

并行与分布式计算 Parallel & Distributed Computing

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Lecture 9 — Programming with MPI

- Matrix-Vector Multiplication and MPI + OpenMP

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Outline:

- > Example: matrix-vector multiplication
 - **□** Sequential algorithm;
 - **□** Design, analysis, and implementation of three parallel programs;
 - Rowwise block striped
 - Columnwise block striped
 - Checkerboard block
- > MPI + OpenMP

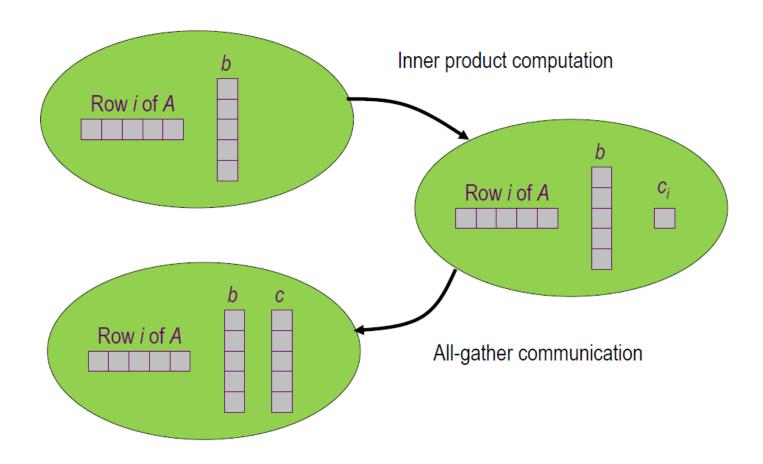
Sequential Algorithm

2	1	0	4	×	1	=	9
3	2	1	1		3		14
4	3	1	2		4		19
3	0	2	0		1		11

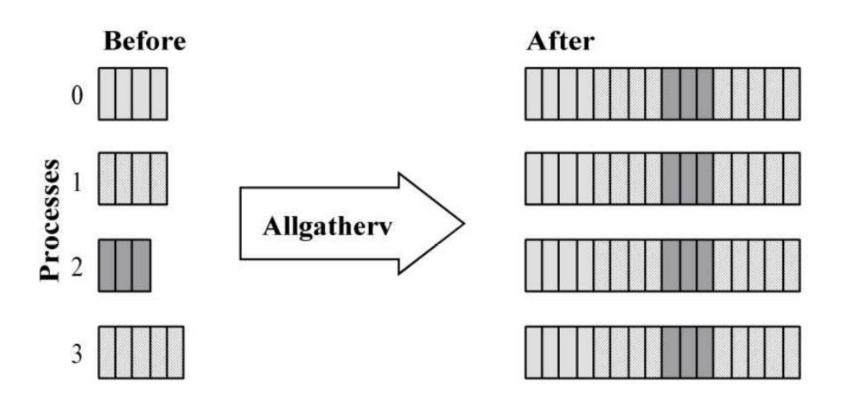


- > Partitioning through domain decomposition
- > Primitive task associated with
 - **□** Row of matrix
 - **■** Entire vector

Phases of Parallel Algorithm



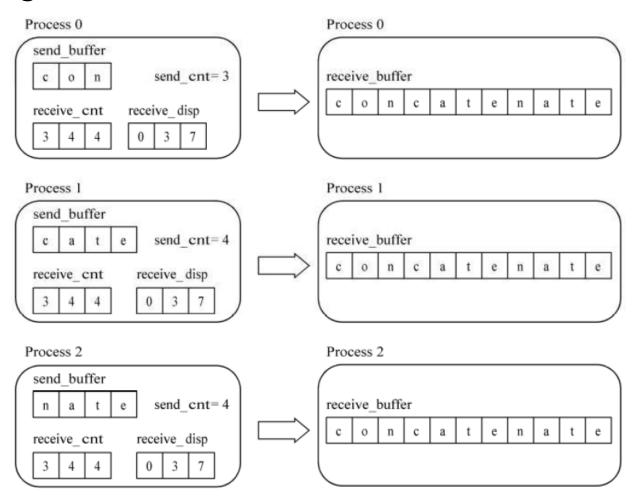
MPI_Allgatherv



MPI_Allgatherv

```
int MPI Allgatherv (
void *send buffer,
int send cnt,
MPI Datatype send type,
void *receive buffer,
int *receive cnt,
int *receive disp,
MPI Datatype receive type,
MPI Comm communicator)
Use a simpler function MPI Allgather (...)
when the number of elements per processor
is a constant
```

