Parallelization Strategies
ASD Distributed Memory HPC Workshop

Computer Systems Group

Research School of Computer Science
Australian National University
Canberra, Australia

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Day 3 – Schedule

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Distributed Memory HPC

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DISTRIBUTED MEMORY HPC

1. Messaging and Networks
2. Advanced Messaging
3. Parallelization Strategies
4. PGAS Paradigm
5. Distributed HPC Systems

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Day 3: Parallelization Strategies

Time	Lecture Topics	Hands-On Exercise	Instructor
9:00	Embarrassingly Parallel Problems	Load Balancing Embarrassingly Parallel Problems	Peter Strazdins
10:30	COFFEE BREAK		
11:00	Parallelisation via Data Partitioning	Bucket Sort	
12:30	LUNCH		
13:30	Synchronous Computations	Synchronous Computations	
15:00	AFTERNOON TEA		
15:30	Parallel Matrix Algorithms	Matrix Multiply	

Parallelization Strategies lecture slides (pdf)

Outline

Outline: Embarrassingly Parallel Problems

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- what they are
- Mandelbrot Set computation
  - cost considerations
  - static parallelization
  - dynamic parallelizations and its analysis
- Monte Carlo Methods
- parallel random number generation

Embarrassingly Parallel Problems

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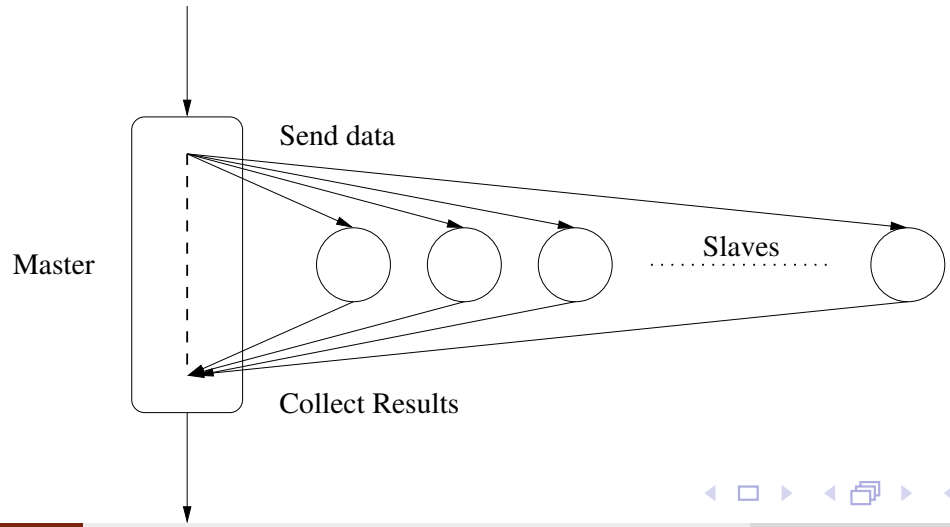
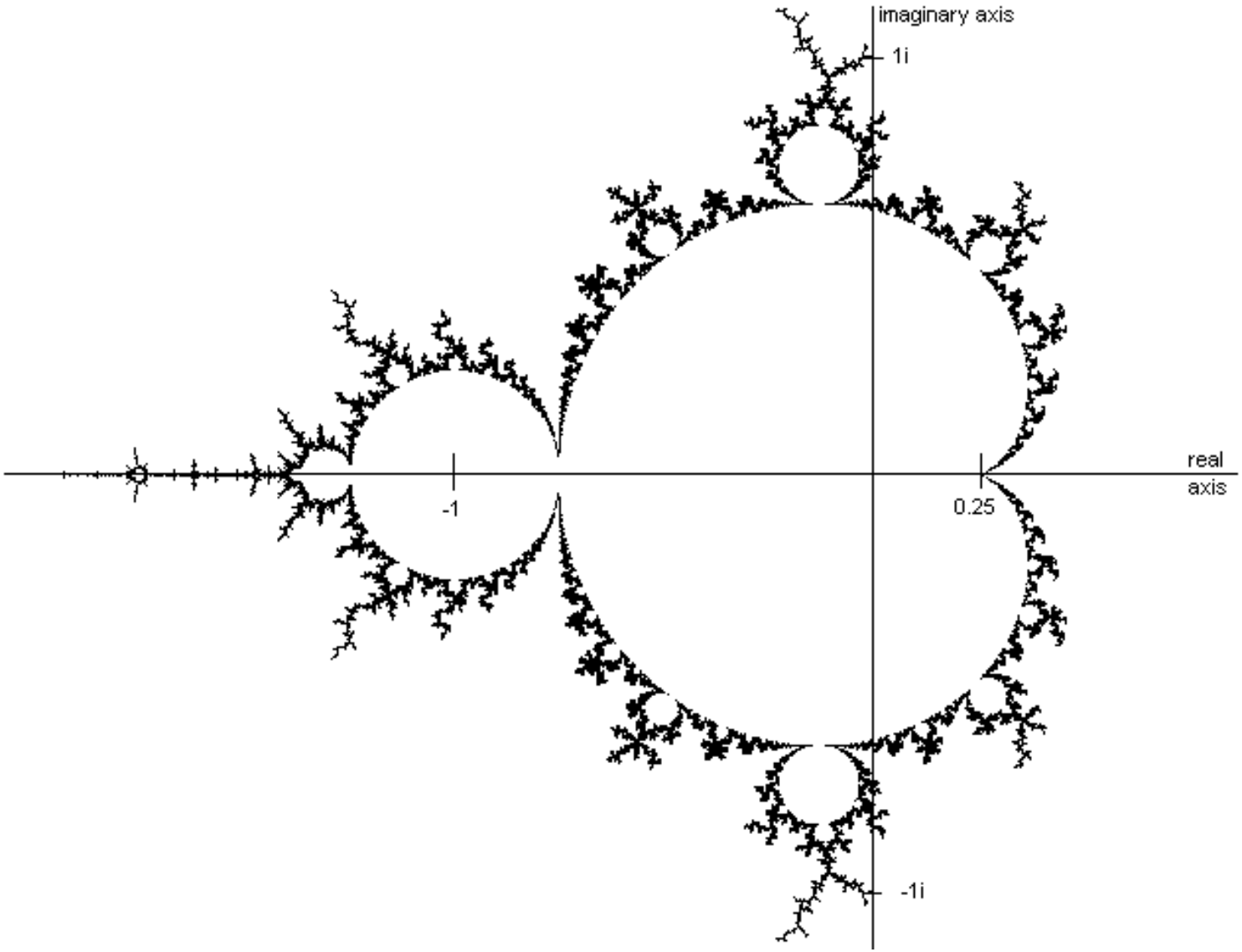
- computation can be divided into completely independent parts for execution by separate processors (correspond to totally disconnected computational graphs)
  - infrastructure: Blocks of Independent Computations (BOINC) project
  - SETI@home and Folding@Home are projects solving very large such problems
- part of an application may be embarrassingly parallel
- distribution and collection of data are the key issues (can be non-trivial and/or costly)
- frequently uses the **master/slave** approach ($p - 1$ speedup)



Example#1: Computation of the Mandelbrot Set



The Mandelbrot Set

- set of points in complex plane that are quasi-stable
- computed by iterating the function

$$z_{k+1} = z_k^2 + c$$

  - z and c are complex numbers ($z = a + bi$)
  - z initially zero
  - c gives the position of the point in the complex plane
- iterations continue until $|z| > 2$ or some arbitrary iteration limit is reached

$$|z| = \sqrt{a^2 + b^2}$$

- enclosed by a circle centered at (0,0) of radius 2

Evaluating 1 Point

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```
typedef struct complex{float real, imag;} complex;
const int MaxIter = 256;

int calc_pixel(complex c){
  int count = 0;
  complex z = {0.0, 0.0};
  float temp, lengthsq;
  do {
    temp = z.real * z.real - z.imag * z.imag + c.real
    z.imag = 2 * z.real * z.imag + c.imag;
    z.real = temp;
    lengthsq = z.real * z.real + z.imag * z.imag;
    count++;
  } while (lengthsq < 4.0  &&  count < MaxIter);
  return count;
}
```

Building the Full Image

Define:

- min. and max. values for c (usually -2 to 2)
- number of horizontal and vertical pixels

```
for (x = 0; x < width; x++)
  for (y = 0; y < height; y++){
    c.real = min.real + ((float) x * (max.real - min.real)/width);
    c.imag = min.imag + ((float) y * (max.imag - min.imag)/height);
    color = calc_pixel(c);
    display(x, y, color);
}
```

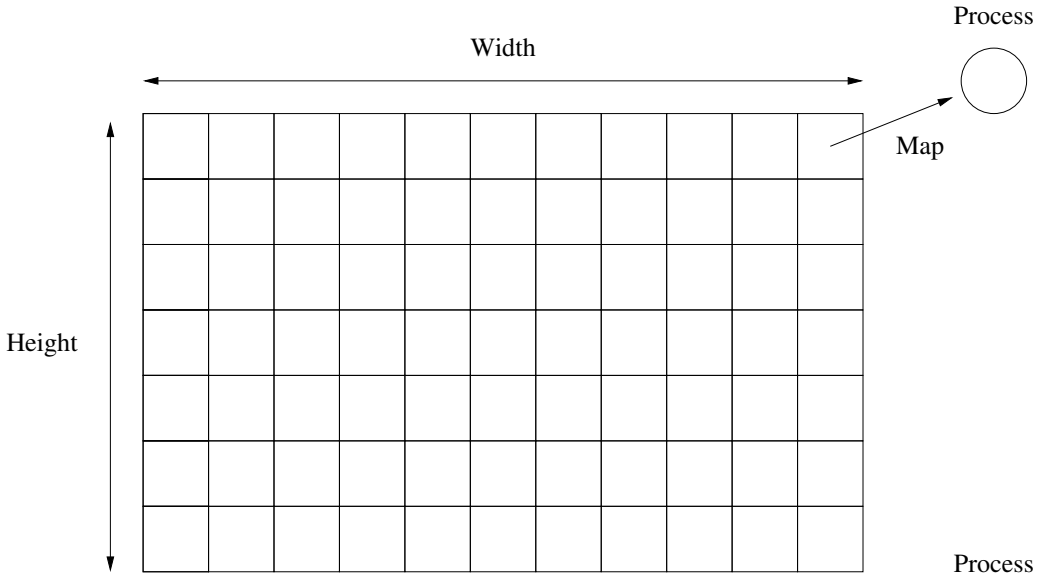
Summary:

- `width` × `height` totally independent tasks
- each task can be of different length

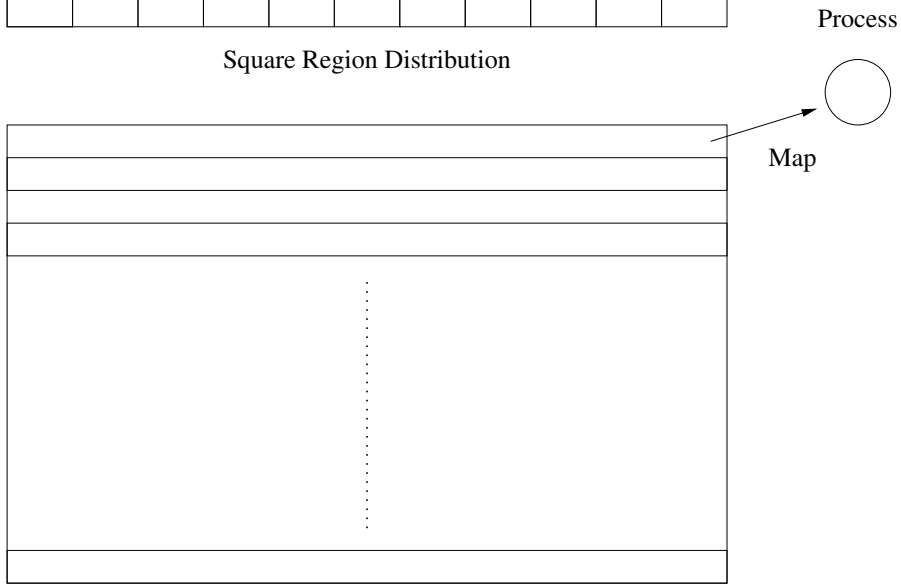
Cost Considerations on NCI's Raijin

- 10 flops per iteration
- maximum 256 iterations per point
- approximate time on one Raijin core:
  $10 \times 256/(8 \times 2.6 \times 10^9) \approx 0.12\text{usec}$
- between two nodes the time to communicate single point to slave and receive result $\approx 2 \times 2\text{usec}$ (latency limited)
- conclusion: cannot parallelize over individual points
- also must allow time for master to send to all slaves before it can return to any given process

Parallelisation: Static



Square Region Distribution



Row Distribution

Static Implementation

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Master:

```
for (slave = 1, row = 0; slave < nproc; slave++) {
  send(&row, slave);
  row = row + height/nproc;
}
for (npixel = 0; npixel < (width * height); npixel++) {
  recv(&x, &y, &color, any_processor);
  display(x, y, color);
}
```

Slave:

```
const int master = 0; // proc. id
recv(&firstrow, master);
lastrow = MIN(firstrow + height/nproc, height);
for (x = 0; x < width; x++)
  for (y = firstrow; y < lastrow; y++) {
    c.real = min.real + ((float) x * (max.real - min.real)/width);
    c.imag = min.imag + ((float) y * (max.imag - min.imag)/height);
    color = calc_pixel(c);
    send(&x, &y, &color, master);
  }
```

Dynamic Task Assignment

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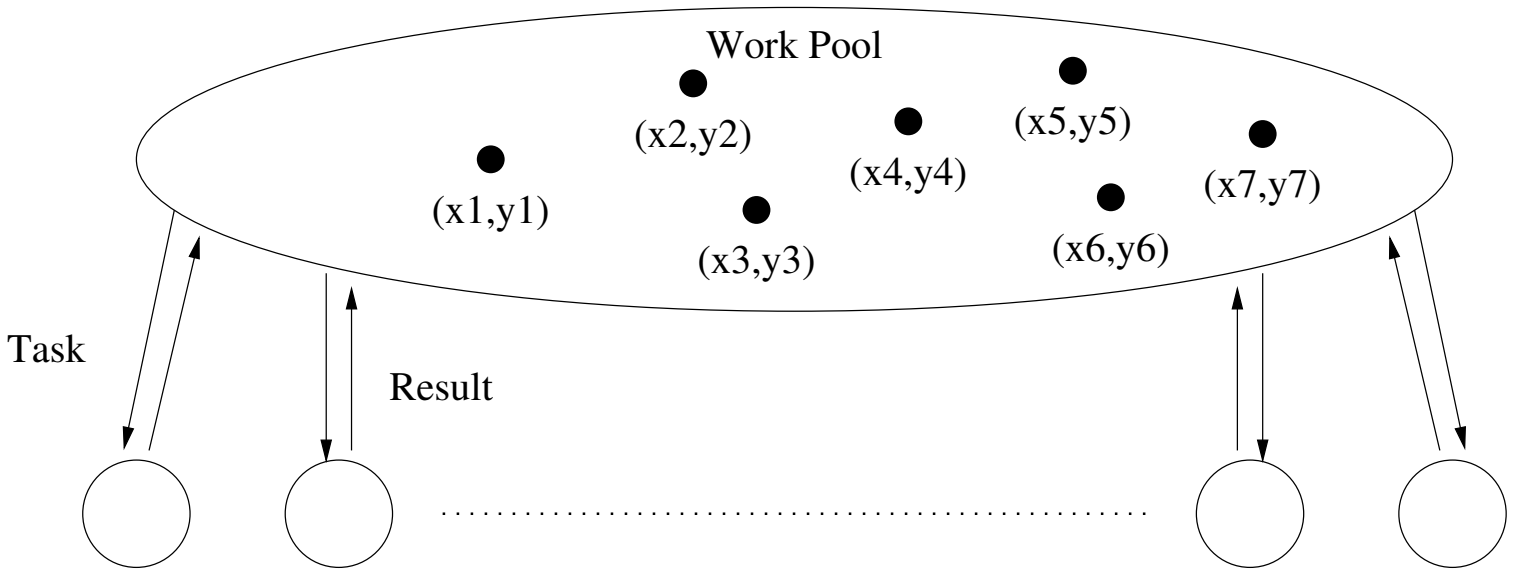
- discussion point: why would we expect static assignment to be sub-optimal for the Mandelbrot set calculation? Would any regular static decomposition be significantly better (or worse)?
- usa a pool of **over-decomposed** tasks that are dynamically assigned to next requesting process:



Processor Farm: Master


