AMATH 483/583 High Performance Scientific Computing

Lecture 19: Advanced Message Passing, Collectives, Performance Models, Eigenfaces

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Administrative

- Fill out course evaluations!
- Final assignment is out, due Friday midnight June 10th
- No physical office hours at LEW 315
- Zoom office hours instead
- Link will be posted through announcement

Top500 As of May 30th, 2022 (top500.org)

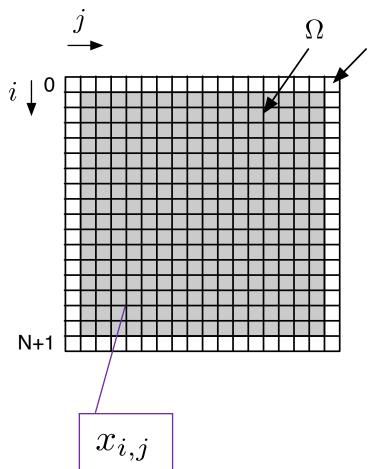
- ORNL's Frontier First to Break the Exaflop Ceiling!
 - HPE Cray EX architecture
 - 1.102 Exaflop/s
 - 8,730,112 total AMD EPYC 64C 2GHz processors
 - AMD Instinct™ 250X accelerators
 - Slingshot-11 interconnect

	Rank	System	Cores	(PFlop/s)	(PFlop/s)	(kW)
	1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
	2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
	3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942
	4	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States AMATH 483/583 Sp 22 U of Washington Xu Tony Liu	2,414,592	148.60	200.79	10,096

Outline

- Previously
 - Laplace's equation on a regular grid
- Non-blocking operations
- Collectives
- Performance models
- Eigenfaces

Laplace's Equation on a Regular Grid



$$\partial\Omega$$

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

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

Discretization



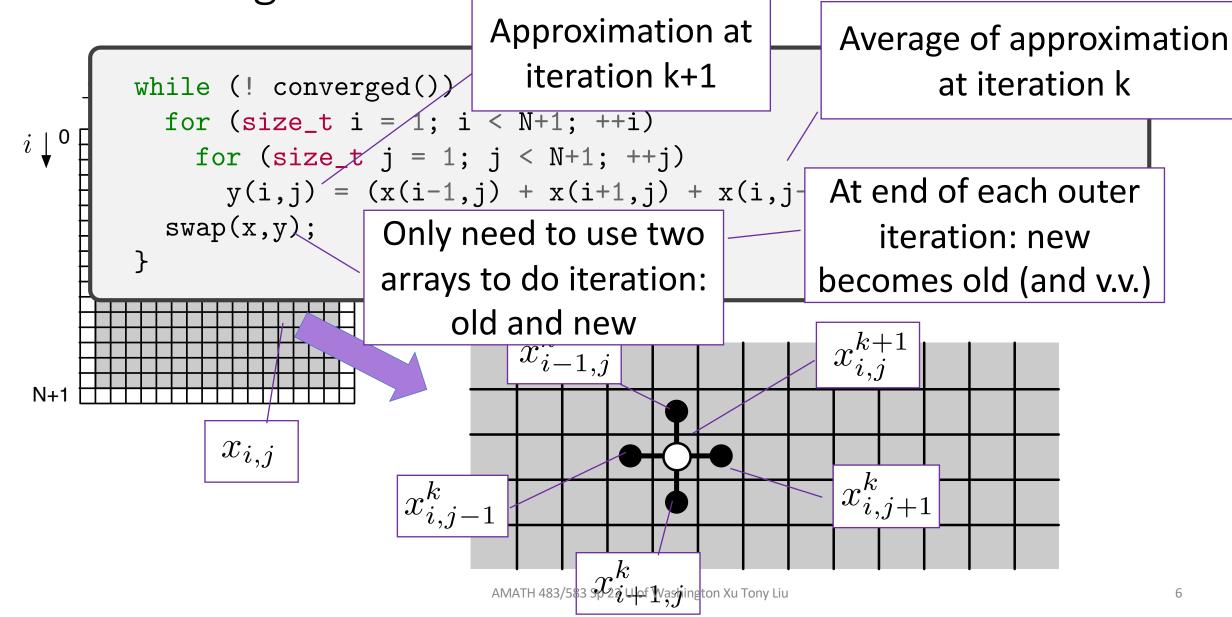
$$x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} - 4x_{i,j} = 0$$

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

The value of each point on the grid

The average of its neighbors

Iterating for a solution



class Grid

```
Grid is a 2D
class Grid {
                                                Constructor
                         array
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]; }
                                                      Accessor
  size_t numX() const { return xPoints; }
  size_t numY() const { return yPoints; }
private:
  size_t xPoints, yPoints;
  std::vector<double> arrayData;
                                      Storage
};
```

