### Parallel algorithms for Dense Matrix Problems

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### Logistics

### Assignments

- A1 grades released
- ▶ Then Mini-Exam 1 grading have commenced
- ▶ Goal to have all grading done by Mon 10/11
- A2 is delayed: apologies

### Reading

Grama Ch 8 on Dense Matrix Algorithms

- Naive Matrix Multiply
- Cannon's Algorithm
- LU Decomposition

### Today

- Matrix algorithms
- ► Facebook?

### Recall Matrix Transpose

- ightharpoonup Common operation on matrices is a **transpose** notated  $A^T$
- ► Interchanges rows/columns of A:  $a_{ij} \rightarrow a_{ji}$
- ▶ Diagonal elements stay the same
- Algorithms that perform operations on A can often be performed on  $A^T$  without re-arranging A how? Hint: consider summing rows of A vs summing rows of  $A^T$

#### Original matrix A

0	5	10	15
20	) 25	30	35
40	45	5 50	55

#### transpose(A)

0	20	40	60
5	25	45	65
10	30	50	70
15	35	55	75

### **Exercise:** Matrix Partitioning Across Processors

Row Partition				
00	01	02	03	
10	11	12	13	
20	21	22	23	
30	31	32	33	

<b>Column Partition</b>				
00	01	02	03	
10	11	12	13	
20	21	22	23	
30	31	32	33	

Block Partition				
01	02	03		
11	12	13		
21	22	23		
31	32	33		
	11 21	11 12 21 22		

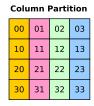
Proc Location		
	P0 / P00	
	P1 / P01	
	P2 / P10	
	P3 / P11	

- Recall several ways to partition matrices across processors
- Diagram shows these
  - Entry ij may be an individual element OR...
  - ► Entry ij may be a **Block**: ex. Block (2,3) is the submatrix from rows 200-299 and cols 300-399
- ► Assume **square** matrices : #rows = #cols
- ▶ Common to multiply to compute product:  $C = A \times B$
- ▶ Ideal partitioning for A and B in matrix multiply?
- ▶ Ideal partitioning for  $C = A^T \times B$
- $\blacktriangleright \ \ \text{Ideal partitioning for} \ C = A \times B^T$

4

# **Answers**: Matrix Partitioning Across Processors

<b>Row Partition</b>				
00	01	02	03	
10	11	12	13	
20	21	22	23	
30	31	32	33	



Block Partition				
00	01	02	03	
10	11	12	13	
20	21	22	23	
30	31	32	33	

Proc Location		
	P0 / P00	
	P1 / P01	
	P2 / P10	
	P3 / P11	

- $ightharpoonup C = A \times B$ 
  - lacktriangle Ideally A is row-partitioned, B is column partitioned
  - ► Then block-partitioned C could be computed w/o communication
- $ightharpoonup C = A^T \times B$ 
  - ightharpoonup Ideally A and B column-partitioned
- $ightharpoonup C = A \times B^T$ 
  - ightharpoonup Ideally A and B row-partitioned
- ightharpoonup Block-partitioning often used: not ideal for any version but less communication required when both A and  $A^T$  will b used

### Naive Parallel Dense Multiplication: Overview

### **Block Partitioning Appears Frequently**

- Specific applications may be able to select a favorable partitioning (e.g. Row Partition for Page Rank)
- ▶ Many applications use both A and A<sup>T</sup> so employ block-partitioned matrices: middle-way approach which does not favor rows or columns
- Parallel Libraries often use block partitions by default

### Matrix Multiply with Blocks

- ➤ To compute Matrix-Matrix multiply, procs must (eventually) multiply full rows by full columns to compute an output block
- Naive method: each Proc stores full rows/columns needed for it to independently compute output block which it stores

### Naive Parallel Dense Multiplication: Demo

P01

1. Initial data layout: each Proc holds a block of A. B. and C respectively. Processors are arragned in a logical grid that reflects their initial data.

data is bolded.



