Sparse linear solvers: iterative methods, sparse matrix-vector multiplication, and preconditioning

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Plan

Krylov subspace methods
- Conjugate gradient method

Tuning sparse matrix-vector product
- Sequential performance optimization
- Tuning on multicore

Iterative solvers that reduce communication
- CA solvers based on s-step methods
- Enlarged Krylov methods

Preconditioners
- One level preconditioners: CA-ILU0
- Two level preconditioners

Extra slides: one level preconditioners
- One level preconditioners: examples

Plan

Krylov subspace methods
    Conjugate gradient method

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Krylov subspace methods

Solve $Ax = b$ by finding a sequence $x_1, x_2, ..., x_k$ that minimizes some measure of error over the corresponding spaces

$$x_0 + \mathcal{K}_i(A, r_0), \quad i = 1, ..., k$$

.

They are defined by two conditions:

1. Subspace condition: $x_k \in x_0 + \mathcal{K}_k(A, r_0)$
2. Petrov-Galerkin condition: $r_k \perp \mathscr{L}_k$

$$\iff (r_k)^t y = 0, \quad \forall \quad y \in \mathscr{L}_k$$

where

- x_0 is the initial iterate, r_0 is the initial residual,
- $\mathcal{K}_k(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^{k-1} r_0\}$ is the Krylov subspace of dimension k,
- $\mathscr{L}_k$ is a well-defined subspace of dimension k.

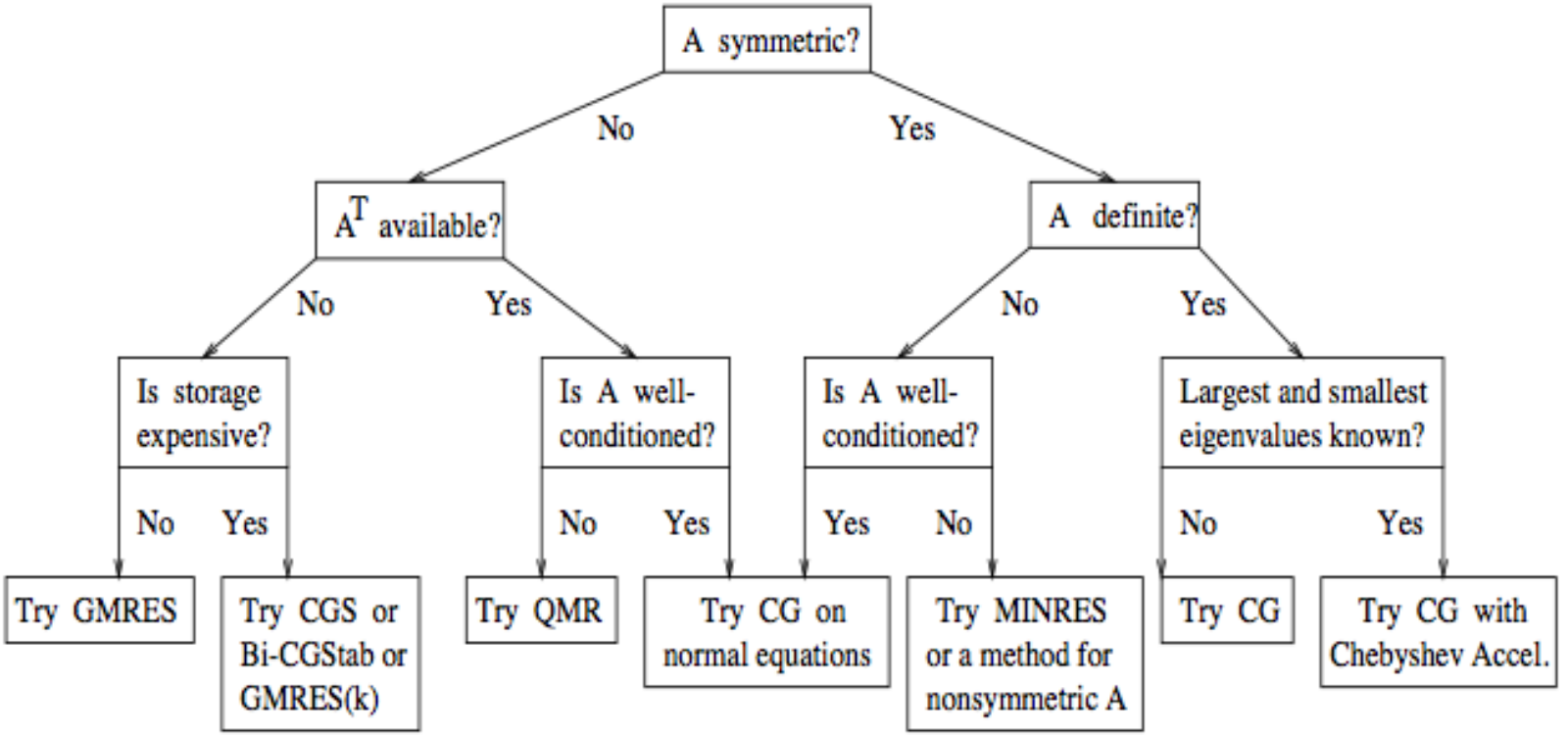
One of Top Ten Algorithms of the 20th Century

From SIAM News, Volume 33, Number 4:
Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of Krylov subspace iteration methods.

- Russian mathematician Alexei Krylov writes first paper, 1931.
- Lanczos - introduced an algorithm to generate an orthogonal basis for such a subspace when the matrix is symmetric.
- Hestenes and Stiefel - introduced CG for SPD matrices.

Other Top Ten Algorithms: Monte Carlo method, decompositional approach to matrix computations (Householder), Quicksort, Fast multipole, FFT.

Choosing a Krylov method



All methods (GMRES, CGS,CG…) depend on SpMV (or variations…)

See www.netlib.org/templates/Templates.html for details

Source slide: J. Demmel

Conjugate gradient (Hestenes, Stieffel, 52)

- A Krylov projection method for SPD matrices where $\mathscr{L}_k = \mathcal{K}_k(A, r_0)$.
- Finds $x^* = A^{-1}b$ by minimizing the quadratic function

$$\begin{aligned} \phi(x) &= \frac{1}{2}(x)^t Ax - b^t x \\ \bigtriangledown\phi(x) &= Ax - b = 0 \end{aligned}$$

- After j iterations of CG,

$$||x^* - x_j||_A \leq 2||x - x_0||_A \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^j,$$

where x_0 is starting vector, $||x||_A = \sqrt{x^T Ax}$ and $\kappa(A) = |\lambda_{max}(A)|/|\lambda_{min}(A)|$.

Conjugate gradient

- Computes A-orthogonal search directions by conjugation of the residuals

$$\left\{ \begin{array}{lcl} p_1 & = & r_0 = - \bigtriangledown \phi(x_0) \\ p_k & = & r_{k-1} + \beta_k p_{k-1} \end{array} \right. \tag{1}$$

- At k-th iteration,

$$x_k = x_{k-1} + \alpha_k p_k = argmin_{x \in x_0 + \mathcal{K}_k(A, r_0)} \phi(x)$$

where α_k is the step along p_k.

- CG algorithm obtained by imposing the orthogonality and the conjugacy conditions

$$\begin{array}{rcl} r_k^T r_i & = & 0, \text{for all } i \neq k, \\ p_k^T A p_i & = & 0, \text{for all } i \neq k. \end{array}$$

CG algorithm

Algorithm 1 The CG Algorithm

1: $r_0 = b - Ax_0$, $\rho_0 = ||r_0||_2^2$, $p_1 = r_0$, $k = 1$
2: **while** ($\sqrt{\rho_k} > \epsilon||b||_2$ and $k < k_{max}$) **do**
3: **if** $(k \neq 1)$ **then**
4: $\beta_k = (r_{k-1}, r_{k-1})/(r_{k-2}, r_{k-2})$
5: $p_k = r_{k-1} + \beta_k p_{k-1}$
6: **end if**
7: $\alpha_k = (r_{k-1}, r_{k-1})/(Ap_k, p_k)$
8: $x_k = x_{k-1} + \alpha_k p_k$
9: $r_k = r_{k-1} - \alpha_k Ap_k$
10: $\rho_k = ||r_k||_2^2$
11: $k = k + 1$
12: **end while**

Challenge in getting efficient and scalable solvers

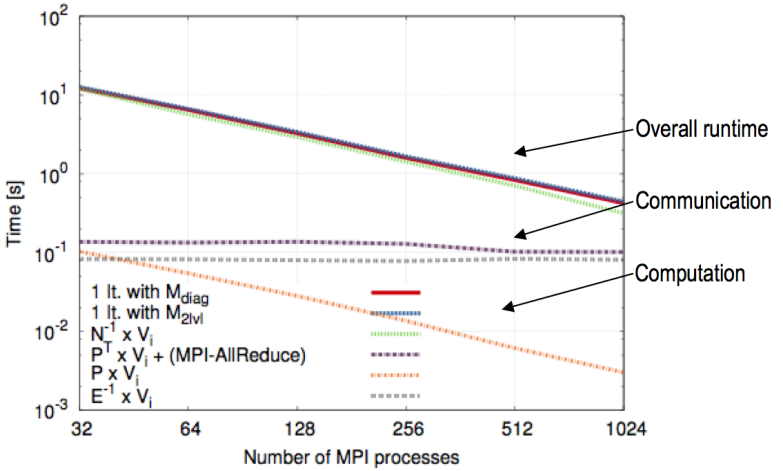
- A Krylov solver finds x_{k+1} from $x_0 + \mathcal{K}_{k+1}(A, r_0)$ where

$$\mathcal{K}_{k+1}(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^k r_0\},$$

  such that the Petrov-Galerkin condition $b - Ax_{k+1} \perp \mathscr{L}_{k+1}$ is satisfied.
- Does a sequence of k SpMVs to get vectors $[x_1, ..., x_k]$
- Finds best solution x_{k+1} as linear combination of $[x_1, ..., x_k]$

Typically, each iteration requires

- Sparse matrix vector product
  $\rightarrow$ point-to-point communication
- Dot products for orthogonalization
  $\rightarrow$ global communication



Map making, with R. Stompor, M. Szydlarski
Results obtained on Hopper, Cray XE6, NERSC

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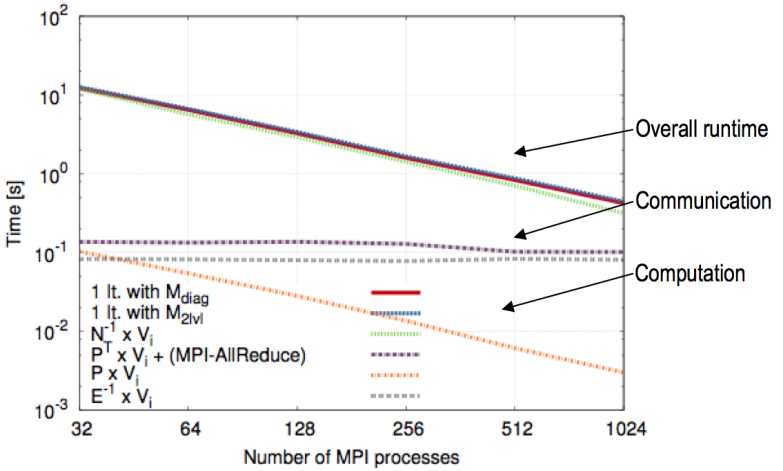

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Ways to improve performance

We will look at three different approaches:

- Improve the performance of sparse matrix-vector product.
- Change numerics - reformulate or introduce Krylov subspace algorithms to:
  - reduce communication,
  - increase arithmetic intensity - compute sparse matrix-set of vectors product.
- Use preconditioners to decrease the number of iterations till convergence.

Plan

Krylov subspace methods

Tuning sparse matrix-vector product
- Sequential performance optimization
- Tuning on multicore

Iterative solvers that reduce communication

Preconditioners

Extra slides: one level preconditioners

Tuning sparse matrix-vector product

- Slides from J. Demmel, lecture on *Automatic Performance Tuning and Sparse-Matrix-Vector-Multiplication (SpMV)*
  `www.cs.berkeley.edu/~demmel/cs267_Spr14`
- Sequential performance optimization
- Tuning SpMV on multicores
- Most of the techniques discussed are available in **OSKI** and **pOSKI**: Optimized Sparse Kernel Interface
  `bebop.cs.berkeley.edu/poski`
  - Provides sparse kernels automatically tuned for user's matrix & machine.

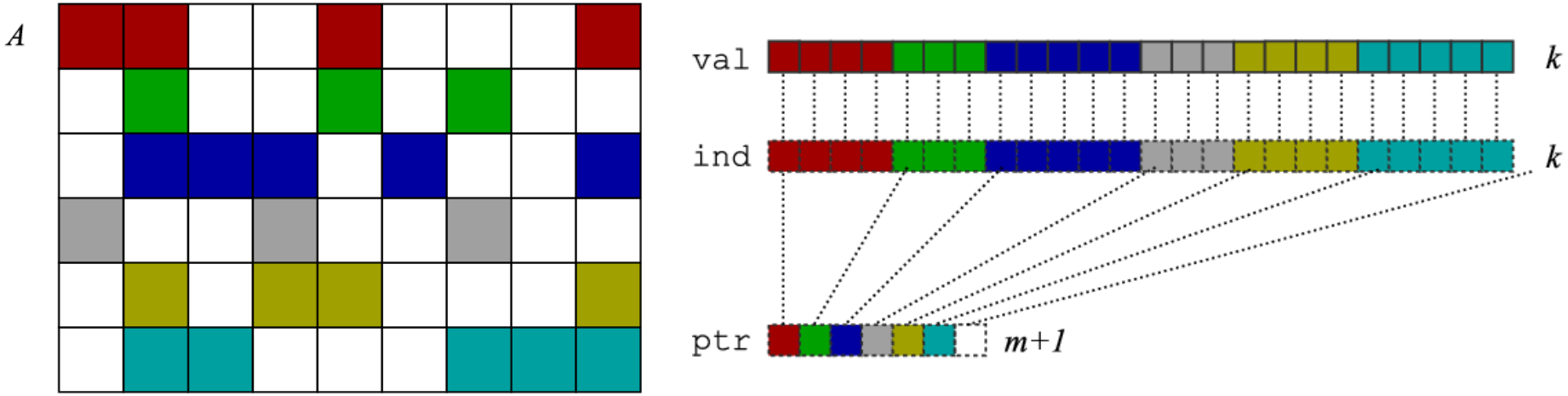
Examples of Automatic Performance Tuning (1)

- Dense BLAS (PHiPAC-UCB, then ATLAS-UTK), FFTs (FFTw – MIT), signal processing(SPIRAL - CMU), MPI reductions
- What do they have in common?
  - Can do the tuning **off-line**: once per architecture, algorithm
  - Can take as much time as necessary (hours, a week…)
  - At run-time, algorithm choice may depend only on few parameters
    - Matrix dimension, size of FFT, etc.

Examples of Automatic Performance Tuning (2)

- What do dense BLAS, FFTs, signal processing, MPI reductions have in common?
  - Can do the tuning **off-line**: once per architecture, algorithm
  - Can take as much time as necessary (hours, a week…)
  - At run-time, algorithm choice may depend only on few parameters
    - Matrix dimension, size of FFT, etc.
- **Can't always do off-line tuning**
  - **Algorithm and implementation may strongly depend on data only known at run-time**
  - **Ex: Sparse matrix nonzero pattern determines both best data structure and implementation of Sparse-matrix-vector-multiplication (SpMV)**
  - **Part of search for best algorithm just be done (very quickly!) at run-time**

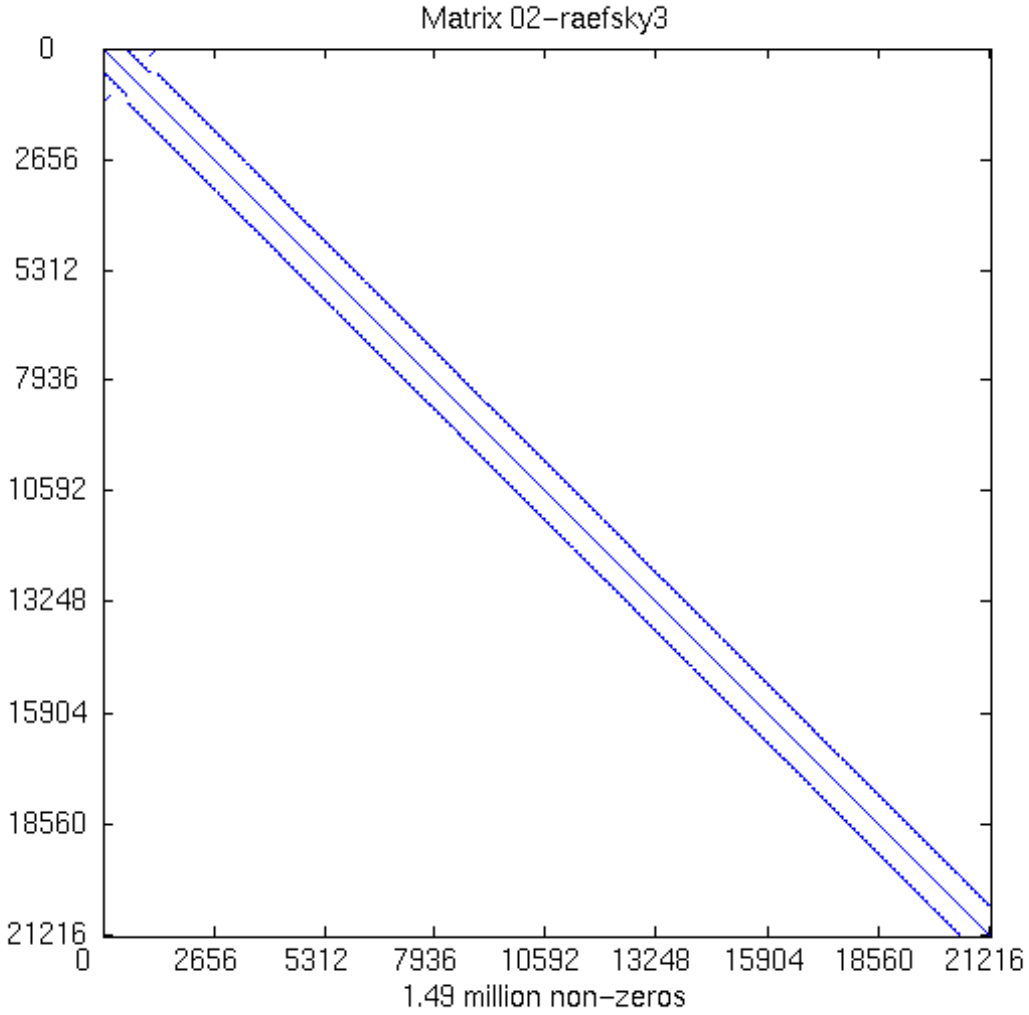
SpMV with Compressed Sparse Row (CSR) Storage



Matrix-vector multiply kernel: y(i) ← y(i) + A(i,j)*x(j)

```
for each row i
   for k=ptr[i] to ptr[i+1]-1 do
       y[i] = y[i] + val[k]*x[ind[k]]
```

Example: The Difficulty of Tuning



- n = 21200
- nnz = 1.5 M
- kernel: SpMV

- Source:

  FEM discretization

  NASA structural analysis problem

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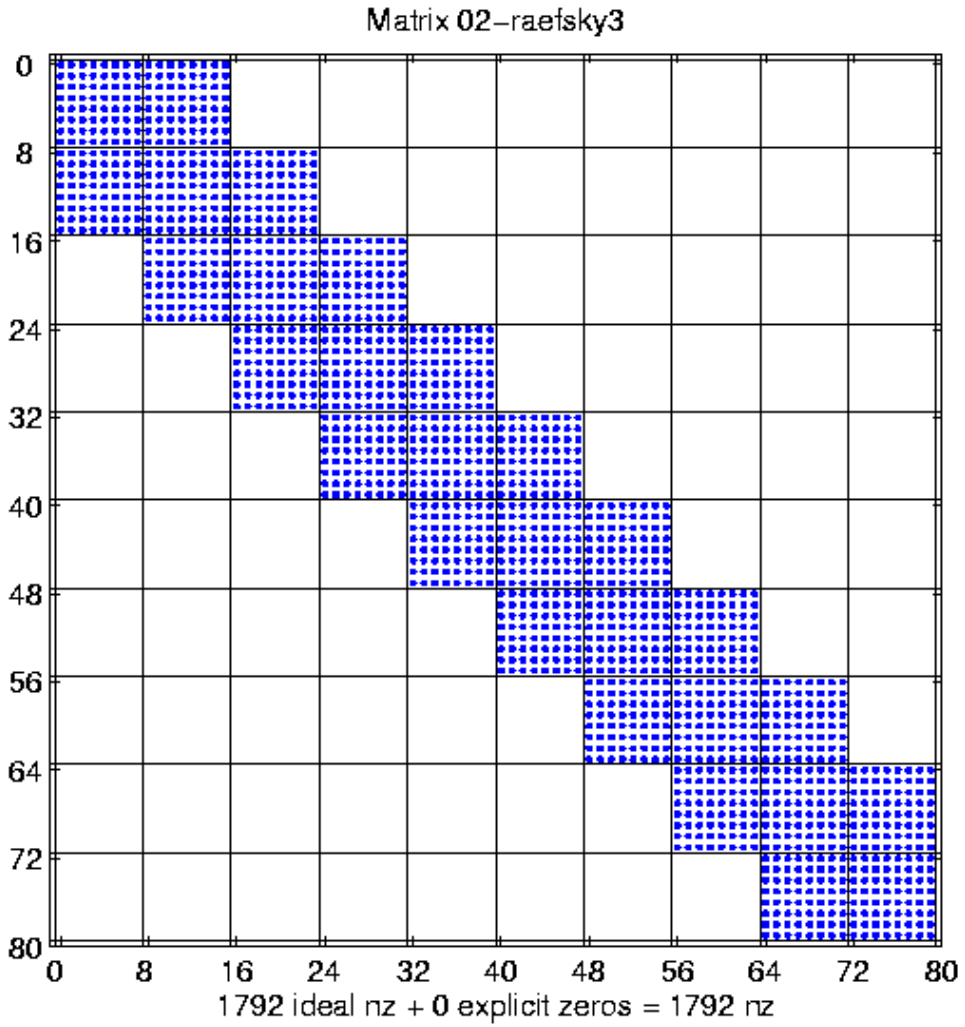


