

# Parallelism (PAR)

## Parallel programming principles: Data decomposition

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# Outline

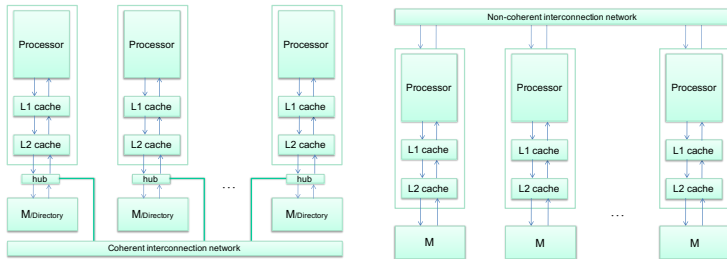
Data decomposition

Distributed-memory architectures

Task interaction in distributed memory architectures

# Why, when and how?

- ▶ Used to derive concurrency for problems that operate on large amounts of data focusing on the multiplicity of data
  - ▶ E.g. Elements in vectors, rows/columns/slices in matrices, elements in a list and subtrees in a tree
- ▶ ... for architectures in which memory plays a performance role



# Motivating example

```
#define n 100
#pragma omp parallel
#pragma omp single
for (iter=0; i<num_iters; iter++) {
    #pragma omp taskloop num_tasks(4)
    for (int i=0; i<n; i++)
        b[i] = foo1(a[i]);

    #pragma omp taskloop num_tasks(4)
    for (int i=0; i<n; i++)
        c[i] = foo2(b[i]);

    #pragma omp taskloop num_tasks(4)
    for (int i=0; i<n; i++)
        a[i] = foo3(c[i]);
}
```

Vectors a, b and c are distributed across the memories of the NUMA system, as follows

M <sub>0</sub>	M <sub>1</sub>	M <sub>2</sub>	M <sub>3</sub>
0..24	25..49	50..74	75..99

Possible assignment of iterations to processors (threads) in the different loops

P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>
25..49	50..74	0..24	75..99
25..49	75..99	0..24	50..74
50..74	25..49	75..99	0..24

# Motivating example (cont.)

```
// Solution based on for work-sharing
#pragma omp parallel
for (iter=0; i<num_iters; iter++) {
    #pragma omp for schedule(static) nowait
    for (int i=0; i<n; i++)
        b[i] = foo1(a[i]);
    #pragma omp for schedule(static) nowait
    for (int i=0; i<n; i++)
        c[i] = foo2(b[i]);
    #pragma omp for schedule(static) nowait
    for (int i=0; i<n; i++)
        a[i] = foo3(c[i]);
}
```

Vectors **a**, **b** and **c** are distributed across the memories of the NUMA system, as follows

M <sub>0</sub>	M <sub>1</sub>	M <sub>2</sub>	M <sub>3</sub>
0..24	25..49	50..74	75..99

Assignment of iterations to processors (threads) based on their thread identifier

P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>
0..24	25..49	50..74	75..99
0..24	25..49	50..74	75..99
0..24	25..49	50..74	75..99

# Why, when and how? (cont.)

- ▶ Step 1: Identify the data used and/or produced in the computations
  - ▶ Output data, input data or both
- ▶ Step 2: Partition this data across various tasks
  - ▶ Linear or geometric decomposition
  - ▶ Recursive decomposition
- ▶ Step 3: Obtain a computational partitioning that corresponds to the data partitioning: owner-computes rule
- ▶ Step 4: In distributed-memory architectures, add the necessary data allocation and movement actions

# Guidelines for data decomposition

- ▶ Data can be partitioned in various ways – this may critically impact performance
  - ▶ Generate comparable amounts of work (for load balancing)
  - ▶ Maximize data locality (or minimize the need for task interactions)
    - ▶ Minimize volume of data involved in task interactions
    - ▶ Minimize frequency of interactions
    - ▶ Minimize contention and hot spots
  - ▶ Overlap computation with interactions to "hide" their effect
- ▶ Parameterizable data partition
  - ▶ number of data chunks, size, ...
- ▶ Simplicity

