Lecture 11:
The Fast Fourier Transform

Outline for today

- Definitions
- A few applications of FFTs
- Sequential algorithm
- Parallel 1D FFT
- Parallel 3D FFT
- Autotuning FFTs: FFTW

Definition of Discrete Fourier Transform (DFT)

- Let $i = \sqrt{-1}$ and index matrices and vectors from 0
- The (1D) DFT of an m-element vector v is:

$$F * v$$

where F is an m-by-m matrix defined as:

$$F[j,k] = \bar{\omega}^{(j*k)}, \quad 0 \le j,k \le m-1$$

and where $\bar{\omega}$ is:

$$\bar{\omega} = e^{2\pi/m} = \cos(2\pi/m) + i * \sin(2\pi/m)$$

- $\bar{\omega}$ is a complex number with whose m^{th} power $\bar{\omega}^{\text{m}} = 1$ and is therefore called an m^{th} root of unity
- E.g., for $m = 4$: $\bar{\omega} = i$, $\bar{\omega}^2 = -1$, $\bar{\omega}^3 = -\text{i}$, $\bar{\omega}^4 = 1$

Definition of Discrete Fourier Transform (DFT)

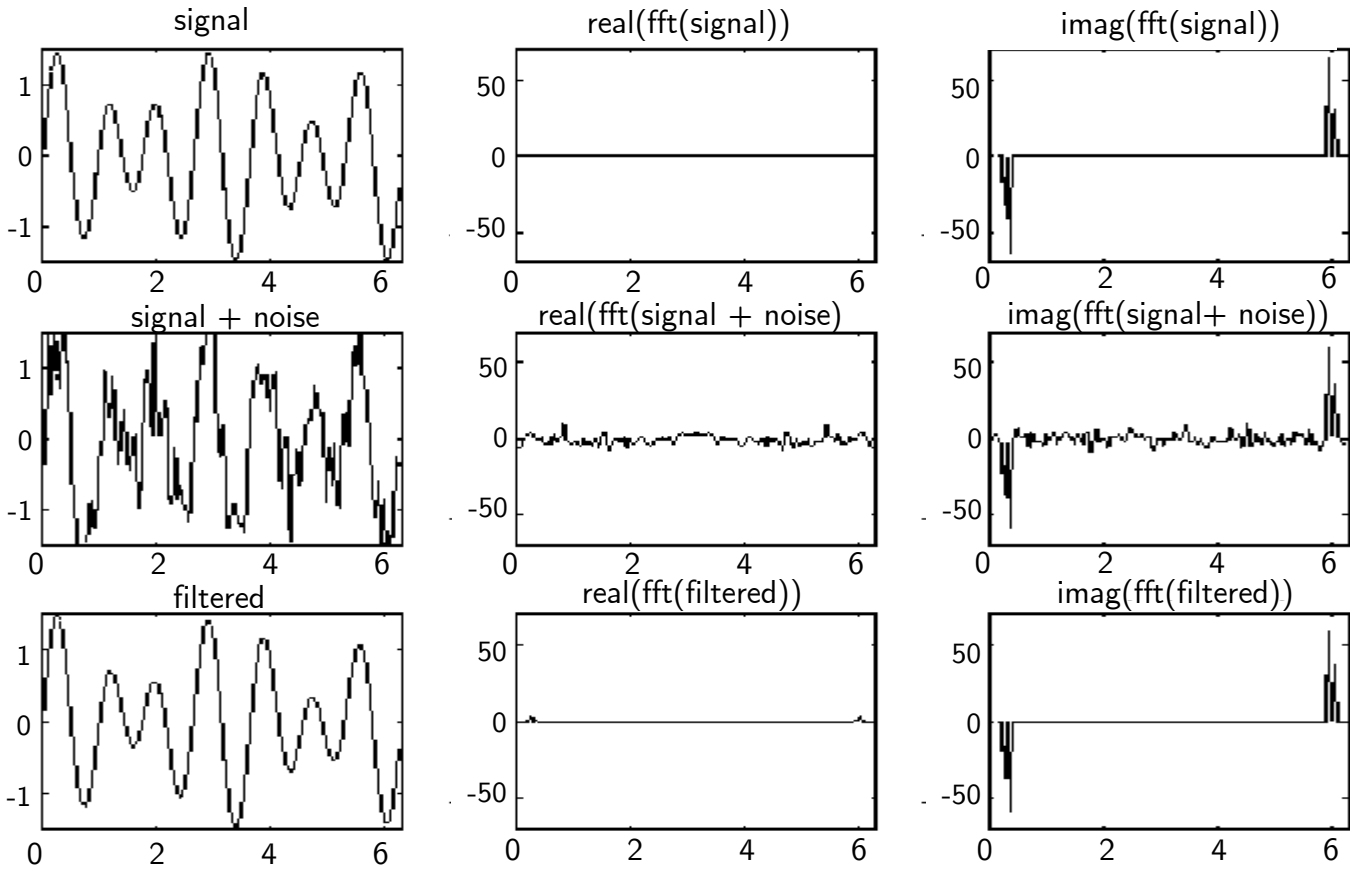
- The 2D DFT of an m-by-m matrix V is $F * V * F$
  - Do 1D DFT on all the columns independently, then all the rows
- Higher dimensional DFTs are analogous

Motivation for *Fast* Fourier Transform (FFT)

- Signal processing
- Image processing
- Solving Poisson's Equation nearly optimally
  - O(N log N) arithmetic operations, N = #unknowns
  - Competitive with multigrid
- Fast multiplication of large integers
- ...

Using the 1D FFT for filtering

- Signal = sin(7t) + .5 sin(5t) at 128 points
- Noise = random number bounded by .75
- Filter by zeroing out FFT components < .25



Using the 2D FFT for image compression

- Image = p_r x p_c matrix of values
- Compress by keeping e.g., largest 2.5% of FFT components
- Similar idea used by jpeg

Recall: Poisson's equation arises in many models

3D: $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \partial^2 u/\partial z^2 = f(x,y,z)$

2D: $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 = f(x,y)$

1D: $d^2 u/dx^2 = f(x)$

f represents the sources; also need boundary conditions

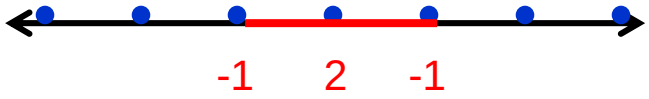
- Electrostatic or Gravitational Potential: Potential(position)
- Heat flow: Temperature(position, time)
- Diffusion: Concentration(position, time)
- Fluid flow: Velocity,Pressure,Density(position,time)
- Elasticity: Stress,Strain(position,time)
- Variations of Poisson have variable coefficients

Solving Poisson Equation with FFT (1/2)

- 1D Poisson equation: solve $L_1 x = b$ where

$$L_1 = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "stencil"



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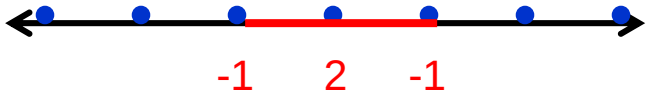
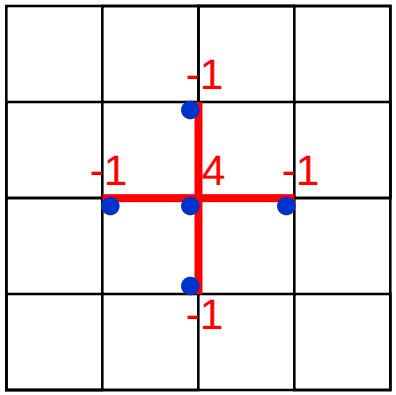


