AMATH 483/583
High Performance Scientific Computing

Lecture 20:
Cannon's Algorithm

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Administrative

- Fill out course evaluations!

Outline

- Previously
  - Collectives
  - Laplace’s equation on a regular grid
- Cannon’s Algorithm
- Summary
- What’s Next

Collectives

- Collective operations are called by ALL processes in a communicator.
- **`MPI_BCAST`** distributes data from one process (the root) to all others in a communicator
- **`MPI_REDUCE`** combines data from all processes in communicator and returns it to one process
- In many numerical algorithms, **`SEND/RECEIVE`** can be replaced by **`BCAST/REDUCE`**, improving both simplicity and efficiency

Collectives

```
void MPI::Comm::Bcast(void* buffer, int count, const MPI::Datatype& datatype,
↪  int root) const = 0
```

```
void MPI::Intracomm::Reduce(const void* sendbuf, void* recvbuf, int count,
↪  const MPI::Datatype& datatype, const MPI::Op& op, int root) const
```

```
void MPI::Comm::Allreduce(const void* sendbuf, void* recvbuf, int count, const
↪  MPI::Datatype& datatype, const MPI::Op& op) const=0
```

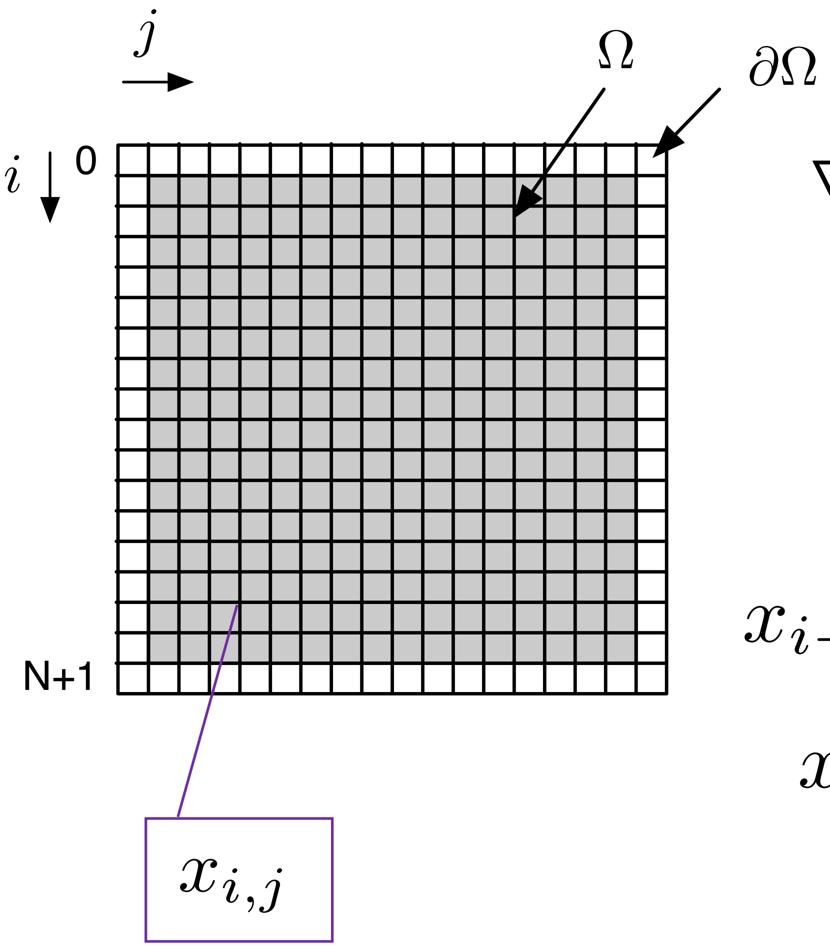
```
void MPI::Comm::Scatter(const void* sendbuf, int sendcount, const MPI::Datatype& sendtype,
↪  void* recvbuf, int recvcount, const MPI::Datatype& recvtype, int root) const
```

```
void MPI::Comm::Gather(const void* sendbuf, int sendcount, const MPI::Datatype& sendtype,
↪  void* recvbuf, int recvcount, const MPI::Datatype& recvtype, int root, const = 0
```

```
void MPI::Comm::Allgather(const void* sendbuf, int sendcount, const MPI::Datatype& sendtype,
↪  void* recvbuf, int recvcount, const MPI::Datatype& recvtype) const = 0
```

```
void MPI::Comm::Alltoall(const void* sendbuf, int sendcount, const MPI::Datatype& sendtype,
↪  void* recvbuf, int recvcount, const MPI::Datatype& recvtype)
```

Laplace's Equation on a Regular Grid



$$\begin{aligned} \nabla^2 \phi &= 0 \quad \text{on } \Omega \\ \phi &= f \quad \text{on } \partial\Omega \end{aligned}$$

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

Discretization

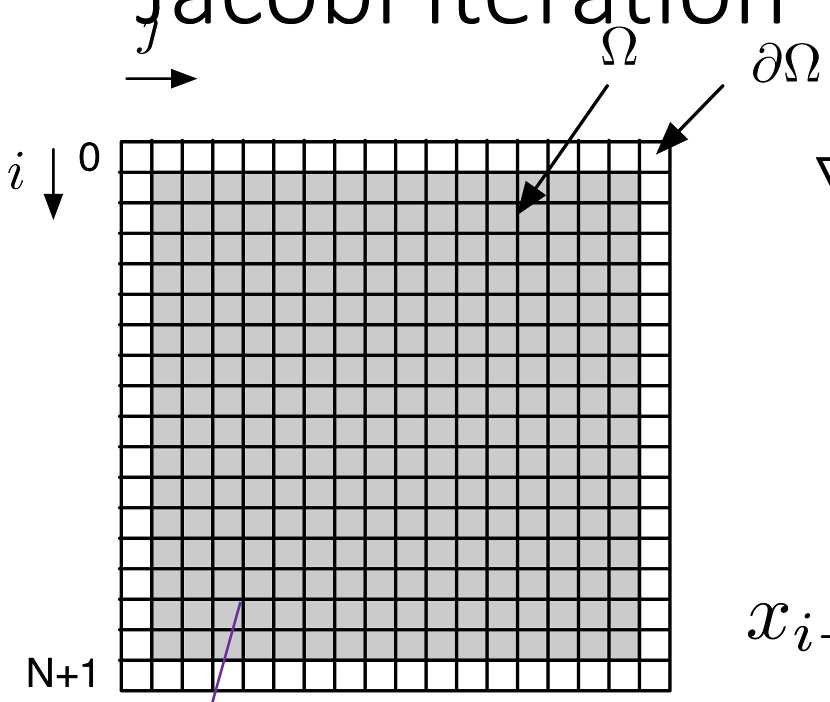
$$x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} - 4x_{i,j} = 0$$

$$x_{i,j} = (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1})/4$$

The value of each point on the grid

The average of its neighbors

Jacobi Iteration



$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

$$\begin{aligned} \nabla^2\phi &= 0 \quad \text{on } \Omega \\ \phi &= f \quad \text{on } \partial\Omega \end{aligned}$$

Discretization

$$x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} - 4x_{i,j} = 0$$

$$x_{i,j}^{k+1} = (x_{i-1,j}^{k} + x_{i+1,j}^{k} + x_{i,j-1}^{k} + x_{i,j+1}^{k})/4$$

$x_{i,j}$

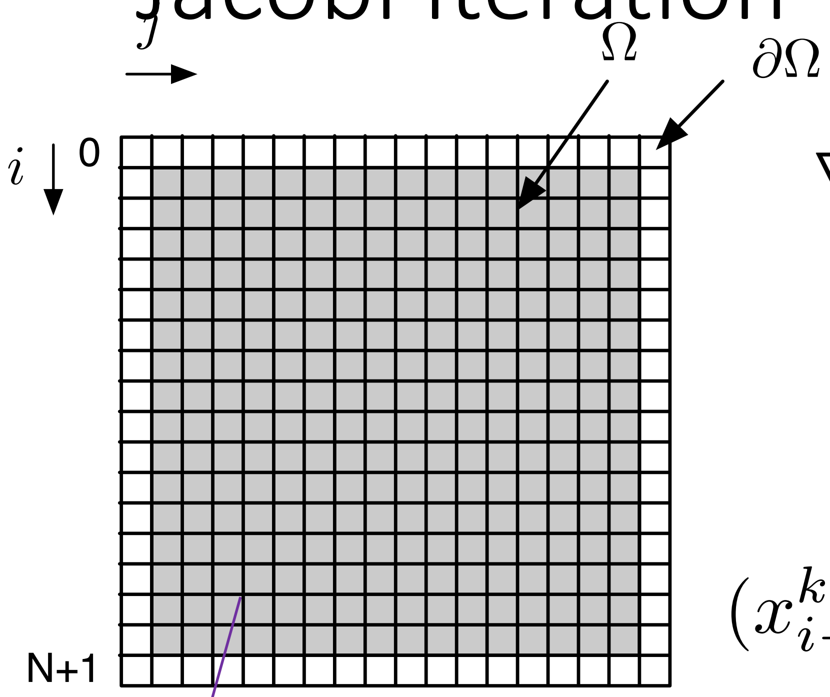
Iteration k+1

The value of each point on the grid

The average of its neighbors

Iteration k

Jacobi Iteration



$$\nabla^2\phi = 0 \quad \text{on } \Omega$$
$$\phi = f \quad \text{on } \partial\Omega$$

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

Discretization

$$(x^k_{i-1,j} + x^k_{i+1,j} + x^k_{i,j-1} + x^k_{i,j+1}) - 4x^{k+1}_{i,j} = 0$$

$$x^{k+1}_{i,j} = (x^k_{i-1,j} + x^k_{i+1,j} + x^k_{i,j-1} + x^k_{i,j+1})/4$$

$x_{i,j}$

Iteration k+1

The value of each point on the grid

The average of its neighbors

Iteration k

Jacobi Iteration

$Ax = b$

A

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

$$4x_{i,j} - (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1}) = 0$$

$$4x_{i,j}^{k+1} - (x_{i-1,j}^{k} + x_{i+1,j}^{k} + x_{i,j-1}^{k} + x_{i,j+1}^{k}) = 0$$

$A = M - N$

$$\frac{1}{h^2}\begin{bmatrix} 4 & 0 & \cdots & 0 & & \\ 0 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & 0 \\ & & 0 & \cdots & 0 & 4 \end{bmatrix} \begin{bmatrix} x_0^{k+1} \\ x_1^{k+1} \\ x_2^{k+1} \\ \vdots \\ \\ \\ \end{bmatrix} - \frac{1}{h^2}\begin{bmatrix} 0 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 0 \end{bmatrix} \begin{bmatrix} x_0^{k} \\ x_1^{k} \\ x_2^{k} \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

M

N

Jacobi Iteration

$Ax = b$

A

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & & \\ -1 & \ddots & \ddots & \ddots & \ddots & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

$$4x_{i,j} - (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1}) = 0$$

$$4x_{i,j}^{k+1} - (x_{i-1,j}^k + x_{i+1,j}^k + x_{i,j-1}^k + x_{i,j+1}^k) = 0$$

$A = M - N$

$$Mx^{k+1} - Nx^k = b$$

$$x_{i,j}^{k+1} = \frac{1}{4}(x_{i-1,j}^k + x_{i+1,j}^k + x_{i,j-1}^k + x_{i,j+1}^k)$$

$$x^{k+1} = M^{-1}(Nx^k + b)$$

Average of neighbors

Still a stencil application

class Grid

```
class Grid {

public:
  explicit Grid(size_t x, size_t y)              :
      xPoints(x+2), yPoints(y+2), arrayData(xPoints*yPoints) {}

        double &operator()(size_t i, size_t j)
            { return arrayData[i*yPoints + j]; }
  const double &operator()(size_t i, size_t j) const
            { return arrayData[i*yPoints + j]; }

  size_t numX() const { return xPoints; }
  size_t numY() const { return yPoints; }

private:
  size_t xPoints, yPoints;
  std::vector<double> arrayData;
};
```

Grid is a 2D array

Constructor

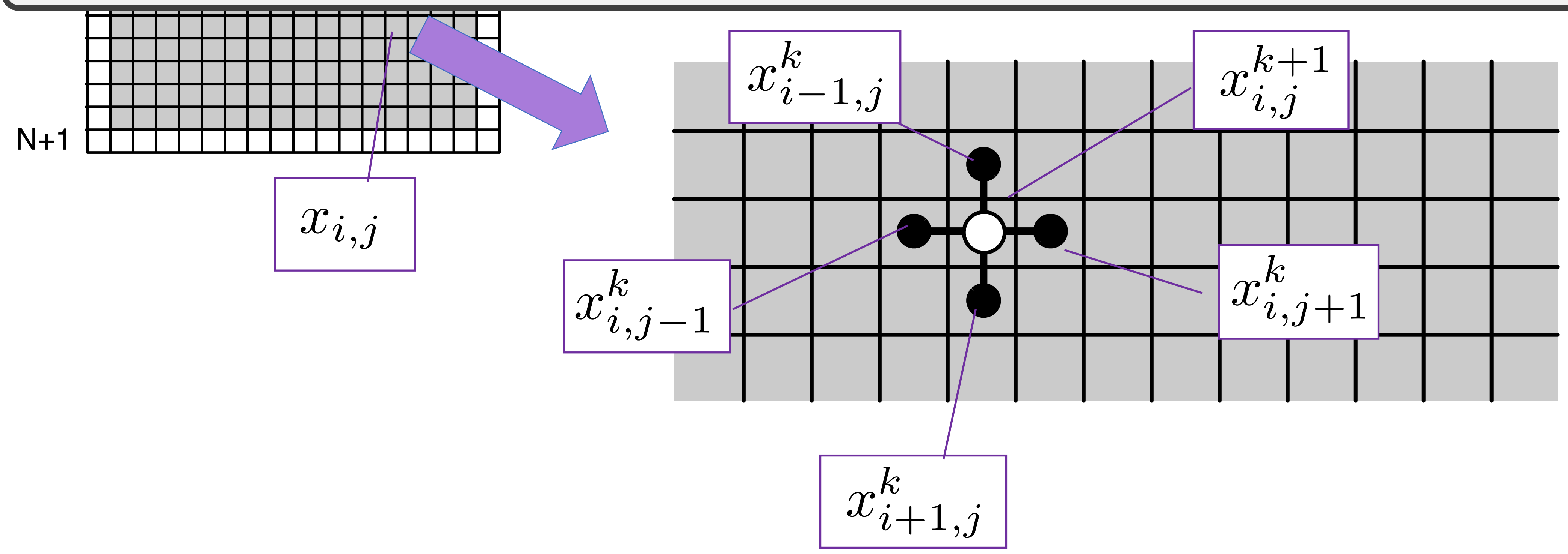
Accessor

Storage

Iterating for a solution

Claim: We only ever need two grids

```
while (! converged()) {
  for (size_t k = 0; k < max_k; ++k) {
    for (size_t i = 1; i < N+1; ++i)
      for (size_t j = 1; j < N+1; ++j)
        x[k+1](i,j) = (x[k](i-1,j) + x[k](i+1,j) + x[k](i,j-1) + x[k](i,j+1))/4.0;
}
```