```
count = 0;
row = 0;
for (slave = 1; slave < nproc; k++){
  send(&row, slave, data_tag);
  count++;
  row++;
}
do {
  recv(&slave, &r, &color, any_proc, result_tag);
  count--;
  if (row < height) {
     send(&row, slave, data_tag);
     row++;
     count++;
  } else
    send(&row, slave, terminator_tag);
  display_vector(r, color);
} while (count > 0);
```

Processor Farm: Slave


```
const int master = 0; //proc id.
recv(&y, master, any_tag, source_tag);
while (source_tag == data_tag) {
  c.imag = min.imag + ((float) y * (max.imag - min.imag)/height);
  for (x = 0; x < width; x++) {
    c.real = min.real + ((float) x * (max.real - min.real)/width);
    color[x] = calc_pixel(c);
  }
  send(&myid, &y, color, master, result_tag);
  recv(&y, master, source_tag);
}
```

Analysis

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Let p, m, n, I denote `nproc`, `height`, `width`, `MaxIter`:

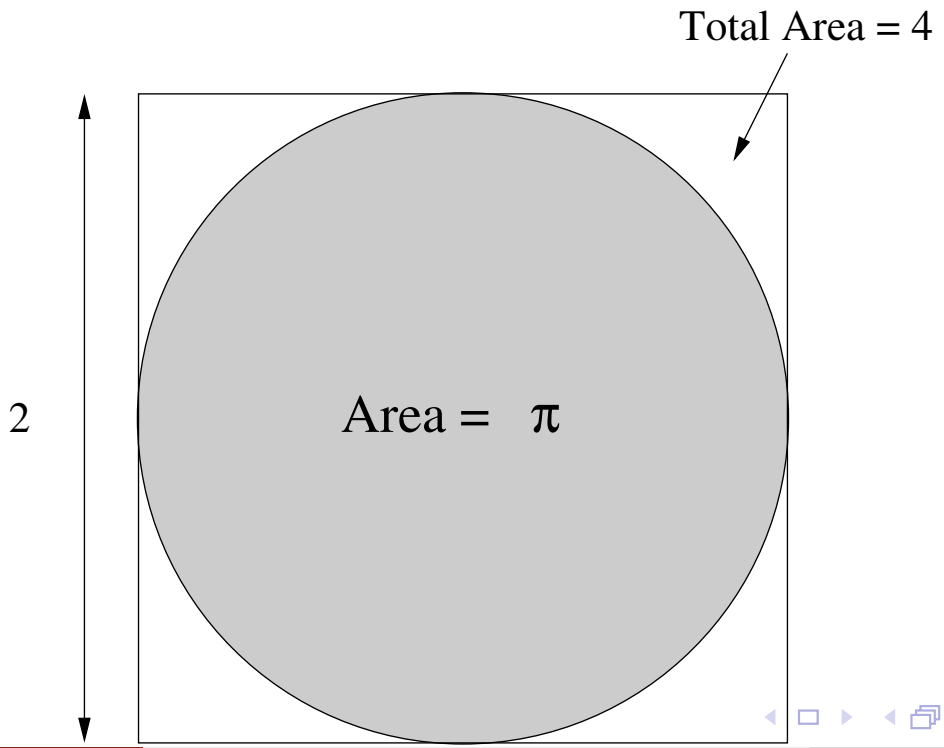
- sequential time: (t_f denotes floating point operation time)
  $t_{\text{seq}} \leq I \cdot mn \cdot t_f = O(mn)$
- parallel communication 1: (neglect t_h term, assume message length of 1 word)
  $t_{\text{com1}} = 2(p-1)(t_s + t_w)$
- parallel computation:
  $t_{\text{comp}} \leq \frac{I \cdot mn}{p-1} t_f$
- parallel communication 2:
  $t_{\text{com2}} = \frac{m}{p-1}(t_s + t_w)$
- overall:
  $t_{\text{par}} \leq \frac{I \cdot mn}{p-1} t_f + (p - 1 + \frac{m}{p-1})(t_s + t_w)$

Discussion point: What assumptions have we been making here? Are there any situations where we might still have poor performance, and how could we mitigate this?

Example#2: Monte Carlo Methods

- use random numbers to solve numerical/physical problems
- evaluation of π by determining if random points in the unit square fall inside a circle

$$\frac{\text{area of circle}}{\text{area of square}} = \frac{\pi(1)^2}{2 \times 2} = \frac{\pi}{4}$$



Monte Carlo Integration

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- evaluation of integral $(x_1 \leq x_i \leq x_2)$

$$\text{area} = \int_{x_1}^{x_2} f(x)\,dx = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(x_i)(x_2 - x_1)$$

- example

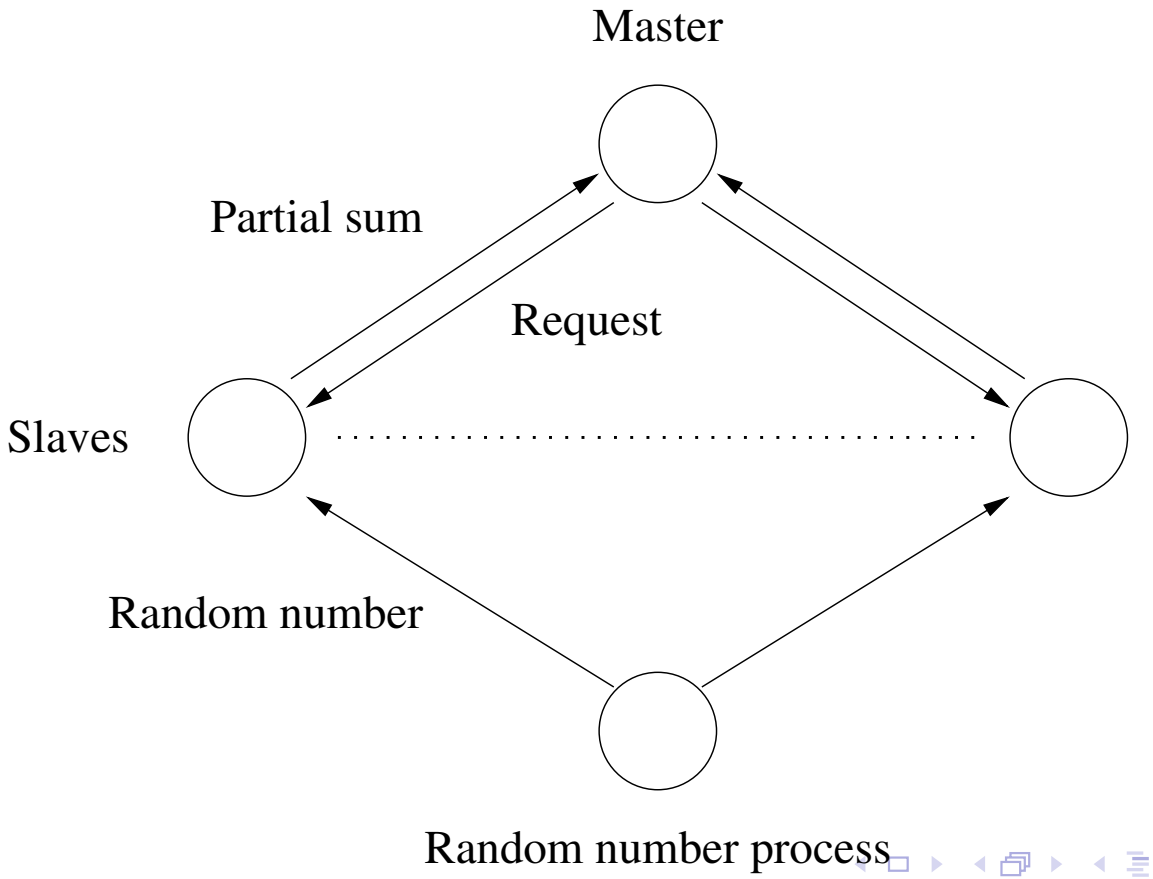
$$I = \int_{x_1}^{x_2} (x^2 - 3x)\,dx$$

```
sum = 0;
for (i = 0; i < N; i++) {
    xr = rand_v(x1, x2);
    sum += xr * xr - 3 * xr;
}
area = sum * (x2 - x1) / N;
```

- where `rand_v(x1, x2)` computes a pseudo-random number between `x1` and `x2`

Parallelization

- only problem is ensuring each process uses a different random number and that there is no correlation
- one solution is to have a unique process (maybe the master) issuing random numbers to the slaves



Parallel Code: Integration

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Master (process 0):

```
for (i = 0; i < N/n; i++) {
  for (j = 0; j < n; j++)
    xr[j] = rand_v(x1, x2);
  recv(any_proc, req_tag, &p_src)
      ;
  send(xr, n, p_src, comp_tag);
}
for (i=1; i < nproc; i++) {
   recv(i, req_tag);
   send(i, stop_tag);
}
sum = 0;
reduce_add(&sum, p_group);
```

Slave:

```
const int master = 0; //proc id.
sum = 0;
send(master, req_tag);
recv(xr, &n, master, tag);
while (tag == comp_tag) {
  for (i = 0; i < n; i++)
    sum += xr[i]*xr[i] - 3*xr[i]
  send(0, req_tag);
  recv(xr, n, master, &tag);
}
reduce_add(&sum, p_group);
```

Question: performance problems with this code?

Parallel Random Numbers

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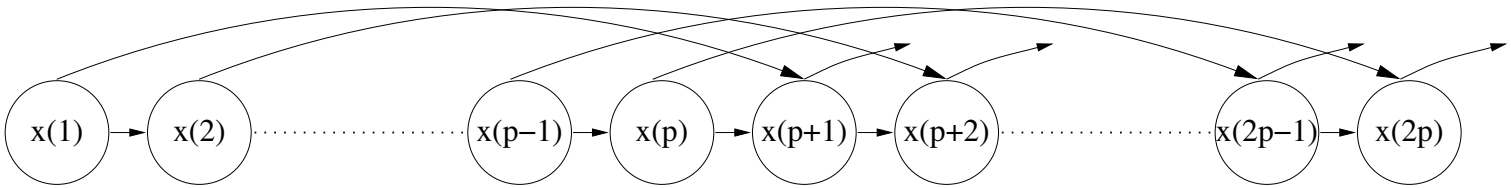
- linear congruential generators $x_{i+1} = (ax_i + c) \bmod m$ (a, c, and m are constants)
- using property $x_{i+p} = (A(a, p, m)x_i + C(c, a, p, m)) \bmod m$, we can generate the first p random numbers sequentially to repeatedly calculate the next p numbers in parallel



Summary: Embarrassingly Parallel Problems

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- defining characteristic: tasks do not need to communicate
- non-trivial however: providing input data to tasks, assembling results, load balancing, scheduling, heterogeneous compute resources, costing
  - **static task assignment** (lower communication costs) vs. **dynamic task assignment** + **overdecomposition** (better load balance)
- **Monte Carlo** or **ensemble simulations** are a big use of computational power!
- the field of grid computing arose to solve this issue

Hands-on Exercise: Embarrassingly || Problems

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Outline

Outline: Parallelisation via Data Partitioning

- partitioning strategies
- vector summation via partitioning, via divide-and-conquer
- binary trees (divide-and-conquer)
- bucket sort
- numerical integration - adaptive techniques
- N-body problems

Challenge from PS1: can you write a well-balanced parallel Mandelbrot set program using static task assignment?

Partitioning Strategies

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- replicated data approach (no partitioning)
  - each process has entire copy of data but does subset of computation
- partition program data to different processes
  - most common
  - strategies: **domain decomposition**, **divide-and-conquer**
- partitioning of program functionality
  - much less common
  - **functional decomposition**
- consider the addition of numbers

$$s = \sum_{i=0}^{n-1} x_i$$

Example#1: Simple Summation of Vector

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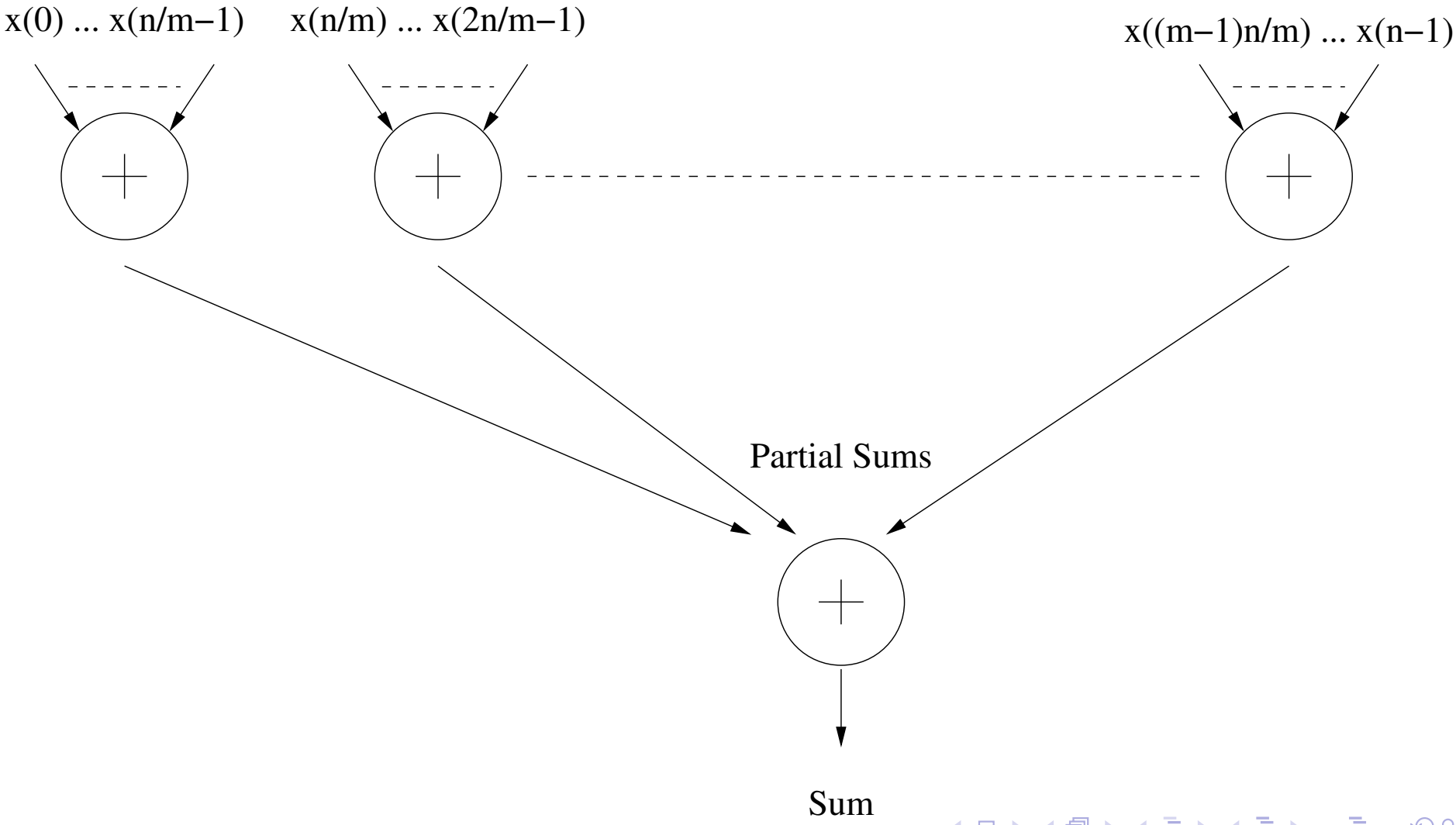
- divide numbers into *m* equal parts



Master/Slave Send/Recv Approach

Master:

