Lecture 13

Matrix Multiplication

Announcements

- Project Progress report, due next Weds 11/28

Today’s lecture

- Cannon’s Matrix Multiplication Algorithm
- 2.5D “Communication avoiding”
- SUMMA

Parallel matrix multiplication

- Assume p is a perfect square
- Each processor gets an $n/\sqrt{p} \times n/\sqrt{p}$ chunk of data
- Organize processors into rows and columns
- Assume that we have an efficient serial matrix multiply (dgemm, sgemm)

p(0,0)	p(0,1)	p(0,2)
p(1,0)	p(1,1)	p(1,2)
p(2,0)	p(2,1)	p(2,2)

Canon's algorithm

- Move data incrementally in √p phases
- Circulate each chunk of data among processors within a row or column
- In effect we are using a ring broadcast algorithm
- Consider iteration i=1, j=2:

C[1,2] = A[1,0]*B[0,2] + A[1,1]*B[1,2] + A[1,2]*B[2,2]

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)

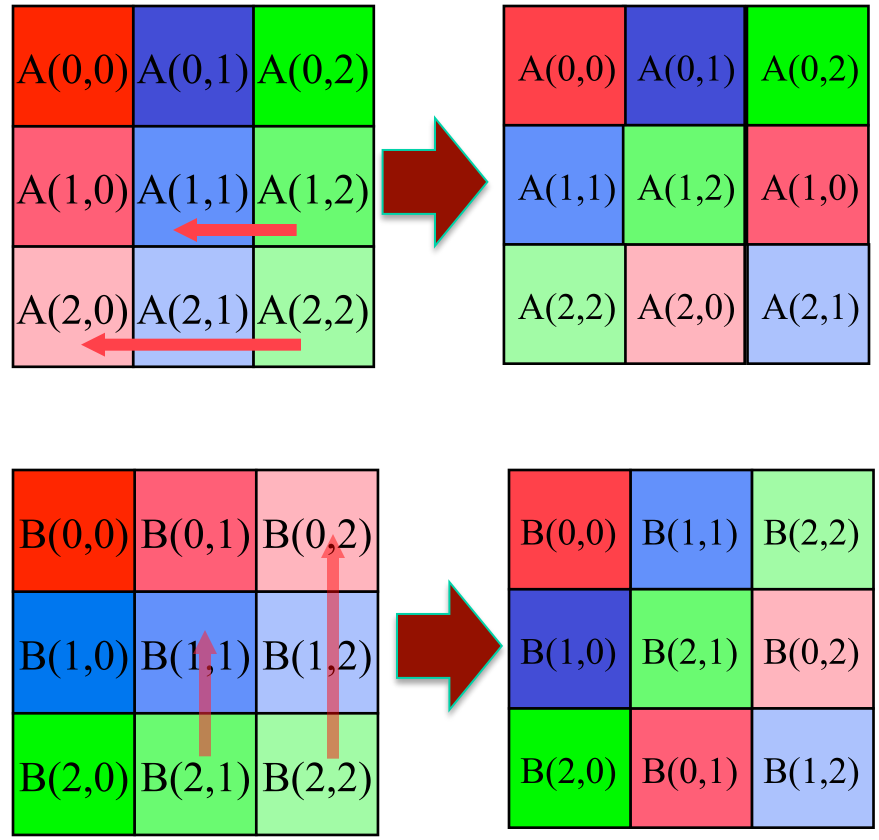
B(0,0)	B(0,1)	B(0,2)
B(1,0)	B(1,1)	B(1,2)
B(2,0)	B(2,1)	B(2,2)

Image: Jim Demmel

Canon’s algorithm

C[1,2] = A[1,0]*B[0,2] + A[1,1]*B[1,2] + A[1,2]*B[2,2]

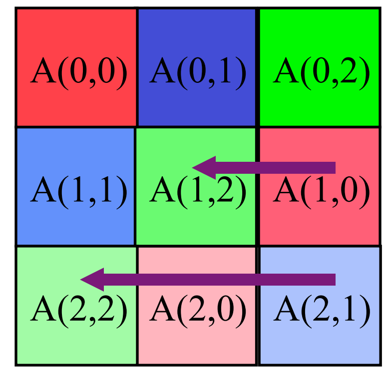
- We want A[1,0] and B[0,2] to reside on the same processor initially
- Shift rows and columns so the next pair of values A[1,1] and B[1,2] line up
- And so on with A[1,2] and B[2,2]

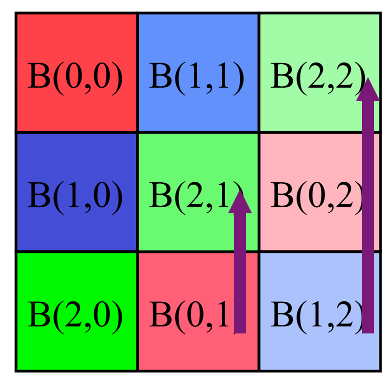


Skewing the matrices

C[1,2] = A[1,0]*B[0,2] + A[1,1]*B[1,2] + A[1,2]*B[2,2]

- We first *skew* the matrices so that everything lines up
- Shift each row *i* by *i* columns to the left using sends and receives
- Communication wraps around
- Do the same for each column

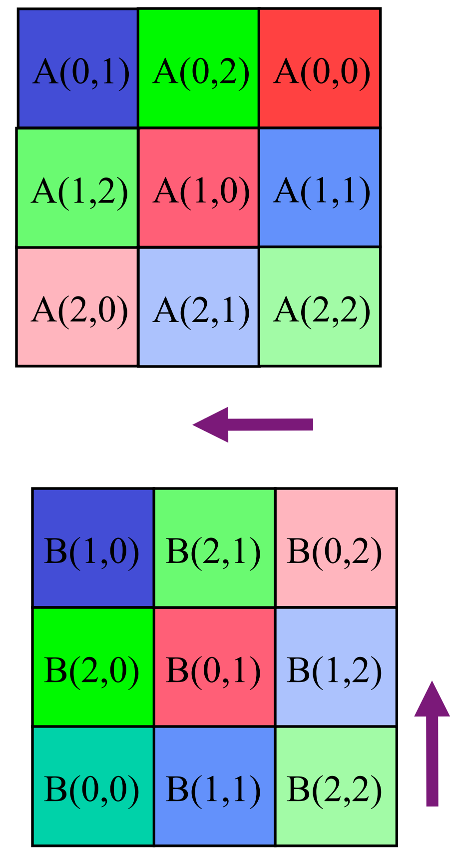




Shift and multiply

C[1,2] = A[1,0]*B[0,2] + A[1,1]*B[1,2] + A[1,2]*B[2,2]

