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

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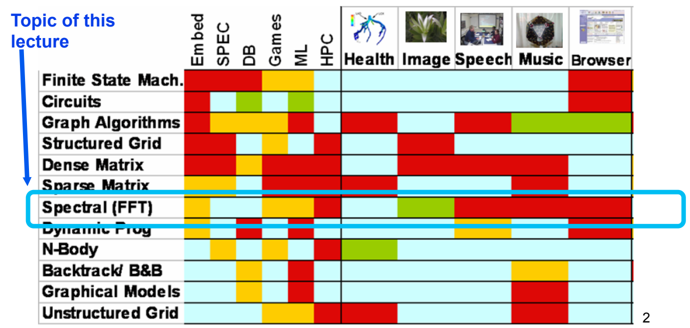
## Motifs

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



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## 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



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## 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:

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

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

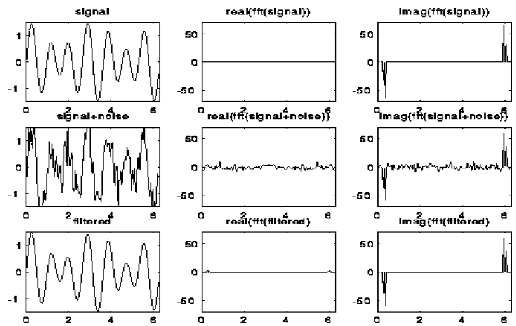
## Motivation for *Fast* Fourier Transform (FFT)

- 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
- …



## Using the 1D FFT for filtering

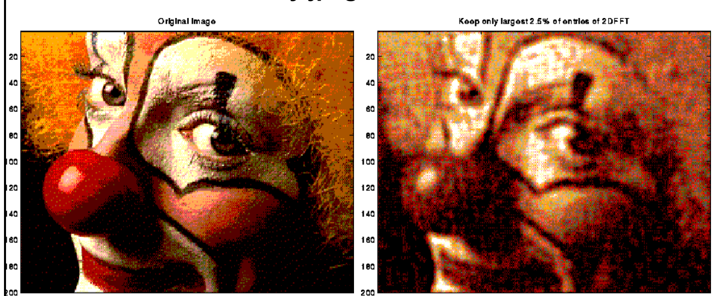
- Signal = sin(7t) + .5 sin(5t) at 128 points
- Noise = random number bounded by .75
- Filter by zeroing out FFT components < .25






## 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 $L_1 x = b$ where

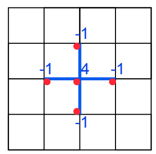
$$L_1 = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "stencil"


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

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

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

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



## Divide and Conquer FFT

- V can be evaluated using divide-and-conquer

$$V(x) = \sum_{k=0}^{m-1} x^k * v(k)$$
$$= v[0] + x^2*v[2] + x^4*v[4] + \dots$$
$$+ x*(v[1] + x^2*v[3] + x^4*v[5] + \dots)$$
$$= V_{even}(x^2) + x*V_{odd}(x^2)$$

- 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)

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

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

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

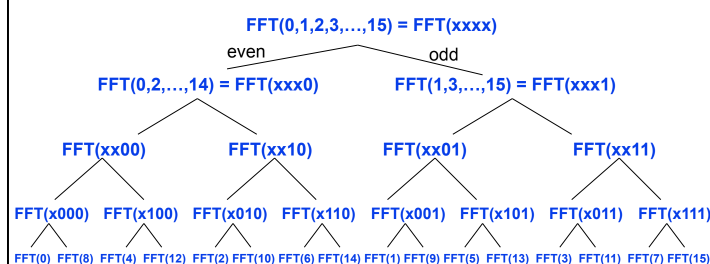
- Matlab notation: ".*" means component-wise multiply.

