# Parallel Spectral Methods: Fast Fourier Transform (FFT) with Applications

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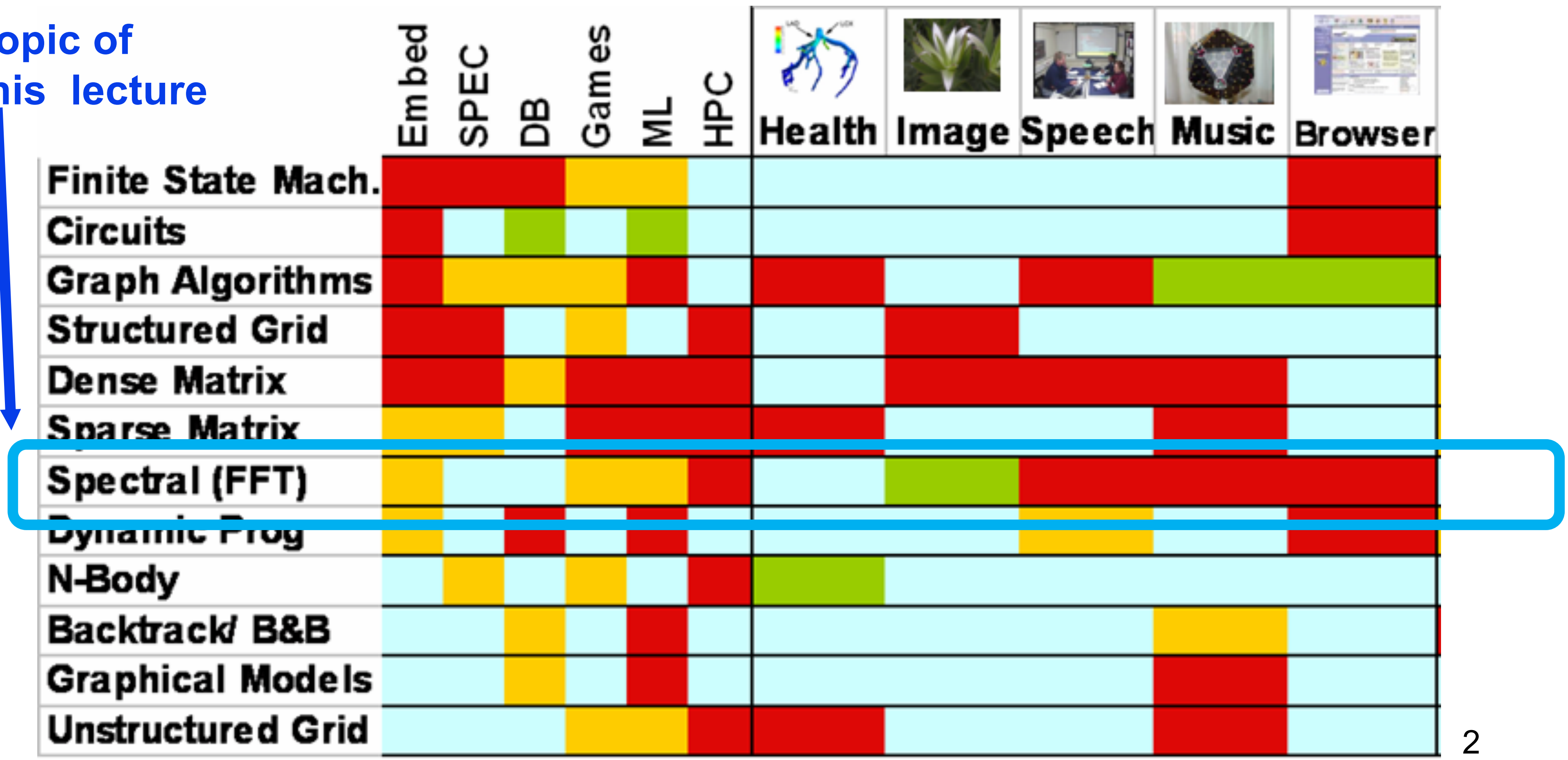
# Motifs

The Motifs (formerly “Dwarfs”) from
“The Berkeley View” (Asanovic et al.)
**Motifs** form key computational patterns

Topic of this lecture



# Ouline and References

## Outline

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

## References

- Previous CS267 lectures
- FFTW project: http://www.fftw.org
- Spiral project: http://www.spiral.net
- LogP: UCB EECS Tech Report UCB/CSD-92-713
- Lecture by Geoffrey Fox:

http://grids.ucs.indiana.edu/ptliupages/presentations/PC2007/cps615fft00.ppt

## 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:

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

and where $\varpi$ is:

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

$\varpi$ is a complex number with whose $m^{th}$ power $\varpi^m = 1$ and is therefore called an $m^{th}$ root of unity

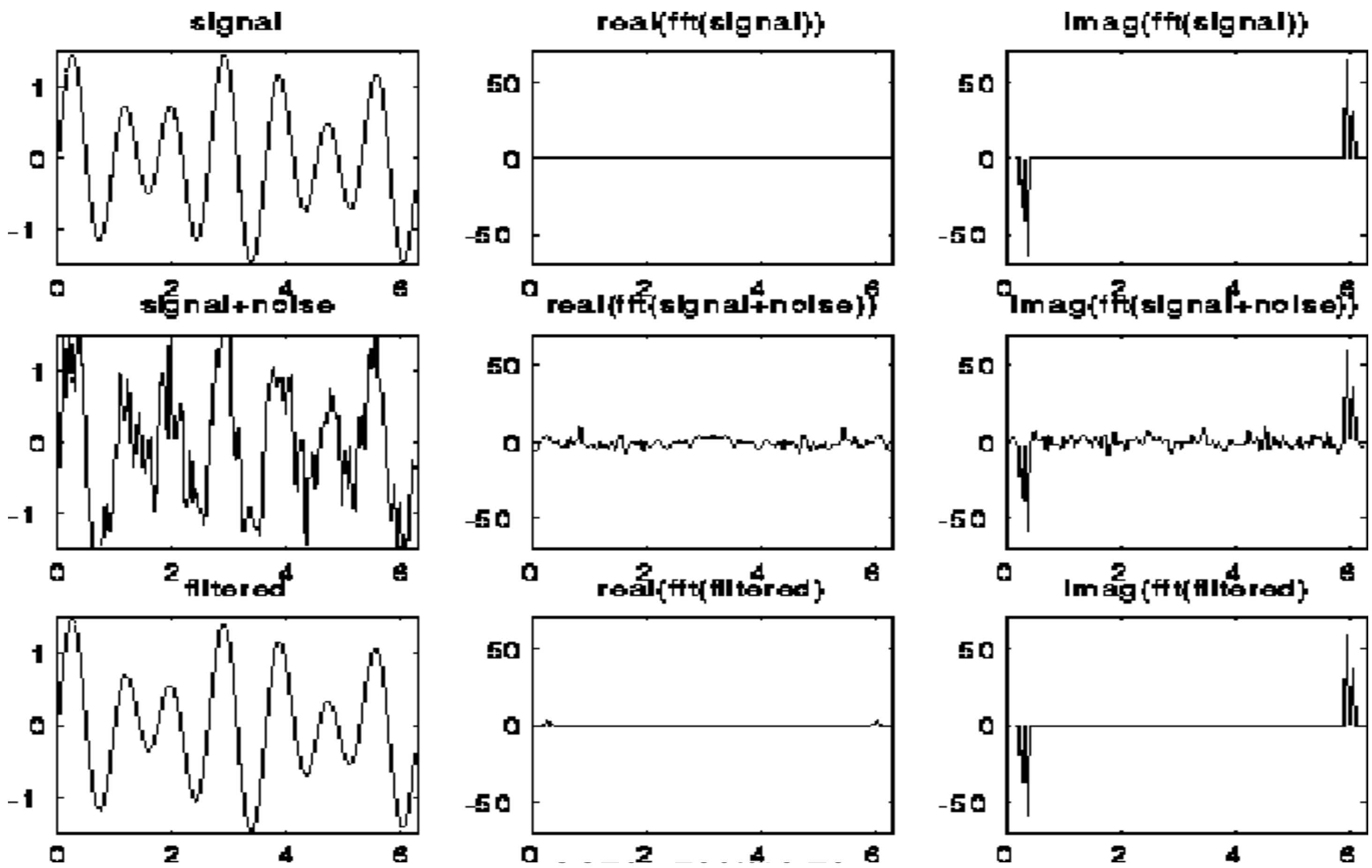
- E.g., for m = 4: $\varpi = i$, $\varpi^2 = -1$, $\varpi^3 = -i$, $\varpi^4 = 1$
- The 2D DFT of an m-by-m matrix V is F*V*F
  - Do 1D DFT on all the columns independently, then all the rows
- Higher dimensional DFTs are analogous

# 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**
  - **Schonhage-Strassen: O(b•log b•log log b) where b = #bits**
- **…**

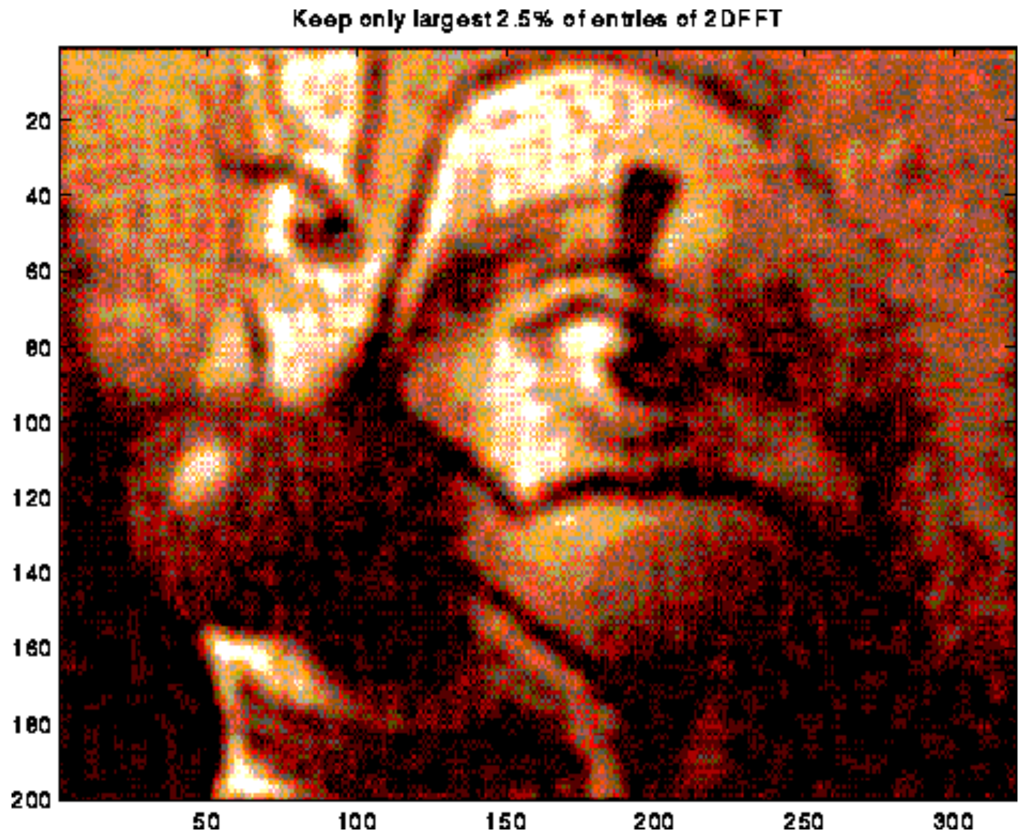
## Using the 1D FFT for filtering

- 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 = 200x320 matrix of values
- Compress by keeping largest 2.5% of FFT components
- Similar idea used by jpeg

# Recall: Poisson's equation arises in many models

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

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

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

f represents the sources; also need boundary conditions

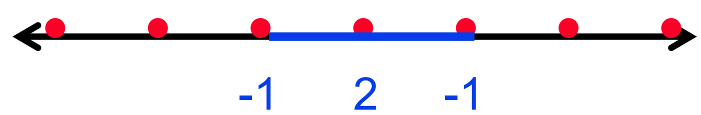
- Electrostatic or Gravitational Potential: Potential(position)
- Heat flow: Temperature(position, time)
- Diffusion: Concentration(position, time)
- Fluid flow: Velocity,Pressure,Density(position,time)
- Elasticity: Stress,Strain(position,time)
- Variations of Poisson have variable coefficients

# Solving Poisson Equation with FFT (1/2)

- **1D Poisson equation: solve $L_1x = b$ where**

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

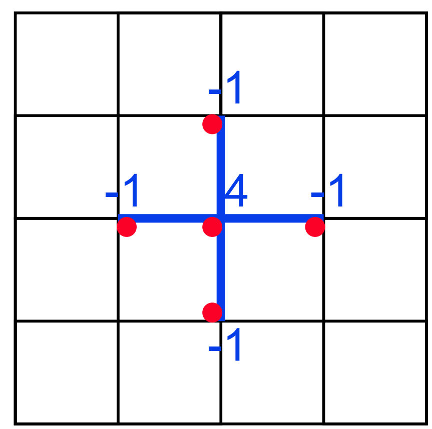
Graph and "stencil"




- **2D Poisson equation: solve $L_2x = b$ where**

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

Graph and "5 point stencil"




3D case is analogous
(7 point stencil)

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

- **Use facts that**
  - $L_1 = F \cdot D \cdot F^T$ is eigenvalue/eigenvector decomposition, where
    - F is very similar to FFT (imaginary part)
      - $F(j,k) = (2/(n+1))^{1/2} \cdot \sin(j\, k\, \pi\ /(n+1))$
    - D = diagonal matrix of eigenvalues
      - $D(j,j) = 2(1 - \cos(j\, \pi\ /\ (n+1))\ )$
  - 2D Poisson same as solving $L_1 \cdot X + X \cdot L_1 = B$ where
    - X square matrix of unknowns at each grid point, B square too
- **Substitute $L_1 = F \cdot D \cdot F^T$ into 2D Poisson to get algorithm**
  1. Perform 2D "FFT" on B to get $B' = F^T \cdot B \cdot F$, or $B = F \cdot B' \cdot F^T$

     Get $FDF^TX+XFDF^T=FB'F^T$ or $F[D(F^TXF)+(F^TXF)D]F^T = F[B']F^T$ or $DX'+X'D=B'$
  2. Solve $D X' + X' D = B'$ for $X'$: $X'(j,k) = B'(j,k)/\ (D(j,j) + D(k,k))$
  3. Perform inverse 2D "FFT" on $X' = F^T \cdot X \cdot F$ to get $X = F \cdot X' \cdot F^T$
- **Cost = 2 2D-FFTs plus $n^2$ adds, divisions = $O(n^2 \log n)$**
- **3D Poisson analogous**