MPI_Allgatherv in Action



Agglomeration and Mapping

- > Static number of tasks
- > Regular communication pattern (all-gather)
- > Computation time per task is constant
- > Strategy:
 - **□** Agglomerate groups of rows
 - ☐ Create one task per MPI process

Columnwise Block Striped Matrix

- > Partitioning through domain decomposition
- > Task associated with
 - □ Column of matrix
 - **□** Vector element

Matrix-Vector Multiplication

$$c_{0} = a_{0,0} b_{0} + a_{0,1} b_{1} + a_{0,2} b_{2} + a_{0,3} b_{3} + a_{4,4} b_{4}$$

$$c_{1} = a_{1,0} b_{0} + a_{1,1} b_{1} + a_{1,2} b_{2} + a_{1,3} b_{3} + a_{1,4} b_{4}$$

$$c_{2} = a_{2,0} b_{0} + a_{2,1} b_{1} + a_{2,2} b_{2} + a_{2,3} b_{3} + a_{2,4} b_{4}$$

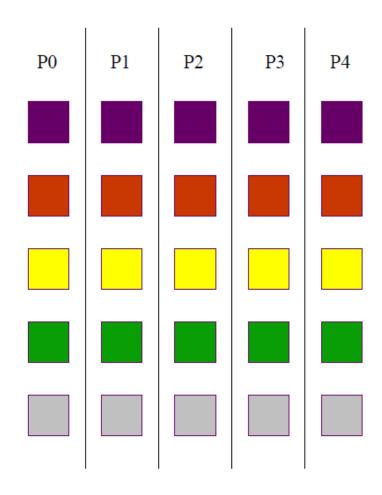
$$c_{3} = a_{3,0} b_{0} + a_{3,1} b_{1} + a_{3,2} b_{2} + a_{3,3} b_{3} + b_{3,4} b_{4}$$

$$c_{4} = a_{4,0} b_{0} + a_{4,1} b_{1} + a_{4,2} b_{2} + a_{4,3} b_{3} + a_{4,4} b_{4}$$
Proc 4

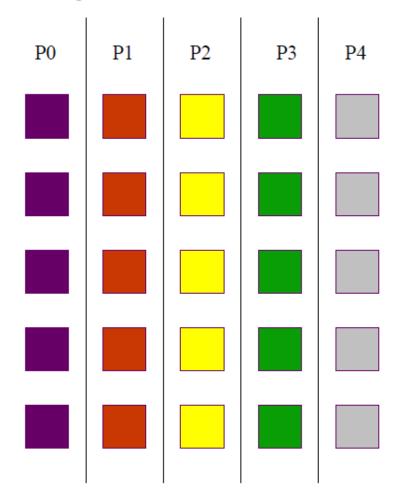
Processor 1's initial computation

Processor 0's initial computation

All-to-all Exchange (Before)



All-to-all Exchange (After)



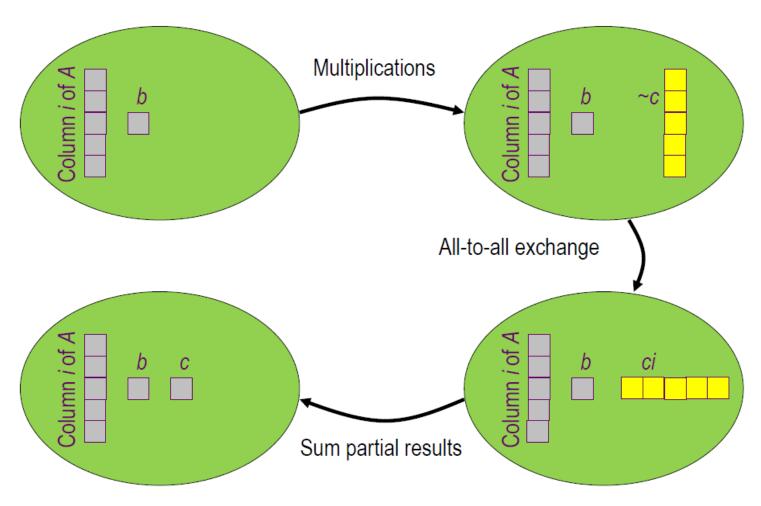
All-to-All Exchange (All-to-All Personalized Communication)