```
s = n / m;
for (i = 0, x = 0; i < m; i++, x = x + s)
  send(&numbers[x], s, i+1 /*slave id*/);

sum = 0;
for (i = 0; i < m; i++) {
  recv(&part_sum, any_proc);
  sum = sum + part_sum;
}
```

Slave:

```
recv(numbers, s, master);
part_sum = 0;
for (i = 0; i < s; i++)
  part_sum = part_sum + numbers[i];
send(&part_sum, master);
```

Using MPI_Scatter and MPI_Reduce

See `man MPI_Scatter` and `man MPI_Reduce`

```
1  s = n/m;
   MPI_Scatter(numbers, s /*sendcount*/, MPI_FLOAT /*send data*/,
3              numbers, s /*recvcount*/, MPI_FLOAT /*recv data*/,
               0 /*root*/, MPI_COMM_WORLD);
5
   for (i = 0; i < s; i++)
7     part_sum = part_sum + numbers[i];

9  MPI_Reduce(&part_sum, &sum, 1 /*count*/, MPI_FLOAT,
              MPI_SUM, 0 /*root*/, MPI_COMM_WORLD);
```

- NOT **master/slave**
- the root sends data to all processes (including itself)
- note related MPI calls:
  - `MPI_Scatterv()`: scatters variable lengths
  - `MPI_Allreduce()`: returns result to all processors

Analysis

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Sequential:

- $n-1$ additions thus $O(n)$

Parallel ($p = \mathtt{m}$):

- communication #1: $t_{\text{scatter}} = p(t_s + \frac{n}{p} t_w)$
- computation #1: $t_{\text{partialsum}} = (\frac{n}{p}) t_f$
- communication #2: $t_{\text{reduce}} = p(t_s + t_w)$
- computation #2: $t_{\text{finalsum}} = (p-1) t_f$
- overall: $t_{\text{p}} = 2pt_s + (n+p)t_w + (n/p + p - 1)t_f = O(n+p)$
- **worse than sequential code!!**

Discussion point: in this example, we are assuming the associative property of addition ($+$)? Is this strictly true for floating point numbers? What impact does this have for such parallel algorithms?

Domain Decomposition via Divide-and-Conquer

- problems that can be recursively divided into smaller problems of the same type
- recursive implementation of the summation problem:

```
int add(int *s) {
  if (numbers(s) == 1)
    return (s[0]);
  else {
    divide(s, s1, s2);
    part_sum1 = add(s1);
    part_sum2 = add(s2);
    return (part_sum1 + part_sum2);
  }
}
```

Binary Tree

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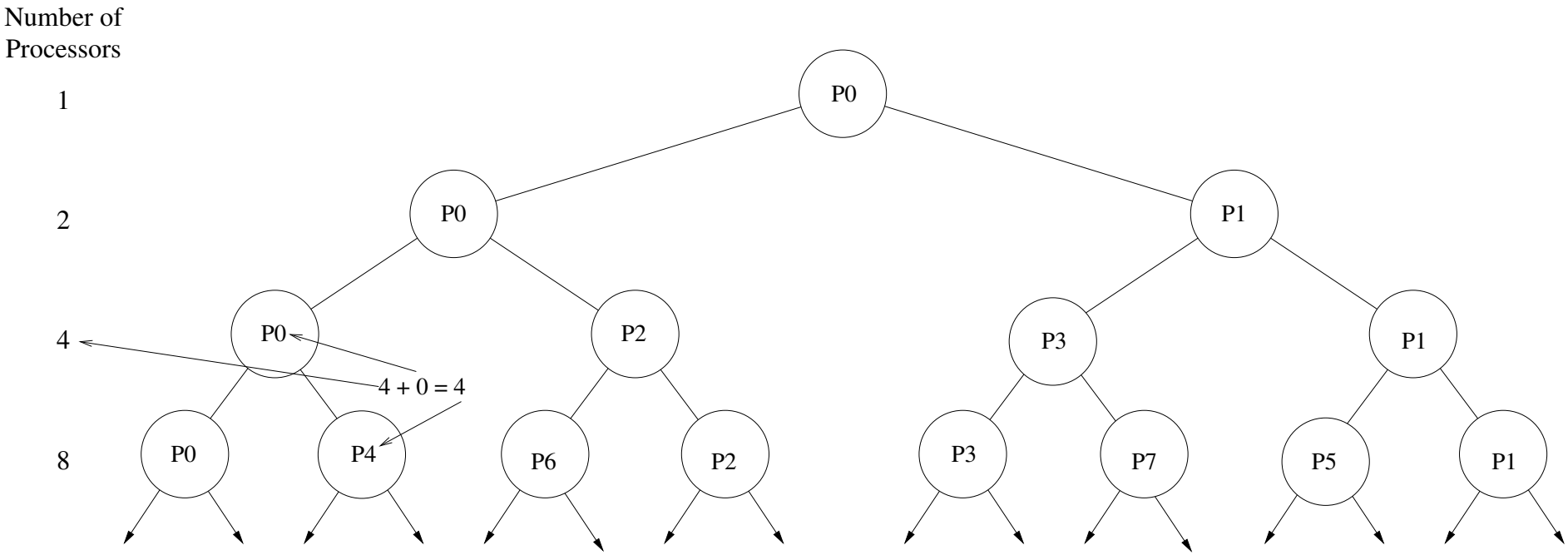
- **divide-and-conquer** with binary partitioning
- note number of working processors decreases going up the tree



Simple Binary Tree Code


```
/* Binary Tree broadcast
  a) 0->1
  b) 0->2, 1->3
  c) 0->4, 1->5, 2->6, 3->7
  d) 0->8, 1->9, 2->10, 3->11, 4->12, 5->13, 6->14, 7->15
*/
  lo = 1;
  while (lo < nproc) {
    if (me < lo) {
      id = me + lo;
      if (id < nproc)
        send(buf, lenbuf, id);
    }
    else if (me < 2*lo) {
      id = lo;
      recv(buf, lenbuf, id);
    }
    lo *= 2;
  }
```

This is used to scatter the vector; the reverse algorithm combines the partial sums.

Analysis

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- assume n is a power of 2 and ignoring t_s
- communication#1: divide
  $t_{\text{divide}} = \frac{n}{2}t_w + \frac{n}{4}t_w + \frac{n}{8}t_w + \cdots \frac{n}{p}t_w = \frac{n(p-1)}{p}t_w$
- communication#2: combine
  $t_{\text{combine}} = \lg p \cdot t_w$
- computation:
  $t_{\text{comp}} = (\frac{n}{p} + \lg p)t_f$
- total:
  $t_{\text{p}} = (\frac{n(p-1)}{p} + \lg p)t_w + (\frac{n}{p} + \lg p)t_f$
- slightly better than before - as $p \to n$, cost $\to O(n)$

Higher Order Trees

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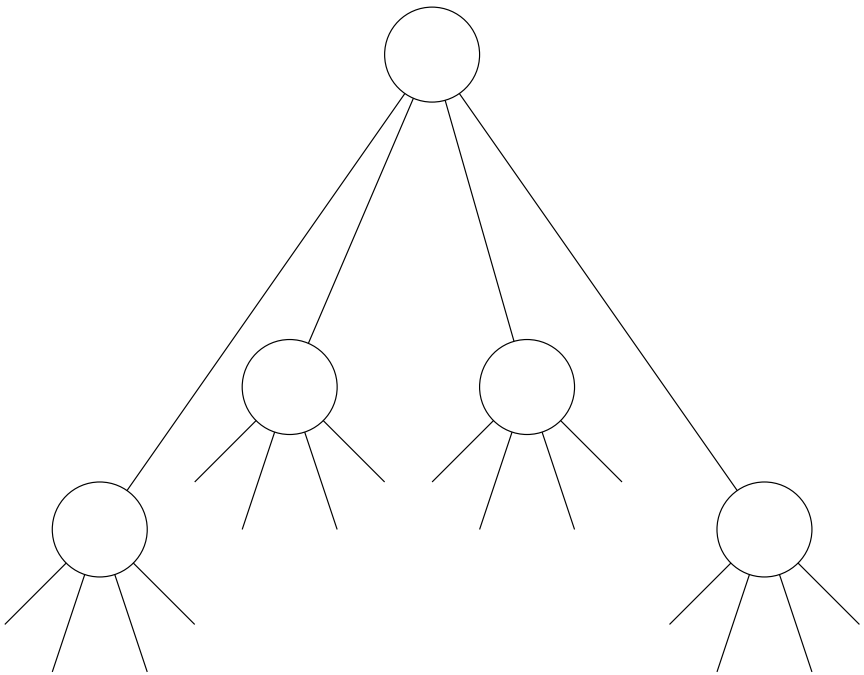
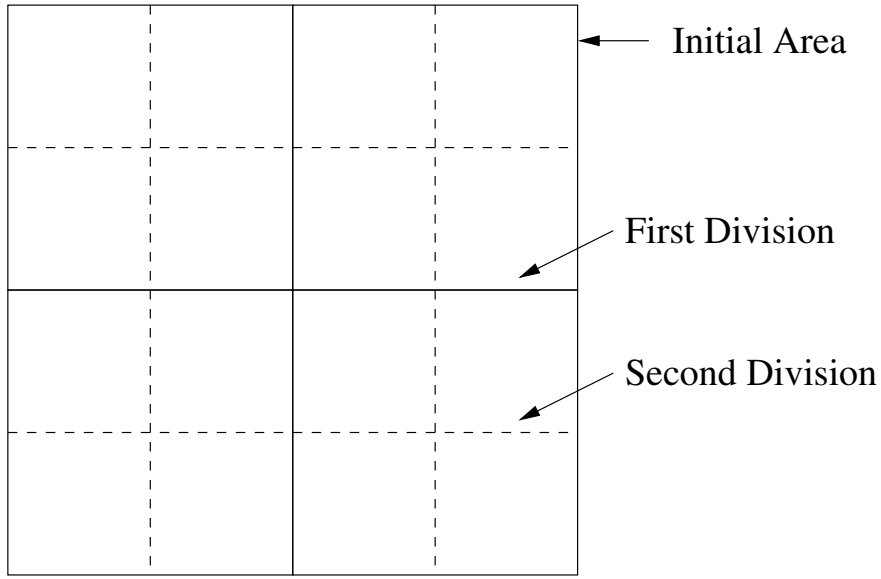
- possible to divide data into higher order trees, e.g. a quad tree





Example#2: Bucket Sort

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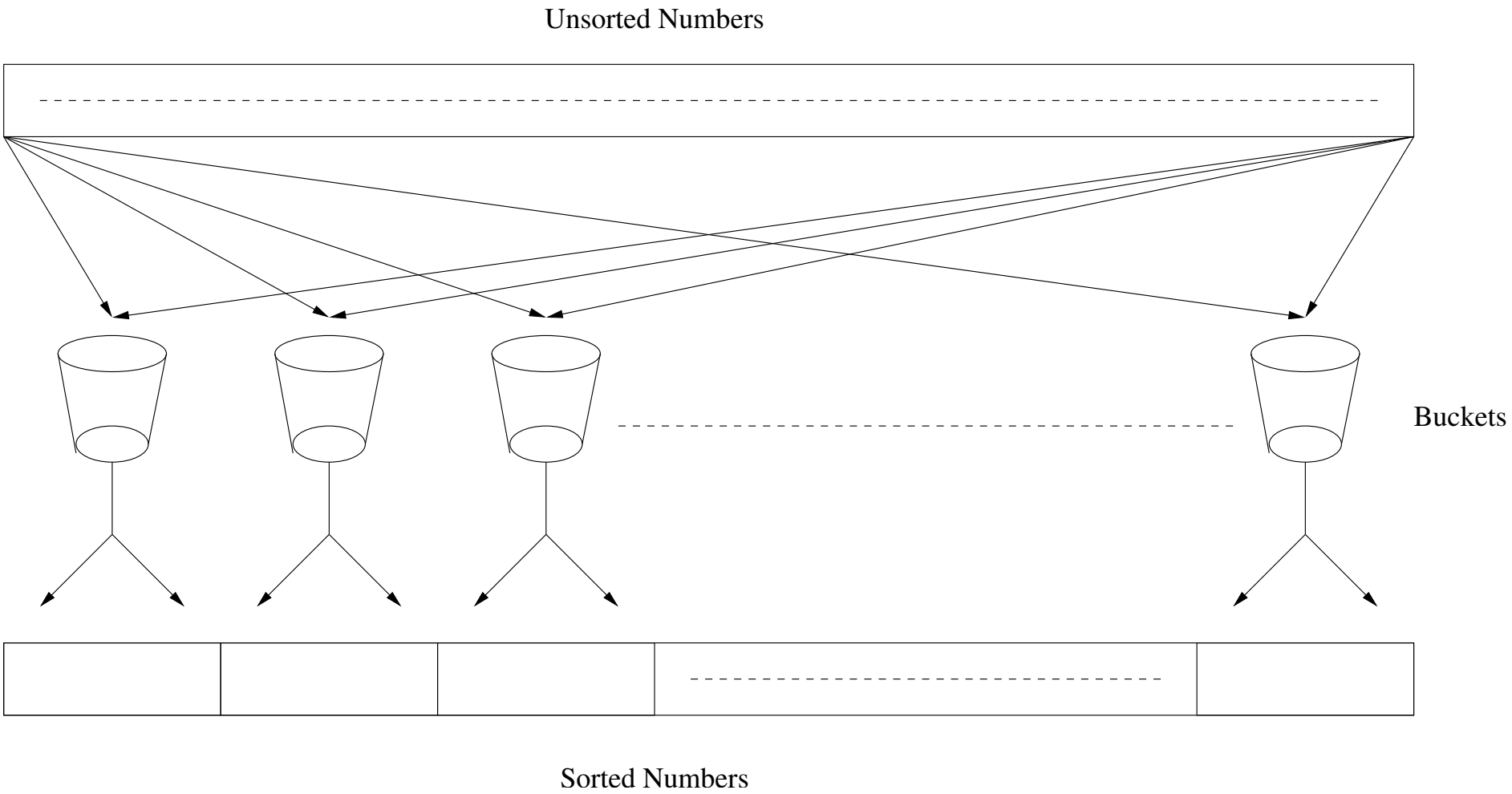
- Divide number range (a) into m equal regions

$$\left(0 \to \frac{a}{m} - 1\right), \left(\frac{a}{m} \to 2\frac{a}{m} - 1\right), \left(2\frac{a}{m} \to 3\frac{a}{m} - 1\right), \cdots$$

- assign one bucket to each region
- stage 1: numbers are placed into appropriate buckets
- stage 2: each bucket is sorted using a traditional sorting algorithm
- works best if numbers are evenly distributed over the range a
- sequential time

$$t_s = n + m((n/m)\lg(n/m)) = n + n\lg(n/m) = O(n\lg(n/m))$$

Sequential Bucket Sort



Parallel Bucket Sort#1

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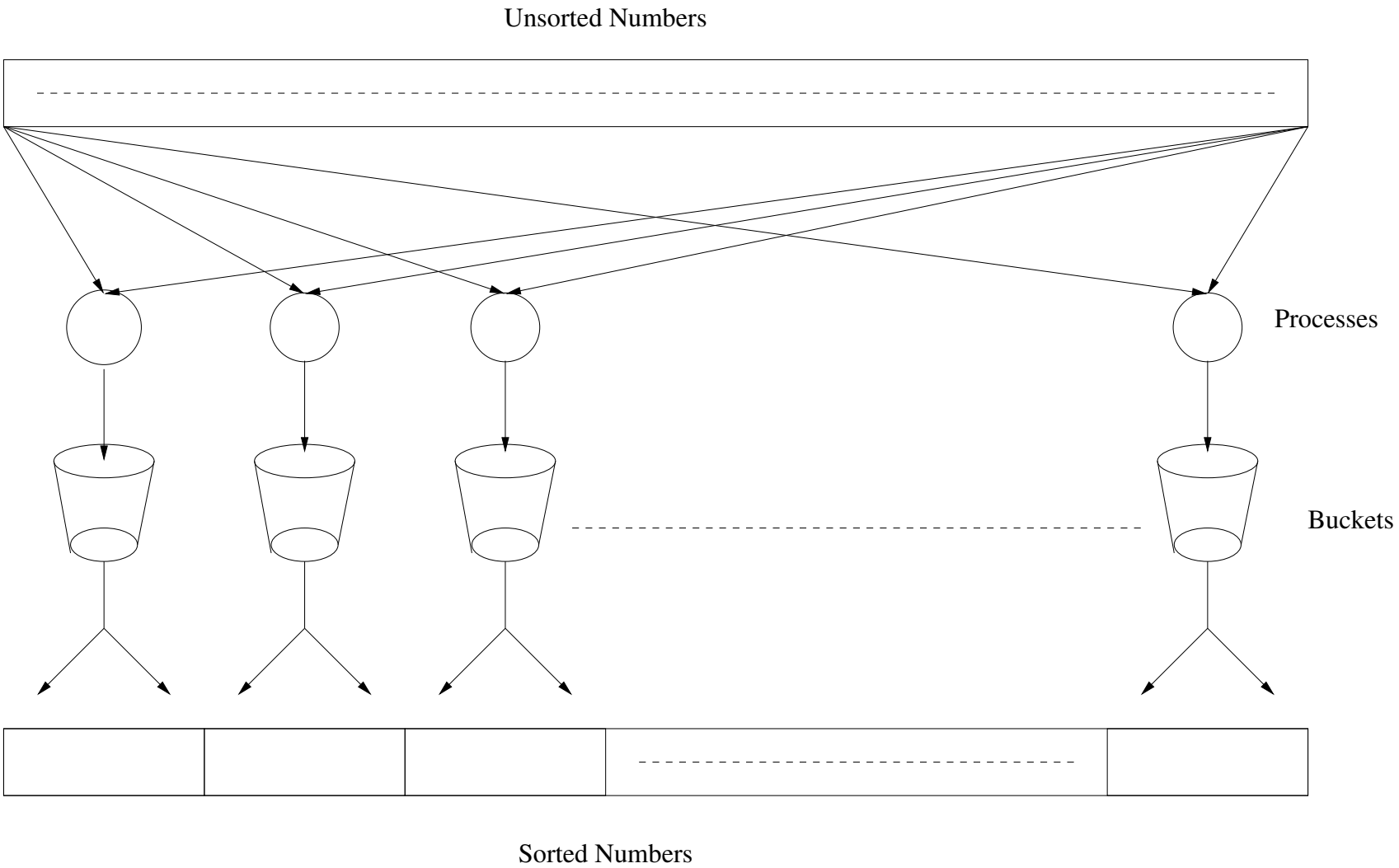
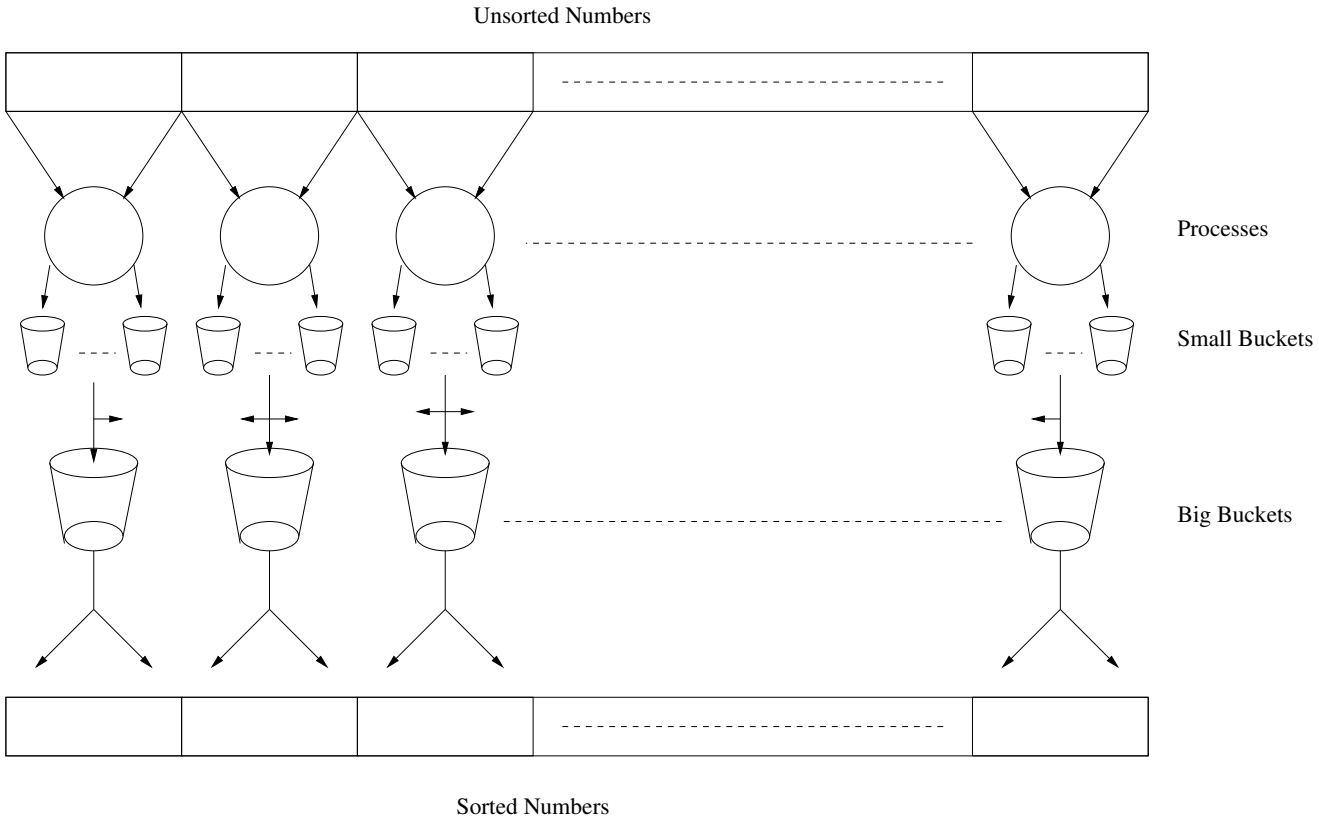
- assign one bucket to each process:



Parallel Bucket Sort#2



- assign p small buckets to each process
- note possible use of `MPI_Alltoall()`