# Example

Counting the instances of given itemsets in a database of transactions

(a) Transactions (input), itemsets (input), and frequencies (output)

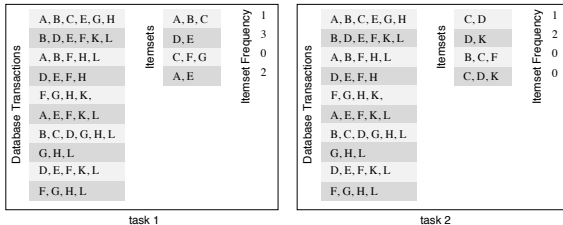
Database Transactions	A, B, C, E, G, H	Itemsets	A, B, C	Itemset Frequency	1
	B, D, E, F, K, L		D, E		3
	A, B, F, H, L		C, F, G		0
	D, E, F, H		A, E		2
	F, G, H, K,		C, D		1
	A, E, F, K, L		D, K		2
	B, C, D, G, H, L		B, C, F		0
	G, H, L		C, D, K		0
	D, E, F, K, L				
	F, G, H, L				



# Output data decomposition

- ▶ Partition of the output data structures across tasks. Input data structures may follow the same decomposition or require replication in order to avoid task interactions
- ▶ Example: the itemset frequencies are partitioned across tasks
  - ▶ The database of transactions needs to be replicated
  - ▶ The itemsets can be partitioned across tasks as well (reduce memory utilization)

(b) Partitioning the frequencies (and itemsets) among the tasks



# Input data decomposition

- ▶ Partition the input data structures across tasks. It may require combining partial results in order to generate the output data structures
- ▶ Example: the database transactions can be partitioned, but it requires the itemsets to be replicated. Final aggregation of partial counts for all itemsets

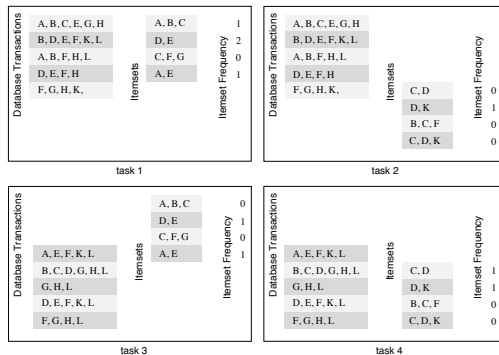
Partitioning the transactions among the tasks

task 1			task 2		
Database Transactions	Itemsets	Itemset Frequency	Database Transactions	Itemsets	Itemset Frequency
A, B, C, E, G, H	A, B, C	1		A, B, C	0
B, D, E, F, K, L	D, E	2		D, E	1
A, B, F, H, L	C, F, G	0		C, F, G	0
D, E, F, H	A, E	1	A, E, F, K, L	A, E	1
F, G, H, K,	C, D	1	B, C, D, G, H, L	C, D	1
	D, K	1	G, H, L	D, K	1
	B, C, F	0	D, E, F, K, L	B, C, F	0
	C, D, K	0	F, G, H, L	C, D, K	0

# Input *and* output data decomposition

- ▶ Input and output data decomposition could be combined
- ▶ Example: the database and itemsets (input) and counts (output) can be decomposed

Partitioning both transactions and frequencies among the tasks



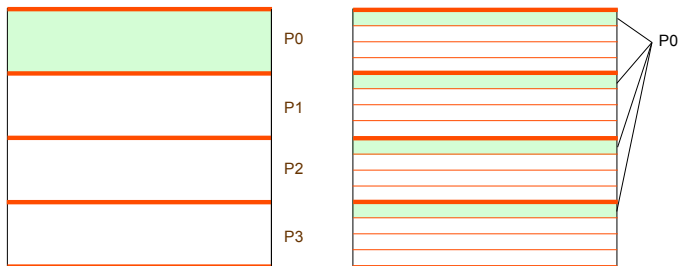
# The Owner Computes rule

It defines who is responsible for doing the computations:

- ▶ In the case of output data decomposition, the owner computes rule implies that the output is computed by the task to which the output data is assigned.
- ▶ In the case of input data decomposition, the owner computes rule implies that all computations that use the input data are performed by the task to which the input is assigned.