Decomposition

Original problem

Index

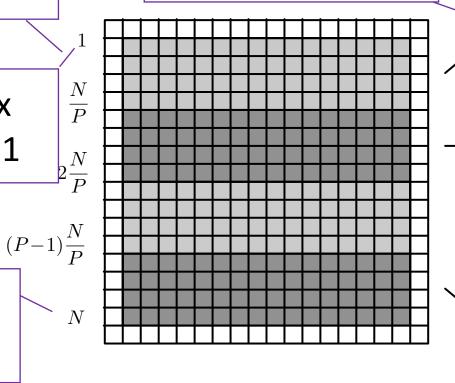
from 1

Index

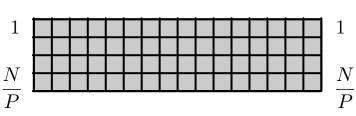
to N

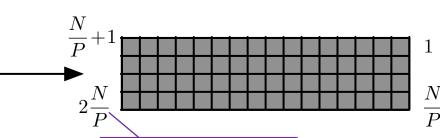
lobal Decompose into P

partitions



Global





Local

SPMD index space

All are identical

Partitioned index space



```
for (size_t i = 1; i < N+1; ++i)

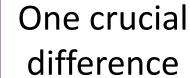
for (size_t j = 1; j < N+1; ++j)

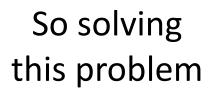
y(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;

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```

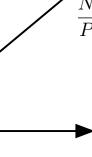
Decomposition **Boundary**

Boundary





To the local / SPMD code, the boundary and as-if are the same





"as-if"

 $\frac{N}{P}+1$

$$\frac{N}{P}+1$$

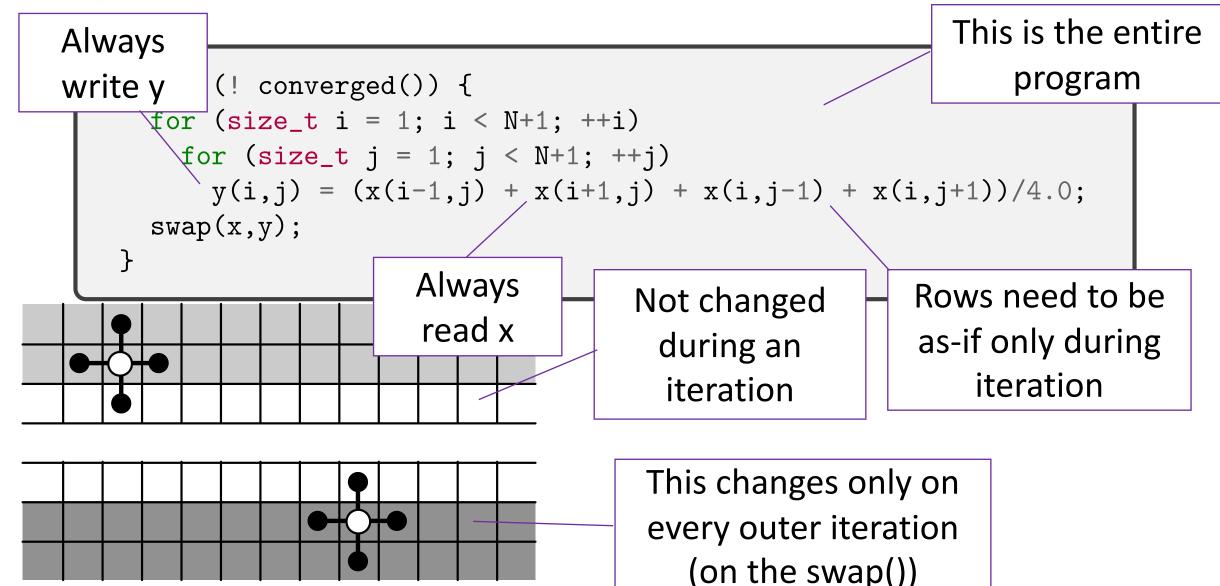
Not part of the original problem



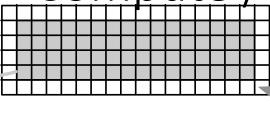
Is the same as solving lots of the same problem but smaller

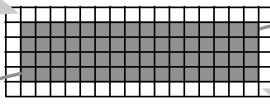
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As-If



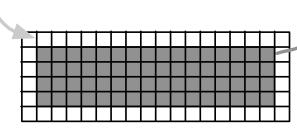
Compute / Communicate





$$K\frac{N}{P}+1$$

To make as-if, we need to update the boundary cells





With their "asif" values

Before they are read at the next outer iteration



Compute / Communicate

ghost

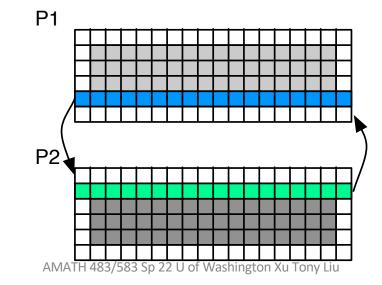
```
while (! converged()) {
for (size_t i = 1; i < N+1; ++i)
    for (size_t j = 1; j < N+1; ++j)
     y(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))/4.0;
 swap(x,y);
```

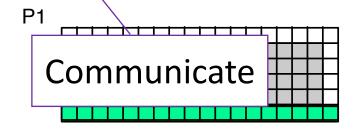
Standard terminology for as-if boundary is "ghost cell" or "halo"

make_as_if(x); // Communicate ghost cells

Compute

ghost

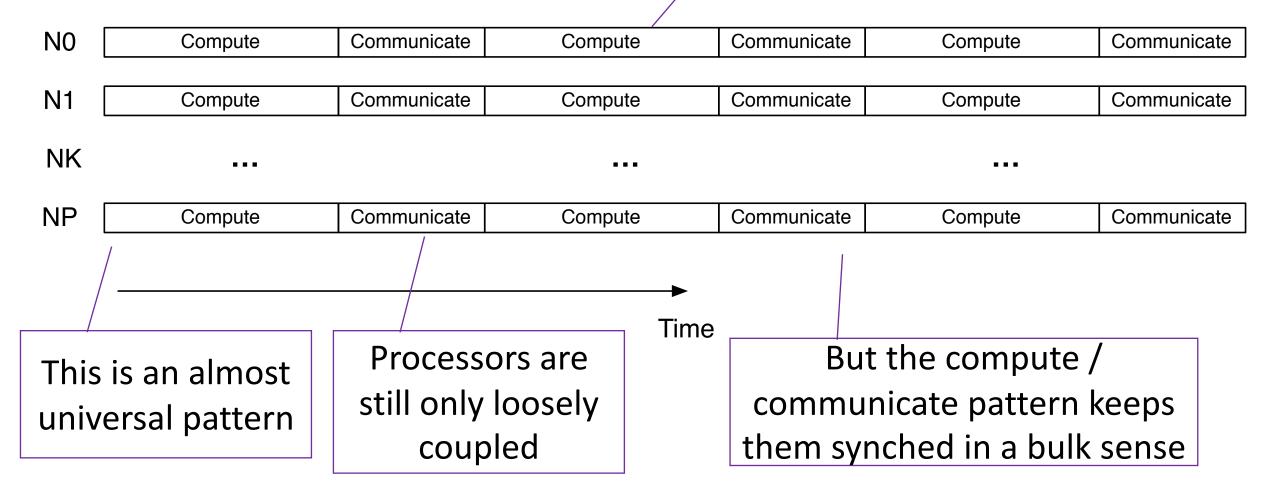






Compute / Communicate

"Bulk Synchronous Parallel" (BSP)



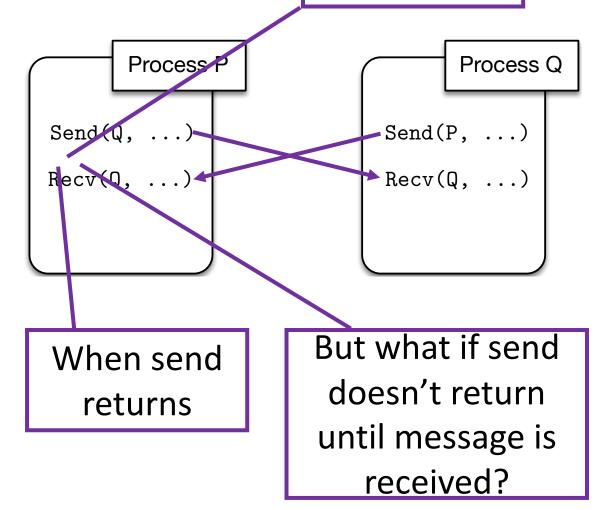
Updating Ghost Cells

ghost ghost P1 P1 P2 P2 P2 Works? MPI_Send(...); // to upper neighbor MPI_Send(...); // to lower neighbor MPI_Recv(...); // from lower neighbor MPI_Recv(...); // from upper neighbor

Exchanging halos (updating ghost cells)

When can we proceed?

- What happens with this set of operations?
- Have we seen this before?
- Behavior depends on implementation of Send (not its semantics)
 - Size of message (use of eager vs rendezvous protocol)
 - System dependent
 - Most MPI implementations have diagnostics for this



Where do messages go when you send t System might not buffer the data System might System might buffer the data w buffer the data Process P Process Q Process P Process Q Good thing or Buffer Buffer bad thing? Data Network Data Data Data Might buffer Not others some message

MPI_Send

```
#include <mpi.h>
void Comm::Send(const void* buf, int count, const Datatype& datatype,

→ int dest, int tag) const
```

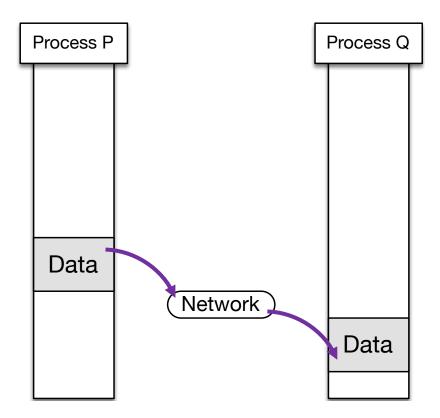
- MPI_Send is sometimes called a "blocking send"
- Semantics (from the standard): Send MPI_Send returns, it is safe to reuse the buffer
- So it only blocks until buffer is safe to reuse
- (Recall we can only specify local semantics)

MPI Recv

- Blocking receive
- Semantics: Blocks until message is received. On return from call, buffer will have message data

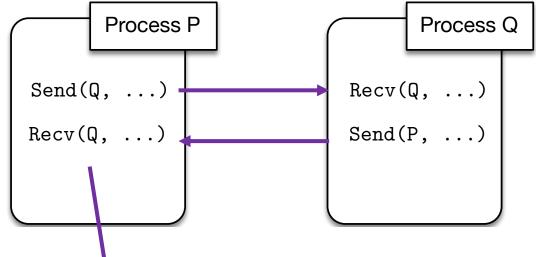
Unbuffered Communication

- Buffering can be avoided
- But we need to make sure it is safe to touch message data
 - Block until it is safe
 - Return before transfer is complete and wait/test later



Some other solutions

Simultaneously send and recv



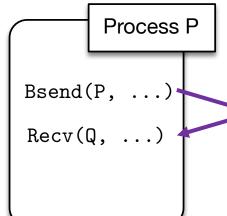
Sendrecv(P, ...)

Sendrecv(Q, ...)

Process Q

Properly order sends and recvs

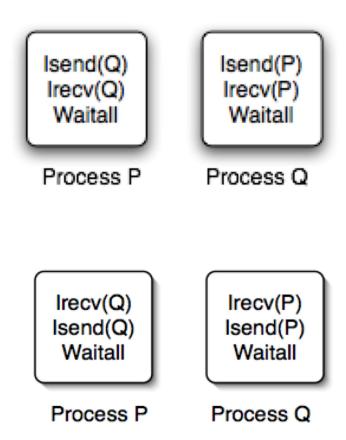
Difficult and breaks spmd



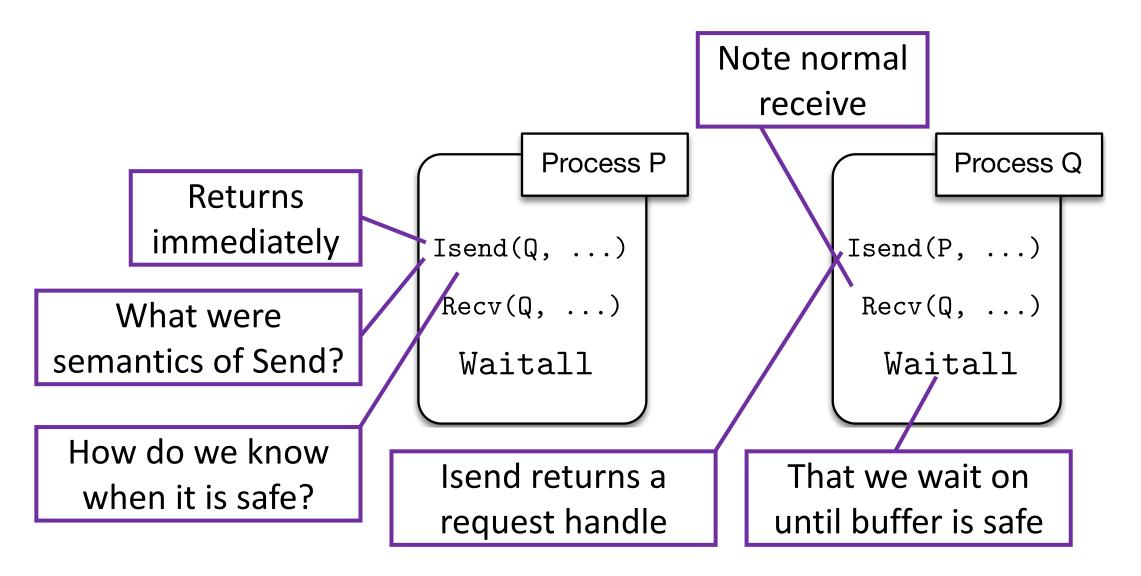
Bsend(Q, ...)
Recv(Q, ...)
Explicitly
buffer

Non-Blocking Operations

- Non-blocking operations (send and receive) return immediately
- Return "request handles" that can be tested or waited on
- Where progress is made (and where communication happens) is implementation specific



Non-blocking (immediate) operations



Non-blocking (immediate) operations

There is also a nonblocking receive

What were semantics of Recv?

Irecv also returns a request handle

Process P

Isend(Q, ...)

Irecv(Q, ...)

Waitall

That can be waited on and will return when data are ready

Process Q

Isend(P, ...)

Irecv(P, ...)

Waitall

We can wait on all requests together (send and recv)

Before

Process P

Isend(Q, ...)

Irecv(Q, ...)

Waitall

Process Q

Isend(P, ...)

Irecv(P, ...)

Waitall

After

Process P

Irecv(Q, ...)

Isend(Q, ...)

Waitall

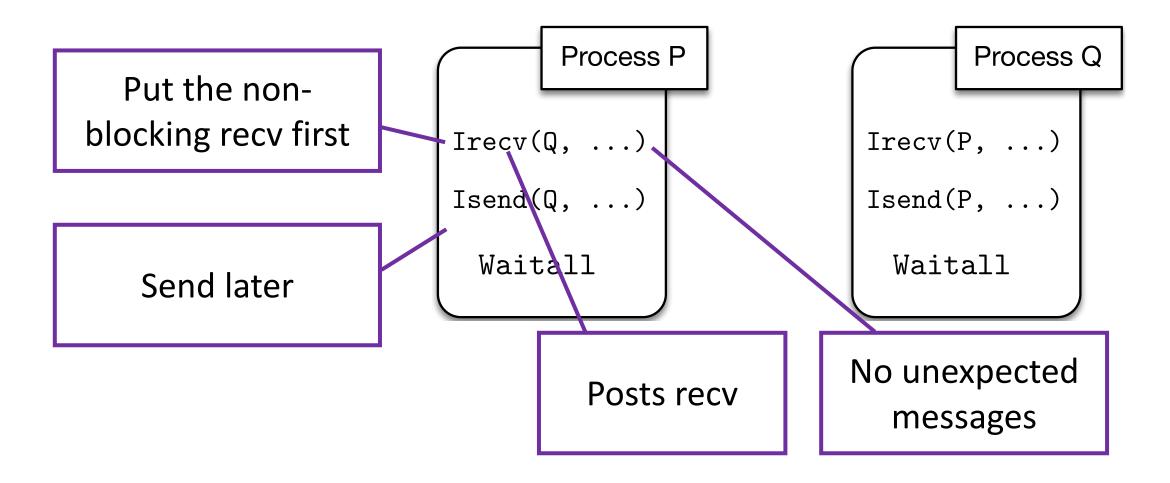
Process Q

Irecv(P, ...)

Isend(P, ...)

Waitall

After



Bindings for non-blocking receive

