



## Code Synthesis for Automatic Tuning

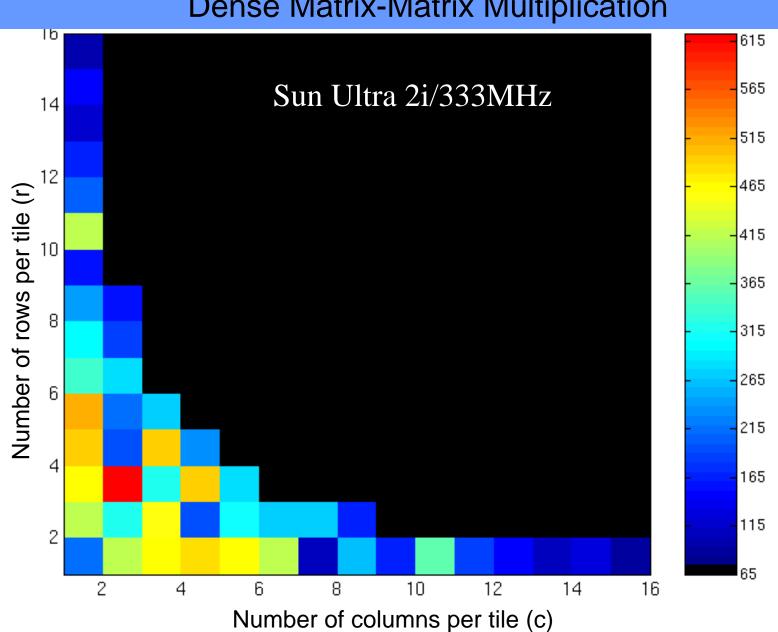
#### Kathy Yelick

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# Automatic Performance Tuning

- Motivation: replace hand tuning of computational kernels
  - Tedious and difficult
  - Too hard to keep up with new architectures, compilers, kernels
  - Sometimes tuning must be done at runtime
- Automatic performance tuning:
  - Approach
    - Generate "space" of candidate algorithms
    - Search space for best one
  - Examples
    - ATLAS adopted by Matlab and elsewhere
    - PHiPAC ATLAS predecessor
    - FFTW 1999 Wilkinson Prize for Numerical Software
    - Spiral signal processing
    - Sparsity/OSKI sparse matrix-vector multiply

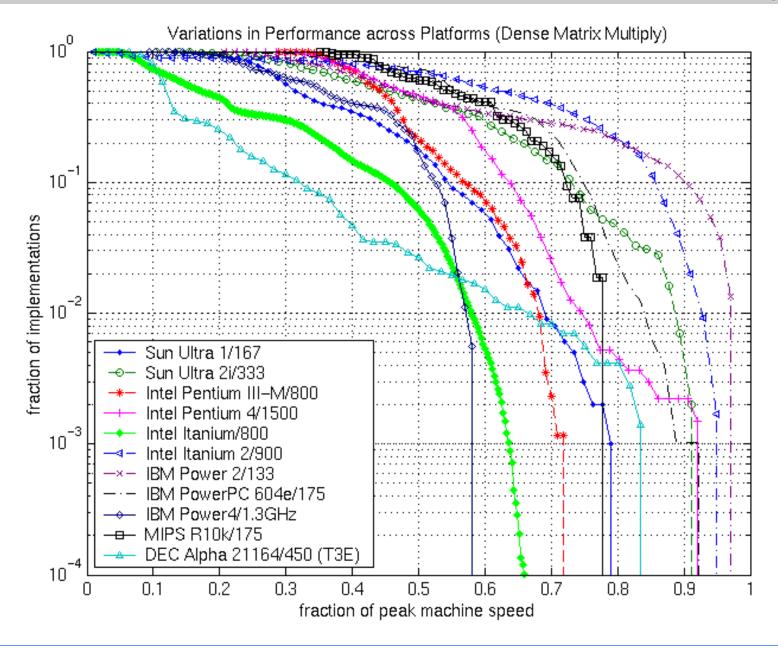


Finding the best block size is like finding a needle in a haystack!

#### **Dense Matrix-Matrix Multiplication**

#### Most Implementations are Not Good

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7 numerical methods domain scientific computing

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Atlas

- 1. Structured Grids (including adaptive)
- 2. Unstructured Grids
- 3. Spectral methods (Fast Fourier Transform) ← FFTW
- 4. Dense Linear Algebra
- 5. Sparse Linear Algebra
- 6. Particle Methods
- 7. Monte Carlo

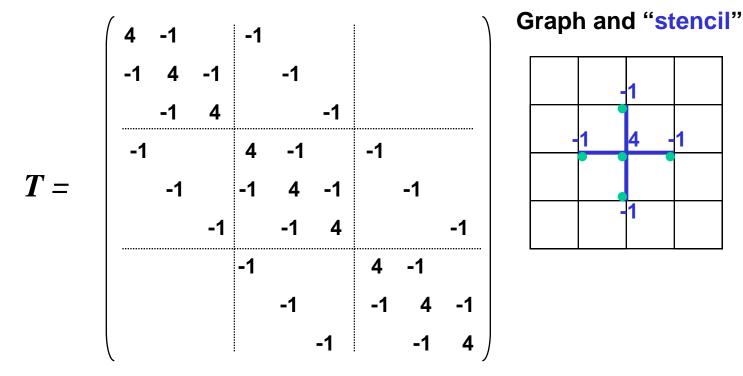
Well-defined targets from algorithmic, software, and architecture standpoint

Slide from "Defining Software Requirements for Scientific Computing", Phillip Colella, 2004



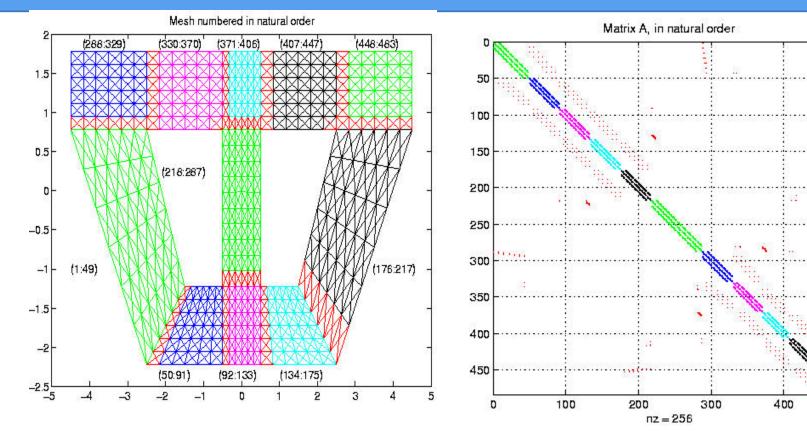
#### Stencil on Grid $\rightarrow$ Matrix Vector Multiply on Matrix

- Shown for the 2D case, the matrix T is now
  - Grid points numbered left to right, top row to bottom row



Similar to "adjacency matrix" for arbitrary graph

#### Conversion between a mesh and matrix

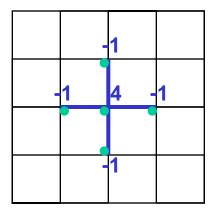


Hidden slide: shown in earlier lecture on sources of parallelism



#### **Project Proposal: Stencil Generator**

- Stencil operations on regular meshes are very common and have many variations
  - Dimension: 1D (e.g. 3pt), 2D (5pt or 9pt), 3D (7pt or 27pt)
  - Shape: 1D (e.g. 3pt), 2D (5pt or 9pt), 3D (7pt or 27pt), they need not be regular
  - Band: just your immediate neighbors (band=1), or their neighbor (band=2), or...
  - Balanced or unbalanced in various directions (isotropic, anisotropic)
  - coefficients (NAS MG)
    - constant, 1 point and all others
    - constant, 1 point and distance-based coefficients
    - variable, relative to each position
  - Update in place vs. 2<sup>nd</sup> grid
  - Colored algorithms (red-black in 2D)





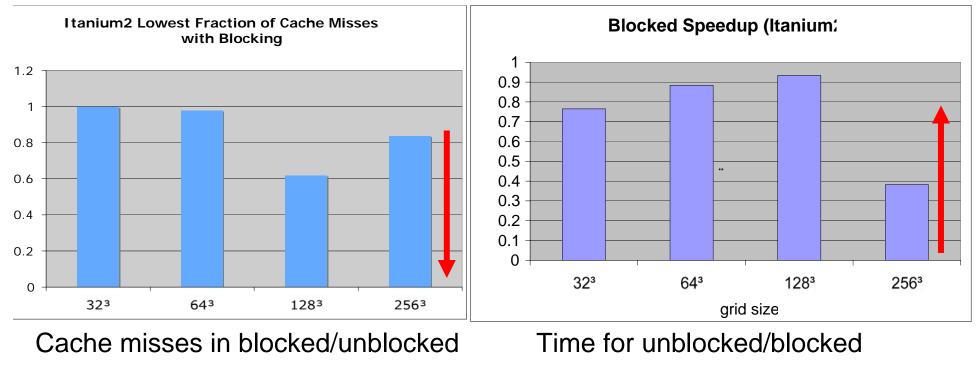
# **Optimizing Stencils**

- Stencil operations have simple structure
  - Loop nest with single assignment in the simple case
  - Real applications use these and more complicated cases
- Low floating point rate:
  - Typically ~1 FLOP per load
  - Good spatial locality, but little temporal locality (re-use)
  - Run at small fraction of peak (<15%)!</p>
- Optimizations:
  - Improve reuse within a sweep through the grid
  - Tile to improve chance that previous plane (or row) is still in cache when the neighboring one is processes

## **Tiling Stencil Computations**

- Several papers on tiling stencil computations
  - E.g., Rivera and Tseng SC2002, ...
- Old Conventional Wisdom

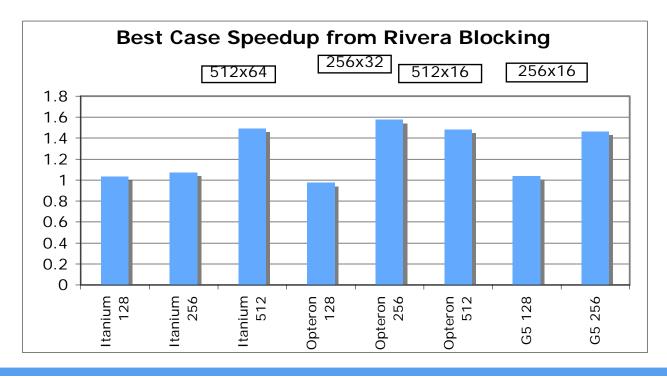
Cache misses are the most important factor



#### **Stencil Probe Cache Blocking Revisited**

New Conventional Wisdom: Prefetching is as important as caching

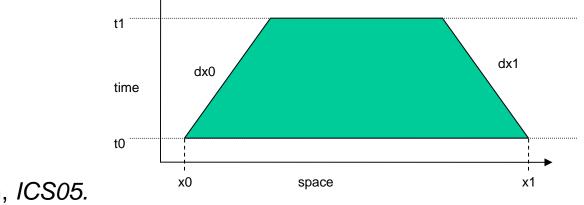
- Little's Law (Bailey '97): need data in-flight = latency \* bandwidth Cache blocking is useful for
- 1. large grid sizes: 3 planes do not fit in cache for 3D problem
- 2. do not cut/block the unit-stride dimension



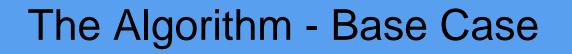


# **Blocking Over Time / Iterations**

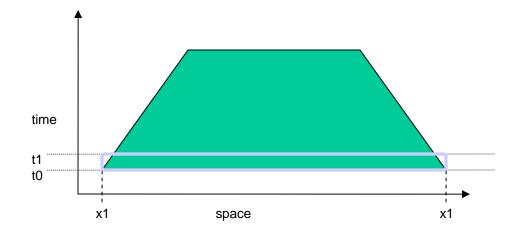
- Can we do better than this?
  - Code is still severely limited by memory bandwidth
- For some computations, you can merge across k sweeps over the grid
  - Re-use data k times (as well as re-use within a plane)
- Dependencies produce pyramid patterns



Frigo & Strumpen, ICS05.



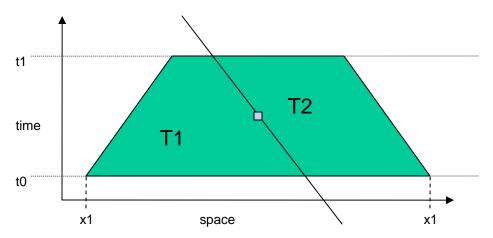
If the height is 1 (ie t1-t0=1) then we simply have a line of points (t0,x) where  $x0 \le x \le x$ . Do the kernel on this set of points. Order does not matter (no interdependencies).





#### The Algorithm - Space Cut

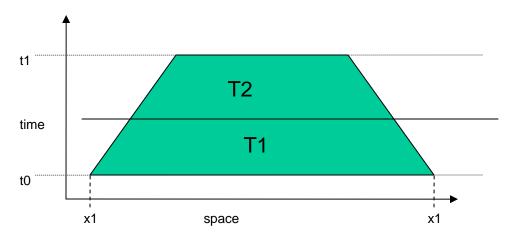
 If the width <= 2\*height, then cut with slope=-1 through the center.



 Do T1, then T2. No point in T1 depends on values from T2.

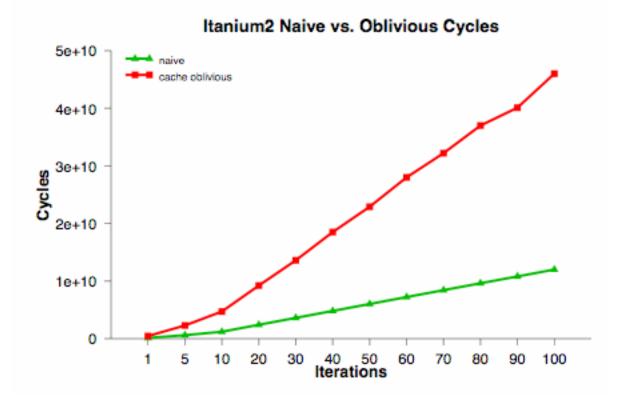
## The Algorithm - Time Cut

• Otherwise, cut trapezoid in half in the time dimension.

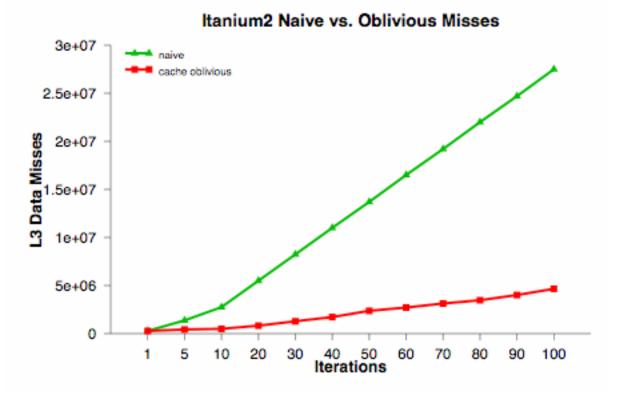


 Do T1, then T2. No point in T1 depends on values of T2.