- Takes √p steps
- Circularly shift
  - each row by 1 column to the left
  - each column by 1 row to the left
- Each processor forms the product of the two local matrices adding into the accumulated sum



Cost of Cannon's Algorithm

forall i=0 **to** √p -1
    CShift-left A[i; :] by i   **// T= α+βn²/p**
forall j=0 **to** √p -1
    Cshift-up B[: , j] by j   **// T= α+βn²/p**
for k=0 **to** √p -1
    forall i=0 **to** √p -1 **and** j=0 to √p -1
        C[i,j] += A[i,j]*B[i,j]   **// T = 2*n³/p^{3/2}**
        CShift-leftA[i; :] by 1   **// T= α+βn²/p**
        Cshift-up B[: , j] by 1   **// T= α+βn²/p**
    end forall
end for

$$T_P = 2n^3/p + 2(\alpha(1+\sqrt{p}) + \beta n^2/(1+\sqrt{p})/p)$$

$$E_P = T_1/(pT_P) = (1 + \alpha p^{3/2}/n^3 + \beta\sqrt{p}/n))^{-1}$$

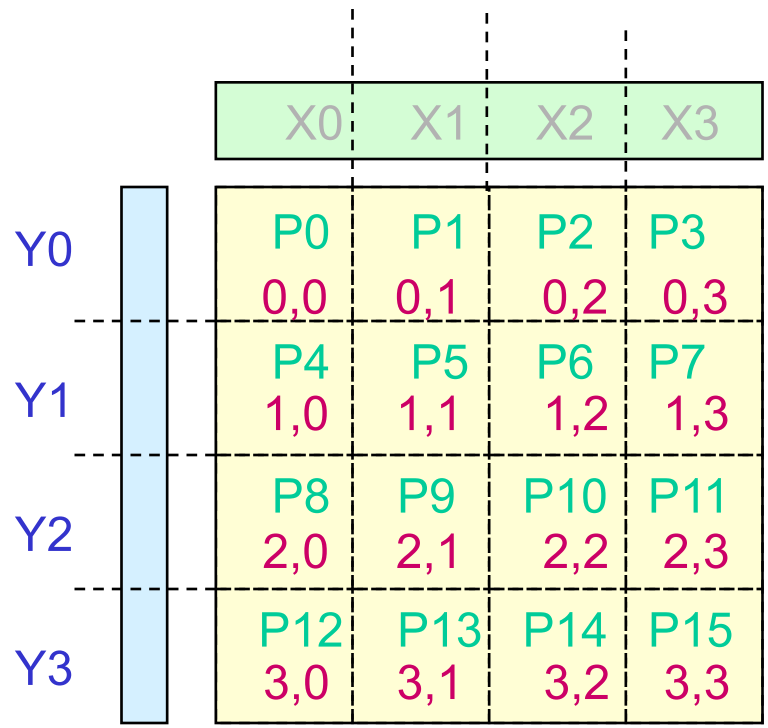
$$\approx (1 + O(\sqrt{p}/n))^{-1}$$

$E_P \rightarrow 1$ as $(n/\sqrt{p})$ grows [sqrt of data / processor]

Implementation

Communication domains

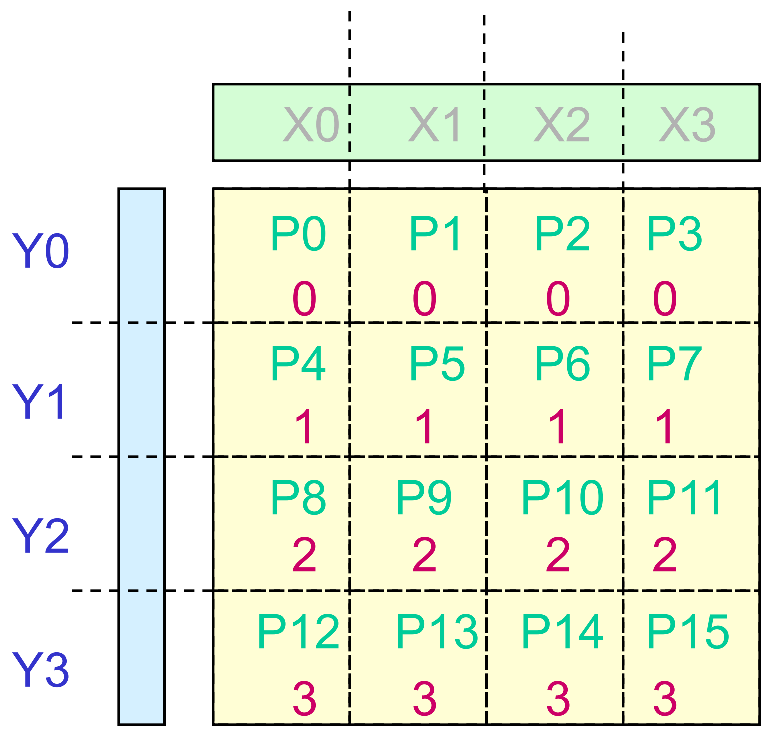
- Cannon's algorithm shifts data along rows and columns of processors
- MPI provides communicators for grouping processors, reflecting the communication structure of the algorithm
- An MPI communicator is a name space, a subset of processes that communicate
- Messages remain within their communicator
- A process may be a member of more than one communicator