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

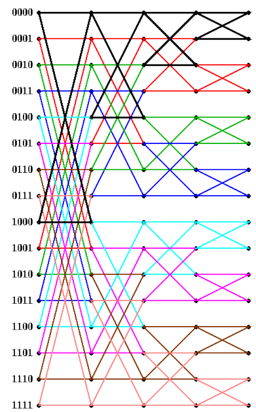



- An iterative algorithm that uses loops rather than recursion, does each level in the tree starting at the bottom
  - Algorithm overwrites v[i] by (F*v)[bitreverse(i)]
- Practical algorithms combine recursion (for memory hierarchy) and iteration (to avoid function call overhead) – more later

## 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

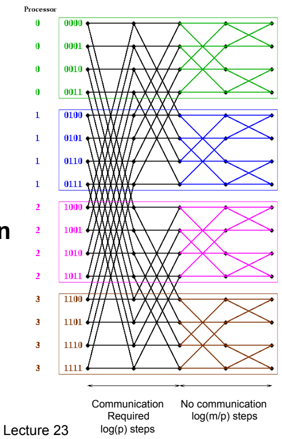





## Block Layout of 1D FFT

- 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

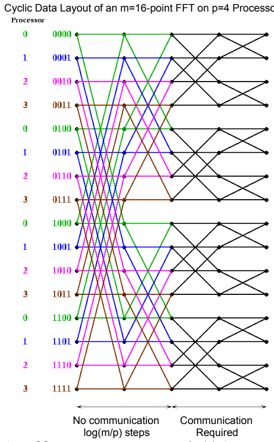





## Cyclic Layout of 1D FFT

- 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



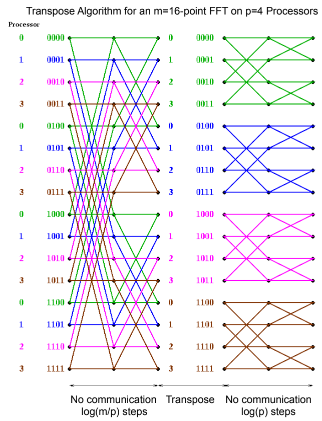



## Parallel Complexity

- 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”

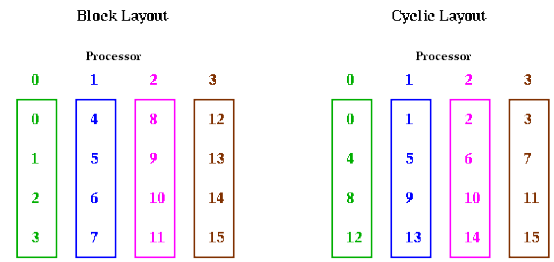
- If we start with a cyclic layout for first log(m/p) steps, there is no communication
- Then **transpose** the vector for last log(p) steps
- All communication is in the transpose
- Note: This example has log(m/p) = log(p)
  - If log(m/p) < log(p) more phases/layouts will be needed
  - We will assume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






## 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
- 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) ≥ log(p)
  - So 2 ≥ log(m) / log(m/p) ≥ 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

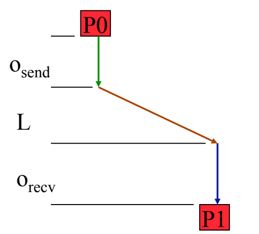


## Bisection Bandwidth

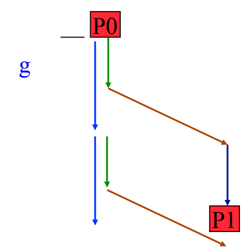
- FFT requires one (or more) transpose operations:
  - Every processor sends 1/p-th of its data to each other one
- Bisection Bandwidth limits this performance
  - Bisection bandwidth is the bandwidth across the narrowest part of the network
  - Important in global transpose operations, all-to-all, etc.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



