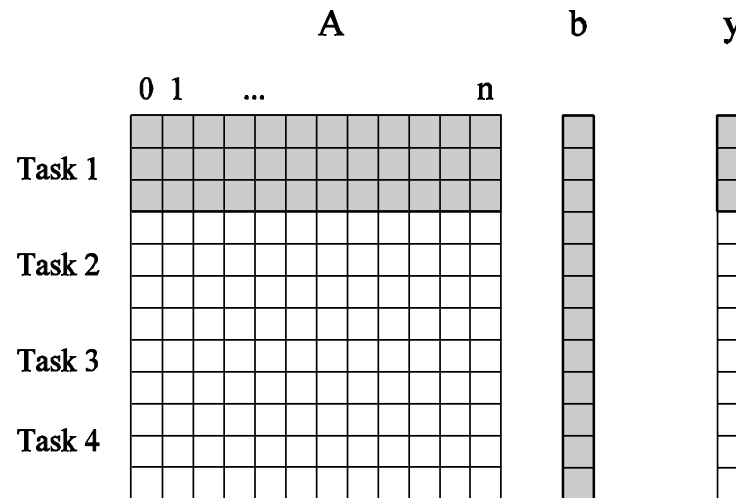
# Replication vs Distribution



Under the hypothesis that the vector  $b$  is replicated, computation of each element of output vector  $y$  is independent of other elements. Based on this, a dense matrix-vector product can be decomposed into  $n$  tasks.

# Granularity of Task Decompositions

- The number of tasks into which a problem is decomposed determines its granularity.
- Decomposition into a large number of tasks results in fine-grained decomposition and that into a small number of tasks results in a coarse grained decomposition.



A coarse grained counterpart to the dense matrix-vector product example. Each task in this example corresponds to the computation of three elements of the result vector.

# Granularity, and Communication

- Finest granularity helps for a larger parallelism and to exploit different levels of parallelism
- But in general, if the granularity of a decomposition is finer, the associated overhead (as a ratio of useful work associated with a task) increases.



# References

- [MPI Documentation](#)
- [MPI APIs \(list\) Documentation](#)



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# Thanks for your attention!!