- 2D Poisson equation: solve $L_2 x = b$ where

$$L_2 = \left(\begin{array}{ccc:ccc:ccc} 4 & -1 & & -1 & & & & & \\ -1 & 4 & -1 & & -1 & & & & \\ & -1 & 4 & & & -1 & & & \\ \hdashline -1 & & & 4 & -1 & & -1 & & \\ & -1 & & -1 & 4 & -1 & & -1 & \\ & & -1 & & -1 & 4 & & & -1 \\ \hdashline & & & -1 & & & 4 & -1 & \\ & & & & -1 & & -1 & 4 & -1 \\ & & & & & -1 & & -1 & 4 \end{array}\right)$$

Graph and "5 point stencil"



3D case is analogous (7 point stencil)

Solving 2D Poisson Equation with FFT (2/2)

- Use facts that:
  - $L_1 = FDF^T$ is eigenvalue/eigenvector decomposition, where
    - F is very similar to FFT (imaginary part)

$$F(j,k) = \left(\frac{2}{n+1}\right)^{1/2} \cdot \sin\left(\frac{jk\pi}{n+1}\right)$$

    - D = diagonal matrix of eigenvalues

$$D(j,j) = 2\left(1 - \cos\left(\frac{j\pi}{n+1}\right)\right)$$

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  - 2D Poisson same as solving $L_1 X + X L_1 = B$ where
    - X square matrix of unknowns at each grid point, B square too

Solving 2D Poisson Equation with FFT (2/2)

$$L_1 X + X L_1 = B$$

Substitute $L_1 = FDF^T$ into 2D Poisson to get algorithm:

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Substitute $L_1 = FDF^T$ into 2D Poisson to get algorithm:

1. Perform 2D FFT on RHS B to get $B' = F^T BF$ or $B = FB'F^T$

Get

$$\begin{aligned} L_1X + XL_1 &= B \\ (FDF^T)X + X(FDF^T) &= FB'F^T \\ F(D(F^TXF) + (F^TXF)D)F^T &= FB'F^T \\ DX' + X'D &= B' \end{aligned}$$

Solving 2D Poisson Equation with FFT (2/2)

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2. Solve $DX' + X'D = B'$ for X': $X'(j,k) = B'(j,k)/\left(D(j,j) + D(k,k)\right)$

Solving 2D Poisson Equation with FFT (2/2)

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Substitute $L_1 = FDF^T$ into 2D Poisson to get algorithm:

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$$\begin{aligned} L_1 X + X L_1 &= B \\ (FDF^T)X + X(FDF^T) &= FB'F^T \\ F(D(F^T XF) + (F^T XF)D)F^T &= FB'F^T \\ DX' + X'D &= B' \end{aligned}$$

2. Solve $DX' + X'D = B'$ for X': $X'(j,k) = B'(j,k)/\left(D(j,j) + D(k,k)\right)$

3. Perform inverse 2D FFT on $X' = F^T XF$ to get $X = FX'F^T$

Solving 2D Poisson Equation with FFT (2/2)

$$L_1 X + X L_1 = B$$

Substitute $L_1 = FDF^T$ into 2D Poisson to get algorithm:

1. Perform 2D FFT on RHS B to get $B' = F^T B F$ or $B = F B' F^T$

   Get

$$\begin{aligned} L_1 X + X L_1 &= B \\ (FDF^T)X + X(FDF^T) &= FB'F^T \\ F(D(F^T X F) + (F^T X F)D)F^T &= FB'F^T \\ DX' + X'D &= B' \end{aligned}$$

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3. Perform inverse 2D FFT on $X' = F^T X F$ to get $X = F X' F^T$

Cost = 2 2D-FFTs (plus n^2 adds, divisions) = $O(n^2 \log n)$

Related Transforms

- Most applications require multiplication by both F and F^{-1}

$$F(j,k) = e^{(2\pi ijk/m)}$$

- Multiplying by F and F^{-1} are essentially the same.

$$F^{-1} = \text{complex\_conjugate}(F) \,/\, m$$

- For solving the Poisson equation and various other applications, we use variations on the FFT
  - The sin transform -- imaginary part of F
  - The cos transform -- real part of F

- Algorithms are similar, so we will focus on F

Serial Algorithm for the FFT

Compute the FFT $(F * v)$ of an m-element vector v

$$
\begin{aligned}
(F * v)[j] &= \sum_{k=0}^{m-1} F(j,k) * v(k) \\
&= \sum_{k=0}^{m-1} \overline{\omega}^{(j*k)} * v(k) \\
&= \sum_{k=0}^{m-1} \left(\overline{\omega}^{j}\right)^{k} * v(k) \\
&= V(\overline{\omega}^{j})
\end{aligned}
$$

where V is defined as the polynomial

$$V(x) = \sum_{k=0}^{m-1} x^{k} * v(k)$$

Divide and Conquer FFT

- V can be evaluated using divide-and-conquer

$$\begin{aligned} V(x) &= \sum_{k=0}^{m-1} x^k * v(k) \\ &= v(0) + x^2 v(2) + x^4 v(4) + \cdots \\ &\quad + x(v(1) + x^2 v(3) + x^4 v(5) + \cdots) \\ &= V_{even}(x^2) + x\, V_{odd}(x^2) \end{aligned}$$

- V has degree $m-1$, so V_{even} and V_{odd} are polynomials of degree $m/2-1$
- We evaluate these at m points: $\left(\bar{\omega}^j\right)^2$ for $0 \leq j \leq m-1$
- But this is really just $m/2$ different points, since

$$\left(\bar{\omega}^{(j+m/2)}\right)^2 = \left(\bar{\omega}^j * \bar{\omega}^{m/2}\right)^2 = \bar{\omega}^{2j} * \bar{\omega}^m = \left(\bar{\omega}^j\right)^2$$

- So FFT on m points reduced to 2 FFTs on $m/2$ points
  - Divide and conquer!