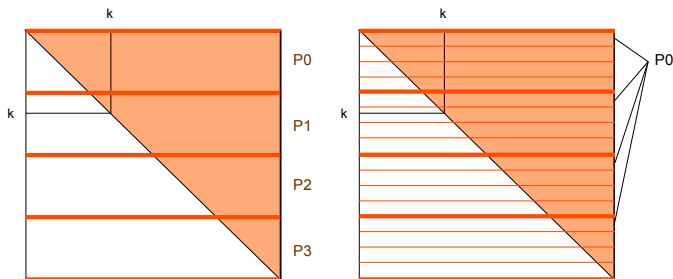
# Data distributions for geometric decomposition

Block (left) and cyclic (right) data decompositions



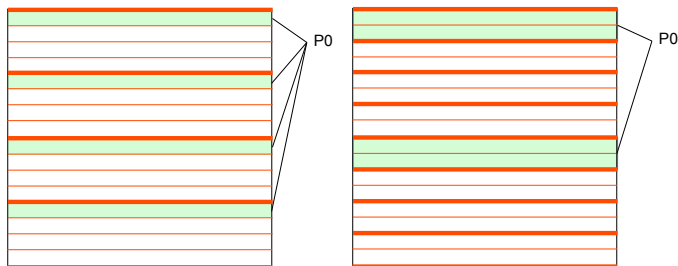
# Data distributions for geometric decomposition

Block (left) and cyclic (right) data decompositions in a triangular iteration space



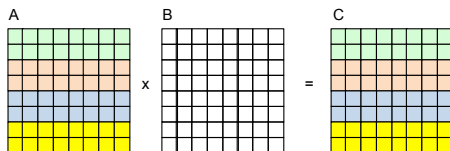
# Data distributions for geometric decomposition

Cyclic (left) and block-cyclic (right) data decompositions



## Example: matrix multiply

```
void matmul (double C[MATSIZE][MATSIZE],  
             double A[MATSIZE][MATSIZE],  
             double B[MATSIZE][MATSIZE])  
{  
    for (int i=0; i<MATSIZE; i++)  
        for (int j=0; j<MATSIZE; j++)  
            for (int k=0; k<MATSIZE; k++)  
                C[i][j] += A[i][k]*B[k][j];  
}
```



$A$  and  $C$  partitioned by rows on 4 processors (logically in shared memory architectures, physically in distributed memory architectures).  $B$  is replicated.



## Example: matrix multiply (OpenMP)

```
void matmul (double C[MATSIZE] [MATSIZE],
             double A[MATSIZE] [MATSIZE],
             double B[MATSIZE] [MATSIZE])
{
    int i, j, k;

#pragma omp parallel
    {
        int myid = omp_get_thread_num();
        int numprocs = omp_get_num_threads();
        int i_start = myid * (MATSIZE/numprocs);
        int i_end = i_start + (MATSIZE/numprocs);
        if (myid == numprocs-1) i_end = MATSIZE;

        for (int i=i_start; i<i_end; i++)
            for (int j=0; j<MATSIZE; j++)
                for (int k=0; k<MATSIZE; k++)
                    C[i][j] += A[i][k]*B[k][j];
    }
}
```