- n = 21200
- nnz = 1.5 M
- kernel: SpMV

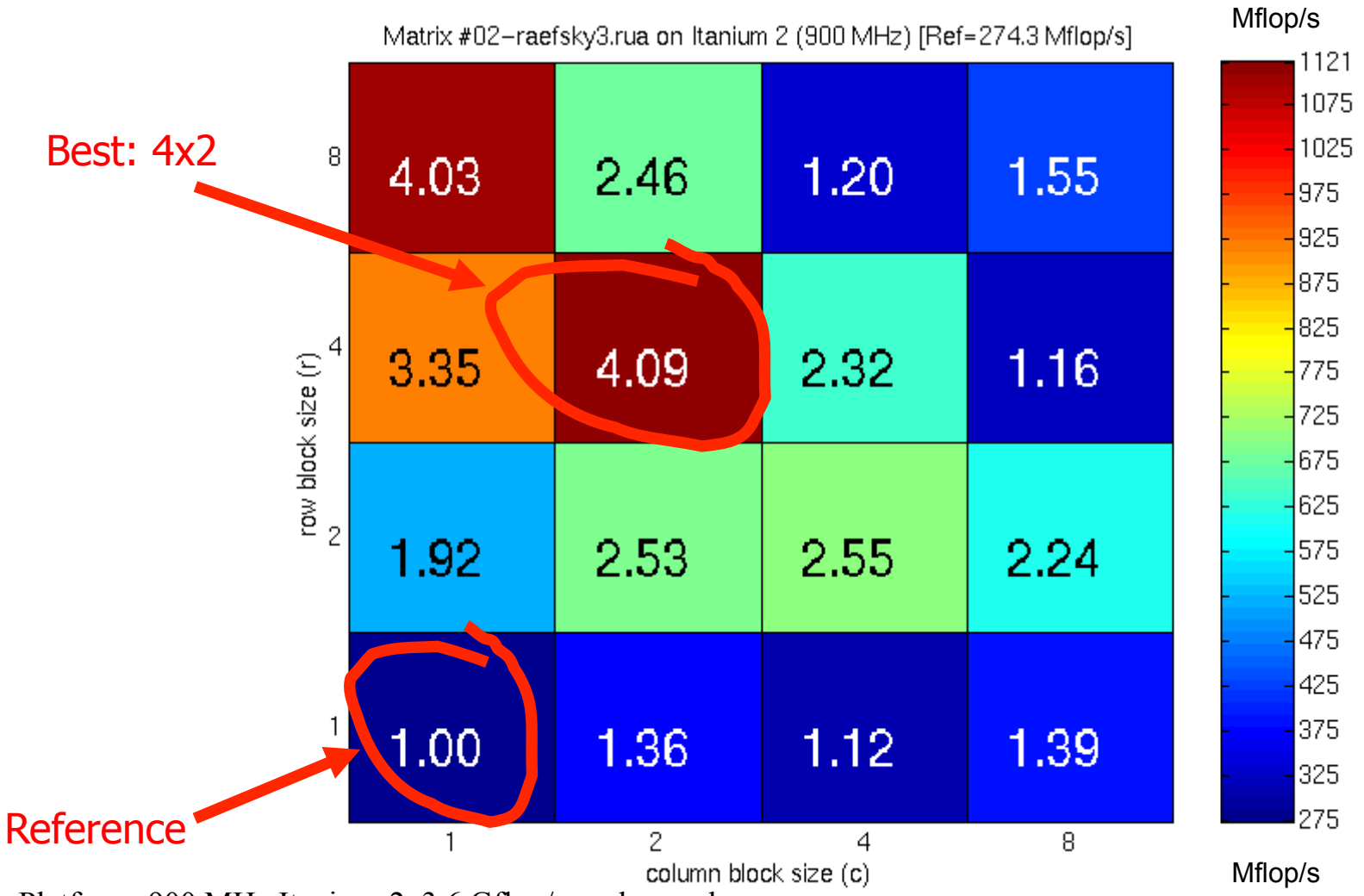
- Source: NASA structural analysis problem

- **8x8** dense substructure

Taking advantage of block structure in SpMV

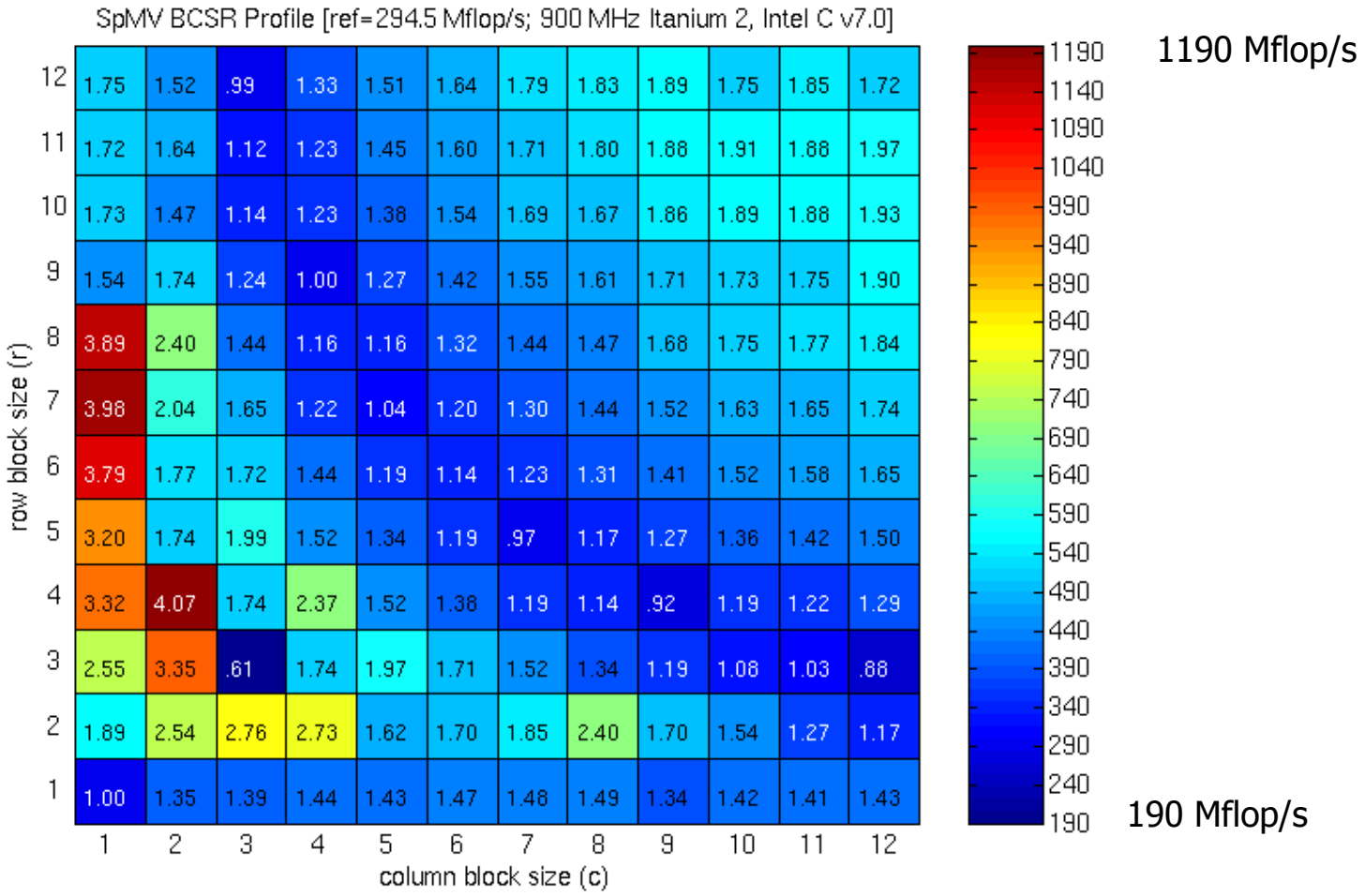
- Bottleneck is time to get matrix from memory
  - Only 2 flops for each nonzero in matrix
- Don't store each nonzero with index, instead store each nonzero r-by-c block with index
  - Storage drops by up to 2x, if rc >> 1, all 32-bit quantities
  - Time to fetch matrix from memory decreases
- Change both data structure and algorithm
  - Need to pick r and c
  - Need to change algorithm accordingly
- In example, is r=c=8 best choice?
  - Minimizes storage, so looks like a good idea…

Speedups on Itanium 2: The Need for Search



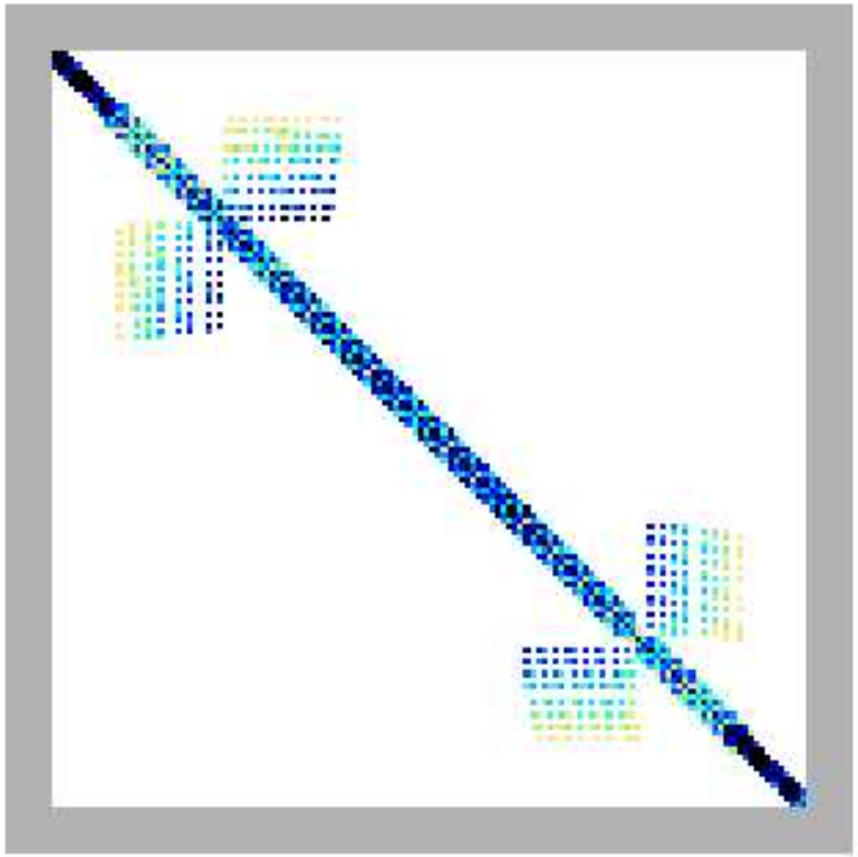
Platform: 900 MHz Itanium-2, 3.6 Gflop/s peak speed.

Register Profile: Itanium 2



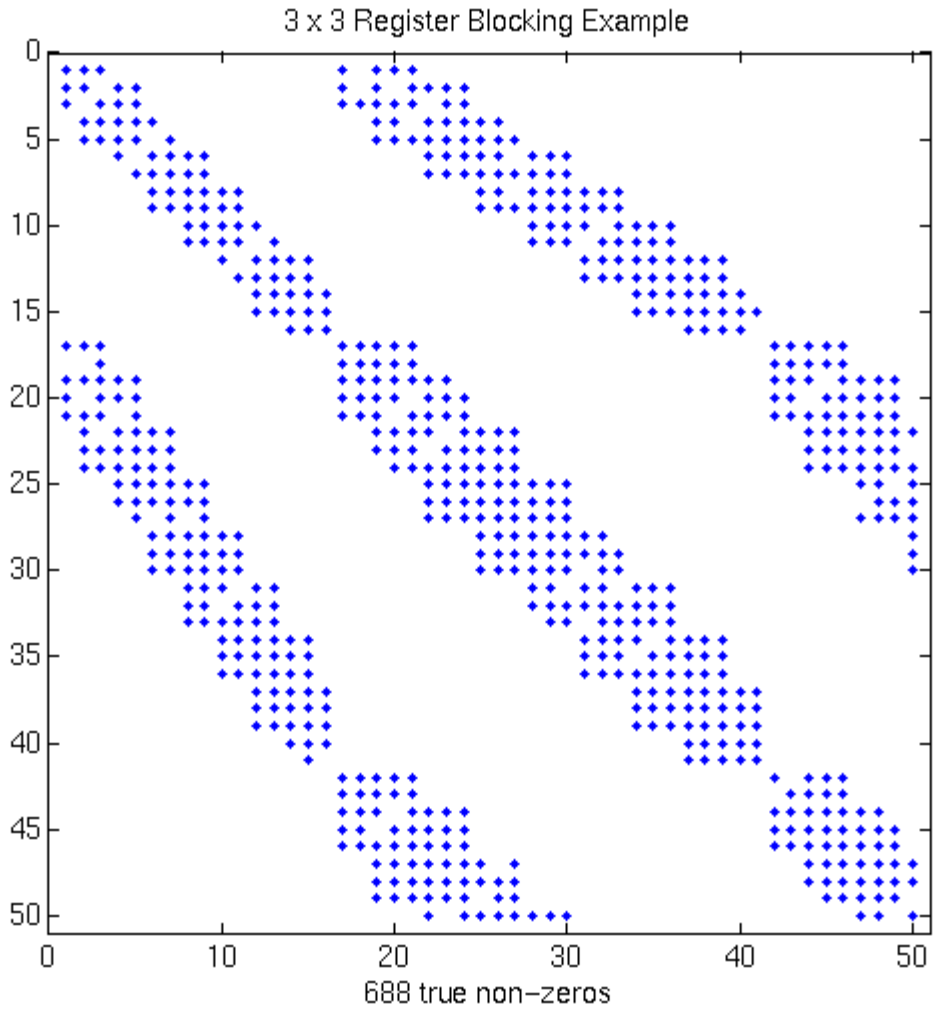
Example of off-line tuning: dense matrix

Another example of tuning challenges



- More complicated non-zero structure in general
- N = 16614
- NNZ = 1.1M
- FEM fluid flow application

Zoom in to top corner



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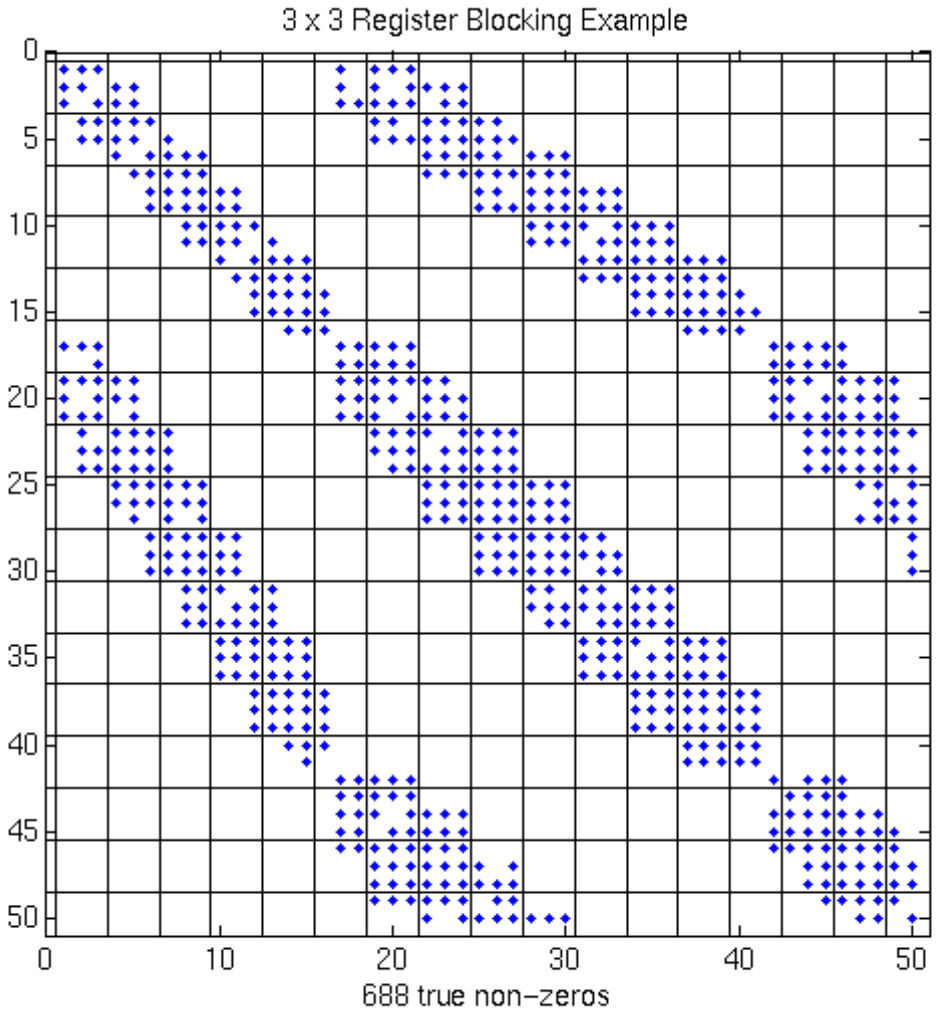
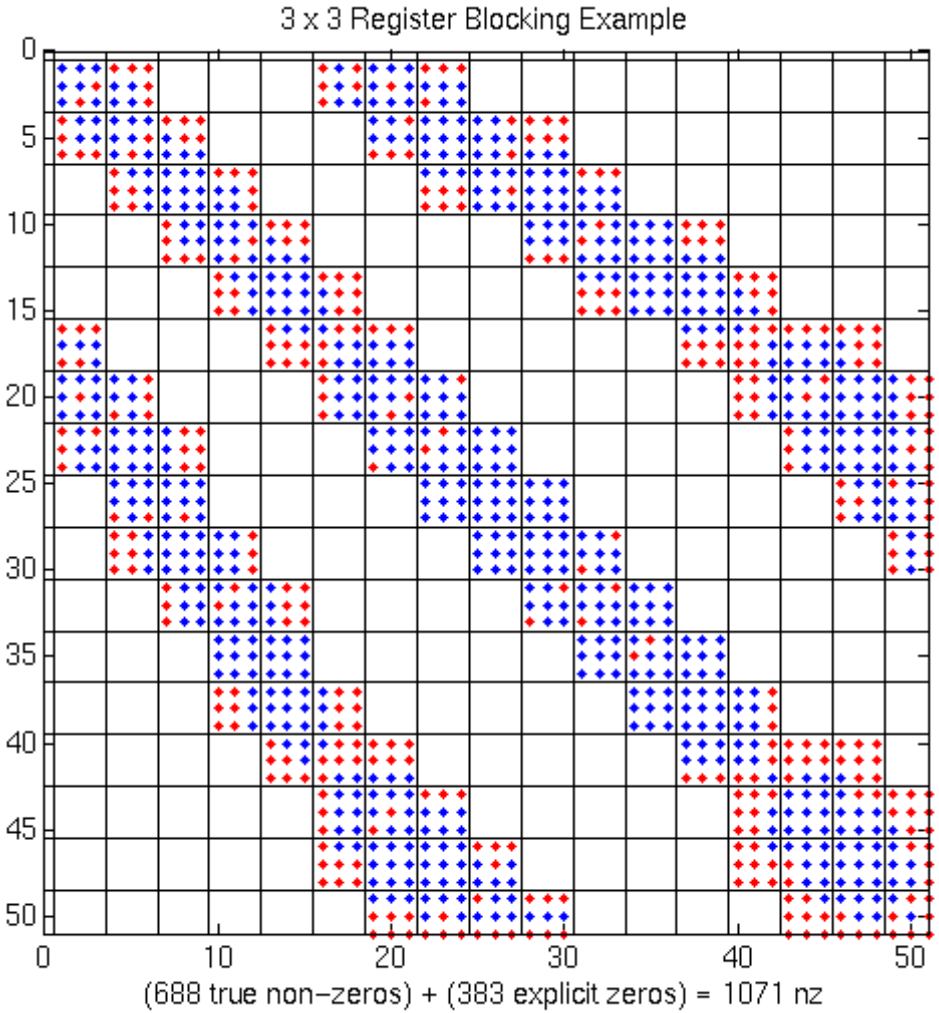
3x3 blocks look natural, but…



- More complicated non-zero structure in general
- Example: 3x3 blocking
  - Logical grid of 3x3 cells
- But would lead to lots of “fill-in”

Extra Work Can Improve Efficiency!