# Algorithms for 2D (3D) Poisson Equation ($N = n^2$ ($n^3$) vars)

| Algorithm | Serial | PRAM | Memory | #Procs |
|---|---|---|---|---|
| ° Dense LU | $N^3$ | $N$ | $N^2$ | $N^2$ |
| ° Band LU | $N^2$ ($N^{7/3}$) | $N$ | $N^{3/2}$ ($N^{5/3}$) | $N$ ($N^{4/3}$) |
| ° Jacobi | $N^2$ ($N^{5/3}$) | $N$ ($N^{2/3}$) | $N$ | $N$ |
| ° Explicit Inv. | $N^2$ | $\log N$ | $N^2$ | $N^2$ |
| ° Conj.Gradients | $N^{3/2}$ ($N^{4/3}$) | $N^{1/2(1/3)} *\log N$ | $N$ | $N$ |
| ° Red/Black SOR | $N^{3/2}$ ($N^{4/3}$) | $N^{1/2}$ ($N^{1/3}$) | $N$ | $N$ |
| ° Sparse LU | $N^{3/2}$ ($N^2$) | $N^{1/2}$ | $N*\log N$ ($N^{4/3}$) | $N$ |
| ° FFT | $N*\log N$ | $\log N$ | $N$ | $N$ |
| ° Multigrid | $N$ | $\log^2 N$ | $N$ | $N$ |
| ° **Lower bound** | **$N$** | **$\log N$** | **$N$** | |

**PRAM is an idealized parallel model with zero cost communication**

**Reference: James Demmel, Applied Numerical Linear Algebra, SIAM, 1997.**

## Related Transforms

° Most applications require multiplication by both F and $F^{-1}$
  - $F(j,k) = \exp(2\pi ijk/m)$

° Multiplying by F and $F^{-1}$ are essentially the same.
  - $F^{-1}$ = 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**

$$(F*v)[j] = \sum_{k=0}^{m-1} F(j,k) * v(k)$$

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

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

$$= V(\varpi^{j})$$

**where V is defined as the polynomial**

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

- **FFT same as evaluating a polynomial V(x) with degree m-1 at m different points**

## Divide and Conquer FFT

° V can be evaluated using divide-and-conquer

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

$$= \quad v[0] + x^2*v[2] + x^4*v[4] + \ldots$$

$$+ x*(v[1] + x^2*v[3] + x^4*v[5] + \ldots )$$

$$= V_{even}(x^2) + x*V_{odd}(x^2)$$

° V has degree m-1, so $V_{even}$ and $V_{odd}$ are polynomials of degree m/2-1

° We evaluate these at m points: $(\varpi^{j})^2$ for $0 \le j \le m-1$

° But this is really just m/2 different points, since

$$(\varpi^{(j+m/2)})^2 = (\varpi^{j} * \varpi^{m/2})^2 = \varpi^{2j} * \varpi^{m} = (\varpi^{j})^2$$

° So FFT on m points reduced to 2 FFTs on m/2 points

- Divide and conquer!

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

FFT($v$, $\varpi$, $m$) … assume $m$ is a power of 2

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

else

$v_{even}$ = FFT($v[0:2:m-2]$, $\varpi^2$, $m/2$)

$v_{odd}$ = FFT($v[1:2:m-1]$, $\varpi^2$, $m/2$)

precomputed

$\varpi$-vec = $[\varpi^0, \varpi^1, \ldots \varpi^{(m/2-1)}]$

return $[v_{even} + (\varpi\text{-vec} .* v_{odd}),$

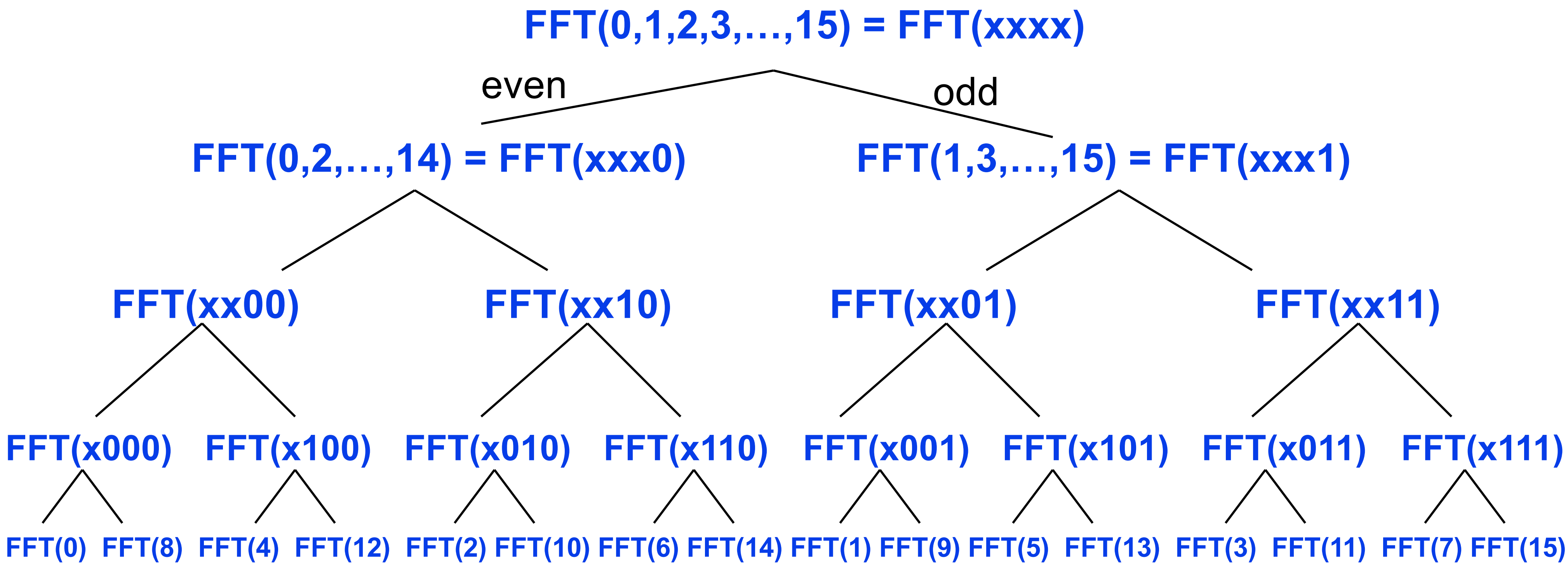
$v_{even} - (\varpi\text{-vec} .* v_{odd})]$

- 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) – more later

# Bit Reversal

- The outputs of the FFT stored in “bit reversed” order

| Decimal | Binary | | Decimal | Binary |
|---|---|---|---|---|
| 0 | 0000 | | 0 | 0000 |
| 1 | 0001 | | 8 | 1000 |
| 2 | 0010 | | 4 | 0100 |
| 3 | 0011 | | 12 | 1100 |
| 4 | 0100 | | 2 | 0010 |
| 5 | 0101 | | 10 | 1010 |
| 6 | 0110 | | 6 | 0100 |
| 7 | 0111 | | 14 | 1110 |
| 8 | 1000 | | 1 | 0001 |
| 9 | 1001 | | 9 | 1001 |
| 10 | 1010 | | 5 | 0101 |
| 11 | 1011 | | 13 | 1101 |
| 12 | 1100 | | 3 | 0011 |
| 13 | 1101 | | 11 | 1011 |
| 14 | 1110 | | 7 | 0111 |
| 15 | 1111 | | 15 | 1111 |

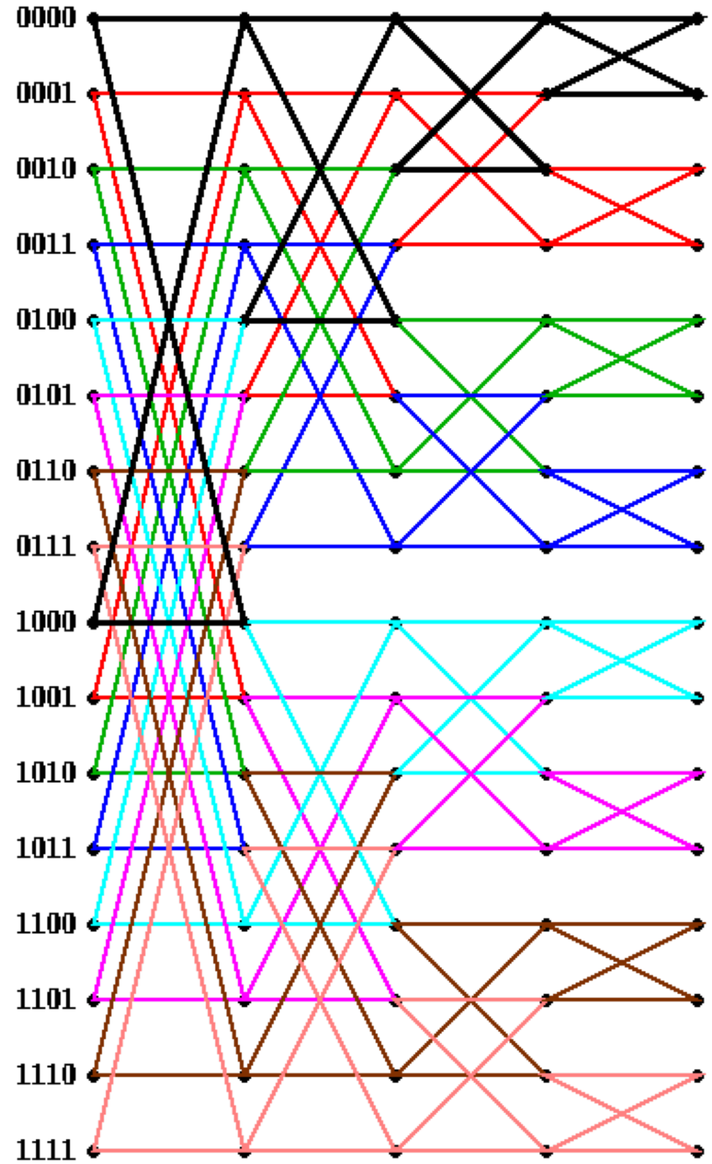
- May need to sort them (which is like transposes at various levels)

- Many FFT applications also do an inverse FFT, and therefore do not require any sorting

# Parallel 1D FFT

- Data dependencies in 1D FFT
  - Butterfly pattern
  - From $v_{even} \pm w .* v_{odd}$
- A PRAM algorithm takes O(log m) time
  - each step to right is parallel
  - there are log m steps
- What about communication cost?
- (See UCB EECS Tech report UCB/CSD-92-713 for details, aka "LogP paper")

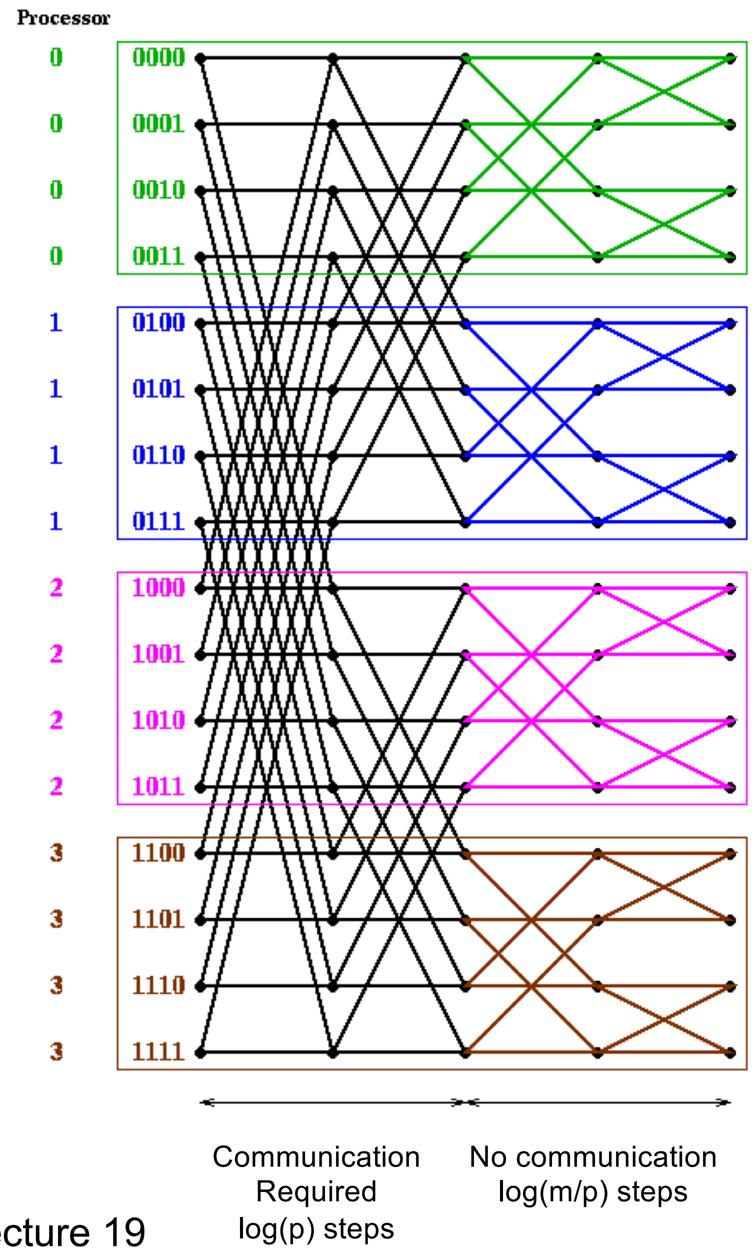
Data dependencies in a 16-point FFT



# 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

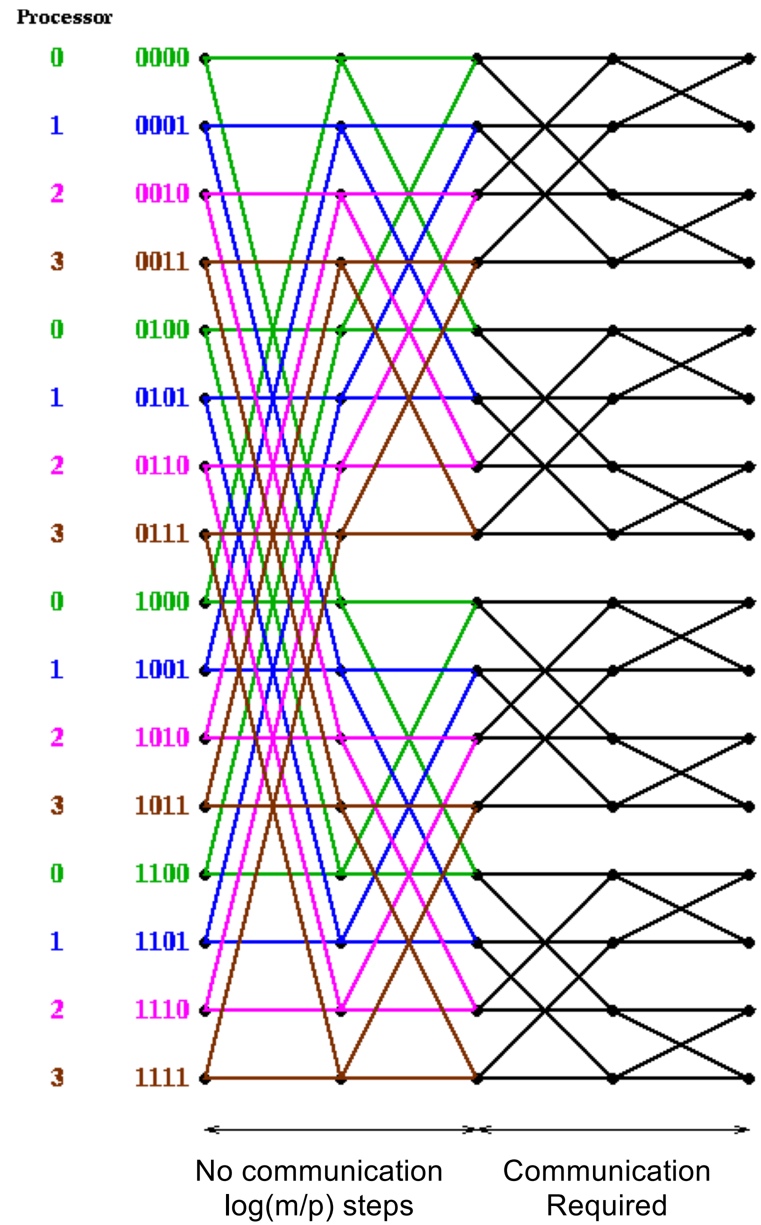
Block Data Layout of an m=16-point FFT on p=4 Processors