```
Request Comm::Isend(const void* buf, int count, const

Datatype& datatype, int dest, int tag) const
```

```
Request Comm::Irecv(void* buf, int count, const

→ Datatype& datatype, int source, int tag) const
```

Communication completion: Wait

```
void Request::Wait(Status& status)
void Request::Wait()
```

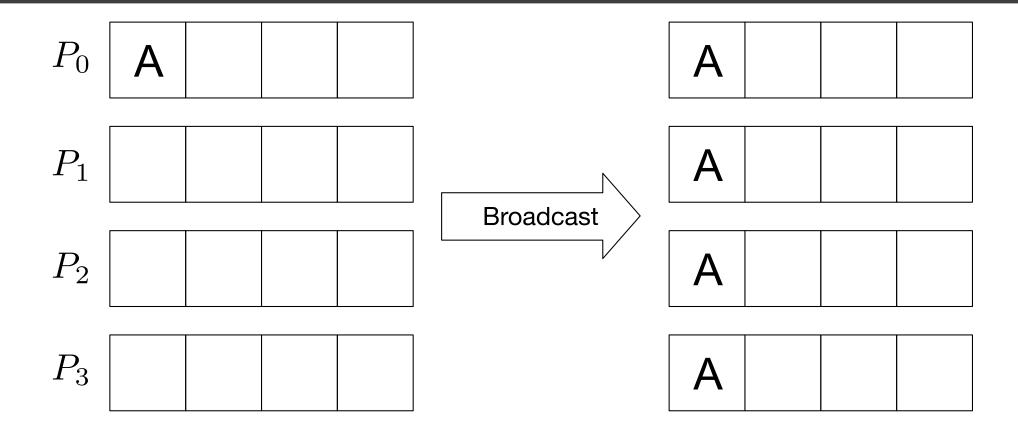
Communication completion: Test