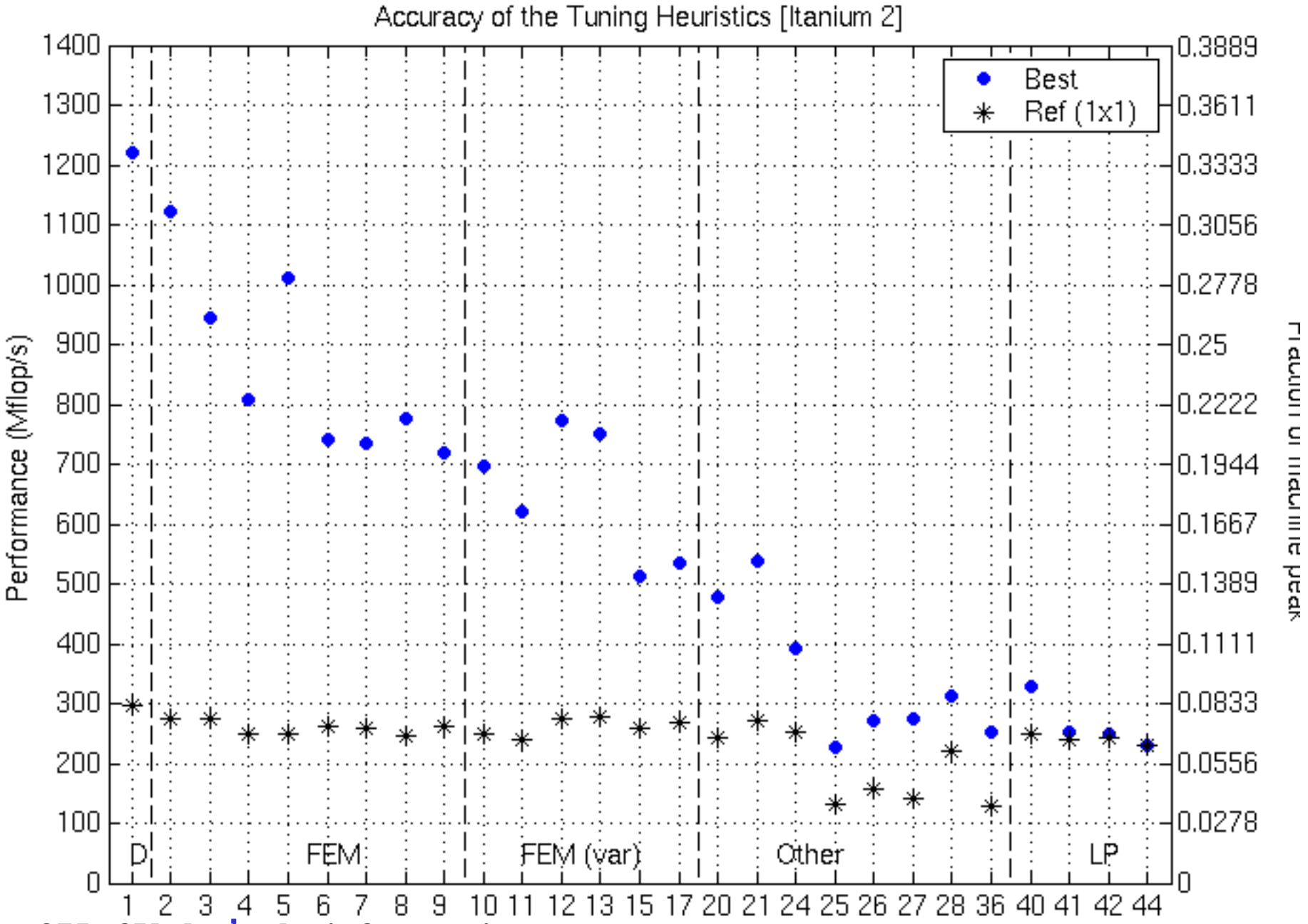
- More complicated non-zero structure in general
- Example: 3x3 blocking
  - Logical grid of 3x3 cells
  - Fill-in explicit zeros
  - Unroll 3x3 block multiplies
  - "Fill ratio" = 1.5
- On Pentium III: 1.5x speedup!
  - Actual mflop rate $1.5^2 = 2.25$ higher

Automatic Register Block Size Selection

- Selecting the r x c block size
  - **Off-line benchmark**
    - Precompute **Mflops(r,c)** using dense A for each r x c
    - Once per machine/architecture
  - **Run-time "search"**
    - Sample *A* to estimate **Fill(r,c)** for each r x c
  - **Run-time heuristic model**
    - Choose r, c to minimize **time ~ Fill(r,c) / Mflops(r,c)**

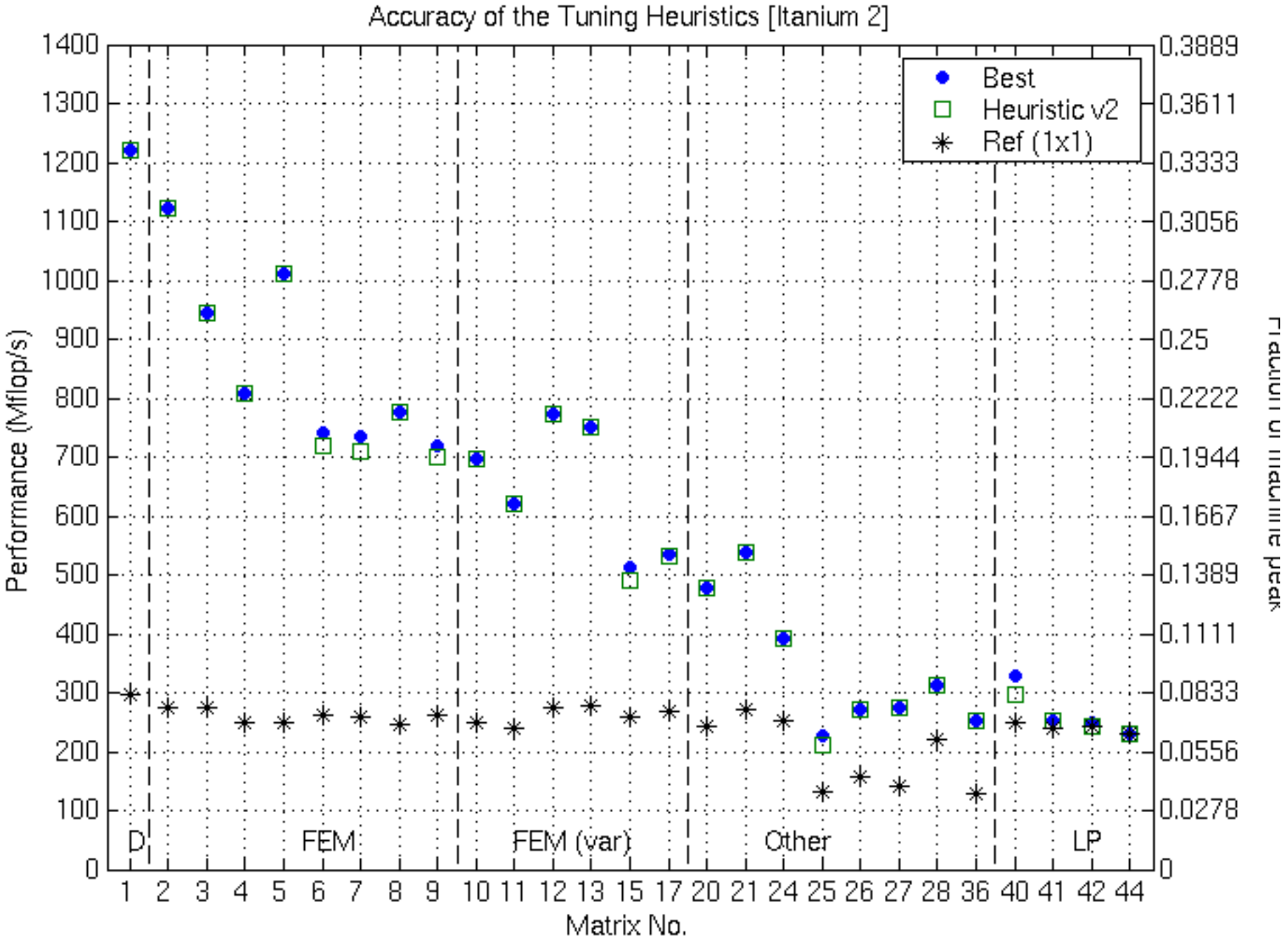
Accurate and Efficient Adaptive Fill Estimation

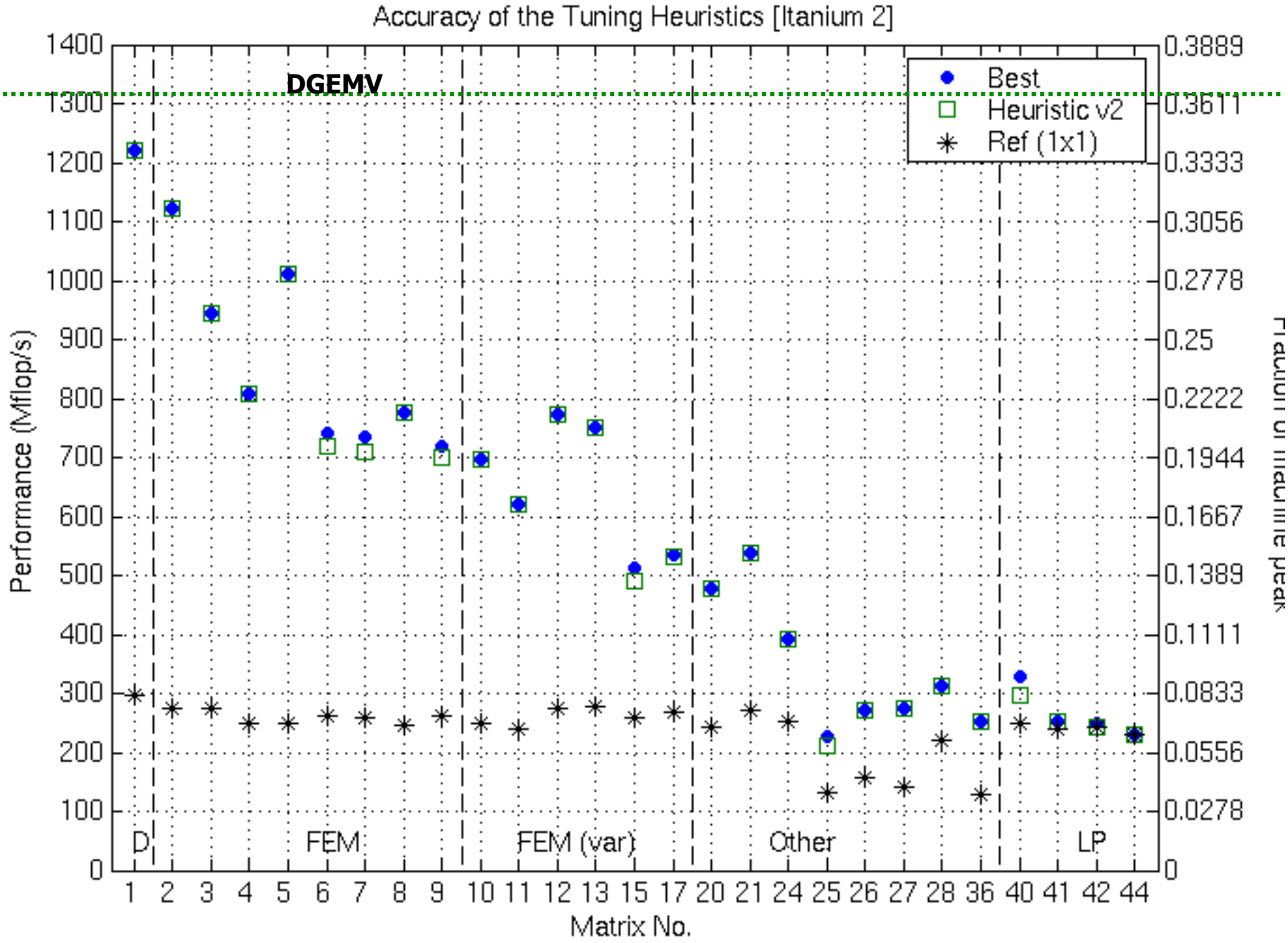
- Idea: Sample matrix
  - Fraction of matrix to sample: $s \in [0,1]$
  - Cost ~ O(s * nnz)
  - Control cost by controlling s
    - Search at run-time: the constant matters!
- Control s automatically by computing statistical confidence intervals
  - Idea: Monitor variance
- Cost of tuning
  - Lower bound: convert matrix in 5 to 40 unblocked SpMVs
  - Heuristic: 1 to 11 SpMVs



See p. 375 of Vuduc's thesis for matrices

NOTE: "Fair" flops used (ops on explicit zeros not counted as "work")


Accuracy of the Tuning Heuristics [Itanium 2]
Performance (Mflop/s)
Fraction of Machine Peak
Matrix No.
Best
Heuristic v2
Ref (1x1)
D
FEM
FEM (var)
Other
LP
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
0.3889
0.3611
0.3333
0.3056
0.2778
0.25
0.2222
0.1944
0.1667
0.1389
0.1111
0.0833
0.0556
0.0278
0
1 2 3 4 5 6 7 8 9 10 11 12 13 15 17 20 21 24 25 26 27 28 36 40 41 42 44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0.3333
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0.3889
1 2 3 4 5 6 7 8 9 10 11 12 13 15 17 20 21 24 25 26 27 28 36 40 41 42 44

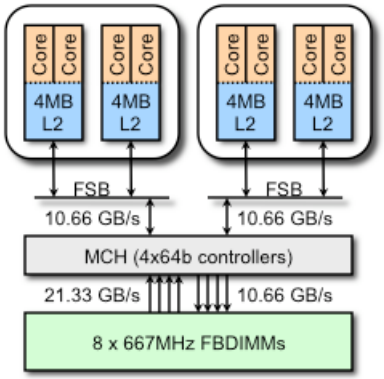
Summary of Other Sequential Performance Optimizations

- Optimizations for SpMV
  - **Register blocking (RB)**: up to **4x** over CSR
  - **Variable block splitting**: **2.1x** over CSR, 1.8x over RB
  - **Diagonals**: **2x** over CSR
  - **Reordering** to create dense structure + **splitting**: **2x** over CSR
  - **Symmetry**: **2.8x** over CSR, 2.6x over RB
  - **Cache blocking**: **2.8x** over CSR
  - **Multiple vectors (SpMM)**: **7x** over CSR
  - And combinations…
- Sparse triangular solve
  - Hybrid sparse/dense data structure: **1.8x** over CSR
- Higher-level kernels
  - $\mathbf{A \cdot A^T \cdot x}$, $\mathbf{A^T \cdot A \cdot x}$: **4x** over CSR, 1.8x over RB
  - $\mathbf{A^2 \cdot x}$: **2x** over CSR, 1.5x over RB
  - $[A \cdot x, A^2 \cdot x, A^3 \cdot x, .. , A^k \cdot x]$

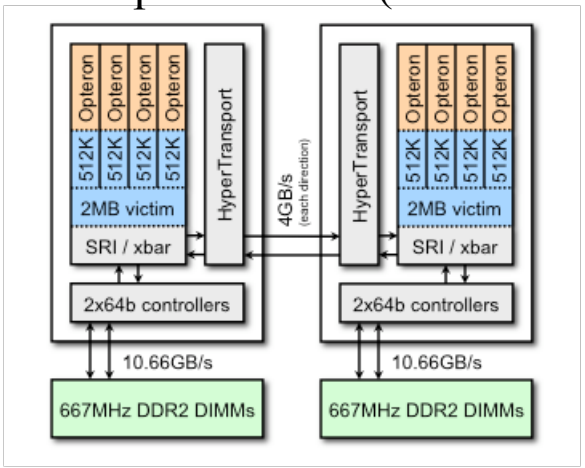
Tuning SpMV on Multicore

Multicore SMPs Used

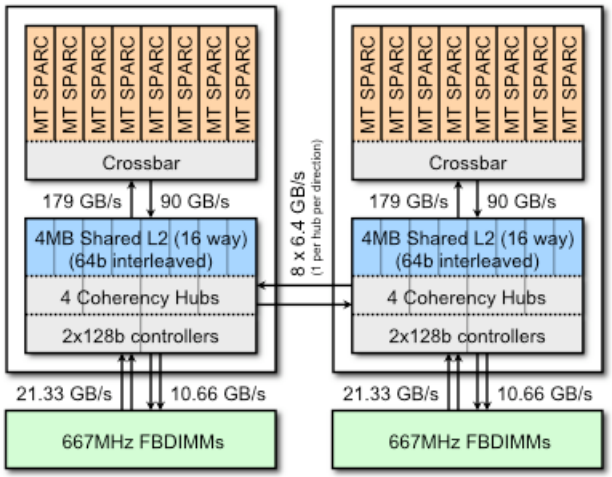
Intel Xeon E5345 (Clovertown)



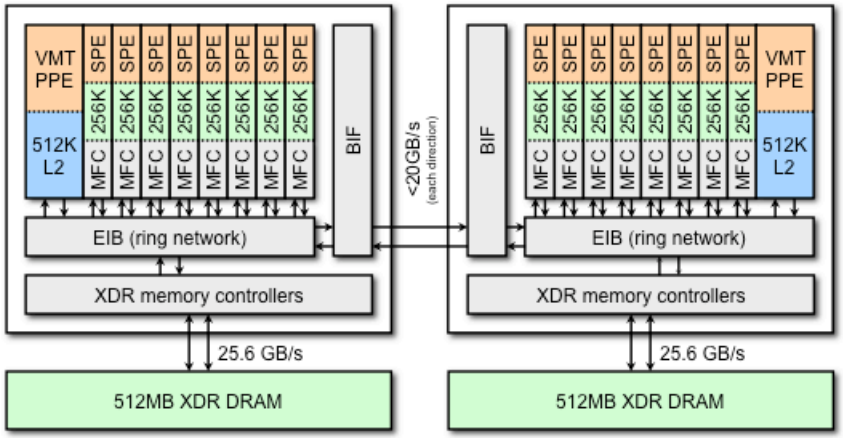
AMD Opteron 2356 (Barcelona)



Sun T2+ T5140 (Victoria Falls)



IBM QS20 Cell Blade

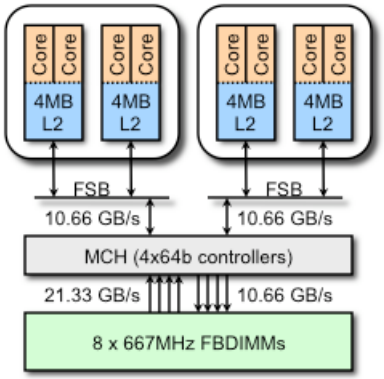


 Source: Sam Williams

Multicore SMPs Used

(Conventional cache-based memory hierarchy)

Intel Xeon E5345 (Clovertown)



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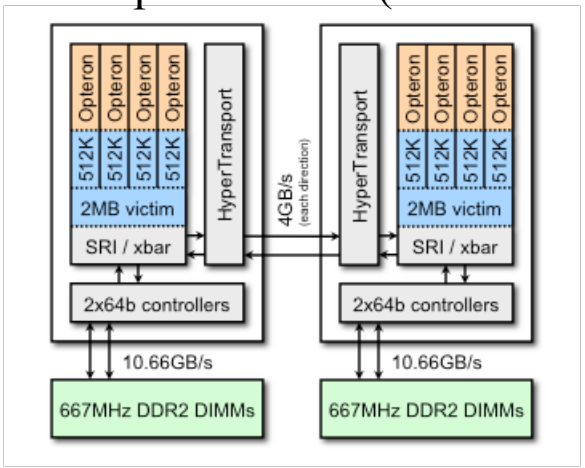

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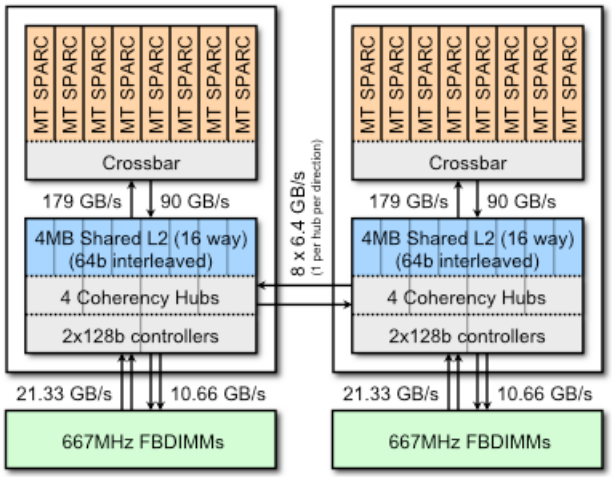

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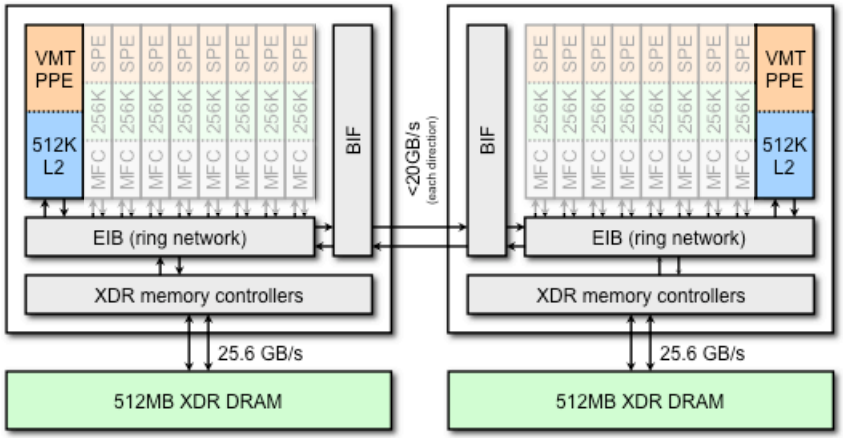
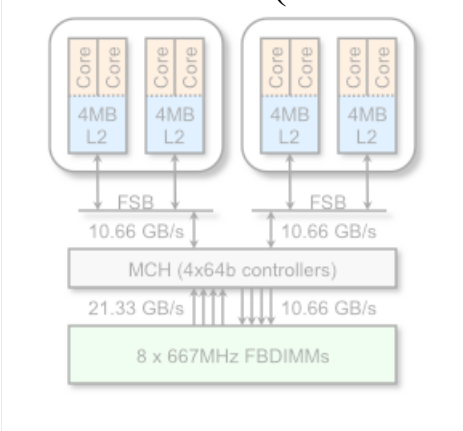


2 such Control processors PPEs on Cell

 Source: Sam Williams

Multicore SMPs Used
(Local store-based memory hierarchy)

Intel Xeon E5345 (Clovertown)



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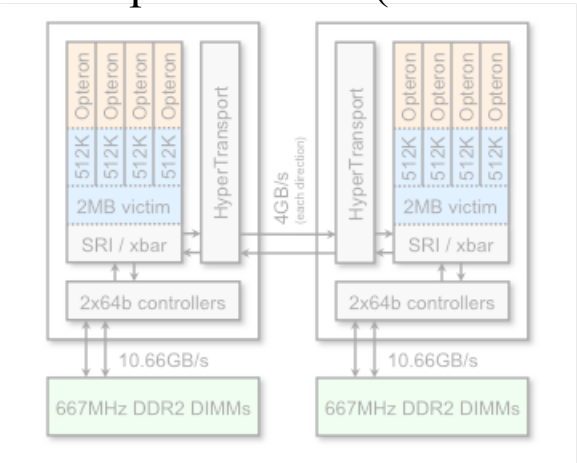
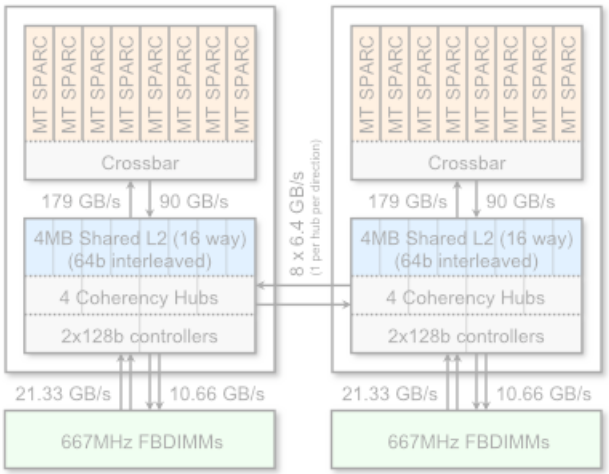