Establishing row communicators

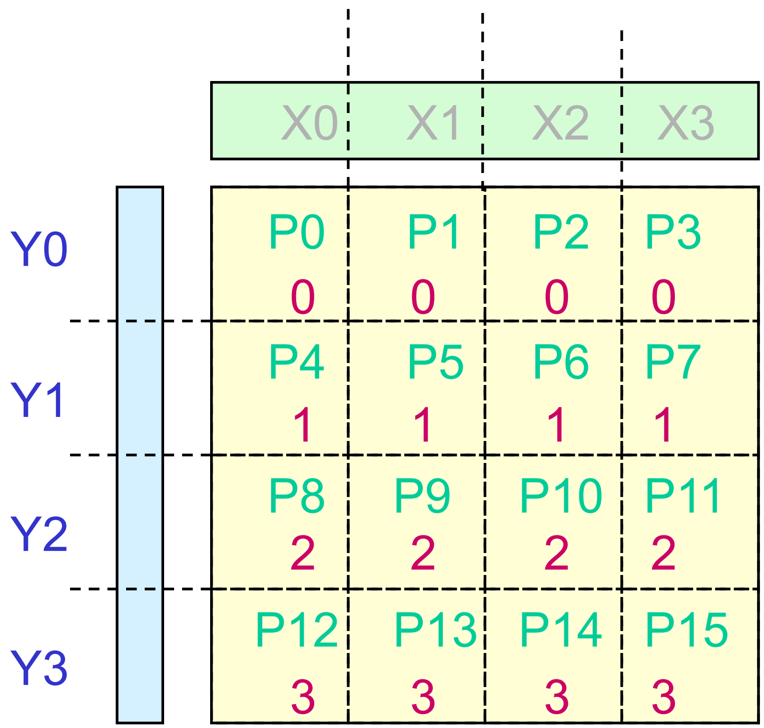
- Create a communicator for each row and column
- By Row

key = myRank div √P



Creating the communicators

MPI_Comm rowComm;
MPI_Comm_split(MPI_COMM_WORLD,
  myRank / √P, myRank, &rowComm);
MPI_Comm_rank(rowComm,&myRow);



- Each process obtains a new communicator
- Each process' rank relative to the new communicator
- Rank applies to the respective communicator only
- Ordered according to myRank

More on Comm_split

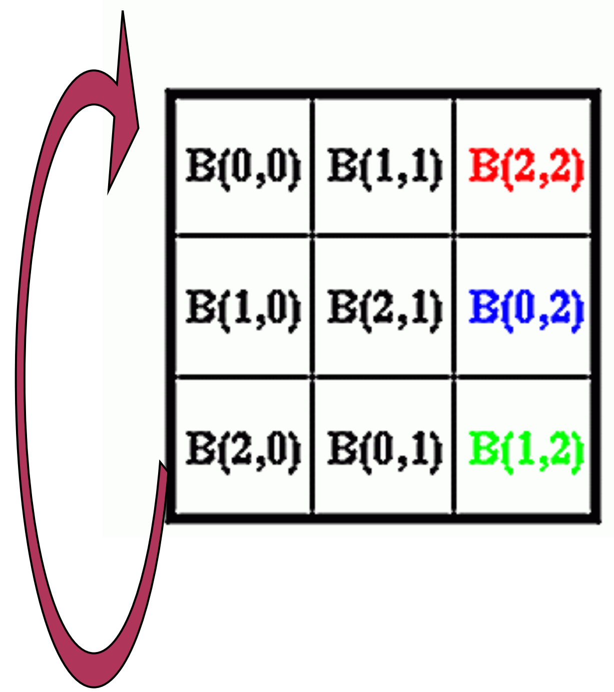
**MPI_Comm_split(MPI_Comm comm, int splitKey,
int rankKey, MPI_Comm* newComm)**

- Ranks assigned arbitrarily among processes sharing the same **rankKey** value
- May exclude a process by passing the constant **MPI_UNDEFINED** as the **splitKey**
- Return a special **MPI_COMM_NULL** communicator
- If a process is a member of several communicators, it will have a rank within each one

Circular shift

- Communication with columns (and rows

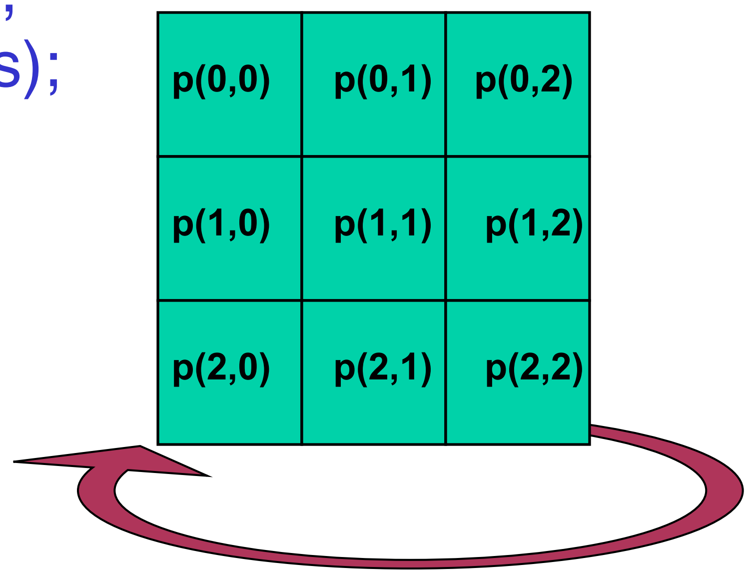
p(0,0)	p(0,1)	p(0,2)
p(1,0)	p(1,1)	p(1,2)
p(2,0)	p(2,1)	p(2,2)



Circular shift

```
MPI_Comm_rank(rowComm,&myidRing);
MPI_Comm_size(rowComm,&nodesRing);
int next = (myidRng + 1 ) % nodesRing;
MPI_Send(&X,1,MPI_INT,next,0, rowComm);
MPI_Recv(&XR,1,MPI_INT,
            MPI_ANY_SOURCE,
            0, rowComm, &status);
```

Processes 0, 1, 2 are in one communicator because they share the same value of key (0)
Processes 3, 4, 5are in another (1), and so on



Today's lecture

- Cannon's Matrix Multiplication Algorithm
- 2.5D "Communication avoiding"
- SUMMA

Motivation

- Relative to arithmetic speeds, communication is becoming more costly with time
- Communication can be data motion on or off-chip, across address spaces
- We seek algorithms that increase the amount of work (flops) relative to the amount of data they move

Communication lower bounds on Matrix Multiplication

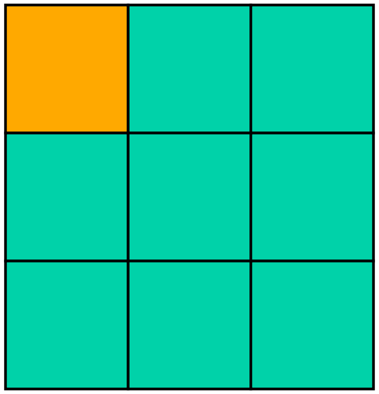
- Assume we are using an $O(n^3)$ algorithm
- Let M = Size fast memory (cache/local memory)
- Sequential case: # slow memory references
  $\Omega(n^3 / \sqrt{M}))$ [Hong and Kung '81]
- Parallel, p = # processors,
  μ = Amount of memory needed to store matrices
  - Refs to remote memory
    $\Omega(n^3 /(p\sqrt{\mu}))$ [Irony, Tiskin, Toledo, '04]
  - If $\mu = 3n^2/p$ (one copy of A, B, C) ⇒
    lower bound = $\Omega(n^2 /\sqrt{p})$ words
  - Achieved by Cannon's algorithm ("2D algorithm")
  - $T_P = 2n^3/p + 4\sqrt{p}\,(\alpha + \beta n^2/p)$