All-to-All Exchange (All-to-All Personalized Communication)



Phases of Parallel Algorithm



Agglomeration and Mapping

- > Static number of tasks
- > Regular communication pattern (all-to-all)
- > Computation time per task is constant
- > Strategy:
 - **□** Agglomerate groups of columns
 - ☐ Create one task per MPI process

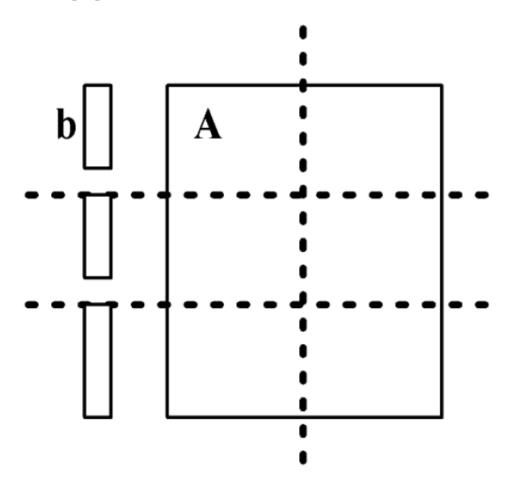
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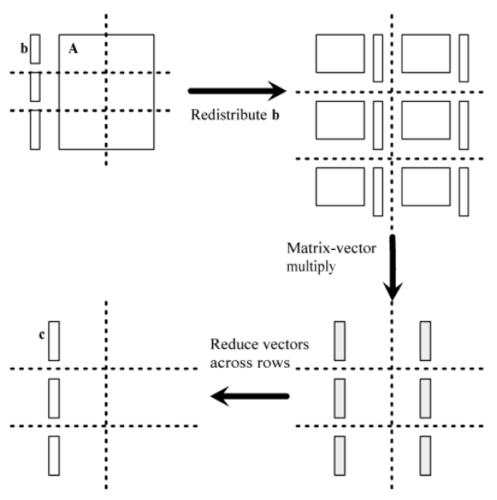
Checkerboard Block Decomposition

- \triangleright Associate primitive task with each element of the matrix A
- > Each primitive task performs one multiply
- > Agglomerate primitive tasks into rectangular blocks
- > Processes form a 2-D grid
- \triangleright Vector b distributed by blocks among processes in first column of grid

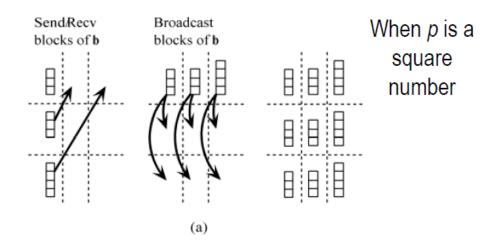
Tasks after Agglomeration



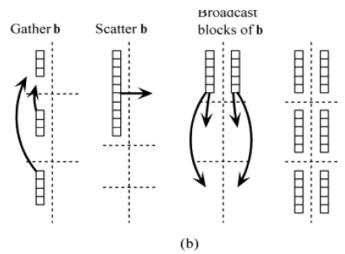
Algorithm's Phases



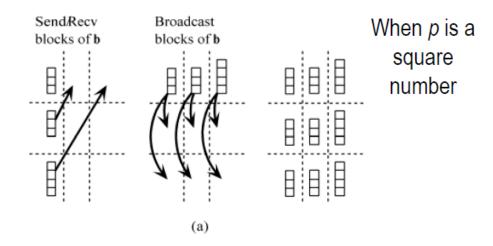
Algorithm's Phases



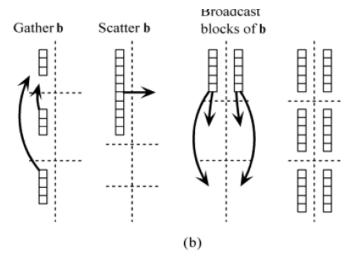
When *p* is not a square number



Algorithm's Phases



When *p* is not a square number



Redistributing Vector b

- \triangleright Step 1: Move b from processes in first row to processes in first column
 - \square If p square
 - First column/first row processes send/receive portions of b
 - \square If p not square
 - Gather b on process 0, 0
 - Process 0, 0 broadcasts to first row procs
- \triangleright Step 2: First row processes scatter b within columns



- **➤** Want processes in a virtual 2-D grid
- > Create a custom communicator to do this
- > Collective communications involve all processes in a communicator
- > We need to do broadcasts, reductions among subsets of processes
- > We will create communicators for processes in same row or same column

What's in a Communicator?