Divide-and-Conquer FFT (D&C FFT)

FFT$(v, \bar{\omega}, m)$ ... assume m is a power of 2

if $m = 1$ return $v[0]$

else

$V_{even} = \text{FFT}(v[0:2:m-2], \bar{\omega}^2, m/2)$

$V_{odd} = \text{FFT}(v[1:2:m-1], \bar{\omega}^2, m/2)$

$\bar{\omega}_{vec} = [\bar{\omega}^0, \bar{\omega}^1, \ldots, \bar{\omega}^{(m/2-1)}]$ ← precomputed

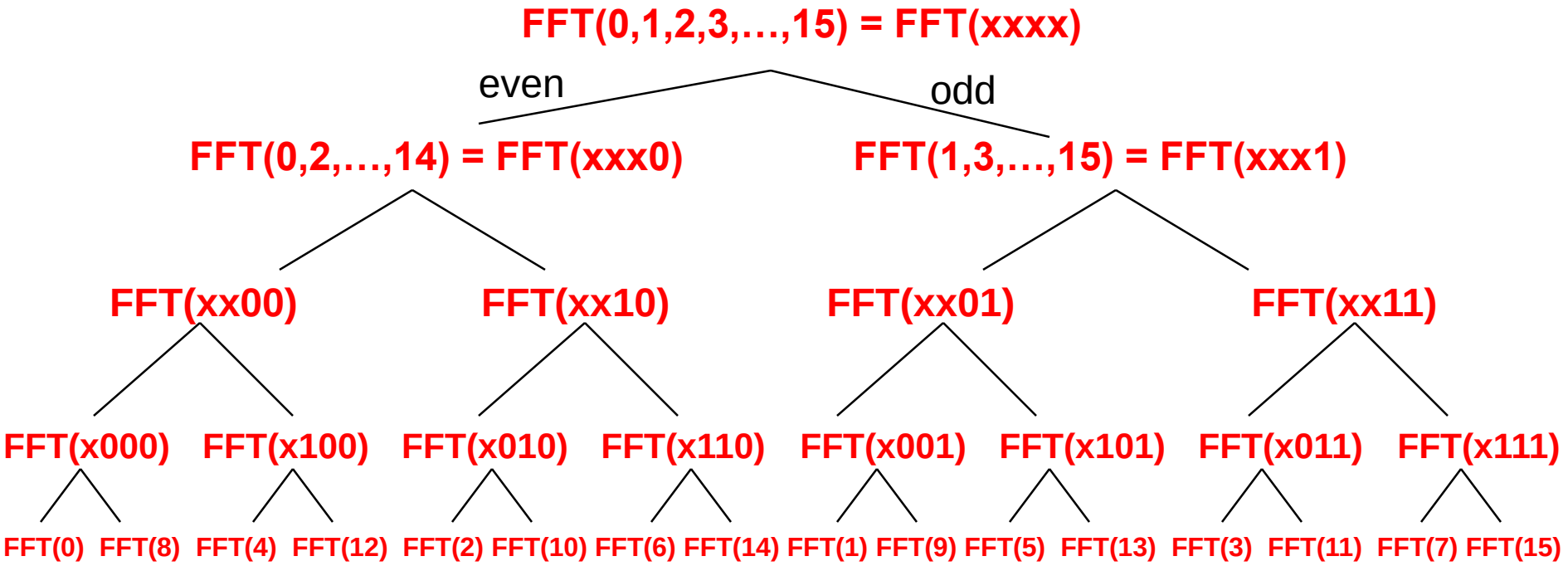
return $[V_{even} + (\bar{\omega}_{vec} .* V_{odd}),\ V_{even} - (\bar{\omega}_{vec} .* V_{odd})]$

- MATLAB notation: ".*" means component-wise multiply.

Cost: $T(m) = 2T(m/2) + O(m) = O(m \log m)$ operations.

An Iterative Algorithm

- The call tree of the D&C FFT algorithm is a complete binary tree of $\log m$ levels

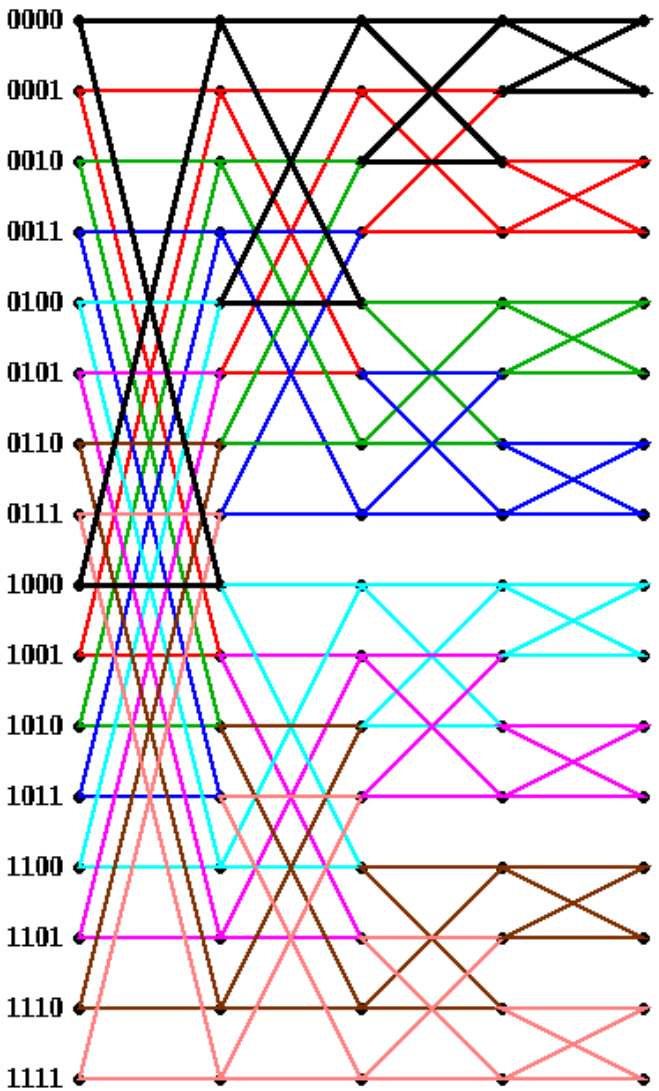


- An iterative algorithm that uses loops rather than recursion, does each level in the tree starting at the bottom
  - Algorithm overwrites v[i] by (F*v)[bitreverse(i)]
- Practical algorithms combine recursion (for memory hierarchy) and iteration (to avoid function call overhead)