```
MPI_Alltoall(void* sendbuf, int sendct, MPI_Datatype sendtype,
2             void* recvbuf, int recvct, MPI_Datatype recvtype,
              MPI_Comm comm)
```

Analysis

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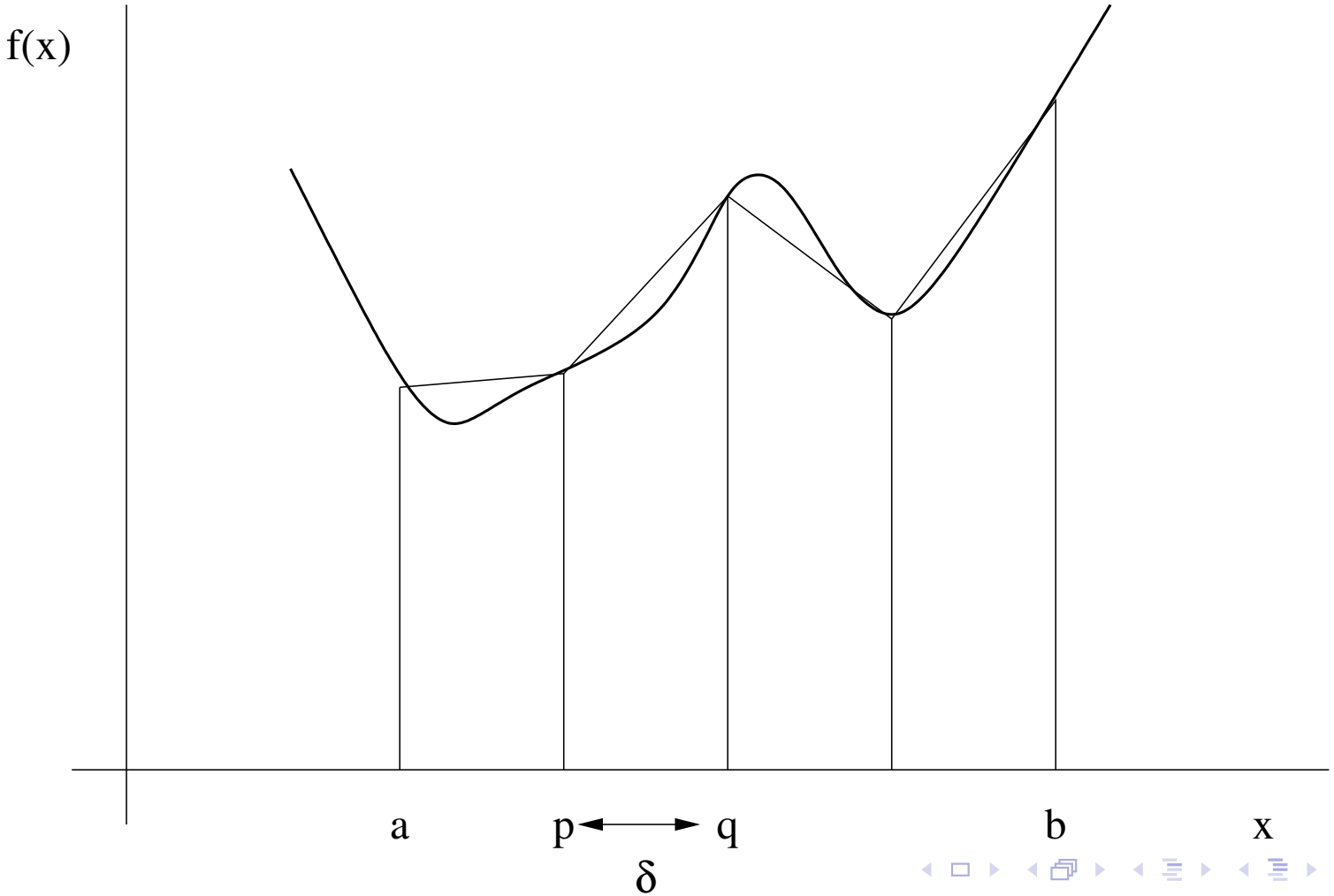
- initial partitioning and distribution
  $t_{\text{comm1}} = pt_s + t_w n$
- sort into small buckets
  $t_{\text{comp2}} = n/p$
- send to large buckets: (overlapping communications)
  $t_{\text{comm3}} = (p-1)(t_s + (n/p^2)t_w)$
- sort of large buckets
  $t_{\text{comp4}} = (n/p)\lg(n/p)$
- total
  $t_{\text{p}} = pt_s + nt_w + n/p + (p-1)(t_s + (n/p^2)t_w) + (n/p)\lg(n/p)$
- at best $O(n)$
- what would be the worse case scenario?

Example#3: Integration

- consider the evaluation of an integral using the trapezoidal rule
  $I = \int_a^b f(x)dx$



Static Distribution: SPMD Model

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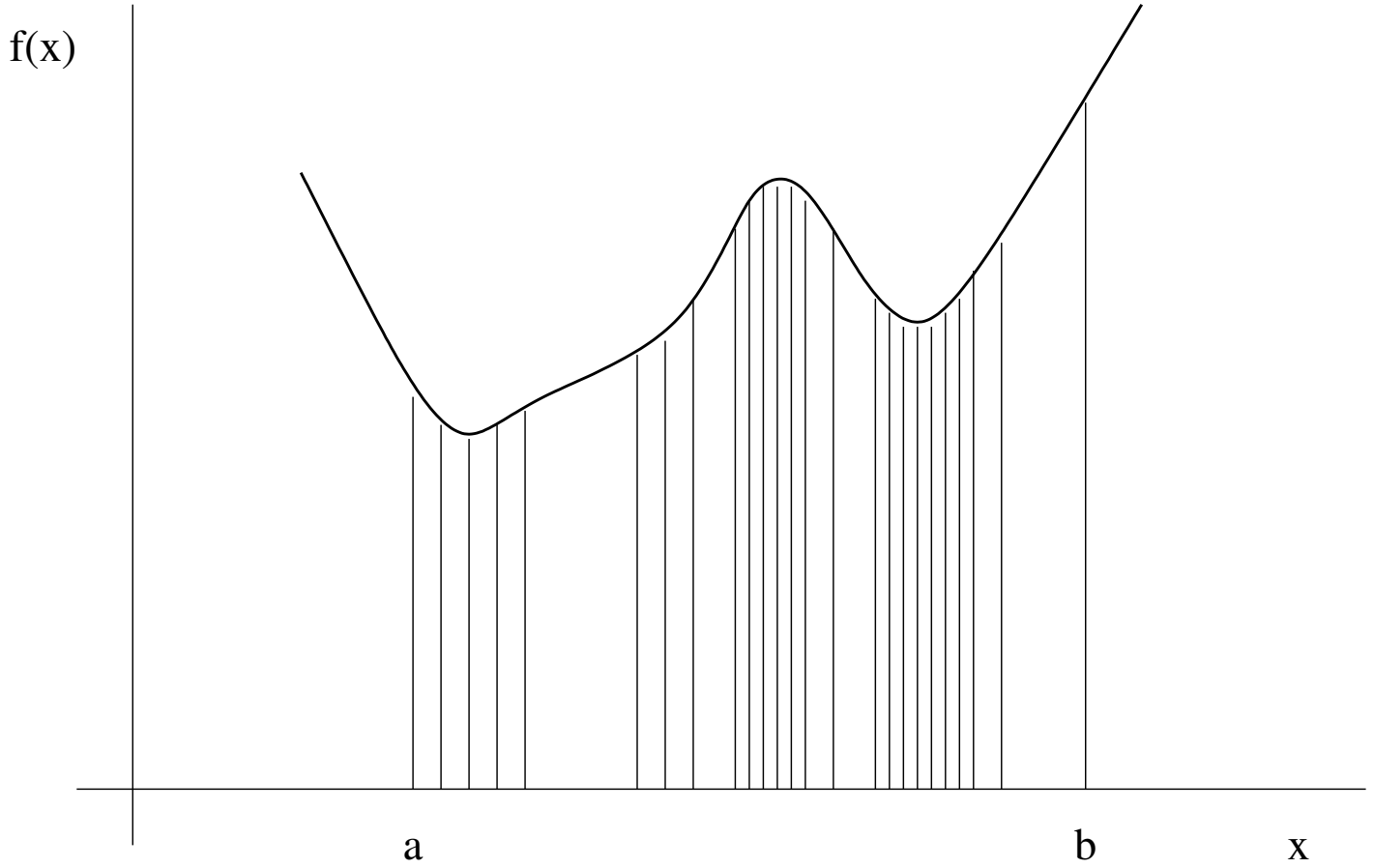
```
1  if (process_id == master) {
     printf("Enter number of regions\n");
3    scanf("%d", &n);
   }
5  broadcast(&n, master, p_group)
   region = (b-a)/p;
7  start = a + region*process_id;
   end = start + region;
9  d = (b-a)/n;
   area = 0.0;
11 for (x = start; x < end; x = x + d)
     area = area + 0.5 * (f(x) + f(x+d)) * d;
13 reduce_add(&area, master, p_group);
```

Adaptive Quadrature

- not all areas require the same number of points
- when to terminate division into smaller areas is an issue
- the parallel code will have uneven workload



Example#4: N-Body Problems

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- summing long-range pairwise interactions, e.g. gravitation
  $F = \frac{Gm_a m_b}{r^2}$
  where G is the gravitational constant, m_a and m_b are the mass of two bodies, and r is the distance between them
- in Cartesian space:

$$F_x = \frac{Gm_a m_b}{r^2}\left(\frac{x_b - x_a}{r}\right)$$
$$F_y = \frac{Gm_a m_b}{r^2}\left(\frac{y_b - y_a}{r}\right)$$
$$F_z = \frac{Gm_a m_b}{r^2}\left(\frac{z_b - z_a}{r}\right)$$

- what is the total force on the sun due to all other stars in the milky way?
- given the force on each star we can calculate their motions
- molecular dynamics is very similar but the long forces are electrostatic

Simple Sequential Force Code

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```
1  for (i = 0; i < n; i++)
     for (j = 0; j < n; j++) {
3      if (i != j) {
         rij2 = (x[i]-x[j])*(x[i]-x[j])
5             + (y[i]-y[j])*(y[i]-y[j])
              + (z[i]-z[j])*(z[i]-z[j]);
7        Fx[i] = Fx[i] + G*m[i]*m[j]/rij2 * (x[i]-x[j]) / sqrt(rij2);
         Fy[i] = Fy[i] + G*m[i]*m[j]/rij2 * (y[i]-y[j]) / sqrt(rij2);
9        Fz[i] = Fz[i] + G*m[i]*m[j]/rij2 * (z[i]-z[j]) / sqrt(rij2);
       }
11   }
```

