### CS410: Parallel Computing

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Applications and Algorithms from Dense Linear Algebra

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credits: James Demmel (CS267), Ananth Grama (slides accompanying the text book)

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#### This class and next...

- Applications and Algorithms from Dense Linear Algebra
  - Matrix multiplication, Matrix-Vector multiplication
  - Solving linear equations using Gauss Elimination
- "Thinking Parallel"
  - Synchronization requirement (have seen this)
  - Load balancing requirement (haven't seen this much)
  - Minimizing communication overhead requirement (haven't seen this much)

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## Matrix Multiplication

- Why study?
  - An important "kernel" in many linear algebra algorithms
  - Most studied kernel in high performance computing
  - Simple. Optimization ideas can be applied to other kernels
- Matrix representation
  - Matrix is a 2D array of elements. Computer memory is inherently linear
  - C++ and Fortran allow for definition of 2D arrays. 2D arrays stored row-wise in C++. Stored column-wise in Fortran. E.g.

```
// stores 10 arrays of 20 doubles each in C++
double** mat = new double[10][20];
```

## Storage Layout - Example

• Matrix (**2D**):A = 
$$\begin{bmatrix} A(0,0) & A(0,1) & A(0,2) \\ A(1,0) & A(1,1) & A(1,2) \\ A(2,0) & A(2,1) & A(2,2) \end{bmatrix}$$

A(i,j) = A(row, column) refers to the matrix element in the i<sup>th</sup> row and the j<sup>th</sup> column

Row-wise (/Row-major) storage in memory:

```
        A(0,0)
        A(0,1)
        A(0,2)
        A(1,0)
        A(1,1)
        A(1,2)
        A(2,0)
        A(2,1)
        A(2,2)
```

• Column-wise (/Column-major) storage in memory:

$$A(0,0)$$
  $A(1,0)$   $A(2,0)$   $A(0,1)$   $A(1,1)$   $A(2,1)$   $A(0,2)$   $A(1,2)$   $A(2,2)$ 

## Matrix Multiplication

- Three fundamental ways to think of the algorithm
  - Dot product / Inner product

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 1.5 + 2.7 & 1.6 + 2.8 \\ 3.5 + 4.7 & 3.6 + 4.8 \end{bmatrix}$$

Linear combination of left matrix columns

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 5 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 7 \begin{bmatrix} 2 \\ 4 \end{bmatrix} \quad 6 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 8 \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

Sum of outer products

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \begin{bmatrix} 5 & 6 \end{bmatrix} + \begin{bmatrix} 2 \\ 4 \end{bmatrix} \begin{bmatrix} 7 & 8 \end{bmatrix}$$

#### Review: Matrix-Matrix Product

Computing Matrix-Matrix product C = C + AB,  $A \in \mathbb{R}^{m \times r}$ ,  $B \in \mathbb{R}^{r \times n}$ ,  $C \in \mathbb{R}^{m \times n}$ 

$$\begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mr} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ b_{r1} & b_{r2} & \cdots & b_{rn} \end{bmatrix}$$

$$\mathsf{A} \times \mathsf{B} \ = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + \ldots + a_{1r}b_{r1} & \ldots & a_{11}b_{1n} + a_{12}b_{2n} + \ldots + a_{1r}b_{rn} \\ \vdots & \vdots & \vdots \\ a_{m1}b_{11} + a_{m2}b_{21} + \ldots + a_{mr}b_{r1} & \ldots & a_{m1}b_{1n} + a_{m2}b_{2n} + \ldots + a_{mr}b_{rn} \end{bmatrix}$$

Notice that:

- subscript on a varies from 1 to m in a column (i.e. m rows exist)
- subscript on a varies from 1 to r in a row (i.e. r columns exist)

If we treat a<sub>i</sub> and b<sub>i</sub> as a vector of size r and for such m vectors:

$$=\begin{bmatrix} a_1^Tb_1 & . & . & a_1^Tb_n \\ . & . & . & . \\ a_m^Tb_1 & . & . & a_m^Tb_n \end{bmatrix} \qquad \begin{array}{c} a_i^T \in \mathbb{R}^{1\times r}, b_j \in \mathbb{R}^{r\times 1} \\ & \text{i ranges from 1 to m} \\ & \text{j ranges from 1 to n} \end{array}$$