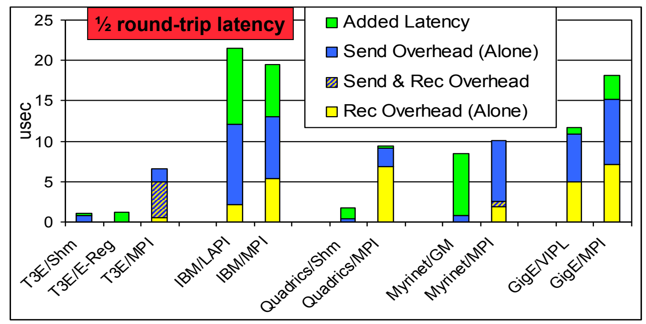

° **LogGP: with overlap**




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



## Historical Perspective




- 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 Communications System

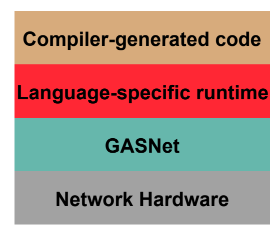
GASNet offers put/get communication

° 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**

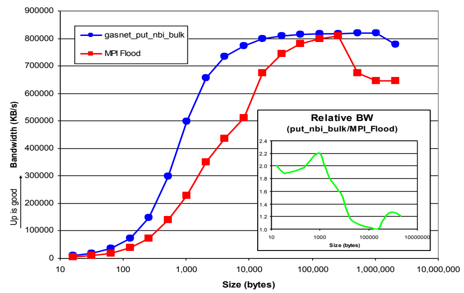
° Used in language runtimes (UPC, etc.)

° Fine-grained and bulk transfers

° Split-phase communication



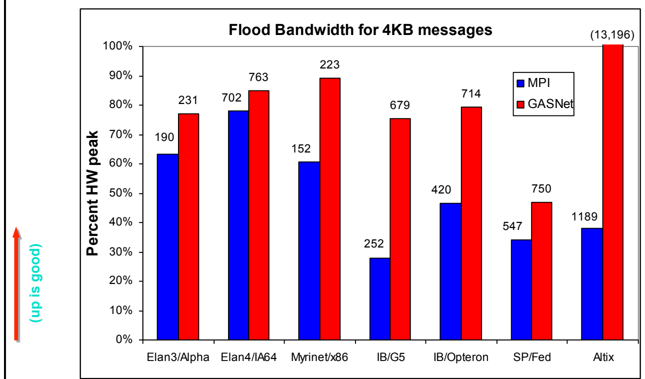
## Performance of 1-Sided vs 2-sided Communication: GASNet vs MPI




- 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



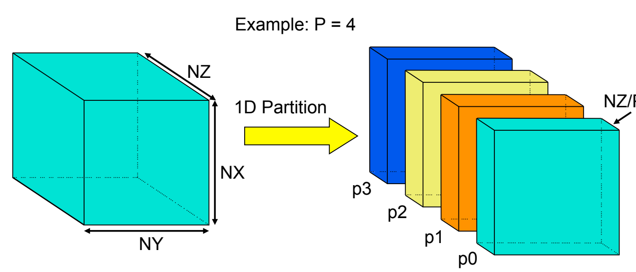
## NAS FT Benchmark Case Study

- 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)

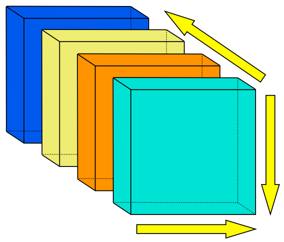
- NX x NY x NZ elements spread across P processors
- Will Use 1-Dimensional Layout in Z dimension
  - Each processor gets NZ / P "planes" of NX x NY elements per plane




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)

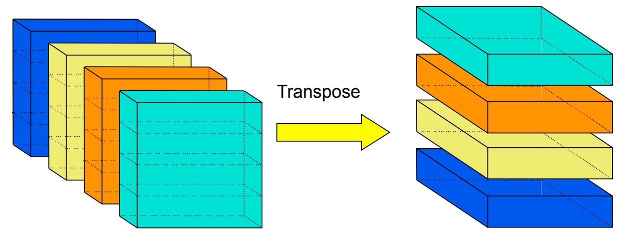
Step 3: FFTs in the Z-dimension
(requires communication)