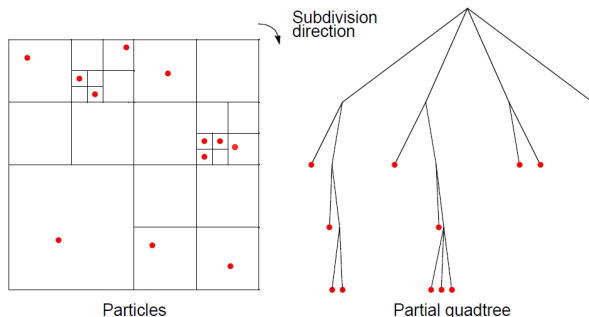
## Example: matrix multiply (OpenMP)

```
void matmul (double C[MATSIZE][MATSIZE],
             double A[MATSIZE][MATSIZE],
             double B[MATSIZE][MATSIZE])
{
    int i, j, k;

    #pragma omp parallel
    {
        int myid = omp_get_thread_num();
        int numprocs = omp_get_num_threads();
        int i_start = myid * (MATSIZE/numprocs);
        int i_end = i_start + (MATSIZE/numprocs);
        int rem = MATSIZE % numprocs;
        if (rem != 0) {
            if (myid < rem) {
                i_start += myid;
                i_end += (myid+1);
            }
            else {
                i_start += rem;
                i_end += rem;
            }
        }
        ...
    }
}
```

# Data distributions for recursive decomposition

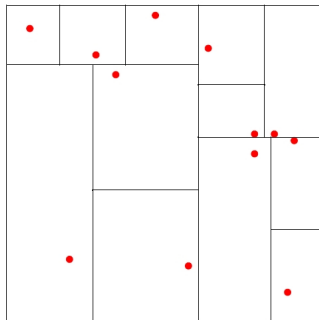
## Quadtree to represent particles in an N-body problem



- ▶ Each leaf node stores position and mass for a body
- ▶ Other nodes store center of mass and total mass for all bodies below

# Data distributions for recursive decomposition

Orthogonal distribution of the particles of an N-body, so that in each bi-partition the number of particles in each side is halved (load balancing)



# Example: N-body computation (sequential)

## Sequential code

```
void main() {
  // Initialize tree
  for (t=0; t<tmax; t++) {
    for (i=0;i<N;i++) doTimeStep(tree, node[i]); // node[i] points to body i in the tree
    // Update the positions and velocities
    // Migrate bodies if required in the tree
  }
}
```

## TreeNode structure

```
typedef struct {
  ...
  char    isLeaf
  TreeNode *quadrant[2][2];
  double  F; // force on node
  double  center_of_mass[3];
  double  mass_of_center;
  ...
} TreeNode;
```

## Calculate forces implementation

```
void doTimeStep(TreeNode* subTree, TreeNode* body) {
  if(subTree) {
    if(!subTree->isLeaf && !distant(subTree, body)) {
      for(int i=0; i<2; i++)
        for(int j=0; j<2; j++)
          doTimeStep(subTree->quadrant[i][j], body);
    }
    else // subtree is a leaf
      calcForces(subTree, body); // update F field for body
  }
}
```

A distant subtree is approximated as a single body with mass/center

## Example: N-body computation (data decomposition)

Each thread computes the forces in each node caused by the sub-tree assigned to it

```
void main() {  
    // initialize tree  
    ...  
    #pragma omp parallel private(subtree) num_threads(4)  
    {  
        // Each thread will get a subtree  
        subtree = partition(tree, omp_get_thread_num(), omp_get_num_threads());  
        for (int t=0; t<tmax; t++) {  
            for (int i=0; i<N; i++) doTimeStep(subtree, node[i]);  
            // Update the positions and velocities  
            ...  
            if (...) { // Migrate bodies if required in the quad-tree  
                ...  
                subtree = partition(tree, omp_get_thread_num(), omp_get_num_threads());  
            }  
        }  
    }  
}
```

# Outline

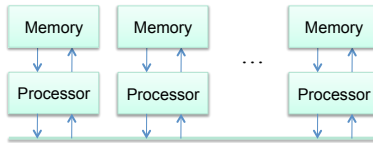
Data decomposition

Distributed-memory architectures

Task interaction in distributed memory architectures

# Why hardware needs to provide data sharing?

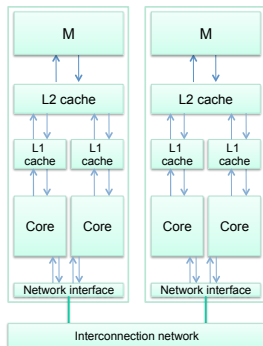
- ▶ Simple design: distributed-memory architectures