# 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
- $\alpha$ = latency for message
- $\beta$ = time per word in a message

- Time(block_FFT) = Time(cyclic_FFT) =

  2*m*log(m)/p … perfectly parallel flops

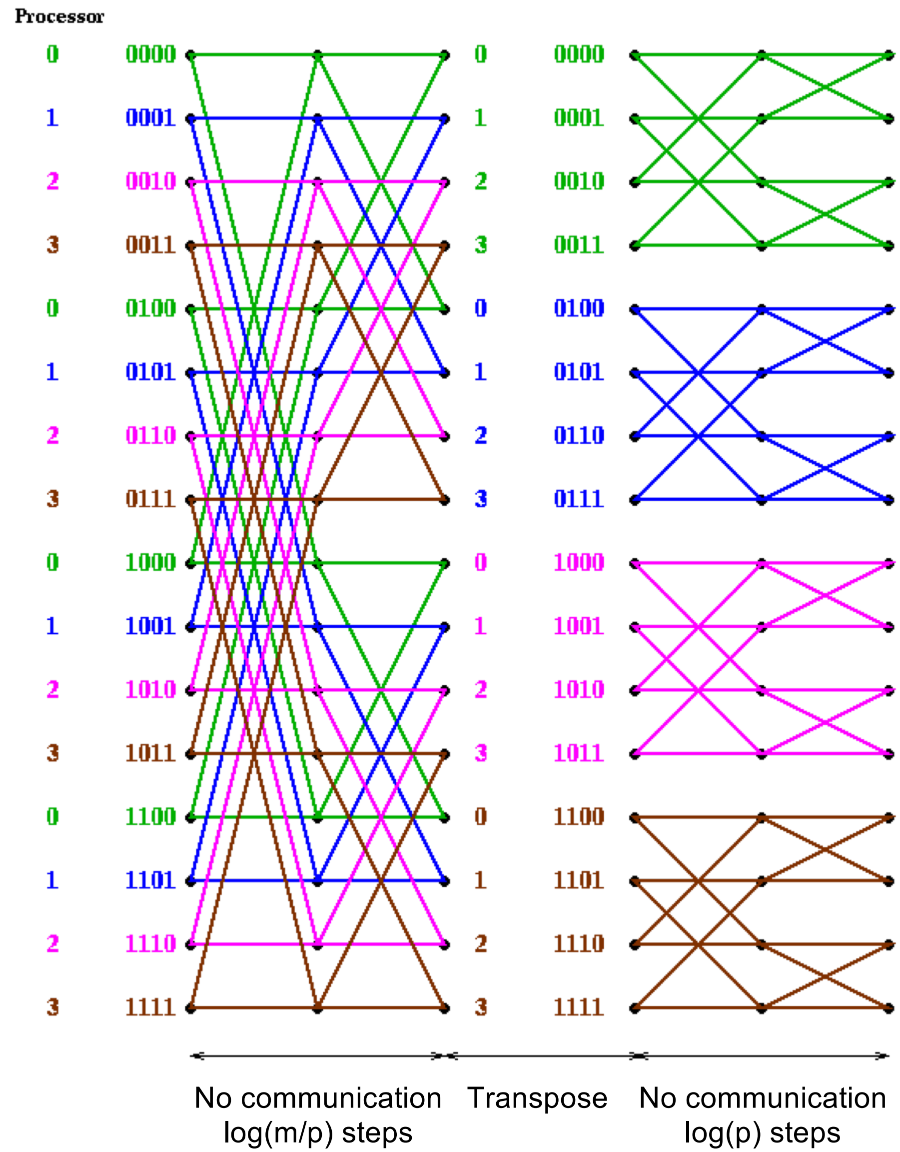
  + log(p) * $\alpha$ ... 1 message/stage, log p stages

  + m*log(p)/p * $\beta$ … m/p words/message

# FFT With "Transpose"

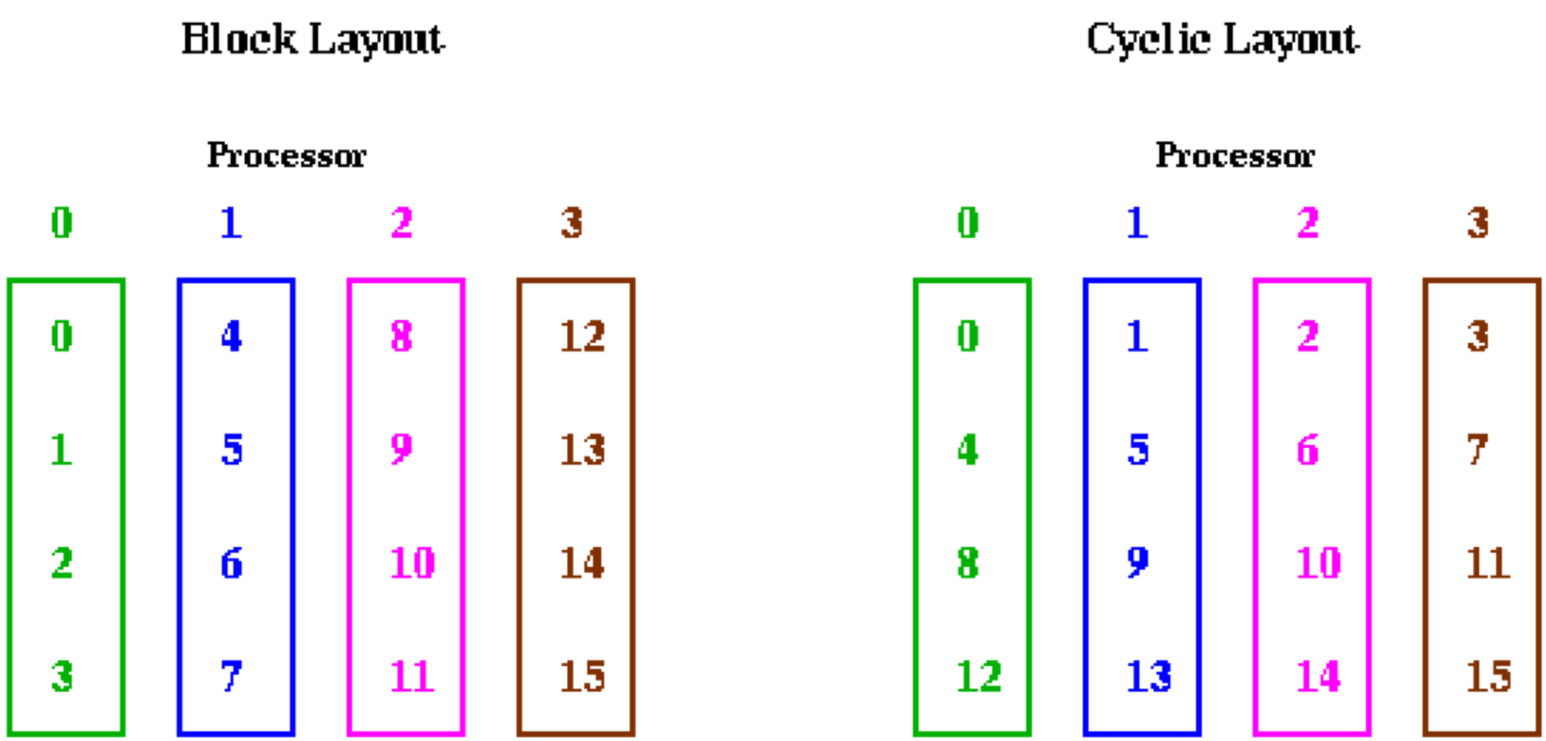
- **If we start with a cyclic layout for first log(m/p) steps, there is no communication**
- **Then transpose the vector for last log(p) steps**
- **All communication is in the transpose**
- **Note: This example has log(m/p) = log(p)**
  - **If log(m/p) < log(p) more phases/layouts will be needed**
  - **We will assume log(m/p) ≥ log(p) for simplicity, i.e. m ≥ p$^2$**

Transpose Algorithm for an m=16-point FFT on p=4 Processors



## Why is the Communication Step Called a Transpose?

- Analogous to transposing an array
- View as a 2D array of m/p by p
- Note: same idea is useful for caches



## Parallel Complexity of the FFT with Transpose

- If 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 $\alpha$, 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; assumes no recomputation
- 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 (FFTW)

# 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): #words = $\Omega(m \log m / (p \log m/p))$
  - 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 #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
    - http://www-math.mit.edu/~edelman
  - Based on the Fast Multipole algorithm
  - Less communication for non-bit-reversed algorithm
  - Approximates FFT

## Higher Dimensional FFTs

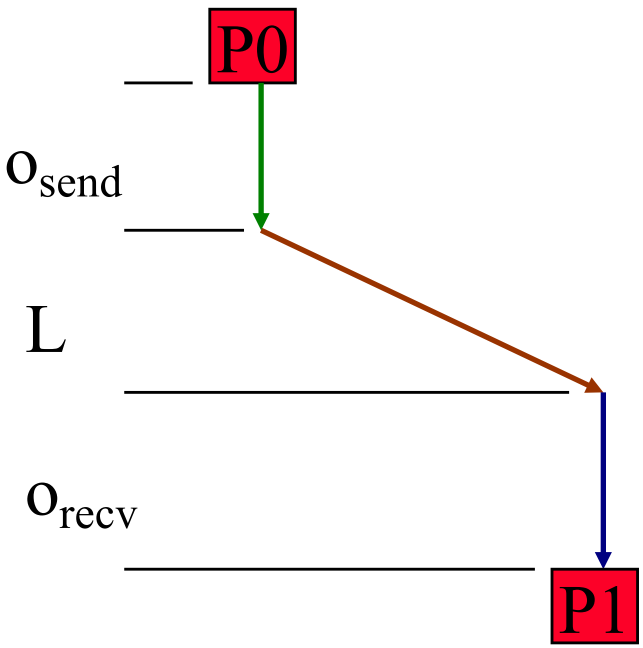
- FFTs on 2 or more dimensions are defined as 1D FFTs on vectors in all dimensions.
  - 2D FFT does 1D FFTs on all rows and then all columns
- There are 3 obvious possibilities for the 2D FFT:
  - (1) 2D blocked layout for matrix, using parallel 1D FFTs for each row and column
  - (2) Block row layout 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

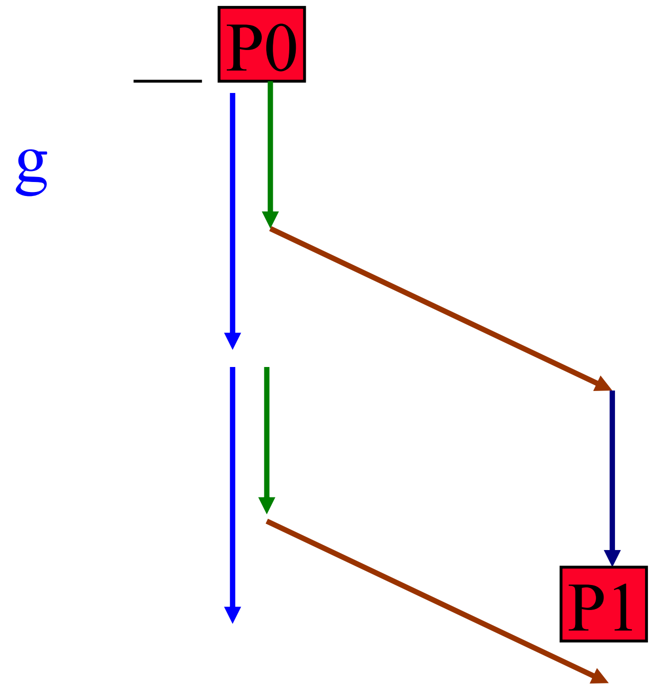
- **FFT requires one (or more) transpose operations:**
  - Every processor sends 1/p-th of its data to each other one
- **Bisection Bandwidth limits this performance**
  - Bisection bandwidth is the bandwidth across the narrowest part of the network
  - Important in global transpose operations, all-to-all, 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**