Canon's Algorithm - optimality

- General result
  - If each processor has M words of local memory …
  - … at least 1 processor must transmit Ω (# flops / $M^{1/2}$) words of data
- If local memory $M = O(n^2/p)$ …
  - at least 1 processor performs $f \geq n^3/p$ flops
  - … lower bound on number of words transmitted by at least 1 processor

$$\Omega\left((n^3/p) / \sqrt{(n^2/p)}\right) = \Omega\left((n^3/p) / \sqrt{M}\right)$$

$$= \Omega\left(n^2 / \sqrt{p}\right)$$



New communication lower bounds – direct linear algebra [Ballard &Demmel '11]

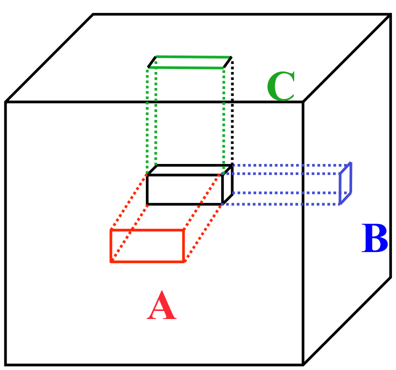
- Let M = amount of fast memory per processor
- Lower bounds
  - # words moved by at least 1 processor

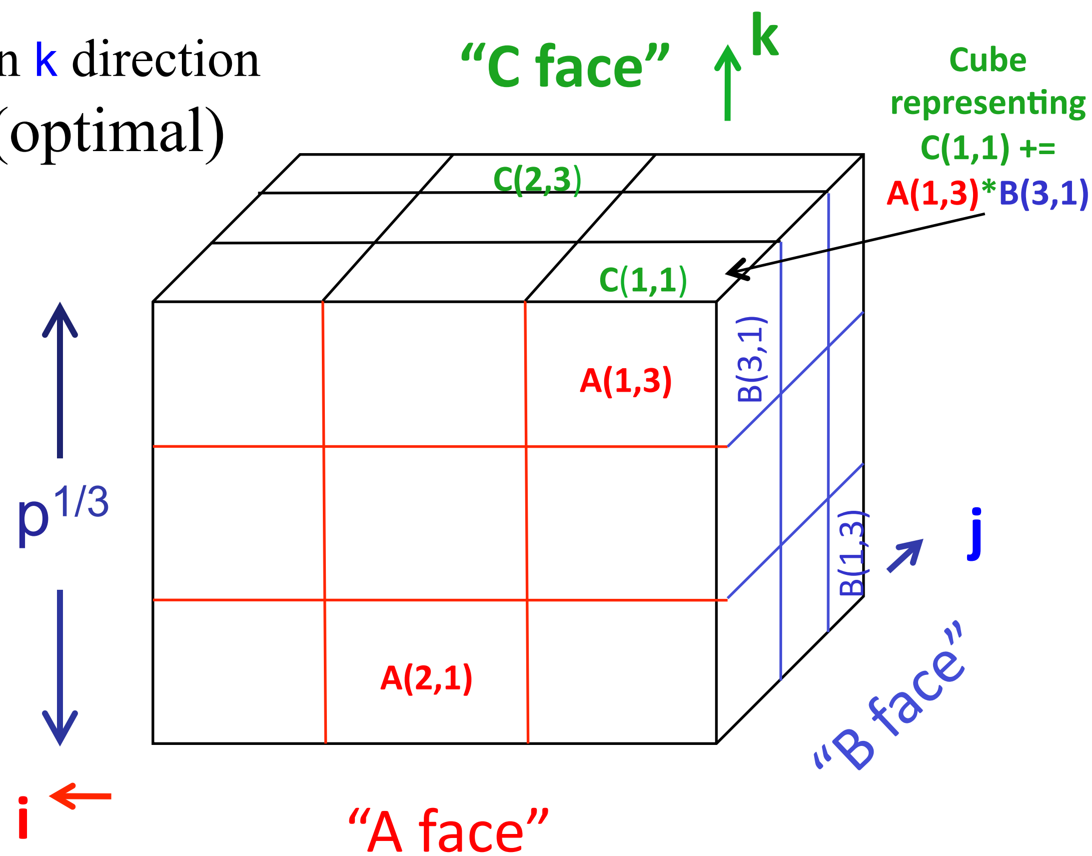
    Ω (# flops / $M^{1/2}$))
  - # messages sent by at least 1 processor

    Ω (# flops / $M^{3/2}$)
- Holds not only for Matrix Multiply but many other "direct" algorithms in linear algebra, sparse matrices, some graph theoretic algorithms
- Identify 3 values of M
  - 2D (Cannon's algorithm)
  - 3D (Johnson's algorithm)
  - 2.5D (Ballard and Demmel)

Johnson's 3D Algorithm

- 3D processor grid: $p^{1/3} \times p^{1/3} \times p^{1/3}$
  - Bcast A (B) in j (i) direction ($p^{1/3}$ redundant copies)
  - Local multiplications
  - Accumulate (Reduce) in k direction
- Communication costs (optimal)
  - Volume = $O(n^2/p^{2/3})$
  - Messages = $O(\log(p))$
- Assumes space for $p^{1/3}$ redundant copies
- Trade memory for communication