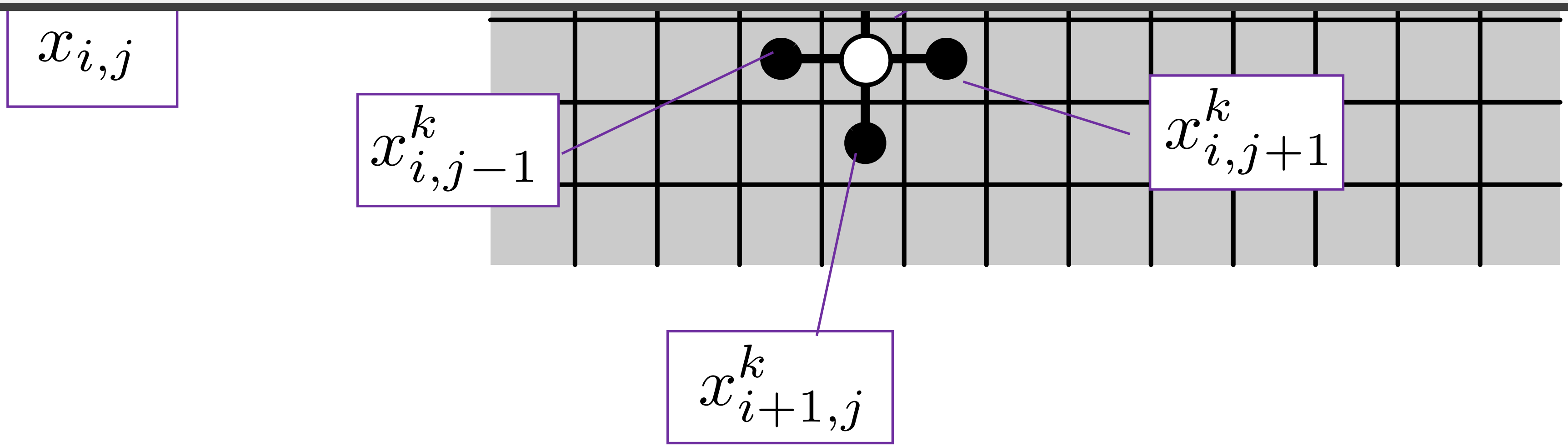
Iterating for a solution

```
while (! converged()) {
  for (size_t i = 1; i < N+1; ++i) {
    for (size_t j = 1; j < N+1; ++j) {
      xp(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
    }
  }
  swap(xp, x);
}
```

Claim: We only ever need two grids

Make current the previous

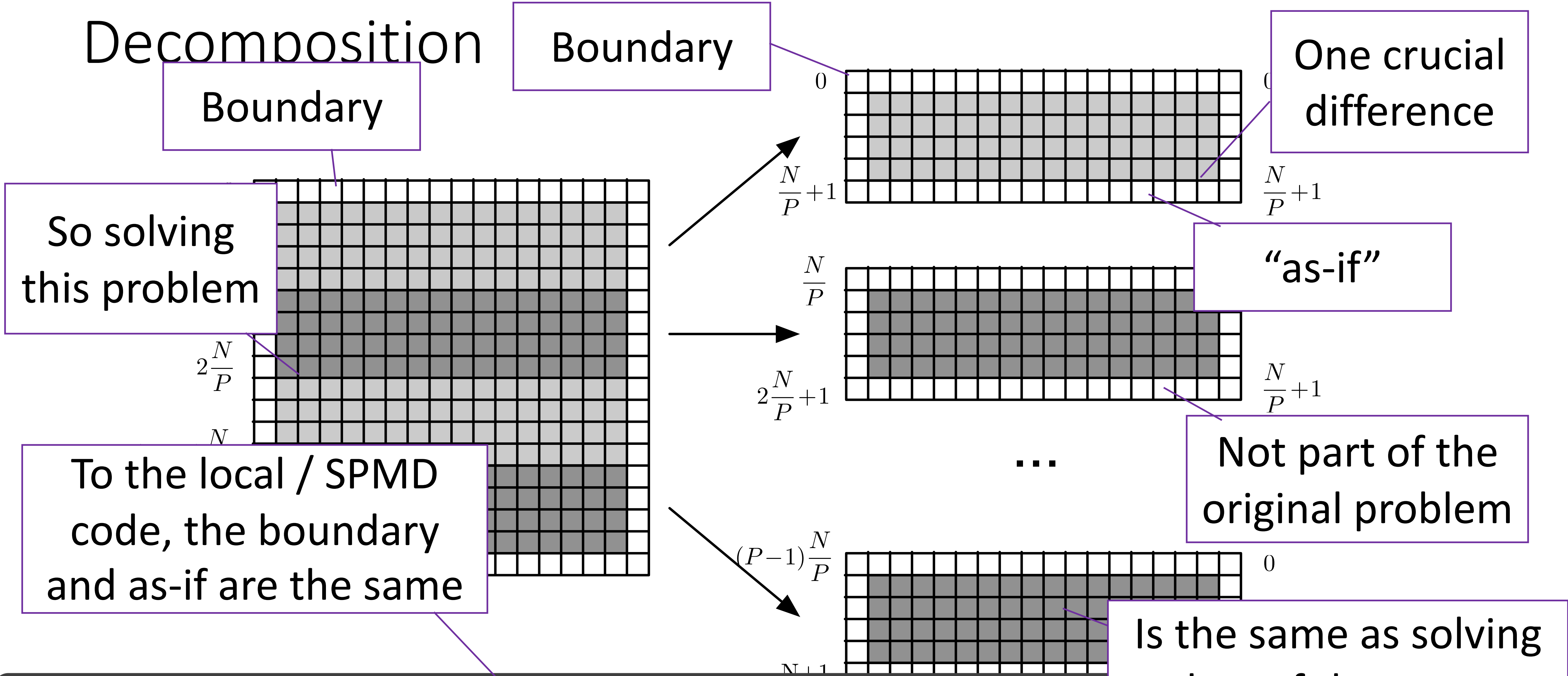
Could copy instead, but…



Sequential

```
void jacobi(Grid& x, Grid& xp) {
  while (! converged()) {
    for (size_t i = 1; i < x.num_x()-1; ++i) {
      for (size_t j = 1; j < x.num_y()-1; ++j) {
        xp(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
      }
    }
    swap(xp, x);
  }
}
```

Decomposition

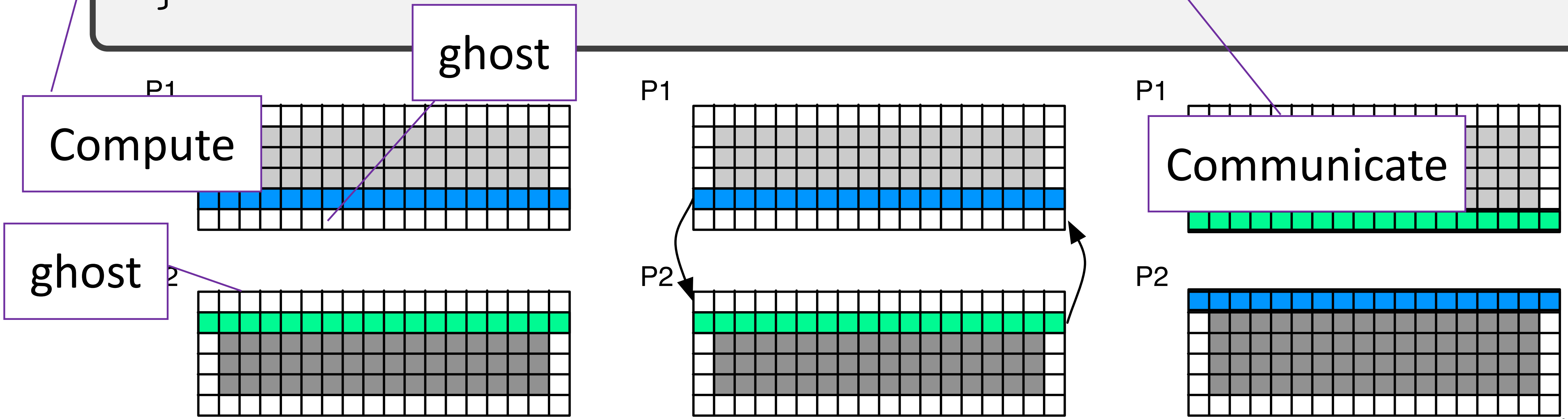



```
for (size_t i = 1; i < N/P+1; ++i)
  for (size_t j = 1; j < N+1; ++j)
    y(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
```

Compute / Communicate

```
while (! converged()) {
  for (size_t i = 1; i < N+1; ++i)
    for (size_t j = 1; j < N+1; ++j)
      y(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
  swap(x,y);
  make_as_if(x); // Communicate ghost cells
}
```

Standard terminology for as-if boundary is "ghost cell" or "halo"



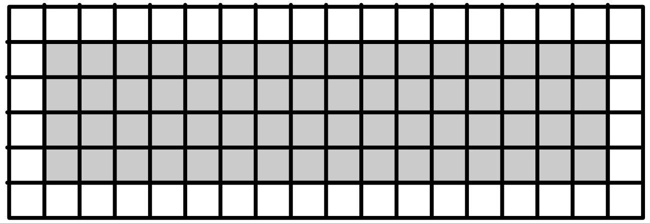
SPMD

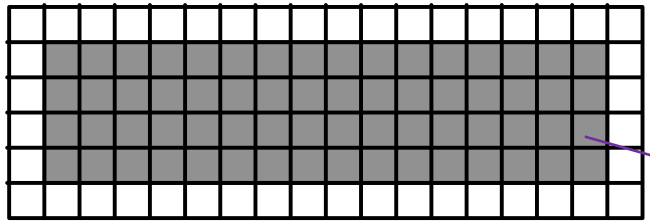
```
void jacobi(Grid& x, Grid& xp) {
  while (! converged()) {
    for (size_t i = 1; i < x.num_x()-1; ++i) {
      for (size_t j = 1; j < x.num_y()-1; ++j) {
        xp(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
      }
    }
    swap(xp, x);
  }
}
```

Or here

Communicate here

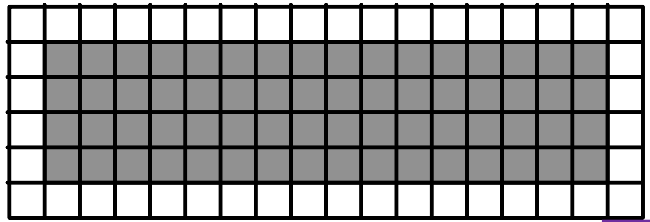
Decomposition





"myrank"

...



```
MPI::COMM_WORLD.Send(to myrank + 1)
MPI::COMM_WORLD.Send(to myrank - 1)
MPI::COMM_WORLD.Recv(from myrank - 1)
MPI::COMM_WORLD.Recv(from myrank + 1)
```

Which match?

Message sent "up"

Received from below

```
MPI::COMM_WORLD.Send(to myrank + 1, uptag)
MPI::COMM_WORLD.Send(to myrank - 1, downtag)
MPI::COMM_WORLD.Recv(from myrank - 1, uptag)
MPI::COMM_WORLD.Recv(from myrank + 1, downtag)
```

Tags really Necessary?

Message sent "up"

Received from below

Details

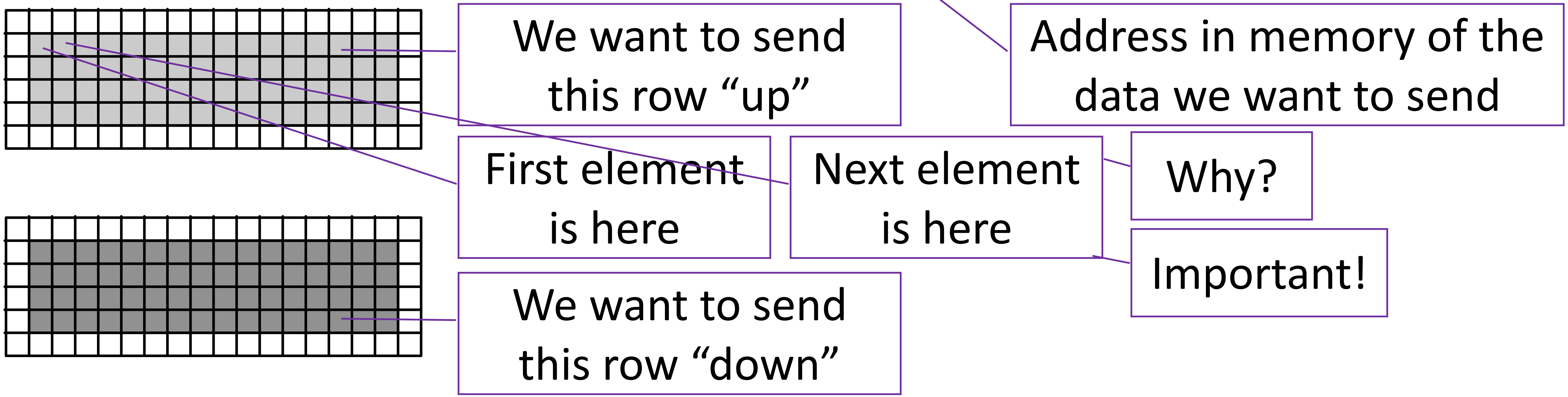
```
MPI::COMM_WORLD.Send(to myrank + 1)
MPI::COMM_WORLD.Send(to myrank - 1)
MPI::COMM_WORLD.Recv(from myrank - 1)
MPI::COMM_WORLD.Recv(from myrank + 1)
```

```
void Comm::Send(const void* buf, int count, const Datatype&
    datatype, int dest, int tag);
```

What are these actually?

Details

```
void Comm::Send(const void* buf, int count, const Datatype&
     datatype, int dest, int tag);
```



Details

```
void Comm::Send(const void* buf, int count, const Datatype&
      datatype, int dest, int tag);
```

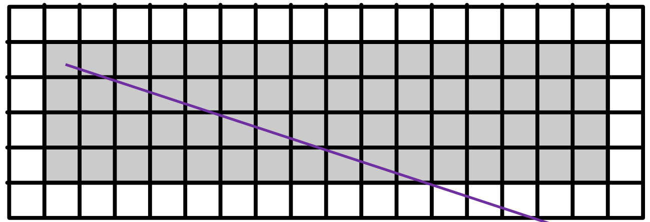
How many?

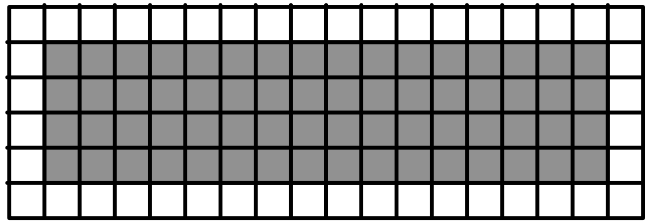
What type?

`x.num_y()`

`MPI::DOUBLE`

Address in memory of the data we want to send





First element is here

What is its address?

How do we access it?

`&x(1,1)`

`x(1,1)`

Address

Details

```
void Comm::Send(const void* buf, int count, const Datatype&
    datatype, int dest, int tag);
```

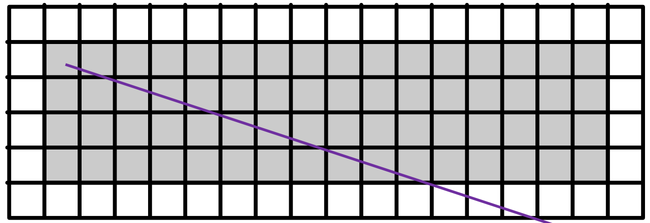
How many?

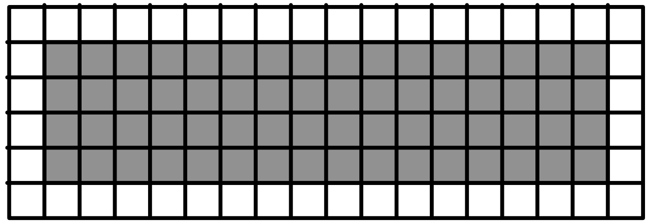
What type?

```
x.num_y()-2
```

```
MPI::DOUBLE
```

Address in memory of the data we want to send





First element is here

What is its address?

How do we access it?

```
&x(1,1)
```

```
x(1,1)
```

Address

Alternatively

```
void Comm::Send(const void* buf, int count, const Datatype&
    datatype, int dest, int tag);
```

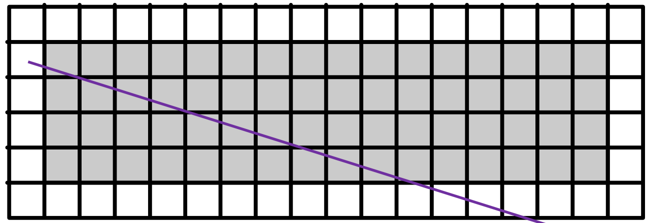
How many?

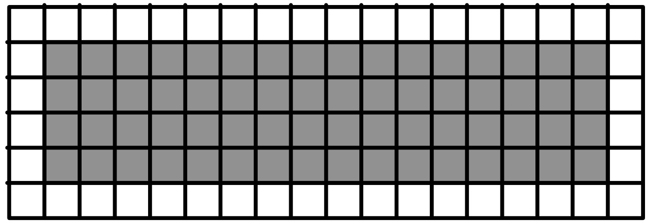
What type?