Sun T2+ T5140 (Victoria Falls)



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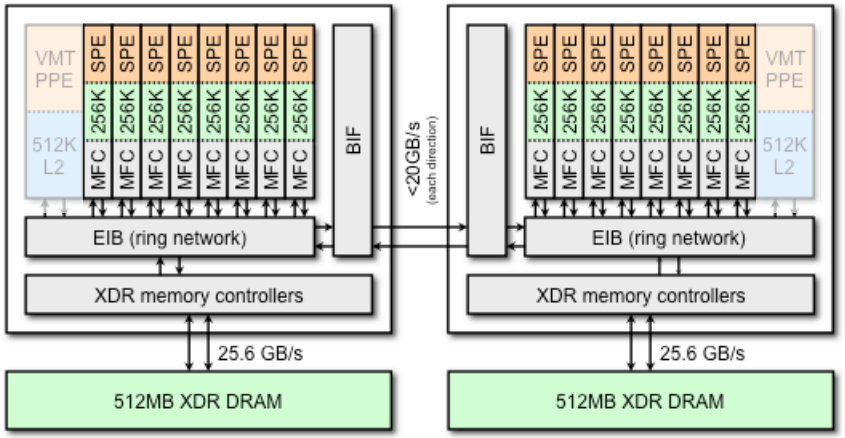
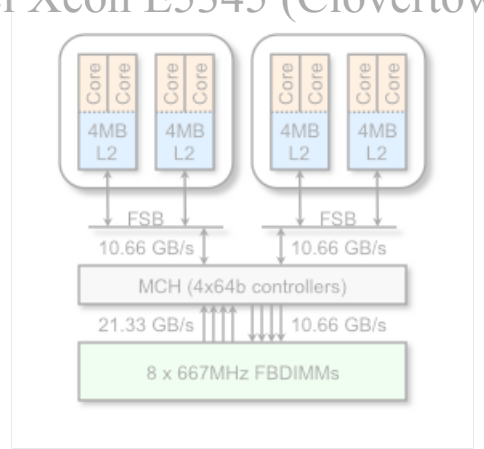


Explicit load and stores (special subroutines) for 16 SPEs
To move data between local memory/DRAM

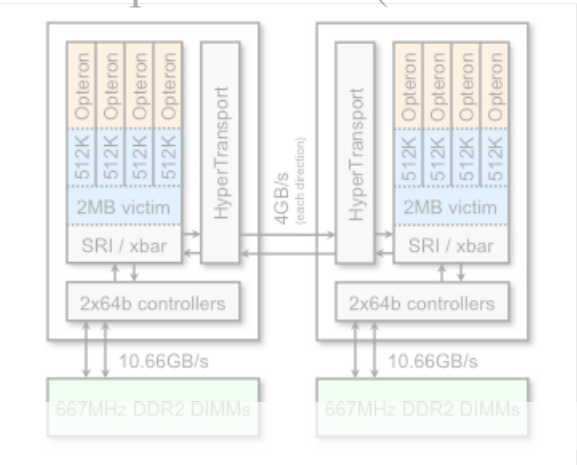
Source: Sam Williams

Multicore SMPs Used
(CMT = Chip-MultiThreading)

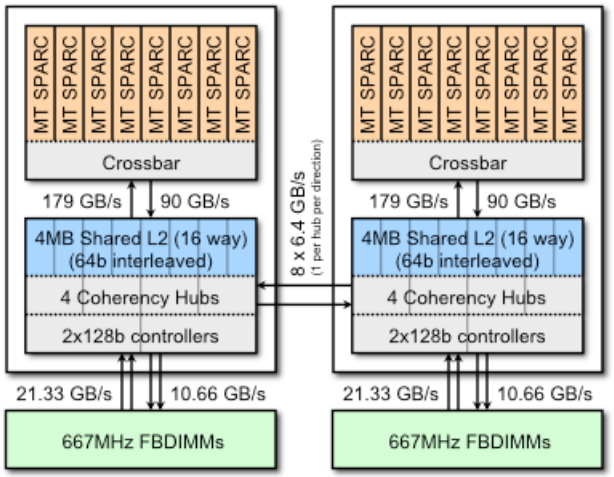
Intel Xeon E5345 (Clovertown)



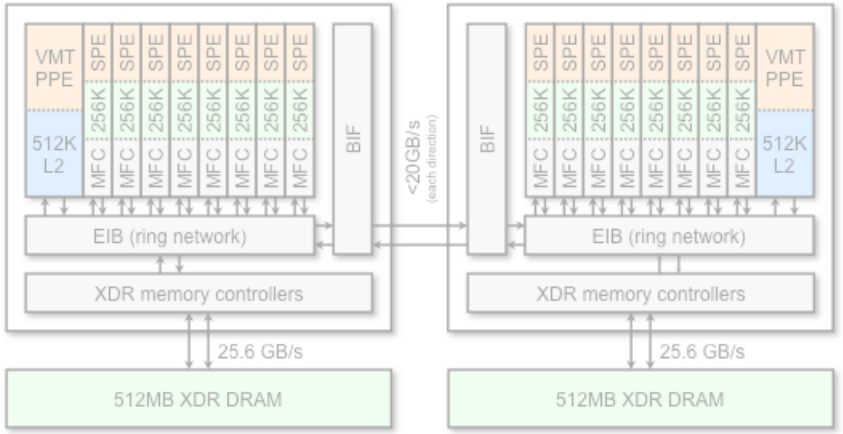
AMD Opteron 2356 (Barcelona)



Sun T2+ T5140 (Victoria Falls)



IBM QS20 Cell Blade

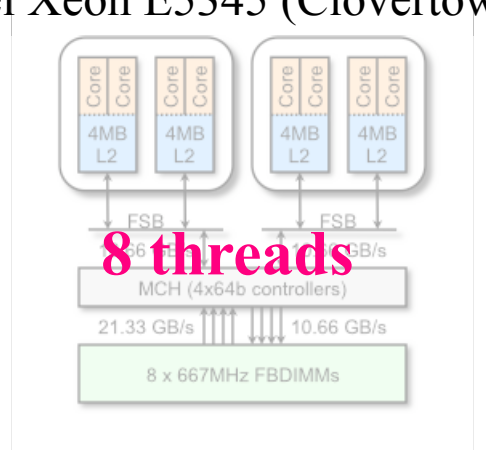


HW switches automatically from thread waiting for memory to another

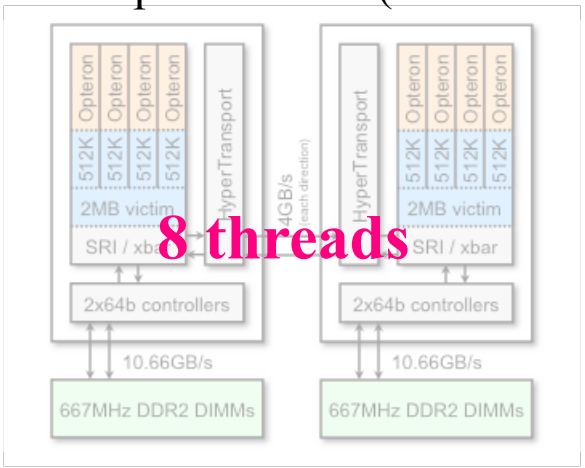
 Source: Sam Williams

Multicore SMPs Used
(threads)

Intel Xeon E5345 (Clovertown)



AMD Opteron 2356 (Barcelona)



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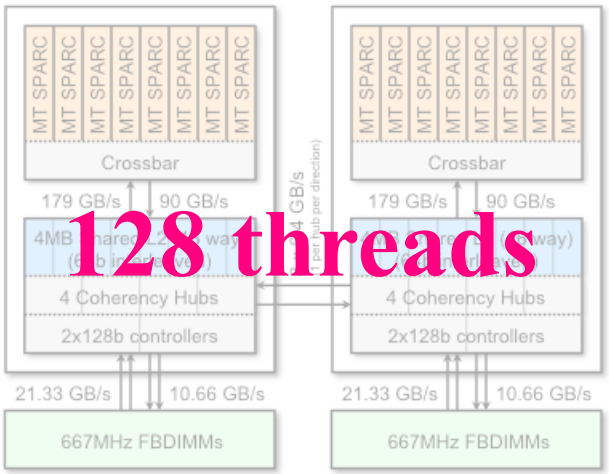
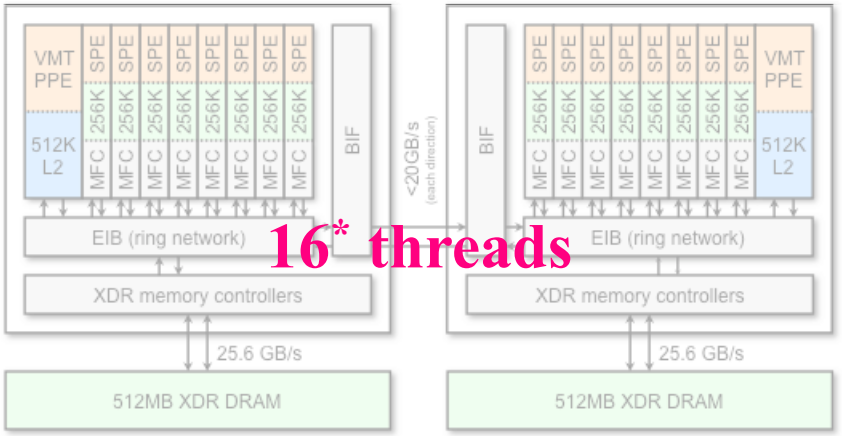


IBM QS20 Cell Blade

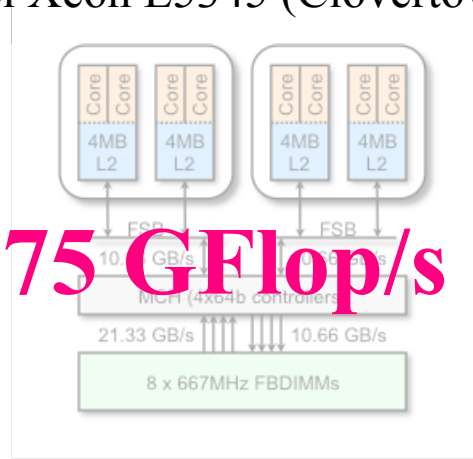


Source: Sam Williams

*SPEs only

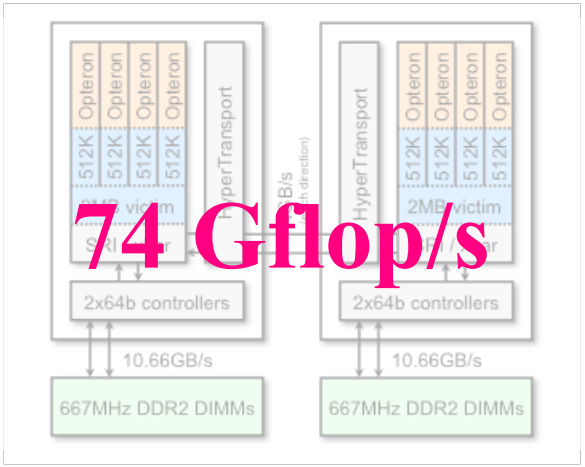
Multicore SMPs Used
(peak double precision flops)

Intel Xeon E5345 (Clovertown)



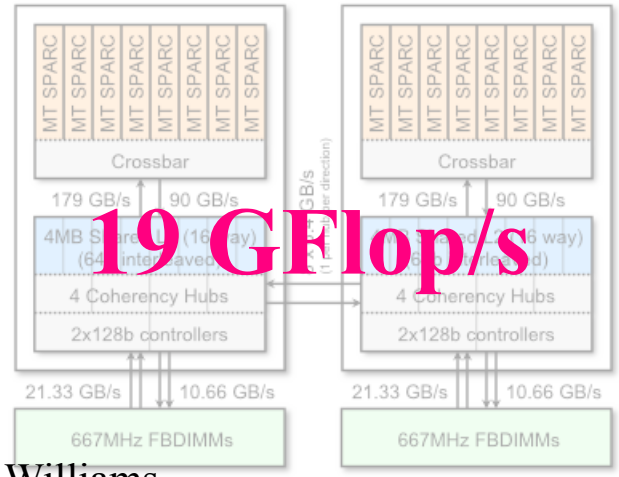
75 GFlop/s

AMD Opteron 2356 (Barcelona)



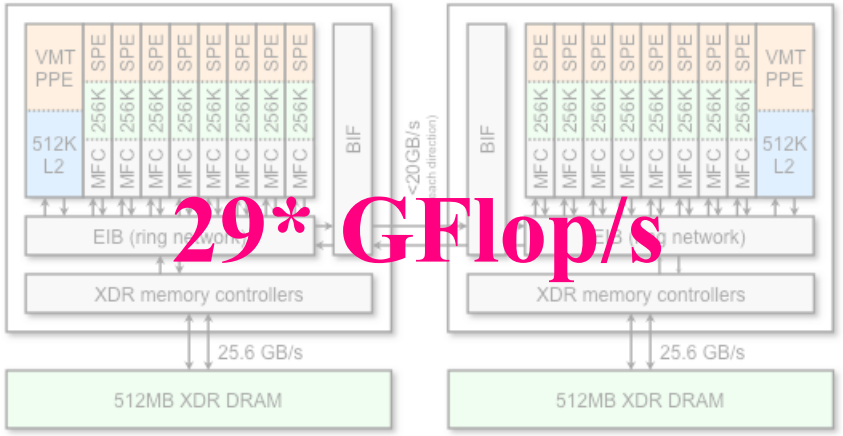
74 Gflop/s

Sun T2+ T5140 (Victoria Falls)



19 GFlop/s

IBM QS20 Cell Blade



29* GFlop/s

Source: Sam Williams

*SPEs only

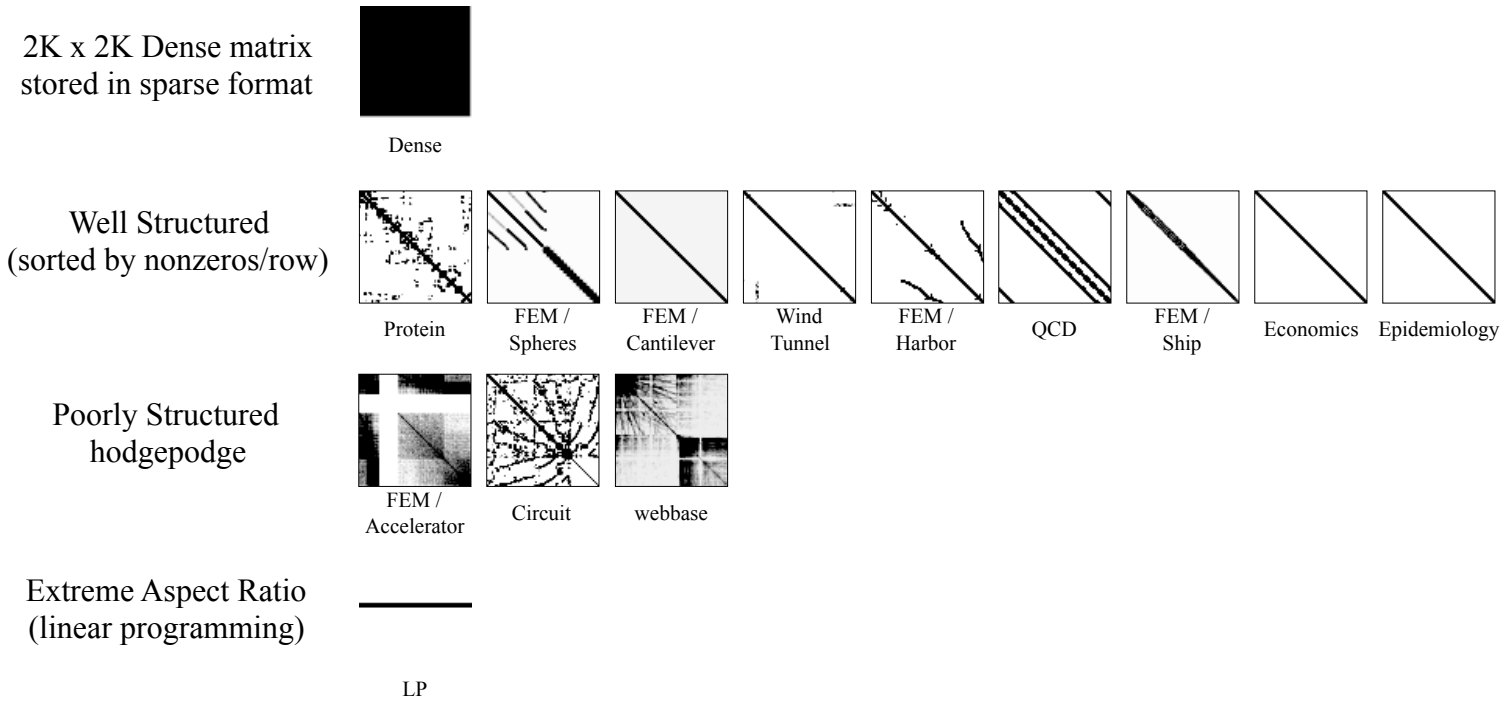
Results from

"Auto-tuning Sparse Matrix-Vector Multiplication (SpMV)"

Samuel Williams, Leonid Oliker, Richard Vuduc, John Shalf, Katherine Yelick, James Demmel, "Optimization of Sparse Matrix-Vector Multiplication on Emerging Multicore Platforms", Supercomputing (SC), 2007.

Test matrices

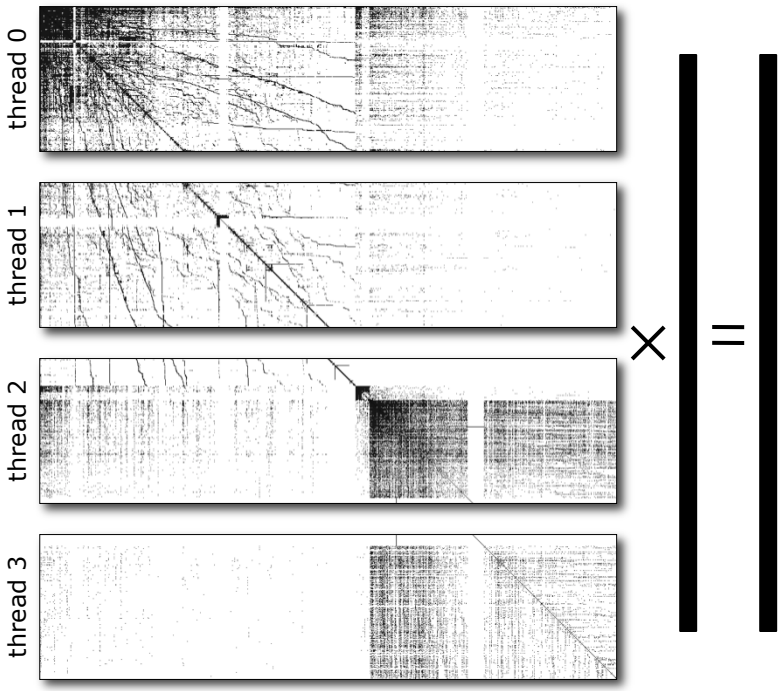
- Suite of 14 matrices
- All bigger than the caches of our SMPs
- We' ll also include a median performance number



Source: Sam Williams

SpMV Parallelization

- How do we parallelize a matrix-vector multiplication ?
- By rows blocks, load balance by number of nonzeros
- No inter-thread data dependencies, but random access to x

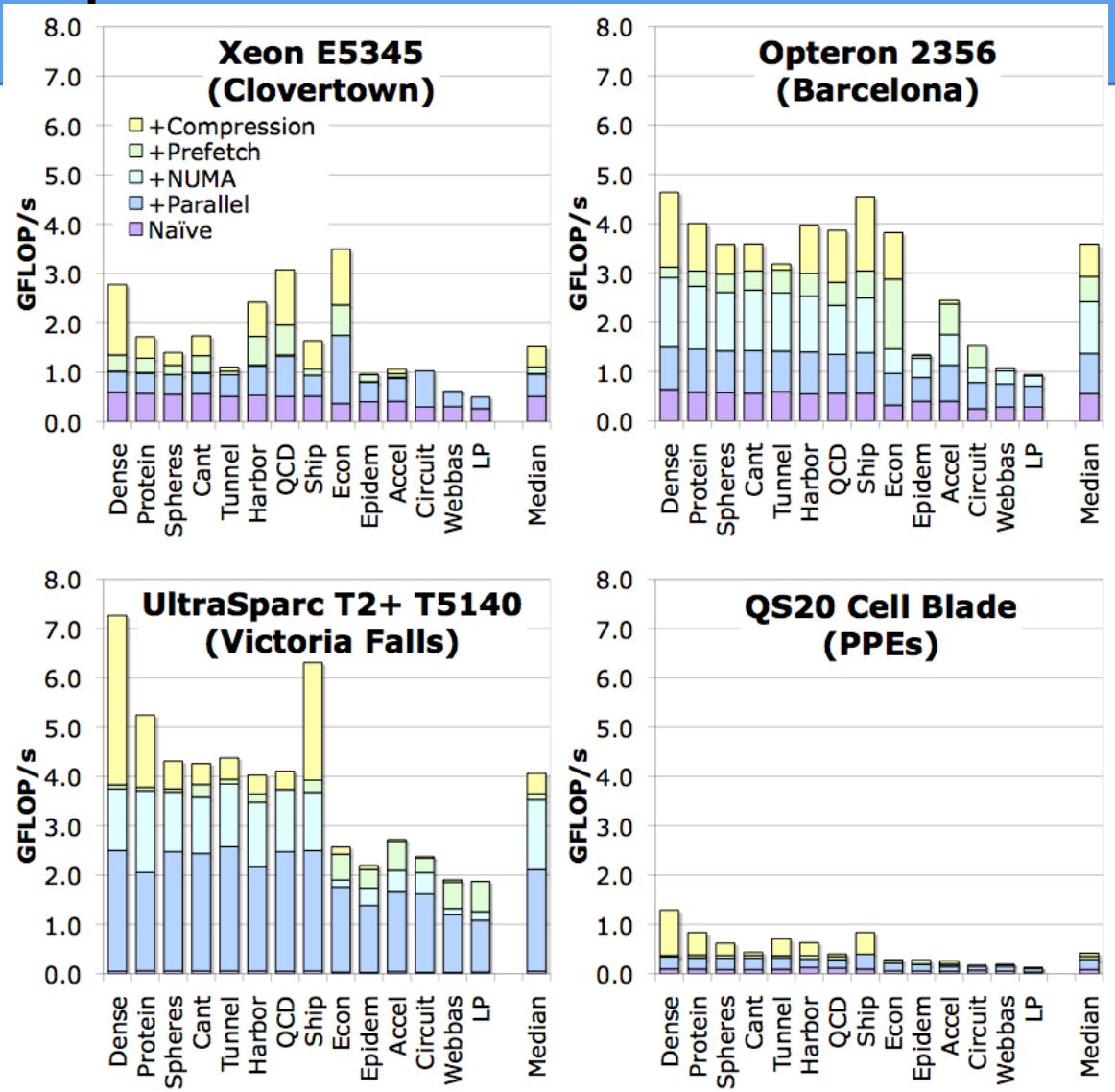


Source: Sam Williams

Summary of Multicore Optimizations

- NUMA - Non-Uniform Memory Access
  - pin submatrices to memories close to cores assigned to them
  - either explicit (malloc, affinity) or implicit (first touch)
- Prefetch – values, indices, and/or vectors
  - Pragma inserted in C code – special HW instructions
  - use exhaustive search on prefetch distance
- Matrix Compression – not just register blocking (BCSR)
  - 32 or 16-bit indices, Block Coordinate format for submatrices
- Cache-blocking
  - 2D partition of matrix, so needed parts of x,y fit in cache