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)
  2. Slabs
  3. Pencils
- 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

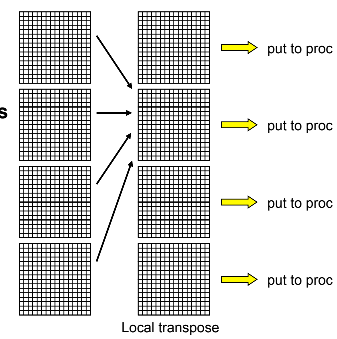
Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick



## 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

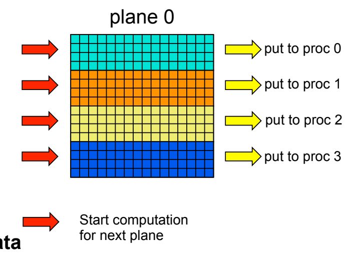
## Bandwidth Utilization

- NAS FT (Class D) with 256 processors on Opteron/InfiniBand
  - Each processor sends 256 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

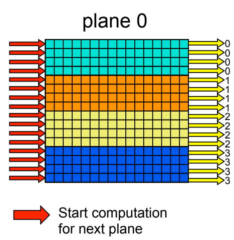



- For $512^3$ grid across 64 processors
  - Send 512-8 messages of 64kB each

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



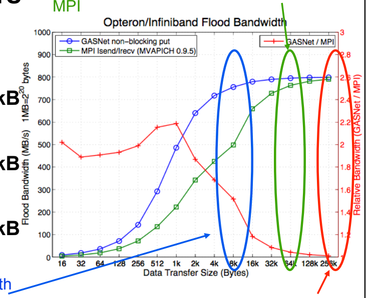

- For $512^3$ grid across 64 processors
  - Send 4096-64 messages of 8kB each

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

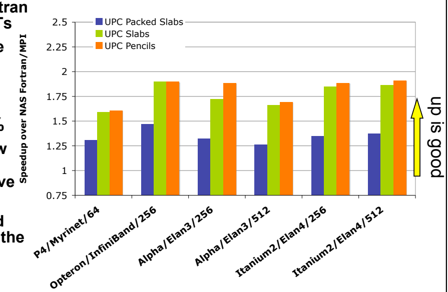
| Name | Processor | Network | Software |
|---|---|---|---|
| Opteron/Infiniband “Jacquard” @ NERSC | Dual 2.2 GHz Opteron (320 nodes @ 4GB/node) | Mellanox Cougar InfiniBand 4x HCA | Linux 2.6.5, Mellanox VAPI, MVAPICH 0.9.5, Pathscale CC/F77 2.0 |
| Alpha/Elan3 “Lemieux” @ PSC | Quad 1 GHz Alpha 21264 (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