#### Initial Results - Itanium2

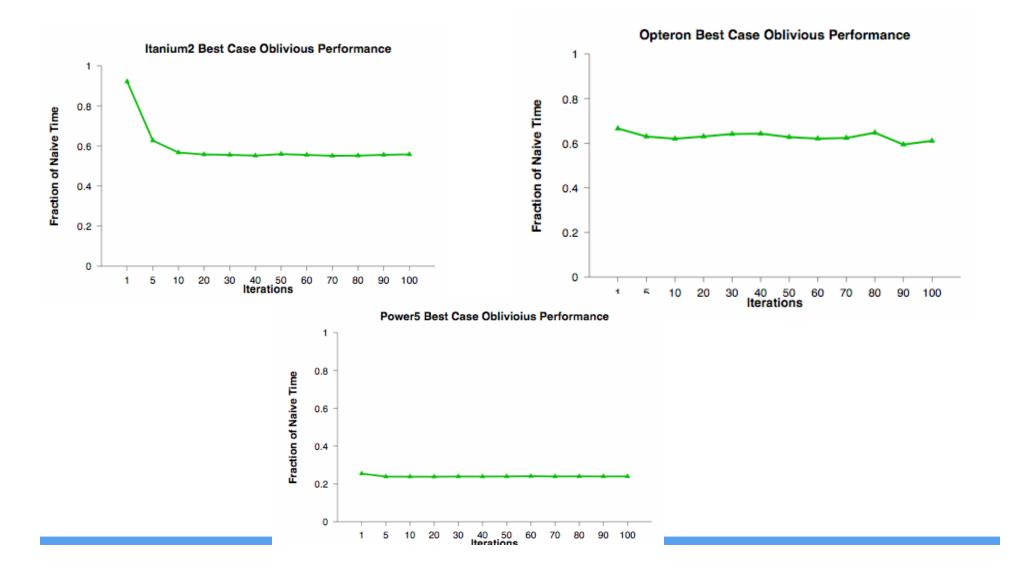


#### Initial Results - Itanium2



#### **Best Performance**





#### **Project Idea Revisited**



- Only limited stencils (3D 7pt)
- Applications use many different stencils
  - Requested work by apps folks
- Paper by S. Kamil, Oliker, Shalf so that many optimizations are needed to make it really work
- Recursion is useful for understanding the algorithm
  - Can't use recursion all the way to the bottom
  - A fixed tiling approach may work as well
  - Key inside is tile shapes: Pyramids and Parallelopipeds

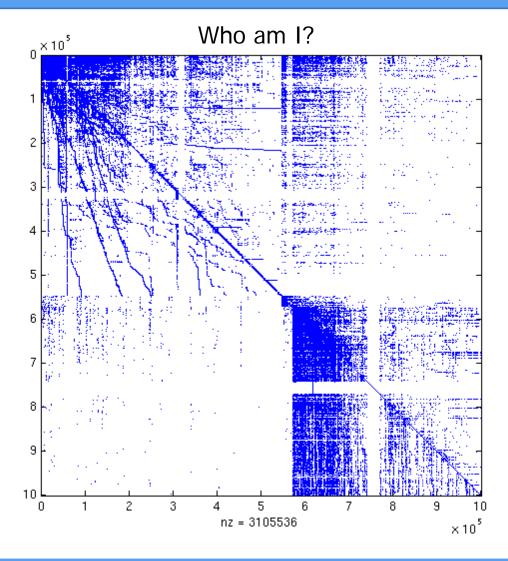




## **General Sparse Matrix Case**

- If this works for stencils, what about arbitrary matrices?
- Tuning arbitrary matrices
  - Project: code generator that is more flexible, maintainable, extensible than current approach
- The time-blocked approach extended to matrices
  - $A^{k} * x$
  - Intuition: most of cost in A\*x is reading matrix A
  - Can we read A once and do k operations with it?
- Notes:
  - "Time" is used loosely; this is typically iterations in a solver
  - Many numerical "details" to make A<sup>k</sup> \* x useful [Hoemmen]

#### A "Familiar" Sparse Matrix





I am a Big Repository Of useful And useless Facts alike.

#### Who am I?

(Hint: Not your e-mail inbox.)

## Motivation for Tuning Sparse Matrices

- Sparse matrix kernels can dominate solver time
  - Sparse matrix-vector multiply (SpMV)
  - SpMV: runs at < 10% of peak</p>
- Improving SpMV's performance is hard
  - Performance depends on machine, kernel, matrix
  - Matrix known only at run-time
  - Best data structure + implementation can be surprising
  - Tuning becoming more difficult over time
- Approach: Empirical modeling and search
  - Off-line benchmarking + run-time models
  - Up to 4x speedups and 31% of peak for SpMV
  - Other kernels: **1.8x** triangular solve, **4x**  $A^{T}A \cdot x$ , **2x**  $A^{2} \cdot x$

## **OSKI: Optimized Sparse Kernel Interface**

- Sparse kernels tuned for user's matrix & machine
  - Hides complexity of run-time tuning
  - Low-level BLAS-style functionality
  - Includes fast locality-aware kernels:  $A^T A \cdot x$ ,  $A^k \cdot x$  ...
  - Initial target: cache-based superscalar uniprocessors
- Target users: "advanced" users & solver library writers
- Current focus on uniprocessor tuning
  - Shared/distributed memory versions in progress
- Open-source (BSD) C library
  - 1.0 available: bebop.cs.berkeley.edu/oski
  - Recently integrated into PETSc

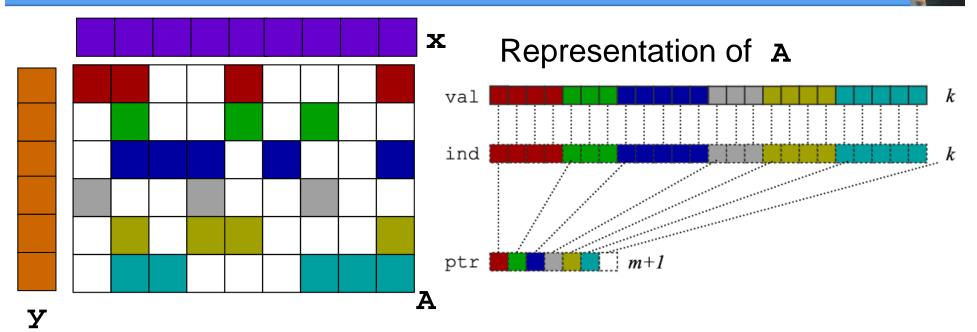




#### **Road Map**

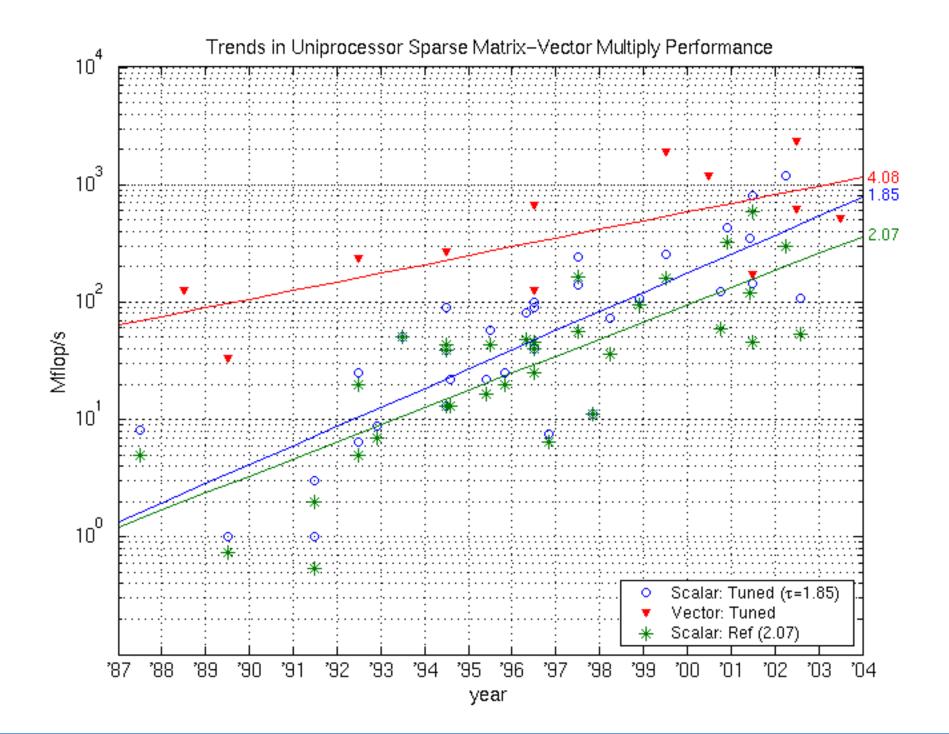
- Sparse matrix-vector multiply (SpMV) review
  - Why doesn't my compiler solve the problem?
- Historical trends
- Automatic tuning in OSKI
- Future work

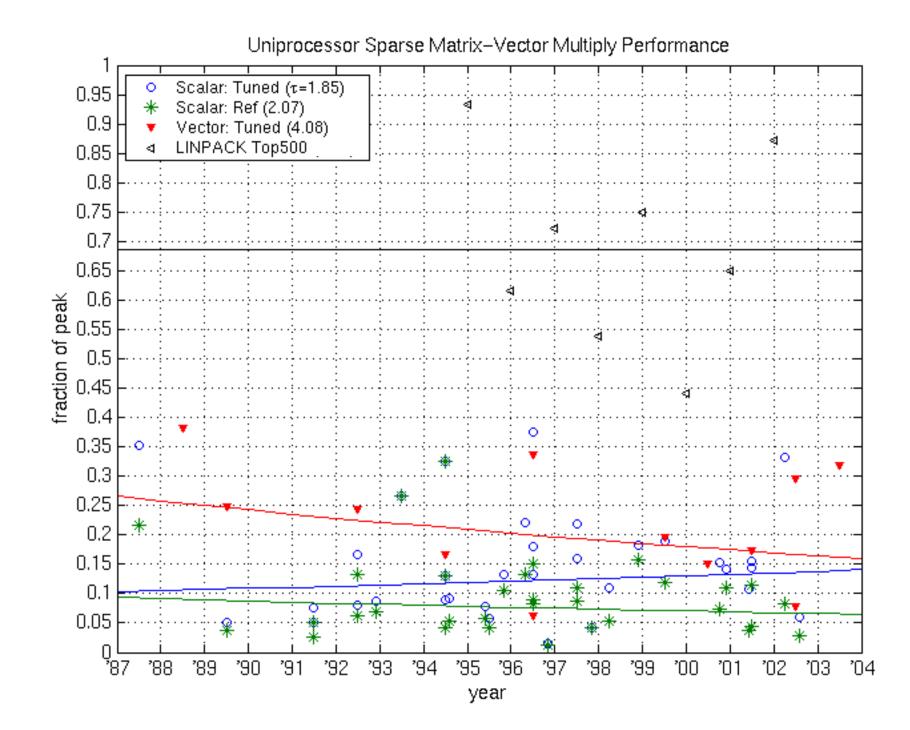
## Compressed Sparse Row (CSR) Storage



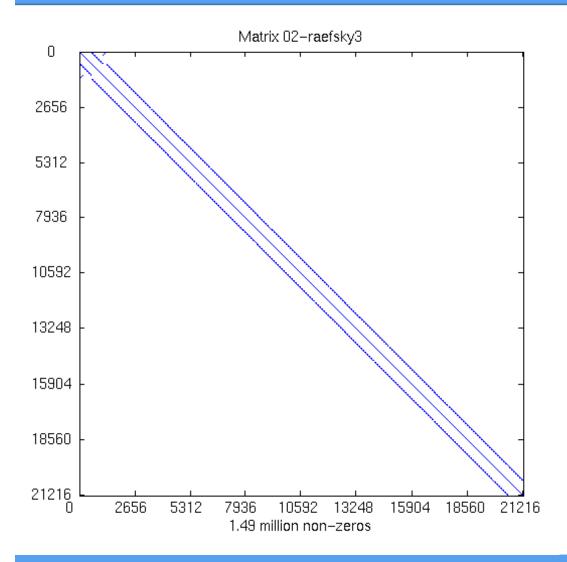
Matrix-vector multiply kernel:  $y(i) \leftarrow y(i) + A(i,j) \cdot X(j)$ 

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





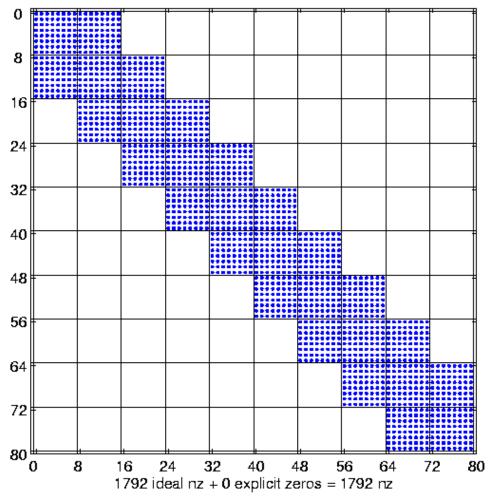
## Example: The Difficulty of Tuning



- n = 21216
- nnz = 1.5 M
- kernel: SpMV
- Source: NASA structural analysis problem



## Example: The Difficulty of Tuning



#### Matrix 02-raefsky3

- n = 21216
- nnz = 1.5 M
- kernel: SpMV
- Source: NASA structural analysis problem
- 8x8 dense substructure



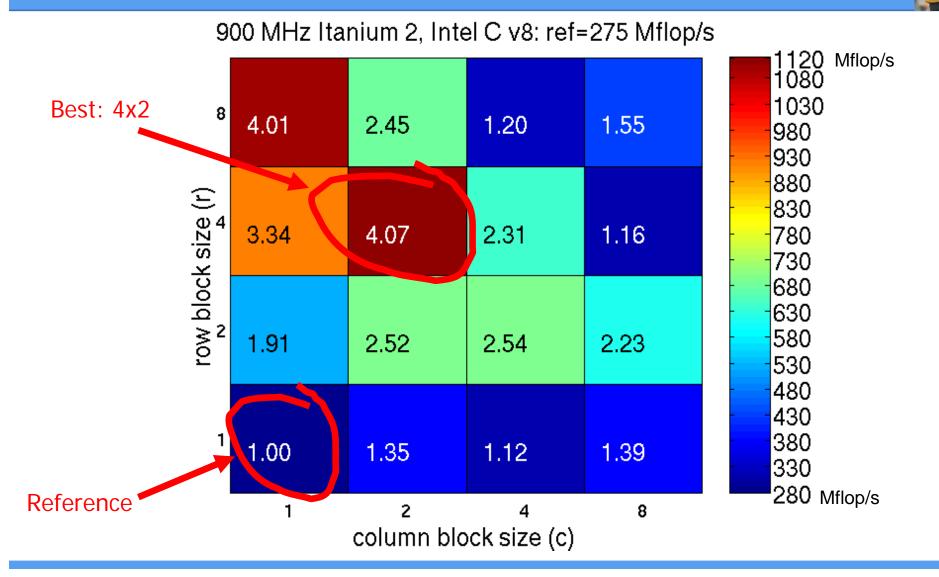
#### What We Expect

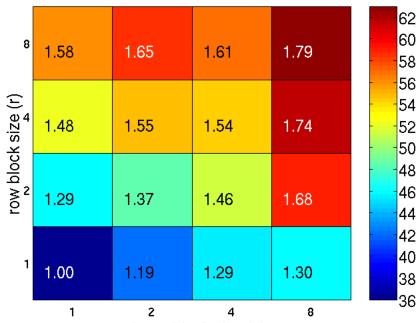
#### Assume

- Cost(SpMV) = time to read matrix
- 1 double-word = 2 integers
- r, c in {1, 2, 4, 8}
- CSR: 1 int / non-zero
- BCSR(r x c): 1 int / (r\*c non-zeros)
- As r\*c increases, speedup should
  - Increase smoothly
  - Approach 1.5

$$Speedup = \frac{T_{CSR}}{T_{BCSR}(r,c)} \approx \frac{1.5}{1 + \frac{1}{rc}} \xrightarrow{r,c=\infty} 1.5$$

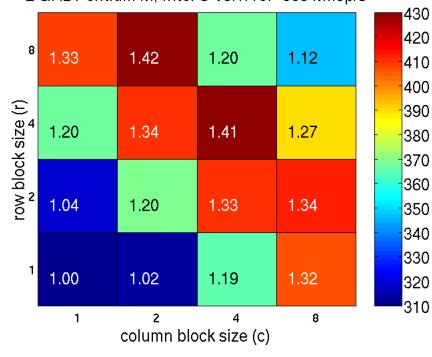
#### What We Get (The Need for Search)



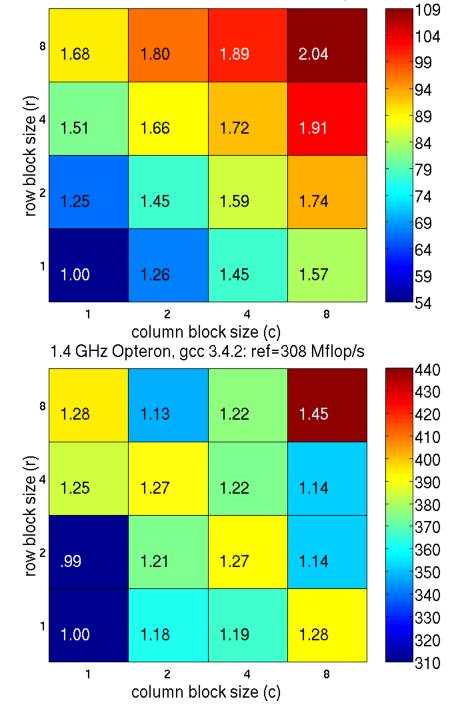


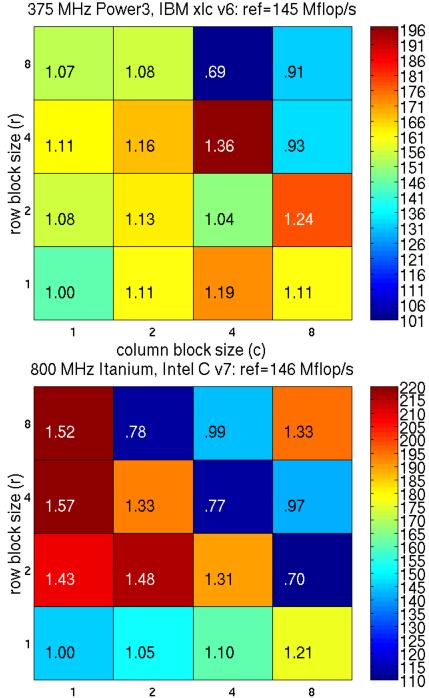
333 MHz Sun Ultra 2i, Sun C v6.0: ref=35 Mflop/s