- ▶ Each node can only access its own (local) memory hierarchy, through load/store instructions
  - ▶ No access to memory locations in other nodes
  - ▶ No cache coherency among nodes
- ▶ Interconnection network to exchange data between nodes through messages



# Why hardware needs to provide data sharing?



- ▶ Each node usually based on a shared-memory multiprocessor architecture (i.e. multi-socket and/or multicore)
- ▶ Network interface in each node to inject/retrieve messages to/from the interconnection network

# Interconnection networks

- ▶ Interconnection networks are build up of switching elements
  - ▶ Switches: devices that contain multiple input and output ports with a crossbar interconnection between them (i.e. any input to any output path available)
- ▶ Topology is the pattern in which the individual switches are connected to other switches and to processors and memories (nodes).
  - ▶ Direct topologies connect each switch directly to the network interface of a node
  - ▶ In indirect topologies at least some of the switches connect to other switches

# Interconnection networks: direct topologies

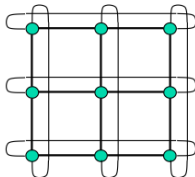
line



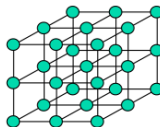
ring (1D torus)



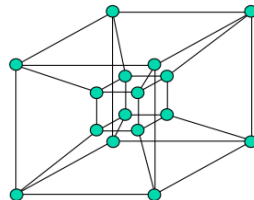
2D torus



3D mesh

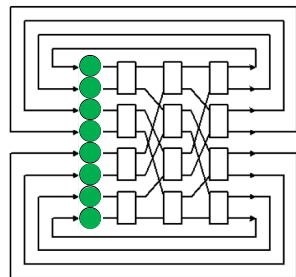
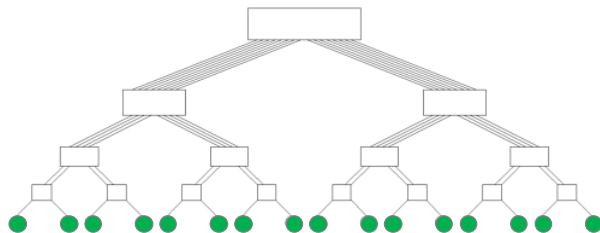


hipercube



# Interconnection networks: indirect topologies

E.g. fat tree (left) and Omega multistage (right) networks



# Communication metrics

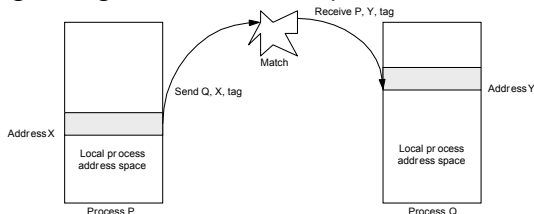
Network topology determines communication metrics (latency and bandwidth) and possibility of contention/congestion

- ▶ Latency: How long (e.g. microseconds) does a single data exchange take?
- ▶ Bandwidth: What data rate (e.g. Mbytes/sec.) can be sustained?

Interconnect	Typical latency	Typical bandwidth
100 Mbps Ethernet	75	8
1Gbit/s Ethernet	60-90	90
10 Gb/s Ethernet	12-20	800
Myricom Myrinet	2.2-3	250-1200
InfiniBand	2-4	900-1400

# Communication model

## Data exchange using send and receive primitives



- ▶ Send specifies buffer to be sent and receiving process
- ▶ Receive specifies sending process and application storage to receive into
- ▶ Optional tag on send and matching rule on receive
- ▶ Optional implicit synchronization (e.g. blocking receive)

# Who does communication?

- ▶ Software DSM (distributed-shared memory)
  - ▶ Software layer that implements data sharing (and coherence)
  - ▶ Transparently to programmer
  - ▶ Usually based on page faults (OS involved, high overhead), which uses the communication model to move pages between nodes
- ▶ Compiler inserts communication based on programmer annotations (e.g. in Unified Parallel C – UPC)
- ▶ Message-passing paradigm (e.g. MPI standard)
  - ▶ User-level library exporting the communication model to the programmer, who moves data when necessary, assuming a data distribution

