

Parallelism (PAR)

Parallel programming principles: Data decomposition

Eduard Ayguadé, José Ramón Herrero and Gladys Utrera

Computer Architecture Department
Universitat Politècnica de Catalunya

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Additional learning material for this lesson

- ▶ Atenea: Unit 5 Data decomposition
 - ▶ Video lessons covering distributed-memory architectures and message passing
 - ▶ Quiz after video lessons
- ▶ Collection of Exercises: problems in Chapter 5

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] = fool(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 ₀	M ₁	M ₂	M ₃
0..24	25..49	50..74	75..99

Possible **assignment of iterations** to processors (threads) in the three loops:

P ₀	P ₁	P ₂	P ₃
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.)

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

    #pragma omp for schedule(static)
    for (int i=0; i<n; i++)
        c[i] = foo2(b[i]);

    #pragma omp for schedule(static)
    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

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0..24	25..49	50..74	75..99
0..24	25..49	50..74	75..99
0..24	25..49	50..74	75..99

Motivating example (cont.)

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

    #pragma omp for schedule(static) nowait
    for (int i=0; i<n/2; i++)
        c[i] = foo2(b[i]);

    #pragma omp for schedule(static)
    for (int i=n/2; i<n; i++)
        c[i] = -foo2(b[i]);

    #pragma omp for schedule(static)
    for (int i=n-1; i>=0; i--)
        a[i] = foo3(c[i]);
}
```

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

M ₀	M ₁	M ₂	M ₃
0..24	25..49	50..74	75..99

Possible **assignment of iterations** to processors (threads) in the three loops:

P ₀	P ₁	P ₂	P ₃
0..24	25..49	50..74	75..99
0..12	13..25	26..37	38..49
50..62	63..75	76..87	88..99
99..75	50..74	25..49	0..24

In this case we need more control on how to assign iterations to threads in order to access data locally

Outline

Data decomposition

Distributed-memory architectures

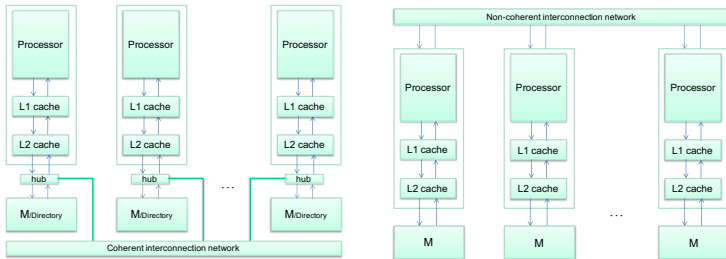
Task interaction in distributed memory architectures

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

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



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

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

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

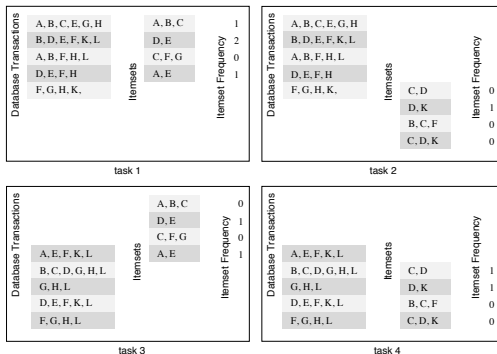
Partitioning the transactions among the tasks

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



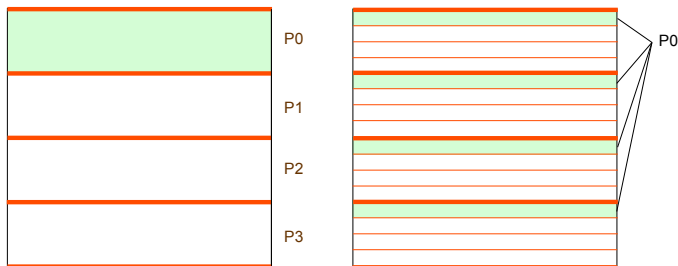
The Owner Computes rule

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.

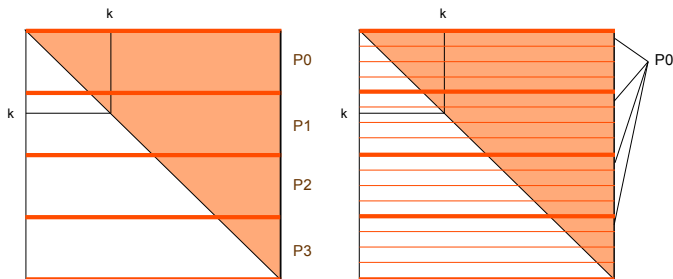
Data distributions for geometric decomposition

Block (left) and cyclic (right) data decompositions



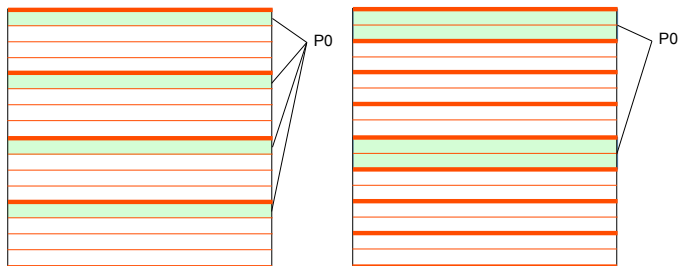
Data distributions for geometric decomposition

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



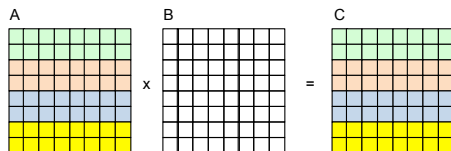
Data distributions for geometric decomposition

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];
    }
}
```