#### column block size (c) 2 GHz Pentium M, Intel C v8.1: ref=308 Mflop/s



900 MHz Ultra 3, Sun CC v6: ref=54 Mflop/s





column block size (c)



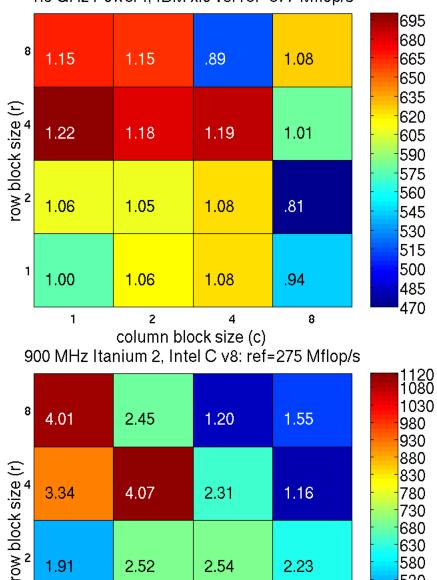
1.91

1.00

1

1

1.3 GHz Power4, IBM xlc v6: ref=577 Mflop/s



280

2 column block size (c)

2.54

1.12

4

2.23

1.39

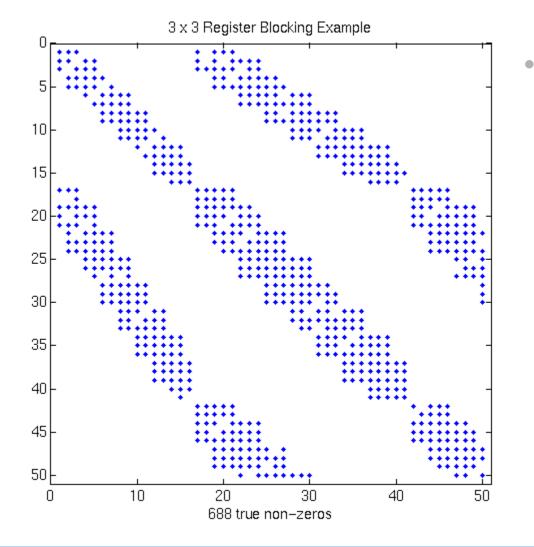
8

2.52

1.35

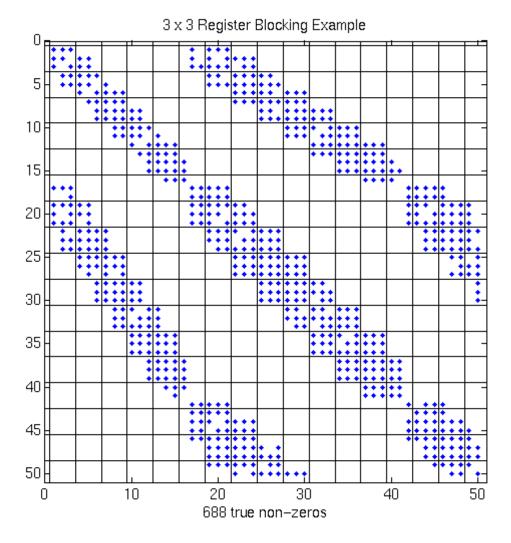


#### **Still More Surprises**



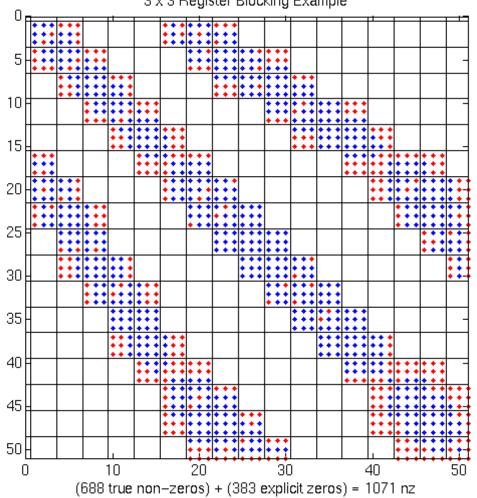
More complicated non-zero structure in general





- More complicated non-zero structure in general
- Example: 3x3 blocking
   Logical grid of 3x3 cells

#### Extra Work Can Improve Efficiency!



3 x 3 Register Blocking Example

- 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!



#### Observations

- ++ Moore's law like behavior
- ----- "Untuned" is 10% peak or less, worsening
- ++ "Tuned" roughly 2x better today, and growing ---- Tuning is complex
- LINPACK not representative of sparse apps



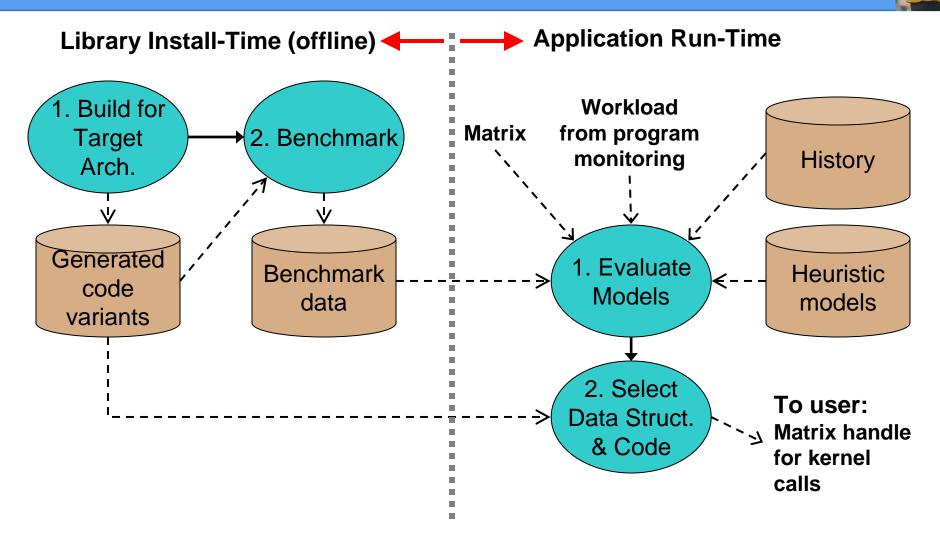






- Historical trends and the need for search
- Automatic tuning in OSKI
  - How does OSKI work?
- Current and future work

### How OSKI Tunes (Overview)



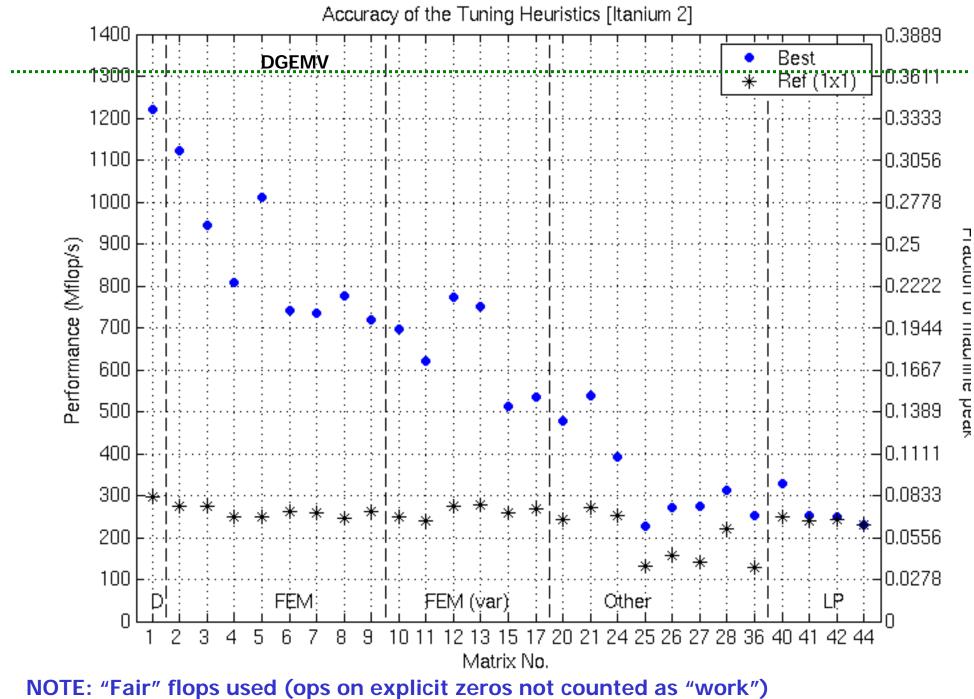
Extensibility: Advanced users may write & dynamically add "Code variants" and "Heuristic models" to system.

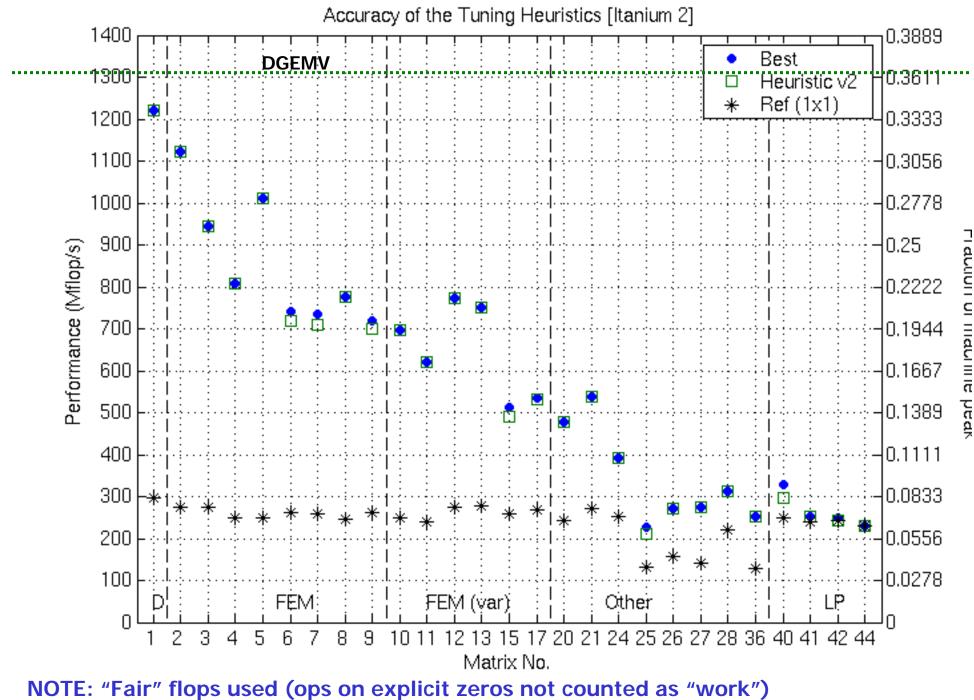
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## **Example of a Tuning Heuristic**

- Example: Selecting the r x c block size
  - Off-line benchmark: characterize the machine
    - Precompute Mflops(r,c) using dense matrix for each r x c
    - Once per machine/architecture
  - Run-time "search": characterize the matrix
    - Sample A to estimate Fill(r,c) for each r x c
  - Run-time heuristic model
    - Choose r, c to maximize Mflops(r,c) / Fill(r,c)
- Run-time costs
  - Up to ~40 SpMVs (empirical worst case)
  - Dominated by conversion
  - May be amortized if pattern fixed





יו מרמחוו חו ווומרווווב נתמי



## Calling OSKI: Interface Design

- Support "legacy applications"
  - Gradual migration of apps to use OSKI
- Must call "tune" routine explicitly
  - Exposes cost of tuning and data structure reorganization
- May provide tuning hints
  - Structural: Hints about matrix
  - Workload: Hints about frequency of calls, to limit tuning time
- May save/restore tuning results
  - To apply on future runs with similar matrix
  - Stored in "human-readable" format



### How to Call OSKI: Basic Usage

- May gradually migrate existing apps
  - Step 1: "Wrap" existing data structures
  - Step 2: Make BLAS-like kernel calls

int\* ptr = ..., \*ind = ...; double\* val = ...; /\* Matrix, in CSR format \*/
double\* x = ..., \*y = ...; /\* Let x and y be two dense vectors \*/

/\* Compute y = β·y + α·A·x, 500 times \*/
for( i = 0; i < 500; i++ )
 my\_matmult( ptr, ind, val, α, x, β, y );</pre>



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/\* Step 1: Create OSKI wrappers around this data \*/
oski\_matrix\_t A\_tunable = oski\_CreateMatCSR(ptr, ind, val, num\_rows,
 num\_cols, SHARE\_INPUTMAT, ...);
oski\_vecview\_t x\_view = oski\_CreateVecView(x, num\_cols, UNIT\_STRIDE);
oski\_vecview\_t y\_view = oski\_CreateVecView(y, num\_rows, UNIT\_STRIDE);

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/\* Compute y =  $\beta \cdot y + \alpha \cdot A \cdot x$ , 500 times \*/
for( i = 0; i < 500; i++ )
 oski MatMult(A\_tunable, OP\_NORMAL,  $\alpha$ , x\_view,  $\beta$ , y\_view);/\* Step 2 \*/

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```
How to Call OSKI: Tune with Explicit Hints
```

```
    User calls "tune" routine
```

May provide explicit tuning hints (OPTIONAL)

```
oski_matrix_t A_tunable = oski_CreateMatCSR( ... );
```

/\* ... \*/

/\* Tell OSKI we will call SpMV 500 times (workload hint) \*/

```
oski_SetHintMatMult(A_tunable, OP_NORMAL, α, x_view, β, y_view, 500);
/* Tell OSKI we think the matrix has 8x8 blocks (structural hint) */
oski_SetHint(A_tunable, HINT_SINGLE_BLOCKSIZE, 8, 8);
```

```
oski_TuneMat(A_tunable); /* Ask OSKI to tune */
```

```
for( i = 0; i < 500; i++ )</pre>
```

```
oski_MatMult(A_tunable, OP_NORMAL, \alpha, x_view, \beta, y_view);
```

# How the User Calls OSKI: Implicit Tuning

#### Ask library to infer workload

- Library profiles all kernel calls
- May periodically re-tune

```
oski_matrix_t A_tunable = oski_CreateMatCSR( ... );
    /* ... */
for( i = 0; i < 500; i++ ) {
    oski_MatMult(A_tunable, OP_NORMAL, α, x_view, β, y_view);
    oski_TuneMat(A_tunable); /* Ask OSKI to tune */
}</pre>
```

# Saving and Restoring Tuning Transformations

 May selecting customized, complex transformations using embedded scripting language (OSKI-Lua)

```
/* In "my_app.c" */
fp = fopen("my_xform.txt", "rt");
fgets(buffer, BUFSIZE, fp);
```