```
bool Request::Test(Status& status)
bool Request::Test()
```

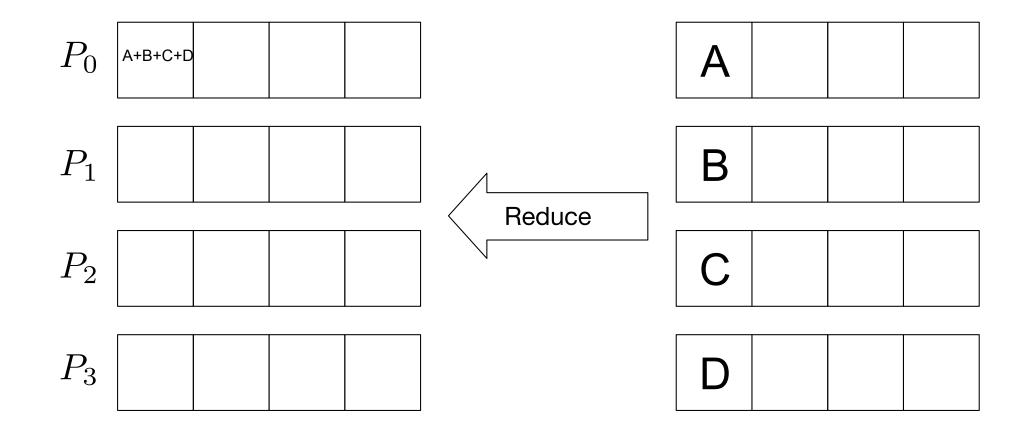
Collectives

- 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

<u>Bcast</u>



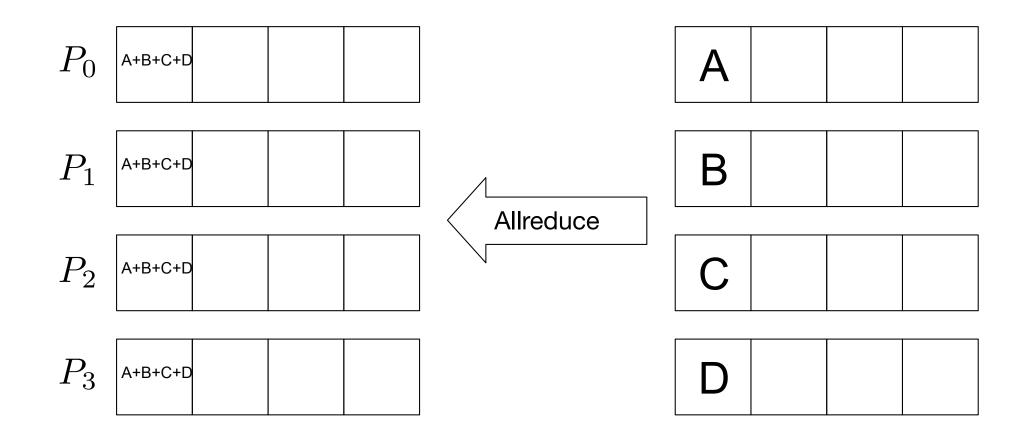
<u>Reduce</u>



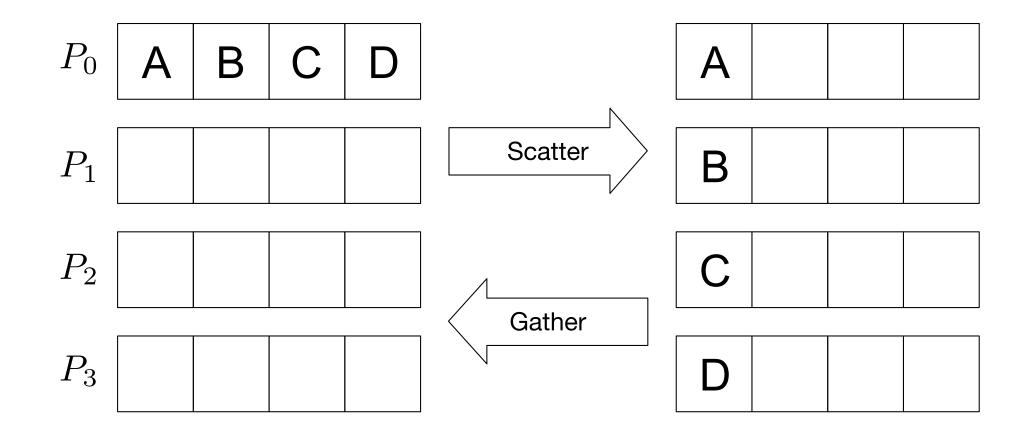
<u>Allreduce</u>

void MPI::Comm::Allreduce(const void* sendbuf, void* recvbuf, int count, const

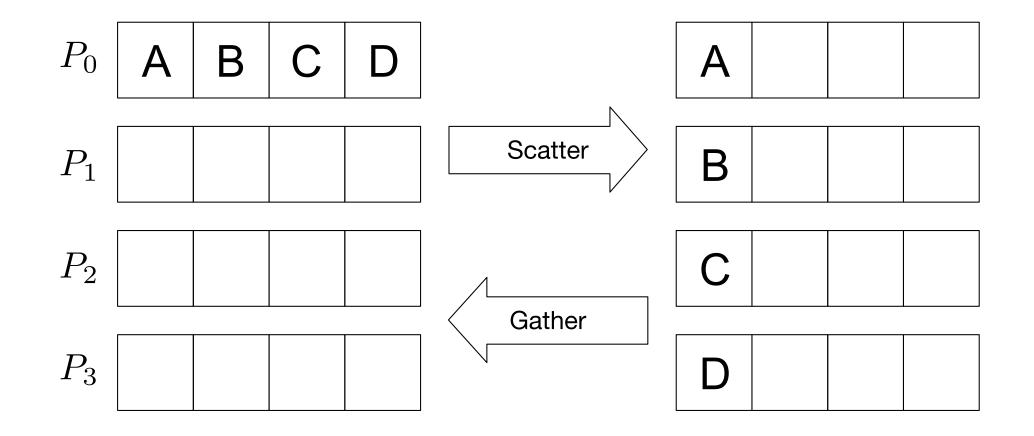
→ MPI::Datatype& datatype, const MPI::Op& op) const=0



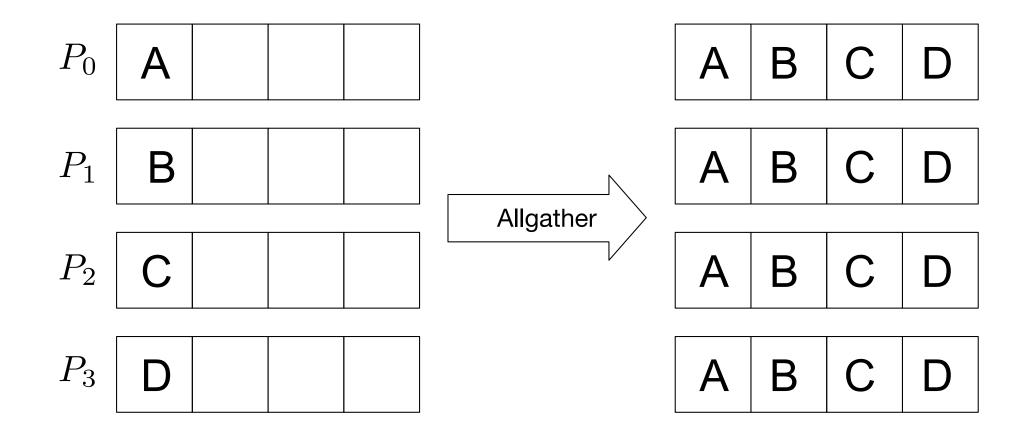
Scatter/Gather



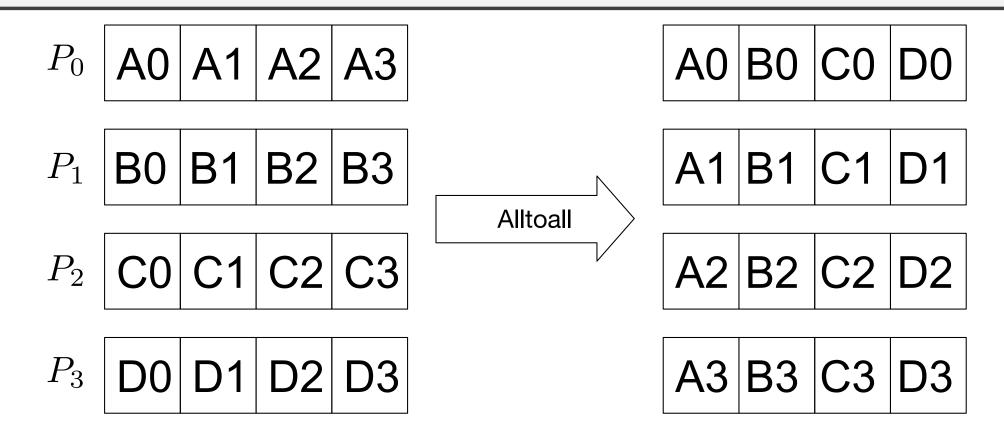
Scatter/Gather



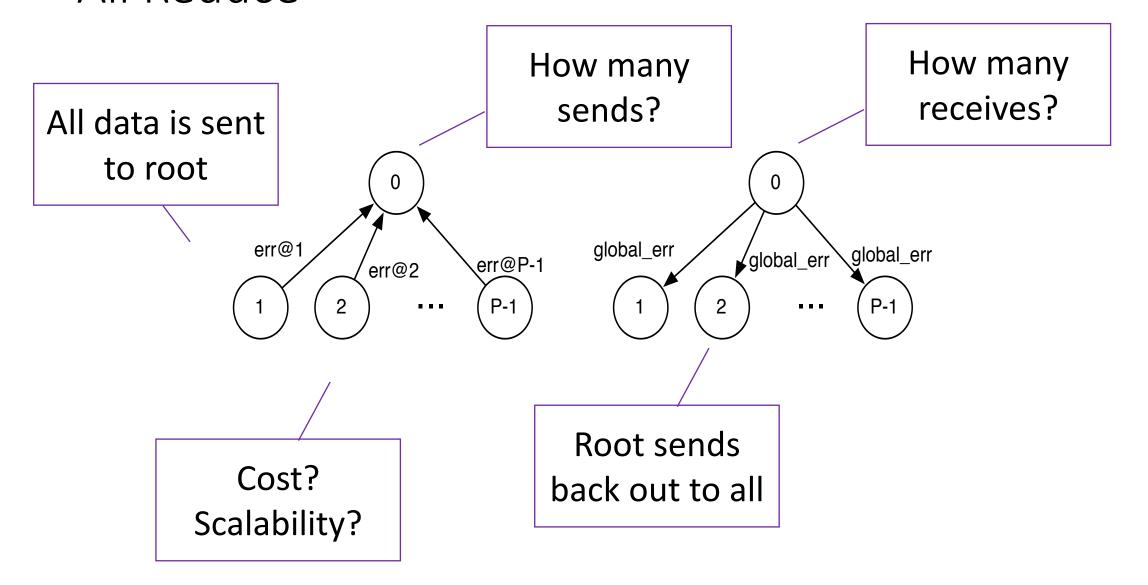
Allgather

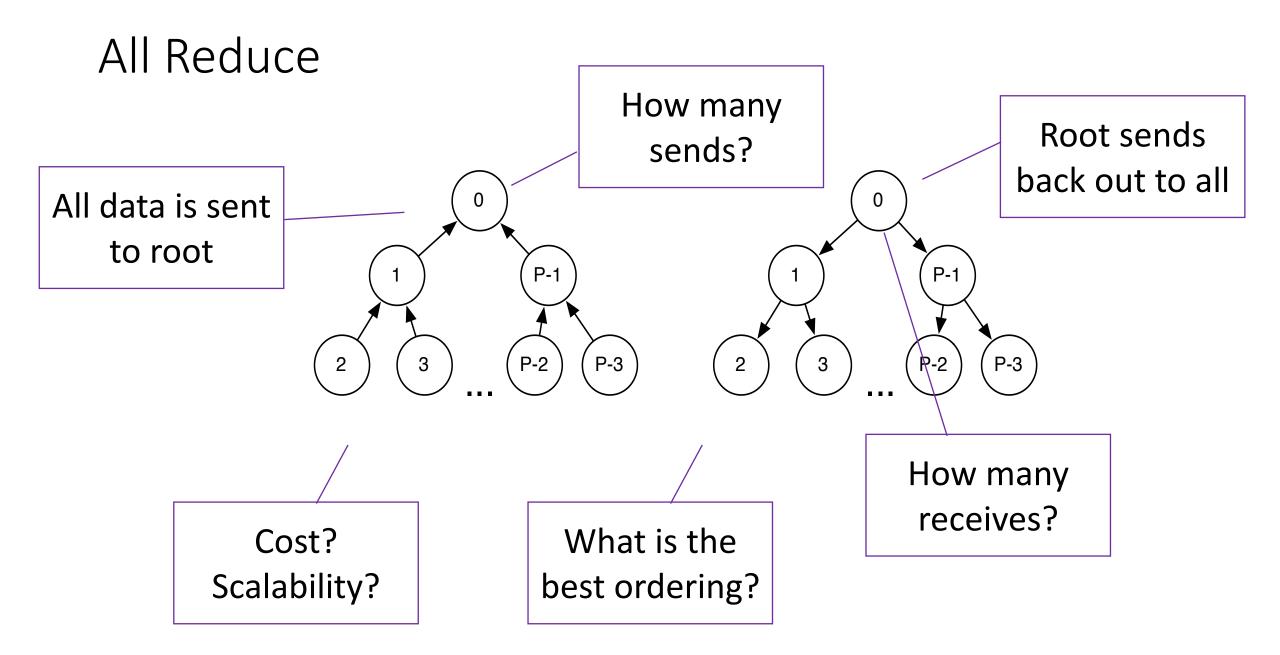


Alltoall



All Reduce





Parallel Random Access Machine

Some number (fixed or infinite) number of processors

Processors all execute same steps in synchrony (but can lay out)

At each cycle, processors read, write, or compute (one operation)

Shared Memory

 P_1 P_2 P_3 P_4 \cdots P_4

Powerful tool for analysis of parallel algorithm

Memory shared by all processes

Completely UMA (O(1) read/write)

Everything interesting in parallel computing is about data dependence

Assume tasks done in parallel are perfectly parallelizable

PRAM cont.

Reads and writes need to be ordered

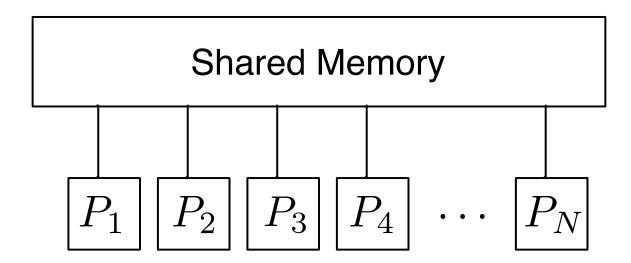
- Several types of PRAM
 - EREW Exclusive Read Exclusive Write
 - CREW Concurrent Read Exclusive Write
 - ERCW Exclusive Read Concurrent Write
 - CRCW Concurrent Read Concurrent Write

Writes need to be ordered

Reads need to be ordered

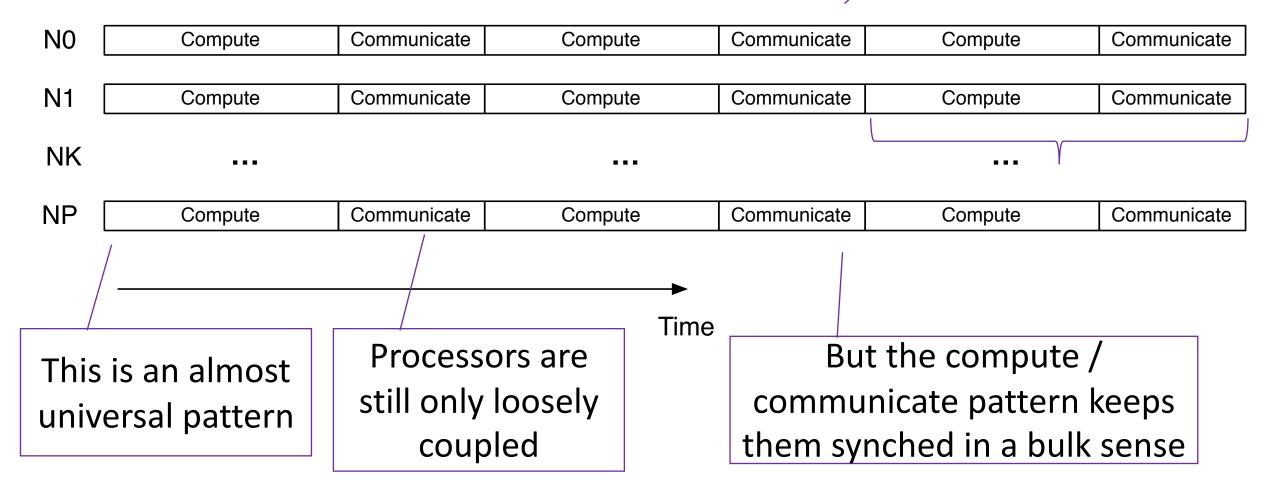
Nothing needs to be ordered

Stronger models can be emulated by weaker models



Compute / Communicate

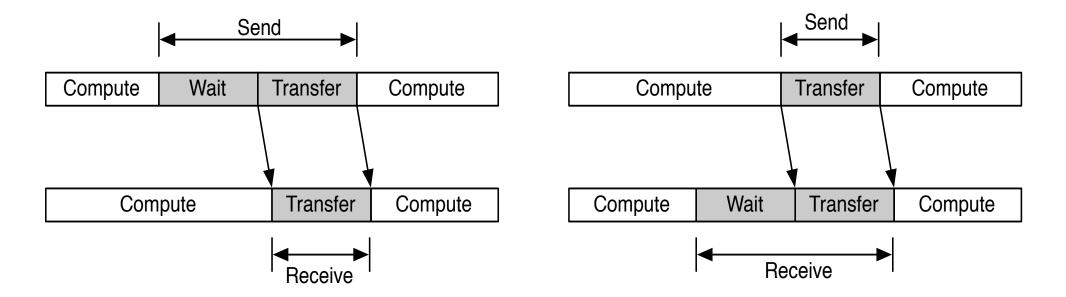
"Bulk Synchronous Parallel" (BSP)



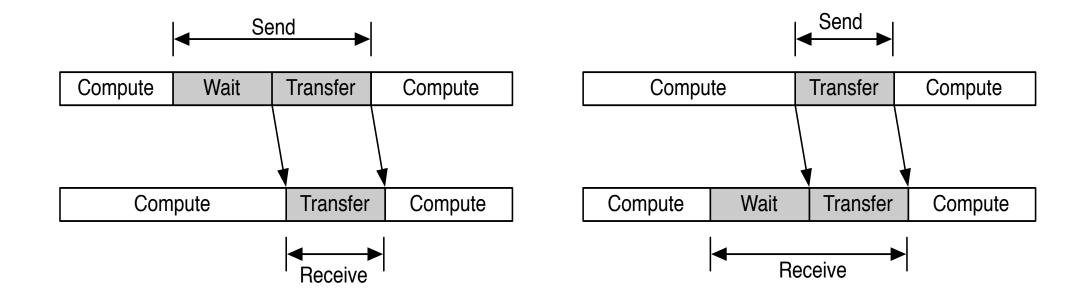
Performance Model

$$T_{communicate} = T_{latency} + T_{bandwidth} = T_L + r_{nic} \cdot Size$$

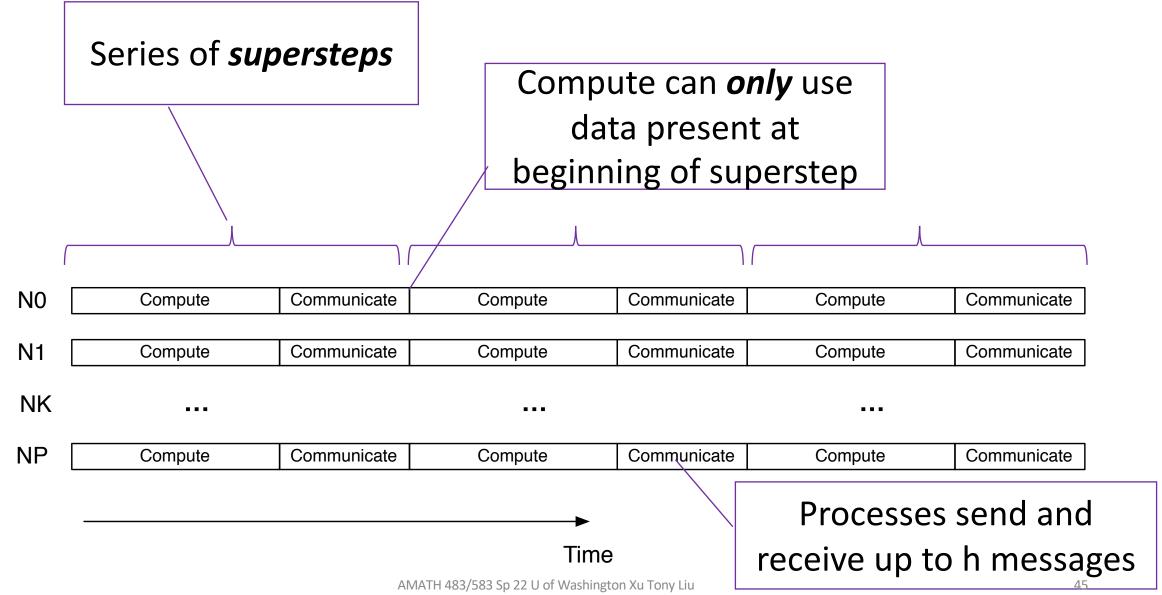
$$Speedup = \frac{T_{seq}}{T_{parallel}} = \frac{T_{seq}}{T_{compute} + T_{bandwidth} + T_{latency}}$$

