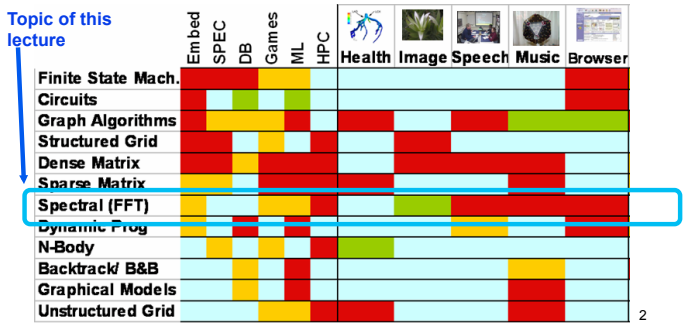
Parallel Spectral Methods: Fast Fourier Transform (FFTs) with Applications

James Demmel

www.cs.berkeley.edu/~demmel/cs267_Spr14

Motifs

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



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:

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

and where ω is:

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

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

° E.g., for m = 4: $\omega = i$, $\omega^2 = -1$, $\omega^3 = -i$, $\omega^4 = 1$

° 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

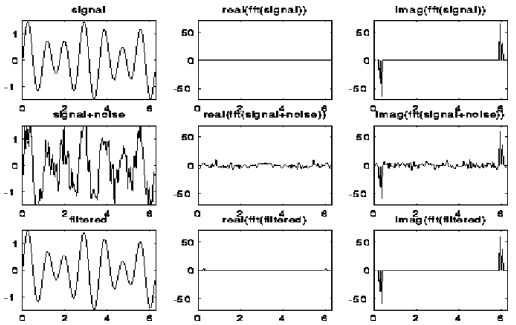
° Higher dimensional DFTs are analogous

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
- …

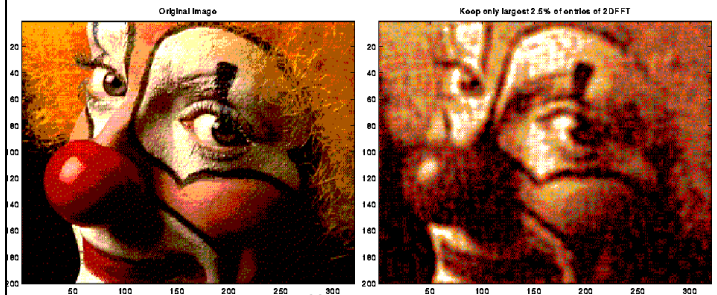
Using the 1D FFT for filtering

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

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)

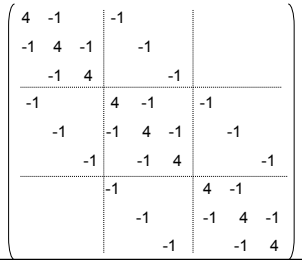
° 1D Poisson equation: solve $L_1 x = b$ where

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

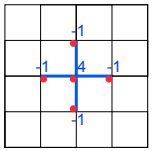
Graph and "stencil"

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

$L_2 =$



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

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

° 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, ϖ, m) … assume m is a power of 2

if m = 1 return v[0]

else

v_{even} = FFT(v[0:2:m-2], ϖ^2, m/2)

v_{odd} = FFT(v[1:2:m-1], ϖ^2, m/2)

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

return [v_{even} + (ϖ-vec .* v_{odd}),

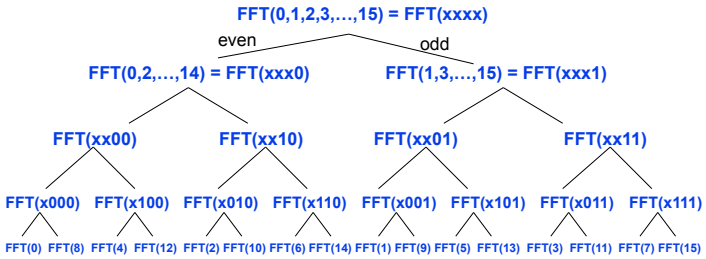
v_{even} - (ϖ-vec .* v_{odd})]

° 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

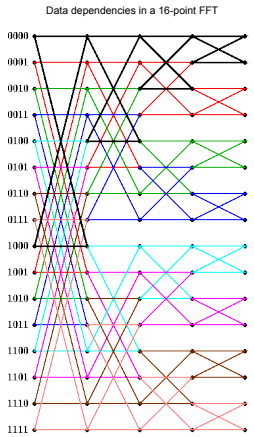
- Algorithm overwrites v[i] by (F*v)[bitreverse(i)]