# Outline

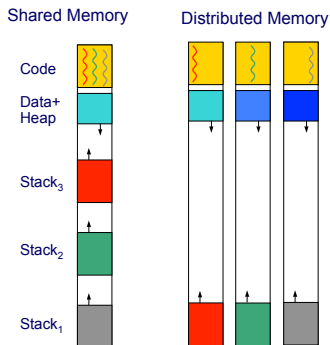
Data decomposition

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Task interaction in distributed memory architectures



# Distributed memory: address space



Programmer needs to

- ▶ Distribute work among tasks
- ▶ Distribute data among nodes
- ▶ Insert task interaction whenever necessary: communication to share data explicitly and synchronization to avoid data races

# Data allocation

- ▶ Tasks will access to data that is resident in the memory of the processor that executes the task
  - ▶ Specified through extensions in the language.

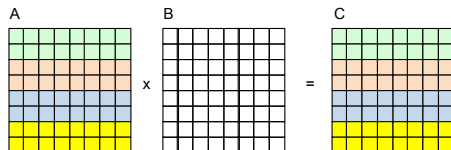
For example in UPC Unified Parallel C:

```
shared [2] int vector[16]; // block cyclic distribution with block size equals 2
```

- ▶ Explicit memory allocation (In MPI standard)

## Example: matrix multiply in MPI

```
void matmul (double C[MATSIZE][MATSIZE],  
             double A[MATSIZE][MATSIZE],  
             double B[MATSIZE][MATSIZE])  
{  
    for (int i=0; i<MATSIZE; i++)  
        for (int j=0; j<MATSIZE; j++)  
            for (int k=0; k<MATSIZE; k++)  
                C[i][j] += A[i][k]*B[k][j];  
}
```



- ▶ Assume that process 0 initially stores  $A$ ,  $B$  and  $C$  complete
- ▶  $A$  and  $C$  are distributed by rows ( $MATSIZE/nproc$  rows per process)
- ▶  $B$  is replicated

## Example: matrix multiply in MPI (cont.)

```
...
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &mpiRank);
MPI_Comm_size(MPI_COMM_WORLD, &mpiSize);
...
n = MATSIZE;
n_local = getRowCount(n, mpiRank, mpiSize);
n_sq     = n * n;
n_sq2    = n * n_local;
...
A = (double *) malloc(sizeof(double) * (mpiRank ? n_sq2 : n_sq));
B = (double *) malloc(sizeof(double) *                n_sq );
C = (double *) malloc(sizeof(double) * (mpiRank ? n_sq2 : n_sq));
...
```

where

```
int getRowCount(int rowsTotal, int mpiRank, int mpiSize) {
    /* Adjust slack of rows in case rowsTotal is not exactly divisible */
    return (rowsTotal / mpiSize) + (rowsTotal % mpiSize > mpiRank);
}
```

# Task interaction

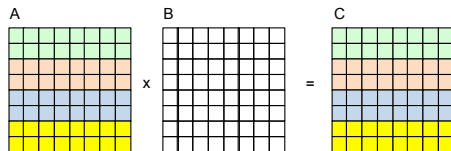
- ▶ Task interaction is necessary whenever a task needs an input (or part of it) that is assigned to another task or generates an output (or part of it) that is assigned to another task
- ▶ All task interactions (read-only, write-only or read/write) require cooperation (orchestration) of two processes: the task that has the data and the task that wants to access the data
- ▶ The message passing model provides the mechanisms to support task interaction

# Task interaction

- ▶ Interaction patterns
  - ▶ Point to Point (one to one)
  - ▶ Scatter and broadcast (one to all)
  - ▶ Gather and Reduce (all to one)
  - ▶ All to All (each processor sends its data to all others)
- ▶ Interactions may imply synchronization, i.e., process waits for interaction to happen (synchronous vs. asynchronous)
- ▶ Example: message-passing interface (MPI)