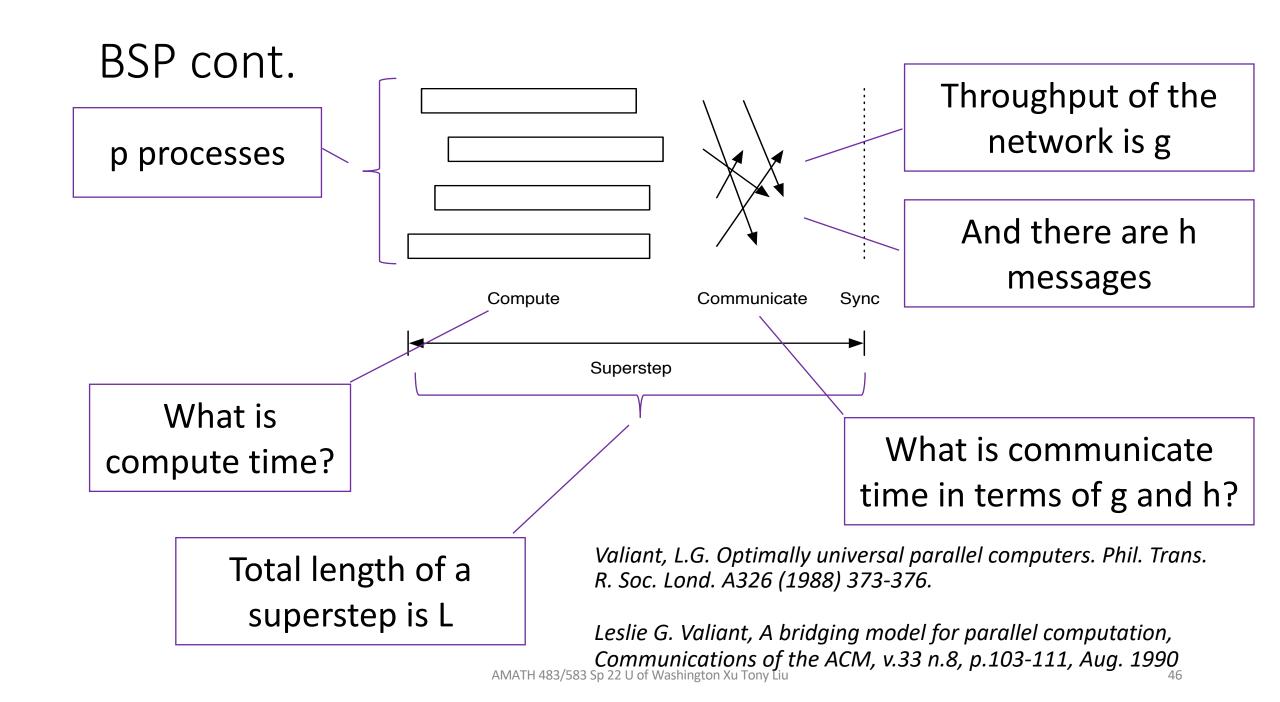


Synchronous vs Asynchronous

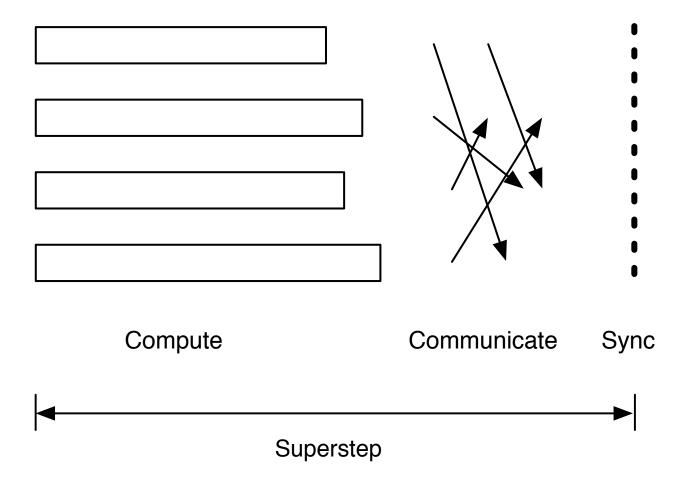


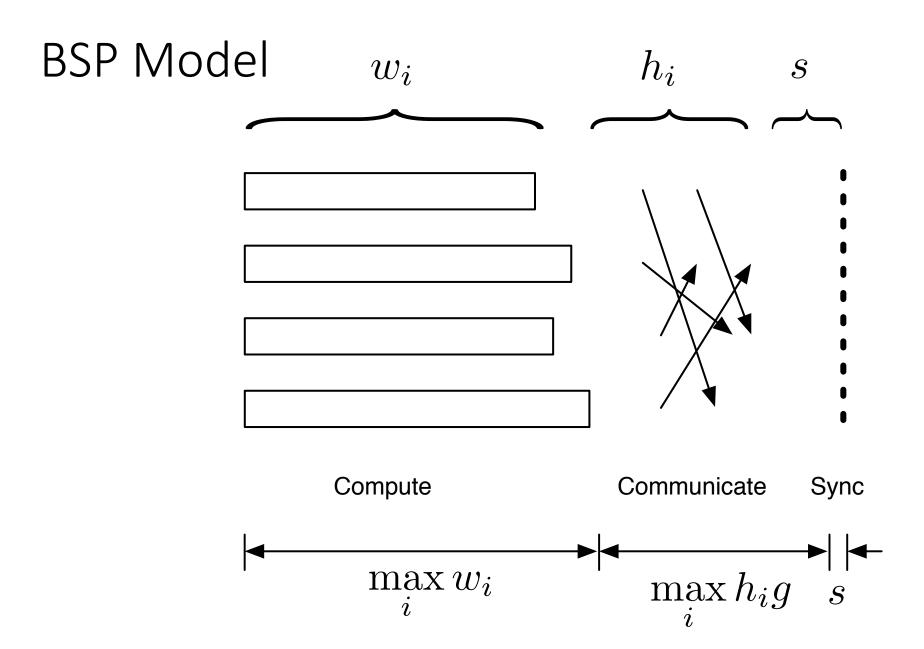
Bulk Synchronous Parallel (BSP)

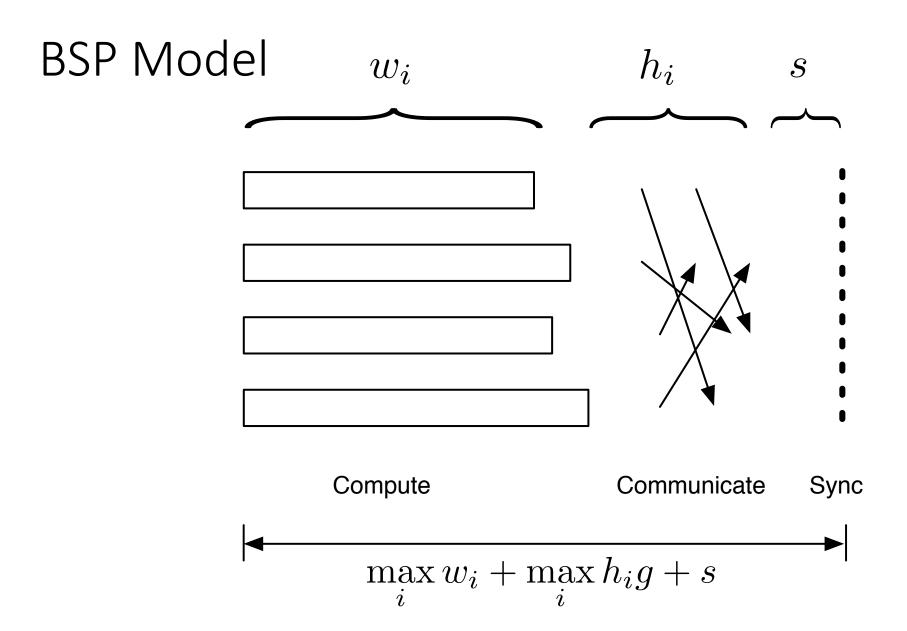




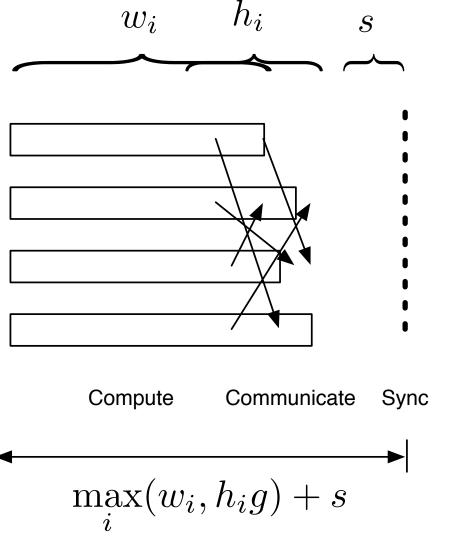
BSP Model





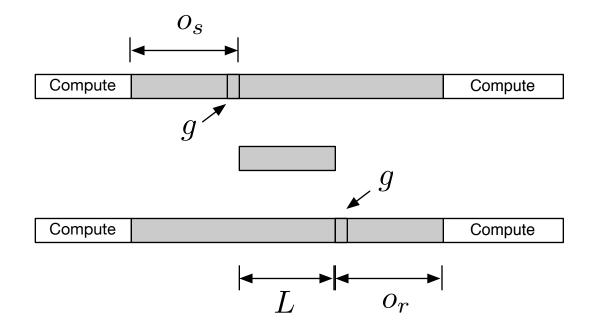


BSP with asynchronous communication



LogP

- Parameters (measured in processor cycles)
 - L upper bound on *latency* for a single message
 - o overhead to transmit or receive a message
 - *g* minimum *gap* between consecutive messages
 - *P* number of processors



- Finite capacity constraint
 - At most \[\int L/g \] messages can be in transit from or to any given processor at one time
 - Processors that attempt to exceed this limit stall until the message can be sent

LogP

Send single message

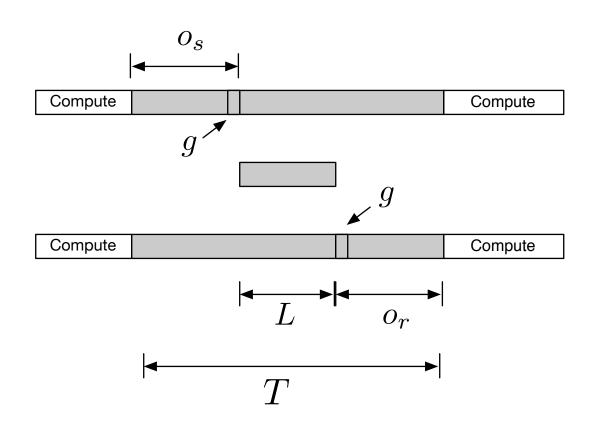
$$T = 2o + L$$

Ping-pong round trip

$$T = 4o + 2L$$

N messages in a row

$$T = L + (n-1)\max(g, o) + 2o$$



Why?

LogP cont.

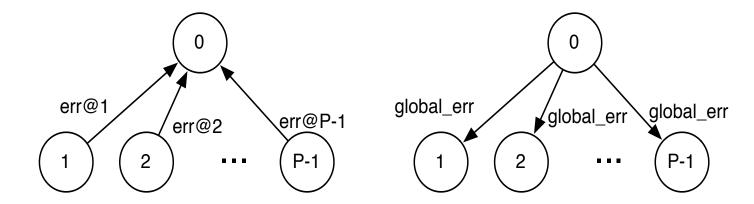
- Allows more precise scheduling of communication
 - Reading a remote memory location
 - BSP next superstep, L cycles
 - LogP *2L + 4o* cycles
- No special synchronization hardware
- Parameters can be experimentally determined for a given machine/architecture
- No special treatment for long messages

Applications: Reduce

- BSP
 - O(log n) supersteps
 - L = time to read two memory locations and write one

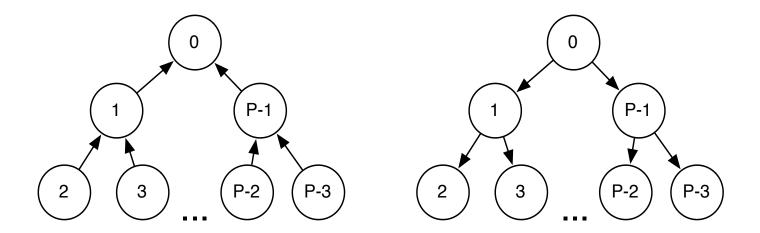
LogP Analysis

- Linear reduce
 - o for each processor to send its value to the root
 - (P-1)o + L for the root to receive them
 - $o + (P-1)*max{g,o} + L$



LogP Analysis

- Binary tree
 - o for each leaf processor to send its value to its parent
 - o + max{g,o} + L + o for each non-leaf processor to receive values from each of its children and send the result to its parent
 - $o + (log P)(o + max{g,o} + L + o)$



Name This Famous Person











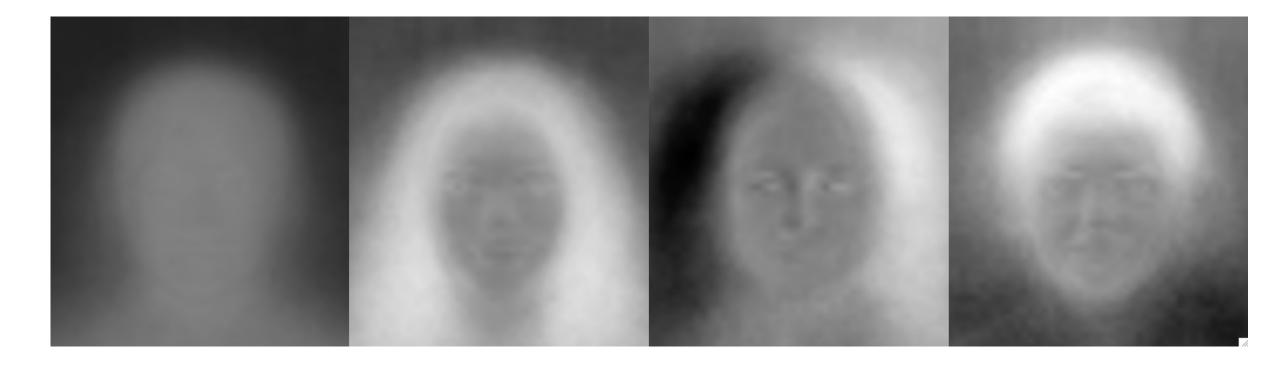








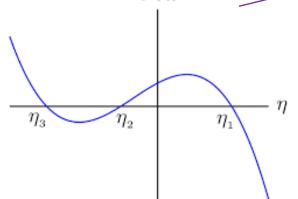
Name This Famous Person



Fundamental Theorems