# Modified LogGP Model

- LogGP: no overlap



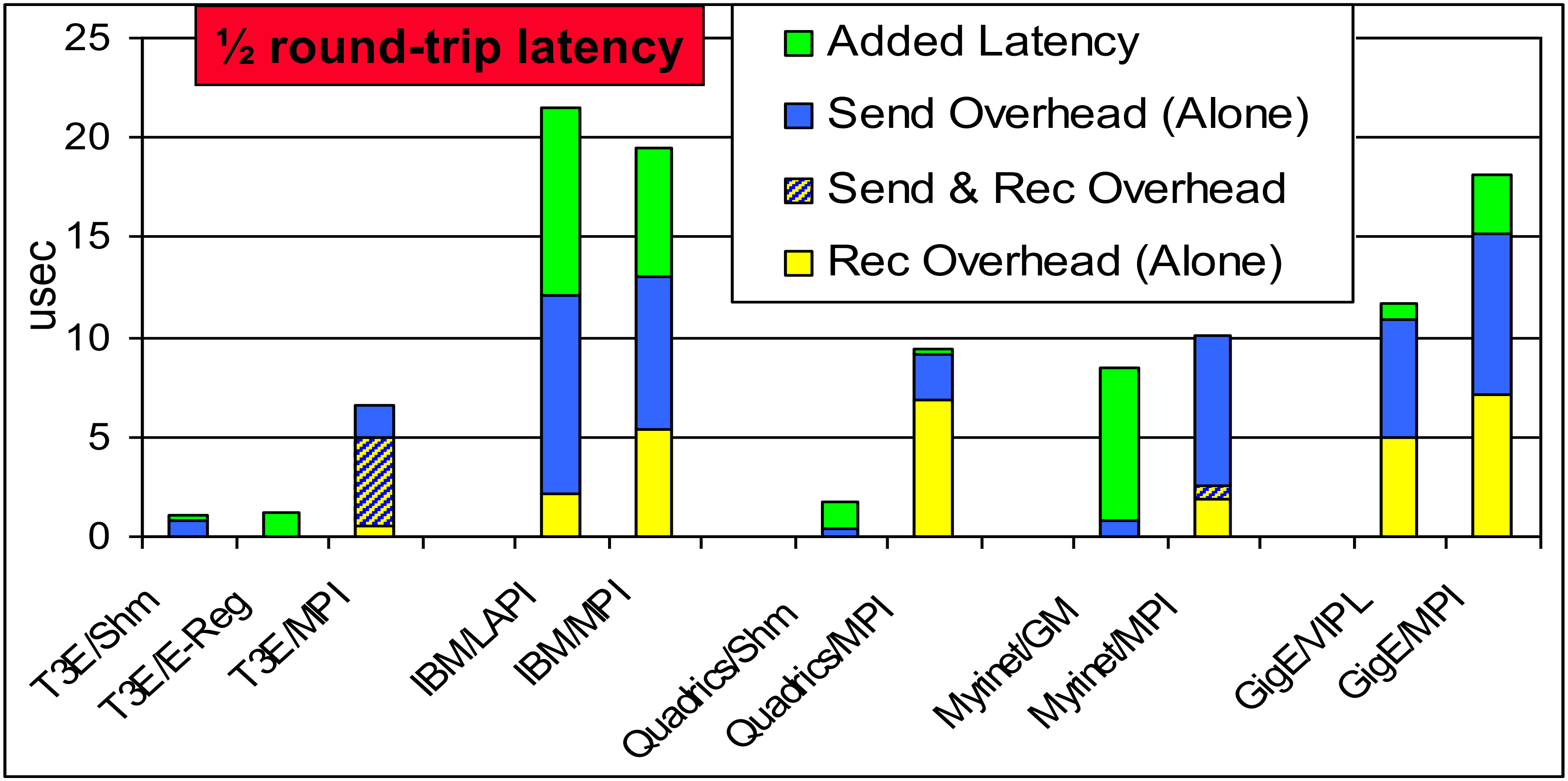

- LogGP: with overlap




EEL: end to end latency (1/2 roundtrip)
g: minimum time between small message sends
G: gap per byte for larger messages

# Historical Perspective

## Green + Yellow = possible comp/comm overlap



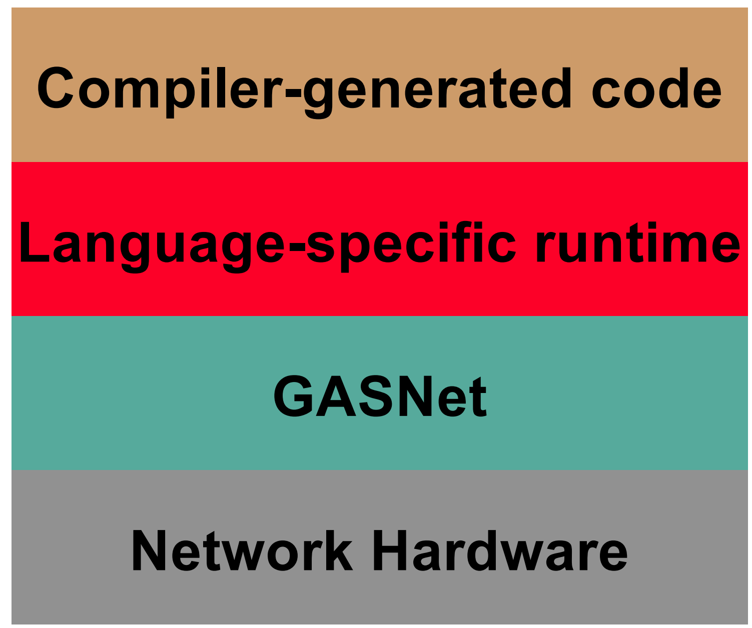

- Potential performance advantage for fine-grained, one-sided programs
- Potential productivity advantage for irregular applications

## General Observations

- "Overlap" means computing and communicating simultaneously, (or communication with other communication, aka pipelining)
- Rest of slide about comm/comp overlap
- The overlap potential is the difference between the gap and overhead
  - No potential if CPU is tied up throughout message send
    - E.g., no send-side DMA
  - Potential grows with message size for machines with DMA (per byte cost is handled by network, i.e. NIC)
  - Potential grows with amount of network congestion
    - Because gap grows as network becomes saturated
- Remote overhead is 0 for machine with RDMA
- Need good SW support to take advantage of this

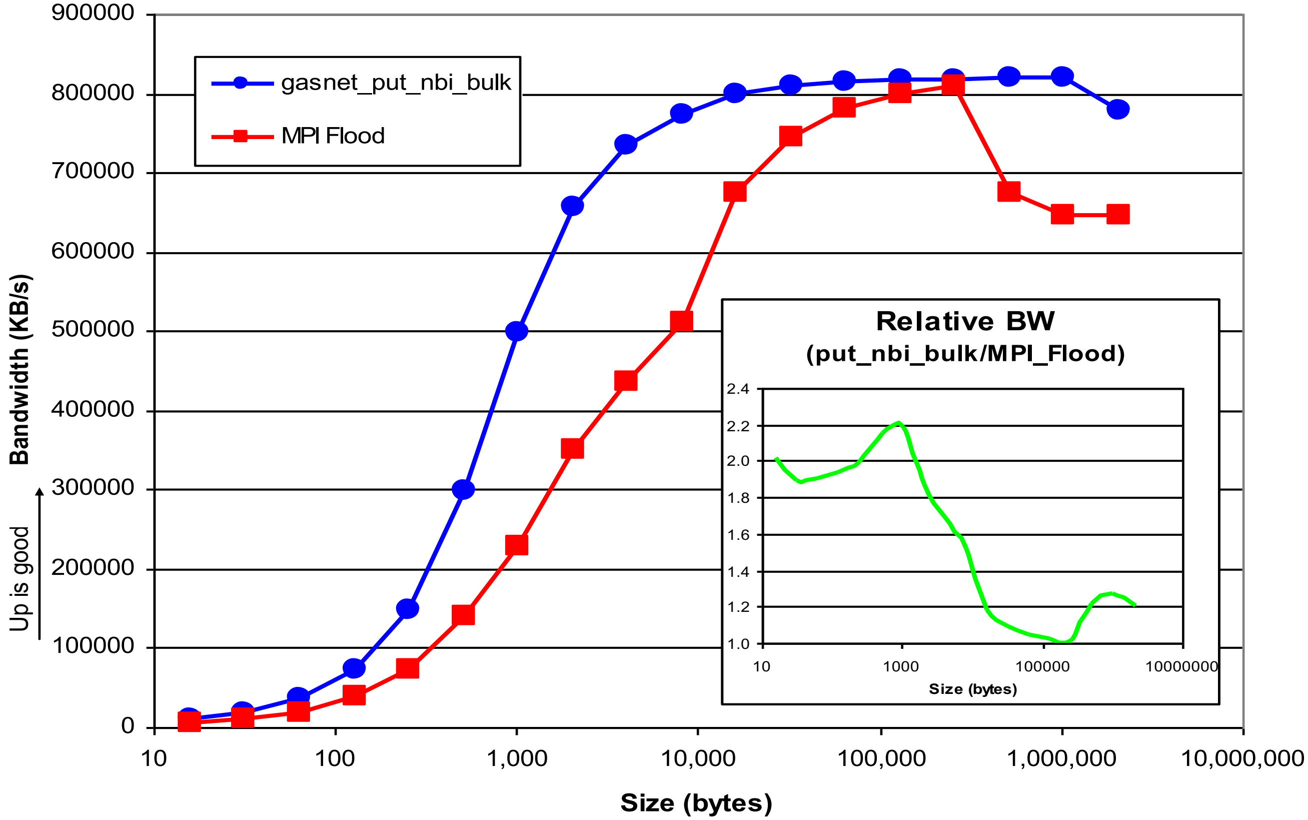
# GASNet offers put/get communication

- One-sided: no remote CPU involvement required in API (key difference with MPI)
  - **Message contains remote address**
  - **No need to match with a receive**
  - **No implicit ordering required**



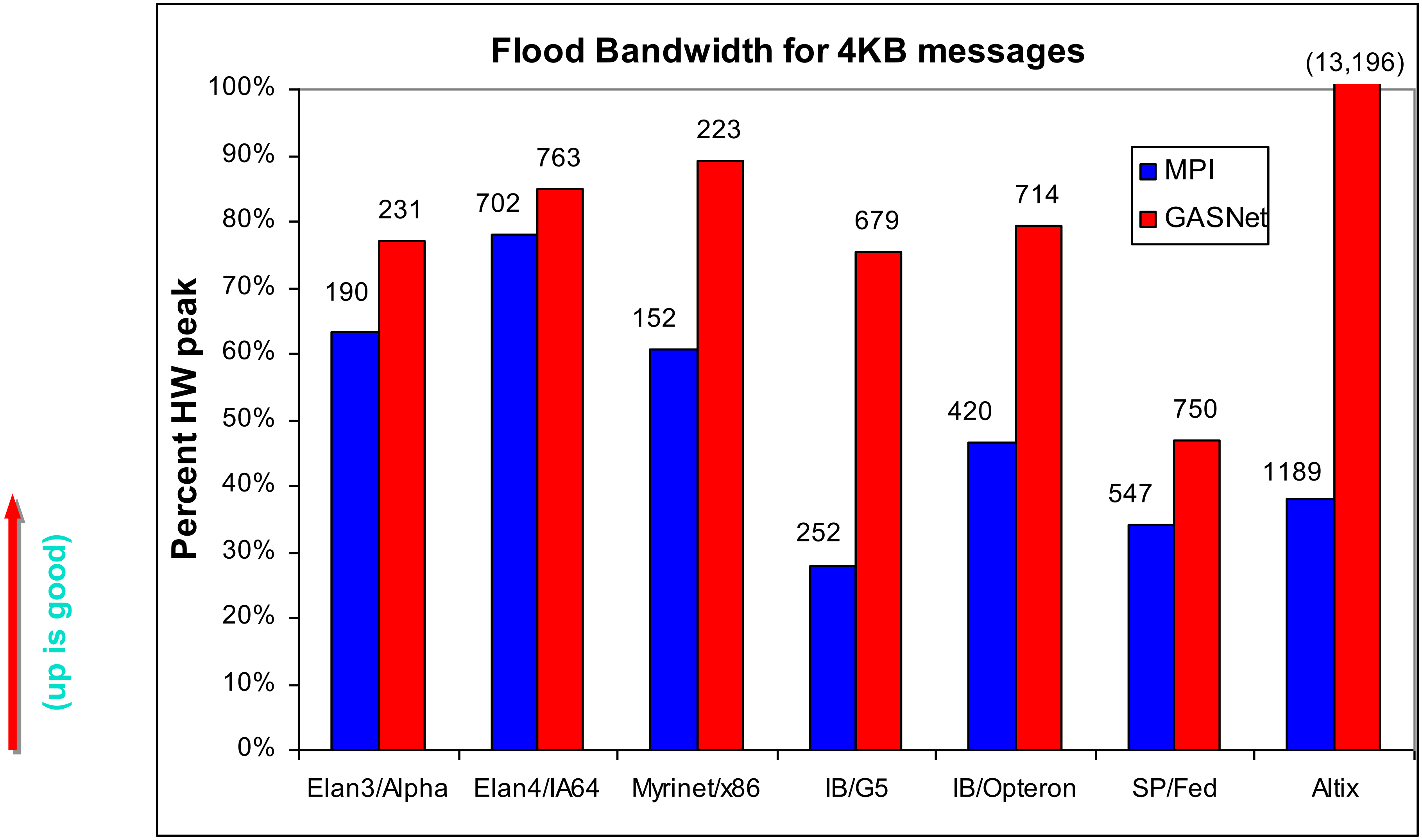

- Used in language runtimes (UPC, etc.)
- Fine-grained and bulk transfers
- Split-phase communication

# Performance of 1-Sided vs 2-sided Communication: GASNet vs MPI




- Comparison on Opteron/InfiniBand – GASNet's vapi-conduit and OSU MPI 0.9.5
- Up to large message size (> 256 Kb), GASNet provides up to 2.2X improvement in streaming bandwidth
- Half power point (N/2) differs by *one order of magnitude*

# GASNet: Performance for mid-range message sizes




GASNet usually reaches saturation bandwidth before MPI - fewer costs to amortize

Usually outperforms MPI at medium message sizes - often by a large margin

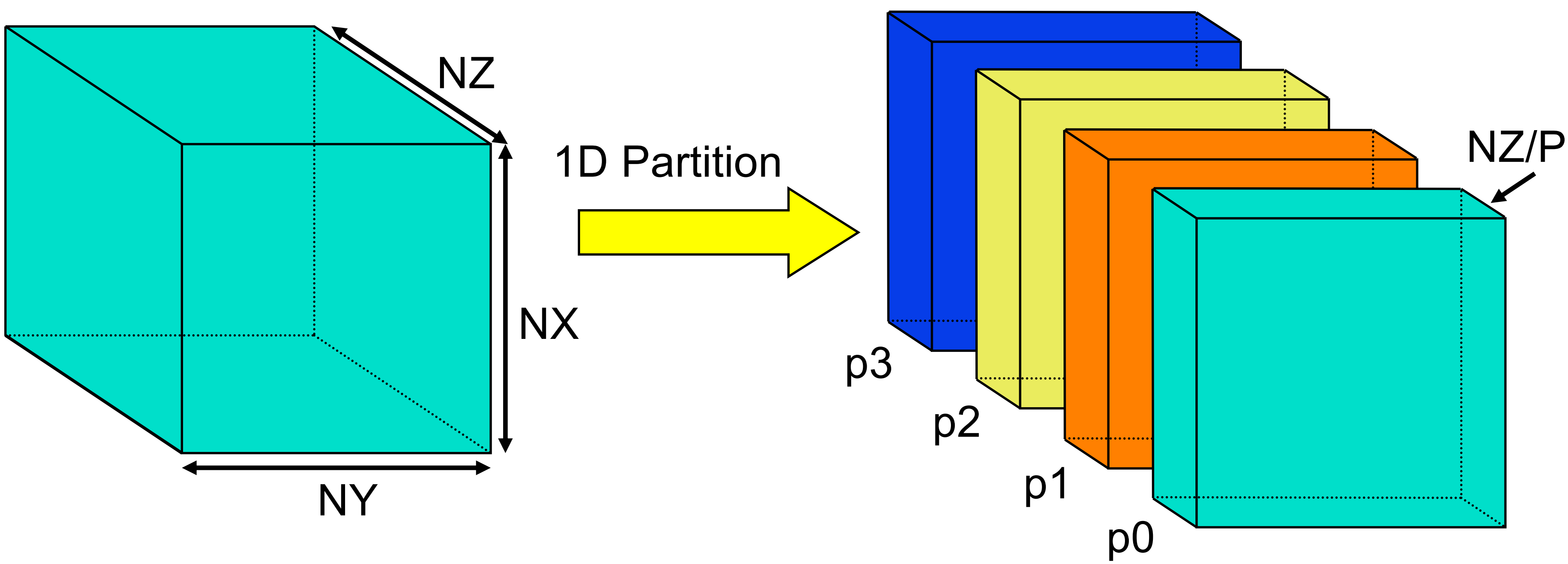
# NAS FT Benchmark Case Study

- **Performance of Exchange (All-to-all) is critical**
  - Communication to computation ratio increases with faster, more optimized 1-D FFTs (used best available, from FFTW)
  - Determined by available bisection bandwidth
  - Between 30-40% of the application's total runtime
- **Assumptions**
  - 1D partition of 3D grid
  - At most N processors for N^3 grid
  - HPC Challenge benchmark has large 1D FFT (can be viewed as 3D or more with proper roots of unity)
- **Reference for details**
  - "Optimizing Bandwidth Limited Problems Using One-side Communication and Overlap", C. Bell, D. Bonachea, R. Nishtala, K. Yelick, IPDPS'06 (www.eecs.berkeley.edu/~rajashn)
  - Started as CS267 project