Parallel 1D FFT

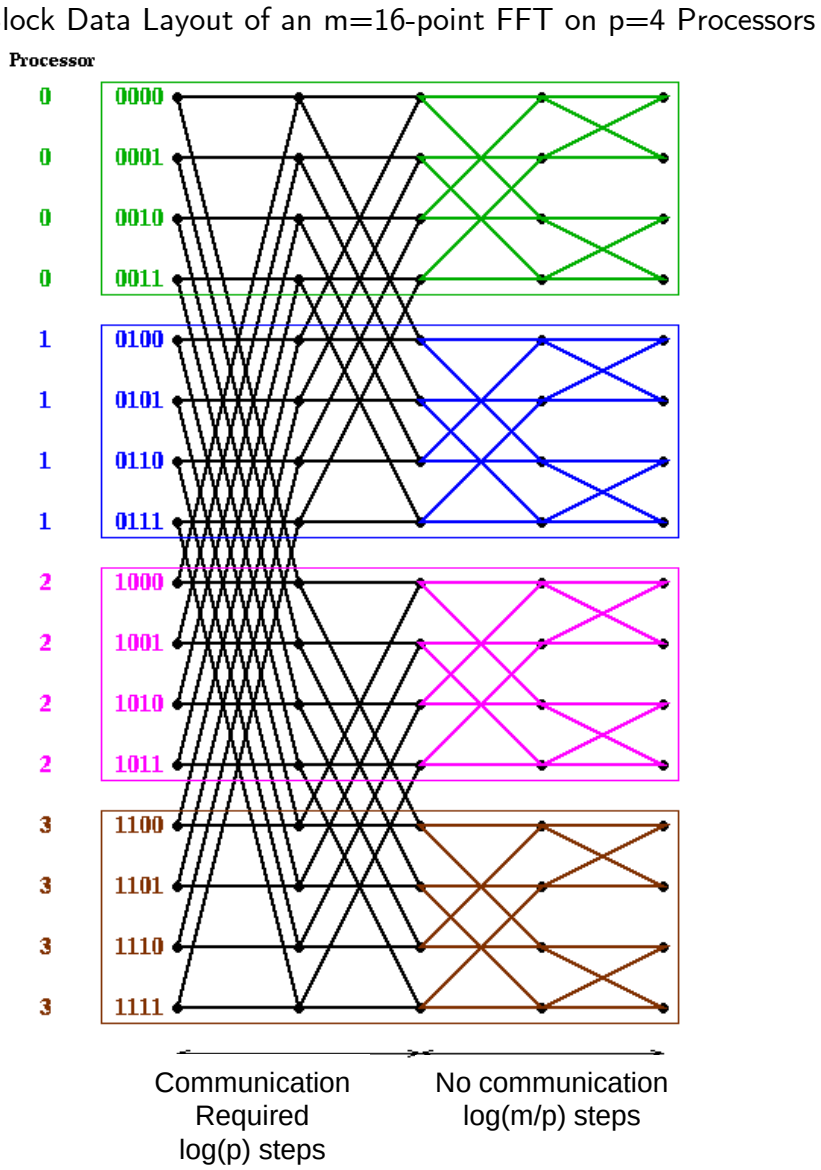
- Data dependencies in 1D FFT
  - Butterfly pattern
  - From $V_{even} \pm \overline{\omega}_{vec} .* V_{odd}$
- A PRAM algorithm takes $O(\log m)$ time
  - each step to right is parallel
  - there are $\log m$ steps
- What about communication cost?

Data dependencies in a 16-point FFT



Block Layout of 1D FFT

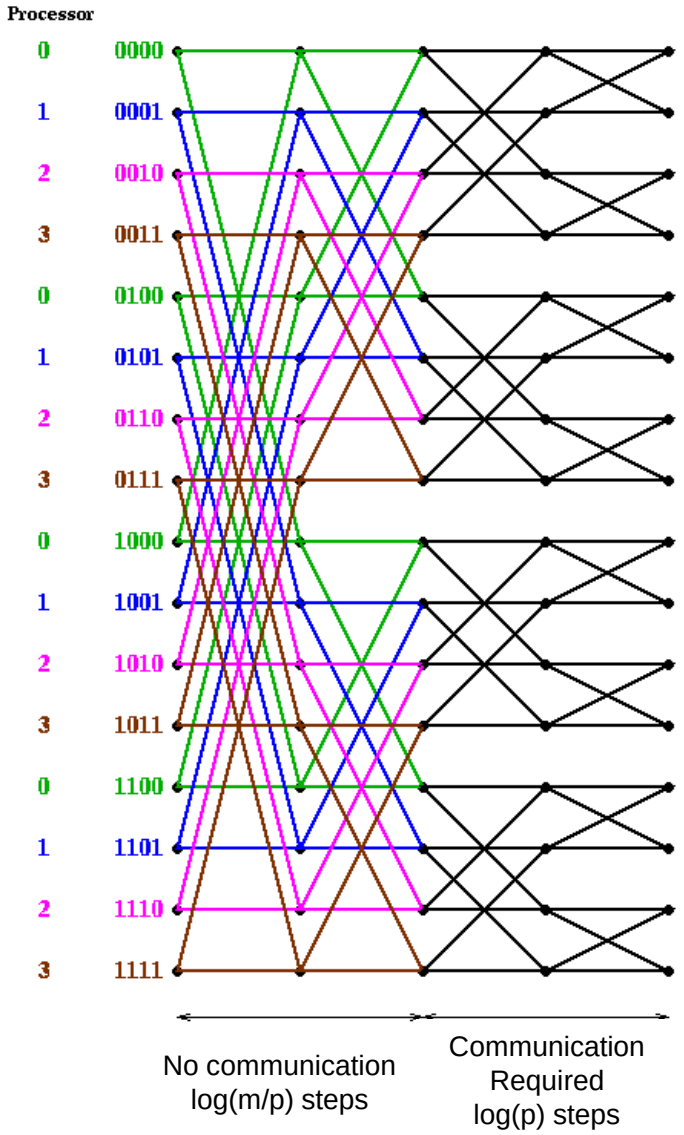
- Using a block layout (m/p contiguous words per processor)
- No communication in last $\log m/p$ steps
- Significant communication in first $\log p$ steps



Cyclic Layout of 1D FFT

- Cyclic layout (consecutive words map to consecutive processors)
- No communication in first $\log(m/p)$ steps
- Communication in last $\log(p)$ steps

Cyclic Data Layout of an m=16-point FFT on p=4 Processors



Parallel Complexity

- m = vector size, p = number of processors
- f = time per flop = 1
- α = latency for message
- β = time per word in a message

- Time(block_FFT) = Time(cyclic_FFT) =

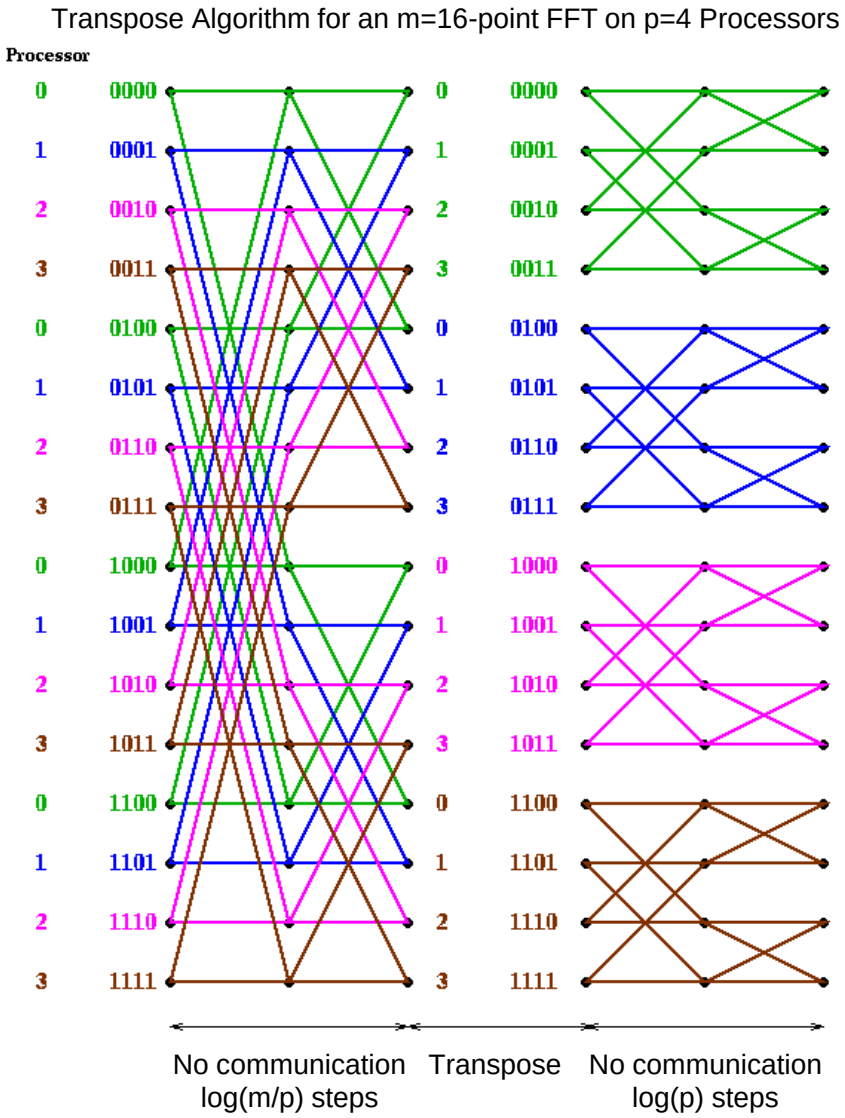
$$2 * m * \log(m)/p \quad \text{... perfectly parallel flops}$$