$$N = \prod_{i=0}^{m} x_i$$

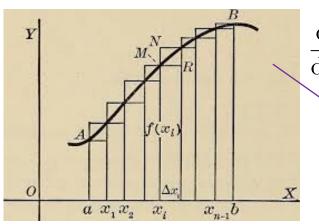
Arithmetic: Every number is a product of primes



 $f(\eta)$

Algebra: Every polynomial has a root





$$\frac{\mathrm{d}}{\mathrm{dt}} \int_0^t f(t)dt = \int_0^t \left[\frac{\mathrm{d}}{\mathrm{dt}} f(t) \right] = f(t)$$

Calculus: The integral of the derivative is the derivative of the integral

Software engineering: We can solve any problem by introducing an extra level of indirection

Linear Systems

Every linear space has a basis

 $e_i = (0, 0, \dots 1 \dots 0)$

Nice orthonormal basis

$$x = \sum_{i=1}^{dim} \alpha_i y_i$$
 Every linear has a base

Any element in the space can be expressed as weighted sums of members of the basis

$$x = (x_0, x_1...x_{N-1})$$

$$\hat{x} = (\alpha_0, \alpha_1, \dots \alpha_{N-1})$$

The same element has multiple representations

Linear Systems

$$e_i = (0, 0, \dots 1 \dots 0)$$

$$x = \sum_{i=0}^{\dim X} \alpha_i y_i$$

$$x = (x_0, x_1...x_{N-1})$$

What is x^?

$$x = \alpha_0(1, 0, \dots, 0) + \alpha_1(0, 1, 0, \dots, 0) + \dots + \alpha_{N-1}(0, 0, \dots, 1)$$

$$\hat{x} = (\alpha_0, \alpha_1, \dots \alpha_{N-1})$$

Which is equal to?

Transforming From One Representation to Another

$$x = (x_0, x_1...x_{N-1})$$

$$\hat{x} = (\alpha_0, \alpha_1, \dots \alpha_{N-1})$$

$$x = \sum_{i=0}^{\dim X} \alpha_i y_i$$

$$x = \alpha_0 y_0 + \alpha_1 y_1 + \dots + \alpha_{N-1} y_{N-1}$$

$$Y = [y_0, y_1, \dots, y_{N-1}]$$
What is this?

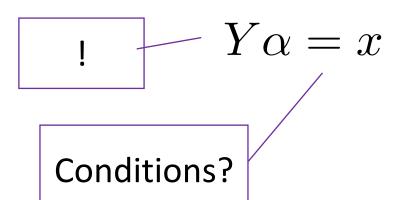
Transforming From One Representation to

Another

$$y_{0,0}$$
 $y_{0,1}$... $y_{0,N-1}$ $y_{1,0}$ $y_{1,1}$... $y_{1,N-1}$... $y_{N-1,0}$ $y_{N-1,1}$... $y_{N-1,N-1}$

$$y_{0,0}$$
 $y_{0,1}$... $y_{0,N-1}$ $y_{1,0}$ $y_{1,1}$... $y_{1,N-1}$...

$$y_{N-1,0}$$
 $y_{N-1,1}$... $y_{N-1,N-1}$



 $\alpha = Y^{-1}x$

$$egin{array}{c} lpha_0 \ lpha_1 \ \ldots \ lpha_{N-1} \end{array}$$

 α_0

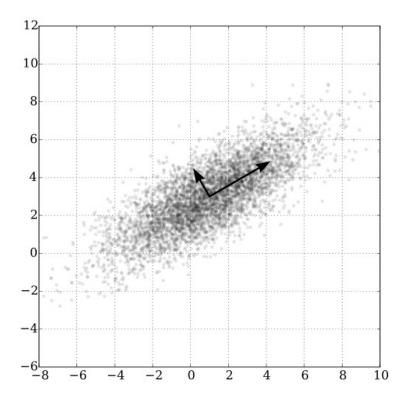
 α_1

 α_{N-1}

$$= \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_{N-1} \end{bmatrix}$$

Principal Components