## Review: Matrix-Matrix Product using Dot Product Formulation

• Pseudocode - Matrix-Matrix product: C = C + AB,  $A \in \mathbb{R}^{m \times r}$ ,  $B \in \mathbb{R}^{r \times n}$ ,  $C \in \mathbb{R}^{m \times n}$ • for i=1 to m for j=1 to n //compute updates involving dot products  $c_{ij} = c_{ij} + a_i^T b_i$ 

## Review: Matrix-Matrix Product using Dot Product Formulation

• Pseudocode - Matrix-Matrix product: C = C + AB,  $A \in \mathbb{R}^{m \times r}$ ,  $B \in \mathbb{R}^{r \times n}$ ,  $C \in \mathbb{R}^{m \times n}$ 

Expanded:

```
for i=1 to m for j=1 to n for k=1 to r c_{ij} = c_{ij} + a_{ik}b_{kj}
```

## Review: Matrix-Matrix Product using Dot Product Formulation

- P Cost? (of C = C + AB,  $A \in \mathbb{R}^{m \times r}$ ,  $B \in \mathbb{R}^{r \times n}$ ,  $C \in \mathbb{R}^{m \times n}$ )

   Per dot-product cost = 2r  $(a_i, b_j \in \mathbb{R}^r)$  Total cost = 2mnr or O(mnr)...

  for i=1 to m

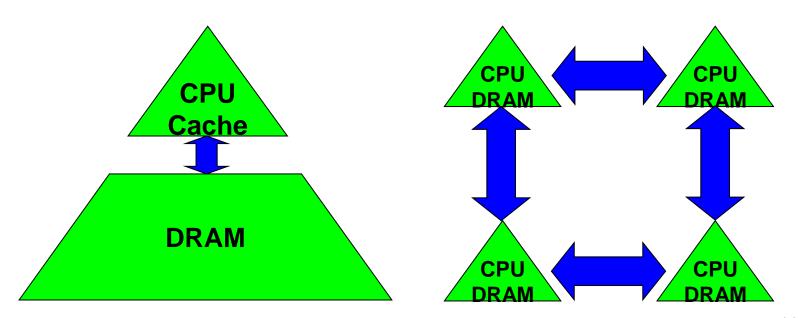
  for j=1 to n

  for k=1 to r  $c_{ij} = c_{ij} + a_{ik}b_{kj}$
- The above is the arithmetic cost. What about other costs?

#### Costs Involved

#### Algorithms have two costs:

- 1.Arithmetic (FLOPS)
- 2. Communication: moving data between
  - levels of a memory hierarchy (sequential case)
  - processors over a network (parallel case).



#### Costs Involved

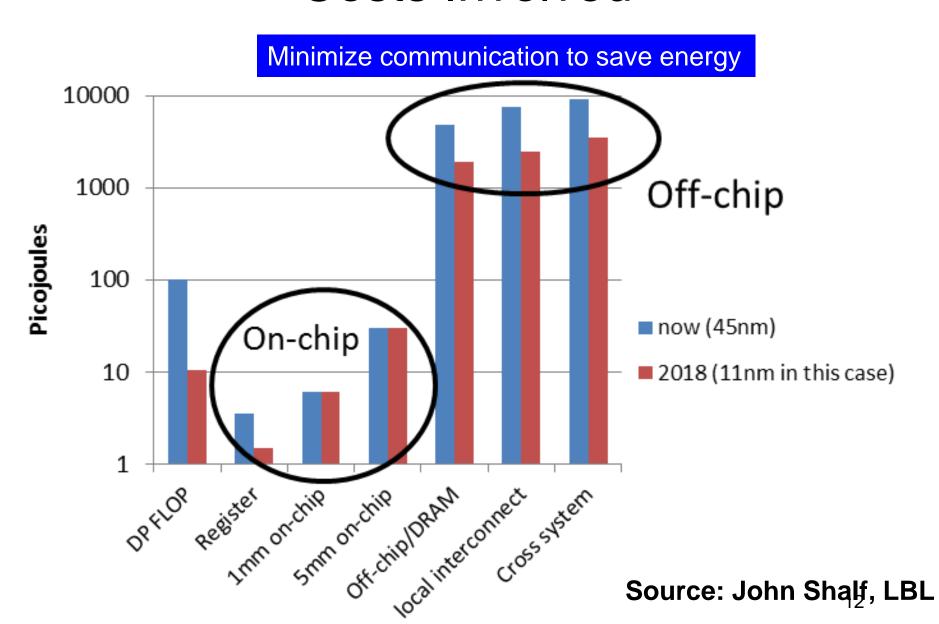
- Running time of an algorithm is sum of 3 terms:
  - 1. # flops \* time\_per\_flop
  - 2. # words moved / bandwidth
  - 3. # messages \* latency