## Example: matrix multiply in MPI (cont.)

```
void matmul (double C[MATSIZE][MATSIZE],  
             double A[MATSIZE][MATSIZE],  
             double B[MATSIZE][MATSIZE])  
{  
    for (int i=0; i<MATSIZE; i++)  
        for (int j=0; j<MATSIZE; j++)  
            for (int k=0; k<MATSIZE; k++)  
                C[i][j] += A[i][k]*B[k][j];  
}
```



$A$  and  $B$  initialised by process 0. Then  $A$  distributed by rows ( $MATSIZE/nproc$  rows per process) and  $B$  replicated.

## Example: matrix multiply in MPI (cont.)

```
...
/* Initialize A and B using some functions */
if (!mpiRank) {
    ReadfromDisk(A, n_sq, 0); /* 0: from beginning; otherwise: from last element read */
    ReadfromDisk(B, n_sq, 0); /* 0: from beginning; otherwise: from last element read */
}

/* Send A by splitting it in row-wise parts */
if (!mpiRank) {
    currentRow = n_sq2;
    for (i=1; i<mpiSize; i++) {
        sizeToBeSent = n * getRowCount(n, i, mpiSize);
        MPI_Send(A + currentRow, sizeToBeSent, MPI_DOUBLE, i, TAG_INIT,
                 MPI_COMM_WORLD);
        currentRow += sizeToBeSent;
    }
}
else { /* Receive parts of A */
    MPI_Recv(A, n_sq2, MPI_DOUBLE, 0, TAG_INIT, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
}
...
```



## Example: matrix multiply in MPI (cont.)

```
...
/* Replicate complete B in each process */
if (!mpiRank) {
    for (i=1; i<mpiSize; i++) {
        MPI_Send(B, n_sq, MPI_DOUBLE, i, TAG_INIT, MPI_COMM_WORLD);
    }
}
else { /* Receive B in each other process */
    MPI_Recv(B, n_sq, MPI_DOUBLE, 0, TAG_INIT, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
}

/* Let each process initialize C to zero */
for (i=0; i<n_sq2; i++)
    C[i] = 0.0;

/* And finally ... let each process perform its own multiplications */
for (i=0; i<nlocal; i++)
    for (j=0; j<MATSIZE; j++)
        for (k=0; k<MATSIZE; k++)
            C[i][j] += A[i][k]*B[k][j];
...
```

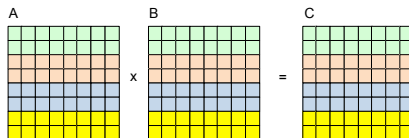
## Example: matrix multiply in MPI (cont.)

```
...
/* Receive partial results from each slave */
if (!mpiRank) {
    currentRow = n_sq2;
    for (i=1; i<mpiSize; i++) {
        sizeToBeSent = n * getRowCount(n, i, mpiSize);
        MPI_Recv(C + currentRow, sizeToBeSent, MPI_DOUBLE, i, TAG_RESULT,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        currentRow += sizeToBeSent;
    }
}
else /* Send partial results to master */
    MPI_Send(C, n_sq2, MPI_DOUBLE, 0, TAG_RESULT, MPI_COMM_WORLD);

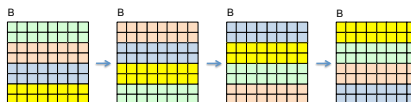
MPI_Finalize();
...
```

# Matrix multiply: stronger memory size constraints

- ▶ What if  $B$  does not fit completely in worker processors?