- > Process group
- > Context
- > Attributes
 - Topology (lets us address processes another way)
 - Others we won't consider

Creating 2-D Virtual Grid of Processes

- ➤ MPI_Dims_create
 - **□** Input parameters
 - Total number of processes in desired grid
 - Number of grid dimensions
 - **□** Returns number of processes in each dim
- > MPI_Cart_create
 - □ Creates communicator with Cartesian topology (笛卡尔拓扑结构)

MPI_Dims_create

dims	function call	dims
before call		on return
(0,0)	MPI_DIMS_CREATE(6, 2, dims)	(3,2)
(0,0)	MPI_DIMS_CREATE(7, 2, dims)	(7,1)
(0,3,0)	MPI_DIMS_CREATE(6, 3, dims)	(2,3,1)
(0,3,0)	l	erroneous call

source: DeinoMPI

MPI_Cart_create (创建笛卡尔拓扑)

```
int MPI Cart create (
  MPI Comm old comm, /* Input - old communicator */
   int dims, /* Input - grid dimensions */
   int *size, /* Input - # procs in each dim */
   int *periodic,
       /* Input - periodic[j] is 1 if dimension j
          wraps around; 0 otherwise */
   int reorder,
       /* 1 if process ranks can be reordered */
  MPI Comm *cart comm)
      /* Output - new communicator */
```

Using MPI_Dims_create **and** MPI_Cart_create

```
MPI Comm cart comm;
int p;
int periodic[2];
int size[2];
size[0] = size[1] = 0;
MPI Dims create (p, 2, size);
periodic[0] = periodic[1] = 0;
MPI Cart create (MPI COMM WORLD, 2, size,
1, &cart comm);
```

Using MPI_Dims_create **and** MPI_Cart_create

```
MPI Comm cart comm;
int p;
int periodic[2];
int size[2];
size[0] = size[1] = 0;
MPI Dims create (p, 2, size);
periodic[0] = periodic[1] = 0;
MPI Cart create (MPI COMM WORLD, 2, size,
1, &cart comm);
```

Useful Grid-related Functions

- > MPI_Cart_rank
 - ☐ Given coordinates of process in Cartesian communicator, returns process rank
- > MPI_Cart_cords
 - ☐ Given rank of process in Cartesian communicator, returns process' coordinates

Header for MPI_Cart_rank

```
int MPI Cart rank (
   MPI Comm comm,
      /* In - Communicator */
   int *coords,
      /* In - Array containing process'
              grid location */
   int *rank)
      /* Out - Rank of process at
         specified coords */
```

Header for MPI_Cart_coords

```
int MPI Cart coords (
  MPI Comm comm,
      /* In - Communicator */
   int rank,
      /* In - Rank of process */
   int dims,
      /* In - Dimensions in virtual grid
*/
   int *coords)
      /* Out - Coordinates of specified
         process in virtual grid */
```

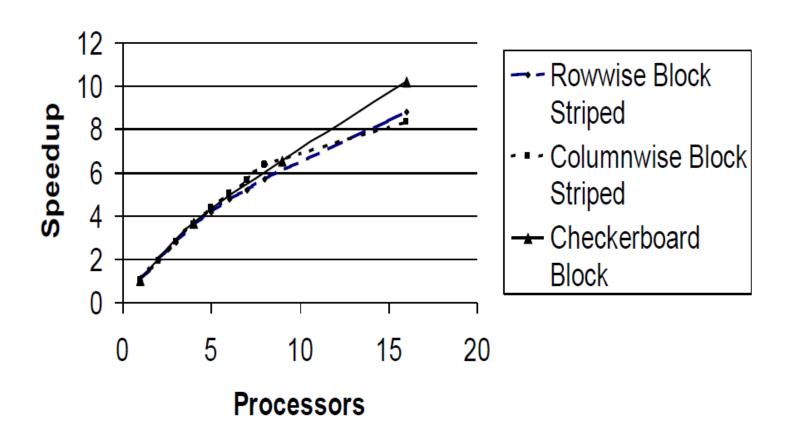
Collective Communications

	Ring	2-D Mesh	Hypercube
One-to-All Broadcast			
All-to-One Reduction			
All-to-All Broadcast			
All-to-All Reduction			
Scatter			
Gather			
All-to-All Personalized Communication			