communication

```
Run on (12 X 2592.01 MHz CPU s)
                                                  Matrix-Matrix Addition
CPU Caches:
 L1 Data 32 KiB (x6)
                                           Minimize communication to save time
 L1 Instruction 32 KiB (x6)
 L2 Unified 256 KiB (x6)
 L3 Unified 12288 KiB (x1)
Load Average: 0.07, 0.02, 0.07
Benchmark
                                  Time
                                                   CPU
                                                         Iterations UserCounters...
BM AddByCol/64/64
                                                             212929 items per second=1.25254G/s
                              3270 ns
                                              3270 ns
BM AddByCol/128/128
                                                              17617 items per second=412.272M/s
                              39741 ns
                                              39741 ns
BM AddByCol/256/256
                            314880 ns
                                             314878 ns
                                                               2241 items per second=208.132M/s
                                                                545 items per second=205.326M/s
BM AddByCol/512/512
                           1276733 ns
                                            1276723 ns
BM AddByRow/64/64
                                                            1042737 items per second=5.91004G/s
                               693 ns
                                                693 ns
                                                             271766 items per second=6.64813G/s
BM AddByRow/128/128
                              2464 ns
                                               2464 ns
BM_AddByRow/256/256
                                                              63210 items_per_second=5.88639G/s
                             11134 ns
                                              11133 ns
  AddRyRgw/513/512
                                                              15576 items per second=5.91041G/s
                             44353 ns
                                              44353 ns
```

(Source code and further reading)

#### Costs Involved



## Computational Intensity

- Connection between computation and communication cost
- Average number of operations performed per data element (word) read/written from slow memory
  - E.g. Read/written m words from memory. Perform f operations on m words.
  - Computational Intensity q = f/m (flops per word).
- Goal: we want to maximize the computational intensity
  - We want to minimize words moved (read/written)
  - We want to minimize messages sent

# Communication Cost – Matrix-Matrix Product

```
//Assume A, B, C are all nxn
for i=1 to n
for j=1 to n
  for k=1 to n
    C(i,j)=C(i,j) + A(i,k)*B(k,j)
```

- loop k=1 to n: read C(i,j) into fast memory and update in fast memory
- End of loop k=1 to n: write C(i,j) back to slow memory

- n<sup>2</sup> words read: each row of A read once for each i.
- Assume that row i of A stays in fast memory during j=2, .. J=n
- Reading a row i of A

n<sup>2</sup> words read and n<sup>2</sup> words written (each entry of C read/written to memory once).
= 2 n<sup>2</sup> words read/written

total cost =  $3 n^2 + n^3$  (if the cache size is n+n+1)

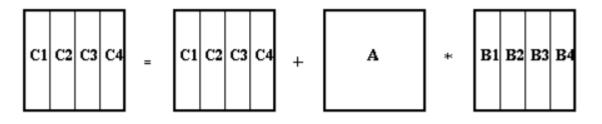
- Reading column j of B
- Suppose there is space in fast memory to hold only one column of B (in addition to one row of A and 1 element of C), then every column of B is read once in inner two loops.
- Each column of B read n times including outer i loop = n<sup>3</sup> words read

# Computational Intensity – Matrix-Matrix Product

- Words moved =  $n^3+3n^2 = n^3+O(n^2)$
- Number of arithmetic operations = 2n<sup>3</sup>
- computational intensity q≈2n³/n³ = 2. (computation to communication ratio)
- Can we do better?