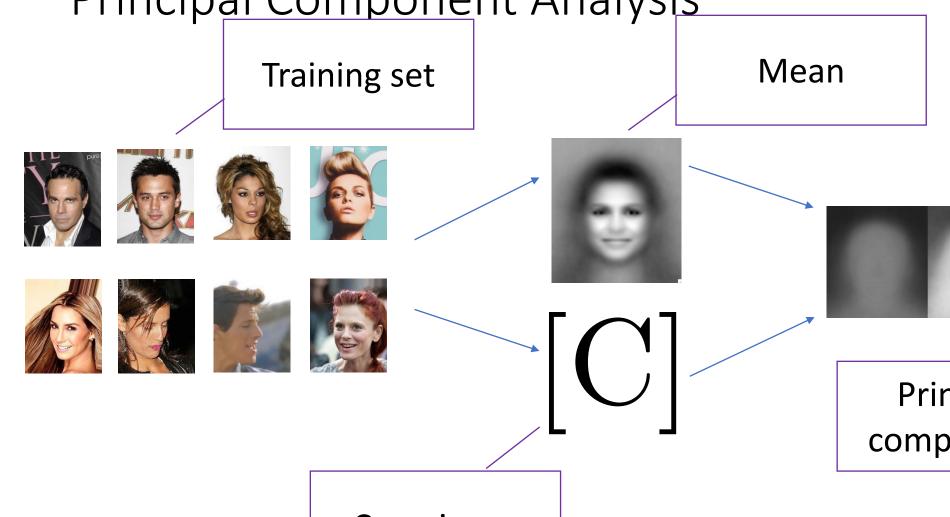
 Given a set of data, what is the best basis for representing elements of that set

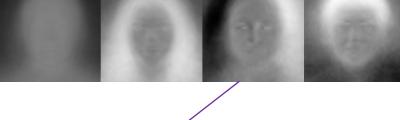


Principal Components Analysis

- We are given a training set X of faces
- We want to find an orthonormal basis that can form an alternate representation of faces with as few dimensions as possible
 - Axes are the "principal components"
 - First axis captures as much of the data set as possible
 - Next axis captures as much of the data that isn't captured by first
 - And so on
- We can represent any face with linear combination of the principal components

Principal Component Analysis





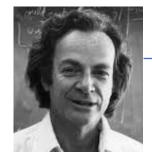
Principal components

Covariance

Principal Component Analysis

Project face onto principal components

Representation in feature space



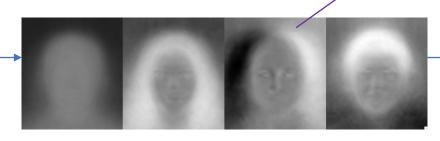


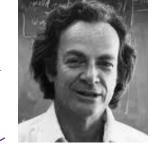
$$\{\phi_0, \phi_1, ..., \phi_{N-1}\}$$

How do we compute these?

$$\{\phi_0, \phi_1, ..., \phi_{N-1}\}$$

Linear combination of principal components





Recreate original face

Computing Principal Components

Let $\{f_0, f_1, \dots f_M\}$ be as set of faces. Each face $f_i \in \mathbb{R}^N$ where N is the total number of pixels in a face image and the elements of each f_i all have the same correspond to the pixels in face image i (without loss of generality, take lexicographical ordering). Let $\mathbf{F} \in \mathbb{R}^{M \times N}$ be a matrix in which every column i consists of f_i .

Let $\Phi \in \mathbb{R}^{N \times N}$ be an orthonormal matrix where each column is a feature vector ϕ_i . For a given face f_i we let $\tilde{f}_i = \sum_{j=0}^{K-1} \alpha_{i,j} \phi_j$ and define Φ such that for each K the difference between f_i and \tilde{f}_i is minimized for $i=0,1,\ldots,N-1$.

Let's start with the case of K=0. Then each $f_i=\alpha_i\phi_0$. The best approximation of f_i will be the projection of f_i onto ϕ_0 , i.e., $\alpha_i=\langle f_i,\phi_0\rangle$.

Computing Principal Components

The sum of squares difference between all of the f_i and their projection onto ϕ_0 is