MPI Names of the Various Operations

Operation	MPI Name	
One-to-all broadcast	MPI_Bcast	
All-to-one reduction	MPI_Reduce	
All-to-all broadcast	MPI_Allgather	
All-to-all reduction	MPI_Reduce_scatter	
All-reduce	MPI_Allreduce	
Gather	MPI_Gather	
Scatter	MPI_Scatter	
All-to-all personalized	MPI_Alltoall	

Comparison of Three Algorithms





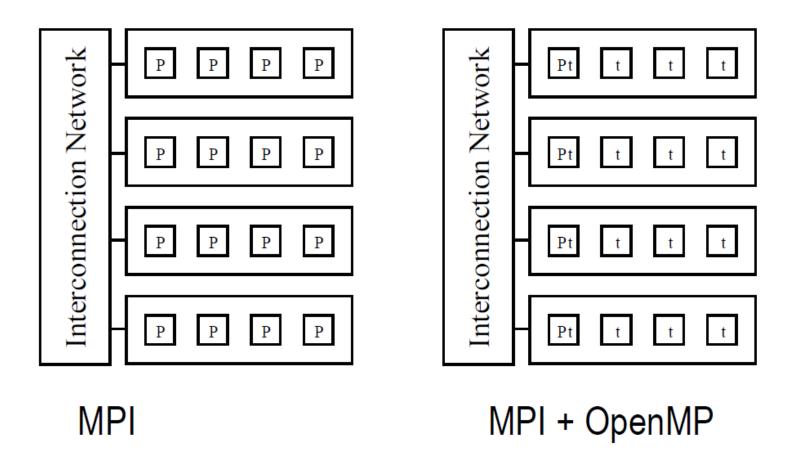
Programming with MPI

MPI + OpenMP

MPI + OpenMP

- > Advantages of using both MPI and OpenMP
 - ☐ Case Study: Jacobi method
 - An iterative methods to solve linear systems

MPI vs. MPI + OpenMP



Why MPI + OpenMP Can Execute Faster?

- > Lower communication overhead
 - **■** Message passing with *mk* processes, versus
 - \square Message passing with m processes with k threads each
- > More portions of program may be practical to parallelize
- > May allow more overlap of communications with computations
 - **□** For example, if 3 MPI processes are waiting for messages, and 1

MPI process is active, it is worthwhile to fork some threads to

speedup the 4th process

Hybrid Light-Weight Threads & Heavier-Weight Processes

- > For example, a serial program runs in 100s
 - ☐ S: 5s is inherent sequential
 - □ P₁: 5s are parallelizable but not worth message passing
 - **□** P₂: 90s are perfectly parallelizable
- > MPI-only with 16 processes
 - **□** Replicate the P₁ part of program on all processes
 - \square Speedup = 1 / (0.10 + 0.90/16) = 6.4
- > Hybrid MPI & threads
 - **■** Execute the replicated P₁ with 2 threads
 - \square Speedup = 1 / (0.05 + 0.05/2 + 0.90/16) = 7.6
 - **□** 19% faster than MPI-only

Code for matrix_vector_product

```
void matrix vector product (int id, int p,
   int n, double **a, double *b, double *c)
  int i, j;
              /* Accumulates sum */
   double tmp;
   for (i=0; i<BLOCK SIZE(id,p,n); i++) {
      tmp = 0.0;
      for (j = 0; j < n; j++)
         tmp += a[i][j] * b[j];
     piece[i] = tmp;
   new replicate block vector (id, p,
     piece, n, (void *) c, MPI DOUBLE);
```

Adding OpenMP Directives

- > Want to minimize fork/join overhead by making parallel the outermost possible loop
- ➤ Outer loop may be executed in parallel if each thread has a private copy of tmp and j

```
#pragma omp parallel for private(j,tmp)
for (i=0; i<BLOCK_SIZE(id,p,n); i++) {</pre>
```