# 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**

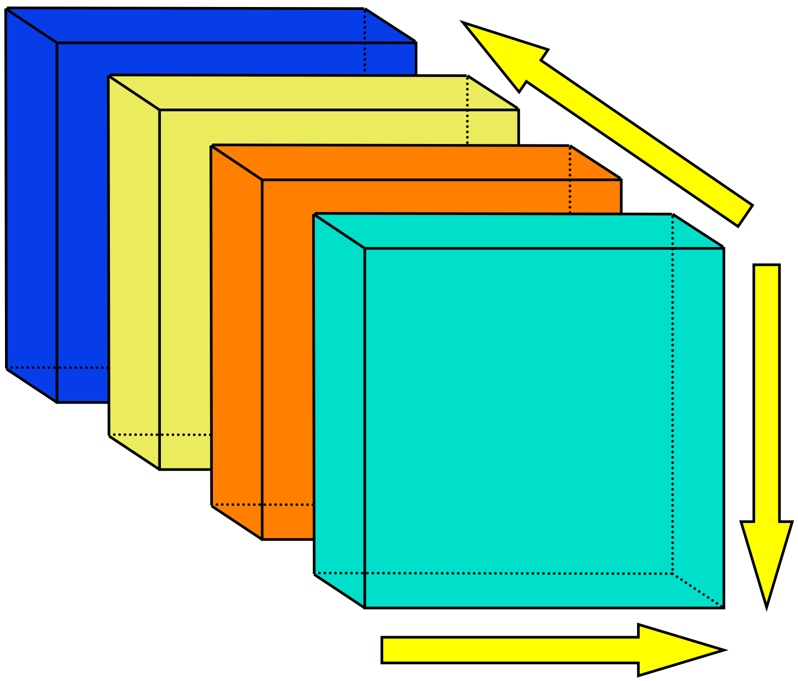
Example: P = 4




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)

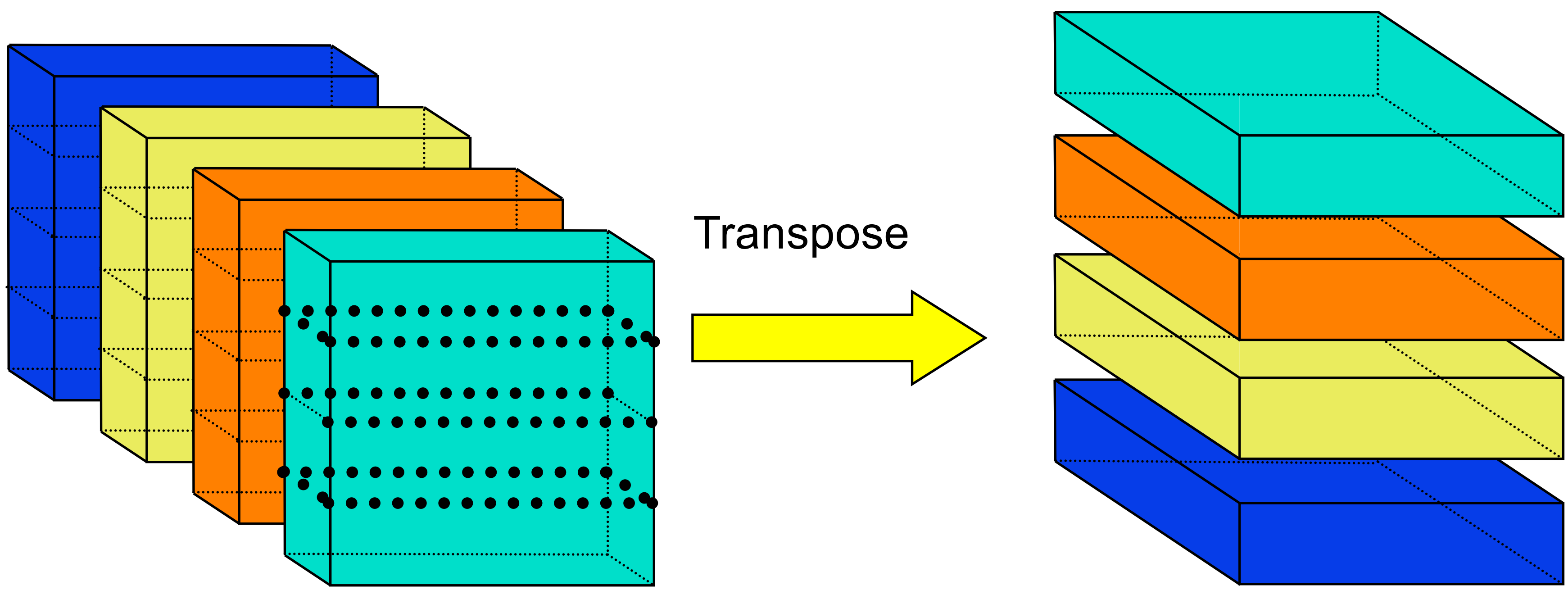
Step 2: FFTs on the rows
(all elements local)

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

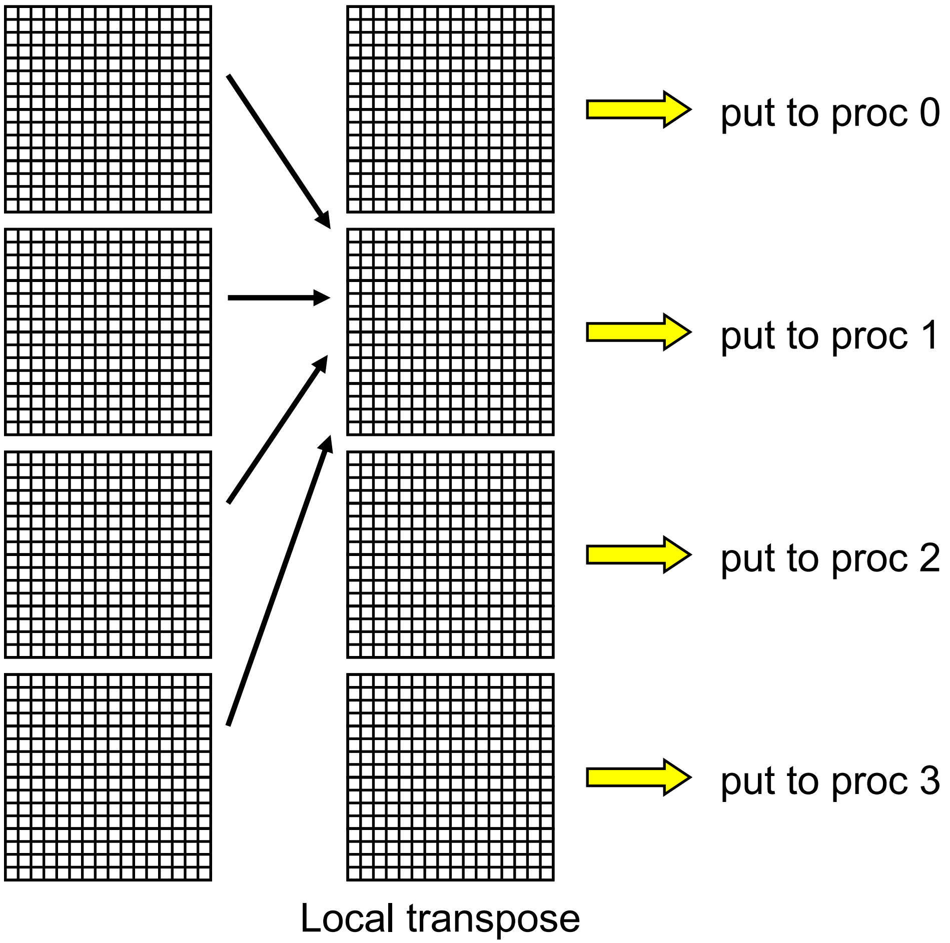
- Each processor has to scatter input domain to other processors
  - Every processor divides its portion of the domain into P pieces
  - Send each of the P pieces to a different processor
- Three different ways to break up the messages
  1. Packed Slabs (i.e. single packed "All-to-all" in MPI parlance) (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 and leverage RDMA support in modern networks

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

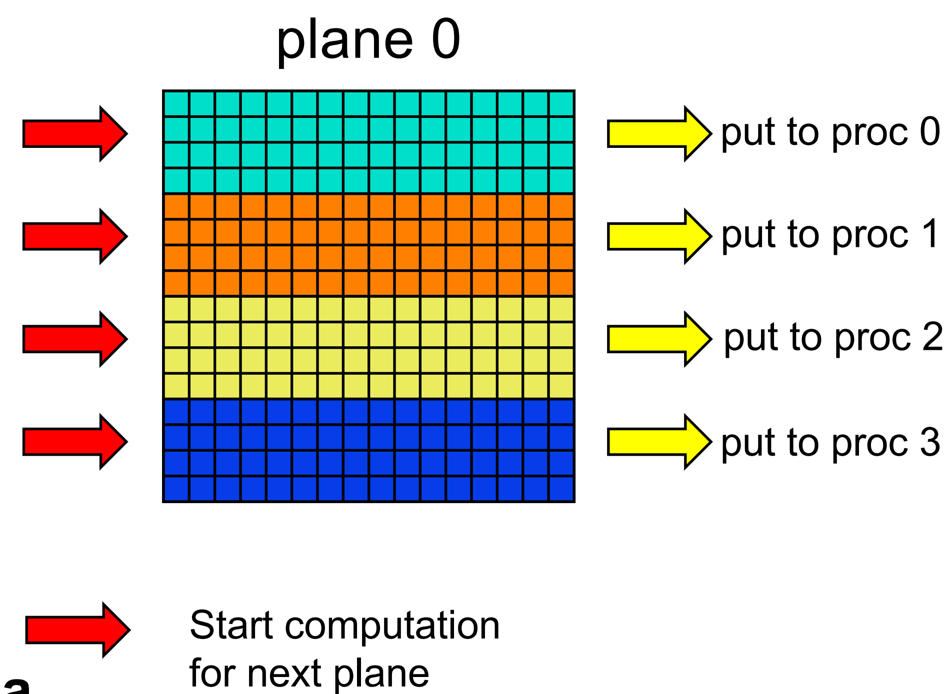
- NAS FT (Class D) with 256 processors on Opteron/InfiniBand
  - Each processor sends 256-1 messages of 512kBytes
  - Global Transpose (i.e. all to all exchange) only achieves 67% of peak point-to-point bidirectional bandwidth
  - Many factors could cause this slowdown
    - Network contention
    -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

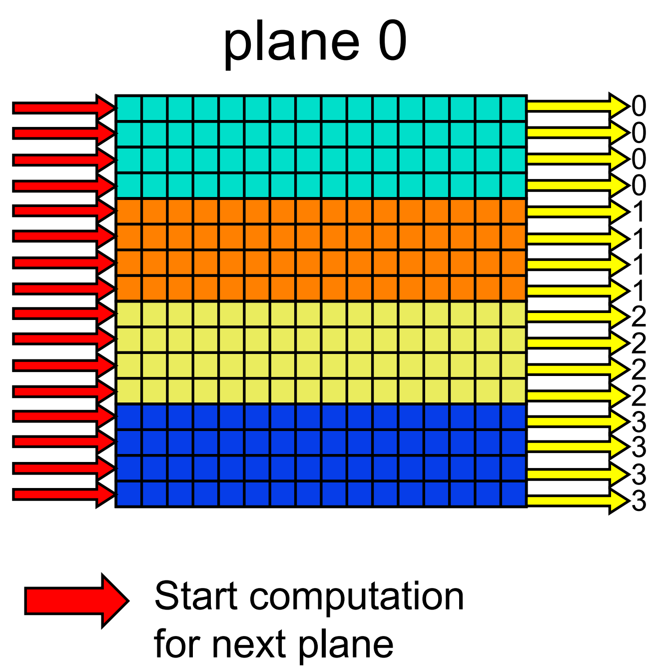



- For $512^3$ grid across 64 processors
  - Send 512-8 messages of 64kB each

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

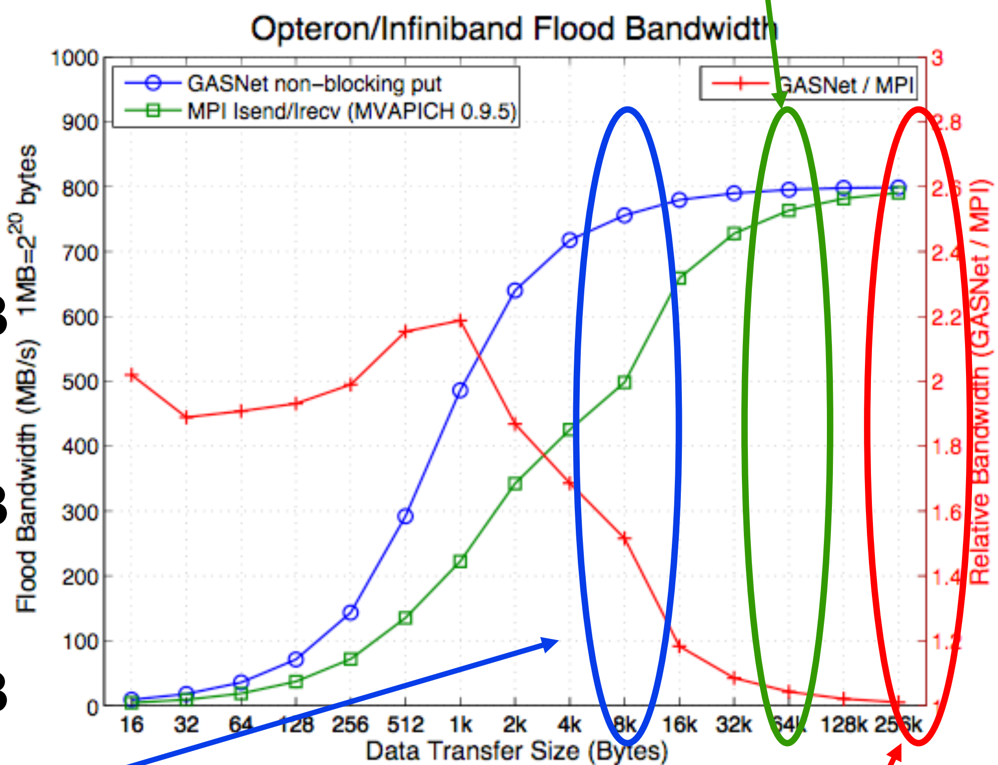
Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