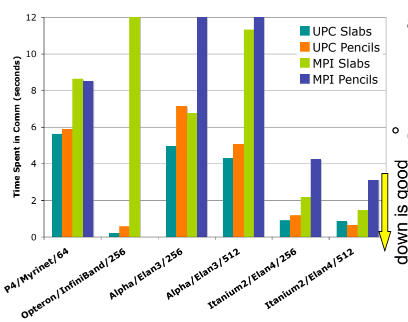
## Comparison of Algorithms

- 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




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

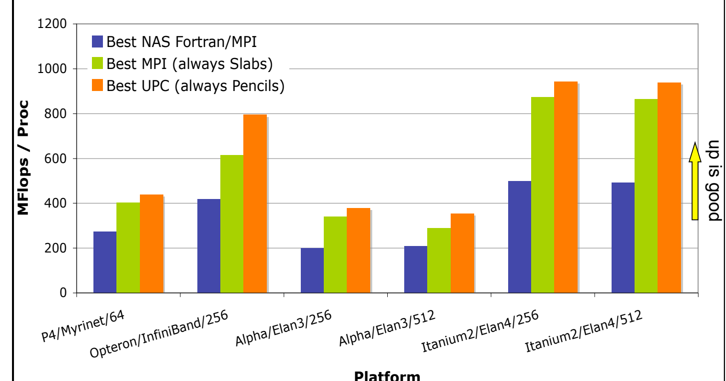
## Time Spent in Communication




- 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

## Performance Summary

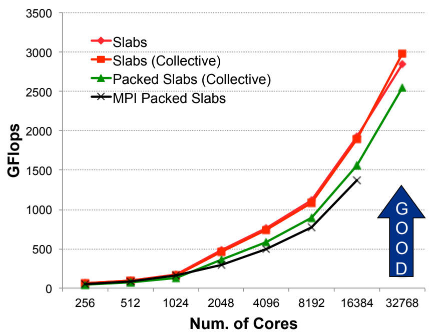



Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

## FFT Performance on BlueGene/P

- PGAS implementations consistently outperform MPI
- Leveraging communication/ computation overlap yields best performance
  - More collectives in flight and more communication leads to better performance
  - At 32k cores, overlap algorithms yield 17% improvement in overall application time
- Numbers are getting close to HPC record
  - Future work to try to beat the record

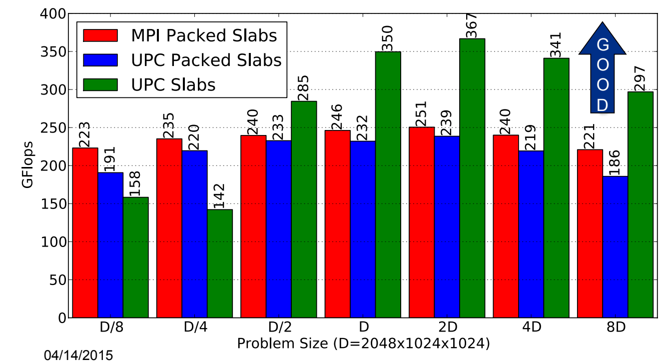
HPC Challenge Peak as of July 09 is ~4.5 Tflops on 128k Cores






## 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
- 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 3.3.4 (Mar 2014), includes threads, OpenMP
  - Added MPI versions in v3.3 Beta 1 (June 2011)
  - Layout constraints from users/apps + network differences are hard to support

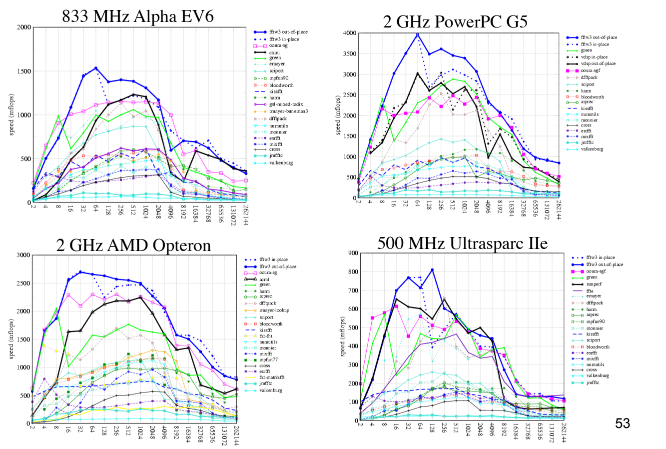


**FFTW** the "Fastest Fourier Tranform in the West"

- 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/`

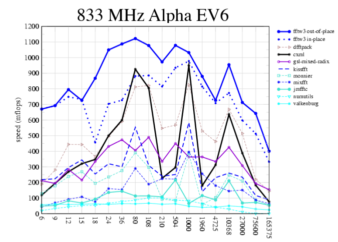
## FFTW performance
power-of-two sizes, double precision