User Control of Threads

- > Want to give user opportunity to specify number of active threads per process
- ➤ Add a call to omp_set_num_threads to function main
- > Argument comes from command line

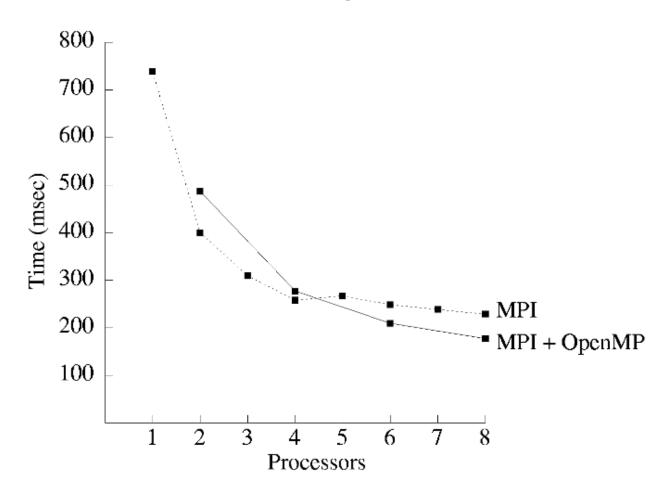
What Happened?

> We transformed a MPI program to a MPI+OpenMP program by adding only two lines to our program!

Benchmarking

- > Target system: a commodity cluster with four dualprocessor nodes
- > MPI program executes on 1, 2, ..., 8 CPUs
 - ☐ On 1, 2, 3, 4 CPUs, each process on different node, maximizing memory bandwidth per CPU
- ➤ MPI+OpenMP program executes on 1, 2, 3, 4 processes
 - **□** Each process has two threads
 - □ C+MPI+OpenMP program executes on 2, 4, 6, 8 threads

Results of Benchmarking



Analysis of Results

- ➤ MPI+OpenMP program slower on 2, 4 CPUs because MPI+OpenMP threads are sharing memory bandwidth, while C+MPI processes are not
- > MPI+OpenMP programs faster on 6, 8 CPUs because they have lower communication cost

Case Study: Jacobi Method

- > Begin with MPI program that uses Jacobi method to solve steady state heat distribution problem
- ➤ Program based on rowwise block striped decomposition of two-dimensional matrix containing finite difference mesh (有限差分网格, FDM)



- \triangleright Used to solve Ax = b when A is dense
- ightharpoonup Reduces Ax = b to upper triangular system Tx = c
- **Back substitution can then solve** Tx = c **for** x

Gaussian Elimination Example (1/4)

$$4x_0 +6x_1 +2x_2 -2x_3 = 8$$

$$2x_0 +5x_2 -2x_3 = 4$$

$$-4x_0 - 3x_1 - 5x_2 + 4x_3 = 1$$

$$8x_0 + 18x_1 - 2x_2 + 3x_3 = 40$$

Gaussian Elimination Example (2/4)

$$4x_0 +6x_1 +2x_2 -2x_3 = 8$$

$$-3x_1 +4x_2 -1x_3 = 0$$

$$+3x_1 -3x_2 +2x_3 = 9$$

$$+6x_1 -6x_2 +7x_3 = 24$$

Gaussian Elimination Example (3/4)

$$4x_0 +6x_1 +2x_2 -2x_3 = 8$$

$$-3x_1 + 4x_2 - 1x_3 = 0$$

$$1x_2 + 1x_3 = 9$$

$$2x_2 + 5x_3 = 24$$

Gaussian Elimination Example (4/4)

$$4x_0 +6x_1 +2x_2 -2x_3 = 8$$

$$-3x_1 +4x_2 -1x_3 = 0$$

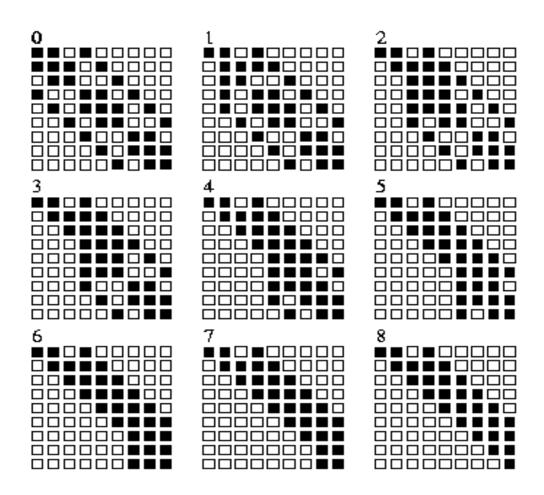
$$1x_2 + 1x_3 = 9$$

$$3x_3 = 6$$

Sparse Systems

- ➤ Gaussian elimination not well-suited for sparse systems
- > Coefficient matrix gradually fills with nonzero elements
 - **□** Increases storage requirements
 - **□** Increases total operation count