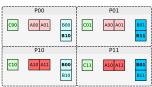
P00

B00

A00

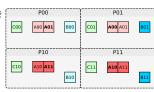
3. Each proc participates in an All-to-All sharing of data for the Column it is

This leaves each row with complete columns as well.

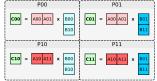


2. Each proc participates in an All-to-All sharing of data for the Row it is in.

This leaves each proc with entire rows of A.



4 Fach Proc now has a unique set of complete Rows and Columns and can independently compute a block of output matrix C through block multiplication.



# Exercise: Analysis of Naive Dense Mult.

#### Assumptions

- ▶ Matrices A and B are size  $N \times N$  so  $N^2$  elements
- ▶ P processors in a  $\sqrt{P} \times \sqrt{P}$  grid (P is a perfect square)
- ▶ Each Proc has block with  $N^2/P$  elements of A,B as a  $(N/\sqrt{P}) \times (N/\sqrt{P})$  submatrix
- Simplified communication cost for All-to-All on a Ring with p #procs in ring,  $t_s$  comm startup time,  $t_w$  per word transfer rate, M message size:

$$t_{comm} = (p-1)(t_s + t_w M)$$

#### Questions

- 1. What is communication cost of this algorithm?
- 2. How much time does the final block matrix multiply take?
- 3. What is the memory requirement for each proc?
- 4. Biggest disadvantage for this algorithm?

### Answers: Analysis of Naive Dense Mult.

- 1. What is communication cost of this algorithm?
  - ▶ #Procs in rows/cols is  $\sqrt{P}$  ~ ring size
  - $ightharpoonup M=N^2/P$  : message size is num elements on each proc
  - ▶ 2 All-to-All shares : 1 for rows, 1 for cols

$$t_{comm} = 2(\sqrt{P} - 1) \times (t_s + t_w(N^2/P))$$

- 2. What is the memory requirement for each proc? E.g. how many submatrices of A,B are on each proc?
  - ► Full rows/cols on each proc
  - Requires  $\sqrt{P}$  submatrices for each Proc
- 3. How much time does the final block matrix multiply take?
  - Each proc has  $\sqrt{P}$  submats of A,B to multiply
  - ▶ MatMult is for size s is  $O(s^3)$ ; submat size  $s = N/\sqrt{P}$

$$t_{mult} = O((\sqrt{P}) \times ((N/\sqrt{P})^3)) = O(N^3/P)$$

- 4. Biggest disadvantage for this algorithm?
  - ▶ Major: The need to store  $\sqrt{P}$  sub matrices on all procs may be prohibitive:  $2\sqrt{P} \times N^2/P$  space on each proc
  - Minor: Not much chance to overlap communication / computation in the algorithm

### Cannon's Algorithm

- Proposed in Lynn Elliot Carter's 1969 thesis
- Target was very small parallel machines implementing a Kalman Filter algorithm in hardware
- "Communication" happening between small Procs with data in registers
- Scales nicely to large machines and overcomes the large memory requirement of the Naive Mat-Mult Algorithm

A CELLULAR COMPUTER TO IMPLEMENT THE KALMAN FILTER ALCORITHM

by

LYNN ELLIOT CANNON

By the conventional definition of matrix product, if A is multiplied by B, the result, call it C, is given by

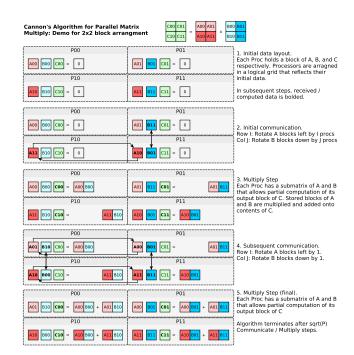
The symmetry of this product can be seen by comparing the ij<sup>th</sup> element with the ji<sup>th</sup> element and noticing that one is obtained from

-24-

- A. 1. The first row of A is left alone.
  - 2. The second row of A is shifted left one column.
  - The third row of A is shifted left two columns.
     (Note, in general the i<sup>th</sup> row of A is shifted left i-l columns for i = 1, ..., n).
- B. 1. The first column of B is left alone.
  - 2. The second column of B is shifted up one row
  - The third column of B is shifted up two rows.
     (Note, in general the j<sup>th</sup> column of B is shifted up j-1 rows for j = 1, ..., n)