```
oski_ApplyMatTransform(A_tunable,
    buffer);
oski MatMult(A tunable, ...);
```

- # In file, "my\_xform.txt"
- # Compute A<sub>fast</sub> = P\*A\*P<sup>T</sup> using Pinar's reordering algorithm
- A\_fast, P =
   reorder\_TSP(InputMat);
- # Split A<sub>fast</sub> = A<sub>1</sub> + A<sub>2</sub>, where A<sub>1</sub> in 2x2 block format, A<sub>2</sub> in CSR
- A1, A2 =
   A fast.extract blocks(2, 2);

return transpose(P)\*(A1+A2)\*P;



## **Additional Features**

- Currently 5 tunable kernels
  - SpMV, triangular solve,  $A \cdot x \& A^T \cdot w$ ,  $A^T A \cdot x$ ,  $A^k \cdot x$
- Support for several scalar type combinations
  - {32-bit, 64-bit int} x {single, double prec.} x {real, complex}
- "Plug-in" extensibility
  - Very advanced users may customize library (at run-time)
    - New heuristics (*e.g.*, Buttari, et al.)
    - Alternative data structures & code variants (*e.g.*, seg-scan for vector architectures)

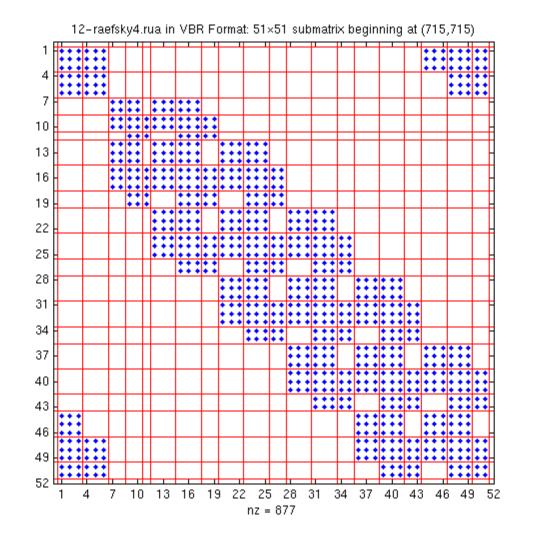


## **Exploiting Problem-Specific Structure**

- Optimizations for SpMV
  - Register blocking (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 (2.2x over CSR)
  - Multiple vectors (7x over CSR)
  - And combinations...
- Sparse triangular solve
  - Hybrid sparse/dense data structure (1.8x over CSR)
- Higher-level kernels
  - $AA^{T} x$ ,  $A^{T}A x$  (4x over CSR, 1.8x over RB)
  - $A^2 \cdot x$  (2x over CSR, 1.5x over RB)



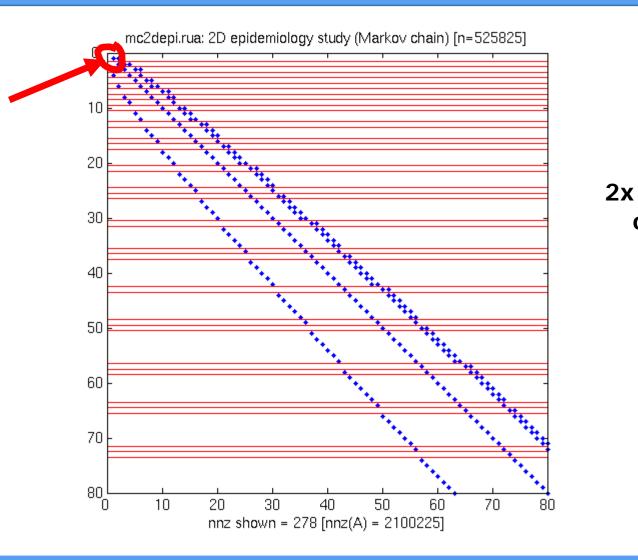
#### **Example: Variable Block Structure**



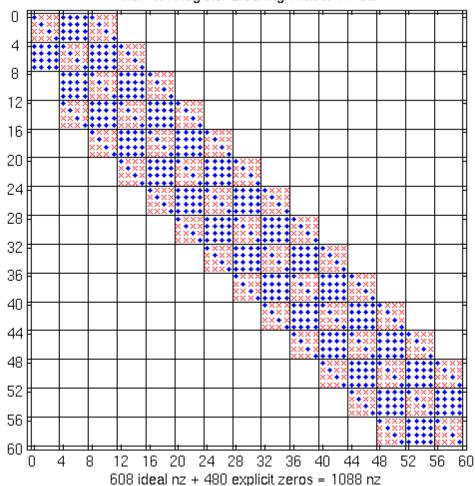
2.1x over CSR 1.8x over RB

over CSR

#### **Example: Row-Segmented Diagonals**



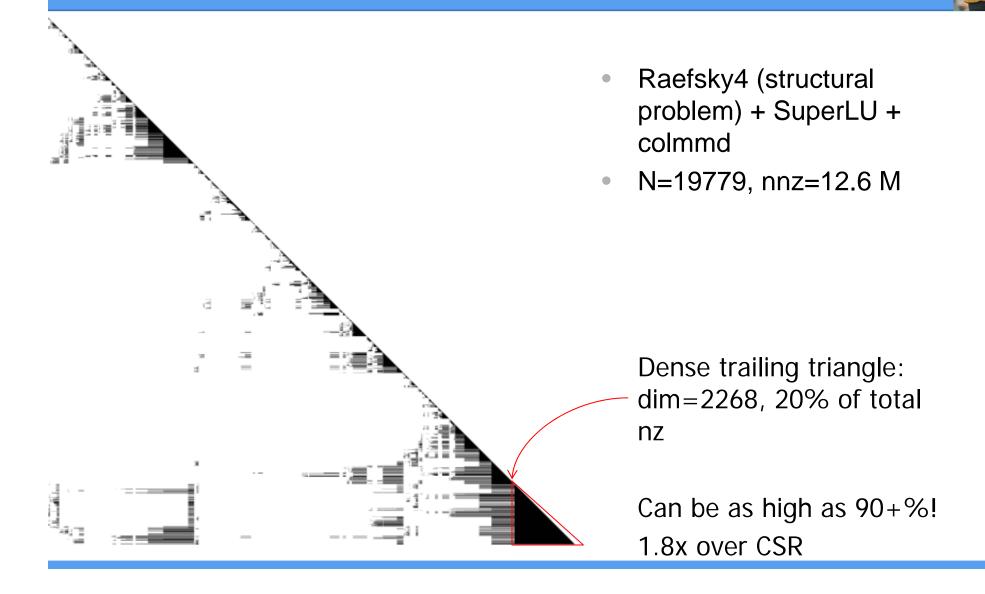
#### **Mixed Diagonal and Block Structure**



After 4x4 Register Blocking: Matrix 11-bai



#### **Example: Sparse Triangular Factor**



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- **Cache-level:** Interleave multiplication by  $A, A^T$
- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning in OSKI
- **Current and future work**

Current and future work
$$AA^{T} \cdot x = \begin{pmatrix} a_{1} \Lambda & a_{n} \end{pmatrix} \begin{pmatrix} a_{1}^{T} \\ M \\ a_{n}^{T} \end{pmatrix} \cdot x = \sum_{i=1}^{n}$$

"axpy"

dot product

- **Register-level**:  $a_i^T$  to be  $r \times c$  block row, or diag row
- Algorithmic-level transformations for A<sup>2</sup>\*x, A<sup>3</sup>\*x, ...

### **Example applications**

- T3P Accelerator Design Ko
  - Register blocking, Symmetric Storage, Multiple vector
  - 1.68x faster on Itanium 2 for one vector
  - 4.4x faster for 8 vectors
- Omega3P Accelerator Design Ko
  - Register blocking, Symmetric storage, Reordering
  - 2.1x faster on Power4
- Semiconductor Industry:
  - 1.9x speedup over SPOOLES in CG at design firm
- Recent integration of OSKI into PETSc



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## Status and Future Work

- OSKI Release 1.0 and docs available
   bebop.cs.berkeley.edu/oski
- Performance bounds modeling (ongoing)
- Future OSKI work
  - Release of PETSc version with OSKI
  - Better "low-level" tuning, including vectors
  - Automatically tuned parallel sparse kernels
- Development of a new HPC Challenge Benchmark
  - Evaluate platforms based on tuned (blocked) SpMV performance
- Tuning higher level algorithms using A<sup>k</sup>x
  - Models indicate large speedups possible





#### **Current SPMV OSKI Code Generator**