# Communication Requirements

° $512^3$ across 64 processors

- **Alg 1: Packed Slabs**
  - Send 64 messages of 512kB
- **Alg 2: Slabs**
  - Send 512 messages of 64kB
- **Alg 3: Pencils**
  - Send 4096 messages of 8kB

With Slabs GASNet is slightly faster than MPI




GASNet achieves close to peak bandwidth with Pencils but MPI is about 50% less efficient at 8k

More overlap possible with 8k messages

With the message sizes in Packed Slabs both comm systems reach the same peak bandwidth

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

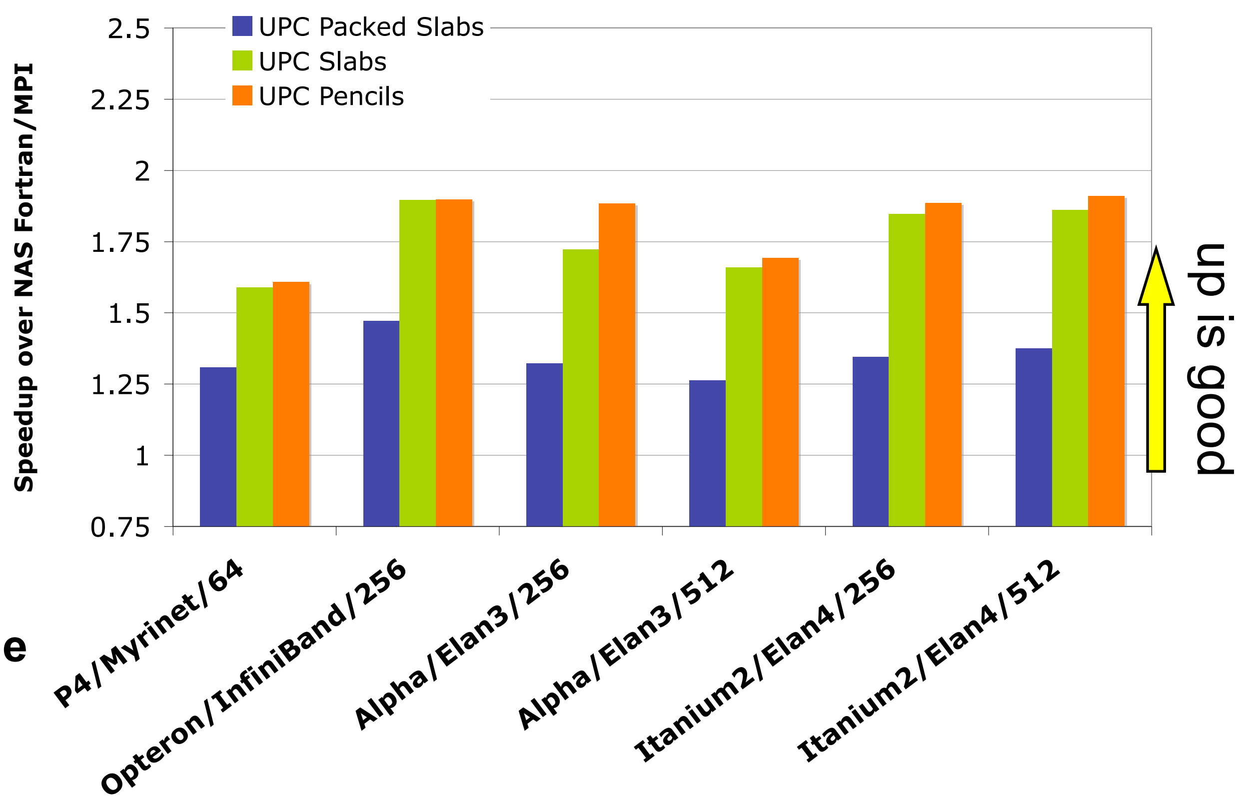
# Platforms

| Name | Processor | Network | Software |
|---|---|---|---|
| Opteron/Infiniband "Jacquard" @ NERSC | Dual 2.2 GHz Opteron (320 nodes @ 4GB/node) | Mellanox Cougar InfiniBand 4x HCA | Linux 2.6.5, Mellanox VAPI, MVAPICH 0.9.5, Pathscale CC/F77 2.0 |
| Alpha/Elan3 "Lemieux" @ PSC | Quad 1 GHz Alpha 21264 (750 nodes @ 4GB/node) | Quadrics QsNet1 Elan3 /w dual rail (one rail used) | Tru64 v5.1, Elan3 libelan 1.4.20, Compaq C V6.5-303, HP Fortra Compiler X5.5A-4085-48E1K |
| Itanium2/Elan4 "Thunder" @ LLNL | Quad 1.4 Ghz Itanium2 (1024 nodes @ 8GB/node) | Quadrics QsNet2 Elan4 | Linux 2.4.21-chaos, Elan4 libelan 1.8.14, Intel ifort 8.1.025, icc 8. 1.029 |
| P4/Myrinet "FSN" @ UC Berkeley Millennium Cluster | Dual 3.0 Ghz Pentium 4 Xeon (64 nodes @ 3GB/node) | Myricom Myrinet 2000 M3S-PCI64B | Linux 2.6.13, GM 2.0.19, Intel ifort 8.1-20050207Z, icc 8.1-20050207Z |

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

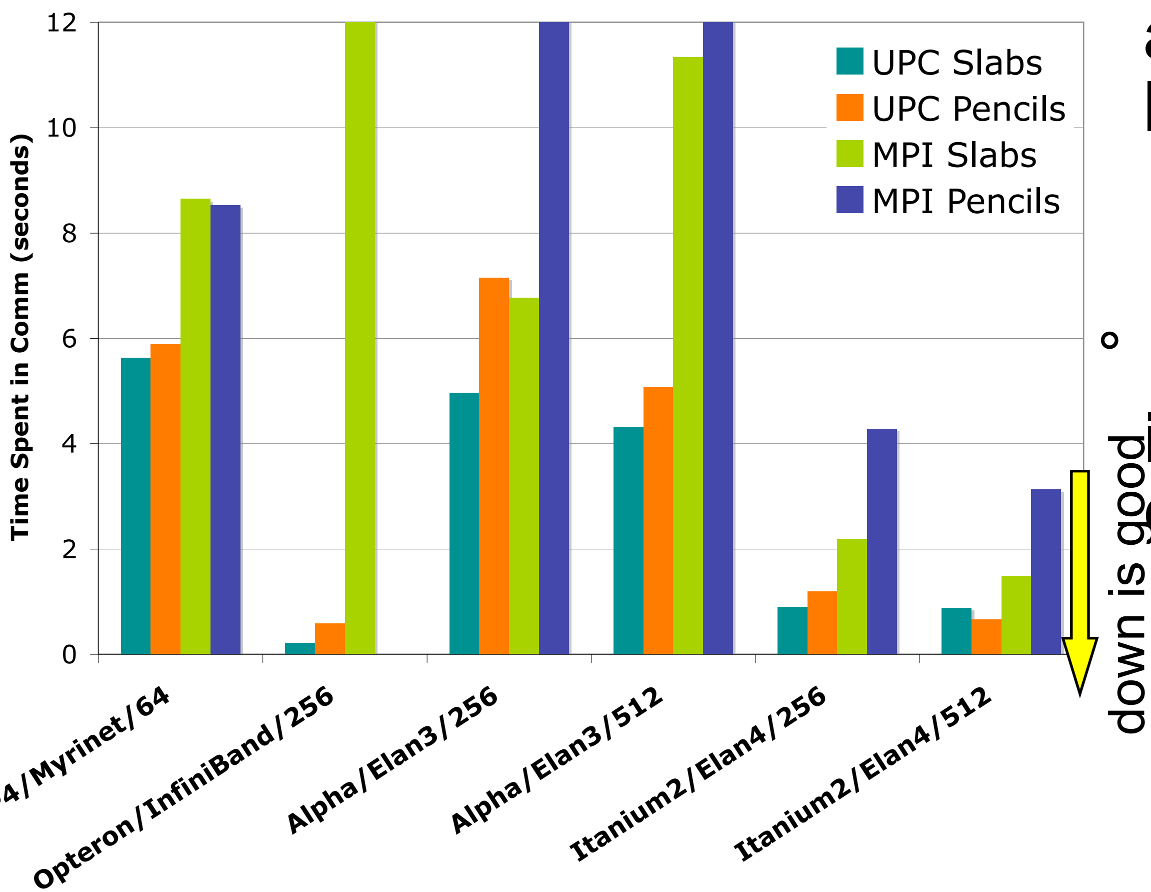
# Comparison of Algorithms

- 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 (out of 2x)




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

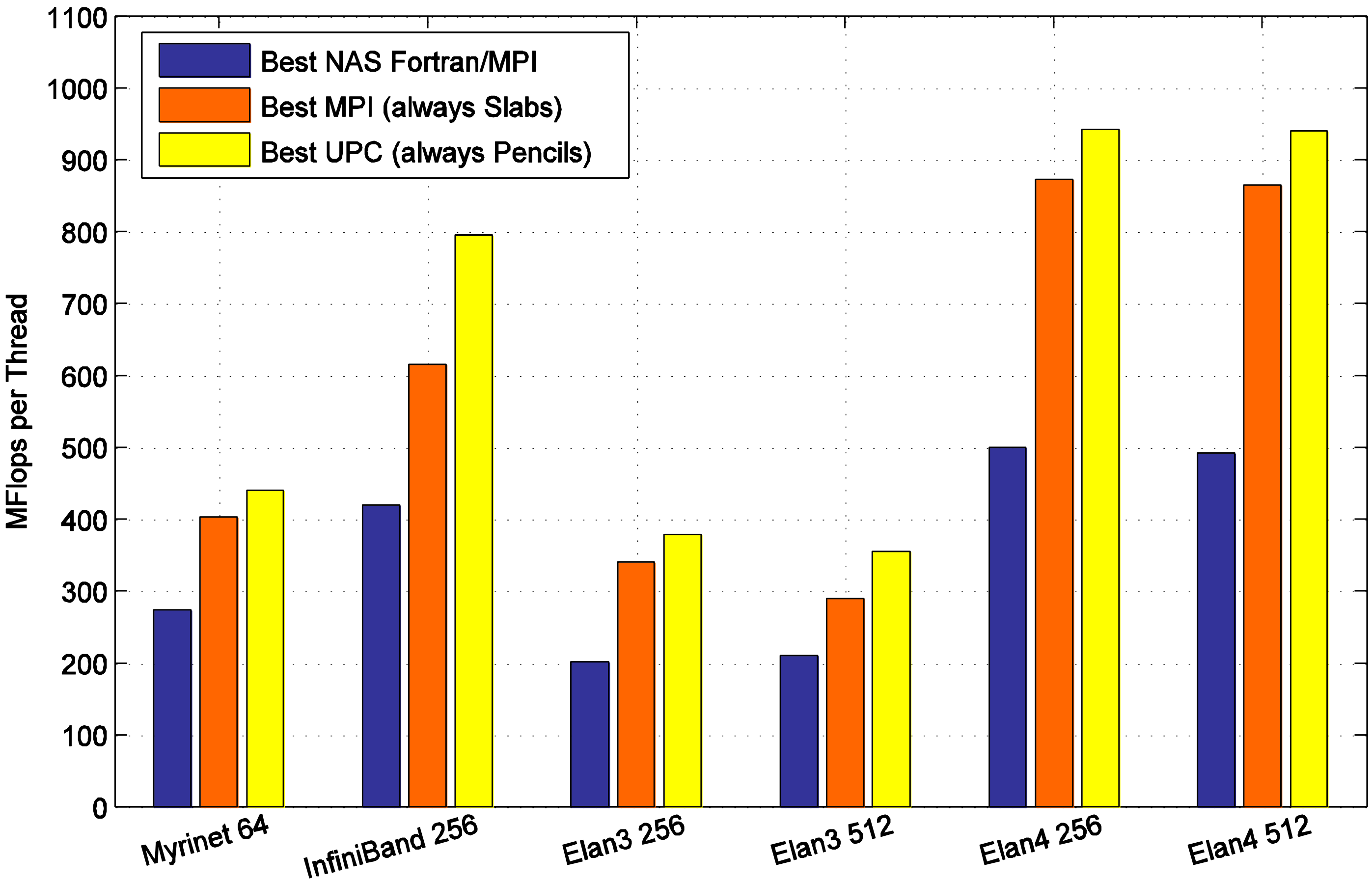
# Time Spent in Communication




- Implemented the 3 algorithms in MPI using Irecvs and Isends
- Compare time spent initiating or waiting for communication to finish
  - UPC consistently spends less time in communication than its MPI counterpart
  - MPI unable to handle pencils algorithm in some cases