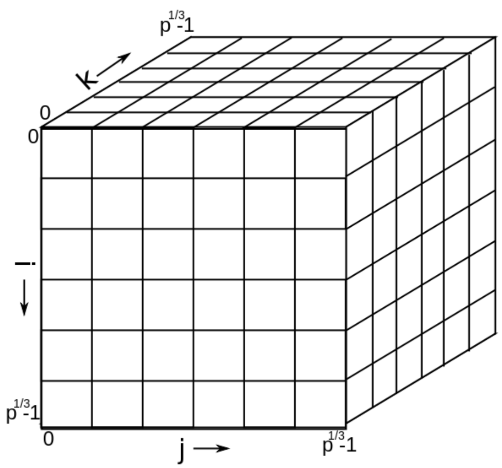


Source: Edgar Solomonik

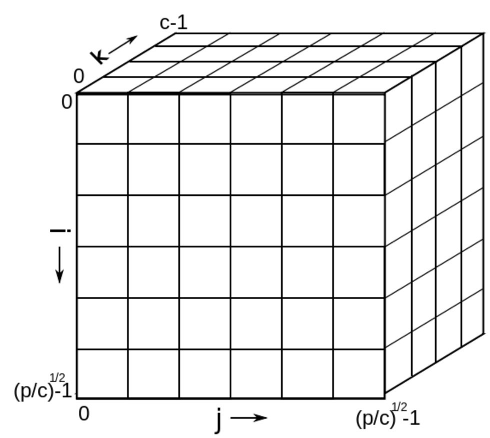
2.5D Algorithm

- What if we have space for only $1 \le c \le p^{1/3}$ copies ?
- $M = \Omega(c \cdot n^2/p)$
- Communication costs : lower bounds
  - Volume = $\Omega(n^2 /(cp)^{1/2})$; Set $M = c \cdot n^2/p$ in Ω (# flops / $M^{1/2}$))
  - Messages = $\Omega(p^{1/2} / c^{3/2})$; Set $M = c \cdot n^2/p$ in Ω (# flops / $M^{3/2}$))
- 2.5D algorithm "interpolates" between 2D & 3D algorithms

3D



2.5D



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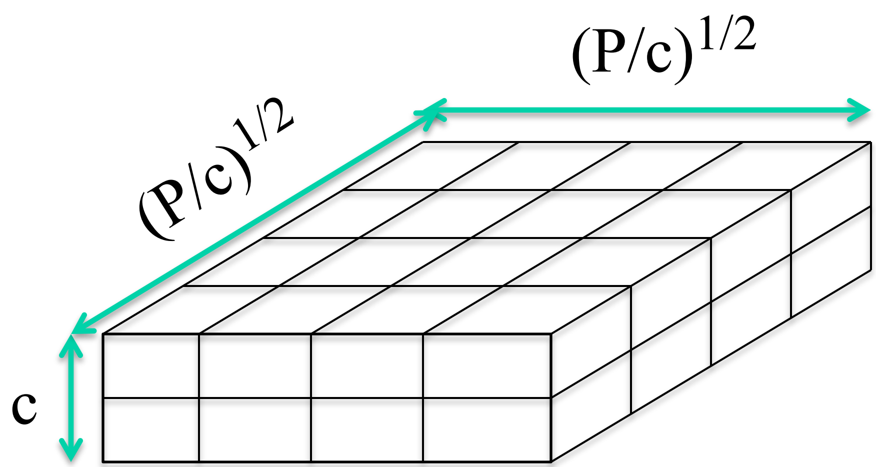
2.5D Algorithm

- Assume can fit cn^2/P data per processor, $c>1$
- Processors form $(P/c)^{1/2}$ x $(P/c)^{1/2}$ x c grid

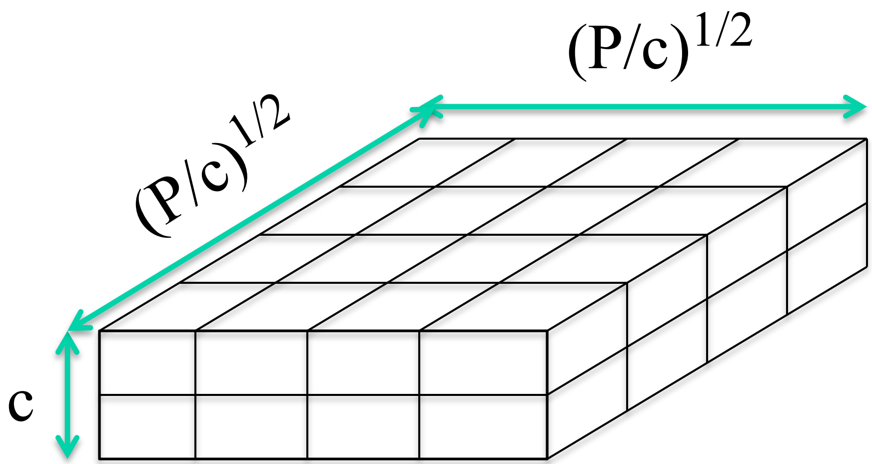


Example: $P = 32$, $c = 2$

Source Jim Demmel

2.5D Algorithm

- Assume can fit cn^2/P data per processor, $c>1$
- Processors form $(P/c)^{1/2}$ x $(P/c)^{1/2}$ x c grid



Initially P(i,j,0) owns A(i,j) &B(i,j) each of size $n(c/P)^{1/2}$ x $n(c/P)^{1/2}$

(1) P(i,j,0) broadcasts A(i,j) and B(i,j) to P(i,j,k)