```
#!/bin/bash
                                                                                 if test ${GENMAKE} = yes ; then
                                                                                        makestub=Make.${mattype}
#
# This script uses some bash extensions.
                                                                                        echo "#
                                                                                 # Automatically generated by $USER@`hostname`
#
                                                                                 # on `date`, running $0
mattype=BCSR
                                                                                 #
                                                                                 " > ${makestub}
if test x" = x; then
                                                                                 fi
       echo ""
       echo "usage: $0 {full, source, makestub}"
                                                                                 for R in 1 2 3 4 5 6 7 8 ; do # row block size
       echo ""
                                                                                 for C in 1 2 3 4 5 6 7 8 ; do # column block size
       exit 1
fi
                                                                                        echo "${MATTYPE} ${R}x${C}..."
GENSOURCE="
                                                                                        outfile=${R}x${C}.c
GENMAKE="
case $1 in
                                                                                        if test ${GENSOURCE} = yes ; then
[fF]*) GENSOURCE=yes ; GENMAKE=yes ;;
                                                                                                     CreateOutfile ${R} ${C} ${outfile}
[sS]*) GENSOURCE=yes ; GENMAKE=no ::
[mM]*) GENSOURCE=no ; GENMAKE=yes ;;
                                                                                                    for OP in normal trans conj herm ; do # transpose option
*) echo "*** Unknown option, '$1' ***" ; exit 1 ;;
                                                                                                    for S in 1 general; do # stride
esac
                                                                                                                       WriteKernel ${R} ${C} ${OP} ${S} ${outfile}
                                                                                                     done # S
CreateOutfile() {
                                                                                                    WriteShell_v1 ${OP} ${outfile}
#-----
                                                                                                    WriteShell ${OP} ${R} ${C} ${outfile}
# args: <R> <C> <outfile>
#
                                                                                                     done # OP
R=$1
C=$2
                                                                                                    WriteMatReprMult ${R} ${C} ${outfile}
outfile=$3
                                                                                                    WriteFooter ${outfile}
                                                                                        fi
echo "/**
* \\file ${mattype}_${R}x${C}.c
* \\brief ${mattype} ${R}x${C} SpMV implementation, for all transpose
                                                                                        if test ${GENMAKE} = yes ; then
                                                                                                    WriteMakeStub ${R} ${C} ${makestub}
       options.
* \\ingroup MATTYPE_${mattype}
                                                                                        fi
                                                                                                                                      750 lines total
*
  Automatically generated by $0 on `date`.
                                                                                 done # C
*/
                                                                                 done # R
                                                                                 exit 0
                                                                                 # eof
```



#### **Project: Improved Code Generation**

- Consider common kernels:
  - Matrix-vector multiply, triangular solve, etc.
- Different emphasis than Bernoulli
  - These are simpler kernels than they were interested in
  - Generate code for many formats, not fixed by programmer
  - Select between them using
    - Performance models
    - Search
- Approach may still apply
  - Use high level language (Matlab?) to "specify" kernels
  - Separate language to specify matrix format

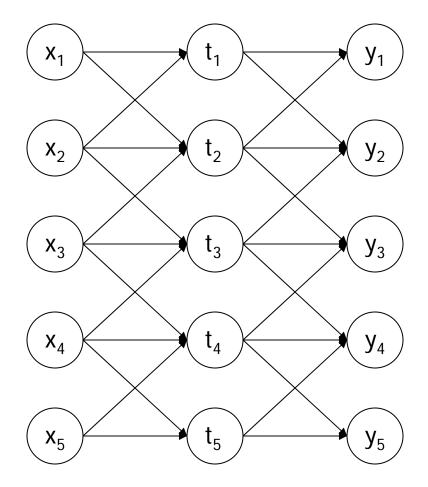


## **Project Idea: Inter Iteration Tiling**

- A<sup>2</sup> \* x is done in Rich Vuduc's PhD thesis
- General case in Michelle Strout's thesis
- Code generation technology would be useful