Example of "Fill" in Gaussian Elimination



Iterative Methods

- > Iterative method: algorithm that generates a series of approximations to solution's value
- > Require less storage than direct methods
- > Since they avoid computations on zero elements, they can save a lot of computations



Let

$$A\mathbf{x} = \mathbf{b}$$

be a square system of *n* linear equations, where:

$$A = egin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \ a_{21} & a_{22} & \cdots & a_{2n} \ dots & dots & \ddots & dots \ a_{n1} & a_{n2} & \cdots & a_{nn} \ \end{pmatrix}, \qquad \mathbf{x} = egin{bmatrix} x_1 \ x_2 \ dots \ x_n \ \end{bmatrix}, \qquad \mathbf{b} = egin{bmatrix} b_1 \ b_2 \ dots \ b_n \ \end{bmatrix}.$$

Then A can be decomposed into a diagonal component D, and the remainder R:

$$A = D + R \qquad ext{where} \qquad D = egin{bmatrix} a_{11} & 0 & \cdots & 0 \ 0 & a_{22} & \cdots & 0 \ dots & dots & \ddots & dots \ 0 & 0 & \cdots & a_{nn} \end{bmatrix} ext{ and } R = egin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \ a_{21} & 0 & \cdots & a_{2n} \ dots & dots & \ddots & dots \ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}.$$

The solution is then obtained iteratively via

$$\mathbf{x}^{(k+1)} = D^{-1}(\mathbf{b} - R\mathbf{x}^{(k)}),$$

where $\mathbf{x}^{(k)}$ is the kth approximation or iteration of \mathbf{x} and $\mathbf{x}^{(k+1)}$ is the next or k+1 iteration of \mathbf{x} . The element-based formula is thus:

$$x_i^{(k+1)} = rac{1}{a_{ii}}\left(b_i - \sum_{j
eq i} a_{ij}x_j^{(k)}
ight), \quad i=1,2,\ldots,n.$$

Values of elements of vector x at iteration k+1 depend upon values of vector x at iteration k

Rate of Convergence

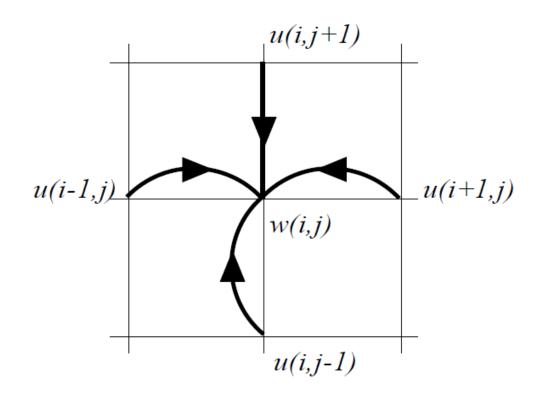
- ➤ Even when Jacobi method, rate of convergence often too slow to make them practical
- > We will move on to an iterative method with much faster convergence

Methodology

- > Profile execution of MPI program
- ➤ Focus on adding OpenMP directives to most compute-intensive function

Heart of Sequential C Program

$$w[i][j] = (u[i-1][j] + u[i+1][j] + u[i][j-1] + u[i][j+1]) / 4.0;$$





Function	1 CPU	8 CPUs
initialize_mesh	0.01%	0.03%
find_steady_state	98.48%	93.49%
print_solution	1.51%	6.48%

Function find_steady_state (1/2)

```
its = 0;
for (;;) {
   if (id > 0)
      MPI Send (u[1], N, MPI DOUBLE, id-1, 0,
         MPI COMM WORLD);
   if (id < p-1) {
      MPI Send (u[my rows-2], N, MPI DOUBLE, id+1,
         0, MPI COMM WORLD);
      MPI Recv (u[my rows-1], N, MPI DOUBLE, id+1,
         0, MPI COMM WORLD, &status);
   if (id > 0)
      MPI Recv (u[0], N, MPI DOUBLE, id-1, 0,
         MPI COMM WORLD, &status);
```