Once the registers have been shifted the multiplication pr

#### Demo



# Cannon's Algorithm Pseudocode

```
Cannon_MM(i, j, Q){
  PE(i,j) has blocks A1=A(i,j) and B1=B(i,j)
  Q is the Block Dimension: A is Q*Q blocks
  Allocate space A2, B2, Cij sized as A1
  doboth send A1 to PE(i, j-i+Q % Q)
        recv A2 from PE(i, j+i+Q % Q)
  doboth send B1 to PE(i-j+Q % Q, j)
         recv B2 from PE(i+j+Q % Q, j)
  for(k=1 to 0){
    copy A2 into A1, B2 into B1
    Cij += A1 * B1
    doboth send A1 to PE(i, j-1+Q % Q)
           recv A2 from PE(i, j+1+Q % Q)
    doboth send B1 to PE(i-1+Q % Q, j)
           recv B2 from PE(i+1+Q % Q, j)
    // optionally skip last comm
  Cij now contains output block of C(i,j)
```

$A_{0,0}$	$A_{0,1}$	A <sub>0,2</sub>	A <sub>0,3</sub>
A <sub>1,0</sub>	A <sub>1,1</sub>	A <sub>1,2</sub>	A <sub>1,3</sub>
A <sub>2,0</sub>	A <sub>2.1</sub>	A <sub>2,2</sub>	A <sub>2,3</sub>
A <sub>3,0</sub>	A <sub>3,1</sub>	A <sub>3,2</sub>	A <sub>3,3</sub>

B <sub>0,0</sub>	B <sub>0,1</sub>	B <sub>0,2</sub>	B <sub>0,3</sub>
B <sub>1,0</sub>	B <sub>1,1</sub>	B <sub>1,2</sub>	B <sub>1,3</sub>
B <sub>2.0</sub>	B <sub>2,1 &amp;</sub>	ў В <sub>2,2</sub>	B <sub>2,3</sub>
B <sub>3,0</sub>	B <sub>3,1</sub>	B <sub>3,2</sub>	B <sub>3,3</sub>

	1	4	1	4
ş -	A <sub>0,0</sub> ⋖	A <sub>0.1</sub> ~	A <sub>0,2</sub> ~	A <sub>0,3</sub> ~
	B <sub>0,0</sub>	B <sub>1,1</sub>	B <sub>2,2</sub>	B <sub>3,3</sub>
	A <sub>1,1</sub> ~	A <sub>1,2</sub> ~	A <sub>1,3</sub> ~	A <sub>1,0</sub>
	B <sub>1,0</sub>	B <sub>2,1</sub>	B <sub>3,2</sub>	B <sub>0,3</sub>
	A <sub>2,2</sub>	A23	A <sub>2,0</sub>	A <sub>2,1</sub>

(a) Initial alignment of A

$B_{0,0}$	B <sub>0,1</sub>	B <sub>0,2</sub>	B <sub>0,3</sub>
B <sub>1,0</sub>	B <sub>1,1</sub>	B <sub>1,2</sub>	в <sub>1,3</sub>
B <sub>2,0</sub>	В <sub>2,1 в</sub>	ў В <sub>2,2</sub>	в <sub>2,3</sub>
B <sub>3,0</sub>	В <sub>3,1</sub>	B <sub>3,2</sub>	В <sub>3,3</sub>