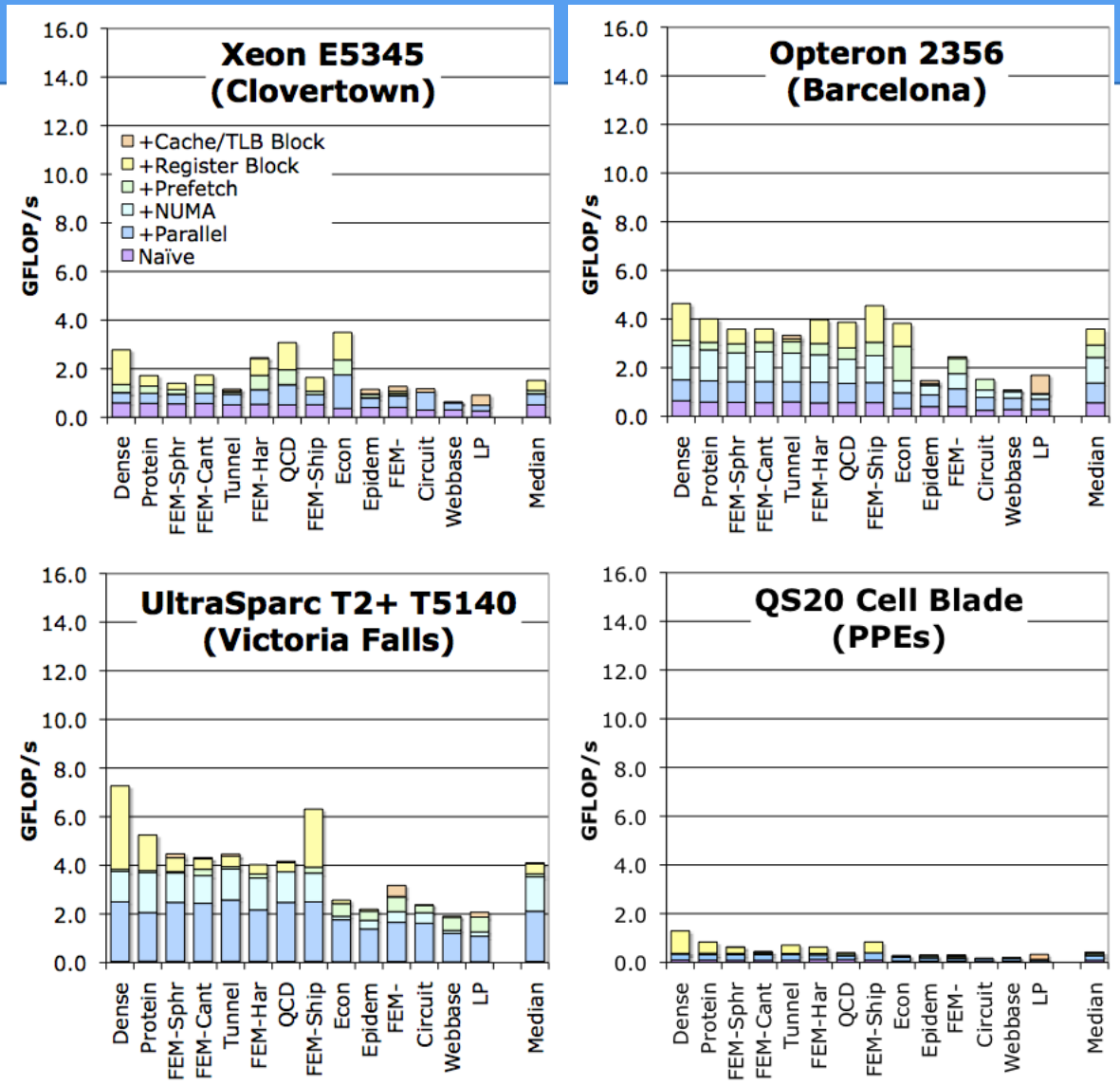
SpMV Performance



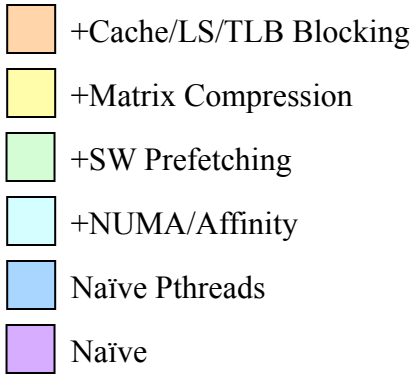
- After maximizing memory bandwidth, the only hope is to minimize memory traffic.
- Compression: exploit
  - register blocking
  - other formats
  - smaller indices
- Use a traffic minimization **heuristic** rather than search
- Benefit is clearly matrix-dependent.
- Register blocking enables efficient software prefetching (one per cache line)

Source: Sam Williams

Auto-tuned SpMV Performance
(cache and TLB blocking)

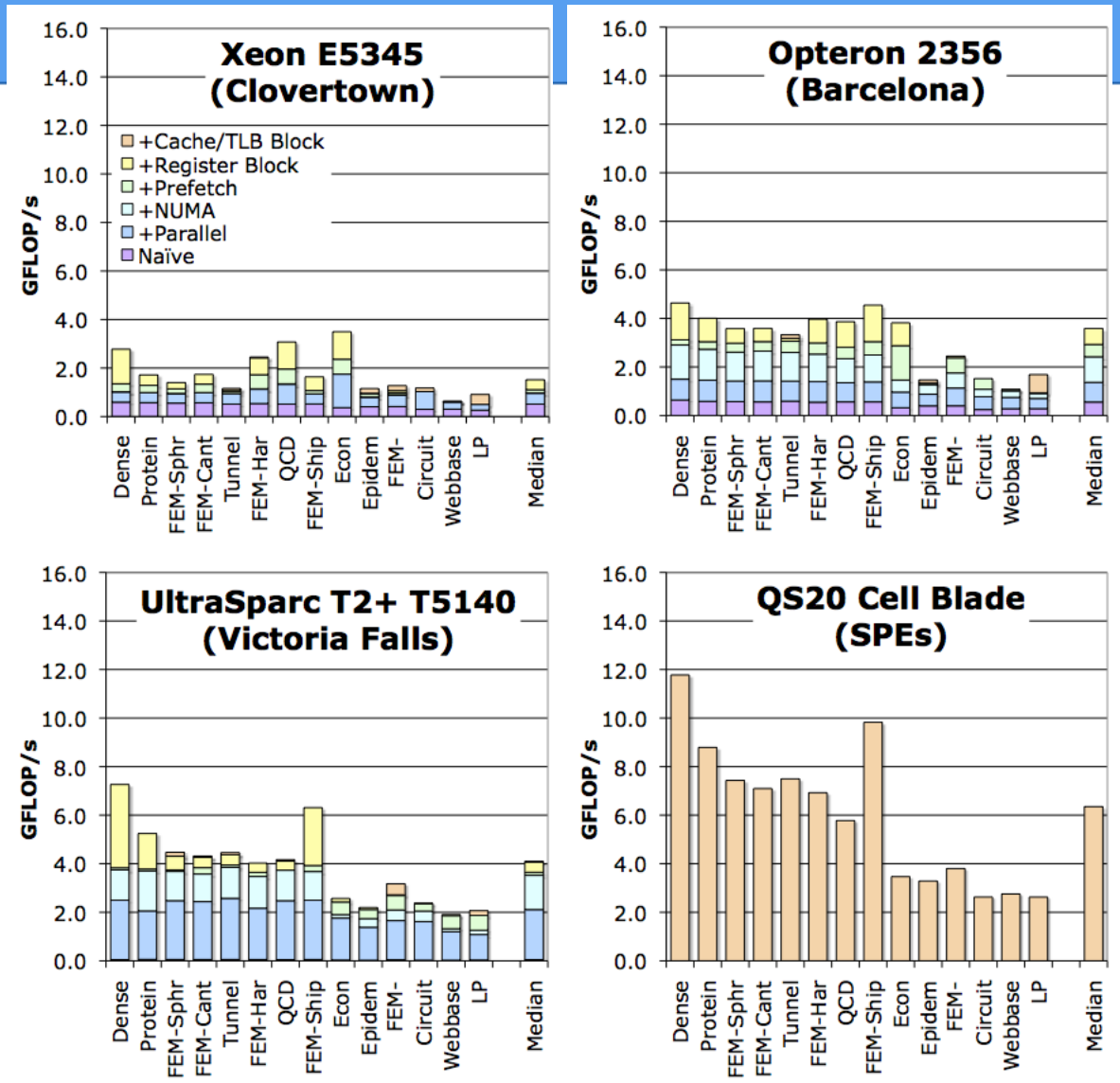


- Fully auto-tuned SpMV performance across the suite of matrices
- Why do some optimizations work better on some architectures?
- **matrices with naturally small working sets**
- **architectures with giant caches**



Source: Sam Williams

Auto-tuned SpMV Performance
(architecture specific optimizations)

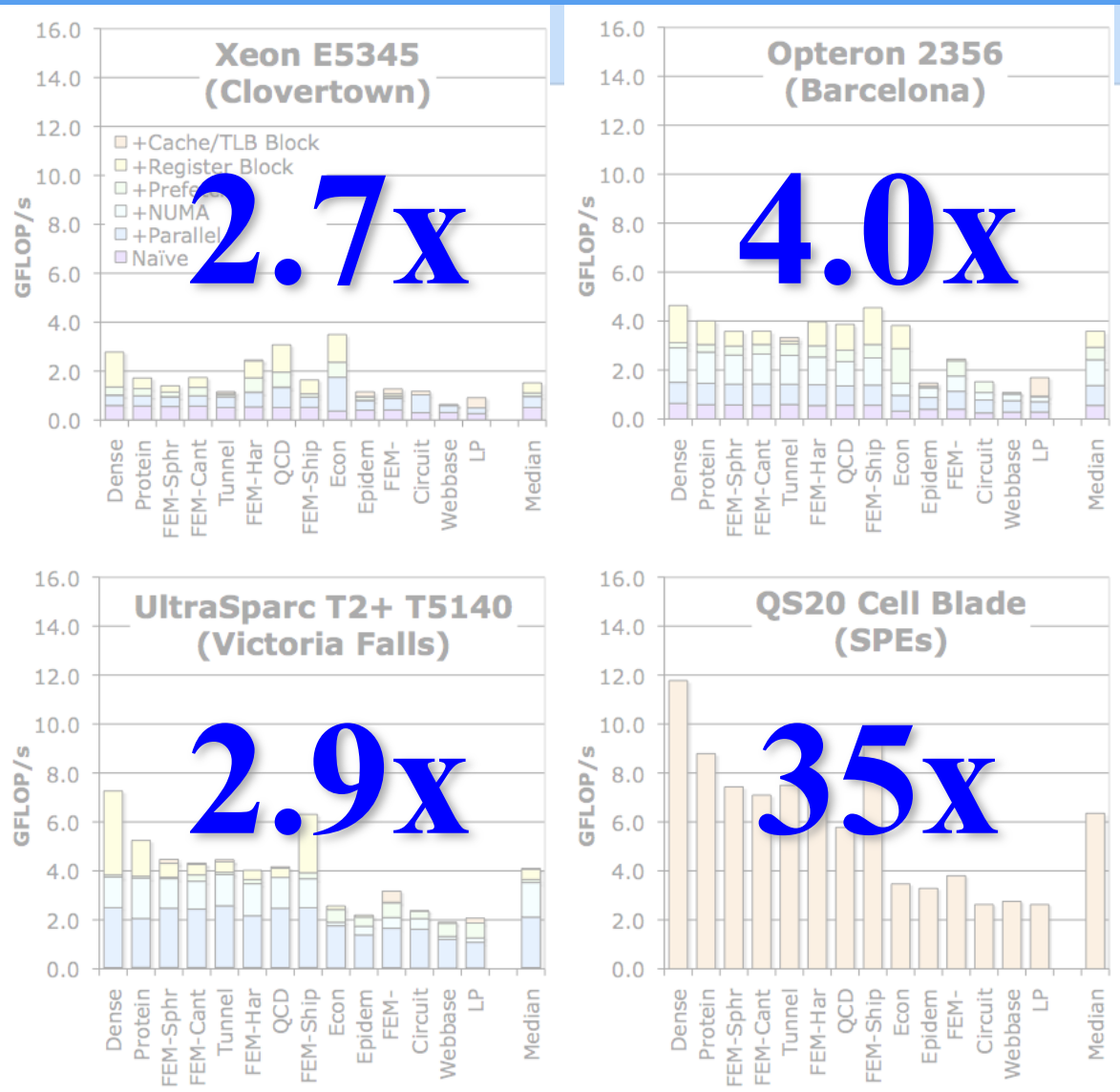


- Fully auto-tuned SpMV performance across the suite of matrices
- Included SPE/local store optimized version
- Why do some optimizations work better on some architectures?

+Cache/LS/TLB Blocking
+Matrix Compression
+SW Prefetching
+NUMA/Affinity
Naïve Pthreads
Naïve

Source: Sam Williams

Auto-tuned SpMV Performance
(max speedup)



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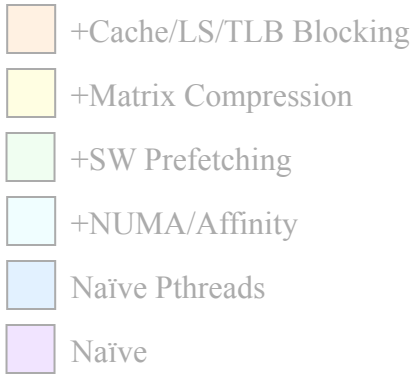

Source: Sam Williams

Plan

Krylov subspace methods

Tuning sparse matrix-vector product

Iterative solvers that reduce communication
- CA solvers based on s-step methods
- Enlarged Krylov methods

Preconditioners

Extra slides: one level preconditioners

Iterative solvers that reduce communication

Communication avoiding based on s-step methods

- Unroll k iterations, orthogonalize every k steps.
- A factor of $O(k)$ less messages and bandwidth in sequential.
- A factor of $O(k)$ less messages in parallel (same bandwidth).

Enlarged Krylov methods

- Decrease the number of iterations to decrease the number of global communications.
- Increase arithmetic intensity.

Other approaches available in the litterature, but not presented here.

CA solvers based on s-step methods: main idea

To avoid communication, unroll k-steps, ghost necessary data,

- generate a set of vectors W for the Krylov subspace $\mathcal{K}_k(A, r_0)$,
- (A)-orthogonalize the vectors using a communication avoiding orthogonalization algorithm (e.g. TSQR(W)).

References

- Van Rosendale '83, Walker '85, Chronopoulous and Gear '89, Erhel '93, Toledo '95, Bai, Hu, Reichel '91 (Newton basis), Joubert and Carey '92 (Chebyshev basis), etc.
- Recent references: G. Atenekeng, B. Philippe, E. Kamgnia (to enable multiplicative Schwarz preconditioner), J. Demmel, M. Hoemmen, M. Mohiyuddin, K. Yellick (to minimize communication, next slides), Carson, Demmel, Knight (CA and other Krylov solvers, preconditioners)

CA-GMRES

GMRES: find x in $span\{b, Ab, ..., A^k b\}$ minimizing $||Ax - b||_2$
Cost of k steps of standard GMRES vs new GMRES

Standard GMRES
for i=1 to k
w = A · v(i-1)
MGS(w, v(0),...,v(i-1))
update v(i), H
endfor
solve LSQ problem with H

Sequential: #words_moved =
O(k·nnz) from SpMV
+ O(k^2·n) from MGS
Parallel: #messages =
O(k) from SpMV
+ O(k^2 · log p) from MGS

Slide source: J. Demmel

CA-GMRES

GMRES: find x in $span\{b, Ab, ..., A^k b\}$ minimizing $||Ax - b||_2$
Cost of k steps of standard GMRES vs new GMRES

Standard GMRES
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w = A · v(i-1)
MGS(w, v(0),...,v(i-1))
update v(i), H
endfor
solve LSQ problem with H

Communication-avoiding GMRES
W = [v, Av, A^2v, ... , A^kv]
[Q,R] = TSQR(W) ... "Tall Skinny QR"
Build H from R, solve LSQ problem

Sequential: #words_moved =
O(k·nnz) from SpMV
+ O(k^2·n) from MGS
Parallel: #messages =
O(k) from SpMV
+ O(k^2 · log p) from MGS

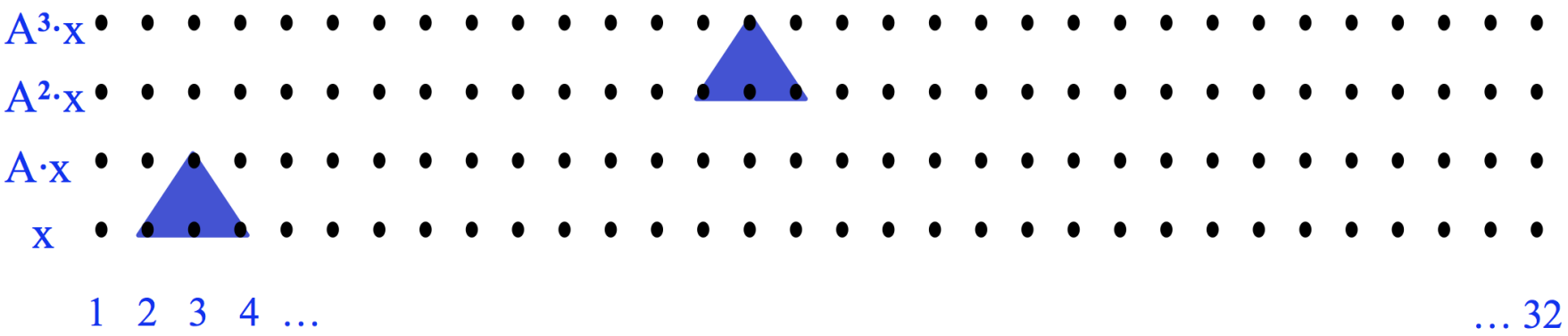
Sequential: #words_moved =
O(nnz) from SpMV
+ O(k·n) from TSQR
Parallel: #messages =
O(1) from computing W
+ O(log p) from TSQR

Slide source: J. Demmel

Matrix Powers Kernel

- Generate the set of vectors $\{Ax, A^2x, \ldots A^kx\}$ in parallel
- Ghost necessary data to avoid communication
- Example: A tridiagonal, $n = 32$, $s = 3$
- Shaded triangles represent data computed redundantly

$$Ax = \begin{pmatrix} * & * & & & & & \\ * & * & * & & & & \\ & * & * & * & & & \\ & & * & * & * & & \\ & & & \ddots & \ddots & \ddots & \end{pmatrix} \cdot \begin{pmatrix} * \\ * \\ * \\ * \\ \vdots \end{pmatrix} = \begin{pmatrix} * \\ * \\ * \\ * \\ \vdots \end{pmatrix}$$



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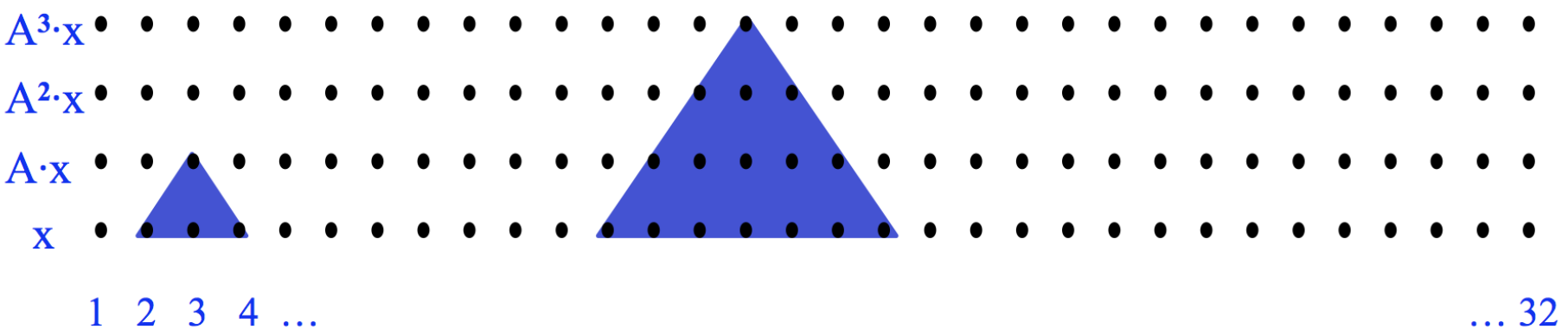