- aside: how could you improve this sequential code?
- $O(n^2)$ - this will get very expensive for large n
- is there a better way?

Clustering

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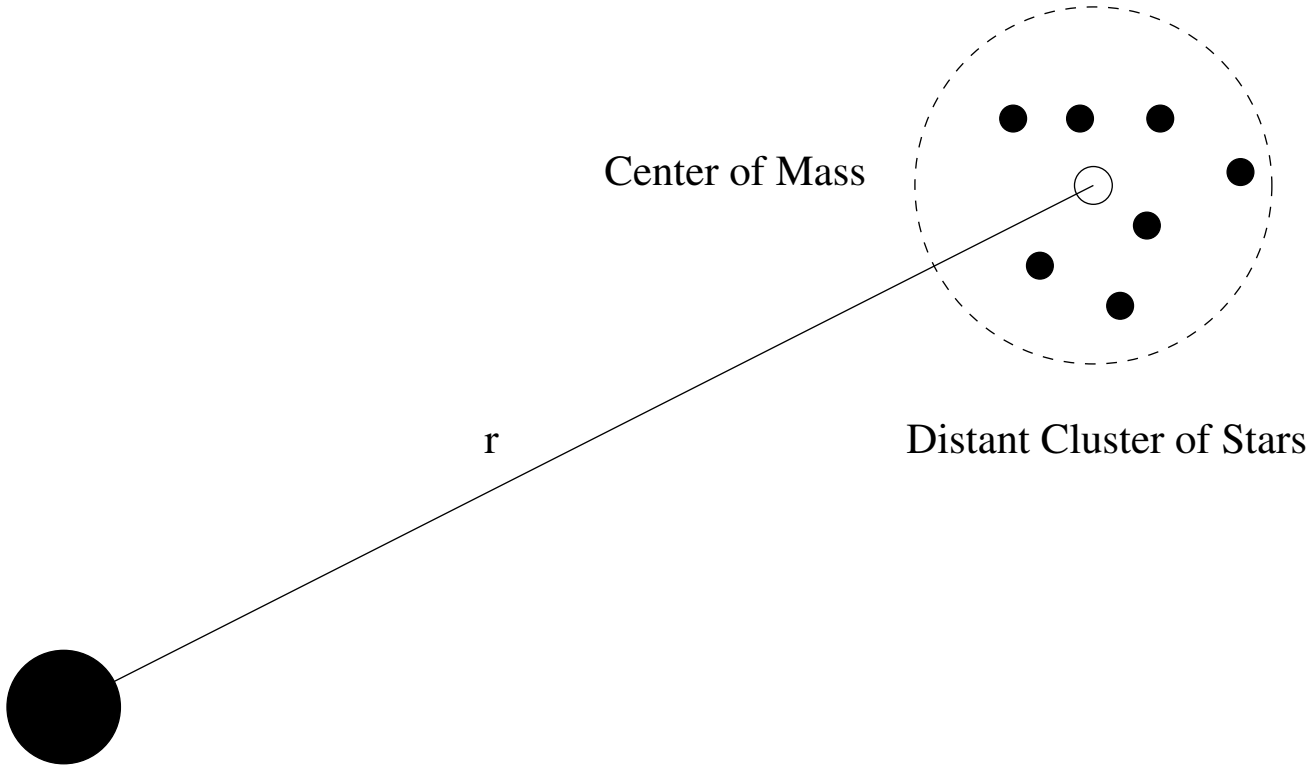
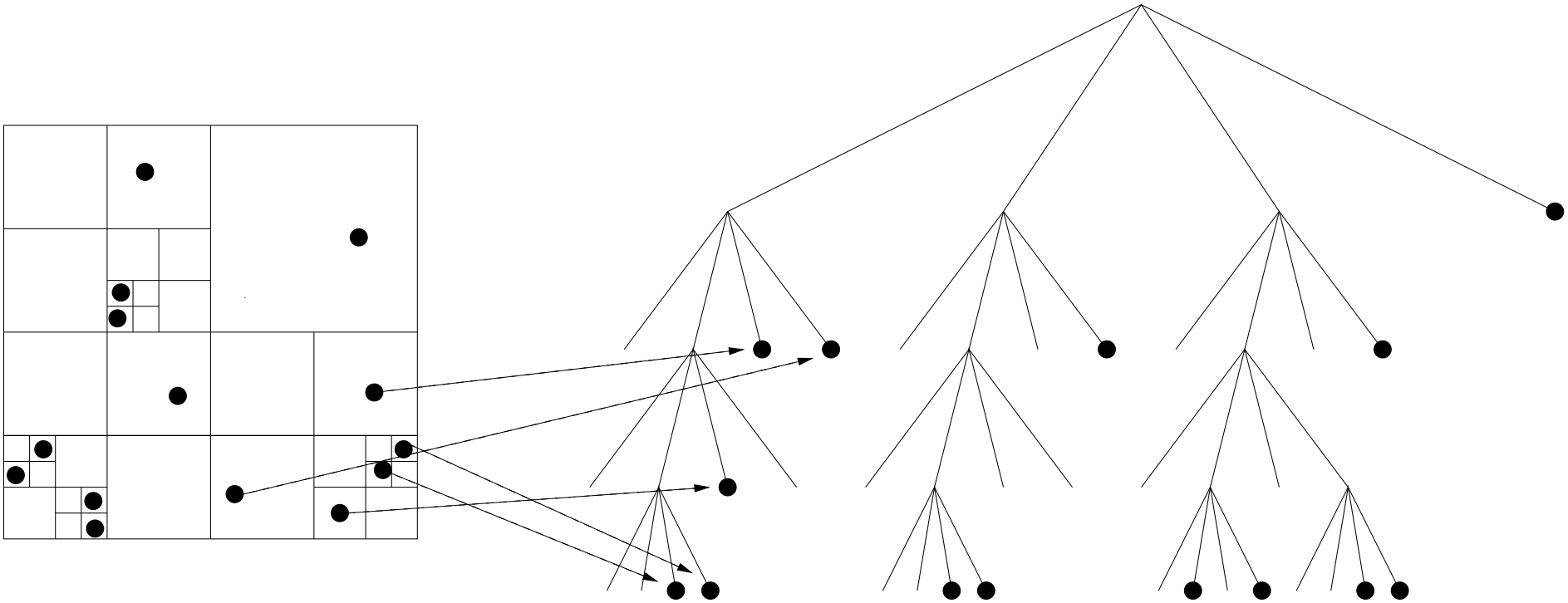
- idea: the interaction with several bodies that are clustered together but are located at large r for another body can be replaced by the interaction with the center of mass of the cluster



Barnes-Hut Algorithm

- start with whole space in one cube
  - divide the cube into 8 sub-cubes
  - delete sub-cubes if they have no particles in them
  - sub-cubes with more than 1 particle are divided into 8 again
  - continue until each cube has only one particle (or none)
- this process creates an **oct-tree**
- total mass and centre of mass of children sub-cubes is stored at each node
- force is evaluated by starting at the root and traversing the tree, BUT stopping at a node if the clustering algorithm can be used
- scaling is $O(n \log n)$
- load balancing likely to be an issue for parallel code

Barnes-Hut Algorithm: 2D Illustration



How to (evenly?) distribute such a structure? How often to re-distribute? (very hard problem!)

Hands-on Exercise: Bucket Sort

Outline

Overview: Synchronous Computations

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- degrees of synchronization
- synchronous example 1: Jacobi Iterations
  - serial and parallel code, performance analysis
- synchronous example 2: Heat Distribution
  - serial and parallel code
  - comparison of block and strip partitioning methods
  - safety
  - ghost points

Ref: Chapter 6: Wilkinson and Allen

Degrees of Synchronization

- from fully to loosely synchronous
  - the more synchronous your computation, the more potential overhead
- **SIMD**: synchronized at the instruction level
  - provides ease of programming (one program)
  - well suited for data decomposition
  - applicable to many numerical problems
  - the `forall` statement was introduced to specify **data parallel** operations

```
forall (i = 0; i < n; i++) {
  data parallel work
}
```

Synchronous Example: Jacobi Iterations

- the Jacobi iteration solves a system of linear equations iteratively

$$
\begin{aligned}
a_{n-1,0}x_0 + a_{n-1,1}x_1 + a_{n-1,2}x_2 + \cdots \quad & a_{n-1,n-1}x_{n-1} = b_{n-1} \\
\vdots & \\
a_{2,0}x_0 + a_{2,1}x_1 + a_{2,2}x_2 + \cdots \quad & a_{2,n-1}x_{n-1} = b_2 \\
a_{1,0}x_0 + a_{1,1}x_1 + a_{1,2}x_2 + \cdots \quad & a_{1,n-1}x_{n-1} = b_1 \\
a_{0,0}x_0 + a_{0,1}x_1 + a_{0,2}x_2 + \cdots \quad & a_{0,n-1}x_{n-1} = b_0
\end{aligned}
$$

where there are n equations and n unknowns $(x_0, x_1, x_2, \cdots x_{n-1})$

Jacobi Iterations

- consider equation i as:

$$a_{i,0}x_0 + a_{i,1}x_1 + a_{i,2}x_2 + \cdots a_{i,n-1}x_{n-1} \quad = \quad b_i$$

  which we can re-cast as: $x_i = (1/a_{i,i})[b_i - (a_{i,0}x_0 + a_{i,1}x_1 + a_{i,2}x_2 + \cdots a_{i,i-1}x_{i-1} + a_{i,i+1}x_{i+1} + \cdots a_{i,n-1}x_{n-1})]$

  i.e.

$$x_i = \frac{1}{a_{i,i}}\left[b_i - \sum_{j \neq i} a_{i,j}x_j\right]$$

- strategy: guess x, then iterate and hope it converges!
  - converges if the matrix is **diagonally dominant**: $\sum_{j \neq i} |a_{i,j}| < |a_{i,i}|$
- terminate when convergence is achieved:

$$|x^t - x^{t-1}| < \text{error tolerance}$$

Sequential Jacobi Code

- ignoring convergence testing:

```
1   for (i = 0; i < n; i++)
      x[i] = b[i];
3   for (iter = 0; iter < max_iter; iter++) {
      for (i = 0; i < n; i++) {
5       sum = -a[i][i]*x[i];
        for (j = 0; j < n; j++){
7           sum = sum + a[i][j]*x[j]
        }
9       new_x[i] = (b[i] - sum) / a[i][i];
      }
11    for (i = 0; i < n; i++)
        x[i] = new_x[i];
13  }
```

Parallel Jacobi Code

- ignoring convergence testing and assuming parallelisation over n processes:

```
1  x[i] = b[i];
   for (iter = 0; iter < max_iter; iter++) {
3    sum = -a[i][i] * x[i];
     for (j = 0; j < n; j++){
5        sum = sum + a[i][j]*x[j]
     }
7    new_x[i] = (b[i] - sum) / a[i][i];
     broadcast_gather(&new_x[i], new_x);
9    global_barrier();
     for (i = 0; i < n; i++)
11     x[i] = new_x[i];
   }
```

- `broadcast_gather()` sends the local `new_x[i]` to all processes and collects their new values

  Question: do we really need the barrier as well as this?

Partitioning

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- normally the number of processes is much less than the number of data items
  - **block partitioning**: allocate groups of consecutive unknowns to processes
  - **cyclic partitioning**: allocate in a round-robin fashion
- analysis: τ iterations, n/p unknowns per process
  - computation – decreases with p

$$t_{\text{comp}} = \tau(2n+4)(n/p)t_f$$

  - communication – increases with p

$$t_{\text{comm}} = p(t_s + (n/p)t_w)\tau = (pt_s + nt_w)\tau$$

  - total - has an overall minimum

$$t_{\text{tot}} = ((2n+4)(n/p)t_f + pt_s + nt_w)\tau$$

  - question: can we do an all-gather faster than $pt_s + nt_w$?