$$+ \log(p) * \alpha \quad \text{... 1 message/stage, log p stages}$$

$$+ (m/p) * \log(p) * \beta \quad \text{... m/p words/message}$$

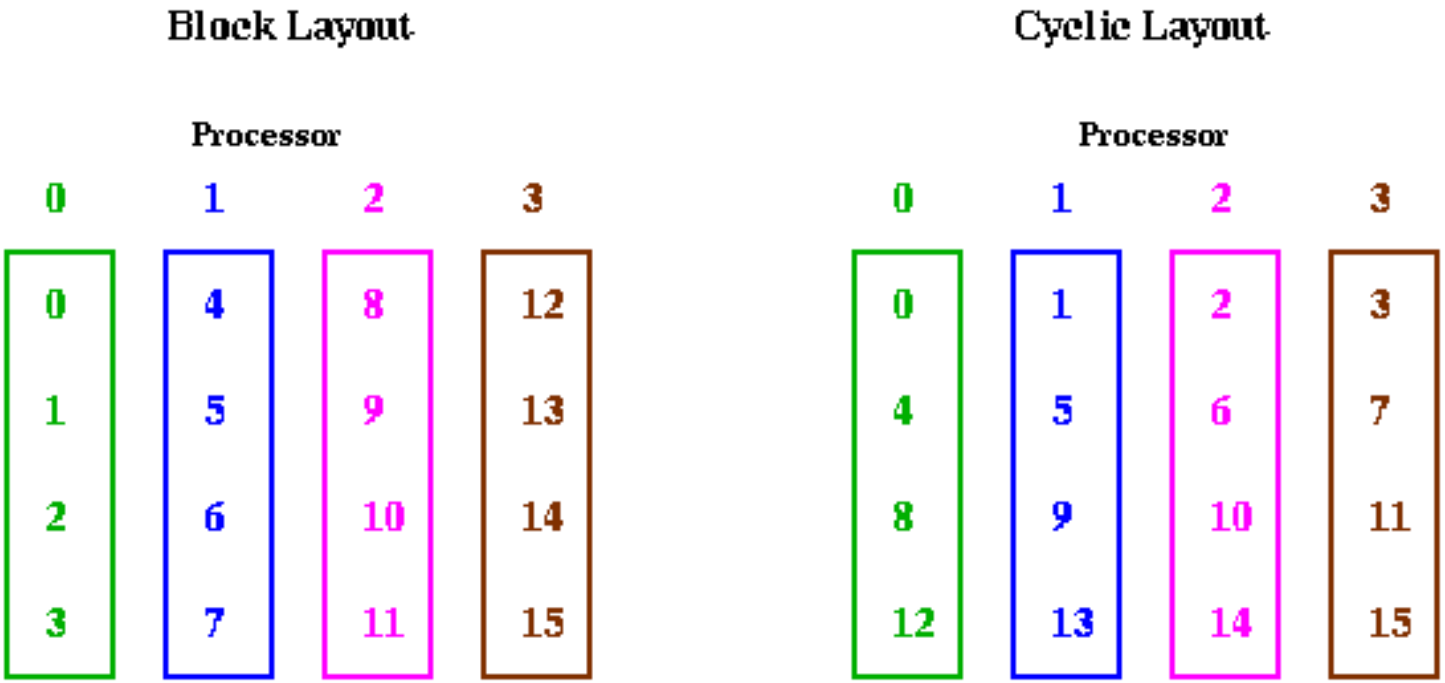
FFT With "Transpose"

- If we start with a cyclic layout for first log(m/p) steps, there is no communication
- Then transpose the vector for last log(p) steps
- All communication is in the transpose
- Note: This example has log(m/p) = log(p)
  - If log(m/p) < log(p) more phases/layouts will be needed
  - We will assume log(m/p) ≥ log(p) for simplicity



Why is the Communication Step Called a Transpose?

- Analogous to transposing an array
- View as a 2D array of m/p by p



Parallel Complexity of the FFT with Transpose

- Assume no communication is pipelined (overestimate!)
- Time(transposeFFT) =

$2 * m * \log(m)/p$ same as before

$+ (p-1) * \alpha$ was $\log(p) * \alpha$

$+ m * (p-1)/p^2 * \beta$ was $m * \log(p)/p * \beta$

- If communication is pipelined, so we do not pay for $p-1$ messages, the second term becomes simply α, rather than $(p-1)\,\alpha$
- This is close to optimal. See LogP paper for details.
- See also following papers
  - A. Sahai, "Hiding Communication Costs in Bandwidth Limited FFT"
  - R. Nishtala et al, "Optimizing bandwidth limited problems using one-sided communication"

Sequential Communication Complexity of the FFT

- How many words need to be moved between main memory and cache of size M to do the FFT of size m, where $m > M$?
- Thm (Hong, Kung, 1981): #words $= \Omega(m \log m / \log M)$
  - Proof follows from each word of data being reusable only $\log M$ times
- Attained by transpose algorithm
  - Sequential algorithm "simulates" parallel algorithm
  - Imagine we have $p = m/M$ processors, so each processor stores and works on $O(M)$ words
  - Each local computation phase in parallel FFT replaced by similar phase working on cache resident data in sequential FFT
  - Each communication phase in parallel FFT replaced by reading/writing data from/to cache in sequential FFT
- Attained by recursive, "cache-oblivious" algorithm

Parallel Communication Complexity of the FFT

- How many words need to be moved between p processors to do the FFT of size m?
- Thm (Aggarwal, Chandra, Snir, 1990):

$$\#\text{words} = \Omega\left(\frac{m \log m}{p \log(m/p)}\right)$$

  - Proof assumes no recomputation
  - Holds independent of local memory size (which must exceed m/p)

- Does TransposeFFT attain lower bound?
  - Recall assumption: $\log(m/p) \geq \log(p)$
  - So $2 \geq \log(m) / \log(m/p) \geq 1$
  - So $\#\text{words} = \Omega(m/p)$
  - Attained by transpose algorithm

Comment on the 1D Parallel FFT

- The above algorithm leaves data in bit-reversed order
  - Some applications can use it this way, like Poisson
  - Others require another transpose-like operation

- Other parallel algorithms also exist
  - A very different 1D FFT is due to Edelman
  - Based on the Fast Multipole algorithm
  - Less communication for non-bit-reversed algorithm
  - Approximates FFT