$$\sum_{i=0}^{N-1} \|f_i - \langle f_i, \phi_0 \rangle \phi_0\|_2^2$$

The best choice for ϕ_0 is thus the one that minimizes this expression, i.e.,

$$\phi_0 = \operatorname{argmin} \sum_{i=0}^{N-1} \|f_i - \langle f_i, \phi_0 \rangle \phi_0\|_2^2 = \operatorname{argmin} \sum_{i=0}^{N-1} \langle f_i - \langle f_i, \phi_0 \rangle \phi_0, f_i - \langle f_i, \phi_0 \rangle \phi_0 \rangle$$
$$= \operatorname{argmin} \sum_{i=0}^{N-1} (\langle f_i, f_i \rangle - \langle f_i, \langle f_i, \phi_0 \rangle \phi_0 \rangle)$$

Computing Principal Components

$$\phi_0 = \operatorname{argmax} \sum_{i=0}^{N-1} \langle f_i, \langle f_i, \phi_0 \rangle \phi_0 \rangle = \operatorname{argmax} \sum_{i=0}^{N-1} \langle \langle \phi_0, f_i \rangle f_i, \phi_0 \rangle$$

$$= \operatorname{argmax} \sum_{i=0}^{N-1} \phi_0^T f_i f_i^T \phi_0 = \operatorname{argmax} \left[\phi_0^T \left(\sum_{i=0}^{N-1} f_i f_i^T \right) \phi_0 \right]$$

 $= \operatorname{argmax} (\langle \phi_0, C\phi_0 \rangle)$

Covariance Matrix Rayleigh Quotient

Constrained Ontimization Lagrangian

$$L(\phi_0) = \langle \phi_0, C\phi_0 \rangle - \sigma_0 \left(1 - \langle \phi_0, \phi_0 \rangle \right)$$

Maximize

$$\langle \phi_0, C\phi_0 \rangle$$

$$\nabla L(\phi_0) = 0^{-1}$$

Will be maximized where gradient is zero

$$\langle \phi_0, \phi_0 \rangle = 1$$

$$\nabla L(\phi_0) = C\phi_0 - \sigma_0\phi_0 = 0$$

Subject to

Gradient of the Lagrangian

$$C\phi_0 = \sigma_0\phi_0$$

Corresponding eigenvector

Largest eigenvalue

Eigenfaces

$$f = \text{read_face}();$$
 $\phi = U^T f$
 $\phi[K:N] = 0$
 $f' = U\phi$

Example



Our Code

- Read in faces data
- Compute mean of all faces
- Subtract mean from every face
- Compute covariance matrix C
- Compute eigendecomposition of matrix C
- Write out eigenface images

$$f = \text{read_face}();$$

$$\phi = U^T f$$

$$\phi[K:N] = 0$$

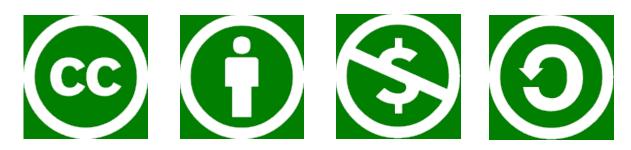
$$f' = U\phi$$

Most computationally expensive step

We want to parallelize this

Thank You!

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