Parallel Jacobi Iteration Time

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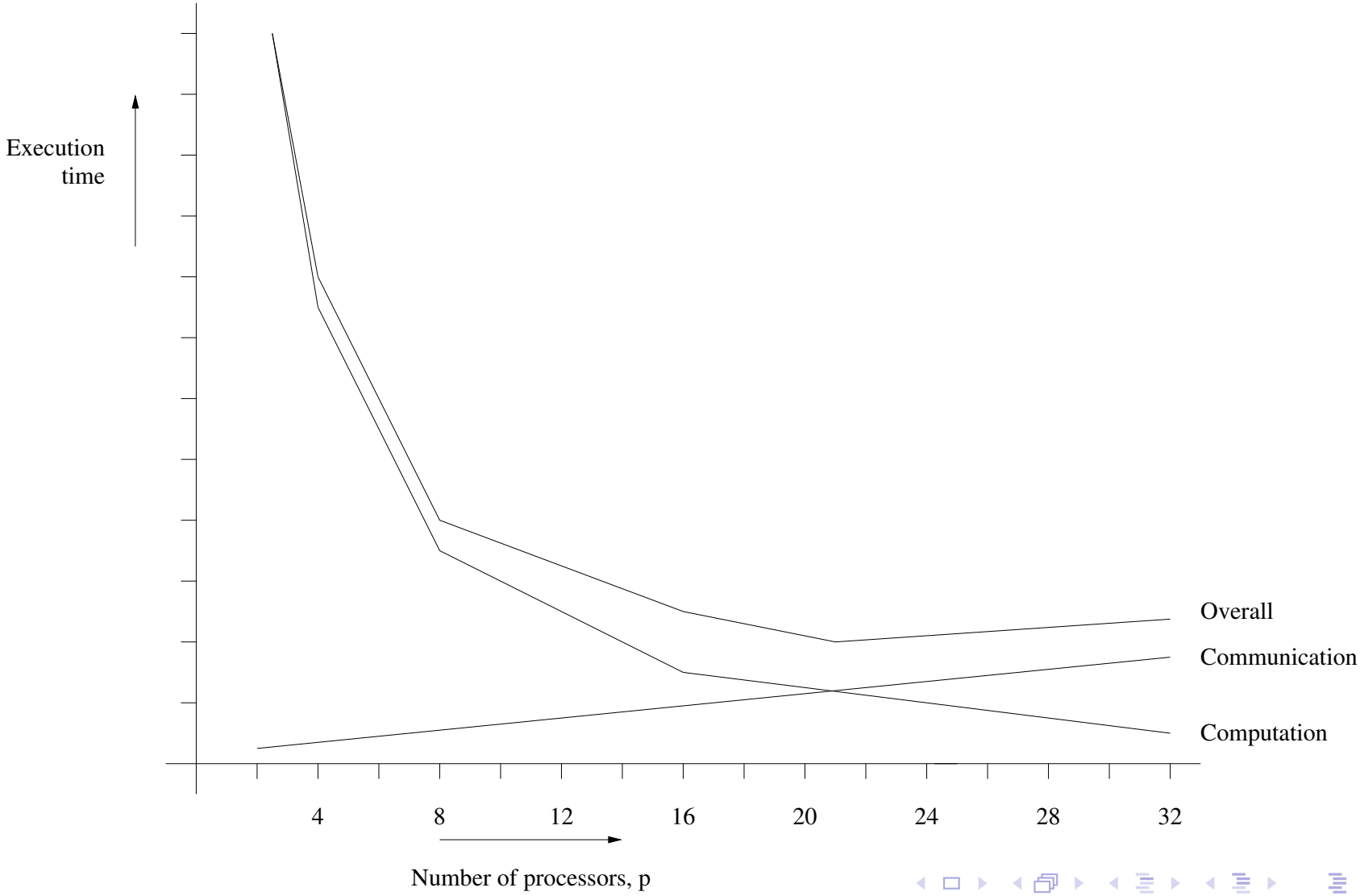
Parameters: $t_s = 10^5 t_f, t_w = 50 t_f, n = 1000$



Locally Synchronous Example: Heat Distribution Problem

Consider a metal sheet with a fixed temperature along the sides but unknown temperatures in the middle – find the temperature in the middle.

- finite difference approximation to the Laplace equation:

$$\frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} = 0$$

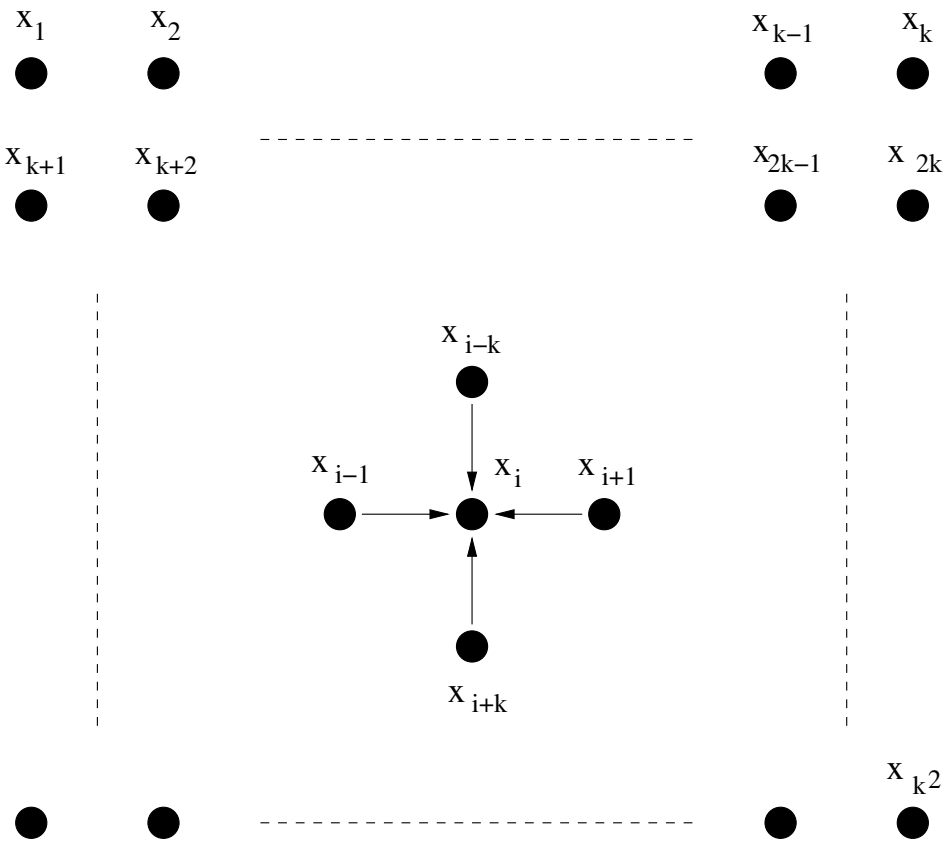
$$\frac{T(x+\delta x,y) - 2T(x,y) + T(x-\delta x,y)}{\delta x^2} + \frac{T(x,y+\delta y) - 2T(x,y) + T(x,y-}{\delta y^2}$$

- assuming an even grid (i.e. $\delta x = \delta y$) of $n \times n$ points (denoted as $h_{i,j}$), the temperature at any point is an average of surrounding points:

$$h_{i,j} = \frac{h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1}}{4}$$

- problem is very similar to the Game of Life, i.e. what happens in a cell depends upon its neighbours

Array Ordering



- we will solve iteratively: $x_i = \frac{x_{i-1}+x_{i+1}+x_{i-k}+x_{i+k}}{4}$
- but this problem may also be written as a system of linear equations:

$$x_{i-k} + x_{i-1} - 4x_i + x_{i+1} + x_{i+k} = 0$$

Heat Equation: Sequential Code

- assume a fixed number of iterations and a square mesh
- beware of what happens at the edges!

```
for (iter = 0; iter < max_iter; iter++) {
  for (i = 1; i < n; i++)
    for (j = 1; j < n; j++)
      g[i][j] = 0.25*(h[i-1][j] + h[i+1][j] +
                      h[i][j-1] + h[i][j+1]);
    for (i = 1; i < n; i++)
      for (j = 1; j < n; j++)
        h[i][j] = g[i][j];
}
```

Heat Equation: Parallel Code

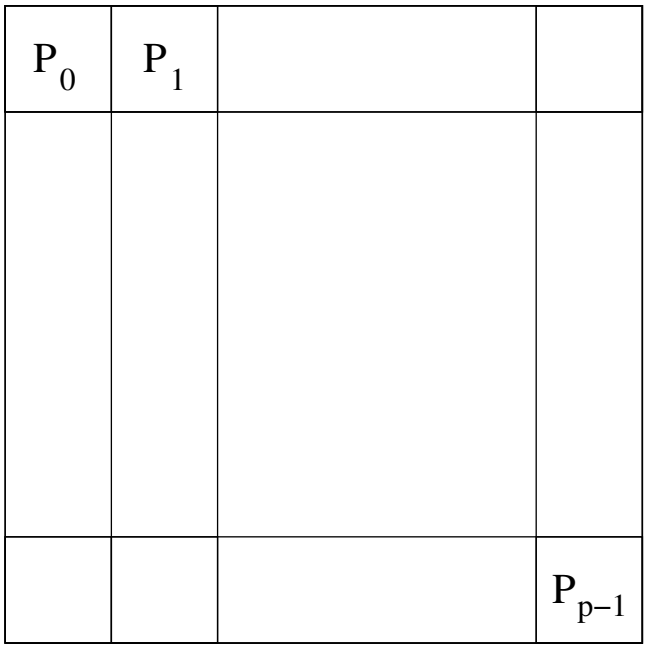
- one point per process
- assuming **locally-blocking sends**:

```
1  for (iter = 0; iter < max_iter; iter++) {
     g = 0.25*(w + x + y + z);
3    send(&g, P(i-1,j));
     send(&g, P(i+1,j));
5    send(&g, P(i,j-1));
     send(&g, P(i,j+1));
7    recv(&w, P(i-1,j));
     recv(&x, P(i+1,j));
9    recv(&y, P(i,j-1));
     recv(&z, P(i,j+1));
11 }
```

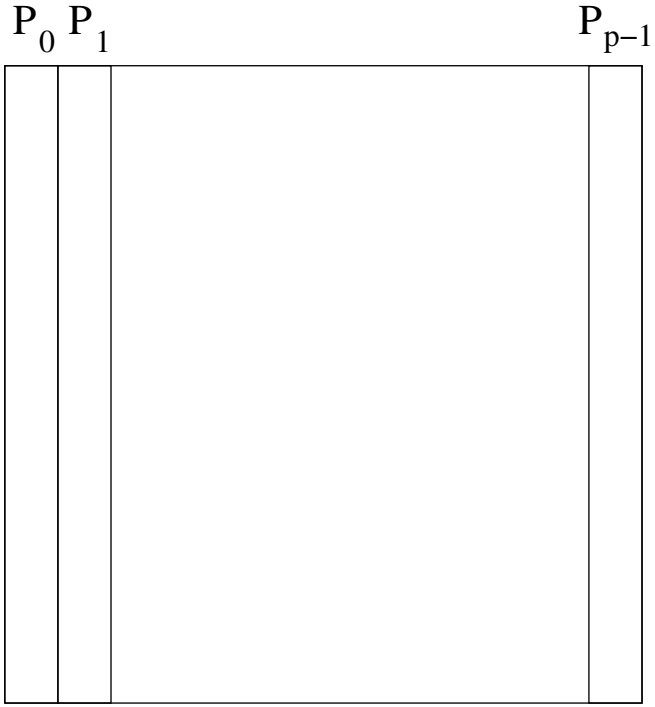
- sends and receives provide a local barrier
  - each process synchronizes with 4 others surrounding processes

Heat Equation: Partitioning

- normally more than one point per process
- option of either **block** or **strip partitioning**



Block Partitioning



Strip Partitioning

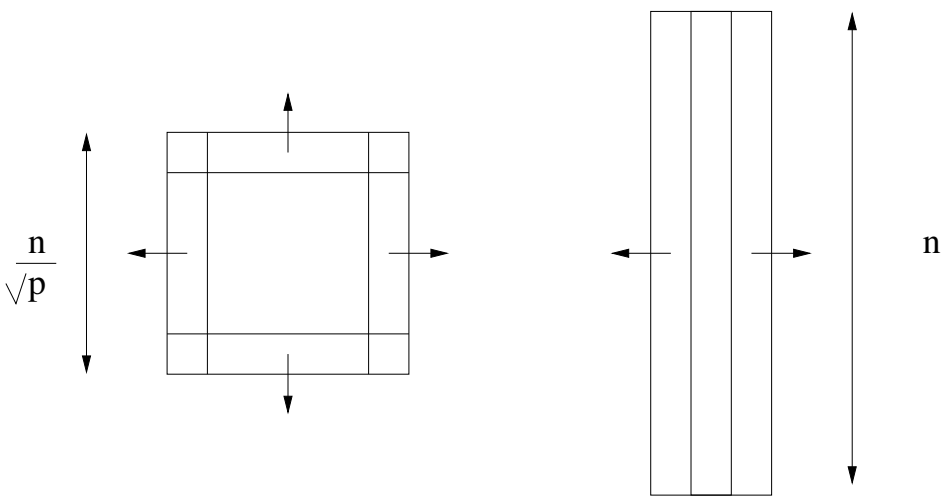
Block/Strip Communication Comparison

- **block partitioning**: four edges exchanged (n^2 data points, p processes)

$$t_{\text{comm}} = 8(t_s + \frac{n}{\sqrt{p}} t_w)$$

- **strip partitioning**: two edges exchanged

$$t_{\text{comm}} = 4(t_s + nt_w)$$



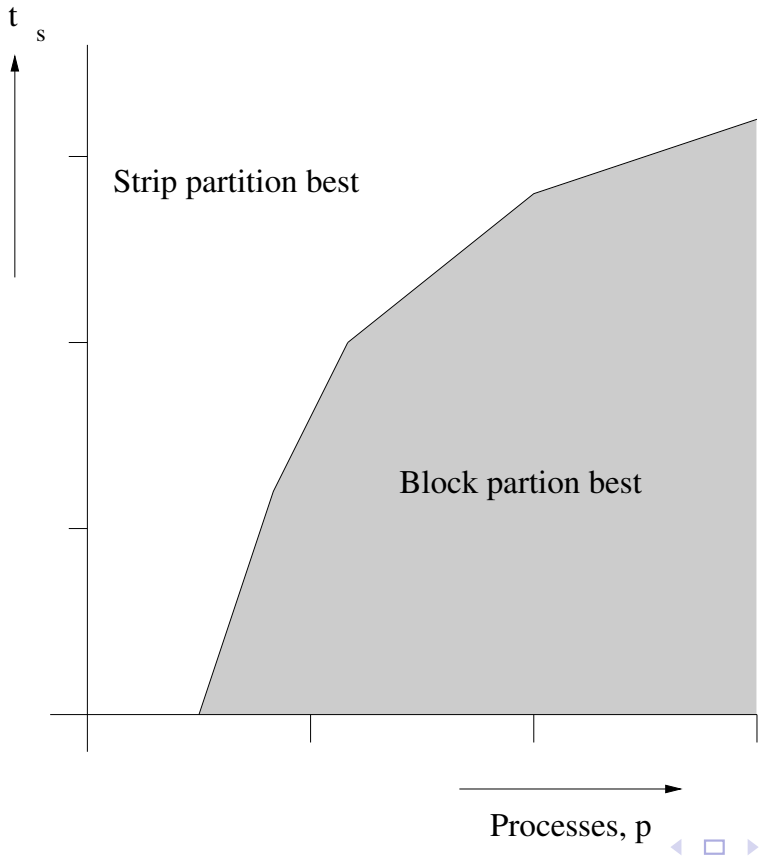
Block Communications Strip Communications

Block/Strip Optimum

- **block** communication is larger than **strip** if:

  $8\left(t_s + \frac{n}{\sqrt{p}}t_w\right) > 4(t_w + nt_w)$

  i.e. if $t_s > n\left(1 - \frac{2}{\sqrt{p}}\right)t_w$



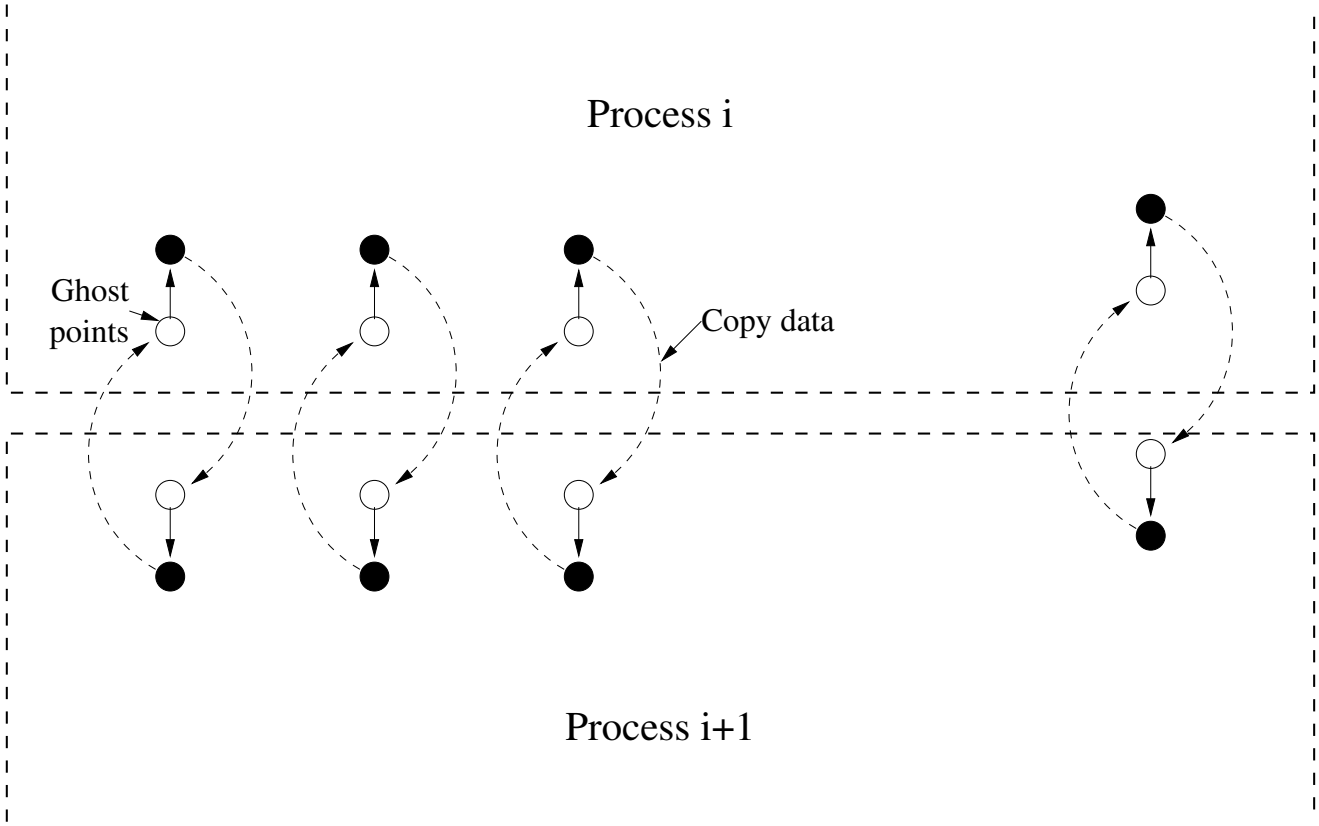
Safety and Deadlock

- with all processes sending and then receiving data, the code is unsafe: it relies on **local buffering** in the `send()` function
  - potential for deadlock (as in Prac 1, Ex 3)!
- alternative #1: re-order sends and receives
  e.g. for **strip partitioning**:

```
if ((myid % 2) == 0){
  send(&g[1][1], n, P(i-1));
  recv(&h[1][0], n, P(i-1));
  send(&g[1][n], n, P(i+1));
  recv(&h[1][n+1], n, P(i+1));
} else {
  recv(&h[1][0], n, p(i-1));
  send(&g[1][1], n, p(i-1));
  recv(&h[1][n+1], n, p(i+1));
  send(&g[1][n], n, p(i+1));
}
```

Alt# 2: Asynchronous Comm. using Ghostpoints

- assign extra receive buffers for edges where data is exchanged
  - typically these are implemented as extra rows and columns in each process' local array (known as a **halo**)
- can use asynchronous calls (e.g. `MPI_Isend()`)



Hands-on Exercise: Synchronous Computations

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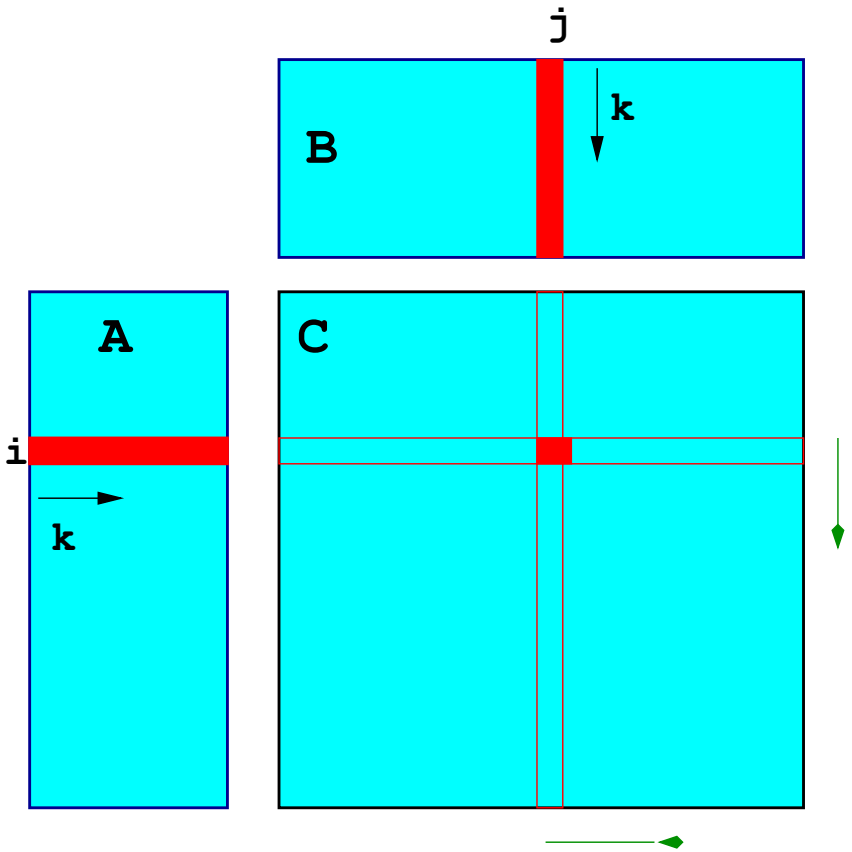
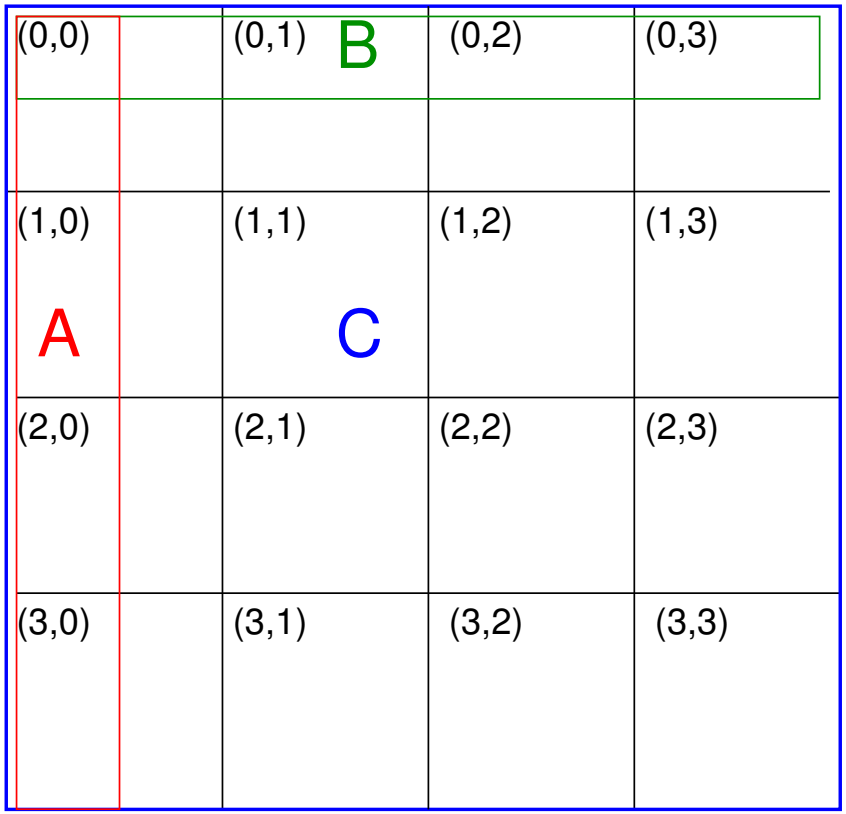
Outline

Matrix Multiplication



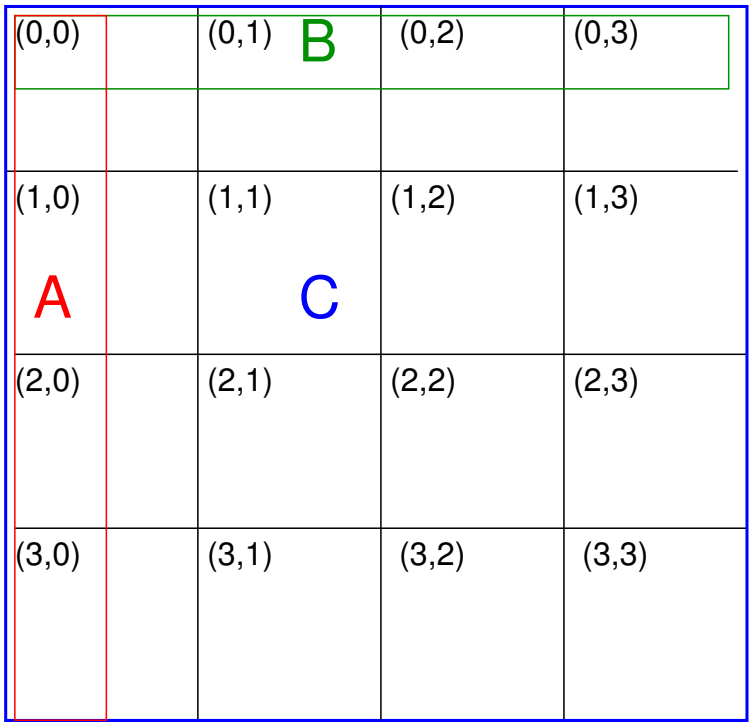
- matrix multiplication is the dominant computation in linear algebra and neural net training
  - tensor operations are broken down to matrix operations on TPUs and GPUs!
- C += AB, where A, B, C are $M \times K, K \times N, M \times N$ matrices, respectively
- $c_{i,j}$ += $\sum_{k=0}^{K-1} a_{i,k} b_{k,j}$, for $0 \leq i < M, 0 \leq j < N$
- we will primarily consider the case $M = N, K < N$

Matrix Process Topologies and Distributions



- use a logical two-dimensional $p = p_y \times p_x$ process grid
  - e.g. a process with ID rank r has a 2D rank (r_y, r_x), where $r = r_y p_x + r_x$, $0 \leq r_x < p_x, 0 \leq r_y < p_y$
  - for performance, $\frac{p_y}{p_x} \approx \frac{M}{N}$ is generally optimal (best local multiply speed, lowest communication volume)
- here, a **block distribution** over the whole 4×4 process grid is used for C
- notice that A (B) must be aligned to be on the same process rows (columns) as C

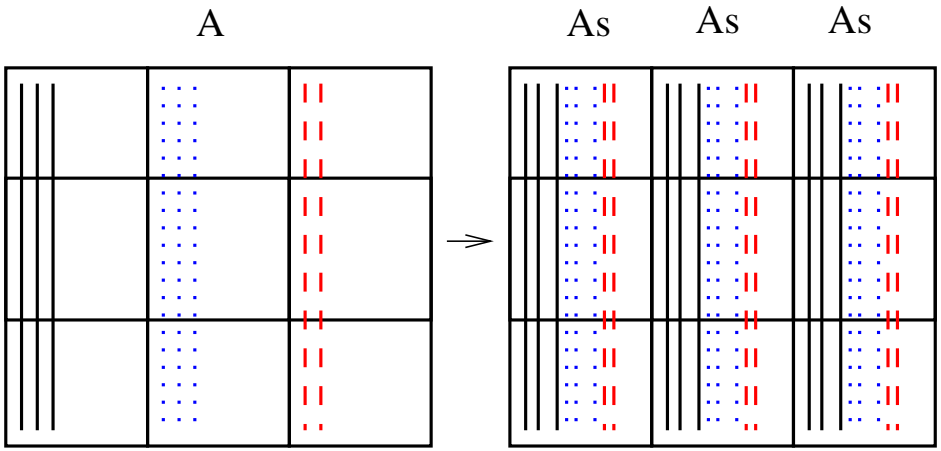
Rank-K Matrix Multiply: Simple Case



- consider the simplest case where K is small enough and $A(B)$ are distributed block-wise over a single process column (row)
- assume local matrix sizes are $m = \frac{M}{p_y}, n = \frac{N}{p_x}$
- denoting `A`, `B`, `C` as local portions of the matrices, the parallel multiply can be done by:
  1. row-broadcast from col $r_x = 0$ of `A` (size $m \times K$ result in `As`)
  2. column-broadcast for row $r_y = 0$ of `B` (size $K \times n$, result in `Bs`)
  3. perform local matrix multiply of `As`, `Bs` and `C`

Rank-K Matrix Multiply: General Case

All processes may have some columns of the distributed matrix A



- e.g. matrix A with $K = 8$, distributed across a 3×3 process grid
- each process column must broadcast its portion, storing result in `As` (a 'spread' of the K-dim. of A)

Algorithm now becomes:

1. row-wise all-gather of `A` (result in `As`, size $m \times K$)
2. column-wise all-gather of `B` (result in `Bs`, size $K \times n$)
3. perform local matrix multiply of `As`, `Bs` and `C`

If $K \not| p_x, p_y$, we can 'pad out' matrices (or use `MPI_Allgatherv()`).
If K is large, we can reduce the size of `As` and `Bs`, by breaking this down into stages.