(b) In	nitial alig	nment of	В
1	1	1	1
~ A <sub>0.1</sub> ~	A <sub>0,2</sub> ~	A <sub>0.3</sub> ~	A <sub>0,0</sub> ~
B <sub>1,0</sub>	B <sub>2,1</sub>	B <sub>3,2</sub>	$B_{0,3}$
A <sub>1,2</sub> ~	A <sub>1,3</sub> ~	A <sub>1,0</sub> ~	A <sub>1,1</sub>
B <sub>2,0</sub>	B <sub>3,1</sub>	B <sub>0,2</sub>	B <sub>1,3</sub>
- A <sub>2,3</sub> -	A <sub>2,0</sub> ~	A <sub>2,1</sub> ~	A <sub>2,2</sub>
B <sub>3,0</sub>	$B_{0,1}$	B <sub>1,2</sub>	B <sub>2,3</sub>
A <sub>3,0</sub> ~	A <sub>3,1</sub> ~	A <sub>3,2</sub> <	A <sub>3,3</sub> <
B <sub>0,0</sub>	B <sub>1,1</sub>	B <sub>2,2</sub>	B <sub>3,3</sub>
1	1	1	

ſ	A <sub>0,3</sub>	A <sub>0,0</sub>	A <sub>0,1</sub>	A <sub>0,2</sub>
	B <sub>3,0</sub>	B <sub>0,1</sub>	B <sub>1,2</sub>	B <sub>2,3</sub>

4	A <sub>0,2</sub> ~	A <sub>0,3</sub> <	A <sub>0.0</sub> ~	A <sub>0.1</sub> ~
	B <sub>2,0</sub>	B <sub>3,1</sub>	B <sub>0,2</sub>	B <sub>1,3</sub>
4	A <sub>1,3</sub> <	A <sub>1,0</sub> <	A <sub>1,1</sub> <	A <sub>1,2</sub> ~
	B <sub>3,0</sub>	B <sub>0,1</sub>	B <sub>1,2</sub>	B <sub>2,3</sub>
ų.	A <sub>2,0</sub> ~	A <sub>2,1</sub> ~	A <sub>2,2</sub> ~	A <sub>2,3</sub> ~
	B <sub>0,0</sub>	$B_{1,1}$	B <sub>2,2</sub>	B <sub>3,3</sub>
٠.	A <sub>3,1</sub> <	A <sub>3,2</sub> ~	A <sub>3,3</sub> <	A <sub>3,0</sub> ~
	B <sub>1,0</sub>	B <sub>2,1</sub>	B <sub>3,2</sub>	B <sub>0,3</sub>

A <sub>0,3</sub>	$A_{0,0}$ $B_{0,1}$	A <sub>0,1</sub>	A <sub>0,2</sub>
B <sub>3,0</sub>		B <sub>1,2</sub>	B <sub>2,3</sub>
A <sub>1,0</sub>	$A_{1,1} \\ B_{1,1}$	A <sub>1,2</sub>	A <sub>1,3</sub>
B <sub>0,0</sub>		B <sub>2,2</sub>	B <sub>3,3</sub>
A <sub>2,1</sub>	A <sub>2,2</sub>	A <sub>2,3</sub>	A <sub>2,0</sub>
B <sub>1,0</sub>	B <sub>2,1</sub>	B <sub>3,2</sub>	B <sub>0,3</sub>
A <sub>3,2</sub>	A <sub>3,3</sub>	A <sub>3,0</sub>	A <sub>3,1</sub>
B <sub>2,0</sub>	B <sub>3,1</sub>	B <sub>0,2</sub>	B <sub>1,3</sub>

(e) Submatrix locations after second shift. (f) Submatrix locations after third shift

Figure 8.3 The communication steps in Cannon's algorithm on 16 processes.

# Exercise: Analysis of Cannon's Algorithm

#### Assumptions

- ▶ Matrices A and B are size  $N \times N$  so  $N^2$  elements
- ▶ P processors with block partitioning: initially  $N^2/P$  elements of A, B on each proc (assume P is a perfect square)
- Simplified communication cost for send/recv on a Ring:

$$t_{comm} = t_s + t_w M$$

with p #procs in ring,  $t_s$  comm startup time,  $t_w$  per word transfer rate, M message size.

#### Questions

- 1. What is communication cost of this Cannon's algorithm?
- 2. Is this any better/worse/same as the Naive algorithm?
- 3. What is the memory requirement for each proc?
- 4. Is this any better/worse/same as the Naive algorithm?