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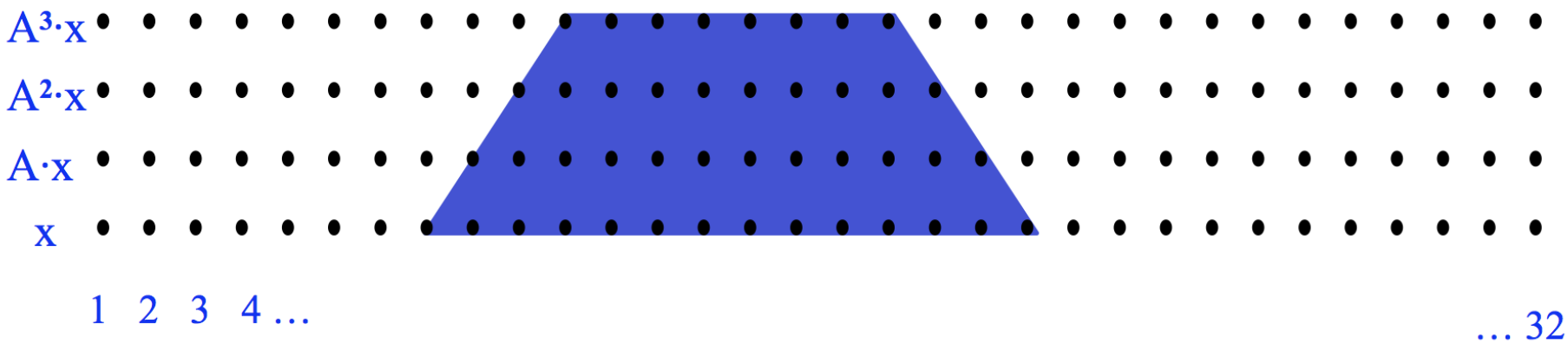

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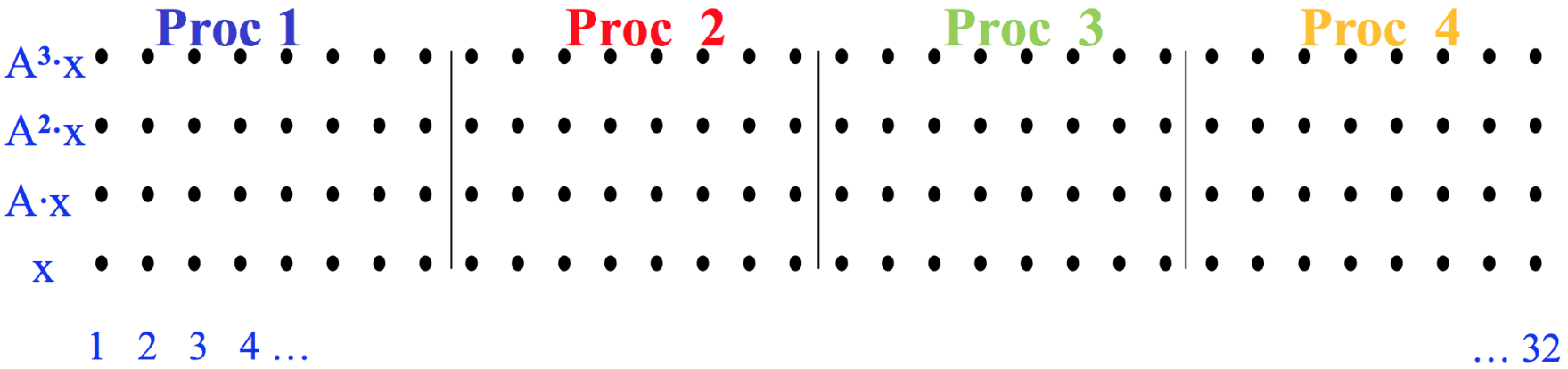

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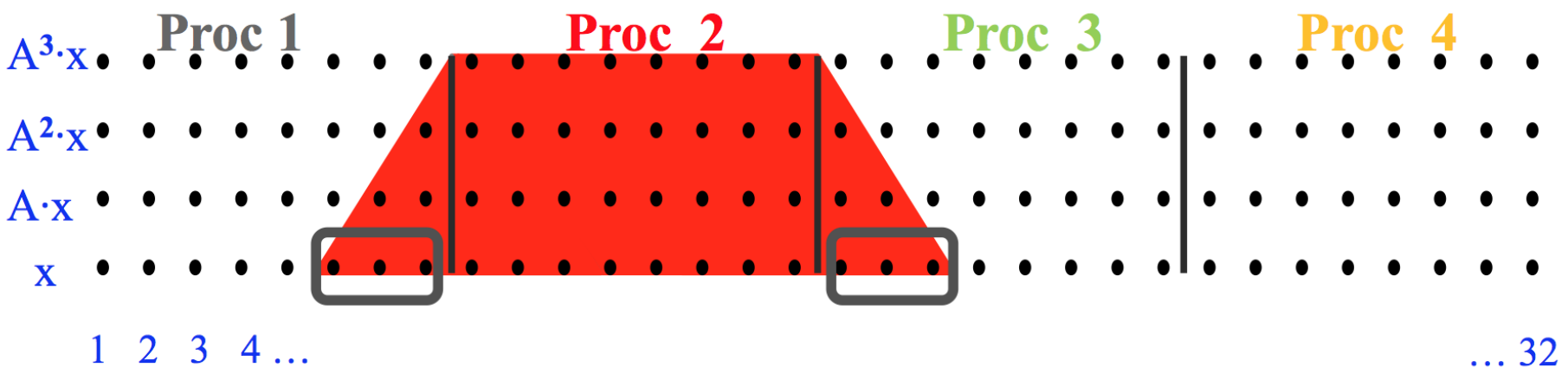

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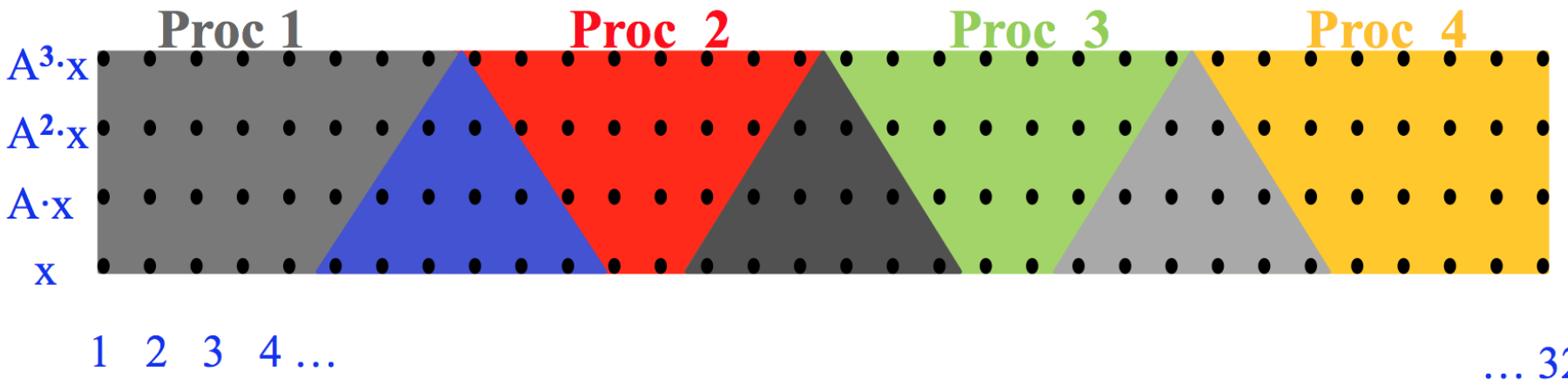
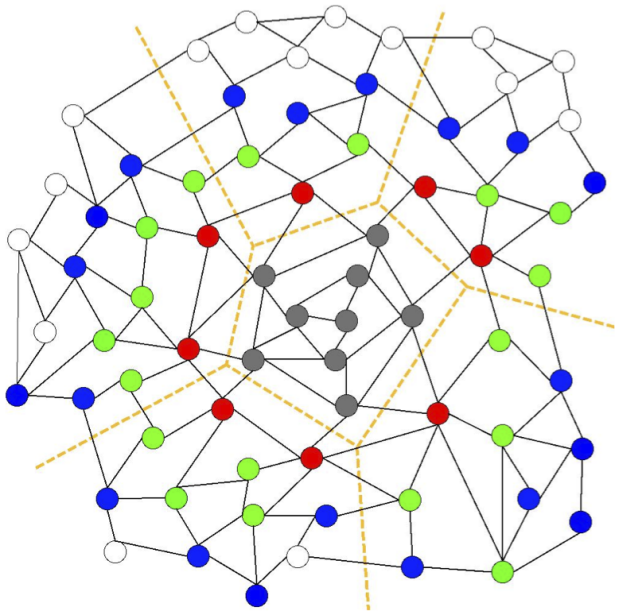


Matrix Powers Kernel (contd)

Ghosting works for structured or well-partitioned unstructured matrices, with modest surface-to-volume ratio.

- Parallel: block-row partitioning based on (hyper)graph partitioning,
- Sequential: top-to-bottom processing based on traveling salesman problem.



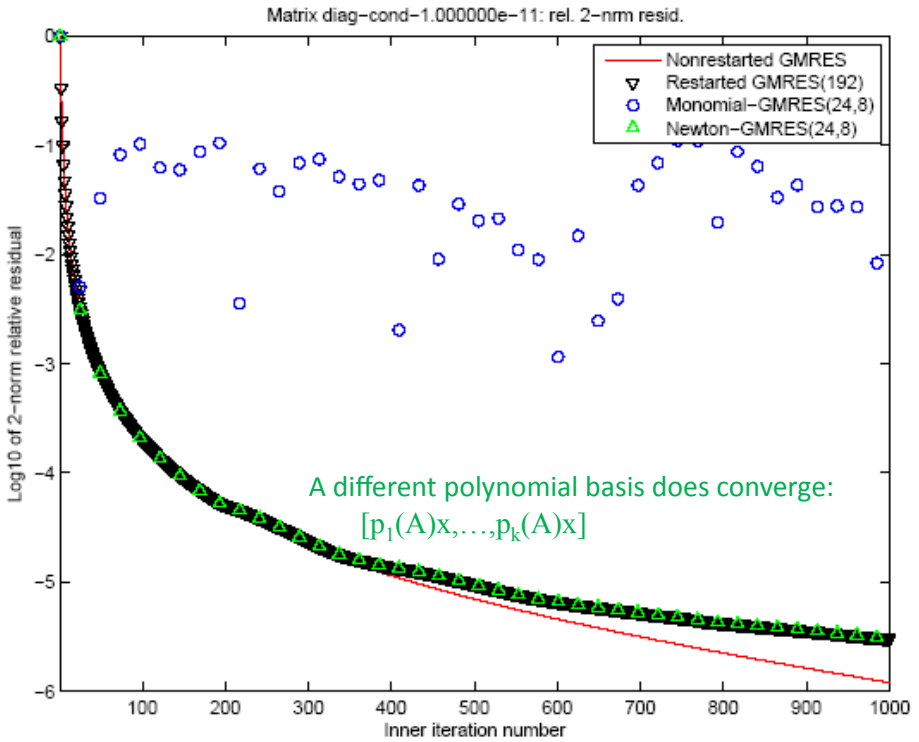
Challenges and research opportunities

Length of the basis k is limited by

- Size of ghost data
- Loss of precision

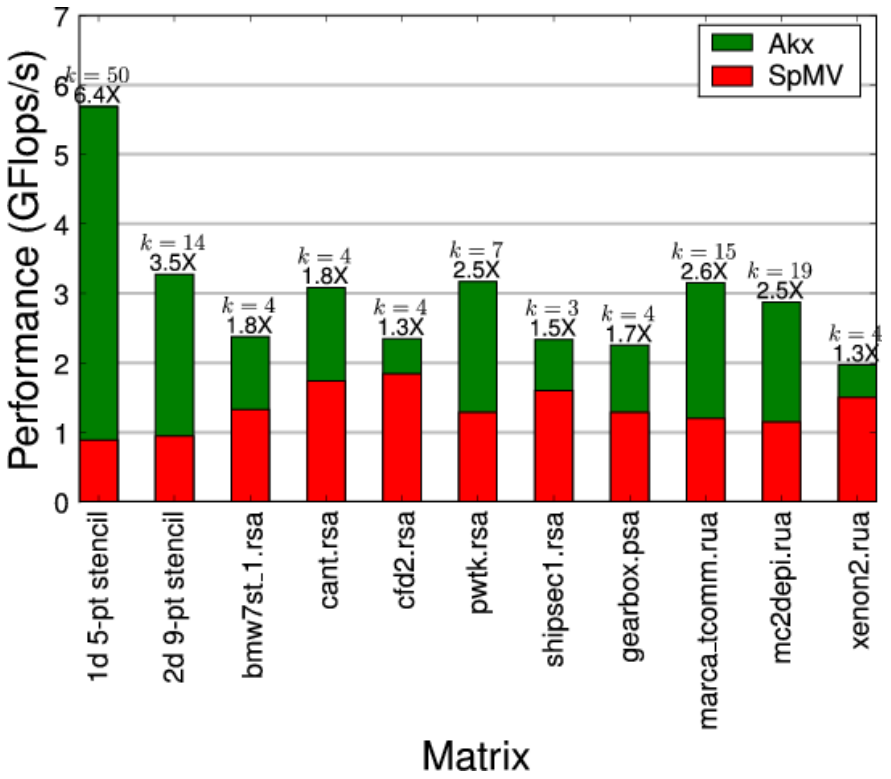
Preconditioners: lots of recent work

- Highly decoupled preconditioners: Block Jacobi
- Hierarchical, semiseparable matrices (M. Hoemmen, J. Demmel)
- CA-ILU0 (extra slides), deflation (Carson, Demmel, Knight)

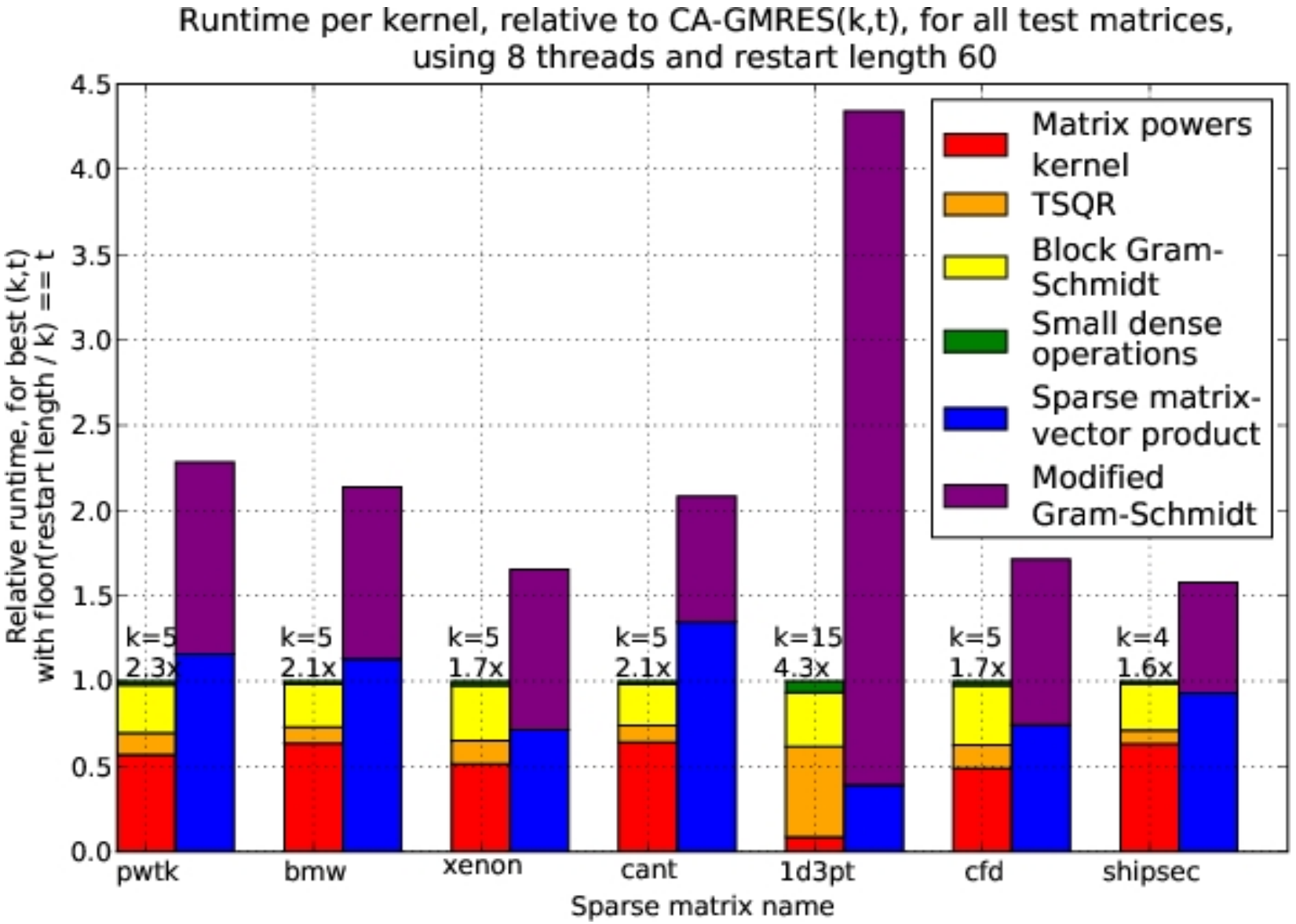


Performance

- Speedups on Intel Clovertown (8 cores), data from [Demmel et al., 2009]
- Used both optimizations:
  - sequential (moving data from DRAM to chip)
  - parallel (moving data between cores on chip)



Performance (contd)



Enlarged Krylov methods [Grigori et al., 2014]

- Partition the matrix into t domains
- At k-th iteration,
  - split the residual r_{k-1} into t vectors corresponding to the t domains,

$$r_{k-1} \rightarrow T(r_{k-1}) = \begin{bmatrix} * & 0 & & 0 \\ \vdots & \vdots & & \vdots \\ * & 0 & & 0 \\ 0 & * & & 0 \\ \vdots & \vdots & & \vdots \\ 0 & * & & 0 \\ & & \ddots & \\ 0 & 0 & & * \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & * \end{bmatrix}, T_s(r_{k-1}) = \{T(r_{k-1})(:,1), \ldots T(r_{k-1})(:,t)$$

  - generate t new basis vectors, obtain an enlarged Krylov subspace

$$\mathscr{K}_{t,k}(A, r_0) \quad = \quad span\{T_s(r_0), AT_s(r_0), A^2 T_s(r0), ..., A^{k-1} T_s(r_0)\}$$

  - search for the solution of the system $Ax = b$ in $\mathscr{K}_{t,k}(A, r_0)$

Properties of enlarged Krylov subspaces

- The Krylov subspace $\mathcal{K}_k(A, r_0)$ is a subset of the enlarged one

$$\mathcal{K}_k(A, r_0) \subset \mathscr{K}_{t,k}(A, r_0)$$

- For all $k < k_{max}$ the dimensions of $\mathscr{K}_{t,k}$ and $\mathscr{K}_{t,k+1}$ are stricltly increasing by some number i_k and i_{k+1} respectively, where

$$t \geq i_k \geq i_{k+1} \geq 1.$$

- The enlarged subspaces are increasing subspaces, yet bounded.

$$\mathscr{K}_{t,1}(A, r_0) \subsetneq \ldots \subsetneq \mathscr{K}_{t,k_{max}-1}(A, r_0) \subsetneq \mathscr{K}_{t,k_{max}}(A, r_0) = \mathscr{K}_{t,k_{max}+q}(A, r_0), \forall q > 0$$

Properties of enlarged Krylov subspaces: stagnation

- Let $\mathcal{K}_{p_{max}} = \mathcal{K}_{p_{max}+q}$ and $\mathscr{K}_{t,k_{max}} = \mathscr{K}_{t,k_{max}+q}$ for $q > 0$. Then

$$k_{max} \leq p_{max}.$$

- The solution of the system $Ax = b$ belongs to the subspace $x_0 + \mathscr{K}_{t,k_{max}}$.

Enlarged Krylov subspace methods based on CG

Defined by the subspace $\mathscr{K}_{t,k}$ and the following two conditions:

1. Subspace condition: $x_k \in x_0 + \mathscr{K}_{t,k}$
2. Orthogonality condition: $r_k \perp \mathscr{K}_{t,k}$

- At each iteration, the new approximate solution x_k is found by minimizing $\phi(x) = \frac{1}{2}(x)^t Ax - b^t x$ over $x_0 + \mathscr{K}_{t,k}$:

$$\phi(x_k) = min\{\phi(x), \forall x \in x_0 + \mathscr{K}_{t,k}(A, r_0)\}$$

Convergence analysis

Given

- A is an SPD matrix, x^* is the solution of $Ax = b$
- $||\overline{e}_k||_A = ||x^* - \overline{x}_k||_A$ is the k^{th} error of CG
- $||e_k||_A = ||x^* - x_k||_A$ is the k^{th} error of enlarged methods
- CG converges in $\overline{K}$ iterations

Result

Enlarged Krylov methods converge in K iterations, where $K \leq \overline{K} \leq n$.

$$||e_k||_A = ||x^* - x_k||_A \leq ||\overline{e}_k||_A$$

LRE-CG: Long Recurrence Enlarged CG

- Use the entire basis to approximate the new solution
- $Q_k = [W_1 W_2 \ldots W_k]$ is an $n \times tk$ matrix containing the basis vectors of $\mathscr{K}_{t,k}$
- At each k^{th} iteration, approximate the solution as

$$x_k = x_{k-1} + Q_k \alpha_k$$

such that

$$\phi(x_k) = min\{\phi(x), \forall x \in x_0 + \mathscr{K}_{t,k}\}$$

- Either x_k is the solution, or t new basis vectors and the new approximation $x_{k+1} = x_k + Q_{k+1}\alpha_{k+1}$ are computed.

SRE-CG: Short recurrence enlarged CG

- By A-orthonormalizing the basis vectors $Q_k = [W_1, W_2, \ldots W_k]$, we obtain a short recurrence enlarged CG.
- Given that $Q_{k-1}^t r_{k-1} = 0$, we obtain the recurrence relations:

$$\begin{aligned} \alpha_k &= W_k^t r_{k-1}, \\ x_k &= x_{k-1} + W_k \alpha_k, \\ r_k &= r_{k-1} - A W_k \alpha_k, \end{aligned}$$

- W_k needs to be A-orthormalized only against W_{k-1} and W_{k-2}.