° Practical algorithms combine recursion (for memory hierarchy) and iteration (to avoid function call overhead) – more later

16

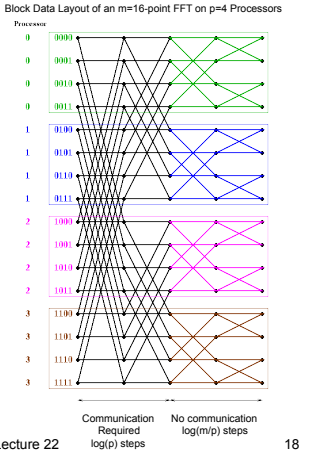
Parallel 1D FFT

° 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")



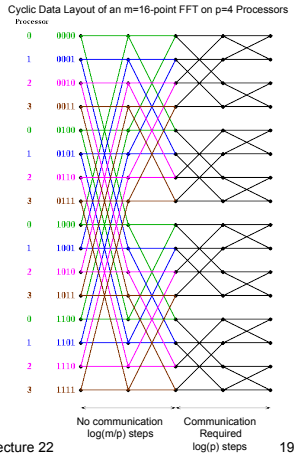
Block Layout of 1D FFT

° 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



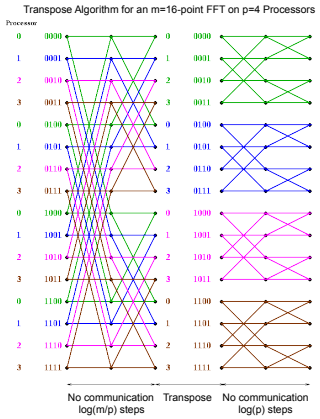
Parallel Complexity

° 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 … perfectly parallel flops
  + log(p) * α … 1 message/stage, log p stages
  + m*log(p)/p * β … m/p words/message

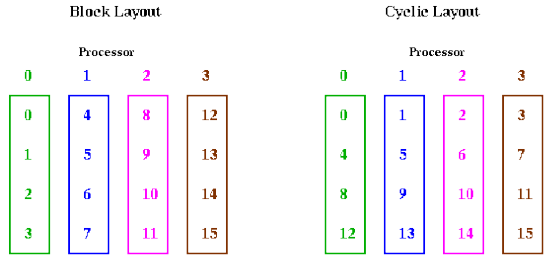
FFT With "Transpose"

- 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 work with this assumption 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 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?
- 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)

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.

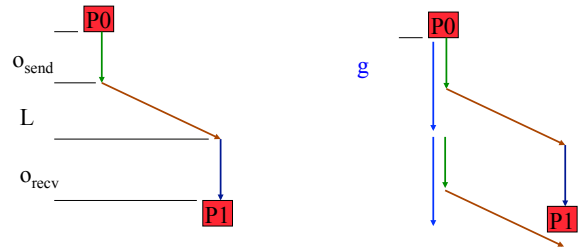
° "Full bisection bandwidth" is expensive
- Fraction of machine cost in the network is increasing
- Fat-tree and full crossbar topologies may be too expensive
- Especially on machines with 100K and more processors
- SMP clusters often limit bandwidth at the node level