# Answers: Analysis of Cannon's Algorithm

- 1. What is communication cost of this Cannon's algorithm?
  - ▶ In each step, each proc performs 2 send/recv ops
  - ▶ Each send/recv is a block of size  $N^2/P$
  - ▶ Block Dim  $Q = \sqrt{P}$  for square 2D Torus
  - $\blacktriangleright$  Total  $\sqrt{P}$  steps : can skip last comm step

$$t_{comm} = 2(\sqrt{P} - 1) \times (t_s + t_w(N^2/P))$$

- 2. Is this any better/worse/same as the Naive algorithm?
  - Same communication cost as Naive algorithm
- 3. What is the memory requirement for each proc?
  - $ightharpoonup O(N^2/P)$ : 5 blocks as stated in pseudcode,
  - ▶ 3 blocks for  $A_{ij}, B_{ij}, C_{ij}$
  - ▶ 2 "workspaces" to allow send/recv of blocks:
  - Eliminate workspace blocks in a refinement
- 4. Is this any better/worse/same as the Naive algorithm?
  - ► Cannon's  $O(N^2/P)$  vs Naive  $O(\sqrt{P} \times N^2/P)$
  - Memory overhead is much better: constant number of blocks rather than the need to store entire rows/cols on single procs

### Lessons from Cannon's Algorithm

- Illustrates "pipelining": blocks used to compute partial results then fed forward other processors
- Benefits greatly from a 2D Grid / Torus network which facilitates local communications that arise in the algorithm
- lacktriangle While not as ideal as row/col partitioning for A,B, realistic and relatively efficient
- Variants of central idea exist in some libraries such as Scalapack which has a parallel xGEMM() using many similar ideas
- Could really use some code support for
  - 2D Coordinates for processors rather than linear rank...
  - Sending/receiving in a ring...

### MPI Tricks for Rings

### Sendrecv in a Ring

MPI\_Sendrecv() allows ring-link partnering

### Sendrecv with Replacement

MPI\_Sendrecv\_replace() allows send/recv in the same buffer

In Cannon's Alg, no longer need A1 / A2: can send/receive block of A with a single buffer.

# MPI Tricks for Grids: MPI\_Cart\_create()

MPI has special support for Grid/Torus network configs; allows creation of a MPI\_Comm that maps processors to a N-D grid

▶ 2D Torus for Cannon's Alg

```
// cartesian comm.c
int dim_len = 2; // Set up the Cartesian topology
int dims[2] = {sqrt(npes), sqrt(npes)}; // # rows/cols
int periods[2] = {1, 1};  // wrap-around rows/cols
// Create the Cartesian topology, with rank reordering
MPI Comm comm 2d;
MPI_Cart_create(MPI_COMM_WORLD, // original comm
               dim_len, dims, periods, // cartesian comm props

    // re-order linear rank if beneficial

               &comm_2d); // new communicator with 2D coords
// Get the rank and coordinates with respect to the new topology
int my2drank = -1; // may be differ from world rank
MPI Comm_rank(comm_2d, &my2drank);
int mycoords[2] = \{-1, -1\}; // (i,j) coords
MPI_Cart_coords(comm_2d, my2drank, 2, mycoords);
printf("Proc %2d (%s): my2drank %3d mycoords (%3d, %3d)\n",
       myrank,processor_name,
       my2drank,mycoords[0],mycoords[1]);
```

# MPI Tricks for Shifting

#### Shifts are eased by the MPI\_Cart\_shift() function

- Calculates linear rank of source/dest procs for shift operations in a Cartesian grid of procs.
- Data exchange via MPI\_Sendrecv() is then direct

### Cannon's Algorithm in MPI

- Grama Program 6.2 is Cannon's Matrix Multiply algorithm implemented via MPI
- Uses the tricks mentioned on the past 2 slides to ease implementation burden
- See cannon\_grama.c for a source code version of it

Note: I haven't tested this code but everything from textbooks always works out the box, right?