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

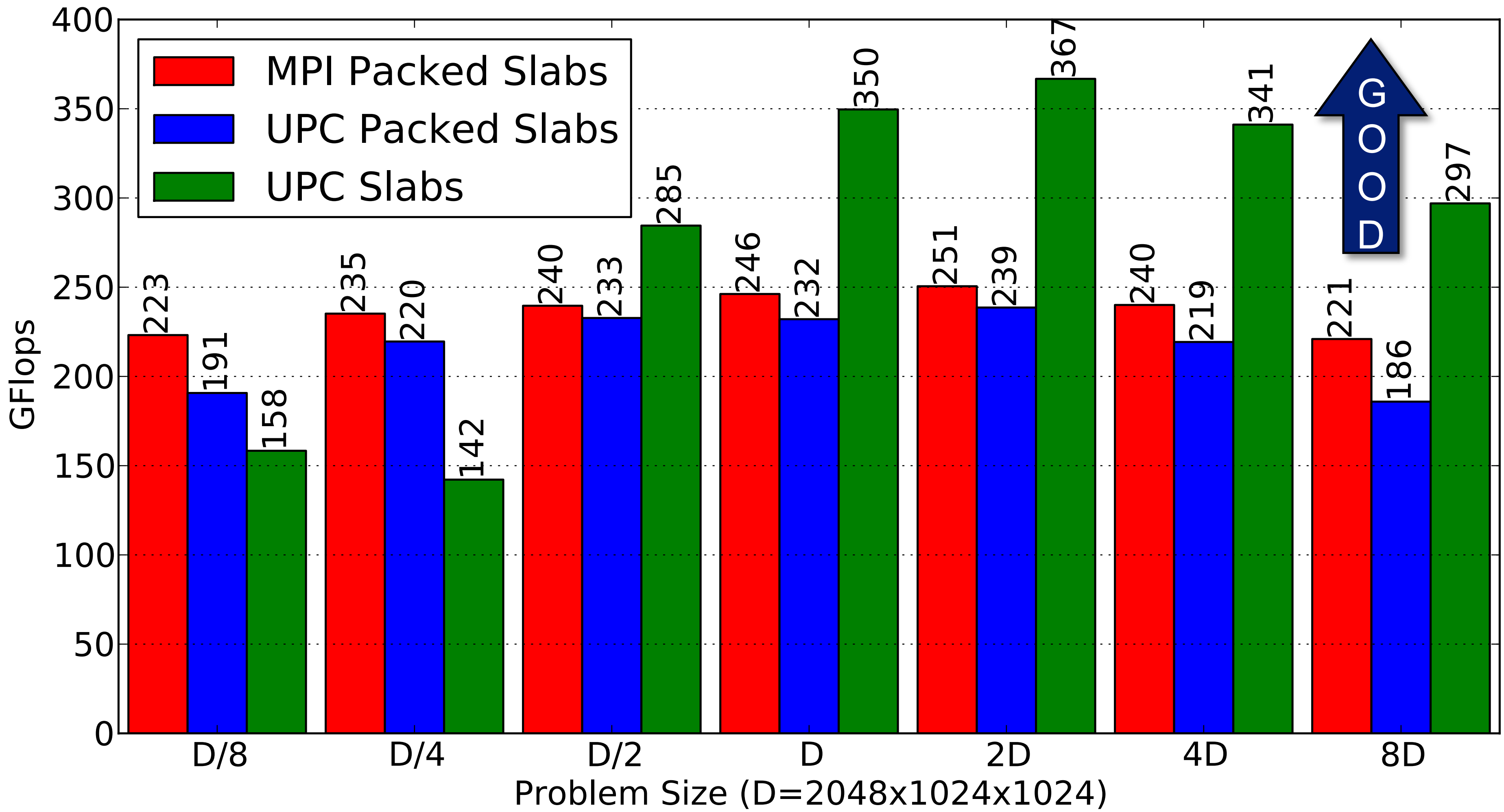
# NAS FT Variants Performance Summary




- Shown are the largest classes/configurations possible on each test machine
- MPI not particularly tuned for many small/medium size messages in flight (long message matching queue depths)

# FFT Performance on Cray XT4 (Franklin)

- 1024 Cores of the Cray XT4
  - Uses FFTW for local FFTs
  - Larger the problem size the more effective the overlap



# FFTW – Fastest Fourier Transform in the West

- [www.fftw.org](http://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 (competes with Spiral)
- **Similar in spirit to PHIPAC/ATLAS/OSKI/Sparsity**
- **Won 1999 Wilkinson Prize for Numerical Software**
- **Widely used**
  - Latest version 3.3.9 (Dec 2020)
  - Includes threads, OpenMP, MPI versions, new architecture support
  - Layout constraints from users/apps + network differences are hard to support

FFTW

the "Fastest
Fourier Tranform
in the West"

- C library for real & complex FFTs (arbitrary size/dimensionality)
  (+ parallel versions for threads & MPI)

- Computational kernels (80% of code) automatically generated

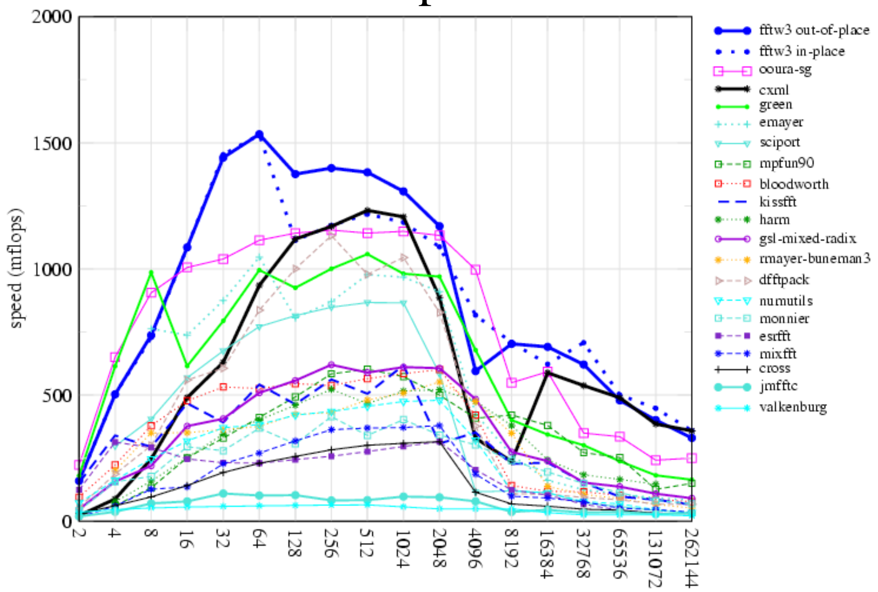
- Self-optimizes for your hardware (picks best composition of steps)
  = **portability + performance**

free software: `http://www.fftw.org/`

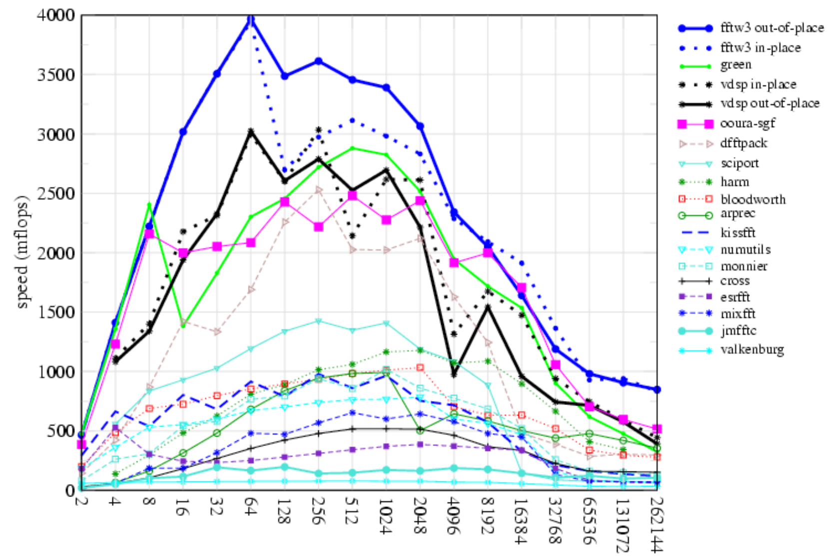
# FFTW performance

## power-of-two sizes, double precision

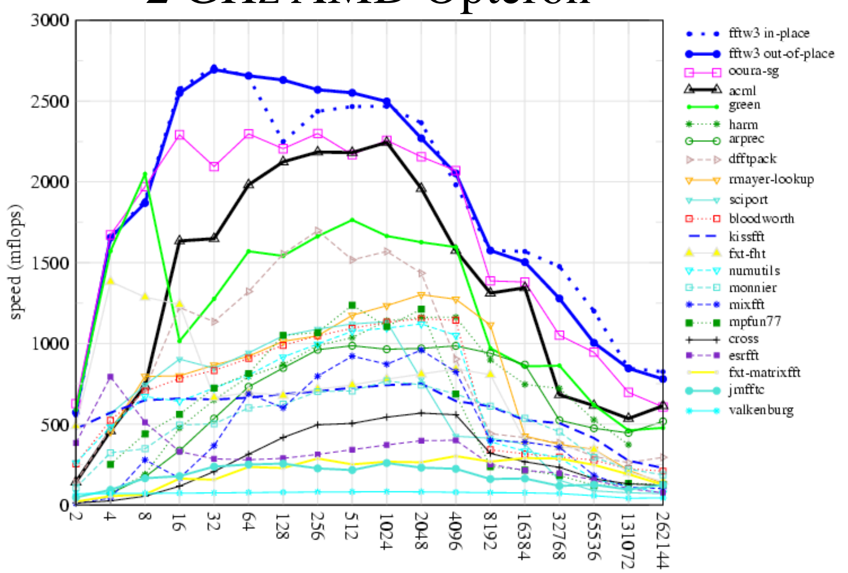
### 833 MHz Alpha EV6



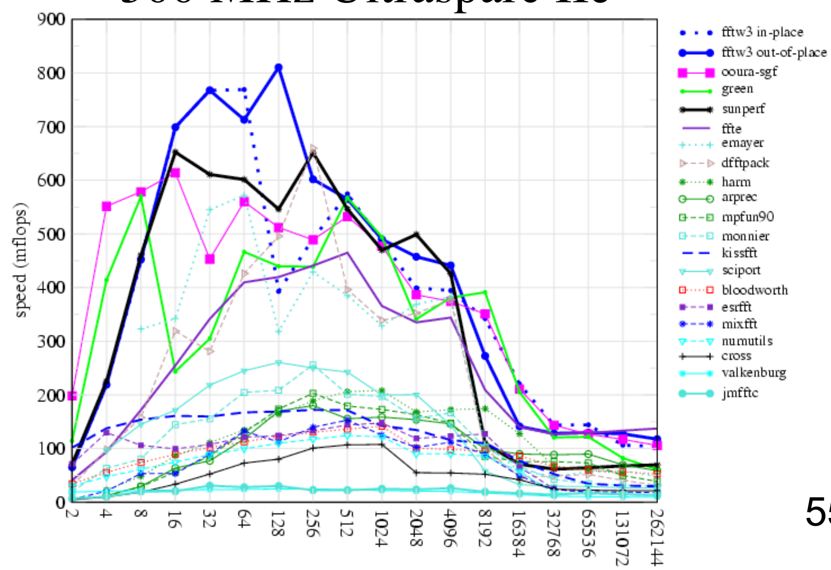

### 2 GHz PowerPC G5




### 2 GHz AMD Opteron




### 500 MHz Ultrasparc IIe

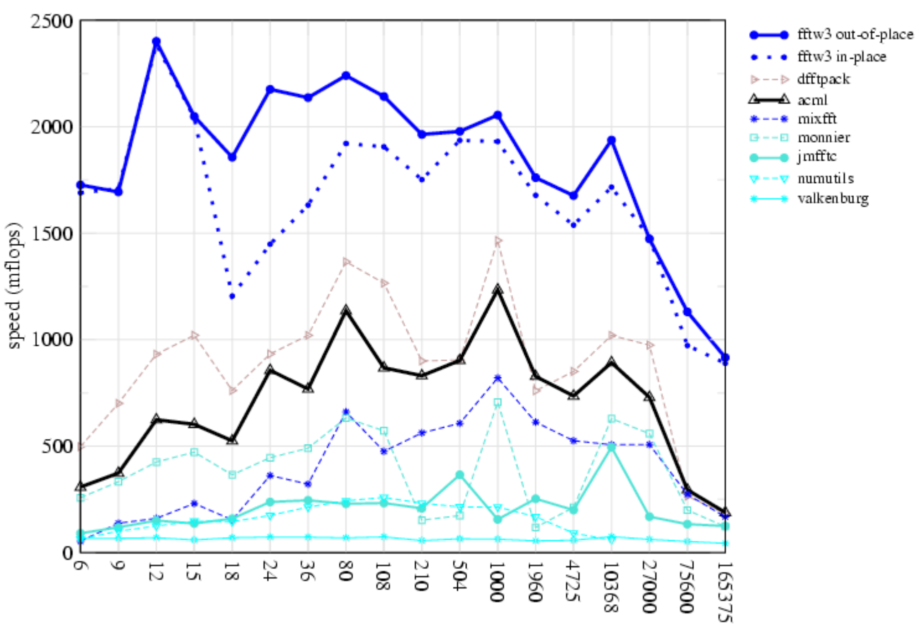


# FFTW performance

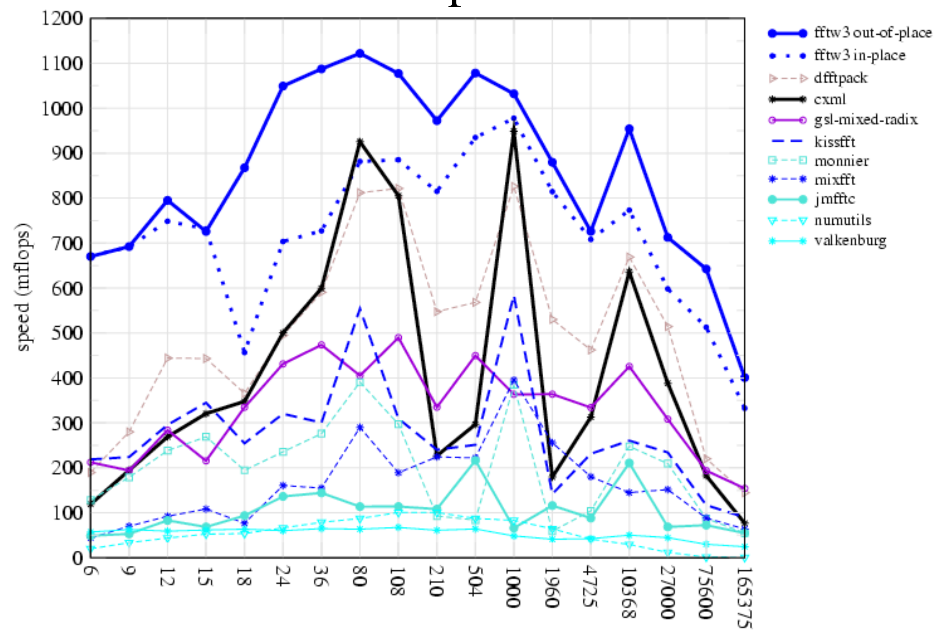
non-power-of-two sizes, double precision