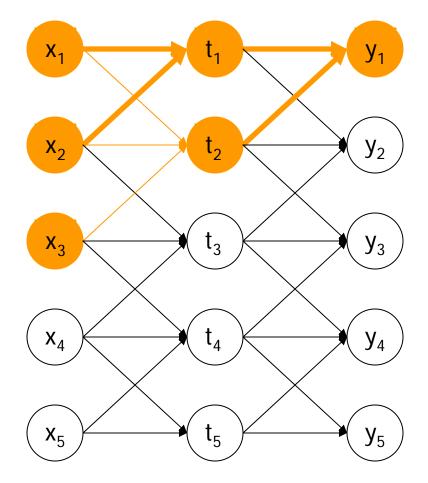
# Inter-Iteration Sparse Tiling (1/3)



- Let A be 6x6 tridiagonal
- Consider y=A<sup>2</sup>x
   t=Ax, y=At
- Nodes: vector elements
- Edges: matrix elements a<sub>ii</sub>

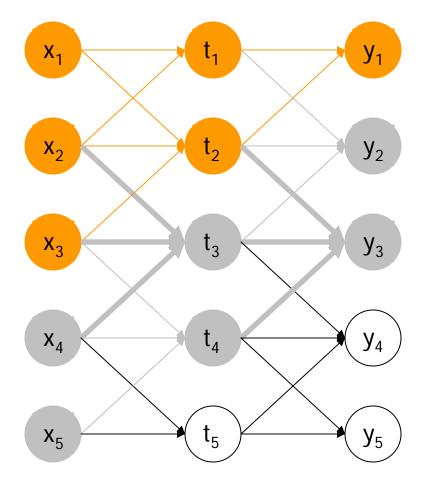


# Inter-Iteration Sparse Tiling (2/3)



- Let A be 6x6 tridiagonal
- Consider y=A<sup>2</sup>x
   t=Ax, y=At
- Nodes: vector elements
- Edges: matrix elements a<sub>ii</sub>
- Orange = everything needed to compute y<sub>1</sub>
  - Reuse a<sub>11</sub>, a<sub>12</sub>

### Inter-Iteration Sparse Tiling (3/3)



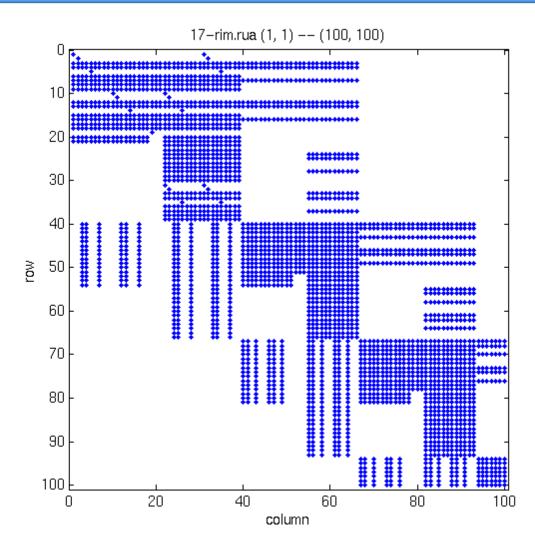
- Let A be 6x6 tridiagonal
- Consider y=A<sup>2</sup>x
   t=Ax, y=At
- Nodes: vector elements
- Edges: matrix elements a<sub>ii</sub>
- Orange = everything needed to compute y<sub>1</sub>
  - Reuse  $a_{11}$ ,  $a_{12}$
- Grey =  $y_2$ ,  $y_3$ 
  - Reuse a<sub>23</sub>, a<sub>33</sub>, a<sub>43</sub>





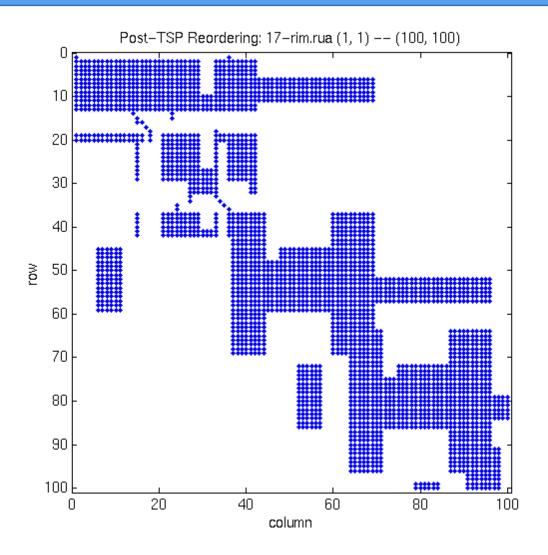
#### Extra slides

### Creating Locality: TSP Reordering (Before)



(Pinar '97; Moon, et al '04)

## Creating Locality: TSP Reordering (After)



(Pinar '97; Moon, et al '04)

Up to 2x speedups over CSR

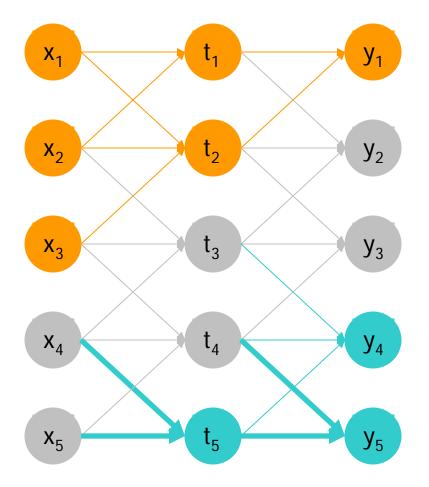




- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning in OSKI
- Current and future work



#### Inter-Iteration Sparse Tiling: Issues



- Tile sizes (colored regions) grow with no. of iterations and increasing out-degree
  - G likely to have a few nodes with high out-degree (e.g., Yahoo)
- Mathematical tricks to limit tile size?
  - Judicious dropping of edges
     [Ng'01]

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## Splitting for Variable Blocks and Diagonals

- Decompose  $A = A_1 + A_2 + \dots A_t$ 
  - Detect "canonical" structures (sampling)
  - Split
  - Tune each  $A_i$
  - Improve performance and save storage
- New data structures
  - Unaligned block CSR
    - Relax alignment in rows & columns
  - Row-segmented diagonals



### Historical Trends in SpMV Performance

- The Data
  - Uniprocessor SpMV performance since 1987
  - "Untuned" and "Tuned" implementations
  - Cache-based superscalar micros; some vectors
  - LINPACK
    - Dense LU factorization
    - Top 500 List



#### Features

- Explicit Hints
  - Can suggest particular tuning technique
- Implicit Tuning: Ask library to infer workload
  - Library profiles all kernel calls
  - May periodically re-tune
- Scripting language for selecting customized transformations
  - Mechanism to save/restore transformations
- "Plug-in" extensibility
  - Very advanced users may customize library (at run-time)



# Summary of High-Level Themes

- "Kernel-centric" optimization
  - Vs. basic block, trace, path optimization, for instance
  - Aggressive use of domain-specific knowledge
- Performance bounds modeling
  - Evaluating software quality
  - Architectural characterizations and consequences
- Empirical search
  - Hybrid off-line/run-time models
- Statistical performance models
  - Exploit information from sampling, measuring



#### **Related Work**



- Sample area 1: Code generation
  - Generative & generic programming
  - Sparse compilers
  - Domain-specific generators

#### Sample area 2: Empirical search-based tuning

- Kernel-centric
  - linear algebra, signal processing, sorting, MPI, ...
- Compiler-centric
  - profiling + FDO, iterative compilation, superoptimizers, selftuning compilers, continuous program optimization





#### **Next Steps**

#### BeBOP Current Work

- Public software release
- Impact on library designs: Sparse BLAS, Trilinos, PETSc, ...
- Integration in large-scale applications
  - Accelerator design, plasma physics (DOE)
  - Geophysical simulation based on Block Lanczos (*A<sup>T</sup>A*\*X; LBL)
- Systematic heuristics for data structure selection?
- Evaluation of emerging architectures
  - Revisiting vector micros
- Other sparse kernels
  - Matrix triple products, A<sup>k\*</sup>x
- Parallelism

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# Future Directions (A Bag of Flaky Ideas)

- Composable code generators and search spaces
- New application domains
  - PageRank: multilevel block algorithms for topic-sensitive search?
- New kernels: cryptokernels
  - rich mathematical structure germane to performance; lots of hardware
- New tuning environments
  - Parallel, Grid, "whole systems"
- Statistical models of application performance
  - Statistical learning of concise parametric models from traces for architectural evaluation
    - Compiler/automatic derivation of parametric models



#### Acknowledgements

- Super-advisors: Jim and Kathy
- Undergraduate R.A.s: Attila, Ben, Jen, Jin, Michael, Rajesh, Shoaib, Sriram, Tuyet-Linh
- See pages *xvi*—*xvii* of dissertation.



#### Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning techniques
- Upper bounds on performance
  - **SC'02**
- Statistical models of performance



#### **Motivation for Upper Bounds Model**

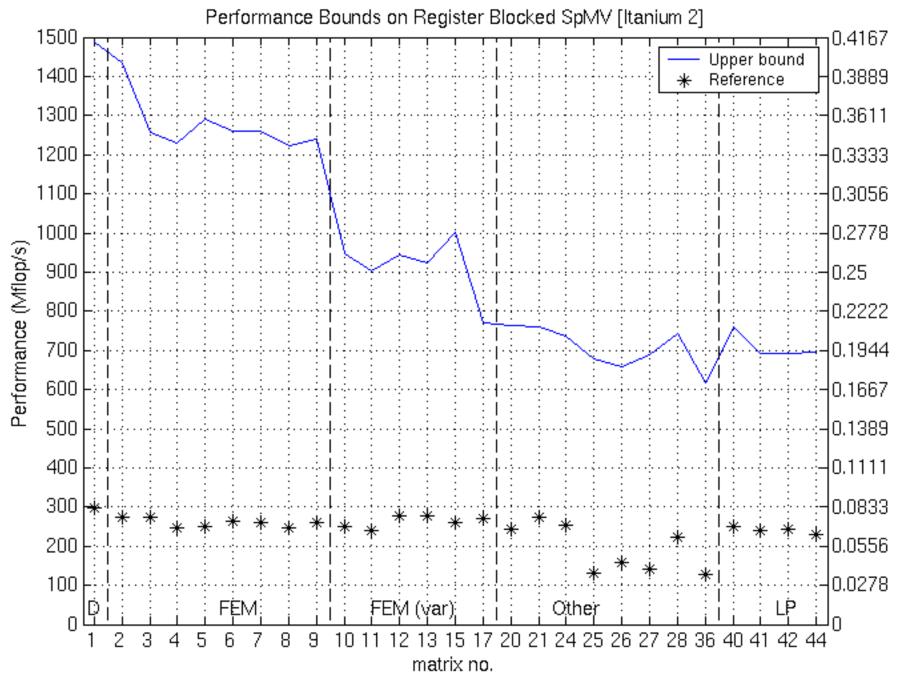
- Questions
  - Speedups are good, but what is the speed limit?
    - Independent of instruction scheduling, selection