`x.num_y()`

`MPI::DOUBLE`

Address in memory of the data we want to send





First element is here

What is its address?

How do we access it?

`&x(1,0)`

`x(1,0)`

Address

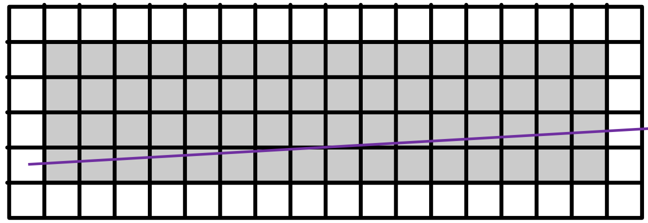
Sending “up”

```
MPI::COMM_WORLD.Send(&x(1, 0)), x.num_y(), MPI::DOUBLE, myrank+1, uptag);
```

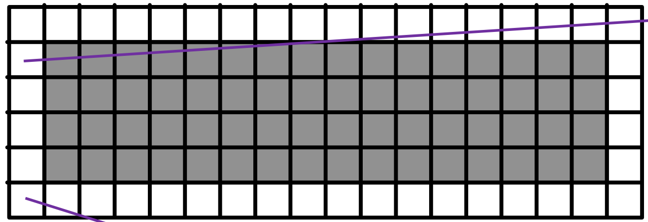
May need const cast

What is corresponding receive?

```
MPI::COMM_WORLD.Recv(&x(x.num_x()-1, 0)), x.num_y(), MPI::DOUBLE, myrank-1, uptag);
```



Send “down”: First element is here



Receive “down”: First element is here

Yes?

Need to handle top and bottom correctly

And not deadlock

First element is here

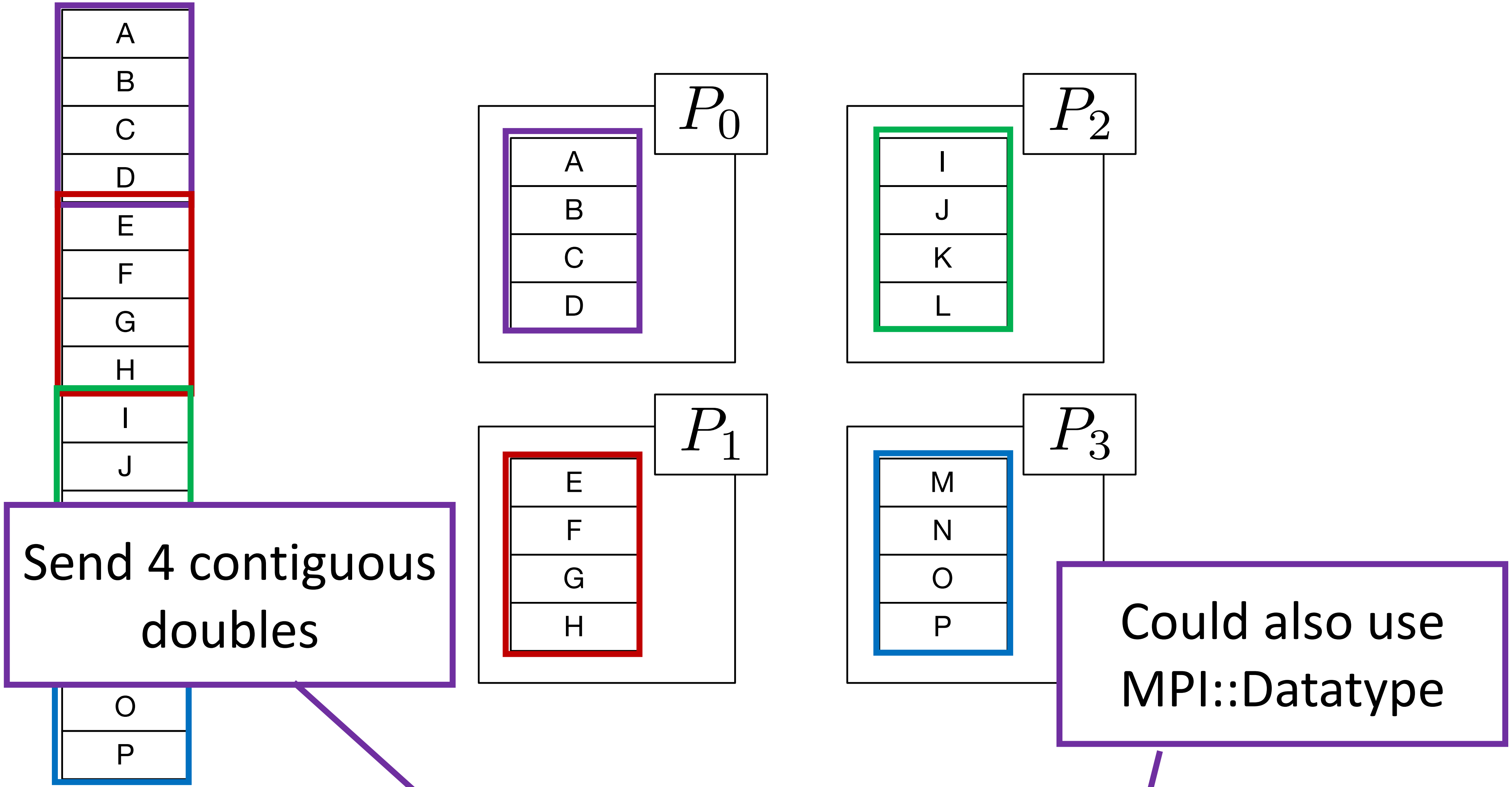
Same size and type

Same tag

Distributed Matrix-Matrix Multiply

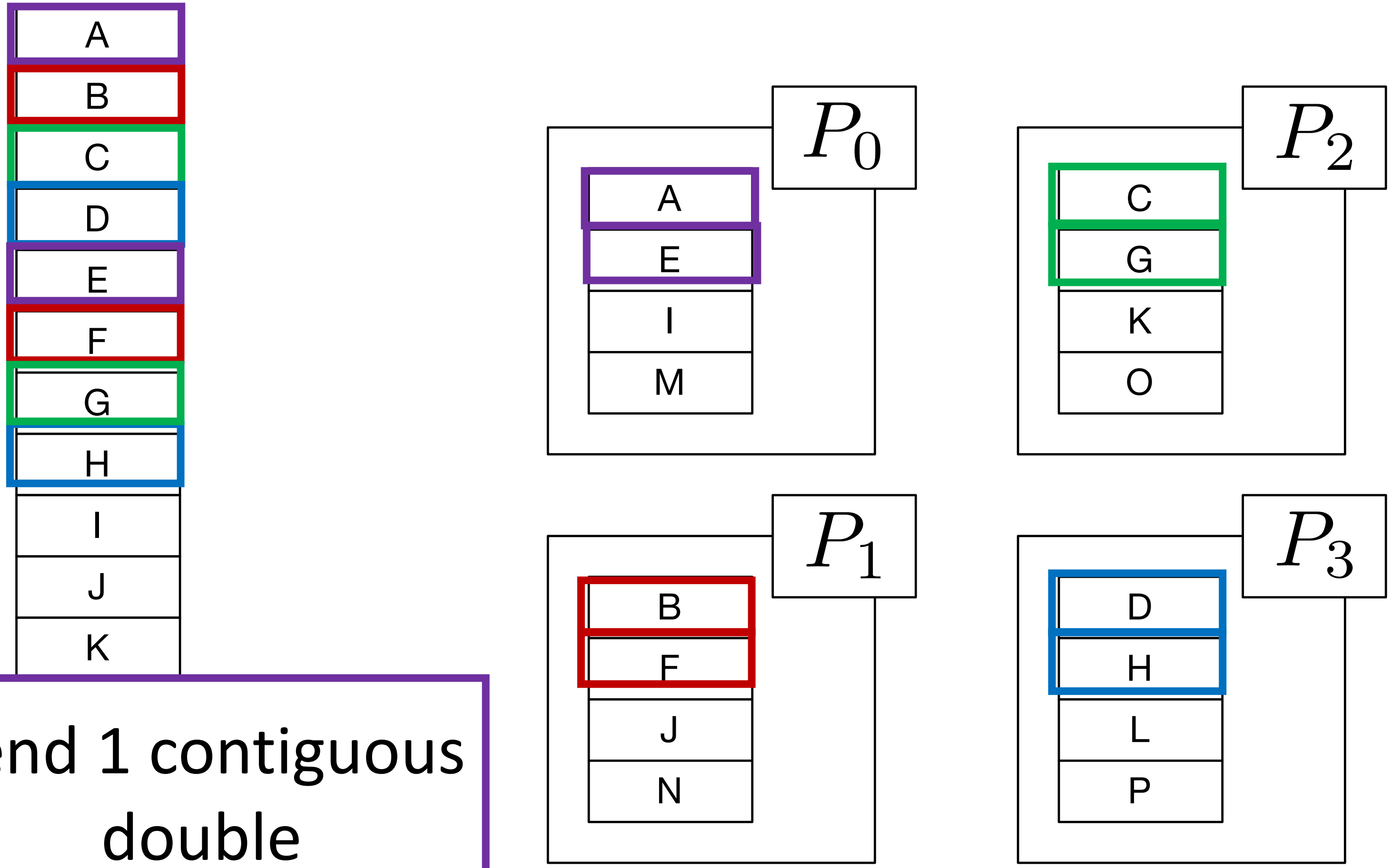
- Use block algorithm
- Partition matrix into blocks
- Assign blocks to ranks
- Orchestrate communication and computation
- ***Owner rank computes***

Block Partitioning




```
MPI::COMM_WORLD.Scatter(&x(0), 4, MPI::DOUBLE, &x(0), 4, MPI::DOUBLE, 0);
```

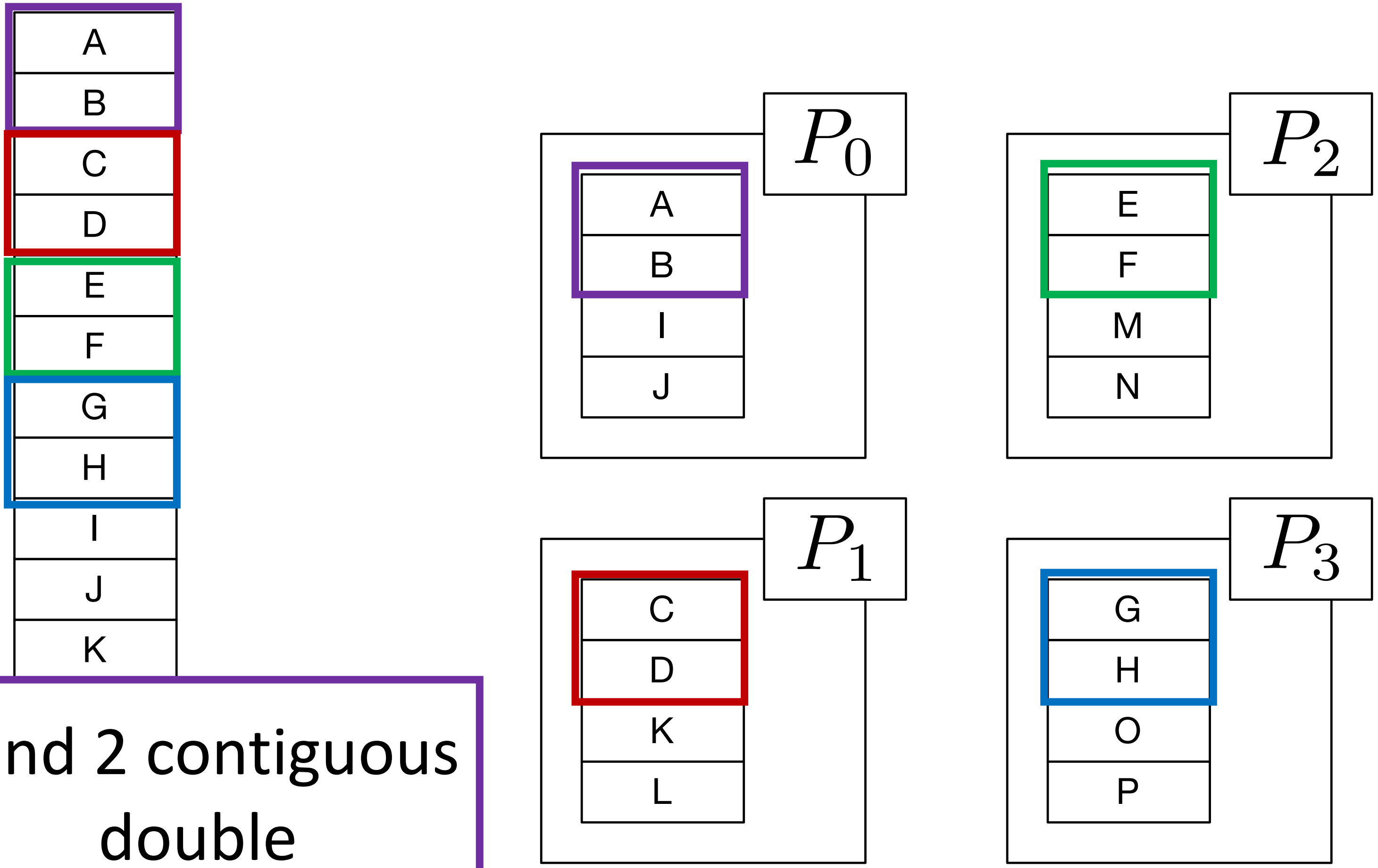
Cyclic Partitioning



Send 1 contiguous double

```
for (size_t i = 0; i < 4; ++i) {
  MPI::COMM_WORLD.Scatter(&x(i*4), 1, MPI::DOUBLE, &x(i*4), 1, MPI::DOUBLE, 0);
}
```

Block Cyclic Partitioning



Send 2 contiguous double

```
for (size_t i = 0; i < 2; ++i) {
  MPI::COMM_WORLD.Scatter(&x(i*8), 2, MPI::DOUBLE, &x(i*8), 2, MPI::DOUBLE, 0);
}
```