## **Blocked Matrix Multiply**

• For N=4:



$$\begin{bmatrix} Cj \\ = \end{bmatrix} \begin{bmatrix} Cj \\ + \end{bmatrix} \begin{bmatrix} A \\ \end{bmatrix} * \begin{bmatrix} Bj \\ \end{bmatrix} = \begin{bmatrix} Cj \\ + \sum \\ k=1 \end{bmatrix} * \begin{bmatrix} A \\ \end{bmatrix} = \begin{bmatrix} A \\ \end{bmatrix}$$

$$A(:,k) \quad Bj(k,:)$$

```
for j=1 to N
//Read entire Bj into fast memory
//Read entire Cj into fast memory
for k=1 to n
    //Read column k of A into fast memory
    Cj=Cj + A(*,k) * Bj(k,*)
    //Write Cj back to slow memory
```

# Computational Intensity - Blocked Matrix Multiply

```
for j=1 to N
//Read entire Bj into fast memory of B read once.
//Read entire Cj into fast memory
for k=1 to n
//Read column k of A into fast memory column of A read N times
C(*,j)=C(*,j) + A(*,k)*Bj(k,*) //outer-product
//Write Cj back to slow memory
• Number of arithmetic operations = <math>2n^3 read/write each entry of C
• q=2n^3/(N+3)n^2=2n/N. Good!
```

### Blocked Matrix Multiply - General

- $A, B, C \in \mathbb{R}^{n \times n}$
- We wish to update C block-by-block:  $C_{ij} = C_{ij} + \sum_{k=1}^{p} A_{ik} B_{kj}$ 
  - Assume that blocks of A, B, and C fit in cache.  $C_{ij}$  is roughly n/q by n/r,  $A_{ij}$  is roughly n/q by n/p,  $B_{ij}$  is roughly n/p by n/r.
  - But how to choose block parameters p, q, r such that assumption holds for a cache of size M?
    - i.e. given the constraint that  $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \le M$

## Blocked Matrix Multiply - General

• Maximize  $\frac{2n^3}{qrp}$  subject to  $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \le M$ 

$$-q_{opt} = p_{opt} = r_{opt} \approx \sqrt{\frac{n^2}{3M}}$$

 Each block should roughly be a square matrix and occupy one third of the cache size

i.e. for a bxb block matrix,  $3b^2 = \text{cache size} = M$ 

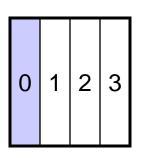
#### **Review: Blocked Matrix Multiply**

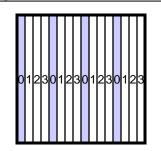
 Blocked Matmul C = A-B breaks A, B and C into blocks with dimensions that depend on cache size

```
... Break A<sup>nxn</sup>, B<sup>nxn</sup>, C<sup>nxn</sup> into bxb blocks labeled A(i,j), etc
... b chosen so 3 bxb blocks fit in cache
for i = 1 to n/b, for j=1 to n/b, for k=1 to n/b
C(i,j) = C(i,j) + A(i,k)-B(k,j) ... b x b matmul, 4b<sup>2</sup> reads/writes
```

- When b=1, get "naïve" algorithm, want b larger ...
- $(n/b)^3 \cdot 4b^2 = 4n^3/b$  reads/writes altogether
- Minimized when  $3b^2$  = cache size = M, yielding  $O(n^3/M^{1/2})$  reads/writes

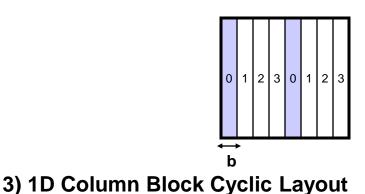
#### Different Parallel Data Layouts for Matrices (not all!)