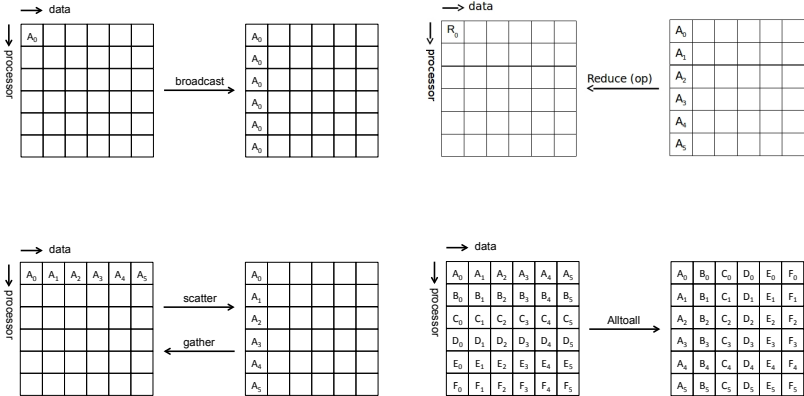


We need to circulate  $B$  among processors in order to do the complete product.



- ▶ What if master has the same memory size constraints as workers?

# Collective communications



## Using collectives in matrix multiply

```
...
/* Replicate complete B in each process */
if (!mpiRank) {
    for (i=1; i<mpiSize; i++) {
        MPI_Send(B, n_sq, MPI_DOUBLE, i, TAG_INIT, MPI_COMM_WORLD);
    }
}
else { /* Receive B in each other process */
    MPI_Recv(B, n_sq, MPI_DOUBLE, 0, TAG_INIT, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
}
...
```

Using a single collective, assuming same number of rows per processor:

```
...
/* Replicate complete B in each process */
MPI_Bcast(B, n_sq, MPI_DOUBLE, 0, MPI_COMM_WORLD);
...
```

## Using collectives in matrix multiply (cont.)

```
...
/* Send A by splitting it in row-wise parts */
if (!mpiRank) {
    currentRow = n_sq2;
    for (i=1; i<mpiSize; i++) {
        sizeToBeSent = n * getRowCount(n, i, mpiSize);
        MPI_Send(A + currentRow, sizeToBeSent, MPI_DOUBLE, i, TAG_INIT,
                 MPI_COMM_WORLD);
        currentRow += sizeToBeSent;
    }
}
else { /* Receive parts of A */
    MPI_Recv(A, n_sq2, MPI_DOUBLE, 0, TAG_INIT, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
}
...
```

Using a single collective, assuming same number of rows per processor:

```
...
sizeToBeSent = n * n/mpiSize;
MPI_Scatter(A, sizeToBeSent, MPI_DOUBLE, A, sizeToBeSent, MPI_DOUBLE, 0, MPI_COMM_WORLD)
...
```

## Using collectives in matrix multiply (cont.)

```
...
/* Receive partial results from each slave */
if (!mpiRank) {
    currentRow = n_sq2;
    for (i=1; i<mpiSize; i++) {
        sizeToBeSent = n * getRowCount(n, i, mpiSize);
        MPI_Recv(C + currentRow, sizeToBeSent, MPI_DOUBLE, i, TAG_RESULT,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        currentRow += sizeToBeSent;
    }
}
else /* Send partial results to master */
    MPI_Send(C, n_sq2, MPI_DOUBLE, 0, TAG_RESULT, MPI_COMM_WORLD);
...
```

Using a single collective, assuming same number of rows per processor:

```
...
sizeToBeSent = n * n/mpiSize;
MPI_Gather(C, sizeToBeSent, MPI_DOUBLE, C, sizeToBeSent, MPI_DOUBLE, 0, MPI_COMM_WORLD)
...
```

# Minimizing interaction overheads

- ▶ Minimize volume of data exchange because of the cost associated with each word that is communicated
- ▶ Minimize frequency of interactions because of the startup cost associated with each interaction (try to merge multiple interactions into one, where possible)
- ▶ Overlap computations with interactions by using non-blocking communications
  - ▶ Non-blocking operations (`MPI_Isend` and `MPI_Irecv`) return (immediately) a "request handler" that can be tested and waited on



# Minimizing interaction overheads (cont.)

- ▶ Use collective communications instead of point-to-point primitives (also programming simplicity)
- ▶ Minimize contention and hot-spots: Use decentralized techniques, replicate data where necessary
- ▶ Replicate computations

# Parallelism (PAR)

## Parallel programming principles: Data decomposition

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