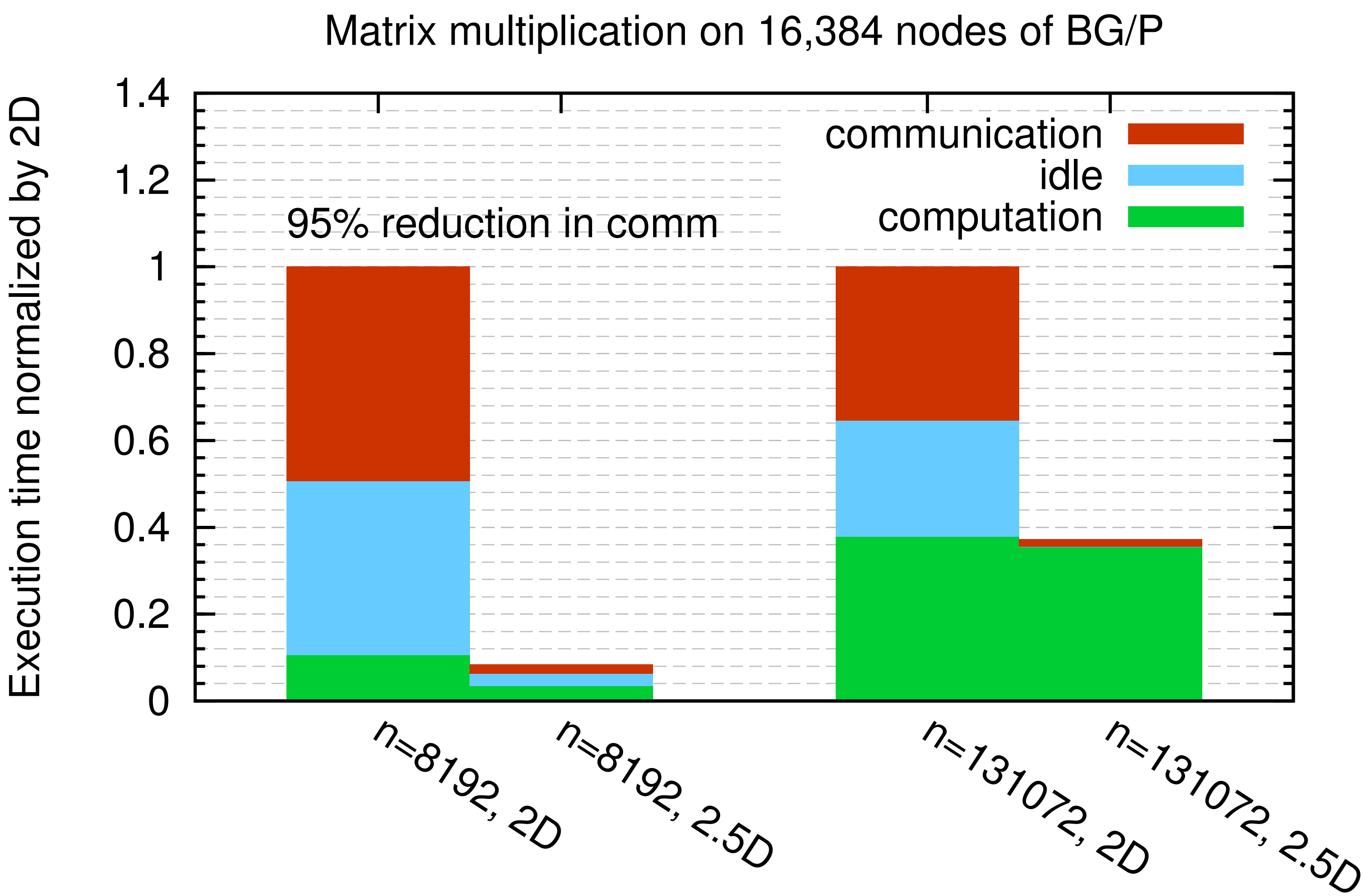
(2) Processors at level k perform 1/c-th of SUMMA, i.e. 1/c-th of Σ_m A(i,m)*B(m,j)

(3) Sum-reduce partial sums Σ_m A(i,m)*B(m,j) along k-axis so that P(i,j,0) owns C(i,j)

Source Jim Demmel

Performance on Blue Gene P

C=16



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2.5D Algorithm

- Interpolate between 2D (Cannon) and 3D
  - *c* copies of A & B
  - Perform $p^{1/2}/c^{3/2}$ Cannon steps on each copy of A&B
  - Sum contributions to C over all *c* layers
- Communication costs (not quite optimal, but not far off)
  - Volume:

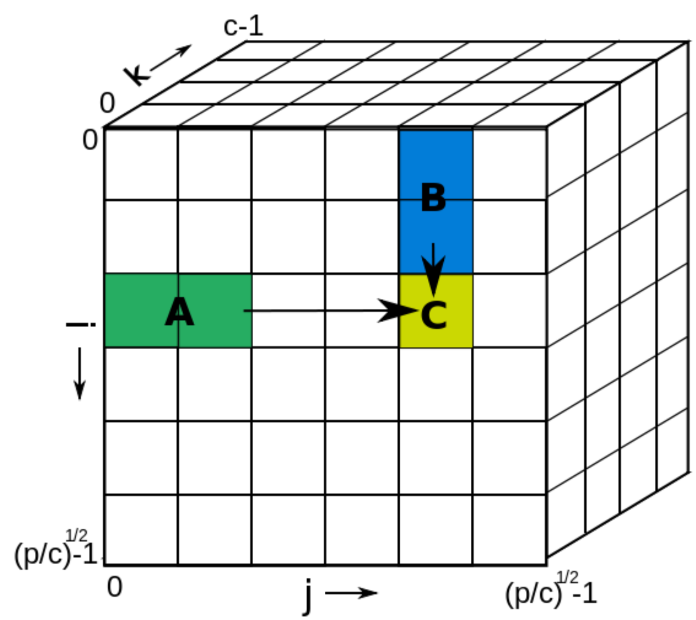
    $O(n^2 /(cp)^{1/2})$

    $[\ \Omega(n^2 /(cp)^{1/2}\ ]$

  - Messages:

    $O(p^{1/2} / c^{3/2} + \log(c))$

    $[\ \Omega(p^{1/2} / c^{3/2})\ ]$



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Today's lecture

- Cannon's Matrix Multiplication Algorithm
- 2.5D "Communication avoiding"
- SUMMA

Outer product formulation of matrix multiply

- Limitations of Cannon's Algorithm
  - P is must be a perfect square
  - A and B must be square, and evenly divisible by √p
- Interoperation with applications and other libraries difficult or expensive
- The SUMMA algorithm offers a practical alternative
  - Uses a shift algorithm to broadcast
  - A variant used in SCALAPACK by Van de Geign and Watts [1997]

Formulation

- The matrices may be non-square (kij formulation)

```
for k := 0 to n3-1
   for i := 0 to n1-1
      for j := 0 to n2-1
         C[i,j] += A[i,k] * B[k,j]
```

C[i,:] += A[i,k] * B[k,:]

- The two innermost loop nests compute n3 *outer products*

```
for k := 0 to n3-1
      C[:,:] +=  A[:,k] • B[k,:]
```

where • is outer product

Outer product

- Recall that when we multiply
  an m×n matrix by an n × p matrix…
  we get an m × p matrix
- Outer product of *column vector* a^T and *vector* b = matrix C
  an m × 1 times a 1 × n

  a[1,3] • x[3,1]

$$(a,b,c) * (x,y,z)^T \equiv \begin{pmatrix} ax & ay & az \\ bx & by & bz \\ cx & cy & cz \end{pmatrix}$$