unusual: non-power-of-two sizes receive as much optimization as powers of two

2 GHz AMD Opteron




833 MHz Alpha EV6

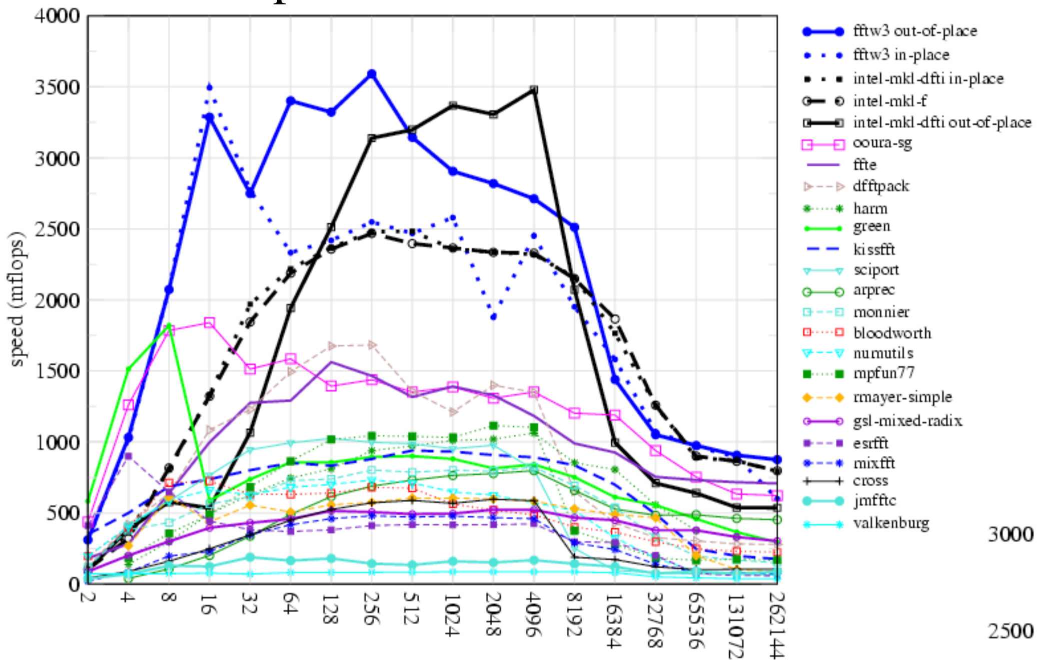



…because we let the code do the optimizing

# FFTW performance

**double precision, 2.8GHz Pentium IV: 2-way SIMD (SSE2)**

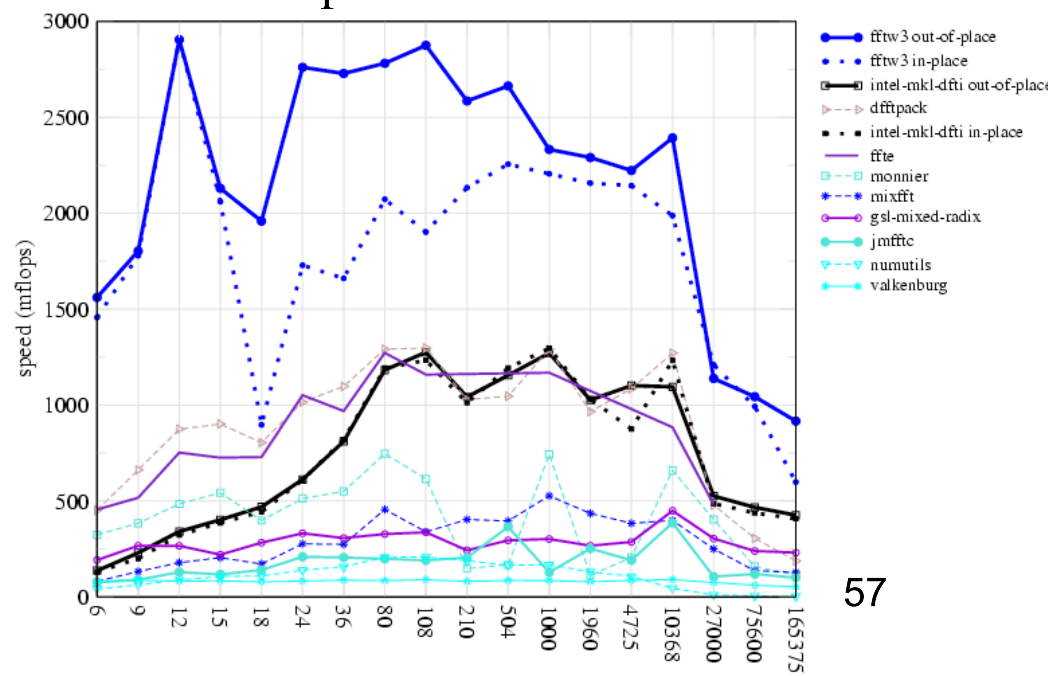
powers of two




exploiting CPU-specific SIMD instructions (rewriting the code) is easy

…because we let the code write itself

non-powers-of-two



# Why is FFTW fast?
## three unusual features

FFTW implements many FFT algorithms:
A planner picks the best composition
by measuring the speed of different combinations.

The resulting *plan* is executed
with explicit recursion:
enhances *locality*

The base cases of the recursion are codelets:
highly-optimized dense code
automatically generated by a special-purpose "compiler"

# FFTW is easy to use

```
{
      complex x[n];
      plan p;

      p = plan_dft_1d(n, x, x, FORWARD, MEASURE);
      ...
      execute(p); /* repeat as needed */
      ...
      destroy_plan(p);
}
```

Key fact: usually,
many transforms of same size
are required.

# Why is FFTW fast?

## three unusual features

3 FFTW implements many FFT algorithms:
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1 The resulting *plan* is executed
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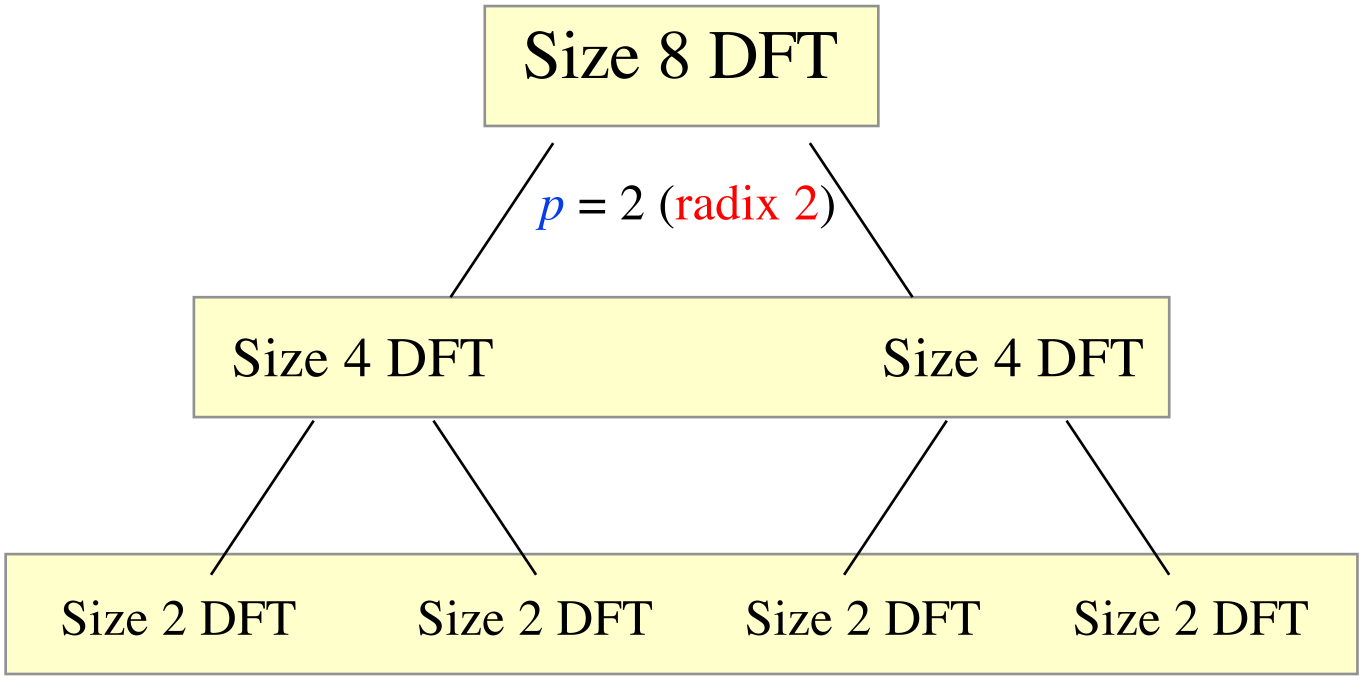
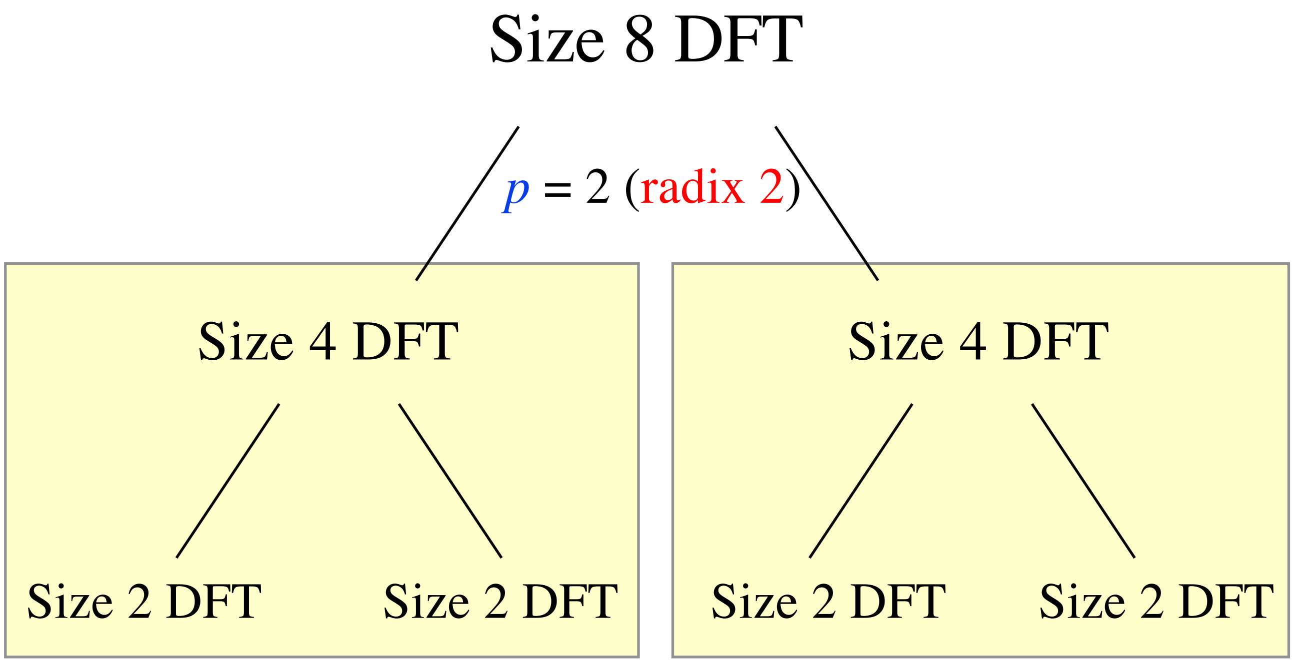
# FFTW Uses Natural Recursion




But traditional implementation is non-recursive, breadth-first traversal:

$\log_2 n$ passes over whole array

# Traditional cache solution: Blocking

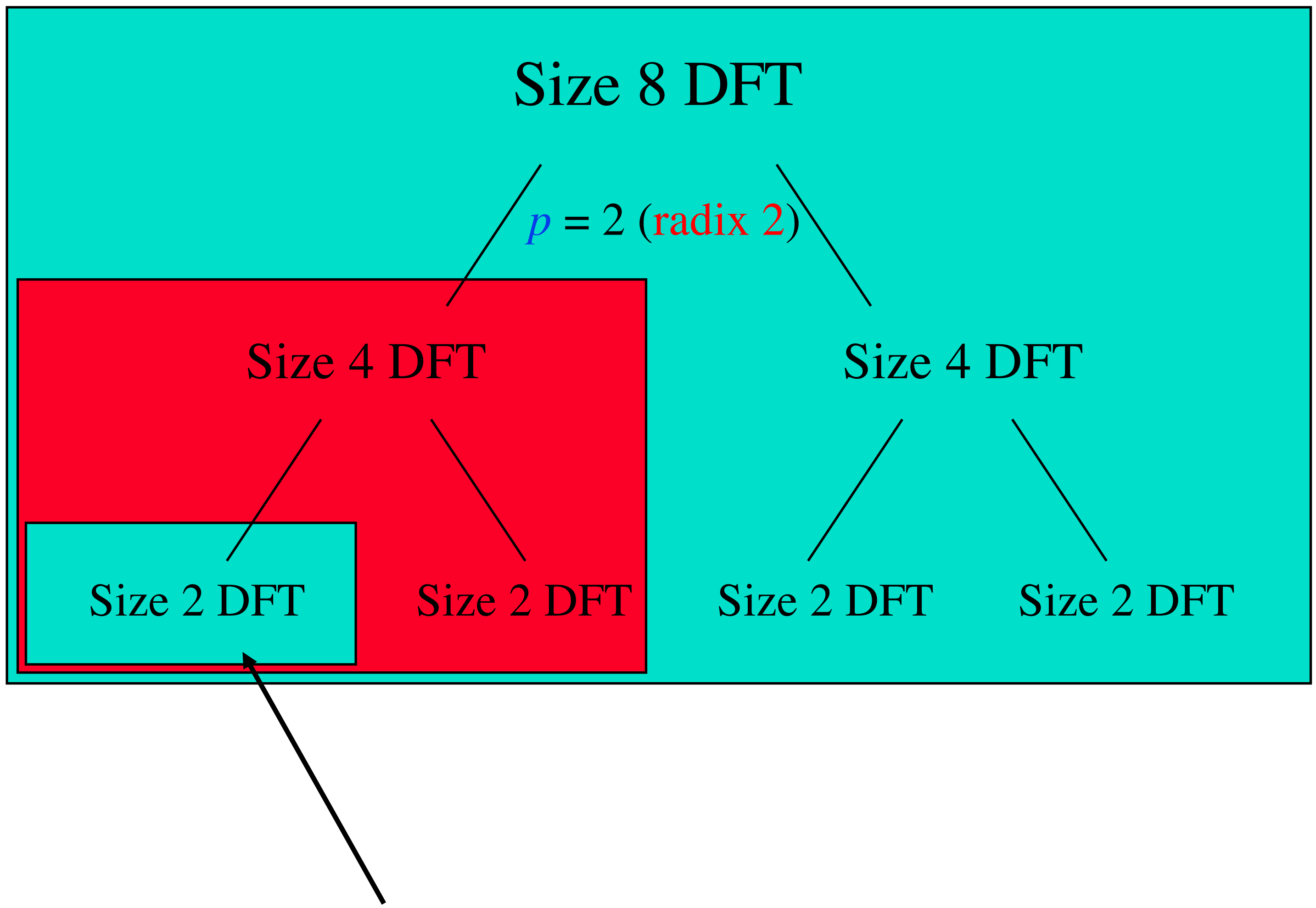



breadth-first, but with *blocks* of size = cache

…requires program specialized for cache size

# Recursive Divide & Conquer is Good

(depth-first traversal) [Singleton, 1967]




eventually small enough to fit in cache
…no matter what size the cache is

## Cache Obliviousness

- A cache-oblivious algorithm does not know the cache size
  — it can be optimal for any machine
  & for all levels of cache simultaneously

- Exist for many other algorithms, too [Frigo *et al*. 1999]
  — all via the recursive divide & conquer approach

## Why is FFTW fast?

### three unusual features

3 FFTW implements many FFT algorithms:
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1 The resulting *plan* is executed
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## Spiral

° Software/Hardware Generation for DSP Algorithms

° Autotuning not just for FFT, many other signal processing algorithms

° Autotuning not just for software implementation, hardware too

° More details at

  - www.spiral.net
  - On-line generators, papers available

# Motifs – so far this semester

The Motifs (formerly “Dwarfs”) from
“The Berkeley View” (Asanovic et al.)
**Motifs** form key computational patterns