Function find_steady_state (2/2)

```
diff = 0.0;
for (i = 1; i < my rows-1; i++)
   for (j = 1; j < N-1; j++) {
      w[i][j] = (u[i-1][j] + u[i+1][j] +
                 u[i][j-1] + u[i][j+1])/4.0;
      if (fabs(w[i][j] - u[i][j]) > diff)
         diff = fabs(w[i][j] - u[i][j]);
for (i = 1; i < my rows-1; i++)
   for (j = 1; j < N-1; j++)
      u[i][j] = w[i][j];
MPI Allreduce (&diff, &global diff, 1,
   MPI DOUBLE, MPI MAX, MPI COMM WORLD);
if (global diff <= EPSILON) break;
its++;
```

Making Function Parallel (1/2)

- > Except for two initializations and a return statement, function is a big for loop
- > Cannot execute for loop in parallel
 - **□** Not in canonical form
 - □ Contains a break statement
 - **□** Contains calls to MPI functions
 - **□** Data dependences between iterations

Making Function Parallel (2/2)

- > Focus on first for loop indexed by i
- ➤ How to handle multiple threads testing/updating diff?
- > Putting if statement in a critical section would increase overhead and lower speedup
- > Instead, create private variable tdiff
- > Thread tests tdiff against diff before call to MPI Allreduce



```
diff = 0.0;
#pragma omp parallel private (i, j, tdiff)
      tdiff = 0.0;
#pragma omp for
      for (i = 1; i < my rows-1; i++)
#pragma omp for nowait
      for (i = 1; i < my rows-1; i++)
#pragma omp critical
      if (tdiff > diff) diff = tdiff;
      MPI Allreduce (&diff, &global diff, 1,
         MPI DOUBLE, MPI MAX, MPI COMM WORLD);
```

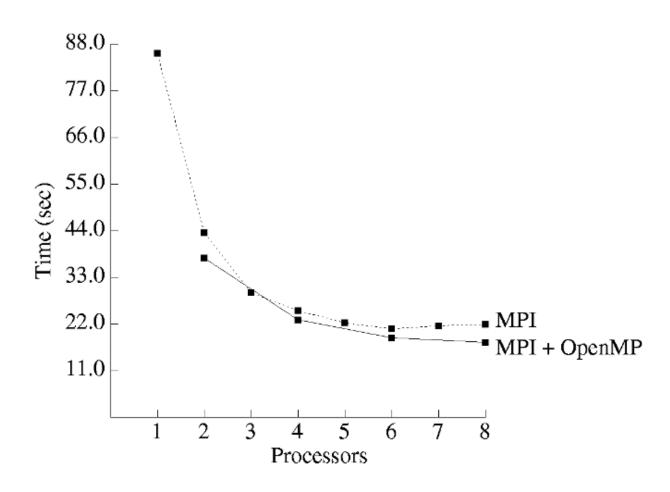
Making Function Parallel (3/3)

- > Focus on second for loop indexed by i
- \succ Copies elements of w to corresponding elements of u: no problem with executing in parallel

Benchmarking

- > Target system: a commodity cluster with four dual-processor nodes
- > C+MPI program executes on 1, 2, ..., 8 processes
 - ☐ On 1, 2, 3, 4 CPUs, each process on different node, maximizing memory bandwidth per CPU
- > C+MPI+OpenMP program executes on 1, 2, 3, 4 processes
 - **□** Each process has two threads
 - □ C+MPI+OpenMP program executes on 2, 4, 6, 8 threads

Benchmarking Results



Analysis of Results

- > Hybrid C+MPI+OpenMP program uniformly faster than C+MPI program
- > Computation/communication ratio of hybrid program is superior
- > Number of mesh points per element communicated is twice as high per node for the hybrid program
- > Lower communication overhead leads to 19% better speedup on 8 CPUs

Summary

- ➤ Hybrid C+MPI+OpenMP program uniformly faster than C+MPI program
- > Computation/communication ratio of hybrid program is superior
- > Number of mesh points per element communicated is twice as high per node for the hybrid program
- > Lower communication overhead leads to 19% better speedup on 8 CPUs

Thank You!