### Linear Equations

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$$

$$\vdots$$

$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_m$$

Summarized in matrix form as

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

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Usually given A, b, must find x. An inordinate amount of CPU cycles are spent on this problem.

### Solving Triangular Systems

#### Easier than a general system via back substitution process

```
2 3 0 | 14 ]
                                [0560|28]
[0567|56]
[0 0 8 9 | 60]
                                [0 0 8 0 | 24]
                                                      60-9*4
                                [0 \ 0 \ 0 \ 1 \ | \ 4] \ x(3) == 4
[0 \ 0 \ 0 \ 1 \ | \ 4] \ x(3) == 4
    2 3 0 | 14 ]
                                           0 | 5 ]
                                                     14-3*3
[0560|28]
                                 [050010]
                                                      28-6*3
   0 \ 1 \ 0 \ | \ 3 \ ] \ x(2) == 3
                                [0 \ 0 \ 1 \ 0 \ | \ 3] \ x(2) == 3
                                 [0\ 0\ 0\ 1\ |\ 4\ ]\ x(3) == 4
[0 \ 0 \ 0 \ 1 \ | \ 4 \ ] \ x(3) == 4
   2 0 0 | 5 ]
[0 \ 1 \ 0 \ 0 \ | \ 2] \ x(1) == 2
                                 [ 0 1 0 0 | 2 ] x(1) == 2
   0 \ 1 \ 0 \ | \ 3 \ ] \ x(2) == 3
                                 [0\ 0\ 1\ 0\ |\ 3\ ]\ x(2) == 3
[0 \ 0 \ 0 \ 1 \ | \ 4] \ x(3) == 4
                                 [0 0 0 1 l
                                                 4] x(3) == 4
         0 \mid 1 \mid x(0) == 1
[0 \ 1 \ 0 \ 0 \ | \ 2] \ x(1) == 2
[0\ 0\ 1\ 0\ |\ 3\ ]\ x(2) == 3
[0 \ 0 \ 0 \ 1 \ | \ 4 \ ] \ x(3) == 4
```

### Standard Code for Back Substitution

```
BACK SUBSTITUTE(A,b,x){
  N = nrows(A)
  for (j=N-1 \text{ downto } 0) {
    x[j] = b[j] / A[j,j]
    for[ i=j-1 downto 0 ] {
      b[i] = b[i] - A[i,j] *x[j]
      A[i,j] = 0 // OPTIONAL
  x \( \) now contains solutions
  b∏ has been modified
  A[] has been modified if OPTIONAL is executed
```

Computational complexity for square matrix of size N?

### Getting a Triangular Matrix via Gaussian Elimination

- ▶ Standard solution algorithm to find x in Ax = b
- ightharpoonup Converts A to U which is upper triangular

```
[ 1 2 3 -4 | -14 ]
[ 2 7 21 10 | 38 ] -2 row0
[ 4 13 43 2 | 24 ] -4 row0
[ -2 -2 7 15 | 60 ] +2 row0
 1 2 3 -4 | -14 ]
0 3 15 18 | 66 ]
0 5 31 18 | 80 ]
0 2 13 7 1
                                                    -5/3 row1
                                                  -2/3 row1
   1 2 3 -4 | -14 ]
0 3 15 18 | 66 ]
0 0 6 -12 | -30 ]
0 0 3 -5 | -12 ]
                                                        -1/2 row3
   1 2 3 -4 | -14 ] [ 1 0 0
0 3 15 18 | 66 ] [ 2 1 0
0 0 6 -12 | -30 ] [ 4 5/3 1
0 0 0 1 | 3 ] [ -2 2/3 1/2
                                                                                           L is formed from negative
                                                                                           coefficients found via
                                                                                0] Gaussian elimination with
                                                                                           unit main diagonal.
                                          b'
```