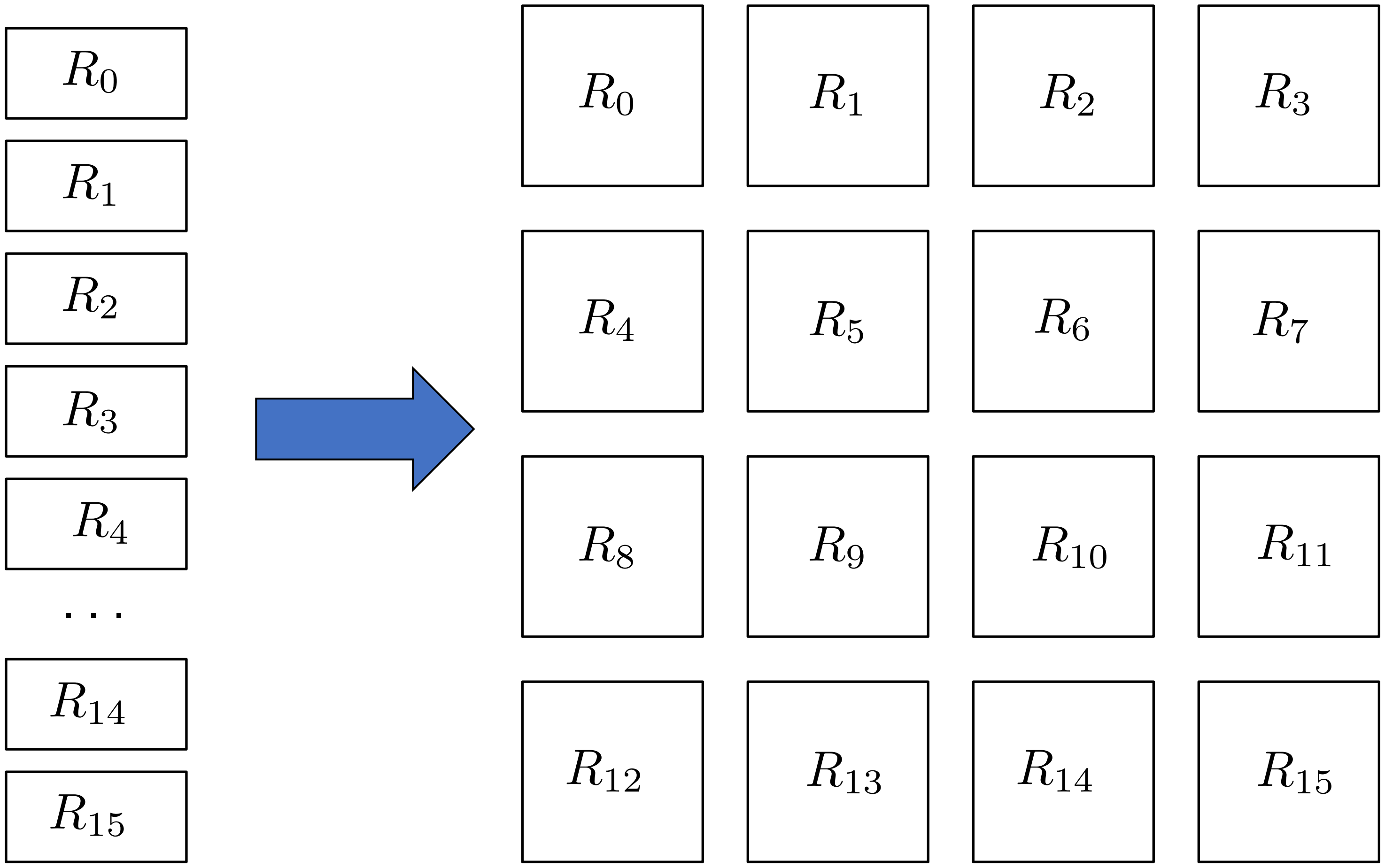
Block Matrix-Matrix Product

$$C_{IJ} = \sum_{K} A_{IK} B_{KJ}$$

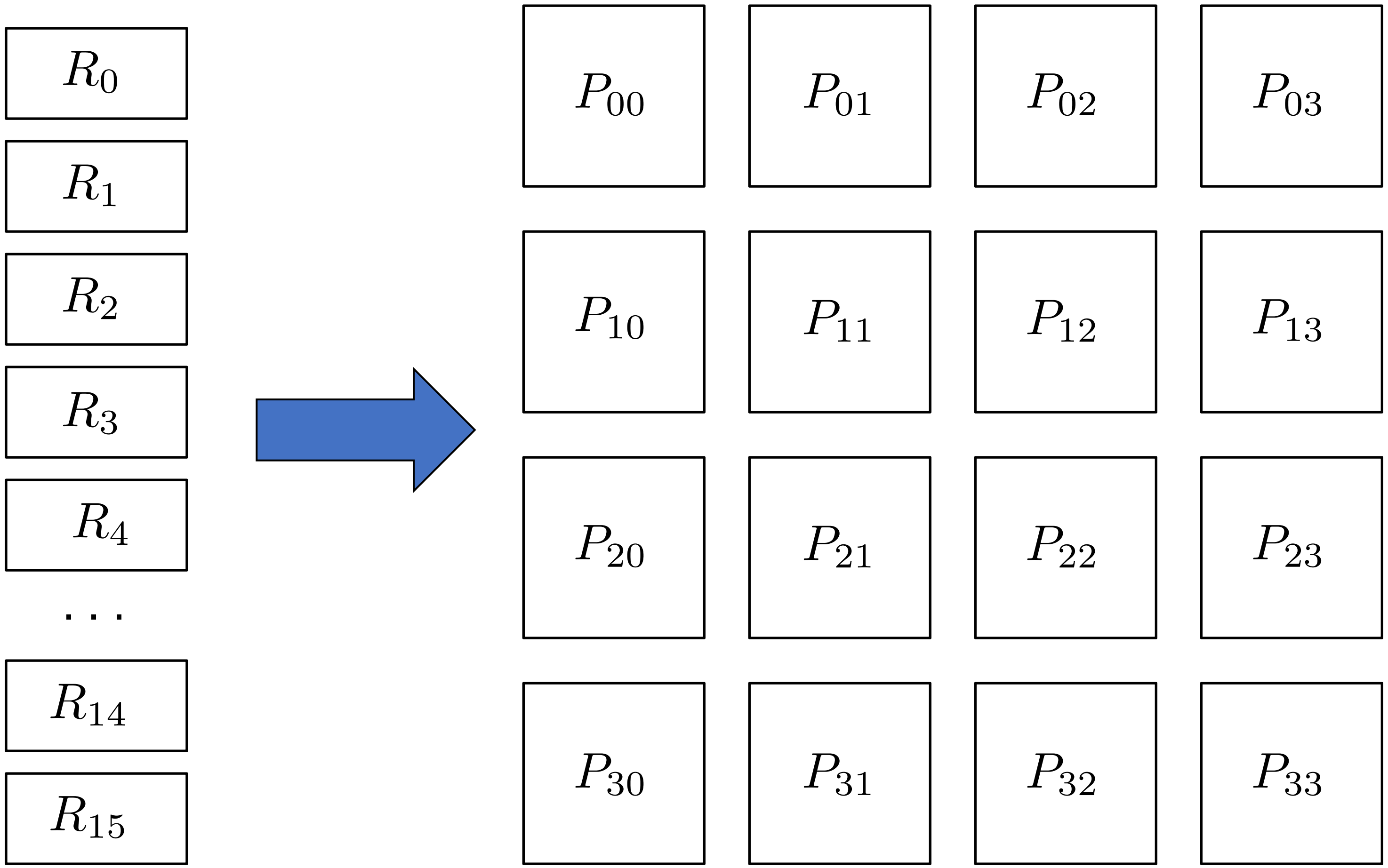
$$\begin{bmatrix} C_{00} & C_{01} & C_{02} & C_{03} \\ C_{10} & C_{11} & C_{12} & C_{13} \\ C_{20} & C_{21} & C_{22} & C_{23} \\ C_{30} & C_{31} & C_{32} & C_{33} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} & A_{02} & A_{03} \\ A_{10} & A_{11} & A_{12} & A_{13} \\ A_{20} & A_{21} & A_{22} & A_{23} \\ A_{30} & A_{31} & A_{32} & A_{33} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} & B_{02} & B_{03} \\ B_{10} & B_{11} & B_{12} & B_{13} \\ B_{20} & B_{21} & B_{22} & B_{23} \\ B_{30} & B_{31} & B_{32} & B_{33} \end{bmatrix}$$

$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

Processor Grid



Processor Grid



Matrix Block Partitioning

A_{00}	A_{01}	A_{02}	A_{03}
A_{10}	A_{11}	A_{12}	A_{13}
A_{20}	A_{21}	A_{22}	A_{23}
A_{30}	A_{31}	A_{32}	A_{33}

Matrix Block Partitioning

A_{00} B_{00}	A_{01} B_{01}	A_{02} B_{02}	A_{03} B_{03}
A_{10} B_{10}	A_{11} B_{11}	A_{12} B_{12}	A_{13} B_{13}
A_{20} B_{20}	A_{21} B_{21}	A_{22} B_{22}	A_{23} B_{23}
A_{30} B_{30}	A_{31} B_{31}	A_{32} B_{32}	A_{33} B_{33}

Matrix Block Partitioning

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{10} B_{10}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{12}	C_{13} A_{13} B_{13}
C_{20} A_{20} B_{20}	C_{21} A_{21} B_{21}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{23}
C_{30} A_{30} B_{30}	C_{31} A_{31} B_{31}	C_{32} A_{32} B_{32}	C_{33} A_{33} B_{33}

Matrix Block Partitioning

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$ (Owner computes)

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{10} B_{10}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{12}	C_{13} A_{13} B_{13}
C_{20} A_{20} B_{20}	C_{21} A_{21} B_{21}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{23}
C_{30} A_{30} B_{30}	C_{31} A_{31} B_{31}	C_{32} A_{32} B_{32}	C_{33} A_{33} B_{33}

$$C_{21} = A_{20} B_{01} + A_{21} B_{11} + A_{22} B_{21} + A_{23} B_{31}$$

Matrix Block Partitioning

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$ (Owner computes)

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{10} B_{10}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{12}	C_{13} A_{13} B_{13}
C_{20} A_{20} B_{20}	C_{21} A_{21} B_{21}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{23}
C_{30} A_{30} B_{30}	C_{31} A_{31} B_{31}	C_{32} A_{32} B_{32}	C_{33} A_{33} B_{33}

$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

Matrix Block Partitioning

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$ (Owner computes)

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{10} B_{10}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{12}	C_{13} A_{13} B_{13}
C_{20} A_{20} B_{20}	C_{21} A_{21} B_{21}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{23}
C_{30} A_{30} B_{30}	C_{31} A_{31} B_{31}	C_{32} A_{32} B_{32}	C_{33} A_{33} B_{33}

$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

Matrix Block Partitioning

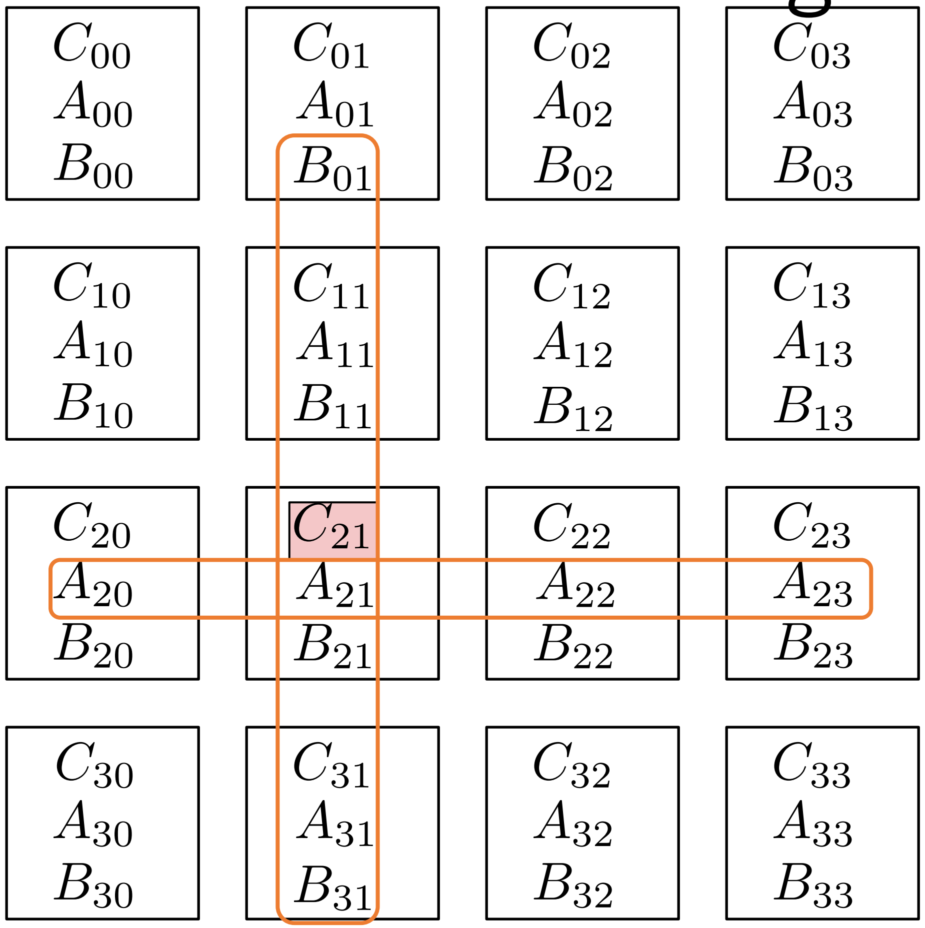
C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{10} B_{10}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{12}	C_{13} A_{13} B_{13}
C_{20} A_{20} B_{20}	C_{21} A_{21} B_{21}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{23}
C_{30} A_{30} B_{30}	C_{31} A_{31} B_{31}	C_{32} A_{32} B_{32}	C_{33} A_{33} B_{33}

$$C_{IJ} = \sum_{K} A_{IK} B_{KJ}$$ (Owner computes)

$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

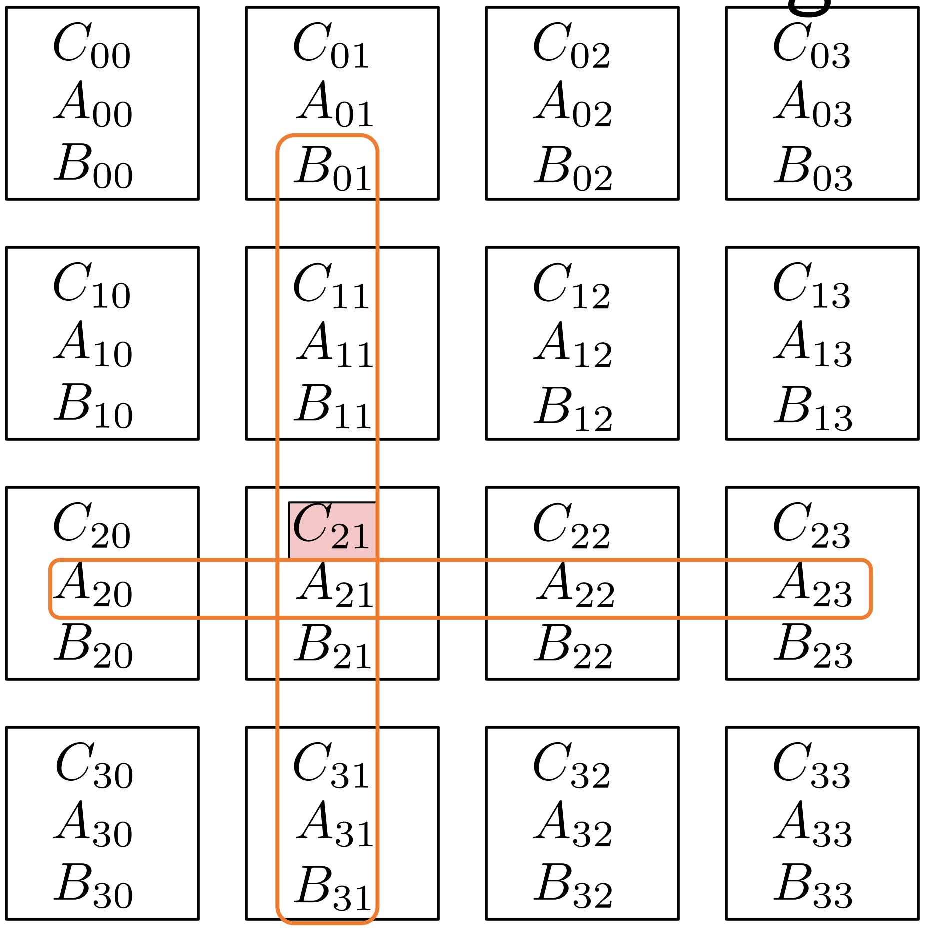
Matrix Block Partitioning

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$ (Owner computes)