Higher Dimensional FFTs

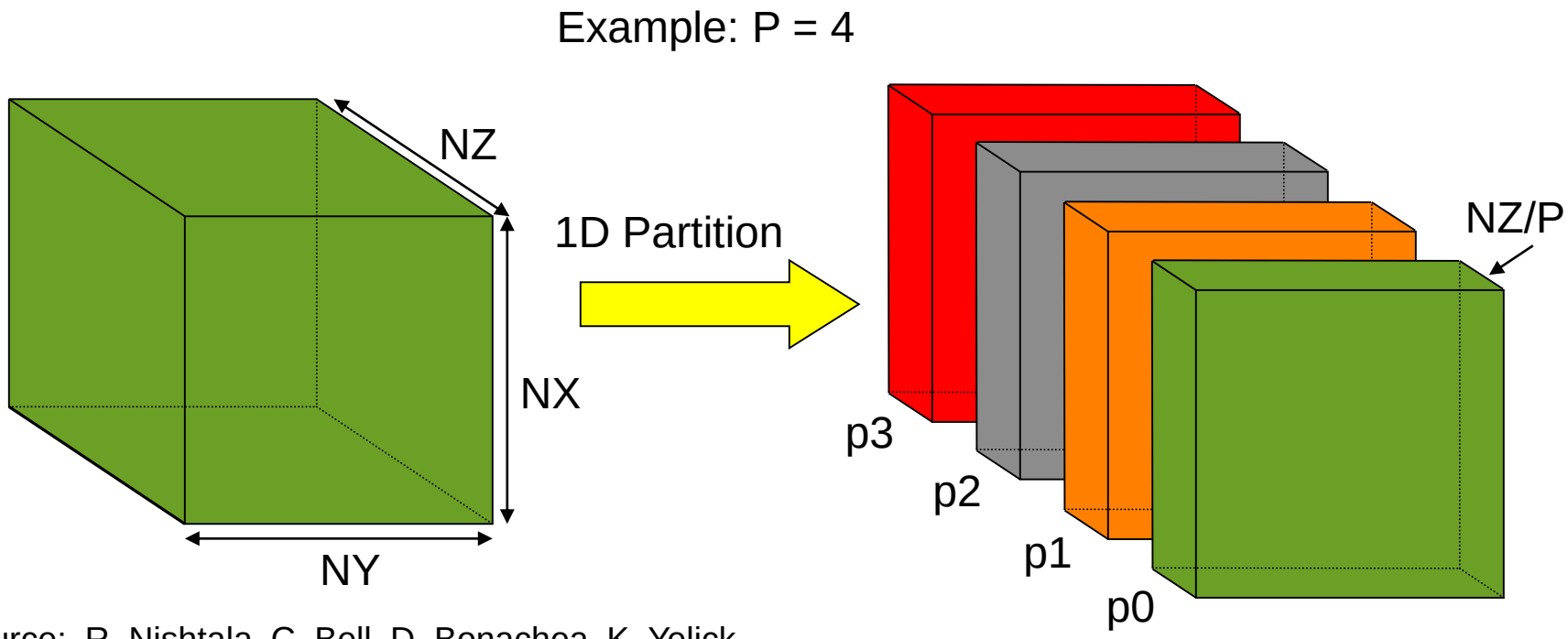
- FFTs on 2 or more dimensions are defined as 1D FFTs on vectors in all dimensions.
  - 2D FFT does 1D FFTs on all rows and then all columns
- There are 3 obvious possibilities for the 2D FFT:
  - (1) 2D blocked layout for matrix, using parallel 1D FFTs for each row and column
  - (2) Block row layout for matrix, using serial 1D FFTs on rows, followed by a transpose, then more serial 1D FFTs
  - (3) Block row layout for matrix, using serial 1D FFTs on rows, followed by parallel 1D FFTs on columns
  - Option 2 is best, if we overlap communication and computation
- For a 3D FFT the options are similar
  - 2 phases done with serial FFTs, followed by a transpose for 3rd
  - can overlap communication with 2nd phase in practice

Bisection Bandwidth

- FFT requires one (or more) transpose operations:
  - Every processor sends 1/p-th of its data to each other one
- Bisection Bandwidth limits this performance
  - Bisection bandwidth is the bandwidth across the narrowest part of the network
  - Important in global transpose operations, all-to-all, etc.
- "Full bisection bandwidth" is expensive
  - Fraction of machine cost in the network is increasing
  - Fat-tree and full crossbar topologies may be too expensive
  - Especially on machines with 100K and more processors
  - SMP clusters often limit bandwidth at the node level
- Goal: overlap communication and computation

Performing a 3D FFT (1/3)

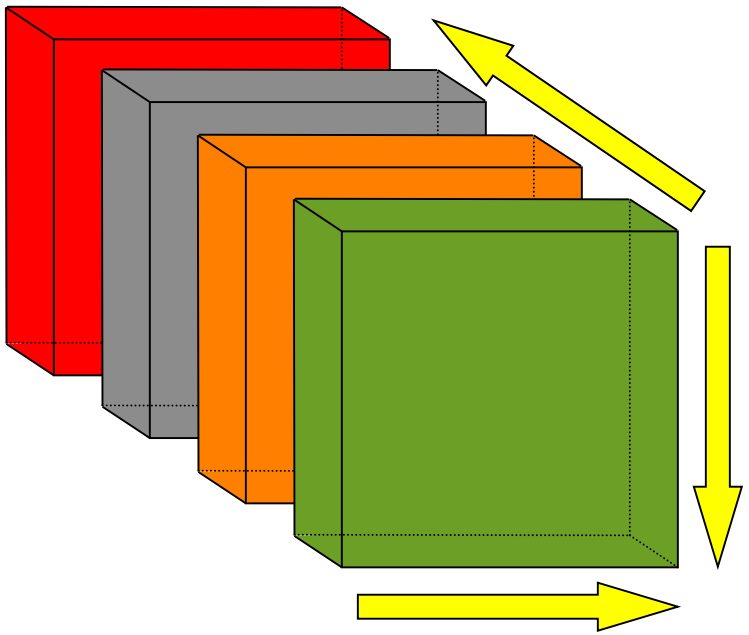
- NX x NY x NZ elements spread across P processors
- Will Use 1-Dimensional Layout in Z dimension
  - Each processor gets NZ / P "planes" of NX x NY elements per plane



Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Performing a 3D FFT (2/3)

- Perform an FFT in all three dimensions
- With 1D layout, 2 out of the 3 dimensions are local while the last Z dimension is distributed



Step 1: FFTs on the columns
(all elements local)