# LU: The Lower Upper Decomposition

- ightharpoonup By tracking the coefficients used during the Gaussian elimination, one gets a matrix L which is lower triangular
- lacktriangle Modifications to A become an upper triangular matrix U
- ▶ One can verify that A = LU

octave> L =	rats	s(L)			octave> U U =
1		0	0	0	1 2 3 -4
2		1	0	0	0 3 15 18
4	5,	/3	1	0	0 0 6 -12
-2	2/	/3	1/2	1	0 0 0 1
octave>	• L *	U			octave> L * U - A
ans =					ans =
1	2	3	-4		0 0 0 0
2	7	21	10		0 0 0 0
4	13	43	2		0 0 0 0
-2	-2	7	15		0 0 0 0

#### Exercise: LU Factorization Pseudocode

```
LU_FACTORS(A[] : square matrix){
      N = nrows(A)
      Allocate L as N*N identity mat
      Allocate U as copy of A
      for (d=0 \text{ to } N-1) {
                                             // leading row d
        for(i=d+1 to N-1){
                                             // remaining rows i
          scale = U[i,d] / U[d,d]
                                             // scale for this row
          L[i.d] = scale
                                             // record scale in L
          for(j=d to N-1){
                                            // iterate over this row j
10
            U[i,j] = U[i,j] - scale*U[d,j] // subtract off scaled leading row
11
12
1.3
14
      }
15
      return
16
        L: a lower triangle matrix with factors and unit diagonal
17
        U: an upper triangle matrix, obeys L*U = A
18
```

- Computational Complexity?
- Could anything go sideways numerically?

### **Answers**: LU Factorization Pseudocode

```
LU_FACTORS(A[] : square matrix){
     N = nrows(A)
     Allocate L as N*N identity mat
     Allocate U as copy of A
 5
6
     for (d=0 \text{ to } N-1)
                                            // leading row d
        for(i=d+1 to N-1){
                                            // remaining rows i
          scale = U[i,d] / U[d,d]
                                            // scale for this row
         L[i,d] = scale
                                       // record scale in L
10
          for(j=r to N-1){
                                          // iterate over this row j
            U[i,j] = U[i,j] - scale*U[d,j] // subtract off scaled leading row
11
12
13
14
      }
15
     return
16
        L: a lower triangle matrix with factors and unit diagonal
        U: an upper triangle matrix, obeys L*U = A
17
18 }
```

- ► Computational Complexity?:  $O(N^3)$  3 nested loops
- Could anything go sideways numerically? Division by 0 at line 8
  - To fix this requires pivoting
  - Robust versions permute rows so the row with the largest U[:,d] element used at iteration d

# Utility of LU Decomposition

#### General Process

- 1. Want x in Ax = b
- 2. Compute LU = A via Gaussian elimination
- 3. Use forward-substitution to find y in Ly = b
- 4. Use back-substitution to find x in Ux = y

Solving in this fashion exploits the following identities

$$Ly = b = Ax$$
 so  $Ax = Ly$   
 $LU = A$  so  $LUx = Ly$ 

$$L^{-1}LUx = L^{-1}Ly \quad \text{so} \qquad Ux = y$$

#### vs Gaussian Elimination

- ► LU factorization costs little more than Gaussian Elim
- Saving the LU Factorization allows solving for a new b with only passes of back/forward substitution

$$Ax_1 = b_1, Ax_2 = b_2, Ax_3 = b_3$$

1 LU decomposition, 3 rounds of back/forward substitution

- ▶ LU Decomp is  $O(N^3)$
- ▶ Back/Forward Sub is  $(N^2)$

#### **Variants**

- ► To save space, overwrite L,U in A
  - Upper triangle of A becomes U including main diagonal
  - ► Lower triangle of A would have been 0's, store L there, implied 1 diagonal
- lackbox Grama's variant makes main diagonal of U all 1's: saves some ops in back/forward substitution
- We are ignoring the need to **pivot** and permute the matrix rows for numerical stability: doing so yields the LUP decomposition with permutation matrix P

### Exercise: Now, about Parallelizing...

```
LU_FACTORS_INPLACE(A[] : square matrix){
      N = nrows(A)
      // Will overwrite A with its L*U factors, no allocation of L or U
 5
      for (d=0 \text{ to } N-1)
                                             // leading row d
        for(i=d+1 to N-1){
                                            // remaining rows i
          scale = A[i,d] / A[d,d]
                                             // scale for this row
          A[i,d] = scale
                                            // record scale in L
          for(j=r to N-1){
                                       // iterate over this row j
            A[i,j] = A[i,j] - scale * A[d,j] // subtract off scaled leading row
10
11
12
13
      }
14
      return; // A now has its L,U factors in its lower/upper triangles
15
```

Assuming an in-place variant how would one go about parallelizing this?