$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

Matrix Block Partitioning



$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

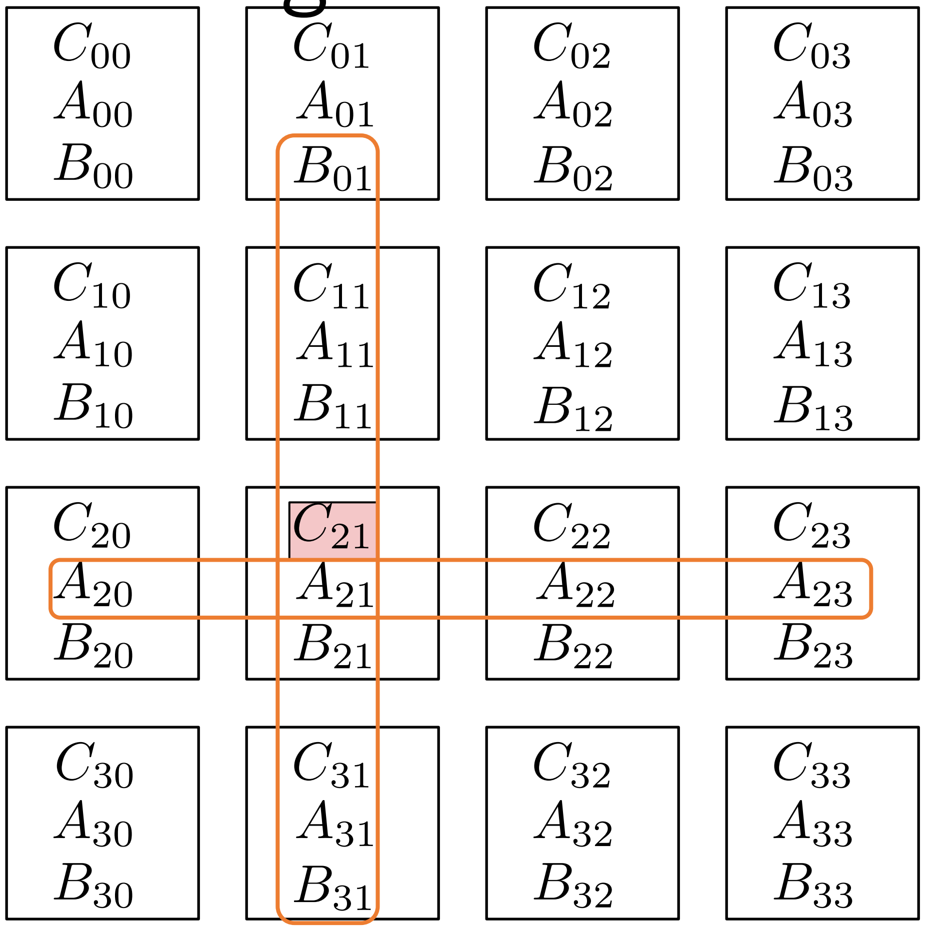
$C_{IJ} = \sum_K A_{IK} B_{KJ}$ (Owner computes)

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J

Cannon's Algorithm



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad B_{(I+J+K),J}$

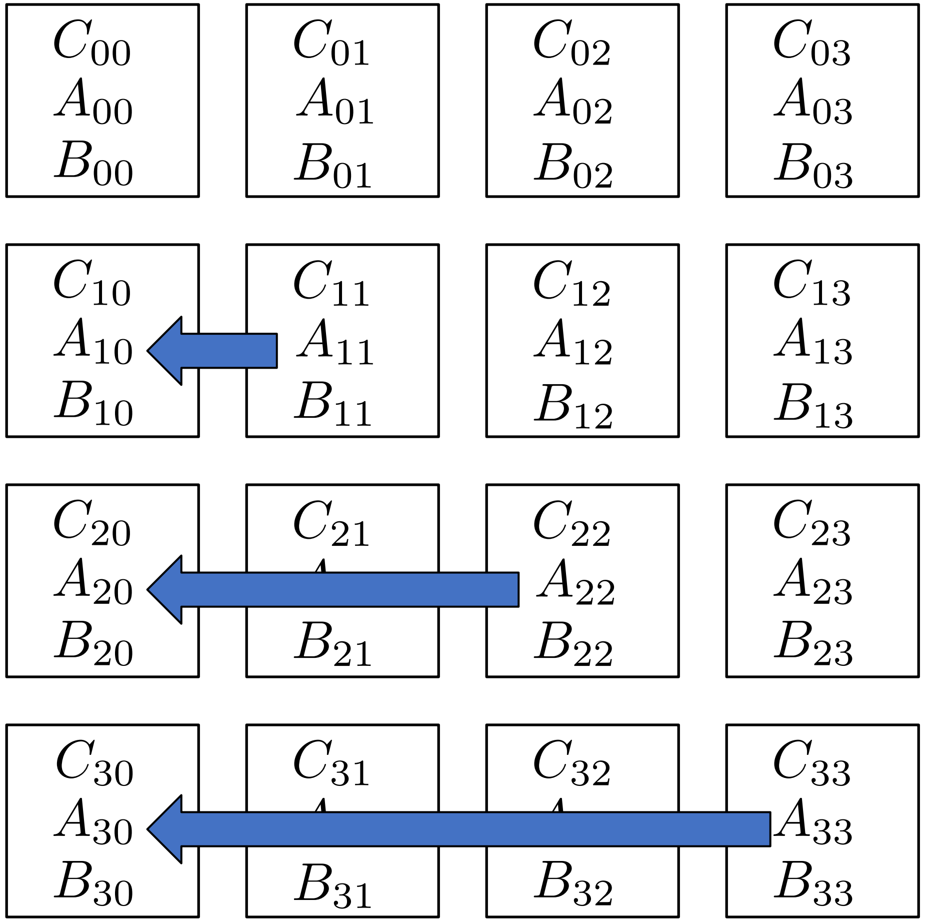
  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

Cannon's Algorithm: Setup (K = 0)



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$

Cannon's Algorithm: Setup (K = 0)

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{01}	C_{02} A_{02} B_{02}	C_{03} A_{03} B_{03}
C_{10} A_{11} B_{10}	C_{11} A_{12} B_{11}	C_{12} A_{13} B_{12}	C_{13} A_{10} B_{13}
C_{20} A_{22} B_{20}	C_{21} A_{23} B_{21}	C_{22} A_{20} B_{22}	C_{23} A_{21} B_{23}
C_{30} A_{33} B_{30}	C_{31} A_{30} B_{31}	C_{32} A_{31} B_{32}	C_{33} A_{32} B_{33}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

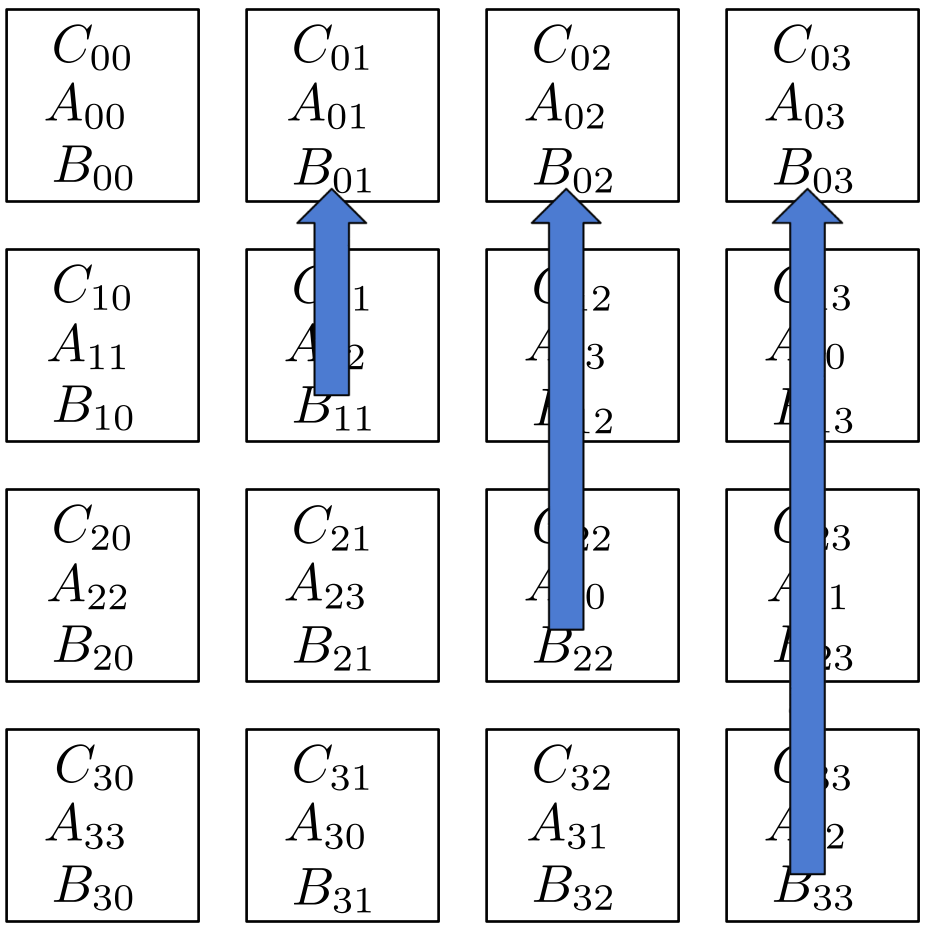
  $A_{I,(I+J+K)}$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: Setup (K = 0)



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J
- Compute

$$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: Setup

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{11}	C_{02} A_{02} B_{22}	C_{03} A_{03} B_{33}
C_{10} A_{11} B_{10}	C_{11} A_{12} B_{21}	C_{12} A_{13} B_{32}	C_{13} A_{10} B_{03}
C_{20} A_{22} B_{20}	C_{21} A_{23} B_{31}	C_{22} A_{20} B_{02}	C_{23} A_{21} B_{13}
C_{30} A_{33} B_{30}	C_{31} A_{30} B_{01}	C_{32} A_{31} B_{12}	C_{33} A_{32} B_{23}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J
- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: K = 0

C_{00} A_{00} B_{00}	C_{01} A_{01} B_{11}	C_{02} A_{02} B_{22}	C_{03} A_{03} B_{33}
C_{10} A_{11} B_{10}	C_{11} A_{12} B_{21}	C_{12} A_{13} B_{32}	C_{13} A_{10} B_{03}
C_{20} A_{22} B_{20}	C_{21} A_{23} B_{31}	C_{22} A_{20} B_{02}	C_{23} A_{21} B_{13}
C_{30} A_{33} B_{30}	C_{31} A_{30} B_{01}	C_{32} A_{31} B_{12}	C_{33} A_{32} B_{23}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

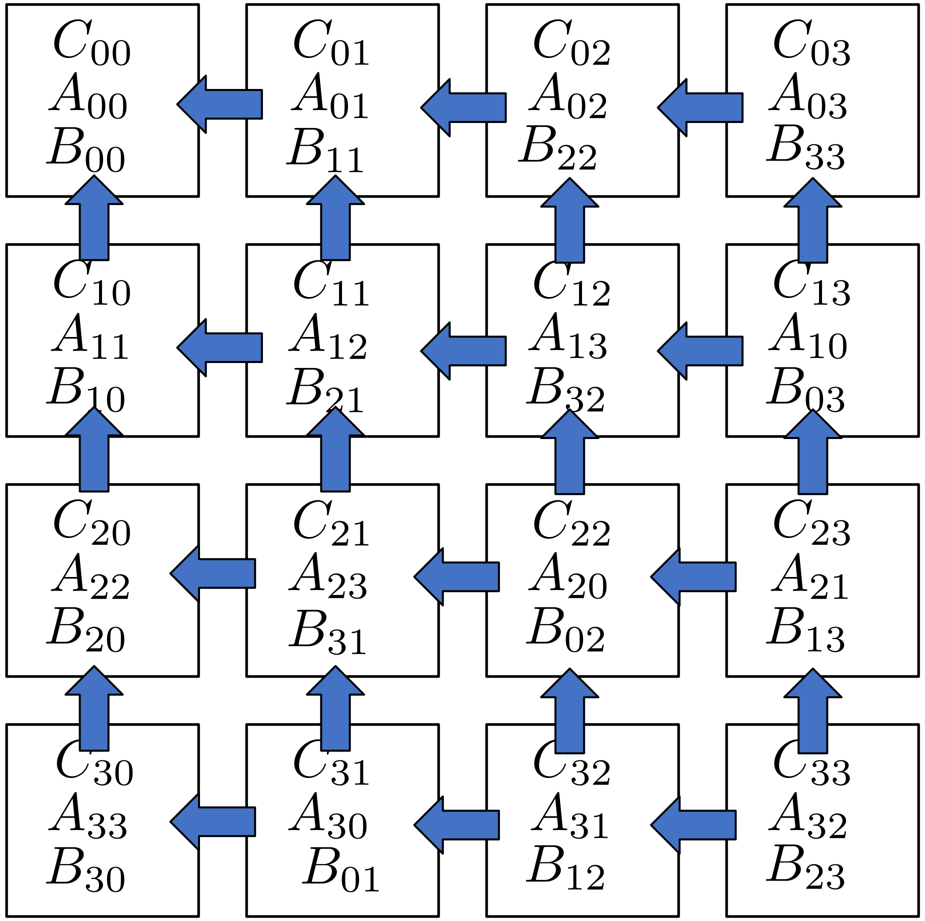
  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: K = 1



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$

Cannon's Algorithm: K = 1

C_{00} A_{01} B_{10}	C_{01} A_{02} B_{21}	C_{02} A_{03} B_{32}	C_{03} A_{00} B_{03}
C_{10} A_{12} B_{20}	C_{11} A_{13} B_{31}	C_{12} A_{10} B_{02}	C_{13} A_{11} B_{13}
C_{20} A_{23} B_{30}	C_{21} A_{20} B_{01}	C_{22} A_{21} B_{12}	C_{23} A_{22} B_{23}
C_{30} A_{30} B_{00}	C_{31} A_{31} B_{11}	C_{32} A_{32} B_{22}	C_{33} A_{33} B_{33}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

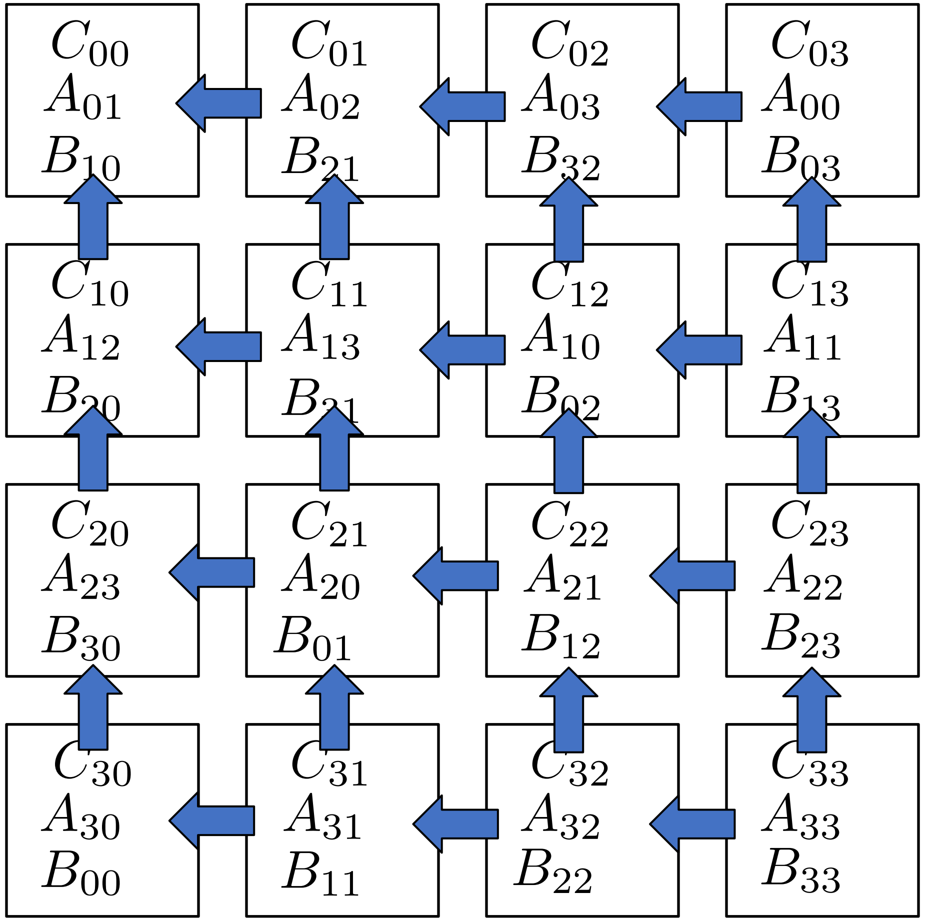
  $A_{I,(I+J+K)}$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$

Cannon's Algorithm: K = 2



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: K = 2

C_{00} A_{02} B_{20}	C_{01} A_{03} B_{31}	C_{02} A_{00} B_{02}	C_{03} A_{01} B_{13}
C_{10} A_{13} B_{30}	C_{11} A_{10} B_{01}	C_{12} A_{11} B_{12}	C_{13} A_{12} B_{23}
C_{20} A_{20} B_{00}	C_{21} A_{21} B_{11}	C_{22} A_{22} B_{22}	C_{23} A_{23} B_{33}
C_{30} A_{31} B_{10}	C_{31} A_{32} B_{21}	C_{32} A_{33} B_{32}	C_{33} A_{30} B_{03}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