  - What machines are "good" for SpMV?

# Upper Bounds on Performance: Blocked SpMV

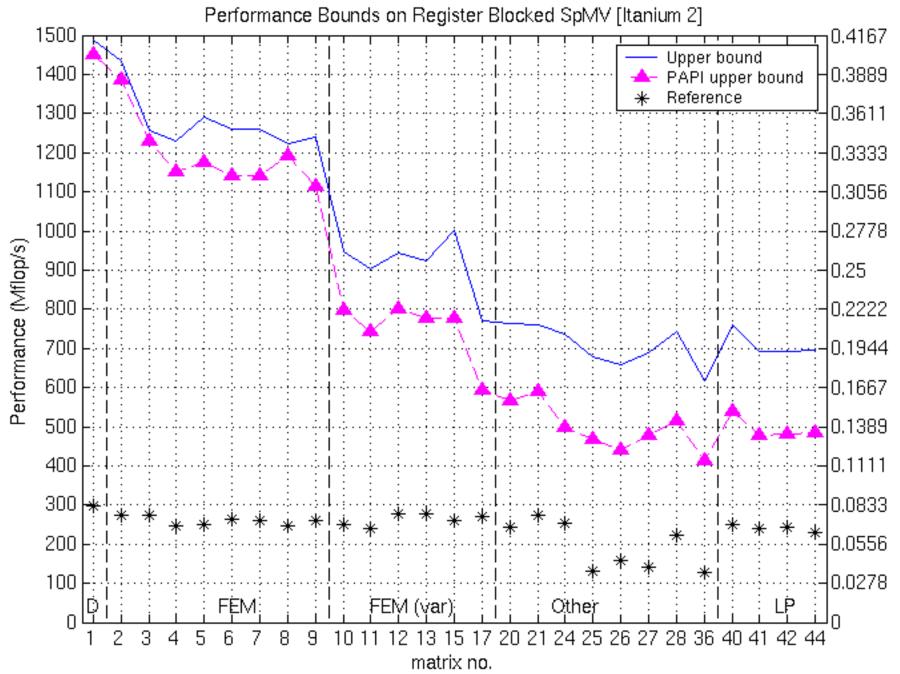
- P = (flops) / (time)
  - Flops = 2 \* nnz(A)
- Lower bound on time: Two main assumptions
  - 1. Count **memory ops only** (streaming)
  - 2. Count only compulsory, capacity misses: ignore conflicts
    - Account for line sizes
    - Account for matrix size and nnz
- Charge min access "latency"  $\alpha_i$  at L<sub>i</sub> cache &  $\alpha_{mem}$

- e.g., Saavedra-Barrera and PMaC MAPS benchmarks

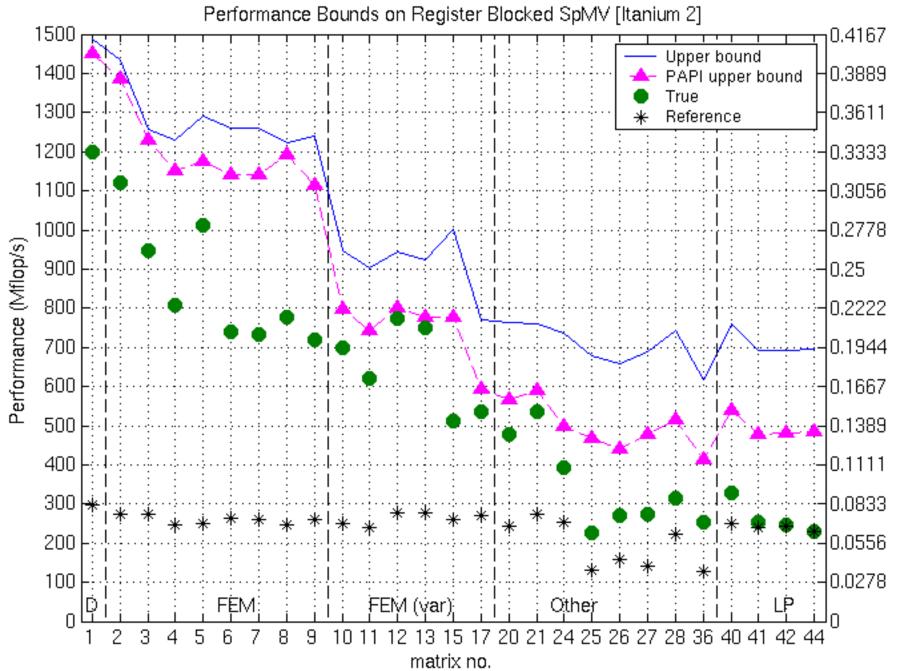
$$\text{Time} \geq \sum_{i=1}^{\kappa} \alpha_i \cdot \text{Hits}_i + \alpha_{\text{mem}} \cdot \text{Hits}_{\text{mem}}$$
$$= \alpha_1 \cdot \text{Loads} + \sum_{i=1}^{\kappa} (\alpha_{i+1} - \alpha_i) \cdot \text{Misses}_i + (\alpha_{\text{mem}} - \alpha_{\kappa}) \cdot \text{Misses}_{\kappa}$$



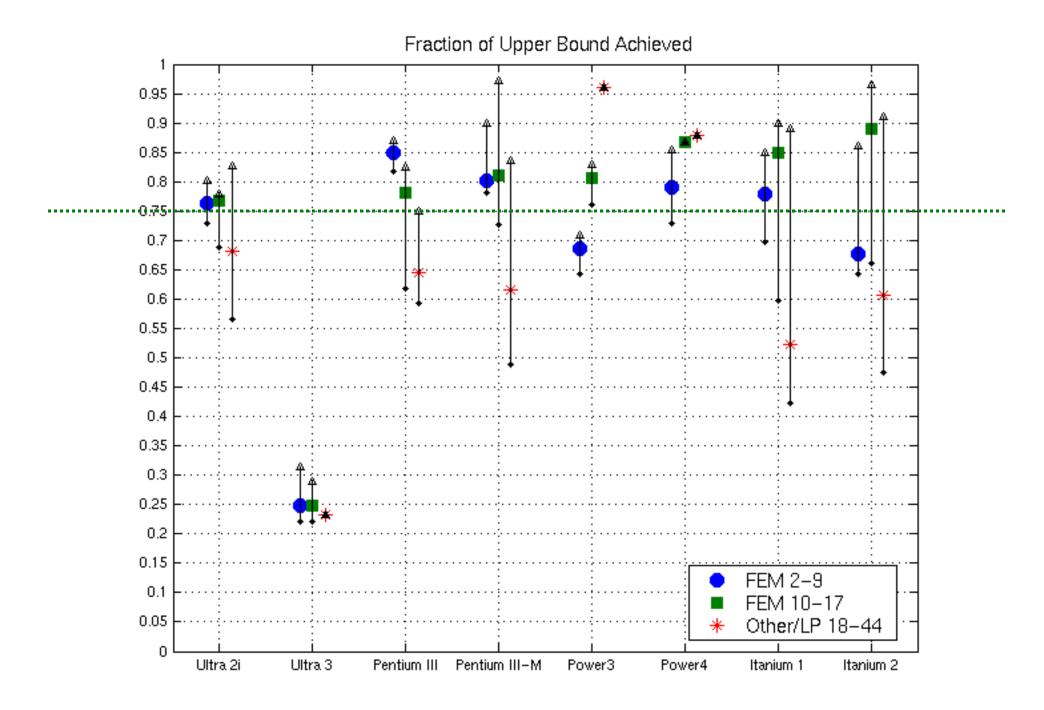
רו מטוווו טו ווומט וווש טדמא



רו מעווטוו טו ווומט ווווש טדמא



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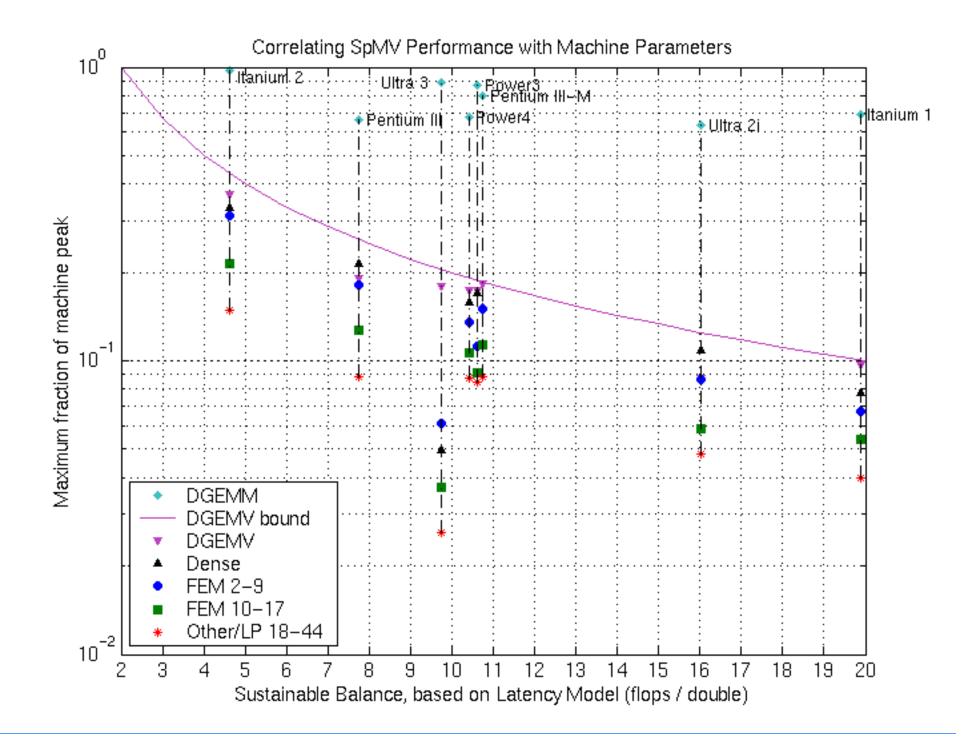


# Achieved Performance and Machine Balance

- Machine balance [Callahan '88; McCalpin '95]
  - Balance = Peak Flop Rate / Bandwidth (flops / double)
- Ideal balance for mat-vec:  $\leq$  2 flops / double
  - For SpMV, even less

Time 
$$\geq \alpha_1 \cdot \text{Loads} + \sum_i (\alpha_{i+1} - \alpha_i) \cdot \text{Misses}_i + (\alpha_{\text{mem}} - \alpha_{\kappa}) \cdot \text{Misses}_{\kappa}$$

- SpMV ~ streaming
  - 1 / (avg load time to stream 1 array) ~ (bandwidth)
  - "Sustained" balance = peak flops / model bandwidth

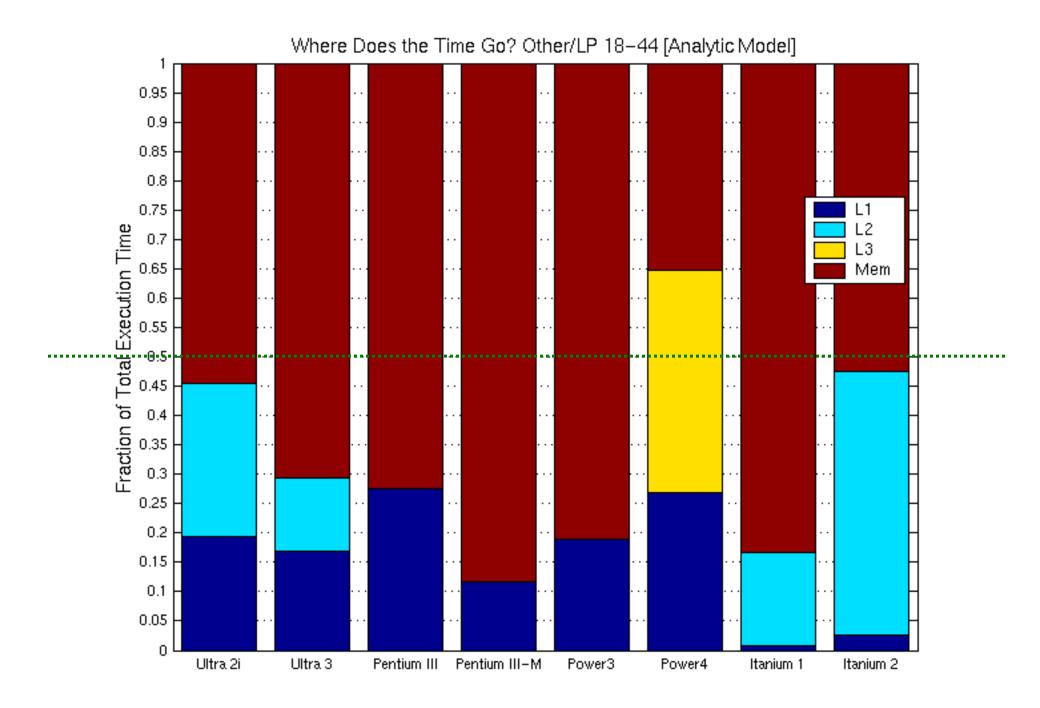


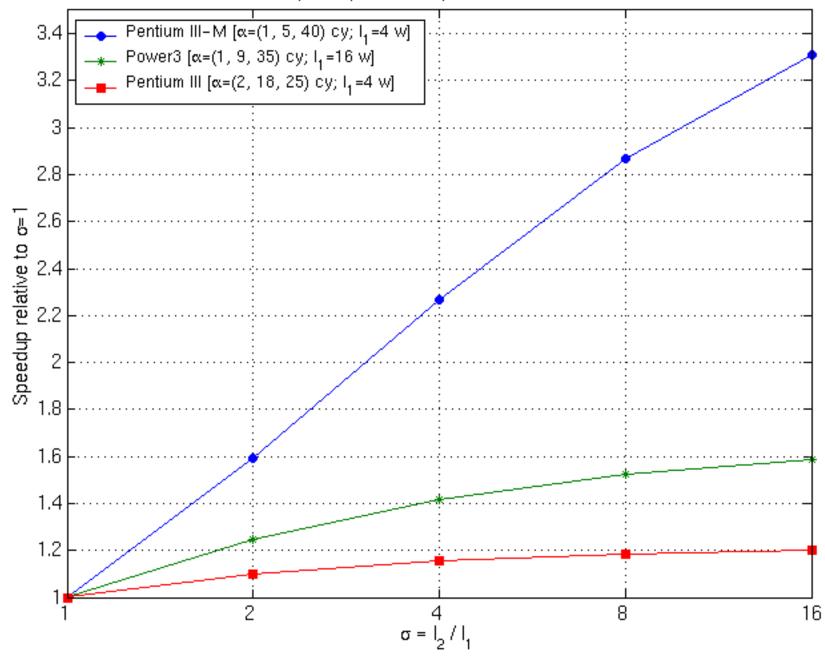


#### Where Does the Time Go?

Time 
$$\geq \sum_{i=1}^{\kappa} \alpha_i \cdot \text{Hits}_i + \alpha_{\text{mem}} \cdot \text{Hits}_{\text{mem}}$$

- Most time assigned to memory
- Caches "disappear" when line sizes are equal
  - Strictly increasing line sizes





Maximum Speedup for 1x1 SpMV as Line Size Increases



#### Summary: Performance Upper Bounds

- What is the best we can do for SpMV?
  - Limits to low-level tuning of blocked implementations
  - Refinements?
- What machines are good for SpMV?
  - Partial answer: balance characterization
- Architectural consequences?
  - Example: Strictly increasing line sizes



#### Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning techniques
- Upper bounds on performance
- Tuning other sparse kernels
- Statistical models of performance
  - FDO '00; IJHPCA '04a

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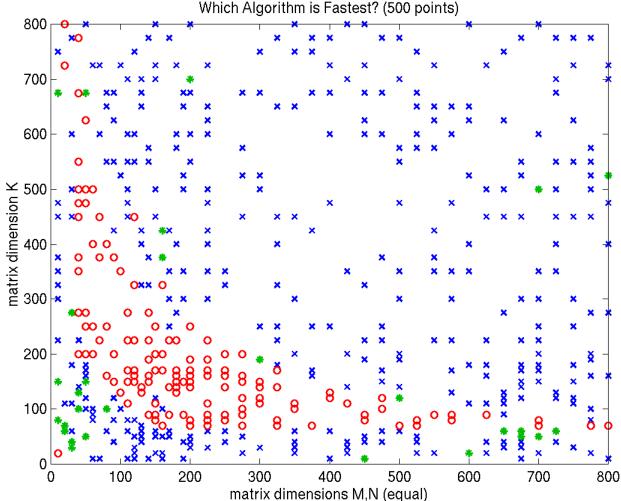
#### Statistical Models for Automatic Tuning

#### Idea 1: Statistical criterion for stopping a search

- A general search model
  - Generate implementation
  - Measure performance
  - Repeat
- Stop when probability of being within  $\varepsilon$  of optimal falls below threshold
  - Can estimate distribution on-line
- Idea 2: Statistical performance models
  - Problem: Choose 1 among *m* implementations at run-time
  - Sample performance off-line, build statistical model

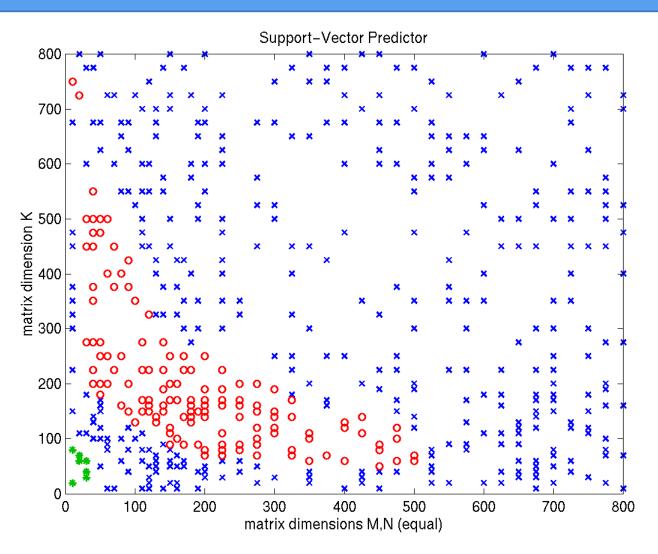
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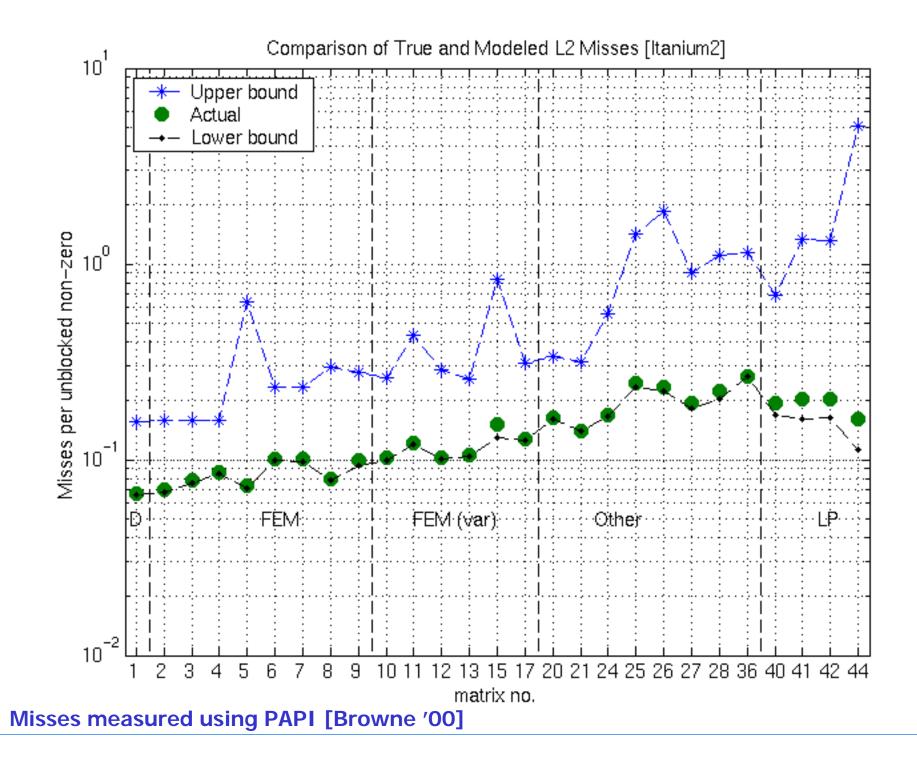
#### **Example: Select a Matmul Implementation**

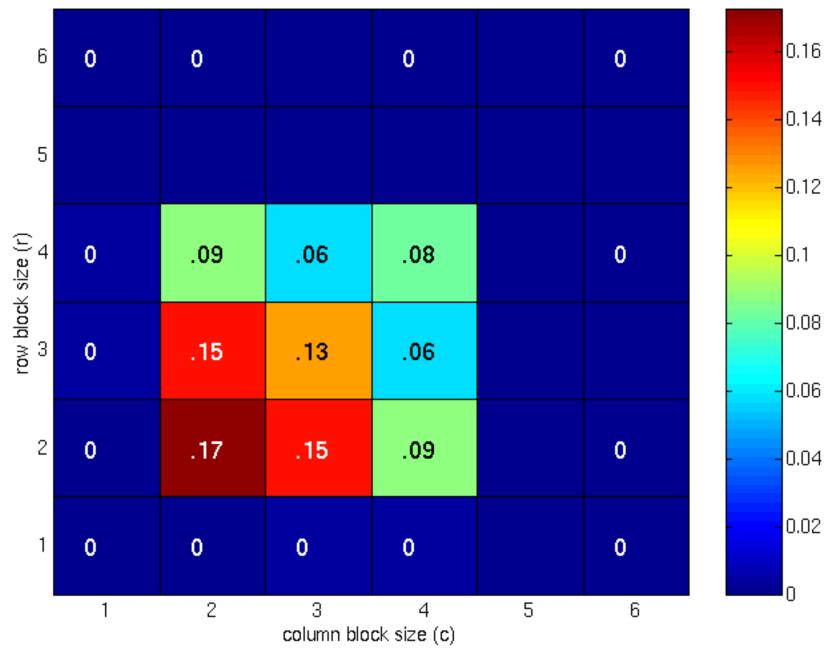


Which Algorithm is Fastest? (500 points)

#### **Example: Support Vector Classification**







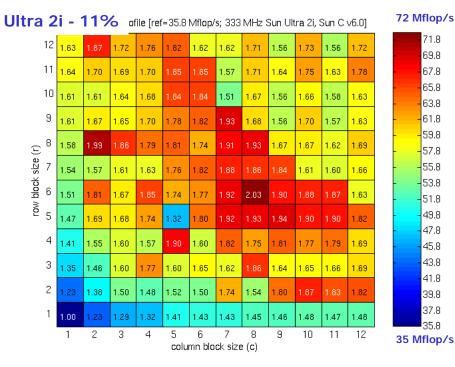
Distribution of Non-zeros: rma10.pua

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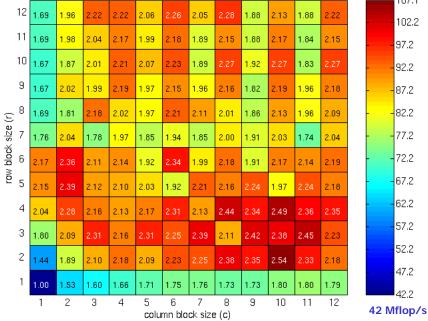
#### Register Profile: Itanium 2

	SpMV BCSR Profile [ref=294.5 Mflop/s; 900 MHz Itanium 2, Intel C v7.0]														1190 Mflop/s
12	1.75	1.52	.99	1.33	1.51	1.64	1.79	1.83	1.89	1.75	1.85	1.72	-	- 1190 - 1140	
11	1.72	1.64	1.12	1.23	1.45	1.60 1.71 1.80 1.8	1.88	1.91	1.88	1.97		- 1090 - 1040			
10	1.73	1.47	1.14	1.23	1.38	1.54	1.69	1.67	1.86	1.89	1.88	1.93	-	- 990	
9	1.54	1.74	1.24	1.00	1.27	1.42	1.55	1.61	1.71	1.73	1.75	1.90	-	- 940 - 890	
۳ 8 ع	3.89	2.40	1.44	1.16	1.16	1.32	1.44	1.47	1.68	1.75	1.77	1.84		-840 -790	
row block size	3.98	2.04	1.65	1.22	1.04	1.20	1.30	1.44	1.52	1.63	1.65	1.74	-	-740	
	3.79	1.77	1.72	1.44	1.19	1.14	1.23	1.31	1.41	1.52	1.58	1.65		-690 -640	
ž 5	3.20	1.74	1.99	1.52	1.34	1.19	.97	1.17	1.27	1.36	1.42	1.50		-590 -540	
4	3.32	4.07	1.74	2.37	1.52	1.38	1.19	1.14	.92	1.19	1.22	1.29	-	- 490	
3	2.55	3.35	.61	1.74	1.97	1.71	1.52	1.34	1.19	1.08	1.03	.88	-	- 440 - 390	
2	1.89	2.54	2.76	2.73	1.62	1.70	1.85	2.40	1.70	1.54	1.27	1.17		- 340 - 290	
1	1.00	1.35	1.39	1.44	1.43	1.47	1.48	1.49	1.34	1.42	1.41	1.43	-	-240	
1 2 3 4 5 6 7 8 9 10 11 12 column block size (c)												190	190 Mflop/s		



#### Pentium III - 21%

=42.1 Mflop/s; 500 MHz Pentium III, Intel C v7.0]



Ultra 3 - 5% Profile [ref=50.3 Mflop/s; 900 MHz Sun Ultra 3, Sun C v6.0]													90 Mflop/s 89.7
12	1.57	1.59	1.61	1.66	1.66	1.63	1.65	1.77	1.76	1.76	1.76	1.78	88.4 86.4
11	1.48	1.59	1.55	1.53	1.66	1.72	1.74	1.74	1.66	1.75	1.74	1.77	<mark>84.4</mark>
10	1.55	1.56	1.63	1.59	1.67	1.71	1.73	1.78	1.75	1.76	1.74	1.77	82.4 80.4