- Decomposition / distribution of A?
- Communication at which steps?

Pitch some ideas

### Answers: Now, about Parallelizing...

- Block decomposition means that some processors idle
- ► Row decomposition also leads to some idling, is described in Grama 8.3
- A cyclic decomposition leads to better balance
  - ► 100 x 100 matrix, 4 Procs, row cyclic
  - P0: rows 4\*i+0 = 0,4,8,12,...
  - P1: rows 4\*i+1 = 1,5,9,13,...
  - etc.
- Broadcast leading row from owning proc to all others

$P_0$	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
$P_1$	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
$P_2$	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
P <sub>3</sub>	0	0	0	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)
$P_4$	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
P <sub>5</sub>	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P <sub>6</sub>	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
$P_7$	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

$P_0$	1	(0,1)	(0,2)	(0,3) (0,4) (0,5) (0,6) (0,7)
P	0	1	(1,2)	(1,3) (1,4) (1,5) (1,6) (1,7)
P <sub>2</sub>	0	0	1	(2,3) (2,4) (2,5) (2,6) (2,7)
P <sub>3</sub>	0	0	0	1 (3,4) (3,5) (3,6) (3,7)
P <sub>4</sub>	0	0	0	(4,3)¥(4,4)¥(4,5)¥(4,6)¥(4,7)
P <sub>5</sub>	0	0	0	(5,3)¥(5,4)¥(5,5)¥(5,6)¥(5,7)
P <sub>6</sub>	0	0	0	(6,3)¥(6,4)¥(6,5)¥(6,6)¥(6,7)
P <sub>7</sub>	0	0	0	(7,3)\$\dagge(7,4)\$\dagge(7,5)\$\dagge(7,6)\$\dagge(7,7)\$
	_			

$P_0$	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
P <sub>1</sub>	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P <sub>2</sub>	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
P <sub>3</sub>	0	0	0	1	(3,4)	(3,5)	(3,6)	(3,7)
$P_4$	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
P <sub>5</sub>	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P <sub>6</sub>	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
$P_7$	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

- (a) Computation:
  - (i) A[k,j] := A[k,j]/A[k,k] for  $k \le j \le j$
  - (ii) A[k,k] := 1

#### (b) Communication:

One-to-all broadcast of row A[k,\*]

#### (c) Computation:

- (i) A[i,j] := A[i,j] A[i,k] × A[k,j]
  for k ≤ i ≤ n and k ≤ i ≤ n
- (ii) A[i,k] := 0 for  $k \le i \le n$

Figure 8.6 Gaussian elimination steps during the iteration corresponding to k = 3 for an 8  $\times$  8 matrix partitioned rowwise among eight processes.

### Analysis of LU Decomposition

- ▶ Serial algorithm runs in  $O(N^3)$
- Parallel approaches use
  - $1. \ N$  iterations of each row as the leading row
  - 2. Broadcast of leading row d to all P procs N broadcasts
  - 3. Parallel modification of N-d lower block of A[] to store L,U factors in it  $O(N^2/P)$
- lacktriangle For a ring of P procs to broad cast length N row

$$t_{broadcast} = (\log_2 P) \times t_s + t_w \times N \times P$$

leading to overall cost of

$$T = N \times (N^2/P + (\log_2 P) \times t_s + t_w \times N \times P)$$

which is  $O(N^3/P)$  overall complexity

- ▶ Main overhead is the need to broadcast at each step
  - Can pipeline Broadcast of the row, overlap with computation
  - ► Likely done by default in good implementations of MPI\_Bcast(): node proceeds with computation as soon as it passes on its messages as part of the broadcast