*	1	2	3
10	11	20	30
20	20	40	60
30	30	60	90

Multiplication table with rows formed by a[:] and the columns by b[:]

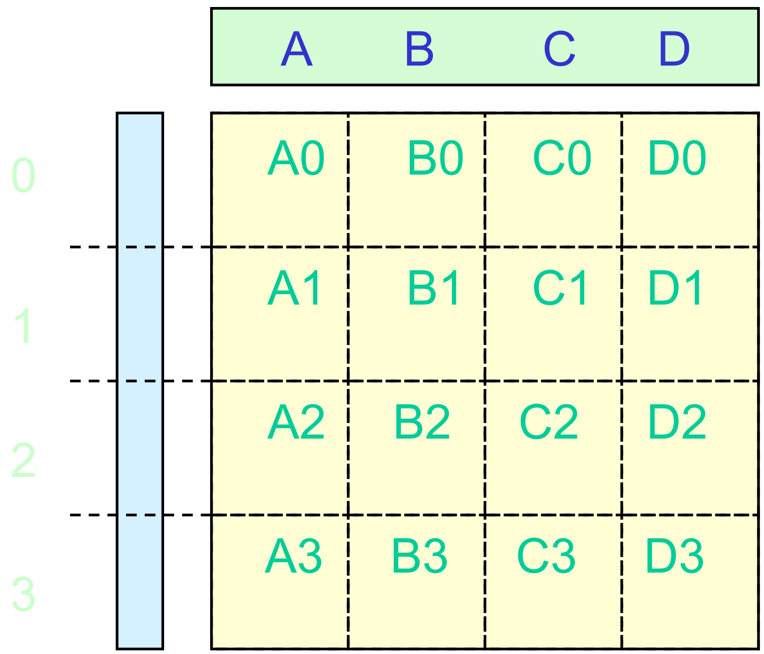
- The SUMMA algorithm computes n partial outer products:

```
for k := 0 to n-1
    C[:,:] +=  A[:,k] • B[k,:]
```

Outer Product Formulation

- The new algorithm computes **n** partial outer products:

for k := 0 to n-1
C[:,:] += A[:,k] • B[k,:]

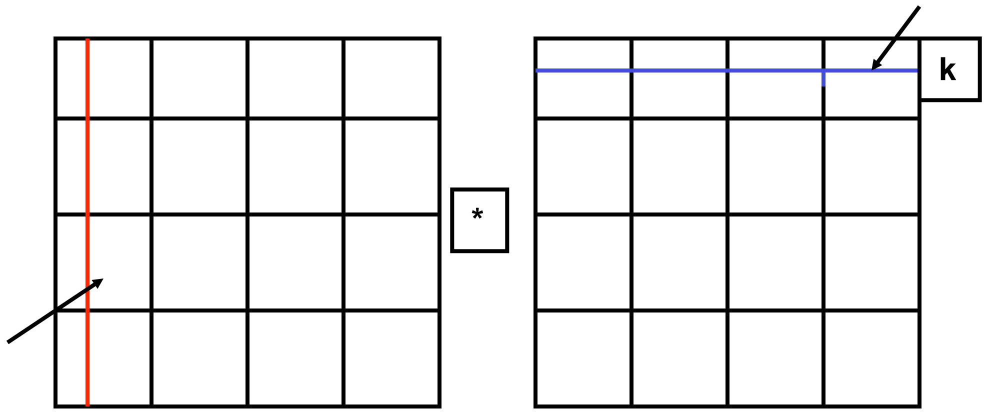


"Inner product" formulation:
for i:= 0 to n-1, j:= 0 to n-1
C[i,j] += A[i,:] * B[:,j]

Serial algorithm

- Each row k of B contributes to the n partial n partial outer products

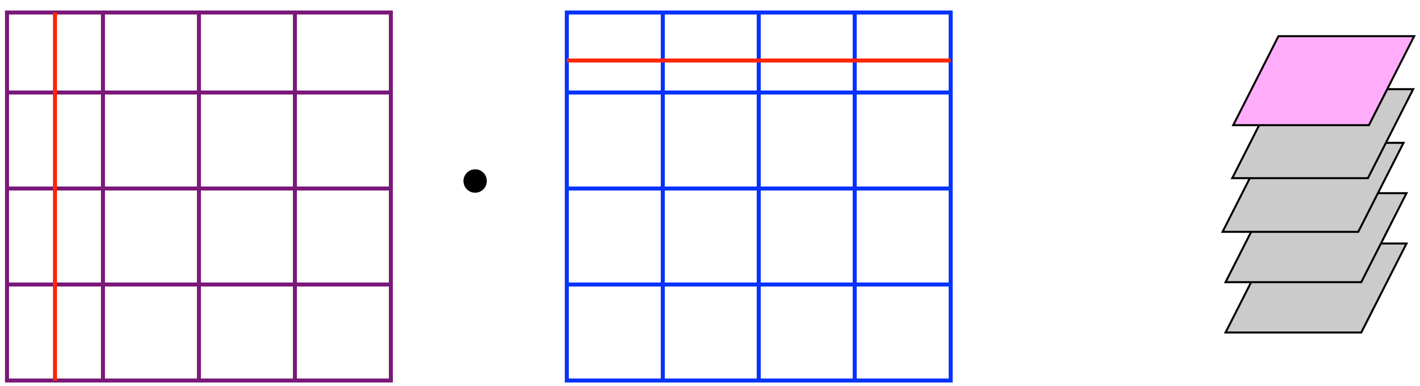
```
for k := 0 to n-1
    C[:,:] += A[:,k] • B[k,:]
```



Animation of SUMMA

- Compute the sum of **n** outer products
- Each row & column **(k)** of A & B generates a single outer product
  - Column vector **A[:,k]** (n × 1) & a vector **B[k,:]** (1 × n)