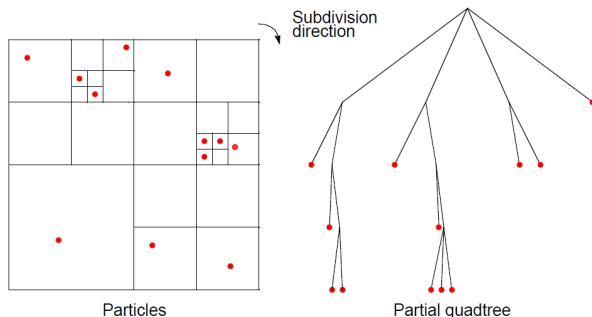
Example: matrix multiply (OpenMP)

```
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

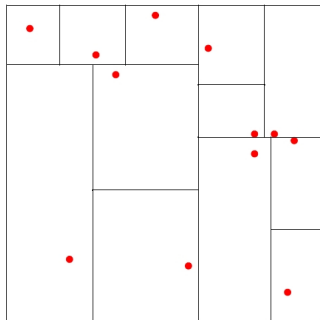
Quadtree to represent particles in an N-body problem



- ▶ 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

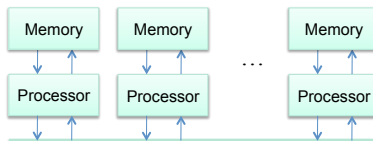
Data decomposition

Distributed-memory architectures

Task interaction in distributed memory architectures

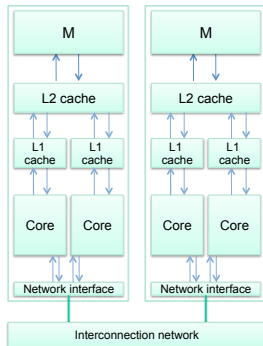
Why hardware needs to provide data sharing?

- ▶ 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

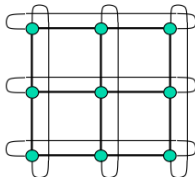
line



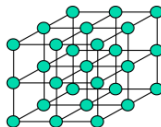
ring (1D torus)



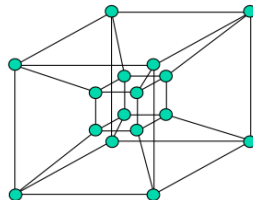
2D torus



3D mesh

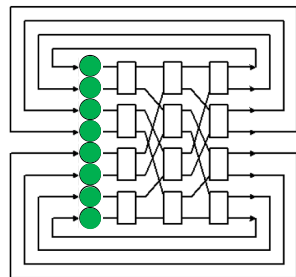
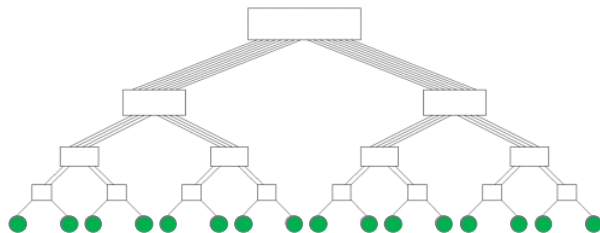


hipercube



Interconnection networks: indirect topologies

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



Communication metrics

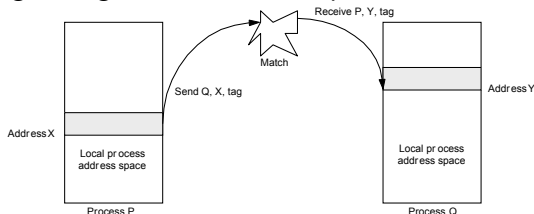
Network topology determines communication metrics (latency and bandwidth) and possibility of contention/congestion

- ▶ 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

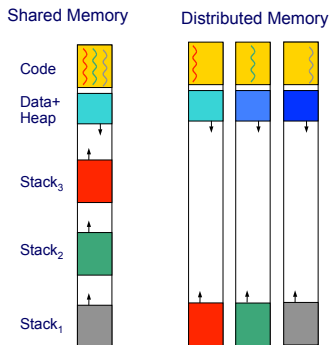
Outline

Data decomposition

Distributed-memory architectures

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.

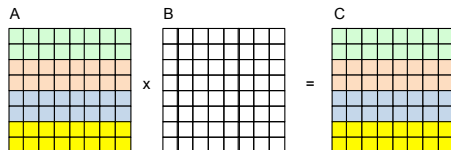
For example in UPC Unified Parallel C:

```
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

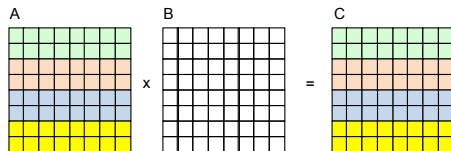
- ▶ Task interaction is necessary whenever a task needs an input (or part of it) that is assigned to another task or generates an output (or part of it) that is assigned to another task
- ▶ All task interactions (read-only, write-only or read/write) require cooperation (orchestration) of two processes: 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 ($MATSIZE/n_{proc}$ 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];
...
```

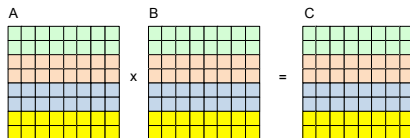
Example: matrix multiply in MPI (cont.)

```
...
/* 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);

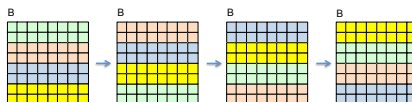
MPI_Finalize();
...
```

Matrix multiply: stronger memory size constraints

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

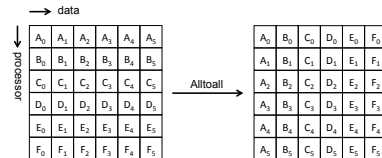
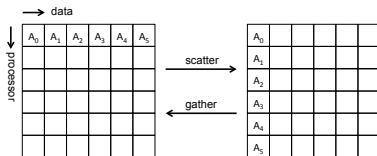
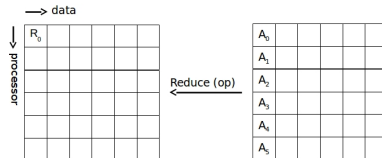
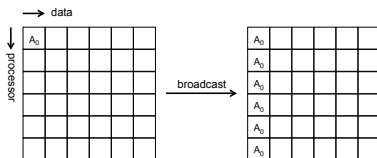


We need to circulate B among processors in order to do the complete product.



- ▶ 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

Eduard Ayguadé, José Ramón Herrero and Gladys Utrera

Computer Architecture Department
Universitat Politècnica de Catalunya

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