2D Process Topology Support in MPI

This involves creating a periodic 2D cartesian topology, followed by row and column communicators:

```
int np, rank, px, py;
MPI_Comm comm2D, commRow, commCol; int dims[2], rank2D, r2D[2];
int periods[] = {1,1}, rowSpec[] = {1,0}, colSpec[] = {0,1};
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_rank(MPI_COMM_WORLD, &np);
px = ...; py = np / px; assert (px * py == np);
dims[0] = px, dims[1] = py;
MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, 0, &comm2D);
MPI_Comm_rank(comm2D, &rank2D); //likely that rank2d==rank
MPI_Cart_coords(comm2D, rank2D, 2, r2D);
// create this process' 1D row / column communicators
MPI_Cart_sub(comm2D, rowSpec, &commRow); //of size px
MPI_Cart_sub(comm2D, colSpec, &commCol); //of size py
MPI_Comm_rank(commRow, &rx); MPI_Comm_rank(commCol, &ry);
assert (rx == r2D[0]  &&  ry == r2D[1]);
```

MPI Rank-K Update Algorithm

- an $m \times n$ local matrix C can be represented as the pair (`C`, `ldC`), where `double *C` points to the 0th element, the leading dimension `int ldC` $\geq m$ and $c_{i,j}$ is stored `C[i + j*ldC]`
- defining a datatype for A will avoid an explicit pack operation:

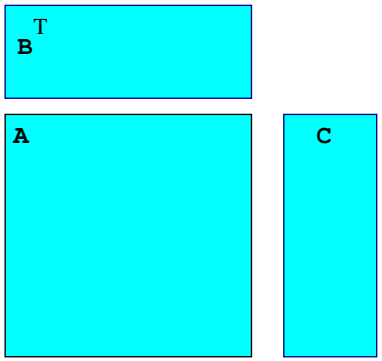
```
MPI_Datatype aCol;
MPI_Type_vector(1, m, ldA, MPI_DOUBLE, &aCol);
MPI_Type_commit(&aCol);
```

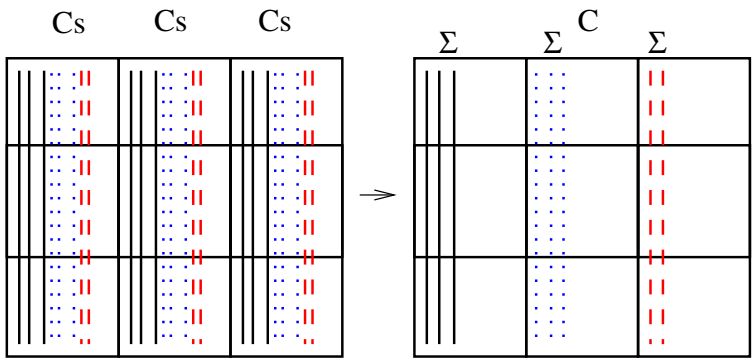
- in order to use `Bs` directly for a local matrix multiply (`dgemm()`) we must transpose and pack B:

```
double Bt[n*kB], As[m*K], Bs[n*K]; int i, j;
for (i=0; i < kB; i++)
  for (j=0; j < n; j++)
    Bt[j + i*n] = B[i + j*ldB];
MPI_Allgather(A, kA, aCol, As, m*kA, MPI_DOUBLE, commRow);
MPI_Allgather(Bt, n*kB, MPI_DOUBLE, Bs, n*kB, MPI_DOUBLE,
    commCol);
dgemm_("NoTrans", "Trans", m, n, K, As, m, Bs, n, C, ldC);
```

(non-unit stride on the K-dim. is generally non-optimal for the multiply)

Matrix Multiplication: AB^T Case





- consider C += AB^T, where $N < K = M$
- this variant of the algorithm is:
  1. column-wise all-gather of `B` (result in `Bs`, size $N \times kB$)
  2. create a workspace `Cs` of size $m \times N$
  3. perform local matrix multiply of `A`, `Bs` and `Cs`
  4. row-wise reduce-scatter of `Cs` (add result to `C`, size $m \times nC$)

- there is an analogous variant for C += $A^T B$, efficient for $M < K = N$
- general matrix multiply algorithm: choose variant involving least data movement, performing a global transposition if needed

Parallel Blocked-Partitioned Matrix Algorithms

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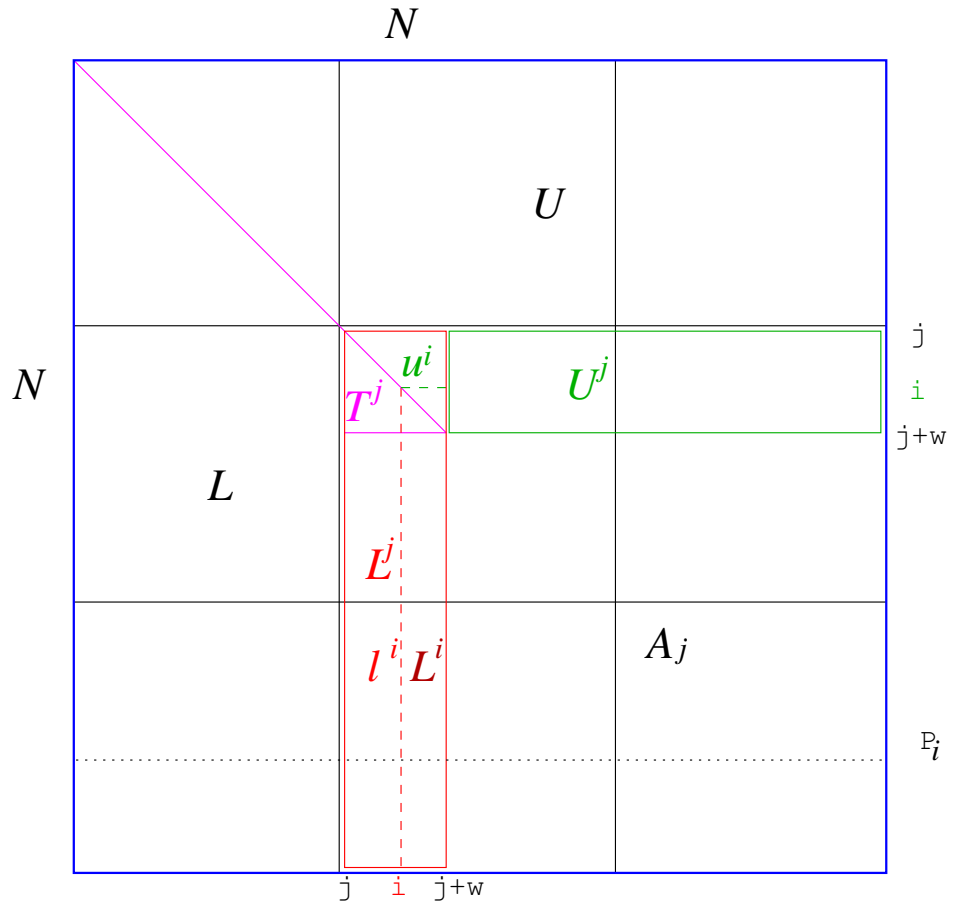
- blocked LU factorization (LINPACK) rated in the Top 10 Algorithms of the 20th Century (CS&E, Jan 2000)
  - symmetric eigenvalue algorithm arguably even more important
  - idea: express vector operations of original algorithm into blocks
    - majority of operations are now matrix-matrix
    - transforms algorithm from data-access to computation bound
  - normal block distribution inadequate for || algorithms!

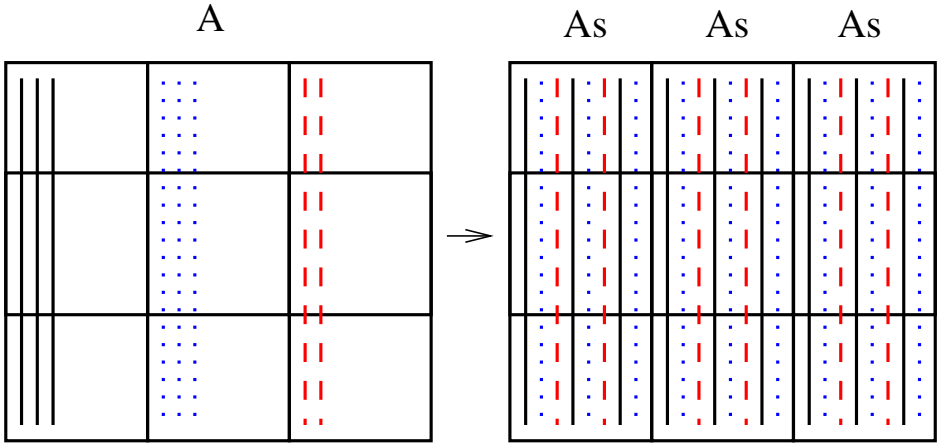


Matrix Distributions: Block-Cyclic

- is 'standard' for || LA (load balance on triangular & sub- matrices)
- divide the global matrix A into $b_y \times b_x$ blocks on a $P \times Q$ array; if block $(0,0)$ is on process (r_y, r_x), block (i,j) is on process $((i + r_y)\%p_y, (j + r_x)\%p_x)$
- e.g. $r_y = r_x = 0, b_y = 3, b_x = 2$ on a 2×3 array, a 10×10 matrix A:

a_{00}	a_{01}	a_{06}	a_{07}	a_{02}	a_{03}	a_{08}	a_{09}	a_{04}	a_{05}
a_{10}	a_{11}	a_{16}	a_{17}	a_{12}	a_{13}	a_{18}	a_{19}	a_{14}	a_{15}
a_{20}	a_{21}	a_{26}	a_{27}	a_{22}	a_{23}	a_{28}	a_{29}	a_{24}	a_{25}
a_{60}	a_{61}	a_{66}	a_{67}	a_{62}	a_{63}	a_{68}	a_{69}	a_{64}	a_{65}
a_{70}	a_{71}	a_{76}	a_{77}	a_{72}	a_{73}	a_{78}	a_{79}	a_{74}	a_{75}
a_{80}	a_{81}	a_{86}	a_{87}	a_{82}	a_{83}	a_{88}	a_{89}	a_{84}	a_{85}
a_{30}	a_{31}	a_{36}	a_{37}	a_{32}	a_{33}	a_{38}	a_{39}	a_{34}	a_{35}
a_{40}	a_{41}	a_{46}	a_{47}	a_{42}	a_{43}	a_{48}	a_{49}	a_{44}	a_{45}
a_{50}	a_{51}	a_{56}	a_{57}	a_{52}	a_{53}	a_{58}	a_{59}	a_{54}	a_{55}
a_{90}	a_{91}	a_{96}	a_{97}	a_{92}	a_{93}	a_{98}	a_{99}	a_{94}	a_{95}

Matrix Multiply on the Block-Cyclic Distribution



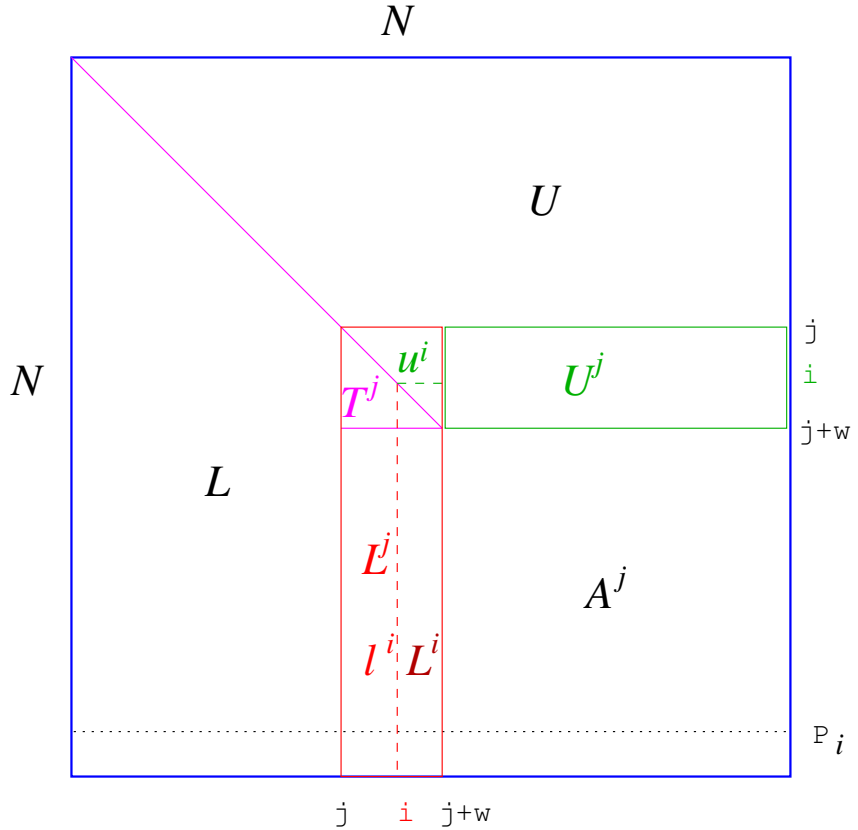
- e.g. matrix A with $K = 8$, distributed across a 3×3 process grid
- each process column must broadcast its portion, storing result in `As` (a 'spread' of the K-dim. of A)

The 'spread' of the K-dim. of A should respect the global order of indices

- `MPI_Allgather()` will not give this order
- unless $p_x = p_y$ and $b_x = b_y$, must re-order columns in `As`, `Bs` before calling `dgemm()`

Blocked LU Factorization Algorithm

- **right-looking** variant using **partial pivoting** on an $N \times N$ matrix A




```
for (j=0; j < N; j+=w)
  for (i=j; i < j+w; i++)
    find P[i] s.t. |A_{P[i], i}| ≥ |A_{i:N-1, i}|
    A_{i, j:j'-1} ↔ A_{P[i], j:j'-1}   (j' = j+w)
    l^i ← l^i / A_{i,i}
    L^i ← L^i − l^i u^i
  for (i = j; i < j+w; i++)
    A_{i,:} ↔ A_{P[i],:}  (outside L^j)
  U^j ← (T^j)^{-1} U^j
  A^j ← A^j − L^j U^j
```

- $l^i = A_{i+1:N-1,\, i}$; $u^i = A_{i,\, i+1:j'-1}$; $L^i = A_{i+1:N-1,\, i+1:j'-1}$
- $(T^j) = A_{j:j'-1,\, j:j'-1}$ (lower triangular matrix, with unit diagonal)
- $L^j = A_{j':N-1,\, j:j'-1}$; $U^j = A_{j:j'-1,\, j':N-1}$; $A^j = A_{j':N-1,\, j':N-1}$

Blocked LU Factorization: Communication

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- let r_x^i (r_y^i) denote the process row (column) rank holding $A_{i,i}$
- assume $w = b_x = b_y$ (one process row (column) holds U^j (L^j) panel)

```
for (j=0; j < N; j+=w)
```

  for (i=j; i < j+w; i++) (note $r_x^i = r_x^j, r_y^i = r_y^j$)

    find $P[i]$ s.t. $|A_{P[i],\,i}| \geq |A_{i:N-1,\,i}|$ (all-reduce on col. r_x^i)

    $A_{i,\,j:j'-1} \leftrightarrow A_{P[i],\,j:j'-1}$ (swap on processes (r_y^i, r_x^i) and $(r_y^{P[i]}, r_x^i)$)

    $l^i \leftarrow l^i / A_{i,i}$ (broadcast $A_{i,i}$ on col. r_x^i from row r_y^i)

    $L^i \leftarrow L^i - l^i u^i$ (broadcast l^i on col. r_x^i from row r_y^i)

  for (i = j; i < j+w; i++)

    $A_{i,:} \leftrightarrow A_{P[i],:}$ (swap on processes (r_y^i, r_x^i) and $(r_y^{P[i]}, r_x^i)$)

  $U^j \leftarrow (T^j)^{-1} U^j$ (broadcast T^j on col. r_x^j from row r_y^j)

  $A^j \leftarrow A^j - L^j U^j$ (row (col.) broadcast L^j (U^j) from col. r_x^j (row r_y^j))

- exercise: implement this using MPI and BLAS!
  - need to calculate local lengths for vector of length say $N - j$ from say process row r_y^j

Parallel Factorization Analysis and Methods

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- performance is determined by **load balance** and **communication overhead** issues
- for an $N \times N$ matrix on a $p_x \times p_x$ process grid, || execution time is:
  $t(N) = c_1 N t_s + c_2 N^2/p_x t_w + c_3 N^3/p_x^2 t_f$
  As $c_1 = O(\lg_2 p_x) > c_2 > c_3$ and typically $\frac{t_s}{f_f} \approx 10^3$,
  the t_s term can be significant for small-moderate N/p_x.
  Note: t_s mainly due to software: several layers of function calls, error checking, message header formation, buffer allocation & search
- **storage blocking**: $(\omega = b_x = b_y)$
  - simplest to implement, minimizes number of messages
  - suffers from $O(b_x + b_y)$ load imbalance on panel formation:
    i.e. one processor column (row) holds L^i (U^i); also in $A^i \leftarrow A^i - L^i U^i$
- **algorithmic blocking**: can use `dgemm`-optimal ω, $b_x = b_y \approx 1$
  - greatly reduces these imbalances, ||izes row swaps
  - introduces $4N$ extra messages; local panel width is small ($\approx \omega/p_x$)
- **lookahead** (High Performance Linpack)
  - eliminates load imbalance in forming L^i by computing it in advance
  - hard to implement; only applicable to some computations

Summary

Topics covered today involve the message passing paradigm:

- issues in parallelizing 'embarrassingly parallel' problems
- parallelizing by domain decomposition
- synchronous computations (mainly using domain decomposition)
- case study: parallel matrix multiply and factorization

Tomorrow - the Partitioned Global Address Space paradigm

Hands-on Exercise: Matrix Multiply