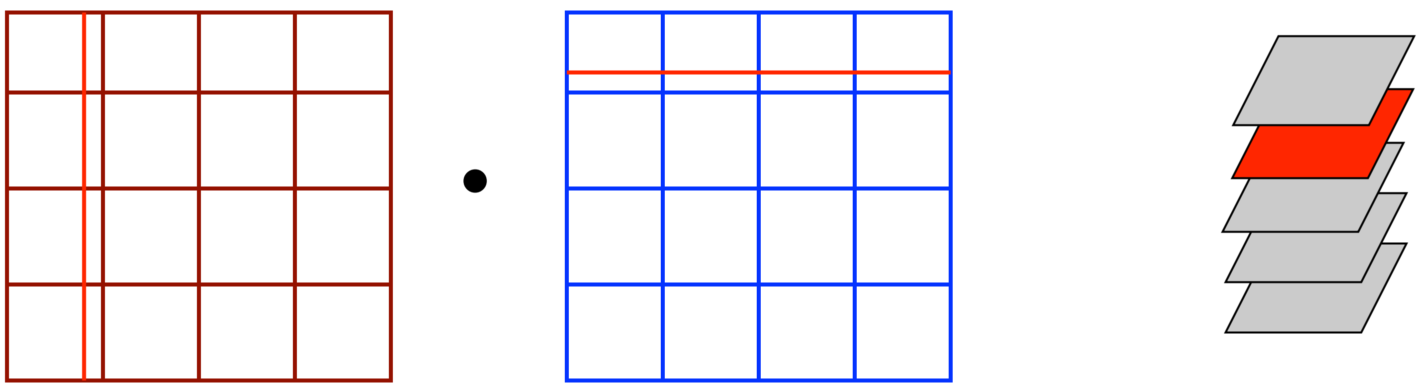
```
for k := 0 to n-1
        C[:,:] += A[:,k] • B[k,:]
```



Animation of SUMMA

- Compute the sum of **n** outer products
- Each row & column **(k)** of A & B generates a single outer product
  - A[:,k+1] • B[k+1,:]

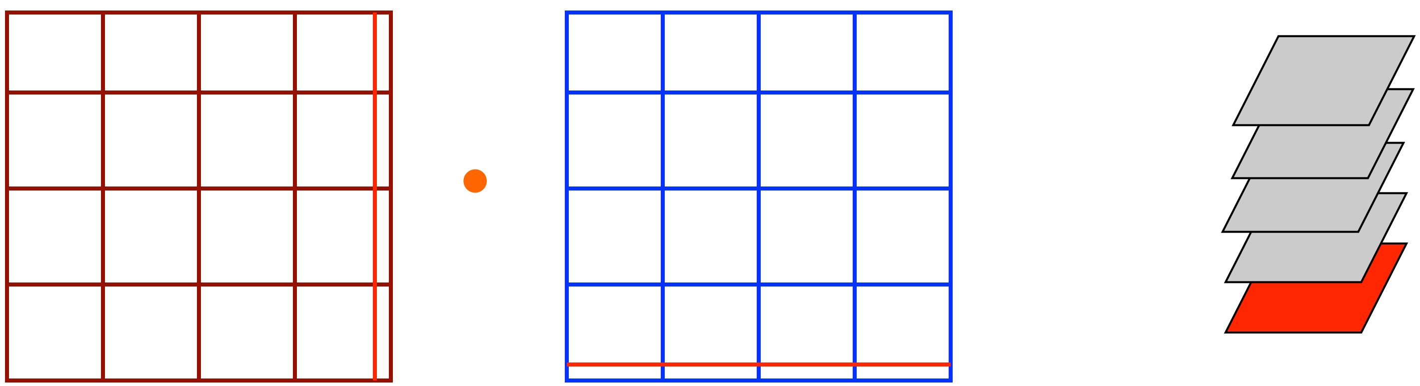
```
for k := 0 to n-1
        C[:,:] +=  A[:,k] • B[k,:]
```



Animation of SUMMA

- Compute the sum of **n** outer products
- Each row & column **(k)** of A & B generates a single outer product
  - **A[:,n-1] • B[n-1,:]**

```
for k := 0 to n-1
        C[:,:] +=  A[:,k] • B[k,:]
```

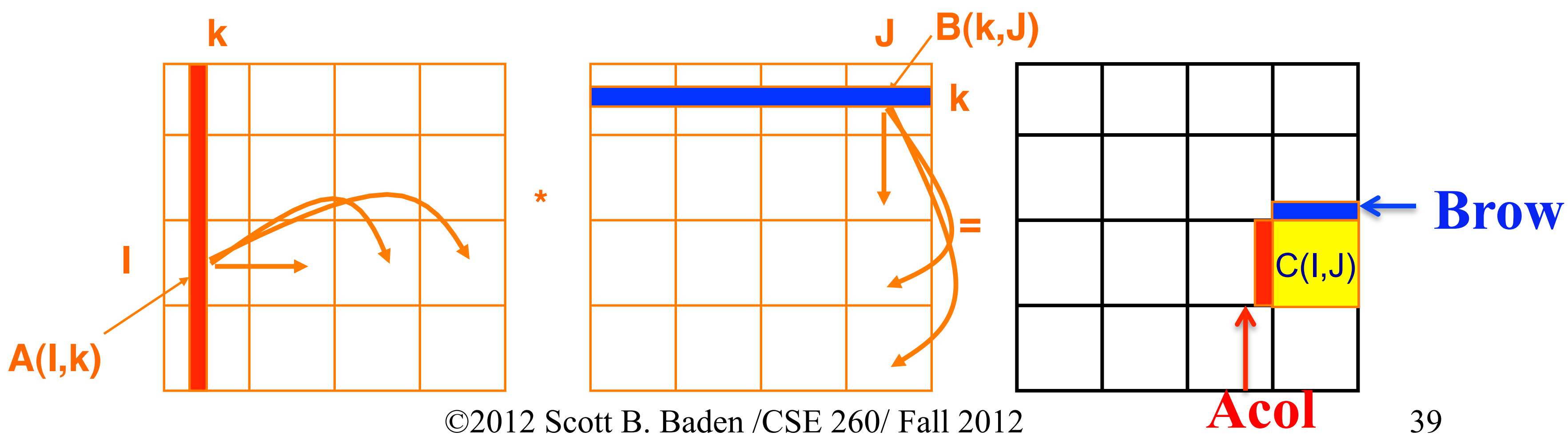


Parallel algorithm

- Processors organized into rows and columns, process rank an ordered pair
- Processor geometry P = px × py
- Blocked (serial) matrix multiply, panel size = b << N/max(px,py)

```
for k := 0 to n-1 by b
    Owner of A[:,k:k+b-1]   Bcasts to ACol    // Along processor rows
    Owner of B[k:k+b-1,:]   Bcasts BRow       // Along processor columns
    C += Serial Matrix Multiply(ACol,BRow )
```

- Each row and column of processors independently participate in a panel broadcast
- Owner of the panel (Broadcast root) changes with k, shifts across matrix



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