SRE-CG Algorithm

Algorithm 2 The SRE-CG algorithm

Input: A, b, x_0, ϵ, k_{max}
Output: x_k, the approximate solution of the system $Ax = b$

$r_0 = b - Ax_0$, $\rho_0 = ||r_0||_2^2$, $k = 1$
while ($\sqrt{\rho_{k-1}} > \epsilon||b||_2$ and $k < k_{max}$) **do**
    if k==1 **then**
        Let $W_1 = T(r_0)$, A-orthonormalise its vectors
    else
        Let $W_k = AW_{k-1}$
        A-orthonormalise W_k against W_{k-1} and W_{k-2} if $k > 2$
        A-orthonormalise the vectors of W_k
    end if
    $\alpha_k = (W_k^t r_{k-1})$
    $x_k = x_{k-1} + W_k \alpha_k$
    $r_k = r_{k-1} - AW_k \alpha_k$
    $\rho_k = ||r_k||_2^2$
    k = k+1
end while

SRE-CG: cost on t processors

Cost of $\bar{k}$ iterations of CG is:

$$\begin{array}{rcl} \text{Total Flops} & \approx & 2nnz \cdot \bar{k}/t + 4n\bar{k}/t \\ \text{\# words} & \approx & O(\bar{k}) \text{ (from SpMV)} \\ \text{\# messages} & \approx & 2 \text{ k log(t)} + \text{O(k) (from SpMV)} \end{array}$$

Cost of k iterations of SRE-CG is:

$$\begin{array}{rcl} \text{Total Flops} & \approx & 2nnz \cdot k + O(ntk) \\ \text{\# words} & \approx & kt^2 log(t) + O(k) \text{ (from SpMV)} \\ \text{\# messages} & \approx & klog(t) + \text{O(k) (from SpMV)} \end{array}$$

Ideally, SRE-CG converges t times faster ($k = \bar{k}/t$)
$\Rightarrow$ SRE-CG has a factor of $\bar{k}/k$ less global communication.

Convergence of different CG versions

	CG		SRE-CG	
Pa	Iter	Err	Iter	Err
SKY3D				
8	902	1E-5	211	1E-5
16	902	1E-5	119	9E-6
32	902	1E-5	43	4E-6
ANI3D				
2	4187	4e-5	875	7e-5
4	4146	4e-5	673	8e-5
8	4146	4e-5	449	1e-4
16	4146	4e-5	253	2e-4
32	4146	4e-5	148	2e-4
64	4146	4e-5	92	1e-4
ELAST3D				
2	1098	1e-7	652	1e-7
4	1098	1e-7	445	1e-7
8	1098	1e-7	321	8e-8
16	1098	1e-7	238	4e-8
32	1098	1e-7	168	5e-8
64	1098	1e-7	116	1e-8

Plan

Krylov subspace methods

Tuning sparse matrix-vector product

Iterative solvers that reduce communication

Preconditioners

- One level preconditioners: CA-ILU0
- Two level preconditioners

Extra slides: one level preconditioners

Preconditioned Krylov subspace methods

- Solve by using iterative methods

$$Ax = b.$$

- Convergence depends on $\kappa(A)$ and the eigenvalue distribution (for SPD matrices).
- To accelerate convergence, solve

$$M^{-1}Ax = M^{-1}b,$$

  where
  - M approximates well the inverse of A and/or
  - improves $\kappa(A)$, the condition number of A.
- Ideally, we would like to bound $\kappa(A)$, independently of the size of the matrix A.

One level preconditioners (two examples)

Incomplete LU factorization

- Computes $A = LU + E$
- Preconditioner $M = LU$
- ILU0 does not introduce any fill in the factors

Block Jacobi preconditioner

Given

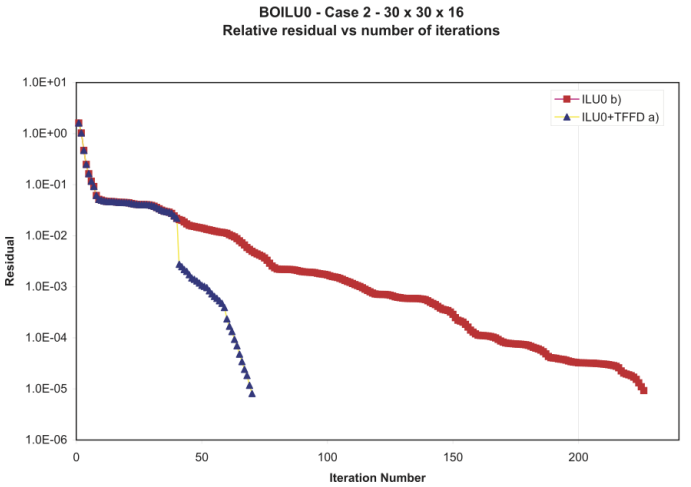
$$A = \begin{pmatrix} A_{11} & \dots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \dots & A_{PP} \end{pmatrix}$$

block Jacobi preconditioner is:

$$M = \begin{pmatrix} A_{11} & & \\ & \ddots & \\ & & A_{PP} \end{pmatrix} = \begin{pmatrix} L_{11}\,U_{11} & & \\ & \ddots & \\ & & L_{PP}\,U_{PP} \end{pmatrix} = LU$$

The need for two level preconditioners

- When solving complex linear systems arising, e.g. from large discretized systems of PDEs with strongly heterogeneous coefficients (high contrast, multiscale).



- Flow in porous media
- Elasticity problems
- CMB data analysys (no PDE)

- Most of the existing preconditioners lack robustness
  - wrt jumps in coefficients / partitioning into irregular subdomains, e.g. one level DDM methods (block Jacobi, RAS), incomplete LU
  - A few small eigenvalues hinder the convergence of iterative methods

Using deflation to deal with low frequency modes

In the unified framework of [Tang et al., 2009], let :

$$P := I - AZE^{-1}Z^T, \quad E := Z^T AZ$$

where

- Z is the deflation subspace matrix of full rank
- E is the coarse grid correction, a small dense invertible matrix
- P is the deflation matrix, $PAZ = 0$

Usage in different classes of preconditioners

- DDM - Z and Z^T are the restriction and prolongation operators based on subdomains, E is a coarse grid, P is a subspace correction
- Deflation - Z contains the vectors to be deflated
- Multigrid - interpretation possible

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Example of preconditioner

$$P_{2lvl}^{-1} = M^{-1}P + ZE^{-1}Z^T,$$

where M is the first level preconditioner (eg based on block Jacobi).

- $P_{2lvl}^{-1}AZ = Z$
- The small eigenvalues are shifted to 1.
- P_{2lvl} is not SPD, even when A is, better choices available, but more expensive.

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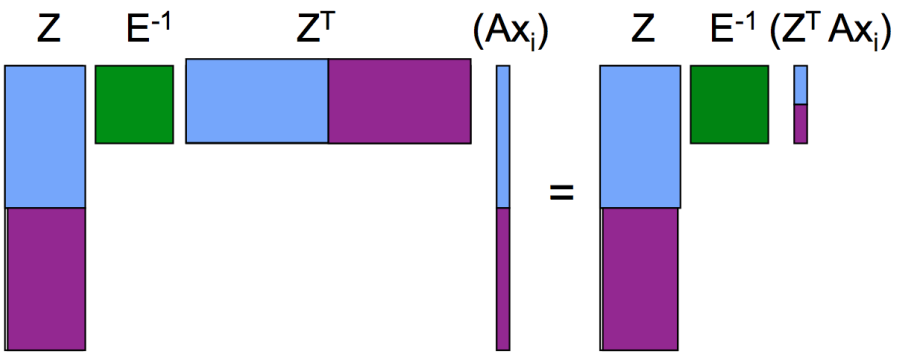
Two level preconditioners (contd)

Computing the preconditioner requires

- Deflation subspace Z, which can be formed by
  - Eigenvectors corresponding to smallest eigenvalues - from previous linear systems solved with different right hand sides, etc.
  - Using knowledge from the physics, partition of the unity, etc.
- Computing AZ and $E = Z^T AZ$.

Applying the preconditioner at each iteration requires

- Computing $y = ZE^{-1}Z^T(Ax_i) = ZE^{-1}Z^T v$
  $\Rightarrow$ involves collective communication when computing $Z^T v$, and solving a linear system with E.



Two level preconditioners (contd)

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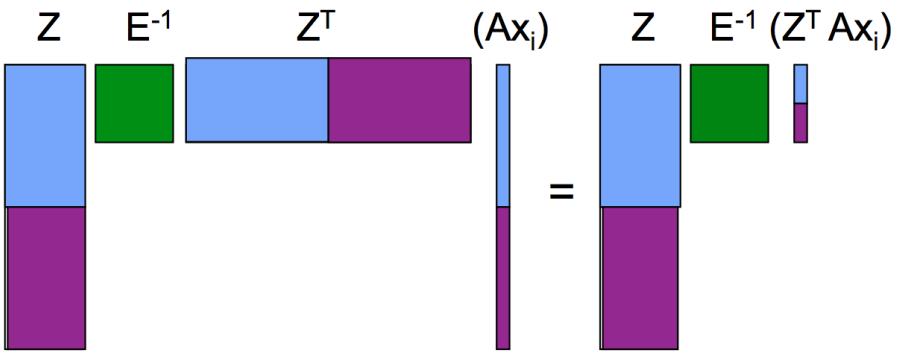


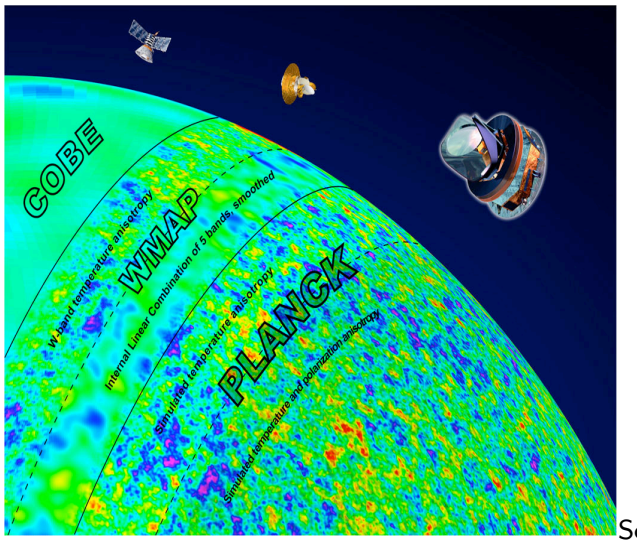
Example of deflation used in CMB data analysis

CMB data analysis

- Study light left over after the ever mysterious Big Bang,
- Produce and analyze multi-frequency 2D images of the universe when it was 5% of its current age.

- COBE (1989) collected 10 gigabytes of data, required 1 Teraflop per image analysis.
- PLANCK (2010) produced 1 terabyte of data, requires 100 Petaflops per image analysis.
- Future experiment (2020) estimated to collect .5 petabytes, require 100 Exaflops per image analysis.

Source: J. Borrill, LBNL, R. Stompor, Paris 7



Source: http://www.epm.ornl.gov/chammp/chammp.html

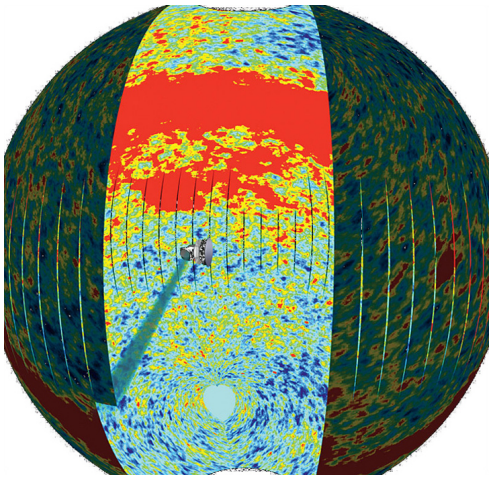
Map-making problem in an (algebraic) nutshell

- Find the best map x from observations d, scanning strategy A, and noise n_t

$$d = Ax + n_t$$

- Assuming the noise properties are Gaussian and piece-wise stationary, the covariance matrix is $N =< n_t n_t^T >$, and N^{-1} is a block diagonal symmetric Toeplitz matrix.
- The solution of the generalized least squares problem is found by solving

$$A^T N^{-1} A x = A^T N^{-1} d$$



Scanning strategy in our experiments:

- 2048 densely crossing circles
- Each circle is scanned 32 times, leading to 10^6 samples
- Piece-wise stationary noise, one Toeplitz block for each circle

Traditional approach used in the CMB community

- Solve the linear system using preconditioned CG:

$$\begin{aligned} M_{diag} S x &= M_{diag} b, \text{ where} \\ S &:= A^T N^{-1} A,\ b := A^T N^{-1} d,\ M_{diag} := (A^T diag(N^{-1}) A)^{-1} \end{aligned}$$

- The diagonal preconditioner M_{diag} does not scale numerically.

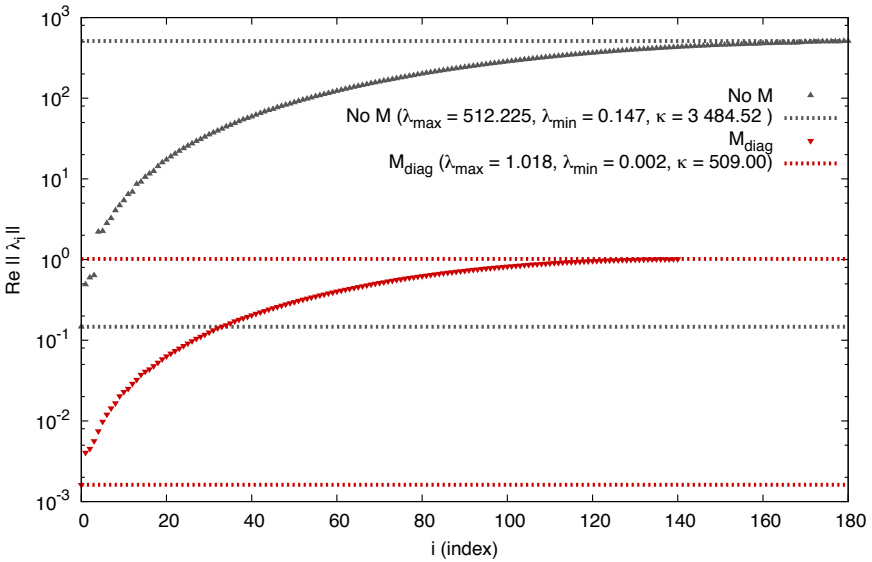


Figure : Eigenvalue distribution of S and $M_{diag}^{-1} S$ (NoM and M_{diag} resp. in the plot).

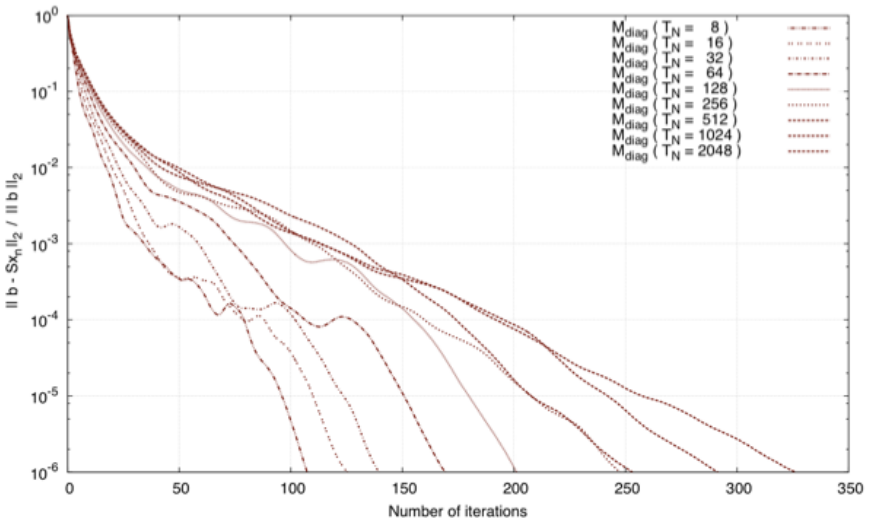


Figure : Convergence of preconditioned CG when increasing the size of the problem, e.g. number of circles T_N.

Two level preconditioner for the map-making problem

- Combine diagonal preconditioner with deflation

$$M_{2lvl} = M_{diag}(I - S(ZE^{-1}Z^T)) + ZE^{-1}Z^T,$$
$$\text{where } M_{diag} = (A^T diag(N^{-1})A)^{-1}, \quad E = Z^T SZ$$

- The efficiency of the preconditioner depends on the choice of Z see for more details [Grigori et al., 2012, Szydlarski et al., 2014].

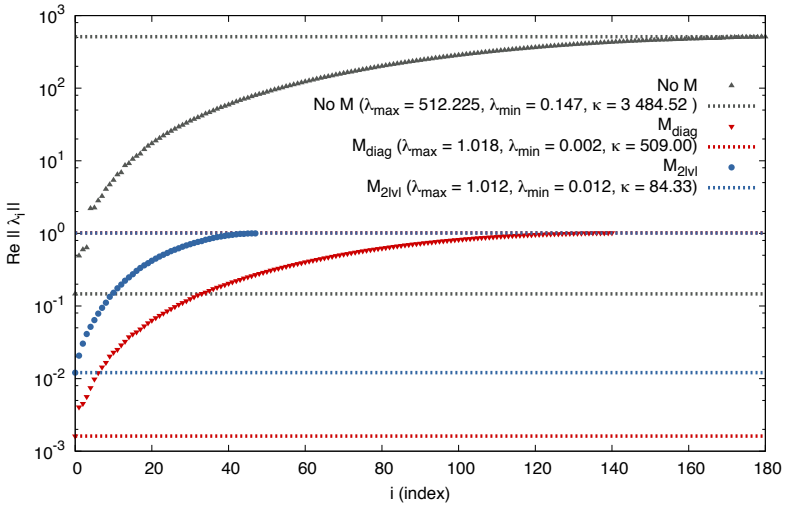


Figure : Eigenvalue distribution of S, $M_{diag}^{-1}S$, $M_{2lvl}^{-1}S$ (NoM, M_{diag}, M_{2lvl} resp. in the plot).

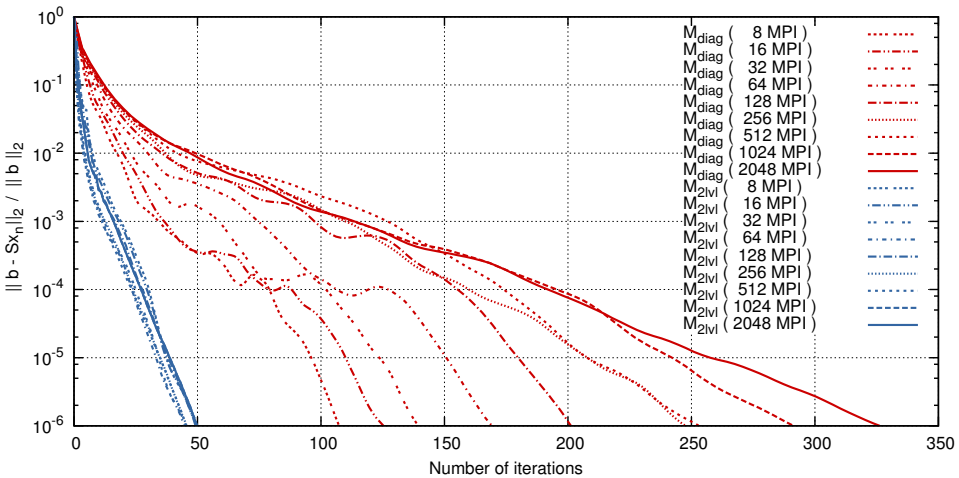
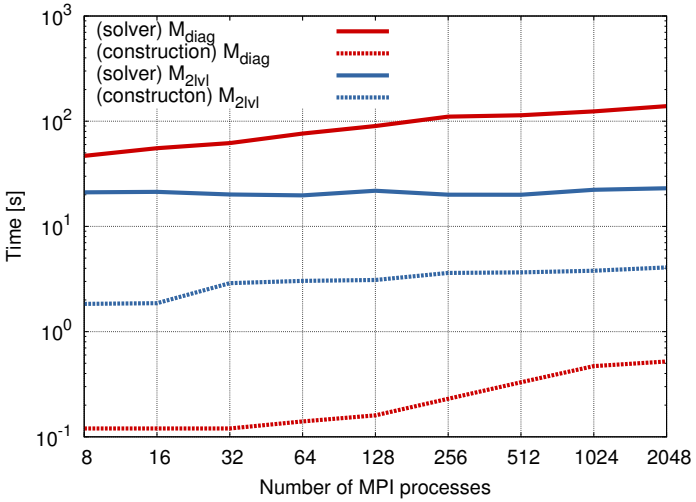
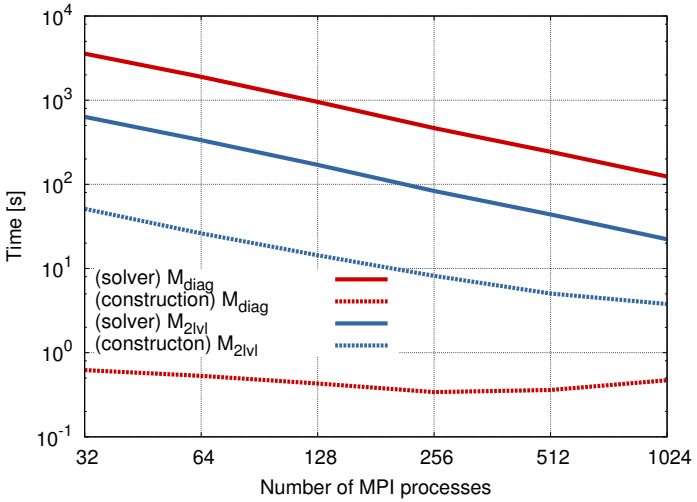


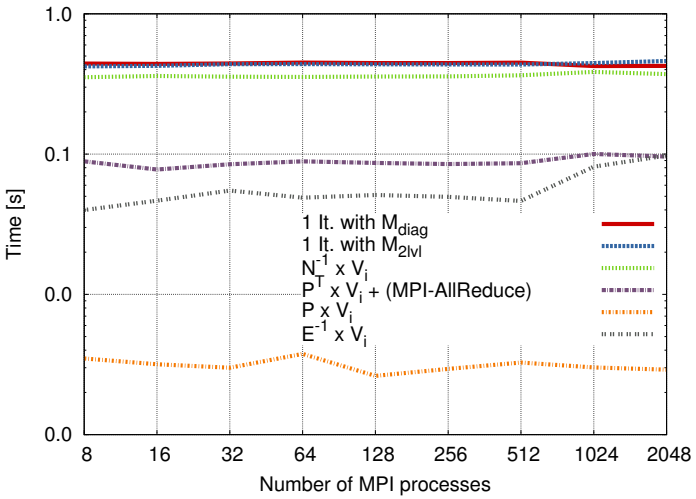
Figure : Convergence of preconditioned CG when increasing the size of the problem, number of circles = no of MPI processes.