° Goal: overlap communication and computation

Modified LogGP Model

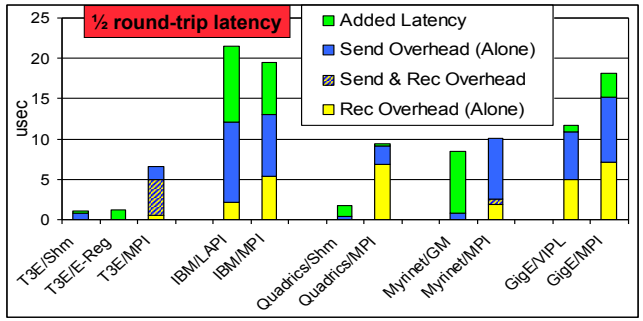
° LogGP: no overlap

° 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

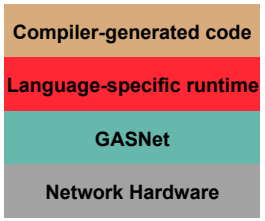
General Observations

- "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

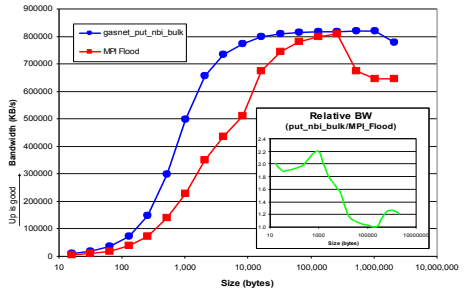
GASNet Communications System

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

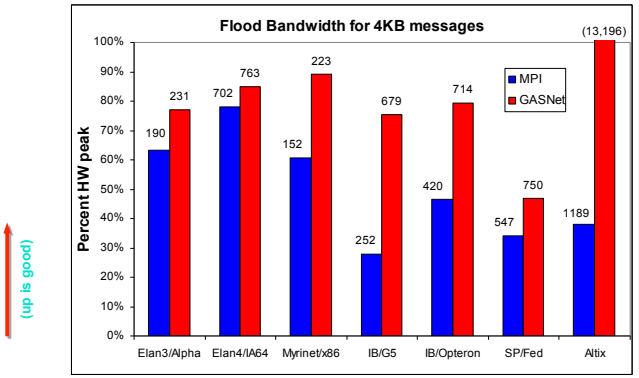


Performance of 1-Sided vs 2-sided Communication: GASNet vs MPI



- 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 applications total runtime

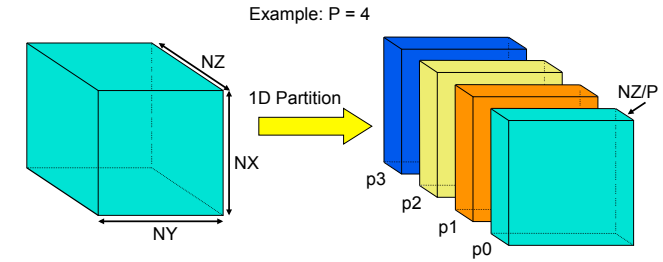
° **Assumptions**
- 1D partition of 3D grid
- At most N processors for N^3 grid
- HPC Challenge benchmark has large 1D FFT (can be viewed as 3D or more with proper roots of unity)

° **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

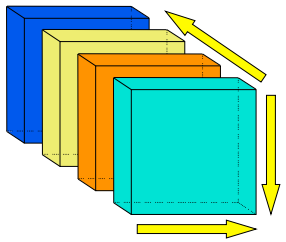


Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

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)

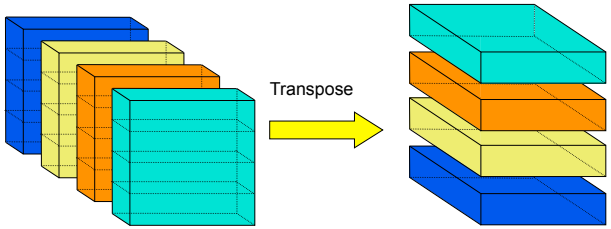
Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

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

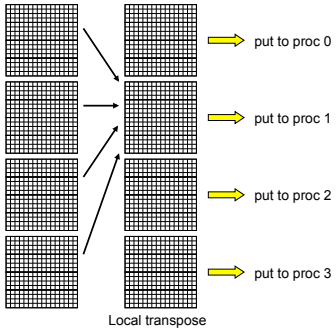
° Why do this? Slabs and Pencils allow overlapping communication and computation and leverage RDMA support in modern networks

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 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

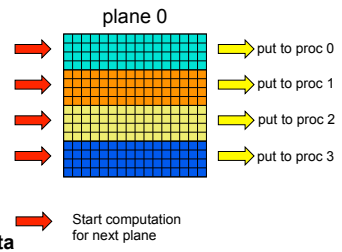
° **Waiting to send all data in one phase bunches up communication events**

° **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 messages of 64kB each

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

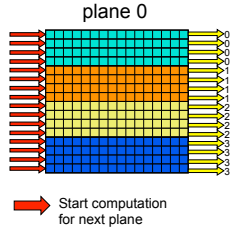
Algorithm 3: Pencils

° **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**



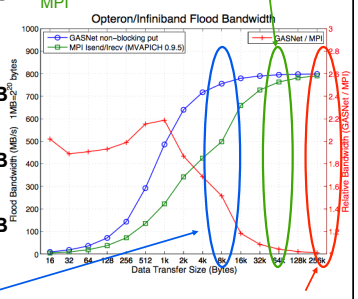
- For 512^3 grid across 64 processors
  - Send 4096 messages of 8kB each