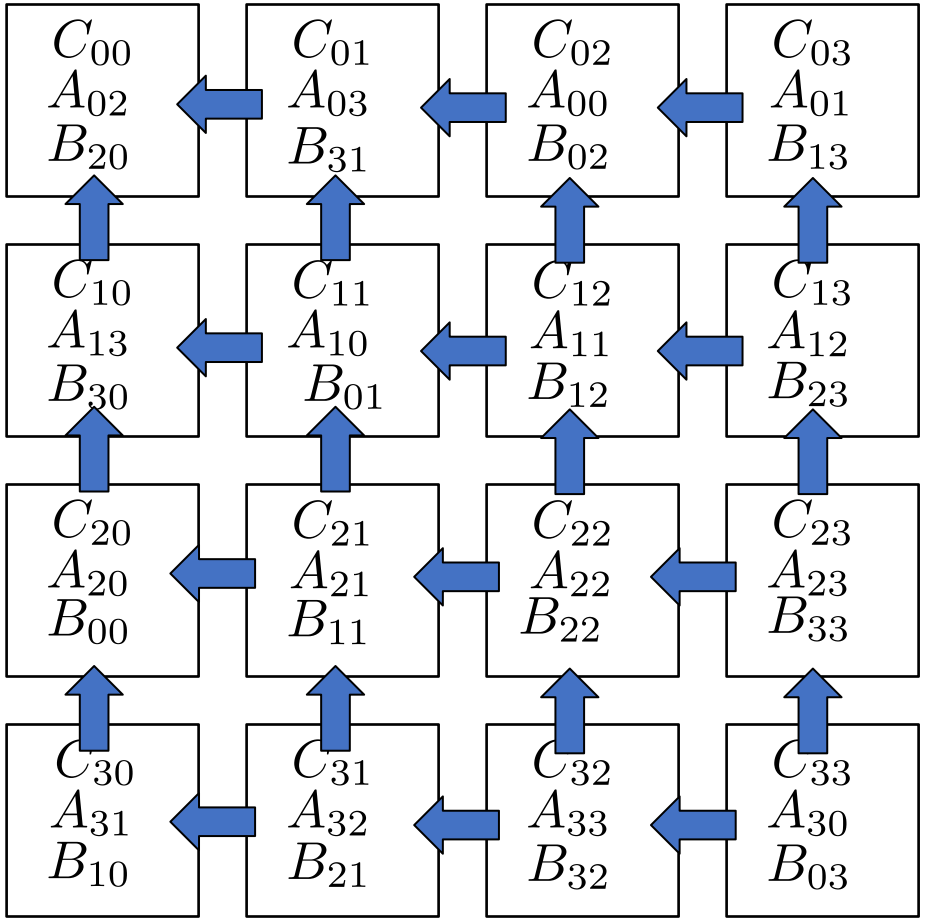
  $A_{I,(I+J+K)}$ $\quad$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Cannon's Algorithm: K = 3



$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$

Cannon's Algorithm: K = 3

C_{00} A_{03} B_{30}	C_{01} A_{00} B_{01}	C_{02} A_{01} B_{12}	C_{03} A_{02} B_{23}
C_{10} A_{10} B_{00}	C_{11} A_{11} B_{11}	C_{12} A_{12} B_{22}	C_{13} A_{13} B_{33}
C_{20} A_{21} B_{10}	C_{21} A_{22} B_{21}	C_{22} A_{23} B_{32}	C_{23} A_{20} B_{03}
C_{30} A_{32} B_{20}	C_{31} A_{33} B_{31}	C_{32} A_{30} B_{02}	C_{33} A_{31} B_{13}

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$

- At each step K, arrange for

  $A_{I,(I+J+K)}$ $\qquad$ $B_{(I+J+K),J}$

  to be on processor I,J

- Compute

  $$C_{IJ} \mathrel{+}= A_{I,(I+J+K)} \times B_{(I+J+K),J}$$

Implementation

- Two-D decomposition of matrices A, B, C
- Move A and B to starting positions
- Local matrix-matrix product
- Shift left
- Shift up
- Move A and B back to initial distributions

MPI Mental Mode

All MPI communication takes place in the context of an ***MPI Communicator***

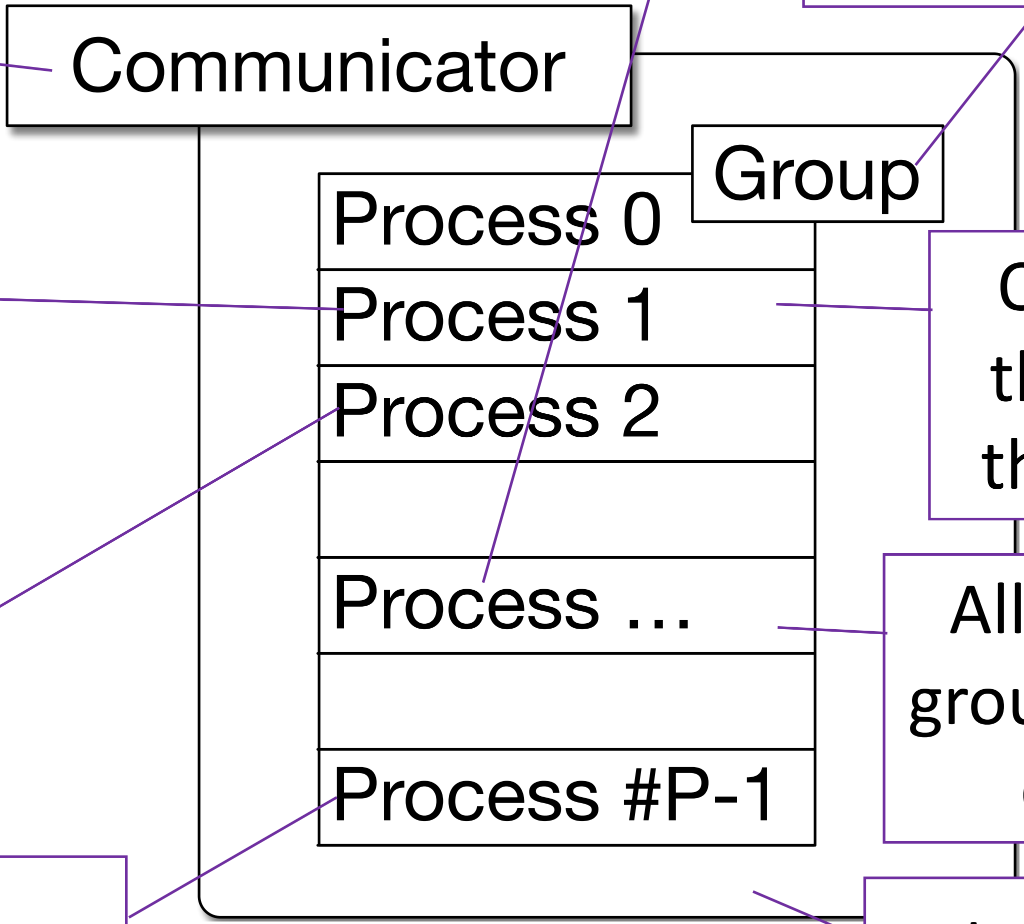
An MPI Group translates from ***rank*** in the group to actual process

We us the index (***rank***) of a process in the group to identify other processes