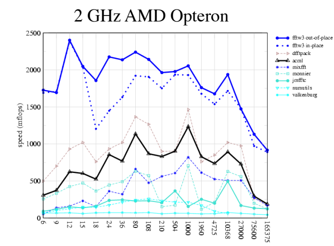





## FFTW performance
non-power-of-two sizes, double precision

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

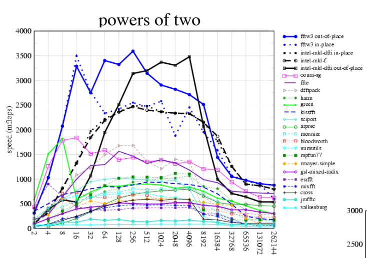


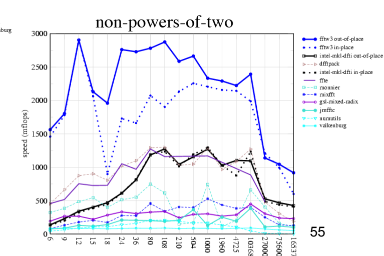

…because we
let the code do the optimizing



## FFTW performance
double precision, 2.8GHz Pentium IV: 2-way SIMD (SSE2)




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




…because we
let the code write itself



## 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

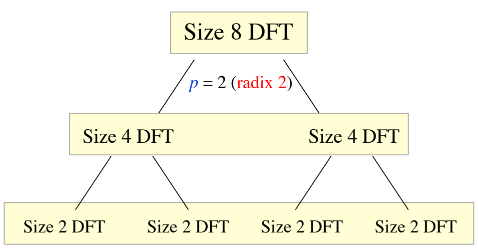
(3) FFTW implements many FFT algorithms: A planner picks the best composition by measuring the speed of different combinations.

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

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



## FFTW Uses Natural Recursion

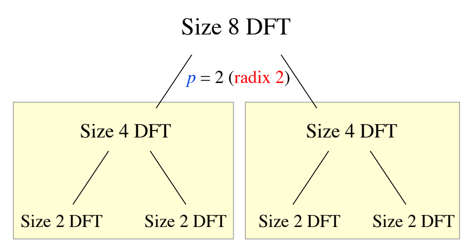



But traditional implementation is non-recursive, breadth-first traversal:

$\log_2 n$ passes over whole array



## Traditional cache solution: Blocking

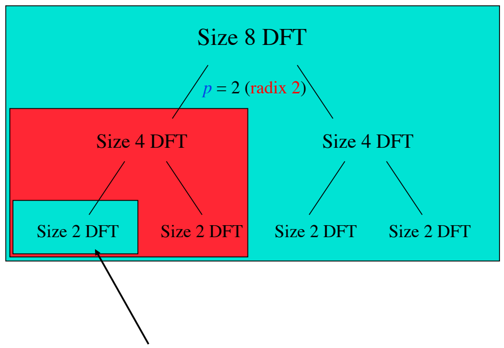



breadth-first, but with *blocks* of size = cache

…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:
A planner picks the best composition
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(1) The resulting *plan* is executed
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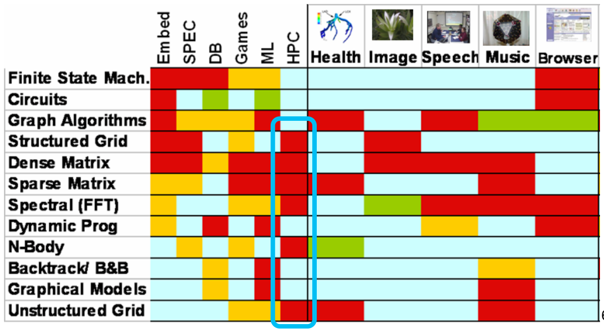
## Spiral

- **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






## Rest of the semester

- Computational Astrophysics (Julian Borrill, LBNL)
- Dynamic Load Balancing (TBD)
- Climate Modeling (Michael Wehner, LBNL)
- Computational Materials Science (Kristin Persson, LBNL)
- Future of Exascale Computing (Kathy Yelick, UCB & LBNL)