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

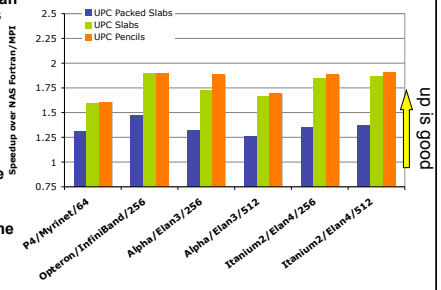
Platforms

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

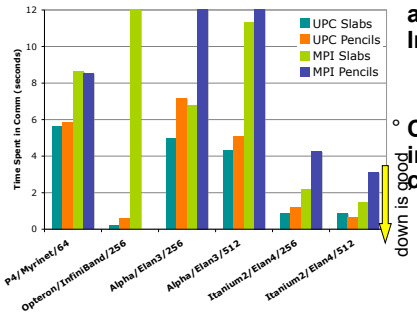
Comparison of Algorithms

- 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

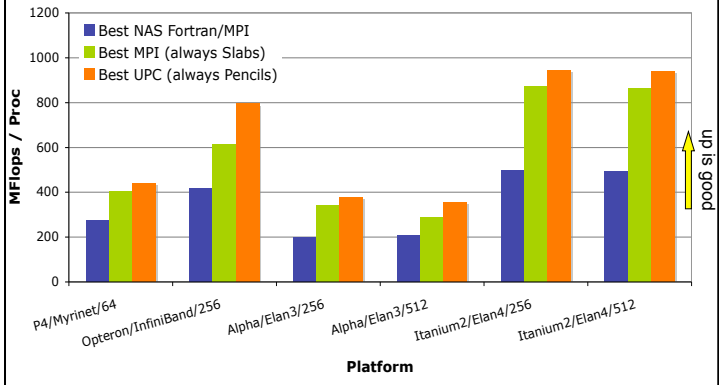
Time Spent in Communication



- 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

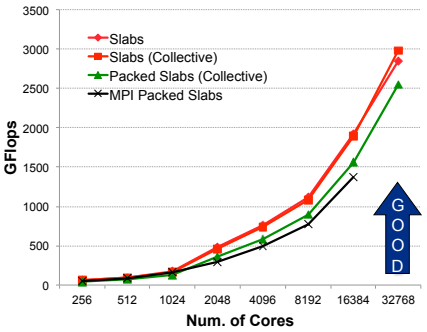


Source: R. Nishtala, C. Bell, D. Bonachea, K. Yelick

FFT Performance on BlueGene/P

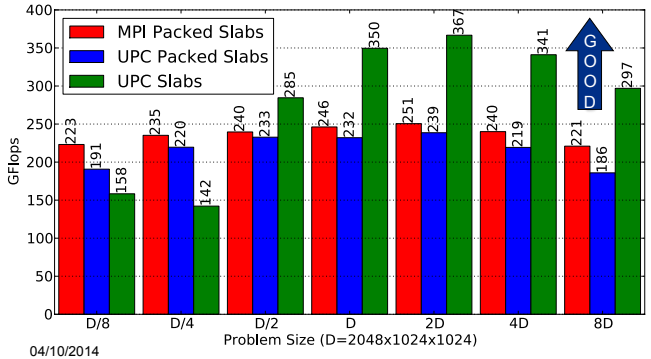
- PGAS implementations consistently outperform MPI
- Leveraging communication/ computation overlap yields best performance
  - More collectives in flight and more communication leads to better performance
  - At 32k cores, overlap algorithms yield 17% improvement in overall application time
- Numbers 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
- 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)

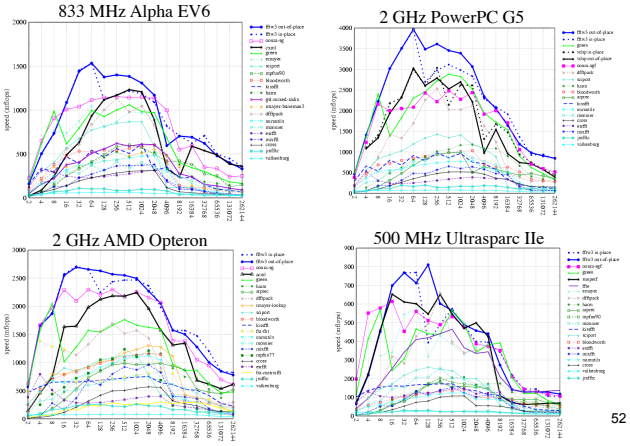
• Computational kernels (80% of code) automatically generated