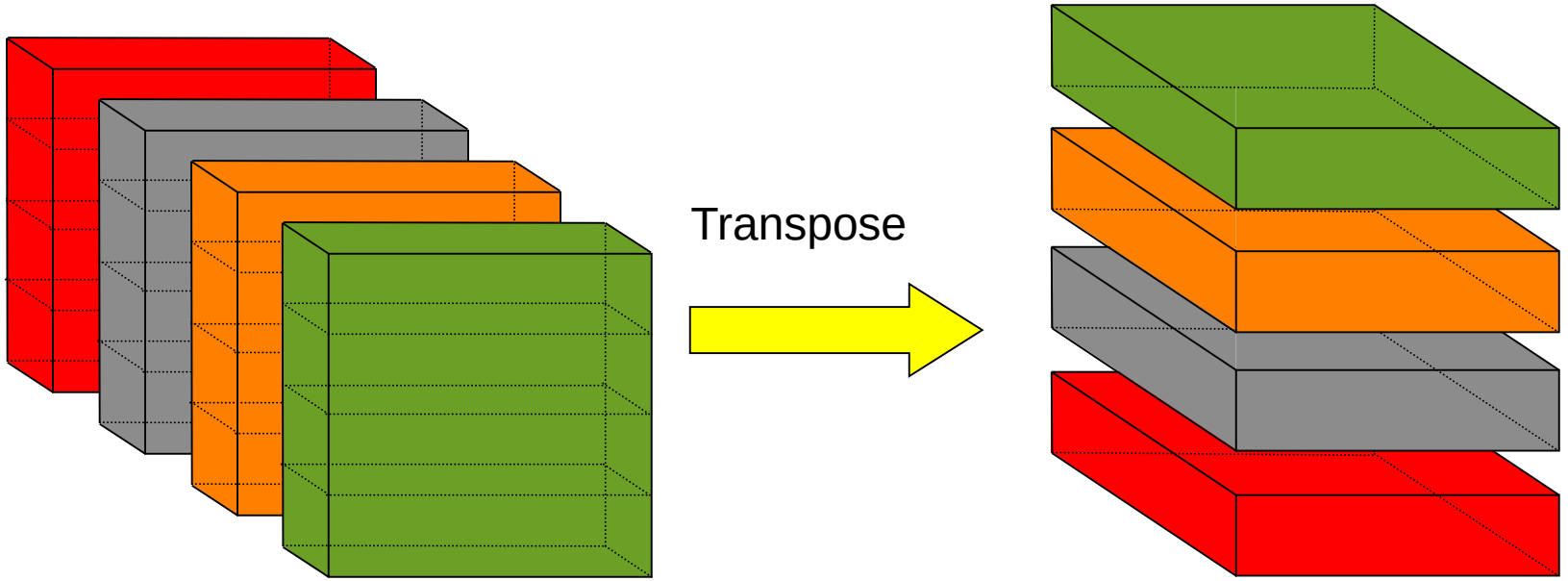
Step 2: FFTs on the rows
(all elements local)

Step 3: FFTs in the Z-dimension
(requires communication)

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Performing the 3D FFT (3/3)

- Can perform Steps 1 and 2 since all the data is available without communication
- Perform a Global Transpose of the cube
  - Allows step 3 to continue



Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

The Transpose

- Each processor has to scatter input domain to other processors
  - Every processor divides its portion of the domain into P pieces
  - Send each of the P pieces to a different processor

- Three different ways to break it up the messages
  1. Packed Slabs (i.e. single packed "All-to-all" in MPI parlance) (3D)
  2. Slabs (2D)
  3. Pencils (1D)

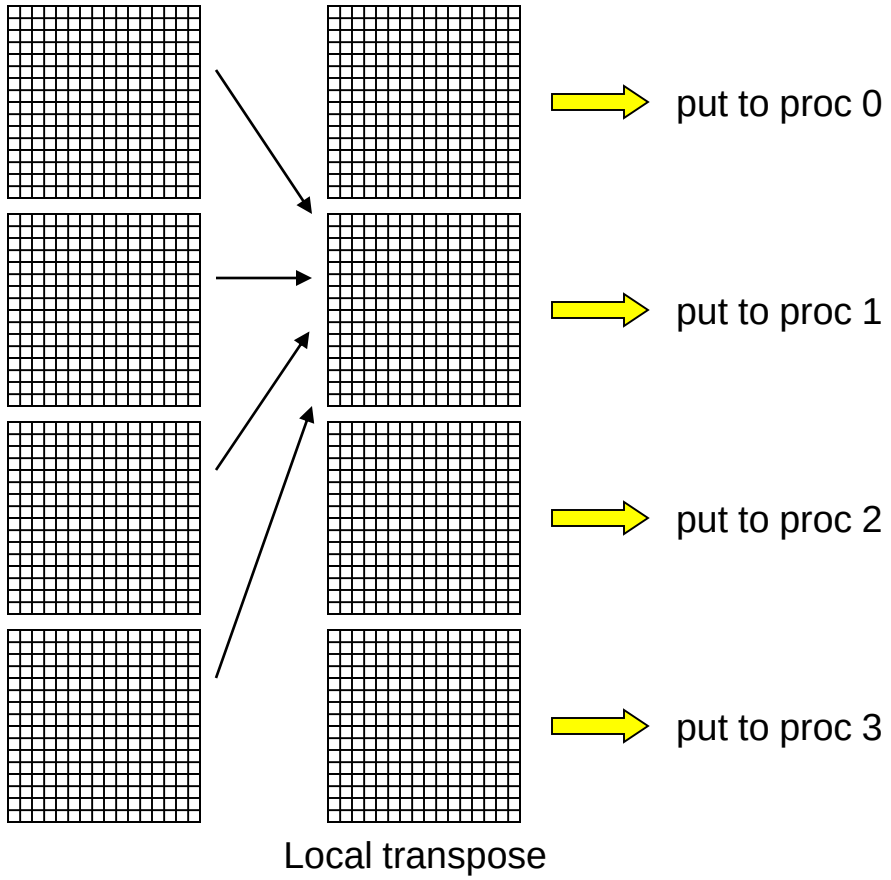
- Going from approach Packed Slabs to Slabs to Pencils leads to
  - An order of magnitude increase in the number of messages
  - An order of magnitude decrease in the size of each message
- Why do this? Slabs and Pencils allow overlapping communication and computation

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Algorithm 1: Packed Slabs

Example with P=4, NX=NY=NZ=16

1. Perform all row and column FFTs
2. Perform local transpose
   - data destined to a remote processor are grouped together
3. Perform P puts of the data



- For 512^3 grid across 64 processors
  - Send 64-1 messages of 512kB each

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Bandwidth Utilization

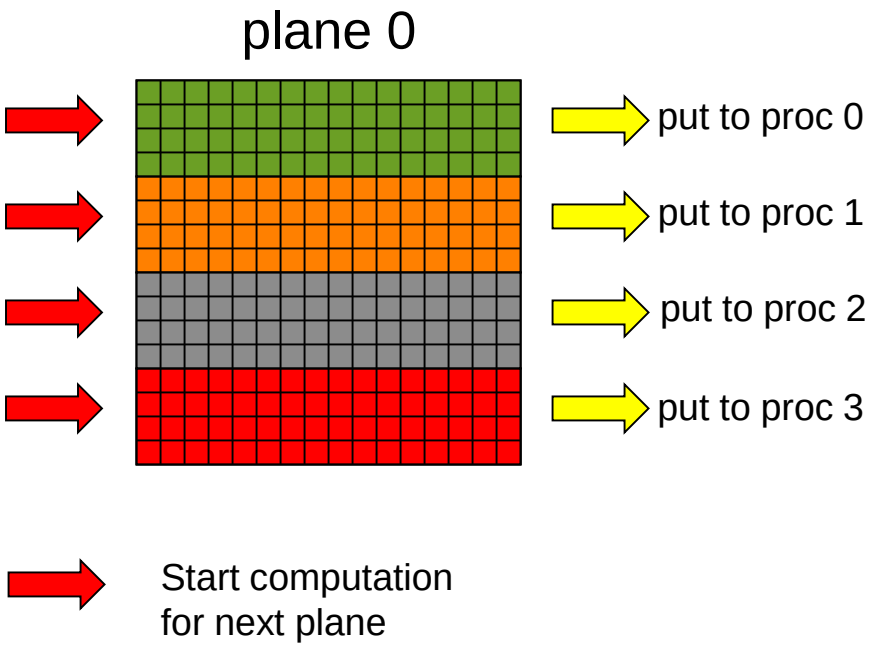
- Benchmark: NAS FT with 256 processors on Opteron/InfiniBand
  - Each processor sends 256-1 messages of 512kBytes
  - Global Transpose (i.e. all to all exchange) **only achieves 67% of peak point-to-point bidirectional bandwidth**
  - Many factors could cause this slowdown
    - Network contention
    - Number of processors with which each processor communicates

- Can we do better?