The ***size*** of a communicator is the size of the group

Processes can query for size and for their own rank in group

An MPI Communicator contains an ***MPI Group***

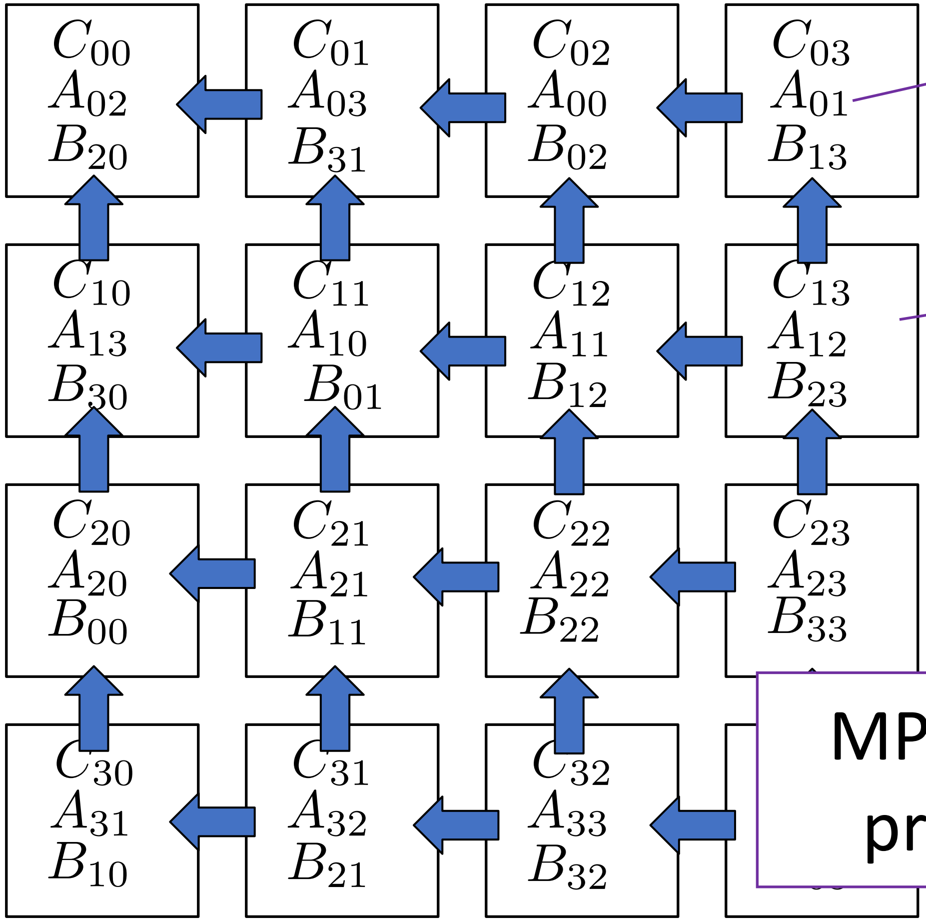


Only processes in the group can use the communicator

All processes in the group see an identical communicator

Behavior is ***as if*** it were global and shared

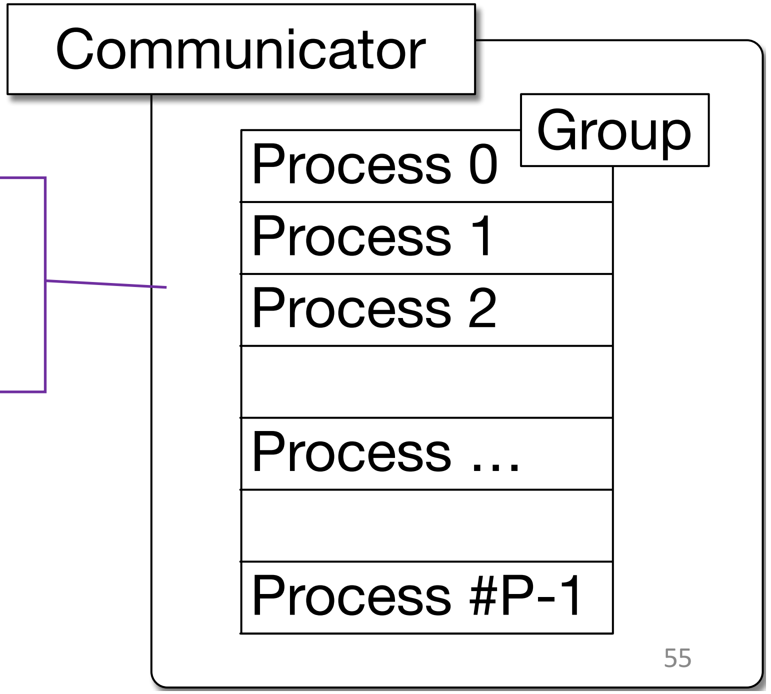
Shifting North, East, West, South



This is a useful way to reason about the algorithm

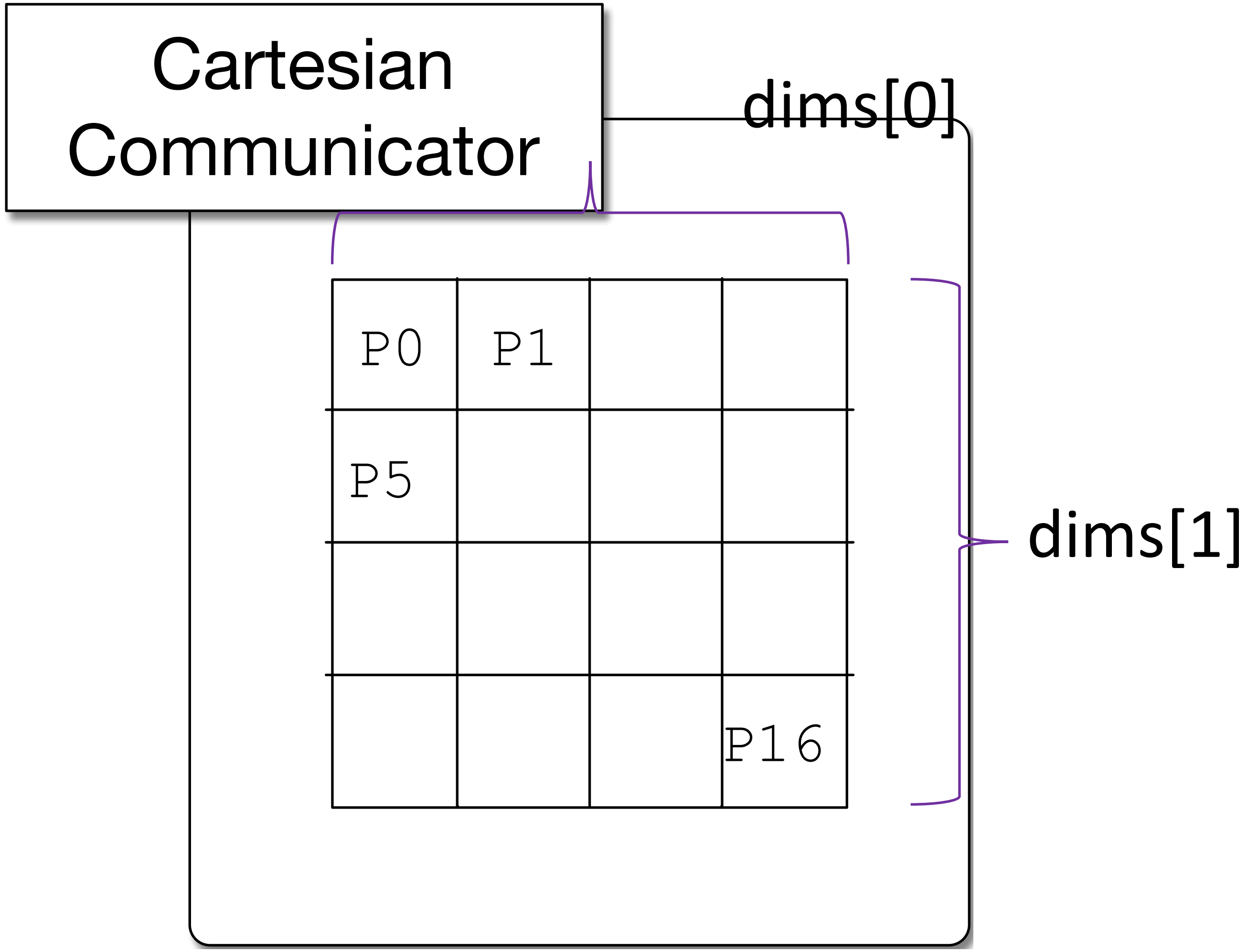
Also turns out to be efficient

MPI communicator has processes in an array



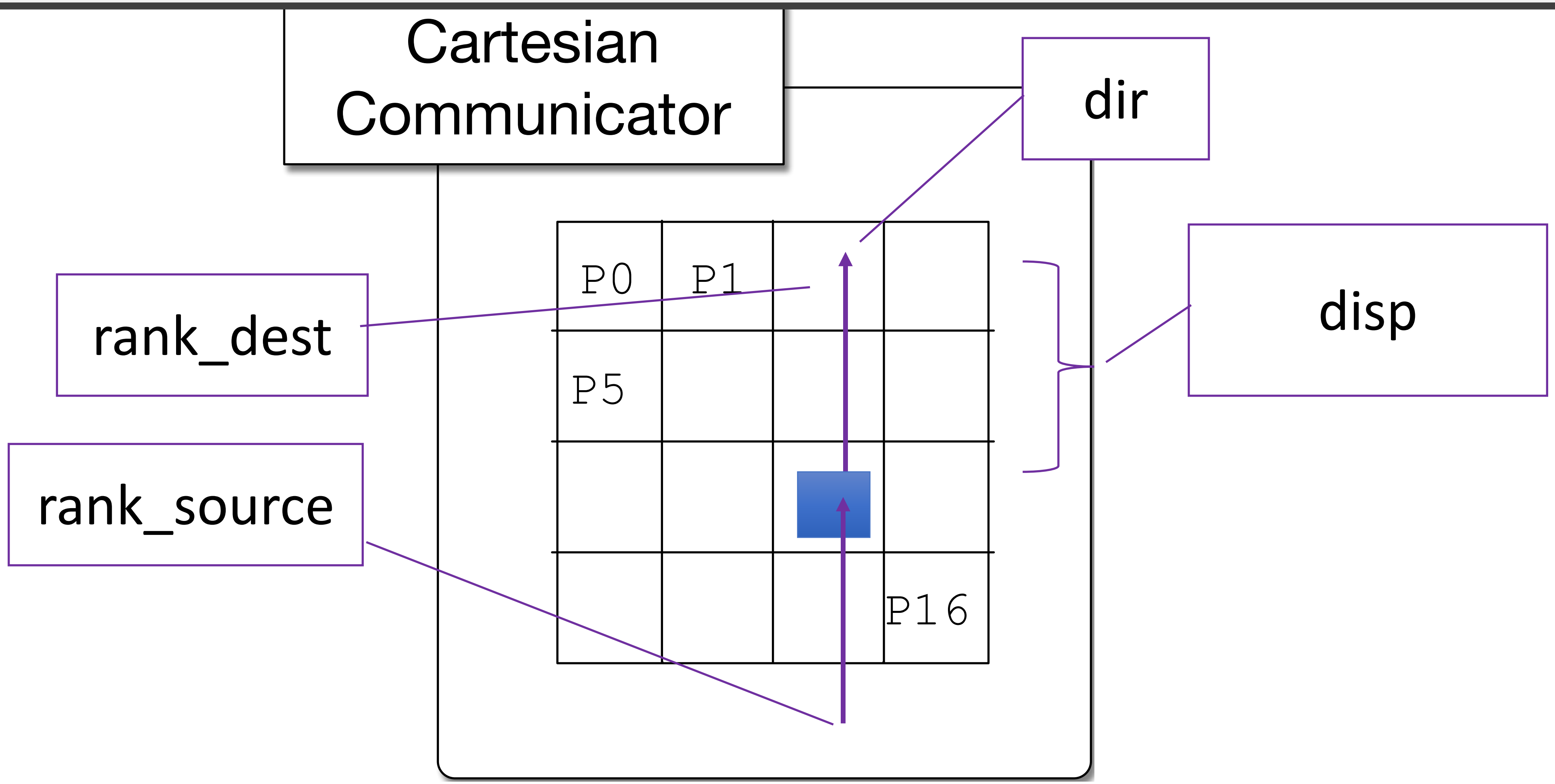
Cartesian Communicator

```
Cartcomm Intracomm.Create_cart(int ndims, int dims[], const bool periods[],
↪ bool reorder) const
```



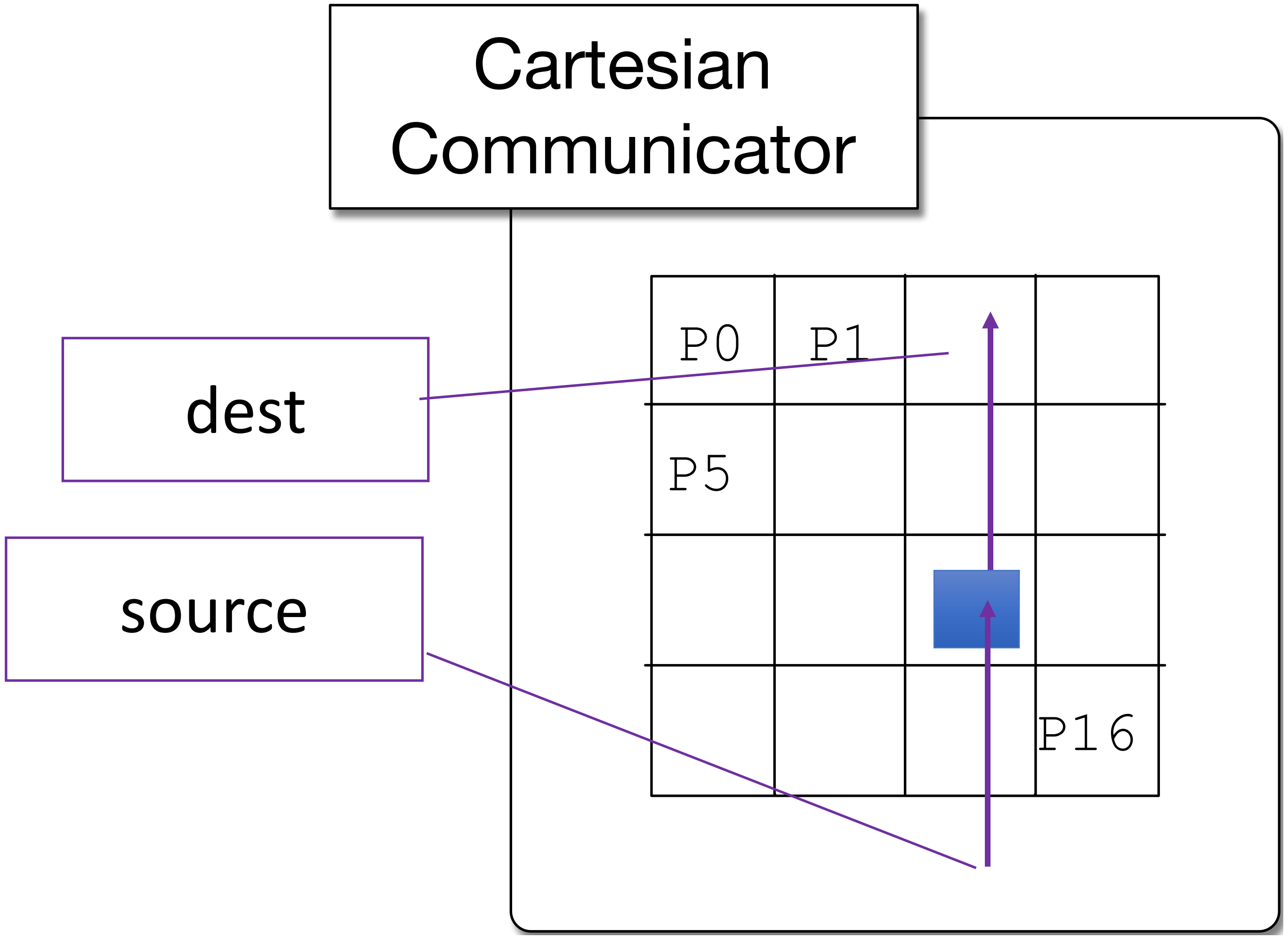
Cartesian Communicator

```
void Cartcomm::Shift(int direction, int disp, int& rank_source,
↪   int& rank_dest) const
```



Cartesian Communicator

```
void Comm::Sendrecv_replace(void* buf, int count, const Datatype& datatype,
↪  int dest, int sendtag, int source, int recvtag) const
```



Implementation

```
void cannonMultiplyMV(const Matrix& A, const Matrix& B, Matrix& C) {
  size_t mysize = MPI::COMM_WORLD.Get_size();

  // Set up grid topology and a grid (Cartesian) communicator
  int dims[2] = { (int) std::sqrt(mysize), (int) std::sqrt(mysize) };
  bool periods[2] = { true, true };

  MPI::Cartcomm gridComm = MPI::COMM_WORLD.Create_cart(2, dims, periods, true);
  size_t myrank = gridComm.Get_rank();

  int mycoords[2];
  gridComm.Get_coords(myrank, 2, mycoords);

  int northRank, eastRank, westRank, southRank;
  gridComm.Shift(0, -1, westRank,  eastRank);
  gridComm.Shift(1, -1, southRank, northRank);

  // Move A and B where they need to be to start
  int shiftSource, shiftDest;
  gridComm.Shift(0, -mycoords[0], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                            MPI::DOUBLE, shiftDest, 314, shiftSource, 314);

  gridComm.Shift(1, -mycoords[1], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                            MPI::DOUBLE, shiftDest, 314, shiftSource, 315);


  // Main loop
  for (int k = 0; k < dims[0]; ++k) {
    hoistedCopyBlockedTiledMultiply2x2(A, B, C); // Local block matmat

    gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                              MPI::DOUBLE, westRank,  316, eastRank,  316);
    gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*A.numCols(),
                              MPI::DOUBLE, northRank, 317, southRank, 317);
  }

  // Restore A and B to initial distribution
  gridComm.Shift(0, +mycoords[0], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                            MPI::DOUBLE, shiftDest, 318, shiftSource, 318);

  gridComm.Shift(1, +mycoords[1], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                            MPI::DOUBLE, shiftDest, 319, shiftSource, 319);

  gridComm.Free();
}
```

Implementation

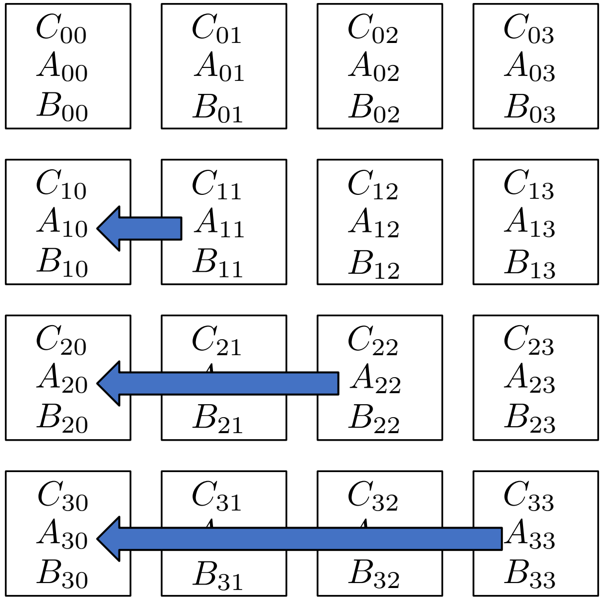
```cpp
void cannonMultiplyMV(const Matrix& A, const Matrix& B, Matrix& C) {
  size_t mysize = MPI::COMM_WORLD.Get_size();

  // Set up grid topology and a grid (Cartesian) communicator
  int dims[2] = { (int) std::sqrt(mysize), (int) std::sqrt(mysize) };
  bool periods[2] = { true, true };

  MPI::Cartcomm gridComm = MPI::COMM_WORLD.Create_cart(2, dims, periods, true);
  size_t myrank = gridComm.Get_rank();

  int mycoords[2];
  gridComm.Get_coords(myrank, 2, mycoords);

  int northRank, eastRank, westRank, southRank;
  gridComm.Shift(0, -1, westRank,  eastRank);
  gridComm.Shift(1, -1, southRank, northRank);

  // Move A and B where they need to be to start
  int shiftSource, shiftDest;
  gridComm.Shift(0, -mycoords[0], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                            MPI::DOUBLE, shiftDest, 314, shiftSource, 314);

  gridComm.Shift(1, -mycoords[1], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                            MPI::DOUBLE, shiftDest, 314, shiftSource, 315);



  // Main loop
  for (int k = 0; k < dims[0]; ++k) {
    hoistedCopyBlockedTiledMultiply2x2(A, B, C); // Local block matmat

    gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                              MPI::DOUBLE, westRank,  316, eastRank,  316);
    gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*A.numCols(),
                              MPI::DOUBLE, northRank, 317, southRank, 317);
  }

  // Restore A and B to initial distribution
  gridComm.Shift(0, +mycoords[0], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                            MPI::DOUBLE, shiftDest, 318, shiftSource, 318);

  gridComm.Shift(1, +mycoords[1], shiftSource, shiftDest);
  gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                            MPI::DOUBLE, shiftDest, 319, shiftSource, 319);

  gridComm.Free();
}
```

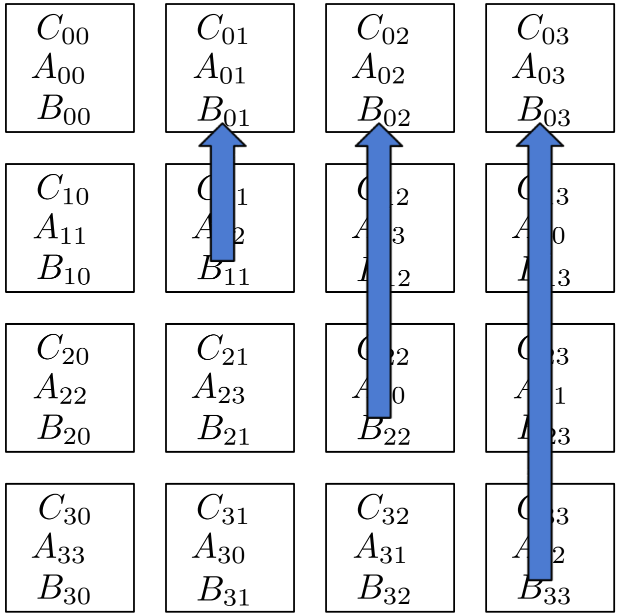
Implementation

```
void cannonMultiplyMV(const Matrix& A, const Matrix& B, Matrix& C) {
  size_t mysize = MPI::COMM_WORLD.Get_size();

  // Set up grid topology and a grid (Cartesian) communicator
  int dims[2] = { (int) std::sqrt(mysize), (int) std::sqrt(mysize) };
  bool periods[2] = { true, true };

  MPI::Cartcomm gridComm = MPI::COMM_WORLD.Create_cart(2, dims, periods, true);
  size_t myrank = gridComm.Get_rank();

  int mycoords[2];
  gridComm.Get_coords(myrank, 2, mycoords);

  int northRank, eastRank, westRank, southRank;
  gridComm.Shift(0, -1, westRank,  eastRank);
  gridComm.Shift(1, -1, southRank, northRank);
```

Implementation

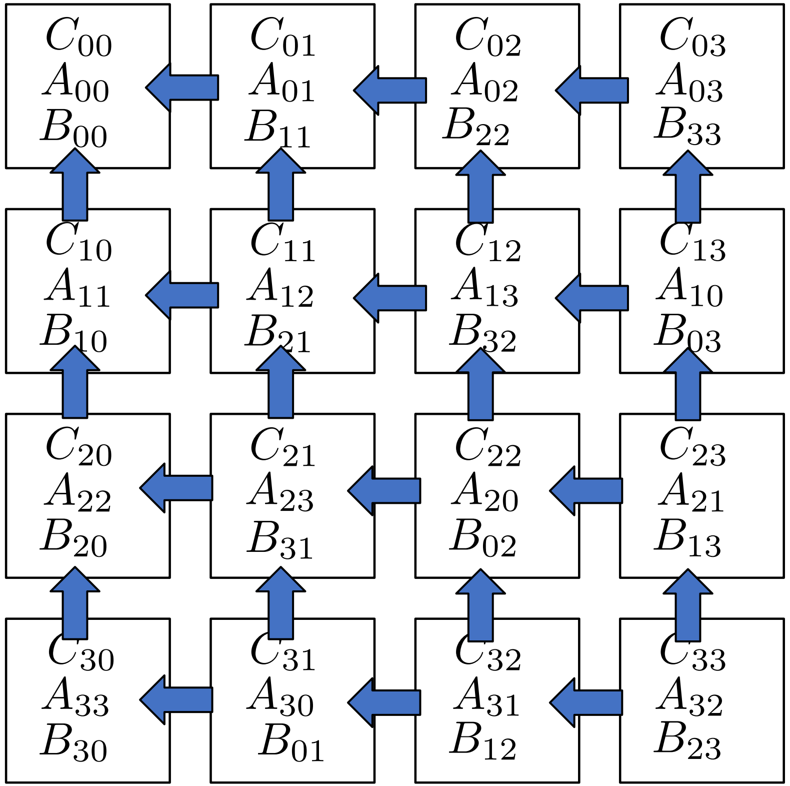
```cpp
// Move A and B where they need to be to start
int shiftSource, shiftDest;
gridComm.Shift(0, -mycoords[0], shiftSource, shiftDest);
gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                          MPI::DOUBLE, shiftDest, 314, shiftSource, 314);

gridComm.Shift(1, -mycoords[1], shiftSource, shiftDest);
gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                          MPI::DOUBLE, shiftDest, 314, shiftSource, 315);
```