• 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

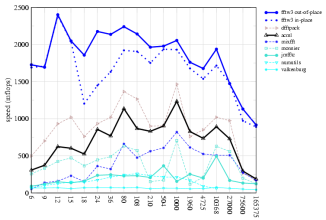


FFTW performance

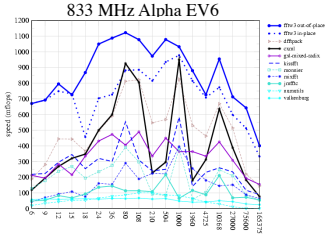
non-power-of-two sizes, double precision

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

2 GHz AMD Opteron



833 MHz Alpha EV6

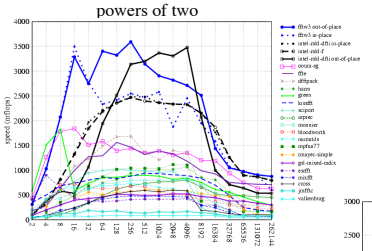


…because we let the code do the optimizing

FFTW performance

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

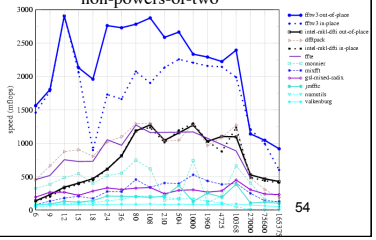
powers of two



…because we let the code write itself

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

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?

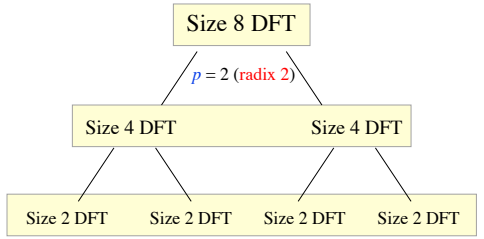
three unusual features

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

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

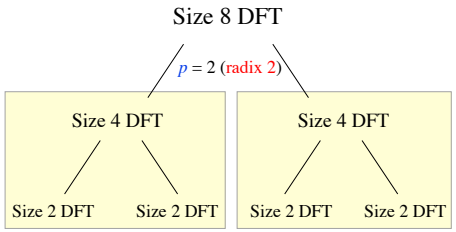
2. The base cases of the recursion are codelets:
   highly-optimized dense code
   automatically generated by a special-purpose "compiler"

FFTW Uses Natural Recursion



But traditional implementation is non-recursive,
breadth-first traversal:
$\log_2 n$ passes over whole array

Traditional cache solution: Blocking

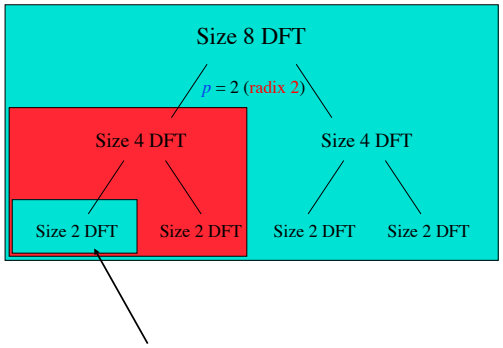


breadth-first, but with *blocks* of size = cache

…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
by measuring the speed of different combinations.

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

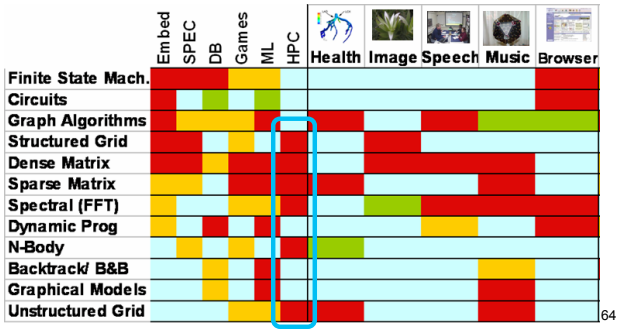
② The base cases of the recursion are codelets:
highly-optimized dense code
automatically generated by a special-purpose "compiler"

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



64

Rest of the semester

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

Extra slides