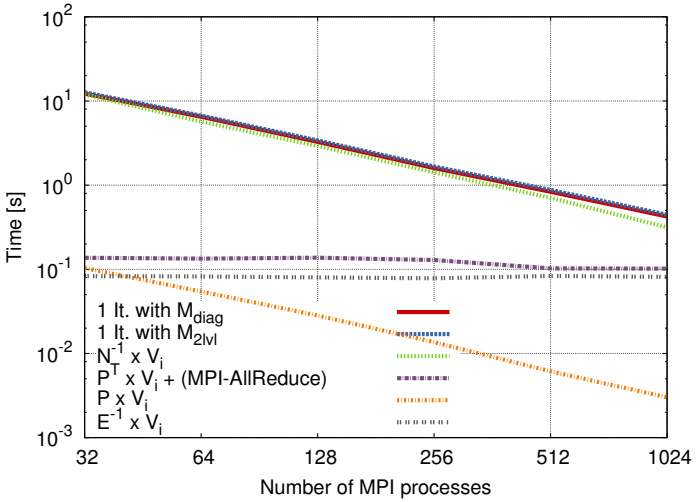
Timings for weak (left) and strong (right) scaling

- 1 or more (for strong scaling) circles per 1 MPI process.
- 1 MPI process mapped on 6 cores of NERSC's Hopper Cray XE6.









Plan

Krylov subspace methods

Tuning sparse matrix-vector product

Iterative solvers that reduce communication

Preconditioners

Extra slides: one level preconditioners

- One level preconditioners: examples

One level preconditioners (two examples)

Incomplete LU factorization

- Computes $A = LU + E$
- Preconditioner $M = LU$
- ILU0 does not introduce any fill in the factors

Block Jacobi preconditioner

Given

$$A = \begin{pmatrix} A_{11} & \dots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \dots & A_{PP} \end{pmatrix}$$

block Jacobi preconditioner is:

$$M = \begin{pmatrix} A_{11} & & \\ & \ddots & \\ & & A_{PP} \end{pmatrix} = \begin{pmatrix} L_{11}\,U_{11} & & \\ & \ddots & \\ & & L_{PP}\,U_{PP} \end{pmatrix} = LU$$

Left-preconditioned system

- A preconditioned matrix powers kernel computes the set basis vectors

$$\{M^{-1}Ay_0, (M^{-1}A)^2y_0, ..., (M^{-1}A)^{s-1}y_0, (M^{-1}A)^s y_0\}$$

  where y_0 is a starting vector and $s \geq 1$.

- The i-th iteration of a Krylov subspace solver preconditioned with $M = LU$ computes $y_i = (LU)^{-1}Ay_{i-1}$ as:

  1. Compute $f = Ay_{i-1}$
  2. Solve $LUy_i = f$ i.e.

     2.1 Solve $Lz = f$ by forward substitution

     2.2 Solve $Uy_i = z$ by backward substitution

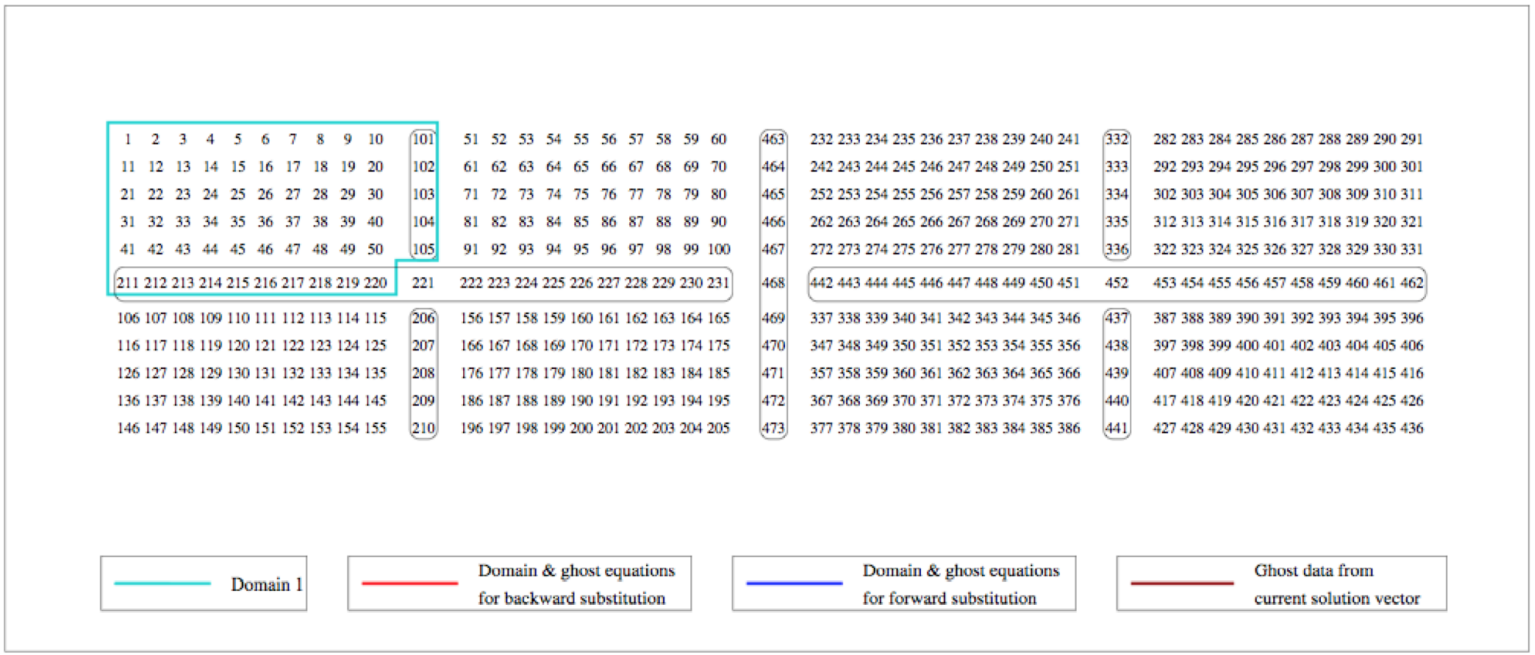
ILU0 with nested dissection

Can we compute s iterations with no communication ?

Compute $y_i = (LU)^{-1} A y_{i-1}$ using 3 steps:

1. Compute $f = A y_{i-1}$
2. Solve $Lz = f$ by forward substitution
3. Solve $U y_i = z$ by backward substitution

$$\begin{pmatrix} A_{11} & & A_{13} & & & & A_{17} \\ & A_{22} & A_{23} & & & & A_{27} \\ A_{31} & A_{32} & A_{33} & & & & A_{37} \\ & & & A_{44} & & A_{46} & A_{47} \\ & & & & A_{55} & A_{56} & A_{57} \\ & & & A_{64} & A_{65} & A_{66} & A_{67} \\ A_{71} & A_{72} & A_{73} & A_{74} & A_{75} & A_{76} & A_{77} \end{pmatrix}$$



Matrix from 5 point stencil on a 2D grid, reordered with nested dissection

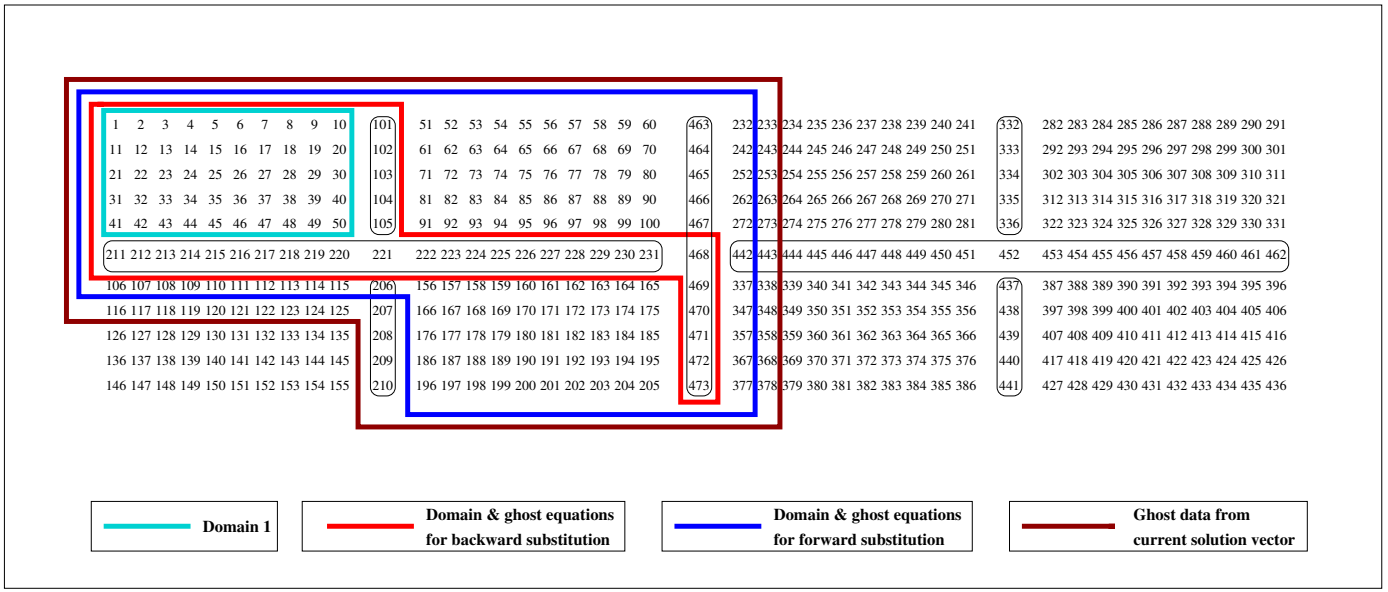
Avoid communication through ghosting

Input: $G(A)$, $G(L)$, $G(U)$,
s, number of steps; α_0, subset of unknowns
Output: Sets β_j, γ_j and δ_j for all $j = 1$ till s
for $i = 1$ *to* s
Find $\beta_i = \mathit{ReachableVertices}(G(U), \alpha_{i-1})$
Find $\gamma_i = \mathit{ReachableVertices}(G(L), \beta_i)$
Find $\delta_i = \mathit{Adj}(G(A), \gamma_i)$
Set $\alpha_i = \delta_i$
end for

Ghost data required for $i = 1 : s$

$$x(\delta_i), A(\gamma_i, \delta_i)$$

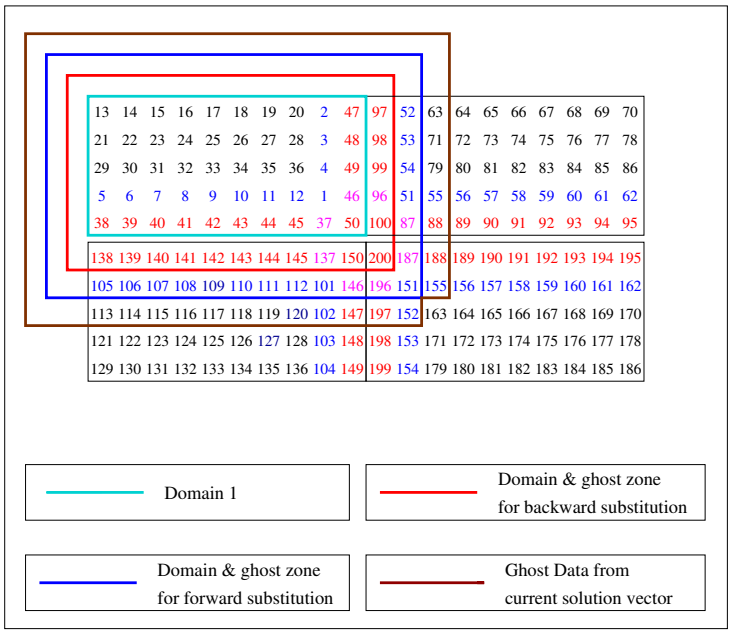
$$L(\gamma_i, \gamma_i), U(\beta_i, \beta_i)$$



⇒ Ghosting not sufficient, one processor does half of the work !

CA-ILU0 with AMML(s) reordering and ghosting

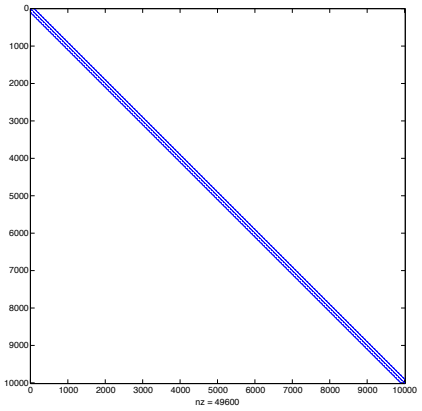
- Reduce volume of ghost data by using Alternating Min-Max Layers (AMML) reordering:
  - First number the vertices at odd distance from the separators,
  - then number the vertices at even distance from the separators.
- No communication required during the construction and the application of CA-ILU0 [Grigori and Moufawad, 2014].

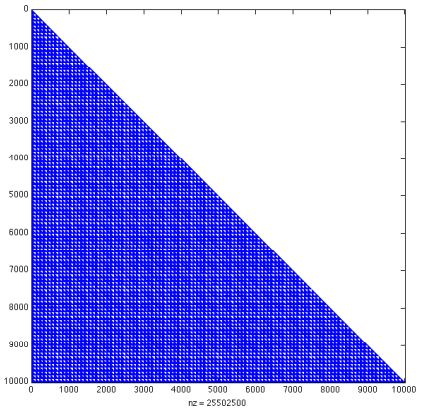


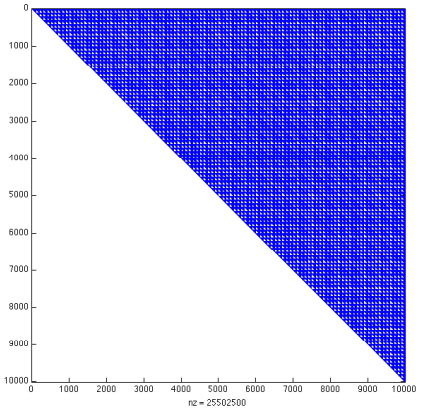
5 point stencil on a 2D grid, nested dissection + AMML(1)

Effect on the inverse of L and U

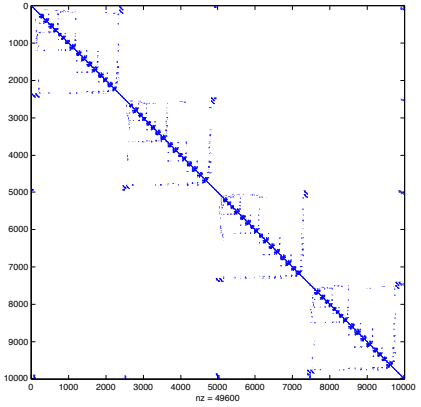
Matrix A in natural order and its L^{-1} and U^{-1} factors

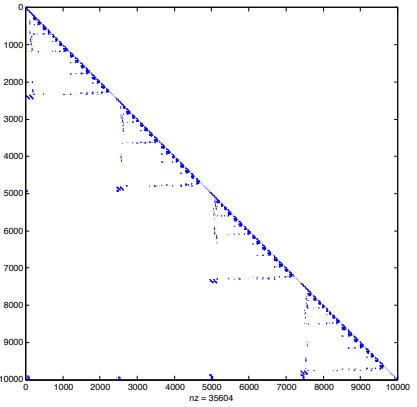


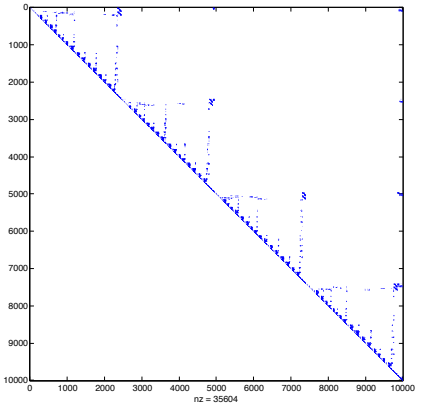




Matrix A with nested dissection and AMML(1) and its L^{-1} and U^{-1} factors







Comparison with block Jacobi

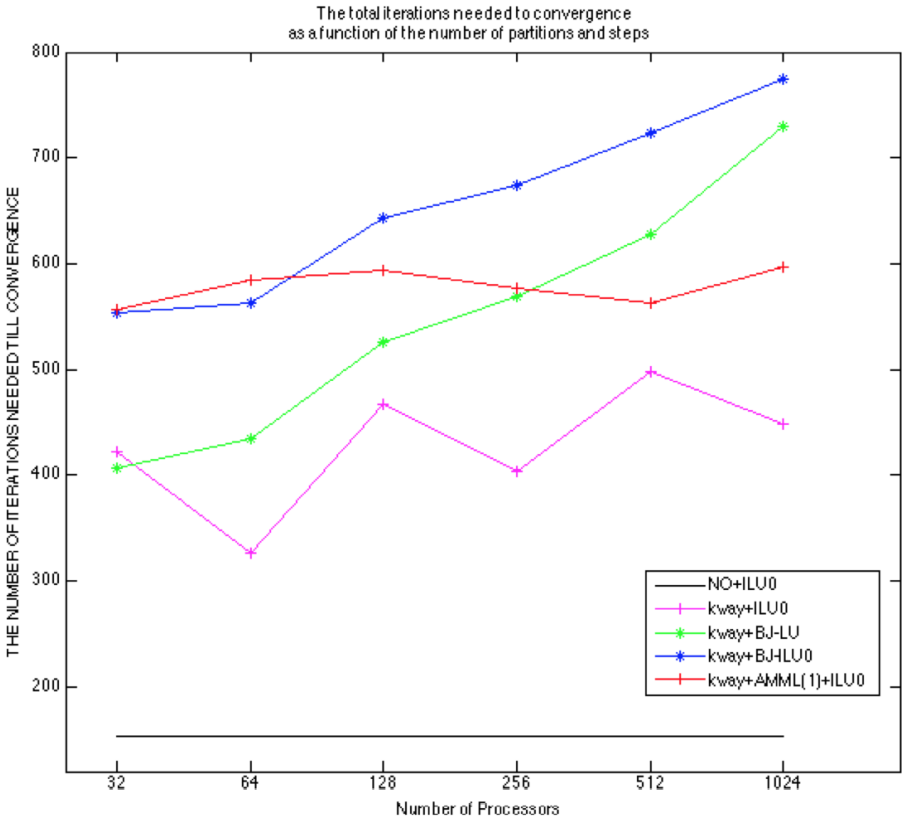
Tests for a boundary value problem (Achdou, Nataf), $40 \times 40 \times 40$ grid

3D Skyscraper Problem - SKY3D

$$
\begin{aligned}
-div(\kappa(x)\nabla u) &= f \text{ in } \Omega \\
u &= 0 \text{ on } \partial\Omega_D \\
\frac{\partial u}{\partial n} &= 0 \text{ on } \partial\Omega_N
\end{aligned}
$$

Methods tested:

- Natural ordering NO+ILU0
- CA-ILU0 - kway+AMML(1)+ILU0
- Block Jacobi using LU - BJ+ILU0
- Block Jacobi using ILU0 - BJ-ILU0



Experimental results

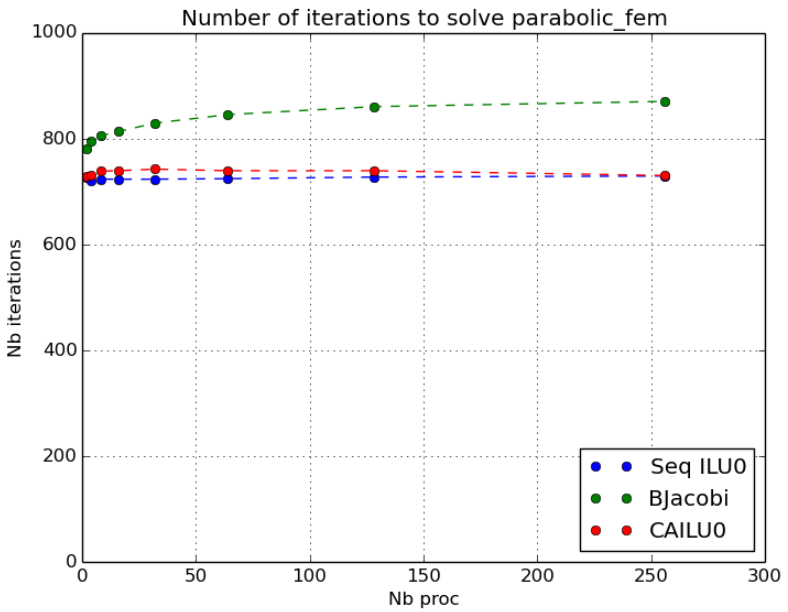


Figure : No of iterations for CA-ILU0 and block Jacobi.

Source: S. Cayrols

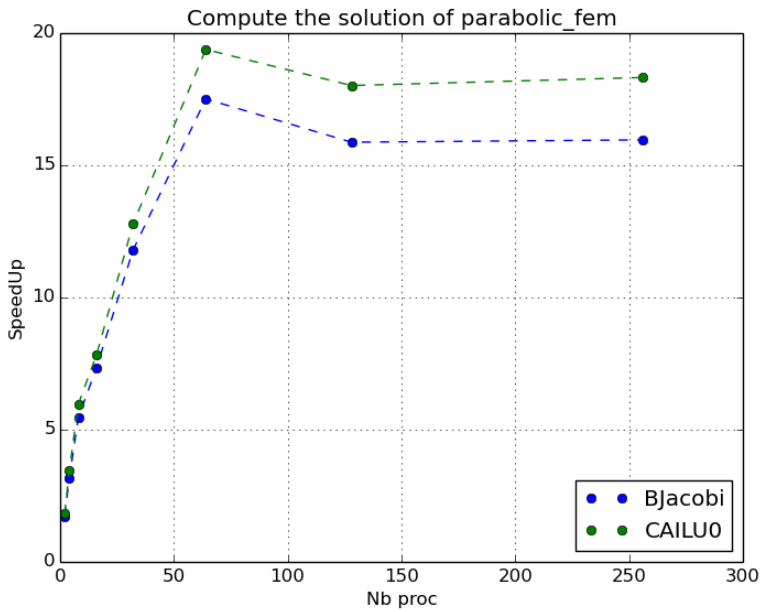


Figure : Speedup with respect to ILU0 from PETSc

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