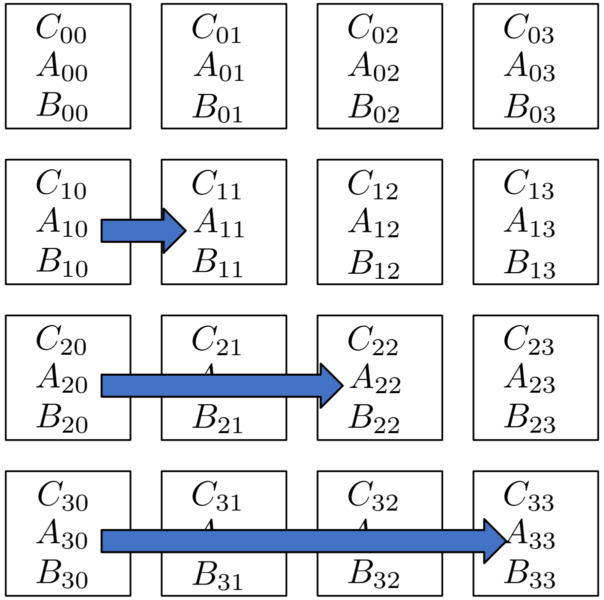
Implementation

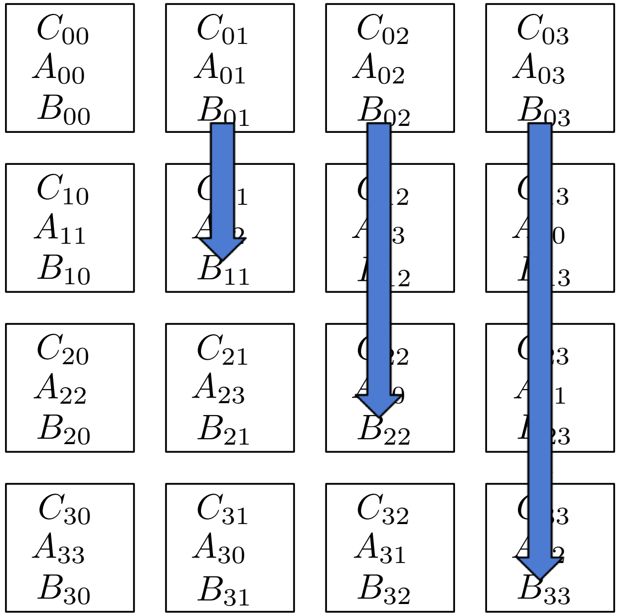
```
// Main loop
for (int k = 0; k < dims[0]; ++k) {
  hoistedCopyBlockedTiledMultiply2x2(A, B, C); // Local block matmat

  gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                            MPI::DOUBLE, westRank,  316, eastRank,  316);
  gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*A.numCols(),
                            MPI::DOUBLE, northRank, 317, southRank, 317);
}
```



Implementation

```
    // Restore A and B to initial distribution
    gridComm.Shift(0, +mycoords[0], shiftSource, shiftDest);
    gridComm.Sendrecv_replace(const_cast<double*>(&A(0,0)), A.numRows()*A.numCols(),
                              MPI::DOUBLE, shiftDest, 318, shiftSource, 318);

    gridComm.Shift(1, +mycoords[1], shiftSource, shiftDest);
    gridComm.Sendrecv_replace(const_cast<double*>(&B(0,0)), B.numRows()*B.numCols(),
                              MPI::DOUBLE, shiftDest, 319, shiftSource, 319);

    gridComm.Free();
}
```





The HP… s of 2022)

Build on each other

We have come to the end of this path

Technology	Paradigm	Hammer
CPU (single core)	Sequential	C++
SIMD/Vector (single core)	Data parallel	
Multicore	Threads	
NUMA shared memory	Threads	
GPU	GPU	CUDA
Clusters	Message passing	MPI

This quarter

Order of evolution (more or less)

Technology and paradigm

In the era of exascale computing

- ORNL – Frontier
  - 8.7M cores, 1.1 exaflop/s

- MPI + X
  - MPI + OpenMP
  - MPI + CUDA
  - MPI + …

Tour of the Course (HPC hardware)

- Basic CPU machine model
- Hierarchical memory (registers, cache, virtual memory)
- Instruction level parallelism
- Multicore processors
- Shared memory parallelism
- GPU
- Distributed memory parallelism

- Use running examples

Tour of the Course (HPC Software)

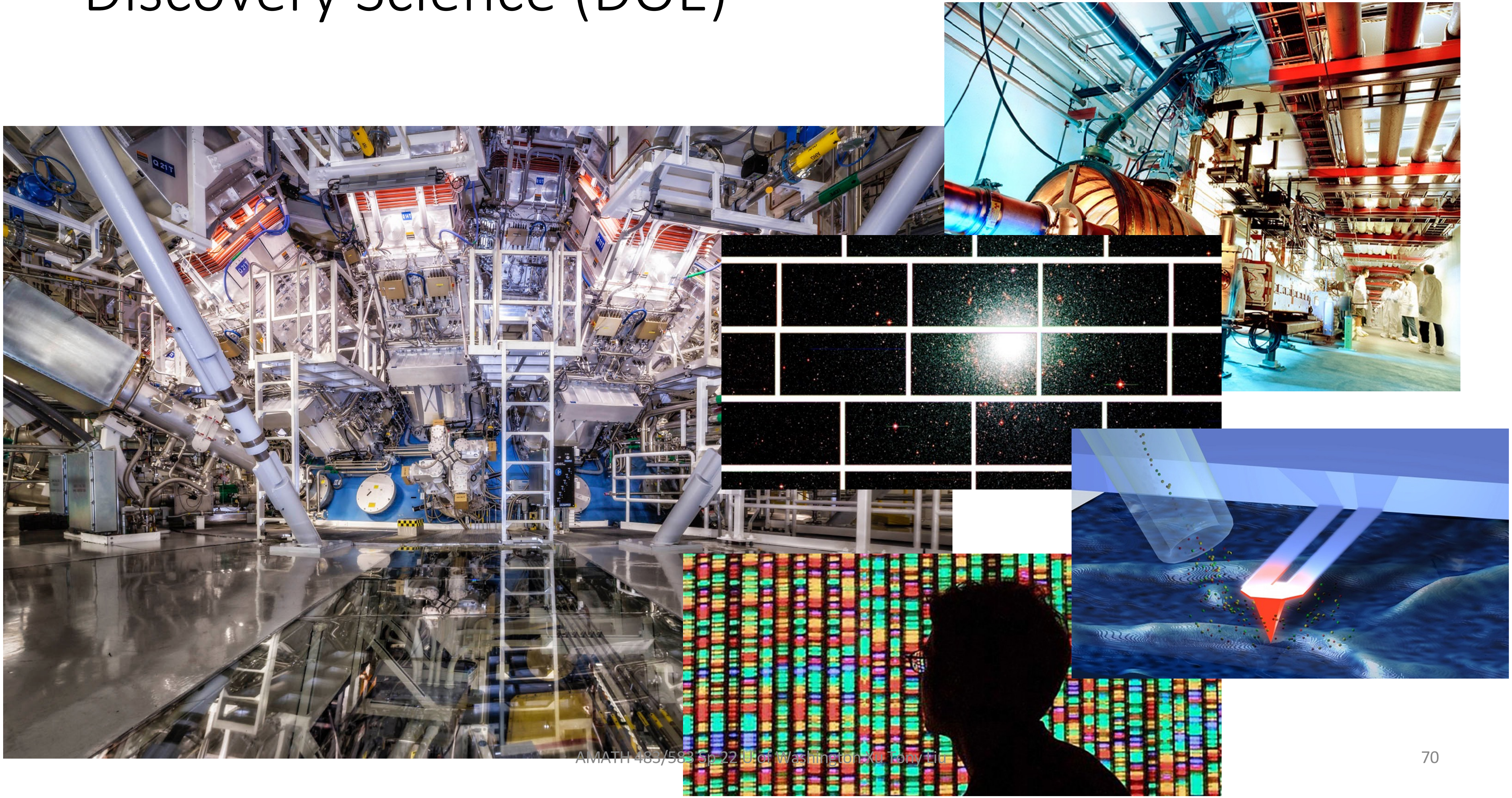
- Elements of C++
- Elements of software organization
- Elements of software practice
- Elements of performance measurement and optimization

What you have learnt

- Ask yourself at the beginning of this quarter
  - What scientific problem you want to solve?
  - What do you want to learn from this course that can prepare you?
  - Can you write a sequential program to solve it?
  - What is the performance of it?
  - …

- Ask yourself at the end of this quarter
  - Do you master the skillset to solve your scientific problem?
  - Can you write a high-performance program to solve it?
  - What is the performance of it?
  - What is the speedup?
    - compare your sequential program with your high-performance program

Discovery Science (DOE)



Uses of HPC (a sample)

- Cosmology
- Earthquake
- Weather
- Climate modeling
- Automobile crash testing
- Aircraft design
- Jet engine design
- Stockpile stewardship
- Nuclear fusion
- Protein folding
- Modeling the brain
- Modeling bloodstream
- Epidemiology
- Rendering (CGI)
- Sigint
- Block chains
- Gene sequencing
- Etc

Where do we go from here?

Clouds = Services

Amazon Web Services

Compute
- EC2 — Virtual Servers in the Cloud
- EC2 Container Service — Run and Manage Docker Containers
- Elastic Beanstalk — Run and Manage Web Apps
- Lambda — Run Code in Response to Events

Storage & Content Delivery
- S3 — Scalable Storage in the Cloud
- CloudFront — Global Content Delivery Network
- Elastic File System PREVIEW — Fully Managed File System for EC2
- Glacier — Archive Storage in the Cloud
- Import/Export Snowball — Large Scale Data Transport
- Storage Gateway — Integrates On-Premises IT Environments with Cloud Storage

Database
- RDS — Managed Relational Database Service
- DynamoDB — Predictable and Scalable NoSQL Data Store
- ElastiCache — In-Memory Cache
- Redshift — Managed Petabyte-Scale Data Warehouse Service

Networking
- VPC — Isolated Cloud Resources
- Direct Connect — Dedicated Network Connection to AWS
- Route 53 — Scalable DNS and Domain Name Registration

Developer Tools
- CodeCommit — Store Code in Private Git Repositories
- CodeDeploy — Automate Code Deployments
- CodePipeline — Release Software using Continuous Delivery

Management Tools
- CloudWatch — Monitor Resources and Applications
- CloudFormation — Create and Manage Resources with Templates
- CloudTrail — Track User Activity and API Usage
- Config — Track Resource Inventory and Changes
- OpsWorks — Automate Operations with Chef
- Service Catalog — Create and Use Standardized Products
- Trusted Advisor — Optimize Performance and Security

Security & Identity
- Identity & Access Management — Manage User Access and Encryption Keys
- Directory Service — Host and Manage Active Directory
- Inspector PREVIEW — Analyze Application Security
- WAF — Filter Malicious Web Traffic

Analytics
- EMR — Managed Hadoop Framework
- Data Pipeline — Orchestration for Data-Driven Workflows
- Elasticsearch Service — Run and Scale Elasticsearch Clusters
- Kinesis — Work with Real-time Streaming data

Internet of Things
- AWS IoT BETA — Connect Devices to the cloud

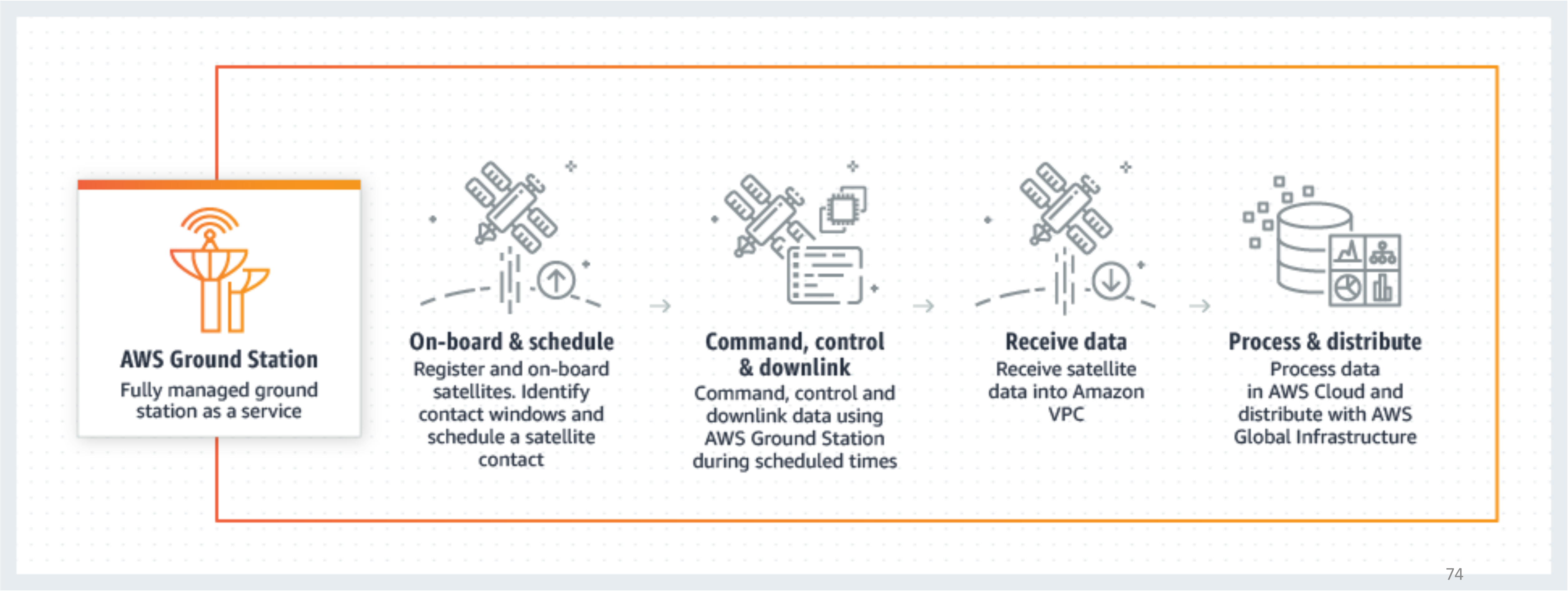
Mobile Services
- Mobile Hub BETA — Build, Test, and Monitor Mobile apps
- Cognito — User Identity and App Data Synchronization
- Device Farm — Test Android, Fire OS, and iOS apps on real devices in the Cloud
- Mobile Analytics — Collect, View and Export App Analytics
- SNS — Push Notification Service

Application Services
- API Gateway — Build, Deploy and Manage APIs
- AppStream — Low Latency Application Streaming
- CloudSearch — Managed Search Service
- Elastic Transcoder — Easy-to-use Scalable Media Transcoding
- SES — Email Sending Service
- SQS — Message Queue Service
- SWF — Workflow Service for Coordinating Application Components

Enterprise Applications
- WorkSpaces — Desktops in the Cloud
- WorkDocs — Secure Enterprise Storage and Sharing Service
- WorkMail PREVIEW — Secure Email and Calendaring Service

Services: On Demand Access

- Data Storage (blob, file, unstructured, SQL, &c)
- Computing (VM, cluster, GPU)



What’s Next

- Machine learning
- Quantum computing
- 5G
- IoT / edge computing

Congratulations!

- You survived HPC course
- Be well
- Do good work
- Stay in touch

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