1) 1D Column Blocked Layout

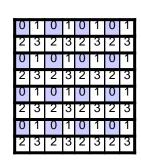
2) 1D Column Cyclic Layout



4) Row versions of the previous layouts

0 1 2 3

5) 2D Row and Column Blocked Layout



**Generalizes others** 

6) 2D Row and Column Block Cyclic Layout

#### Communication Lower Bounds: Prior Work on Matmul

- Assume n<sup>3</sup> algorithm (i.e. not Strassen-like)
- Sequential case, with fast memory of size M
  - Lower bound on #words moved to/from slow memory =  $\Omega$  (n<sup>3</sup> / M<sup>1/2</sup>) [Hong, Kung, 81]
  - Attained using blocked or cache-oblivious algorithms
- Parallel case on P processors:
  - Let M be memory per processor; assume load balanced
  - Lower bound on #words moved =  $\Omega$  ((n<sup>3</sup>/p) / M<sup>1/2</sup>)) [Irony, Tiskin, Toledo, 04]
  - If  $M = 3n^2/p$  (one copy of each matrix), then lower bound =  $\Omega$  ( $n^2/p^{1/2}$ )
  - Attained by SUMMA, Cannon's algorithm

## Load Balancing

- Let a task compute C<sub>ii</sub>
- Divide the task among p<sub>row</sub> x p<sub>col</sub> processors
  - Lay them in 2D and represent a processor in  $x^{th}$  row and  $y^{th}$  column as Proc(x,y).  $1 <= x <= p_{row}$   $1 <= y <= p_{col}$
- Load Balancing (balancing the arithmetic computation assigned to processors)
  - 1. 2D block distribution
    - Assigns continuous block updates
  - 2. 2D block cyclic distribution
    - Assigns blocks of C in strides of p<sub>row</sub> (along y) and p<sub>col</sub> (along x)

## Load Balancing - Block Distribution

• M=8, N=9,  $p_{row} = 2$ ,  $p_{col} = 3$ 

# Load Balancing - Block Cyclic Distribution

Proc(1,1)	Proc(1,2)	Proc(1,3)
$\left\{\begin{array}{cccc} C_{11} & C_{14} & C_{17} \\ C_{31} & C_{34} & C_{37} \\ C_{51} & C_{54} & C_{57} \\ C_{71} & C_{74} & C_{77} \end{array}\right\}$	$ \left\{ \begin{array}{cccc} C_{12} & C_{15} & C_{18} \\ C_{32} & C_{35} & C_{38} \\ C_{52} & C_{55} & C_{58} \\ C_{72} & C_{75} & C_{78} \end{array} \right\} $	$\left\{ \begin{array}{ccc} C_{13} & C_{16} & C_{19} \\ C_{33} & C_{36} & C_{39} \\ C_{53} & C_{56} & C_{59} \\ C_{73} & C_{76} & C_{79} \end{array} \right\}$
$\left\{egin{array}{ll}  ext{Proc}(2,1) \ C_{21} & C_{24} & C_{27} \ C_{41} & C_{44} & C_{47} \ C_{61} & C_{64} & C_{67} \ C_{81} & C_{84} & C_{87} \end{array} ight\}$	$ \left\{ \begin{array}{ccc} C_{22} & C_{25} & C_{28} \\ C_{42} & C_{45} & C_{48} \\ C_{62} & C_{65} & C_{68} \\ C_{82} & C_{85} & C_{88} \end{array} \right\} $	$ \left\{ \begin{array}{ccc} C_{23} & C_{26} & C_{29} \\ C_{43} & C_{46} & C_{49} \\ C_{63} & C_{66} & C_{69} \\ C_{83} & C_{86} & C_{89} \end{array} \right\} $

• M=8, N=9,  $p_{row} = 2$ ,  $p_{col} = 3$ 

#### **Exercise**

- Are the 2D block- and block-cyclic- distribution schemes load balanced for C=C+AB update?
- Scenario 1: A is lower-triangular and B is uppertriangular
  - Block distribution:
    - Load balance depends on number of processors (gets worse with increasing number of processors)
  - Block-cyclic distribution
    - Increasingly balanced as the problem size grows
- Scenario 2: First few rows of A are zeros. First few columns of B are zeros