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Algorithm 2: Slabs

- Waiting to send all data in one phase bunches up communication events
- Algorithm Sketch
  - for each of the NZ/P planes
    - Perform all column FFTs
    - for each of the P "slabs"
      (a slab is NX/P rows)
      - Perform FFTs on the rows in the slab
      - Initiate 1-sided put of the slab
  - Wait for all puts to finish
  - Barrier
- Non-blocking RDMA puts allow data movement to be overlapped with computation.
- Puts are spaced apart by the amount of time to perform FFTs on NX/P rows

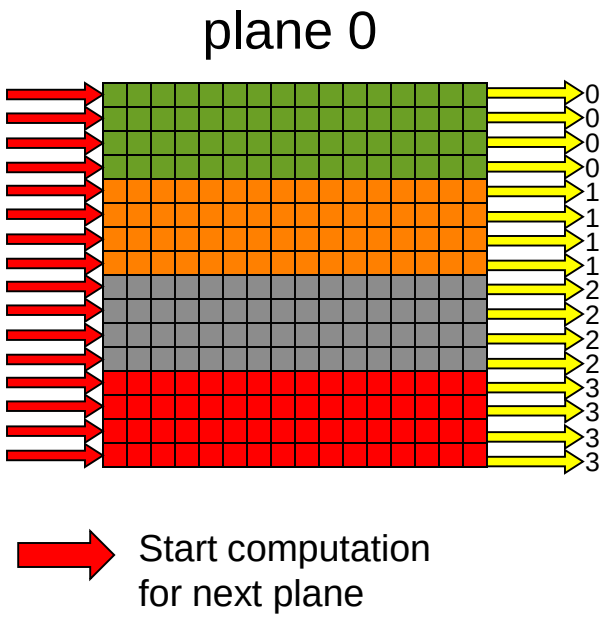


- For 512^3 grid across 64 processors
  - Send 512-8 messages of 64kB each

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Algorithm 3: Pencils

- Further reduce the granularity of communication
  - Send a row (*pencil*) as soon as it is ready
- Algorithm Sketch
  - For each of the NZ/P planes
    - Perform all 16 column FFTs
    - For r=0; r<NX/P; r++
      - For each slab s in the plane
        - Perform FFT on row r of slab s
        - Initiate 1-sided put of row r
  - Wait for all puts to finish
  - Barrier
- Large increase in message count
- Communication events finely diffused through computation
  - Maximum amount of overlap
  - Communication starts early

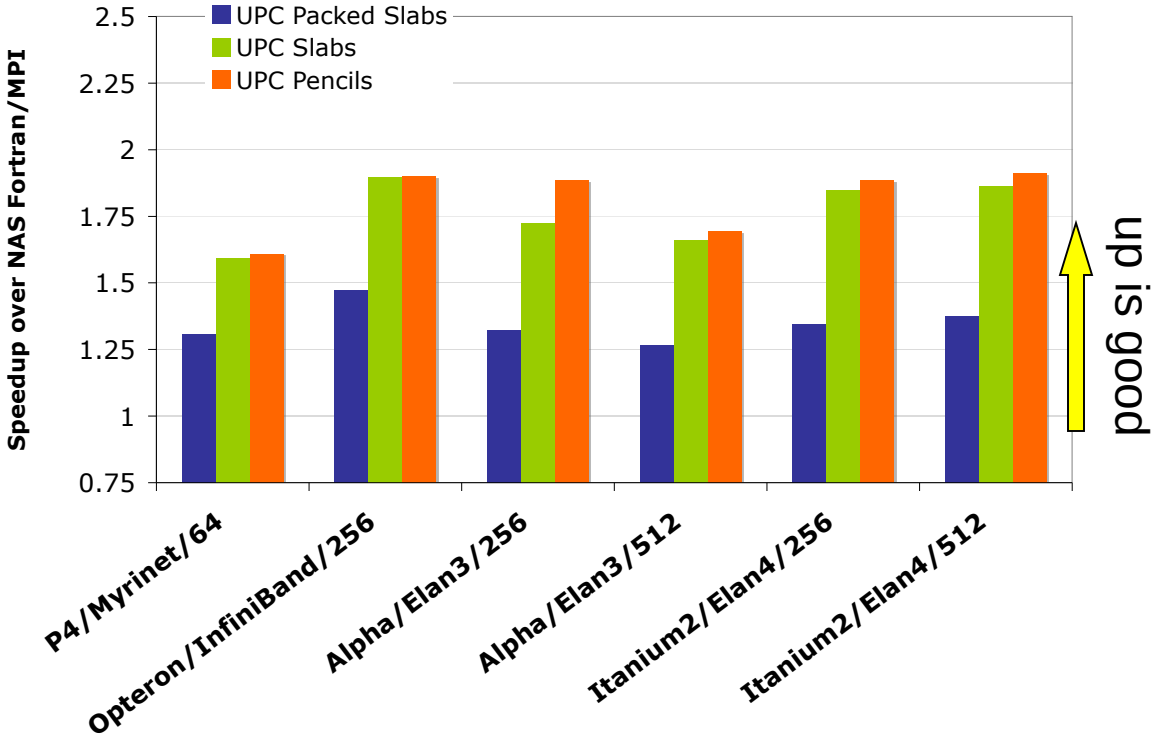


- For 512^3 grid across 64 processors
  - Send 4096-64 messages of 8kB each

Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

Comparison of Algorithms

- Compare 3 algorithms against original NAS FT
  - All versions including Fortran use FFTW for local 1D FFTs
  - Largest class that fit in the memory (usually class D)
- All UPC flavors outperform original Fortran/MPI implantation by at least 20%
  - One-sided semantics allow even exchange based implementations to improve over MPI implementations
  - Overlap algorithms spread the messages out, easing the bottlenecks
  - ~1.9x speedup in the best case



Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

FFTW – Fastest Fourier Transform in the West

- www.fftw.org
- Produces FFT implementation optimized for
  - Your version of FFT (complex, real,...)
  - Your value of n (arbitrary, possibly prime)
  - Your architecture
  - Very good sequential performance
- Won 1999 Wilkinson Prize for Numerical Software
- Widely used
  - Latest version 3.3.10 includes threads, OpenMP
  - Added MPI versions in v3.3
  - supports SSE/SSE2
- GPL license