#### Load Balance and C=AB

When A is lower triangular, and B is upper triangular:

```
C11 C12 C13 C14
A11 0
                      B11 B12 B13 B14
                                                                   P12
A21 A22 0
                           B22 B23 B24
                                                 C21 C22 C23 C24
                                                C31 C32 C33 C34
A31 A32 A33 0
                      0
                           0
                               B33 B34
                                                                   P22
                                           P21
                                                 C41 C42 C43 C44
A41 A42 A43 A44
                               0
                                   B44
```

If Pxy denotes a processor and  $1 <= x <= p_{row}$   $1 <= y <= p_{col}$ , for prow=2, pcol=2, P22 does the most work and P11 does the least work if block-distribution is followed.

#### Load Balance and C=AB

When A is lower triangular, and B is upper triangular:

if block-cyclic distribution is followed:

P11 gets updates C11, C13, C31, and C33 P22 gets updates C22, C42, C24, and C44

- Let there be p processors doing C=C+AB (A=mxr, B=rxn and C=mxn. Also A=MxR, B=RxN, C=MxN)
- Assume block-cyclic distribution (so that arithmetic cost is evenly spread among all processors (i.e. load balanced))
- Let individual processors perform Cij=Cij + Aik \* Bkj @ F flops/sec
- Time to move w words into and out of processor's memory = 1 + b\*w (l=latency b=bandwidth)

Time spent by each processor on doing the computation:  $T_{arith}$  (p)  $\sim$  (2mnr/p) / F

• Let  $T_{data}(p)$  be the time that each processor spends in acquiring the data (communication cost)

Speedup with p processors: 
$$S(P) \approx \frac{T_{arith}(1)}{T_{arith}(p) + T_{data}(p)} = \frac{p}{1 + \frac{T_{data}(p)}{T_{arith}(P)}}$$
 Communication to compute ratio

- An individual processor performing Cij=Cij + Aik \* Bkj would require blocks:
  - Cij (count=Num<sub>Cij</sub>)
  - Ai1, Ai2, . ., AiR (count=Num<sub>Aij</sub>)
  - B1j, B2j, . ., BRj (count=Num<sub>Bij</sub>)
- Suppose each block is uniformly subdivided as: m = m1\*M (i.e. every submatrix in A and C (Aij and Cij) would have m1 rows.). Similarly, r = r1\*R (i.e. every submatrix in A would have r1 columns and submatrix in B would have r1 rows.) and n=n1\*N.
- Then:
  - Time required to bring one block of C (Cij) into fast memory = 1 + b\*m1\*n1
  - Time required to bring one block of B (Bij) into fast memory = 1 + b\*r1\*n1
  - Time required to bring one block of A (Aij) into fast memory = 1 + b\*m1\*r1
- Therefore,  $T_{data}(p) = Num_{Cij}(1 + b*m1*n1) + Num_{Bij}(1 + b*r1*n1) + Num_{Aij}(1 + b*m1*r1)$

The blocked MatMul:

- This algorithm has  $Num_{Cij} = 2MN/p$ ,  $Num_{Aij} = RMN/p$ ,  $Num_{Bij} = RMN/p$
- Communication to compute ratio:  $\frac{T_{data}(p)}{T_{arith}(P)} \approx \frac{F}{2} \left( l \frac{(2+2R)}{m1n1r} + b \left( \frac{2}{r} + \frac{1}{n1} + \frac{1}{m1} \right) \right)$
- Conclusion:
  - Speedup degrades as floprate F increases.
  - Speedup improves if latency and bandwidth (I and b) decrease or m1, n1, r1 increase

#### Observations:

- Communication to compute ratio for the previous matmul method doesn't depend on number of processors
- Fast Memory Capacity vs. Communication cost tradeoff
  - Each submatrix of A loaded N/pcol times
  - Each submatrix of B loaded M/prow times

What if each task computing Cij can get all the required submatrices in fast memory? i.e. the fast memory is big enough so that once loaded, submatrices stay there till end of computation

- Each processor could access C, A, and B matrices.
  - Shared-memory model.

What if A, B, and C together don't fit in RAM?

Even if it fits, it takes enormous amount of time to do the computation?