9	1.54	1.59	1.60	1.61	1.63	1.70	1.73	1.77	1.74	1.74	1.75	1.77	<mark></mark> 78.4
Ξ <sup>8</sup>	1.65	1.58	1.58	1.64	1.65	1.60	1.70	1.76	1.74	1.74	1.74	1.77	76.4 74.4
7 size	1.54	1.52	1.59	1.59	1.62	1.67	1.69	1.76	1.71	1.73	1.71	1.74	72.4 - 70.4
row block size	1.53	1.54	1.55	1.59	1.65	1.69	1.70	1.76	1.73	1.70	1.64	1.72	<mark>68.4</mark>
Ž 5	1.47	1.59	1.57	1.57	1.65	1.59	1.68	1.74	1.72	1.72	1.71	1.72	66.4 64.4
4	1.39	1.53	1.55	1.58	1.55	1.54	1.61	1.69	1.65	1.66	1.59	1.65	<mark>62.4</mark>
3	1.34	1.48	1.51	1.53	1.53	1.58	1.62	1.69	1.68	1.68	1.66	1.66	60.4 58.4
2	1.16	1.38	1.46	1.55	1.45	1.55	1.55	1.60	1.57	1.62	1.60	1.61	<mark>56.4</mark> 54.4
1	1.00	1.21	1.31	1.35	1.39	1.42	1.43	1.44	1.46	1.42	1.47	1.47	- <mark>-</mark> 52.4
													50.4 50 Mflop/s

#### Pentium III-M - 15%

71.8

69.8

67.8

65.8

63.8

61.8

59.8

57.8

49.8

47.8

45.8

43.8

41.8

39.8

37.8

35.8

108 Mflop/s

107.1

102.2

97.2

92.2

87.2

82.2

77.2

72.2

67.2

62.2

57.2

52.2

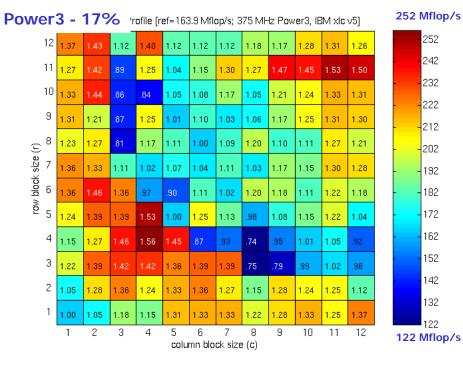
47.2

42.2

flop/s; 800 MHz Pentium III-M, Intel C v7.0] 12 1.70 1.73 2.05 2.06 2.06 2.07 2.04 2.07 1.97 2.06 1.95 2.08 11 1.69 1.77 2.02 2.07 2.03 2.07 1.96 2.07 1.95 2.07 1.92 2.07 10 1.71 1.71 2.05 2.07 2.06 2.08 1.97 2.08 2.00 2.08 1.91 2.09 9 1.73 1.69 1.92 2.06 2.03 2.08 2.06 2.08 2.06 2.08 Ξ8, 1.75 1.62 2.02 2.05 2.06 2.07 2.07 2.08 2.05 2.08 2.07 2.09 size 1.88 1.66 1.84 2.06 2.00 2.07 2.02 2.08 2.07 2.05 2.02 2.08 block. 1.87 1.99 2.05 2.06 2.06 2.07 2.07 2.07 2.08 2.08 2.08 Mo 5 1.73 1.94 2.03 2.05 2.07 2.08 4 1.85 1.96 2.00 1.98 2.04 2.05 2.05 2.06 2.07 2.08 2.07 3 1.74 1.93 1.98 2.01 2.02 2.03 2.05 2.05 2.05 2.06 2.06 2.06 2 1.52 1.84 1.92 1.96 1.99 2.01 2.02 2.02 2.03 2.04 2.04 2.04 1 1.00 1.53 1.58 1.65 1.76 1.78 1.82 1.79 1.89 1.76 1.88 1.83 2 3 4 5 6 7 8 9 10 11 12 1 58 Mflop/s column block size (c)

122 Mflop/s 122 118.6

> 113.6 108.6 103.6 98.6 93.6 88.6 83.6 78.6 73.6 68.6 63.6 58.6







ofile [ref=161.2 Mflop/s; 800 MHz Itanium, Intel C v7]

252

242

232

222

212

202

192

182

172

162

152

142

132

122

247 Mflop/s

247

3.20

3.32

2.55

1

4

3

2 1.89 2.54

1

1.74

3.35 .61

1.35

2 3 4 5 6

1.99

4.07 **1.74** 2.37

1.39 1.44

1.52 1.34

1.74

2.76 2.73

1.52

1.97

1.62

1.43 1.47

1.19 .97

1.71

1.70

1.38 1.19 1.14 .92

1.17 1.27

1.85 2.40 1.70

1.48 1.49

7 8 9

column block size (c)

1.52 1.34 1.19 1.08 1.03

1.34

1.36

1.42

10 11

1.42 1.50

1.54 1.27 1.17

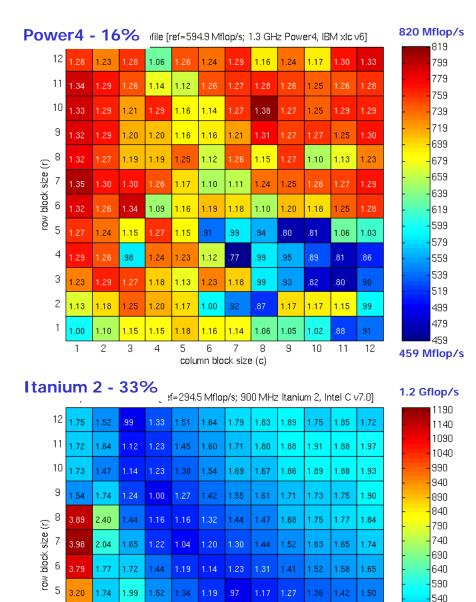
1.41 1.43

.88

12

1.19 1.22

1	2 <mark>.9</mark> 2	2	.77	.99	1.16	1.30	1.35	1.39	1.39	1.45	1.24	1.22	1.32			
1	1 1.8	52	.80	.95	1.11	1.24	1.35	1.39	1.39	1.44	1.24	1.24	1.29			237
1	0 1.3	34	.74	.88	1.04	1.16	1.30	1.36	1.35	1.38	1.22	1.23	1.32			227
9	9 1.2	25	.78	.82	1.01	1.10	1,19	1.34	1.35	1.39	1.21	1.20	1.28			207
_ {			.72	.77	.92	1.05	1.16	1.22	1.31	1.37	1.22	1.15	1.27			197
ize (r)			.80	.76	.82	.98	1.11	1.16	1.26	1.34	1.25	1.18	1.32			187
row block size			.84	.78	.79	.87	.99	1.09	1.18	1.23	1.29	1.14	1.41			177
d wor 2	-															167
	<sup>0</sup> 1.1	10	1.17	.75	.71	.80	.88	.97	1.06	1.09	1.15	1.14	1.29			157
4	<sup>4</sup> 1.8	55	1.30	.80	.72	.71	.77	.80	.94	1.00	1.08	1.11	1.16			147
3	8 1.8	54	1.04	1.15	.80	.71	.66	.76	.77	.81	.87	.95	.98			137
2	2 1.4	48	1.48	1.02	1.27	1.05	.83	.70	.67	.66	.68	.77	.77			127
-	1.0	10	1.07	1.05	1.12	.89	.95	1.07	1.21	1.02	.94	.82	.73			117
	1		2	3	4	5	6	7	8	9	10	11	12			107
	column block size (c)												107	Mflop/s		



240 190 190 Mflop/s

540 490

440

390 340

290



# 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



# Sparse/Dense Partitioning for SpTS

• Partition L into sparse  $(L_1, L_2)$  and dense  $L_D$ :

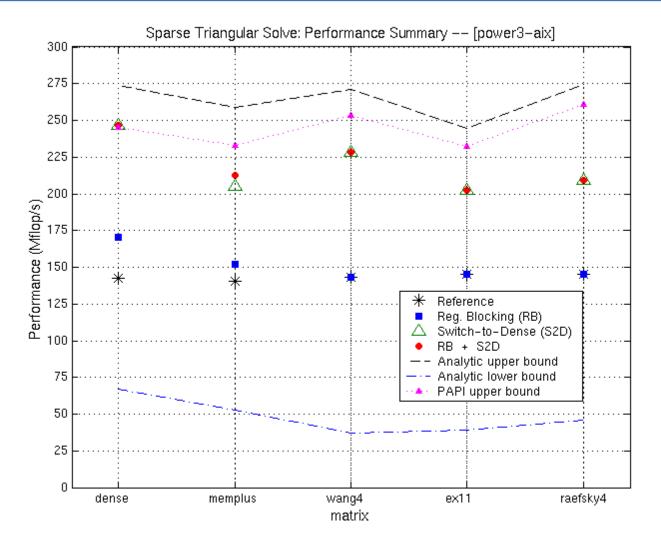
$$\begin{pmatrix} L_1 \\ L_2 \\ L_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

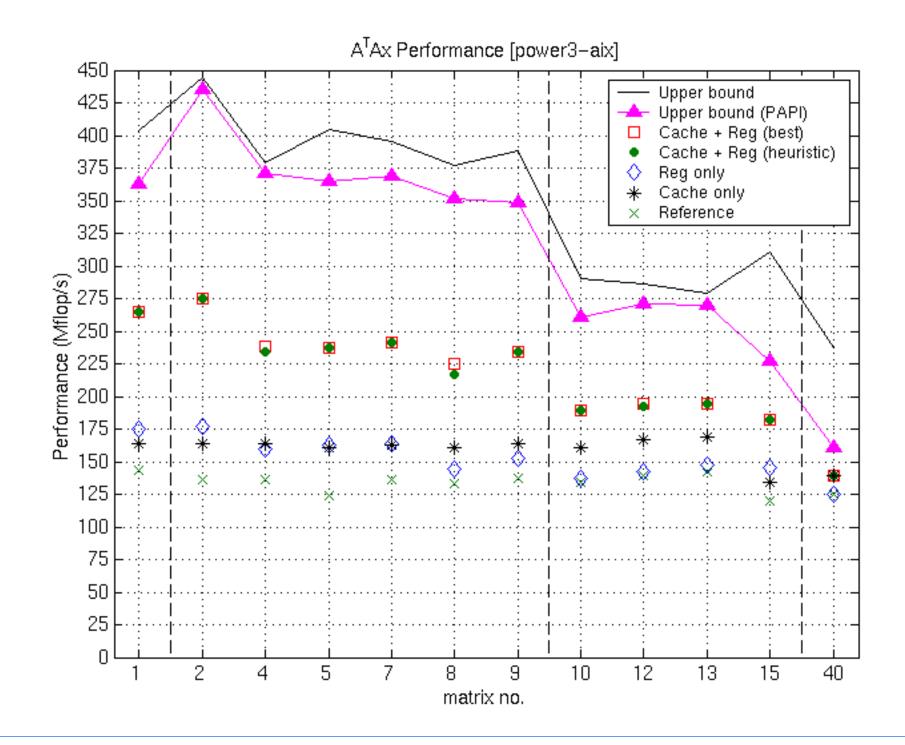
• Perform SpTS in three steps:

(1) 
$$L_1 x_1 = b_1$$
  
(2)  $\hat{b}_2 = b_2 - L_2 x_1$   
(3)  $L_D x_2 = \hat{b}_2$ 

- Sparsity optimizations for (1)—(2); DTRSV for (3)
- Tuning parameters: block size, size of dense triangle

#### SpTS Performance: Power3

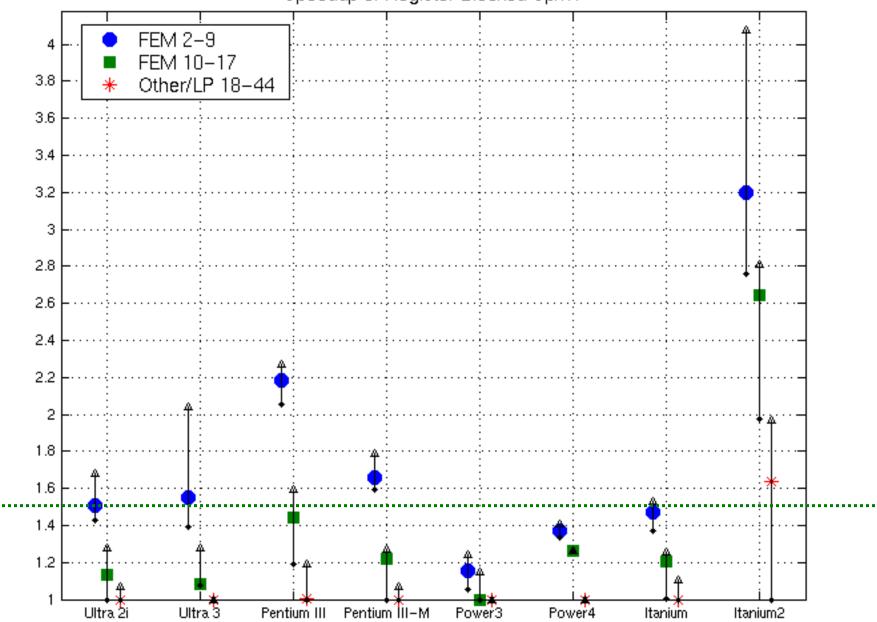




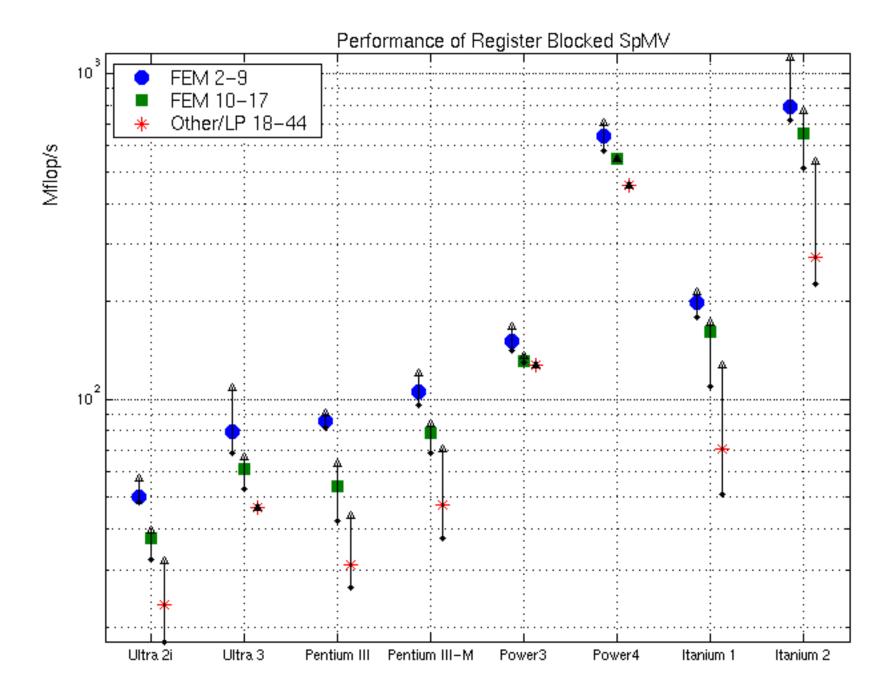


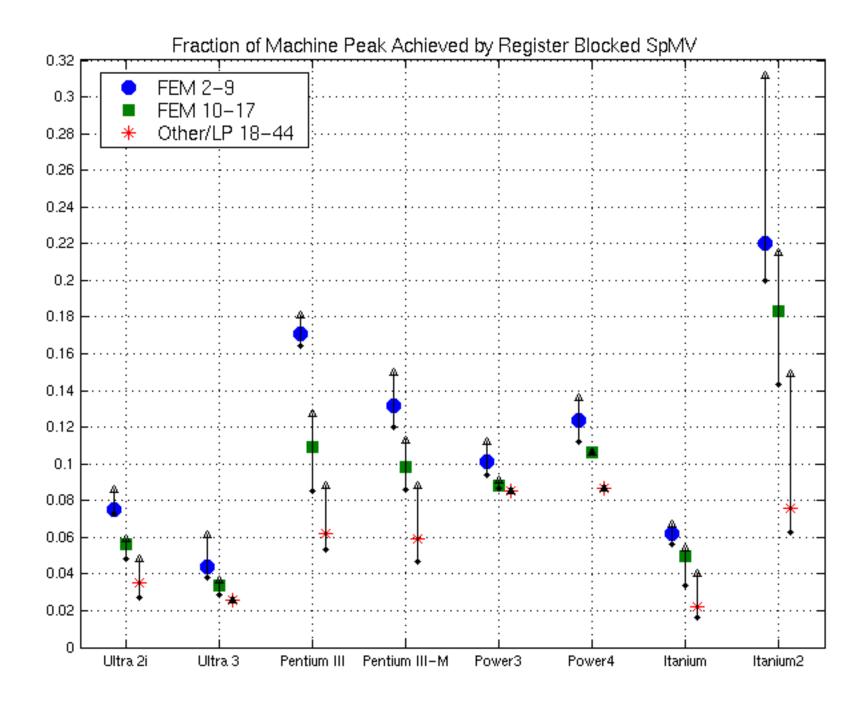
#### Summary of SpTS and AA<sup>T</sup>\*x Results

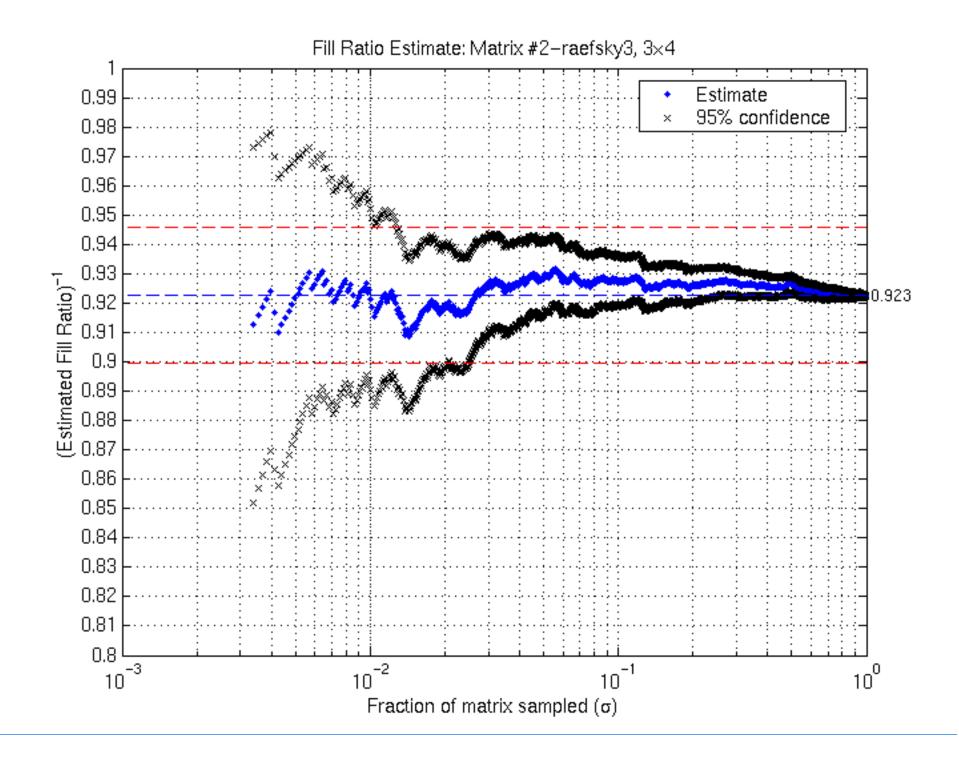
- SpTS Similar to SpMV
  - 1.8x speedups; limited benefit from low-level tuning
- $AA^Tx$ ,  $A^TAx$ 
  - Cache interleaving only: up to 1.6x speedups
  - Reg + cache: up to 4x speedups
    - 1.8x speedup over register only
  - Similar heuristic; same accuracy (~ 10% optimal)
  - Further from upper bounds: 60—80%
    - Opportunity for better low-level tuning *a la* PHiPAC/ATLAS
- Matrix triple products? *A*<sup>*k*</sup>\**x*?
  - Preliminary work

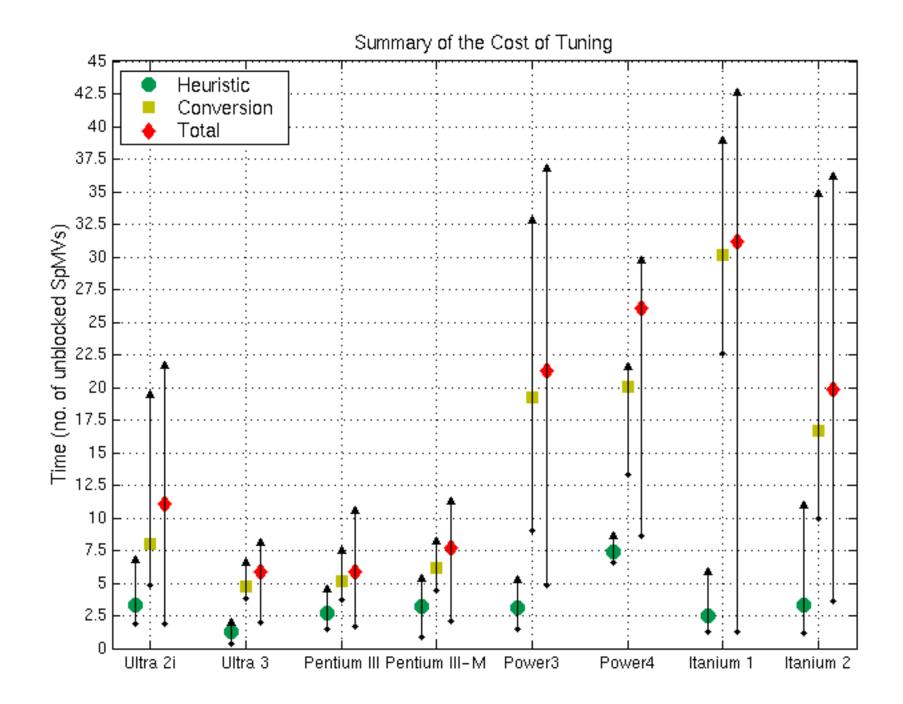


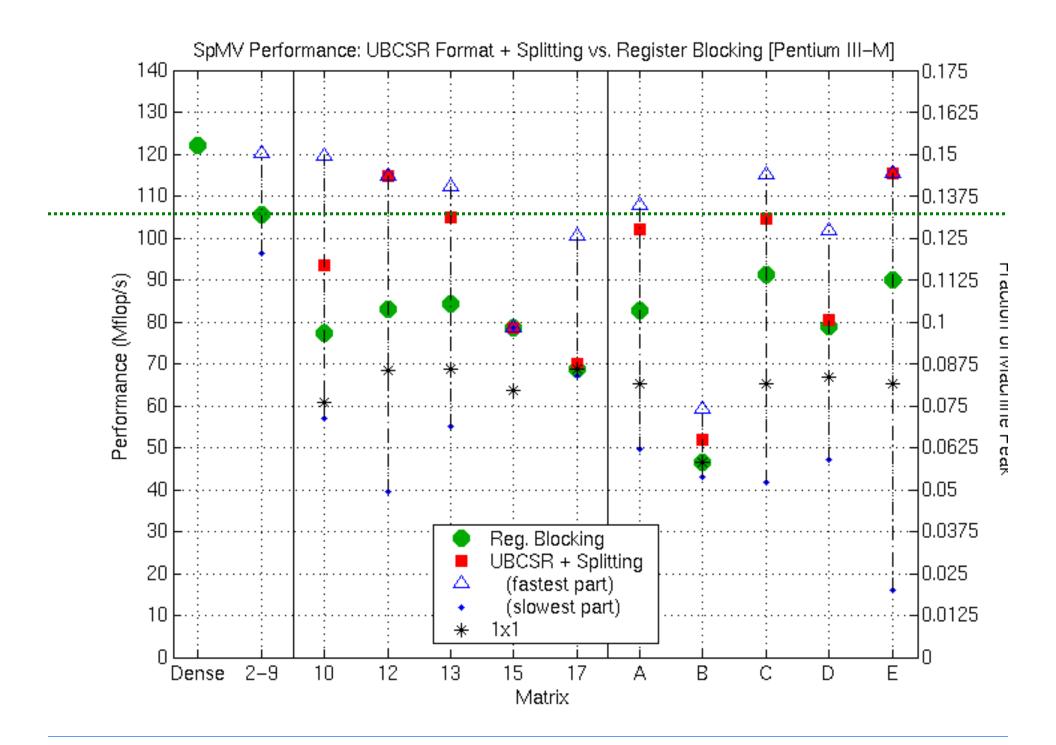
Speedup of Register Blocked SpMV

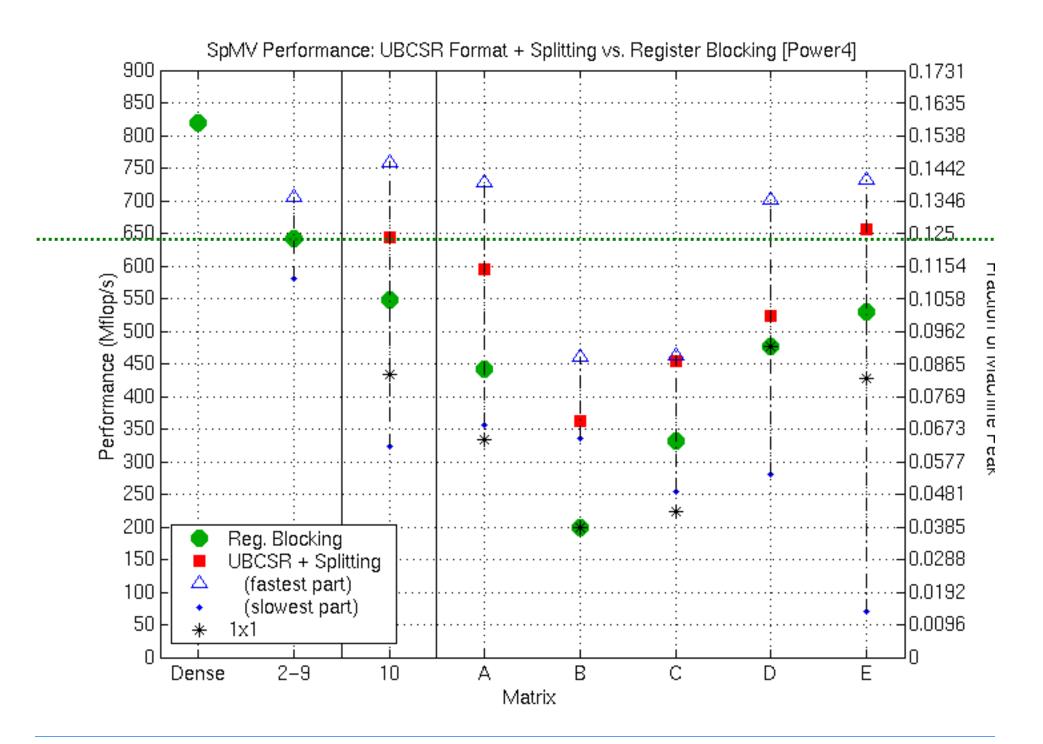


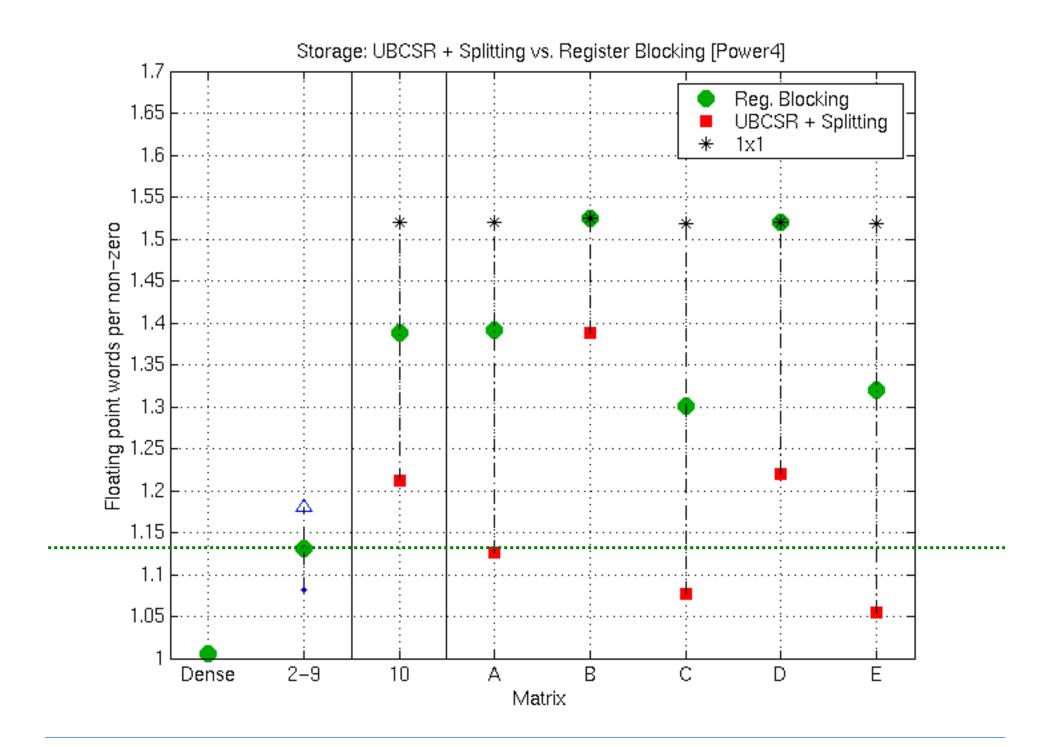


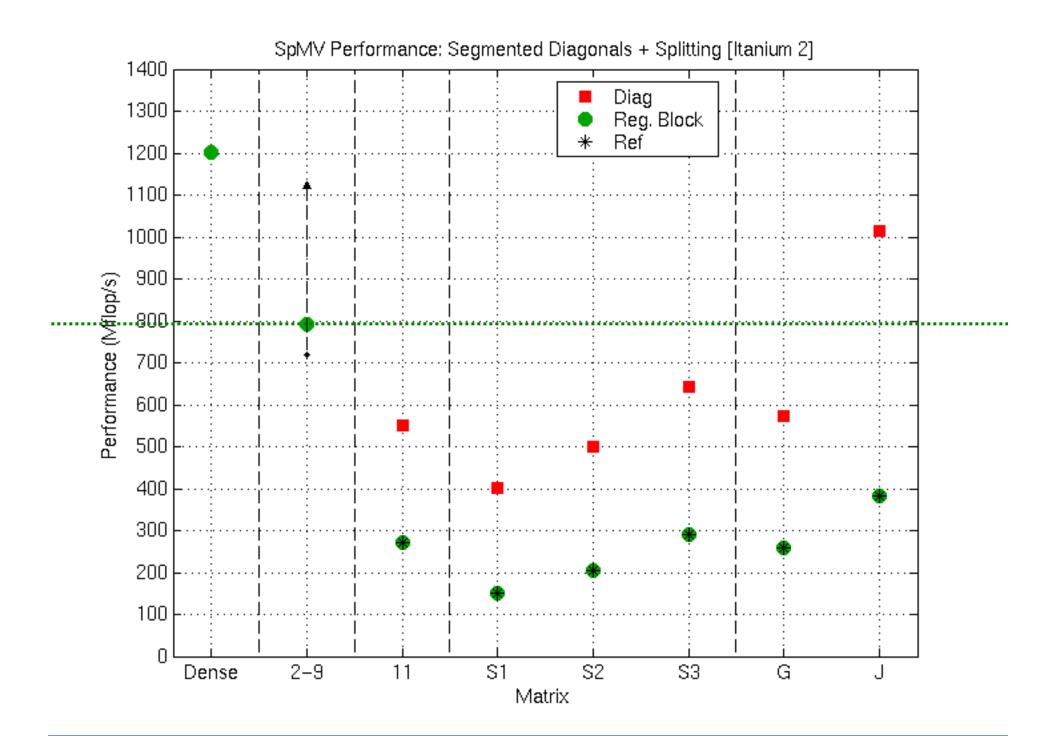


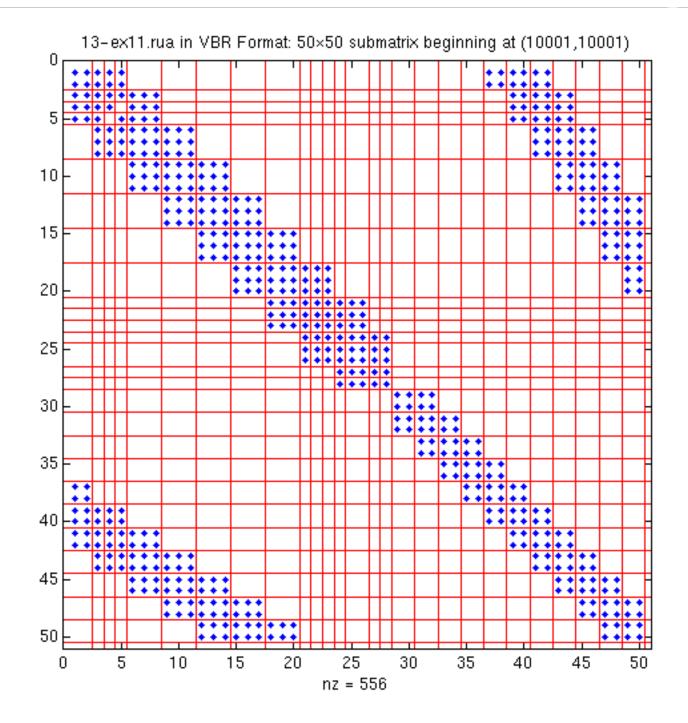








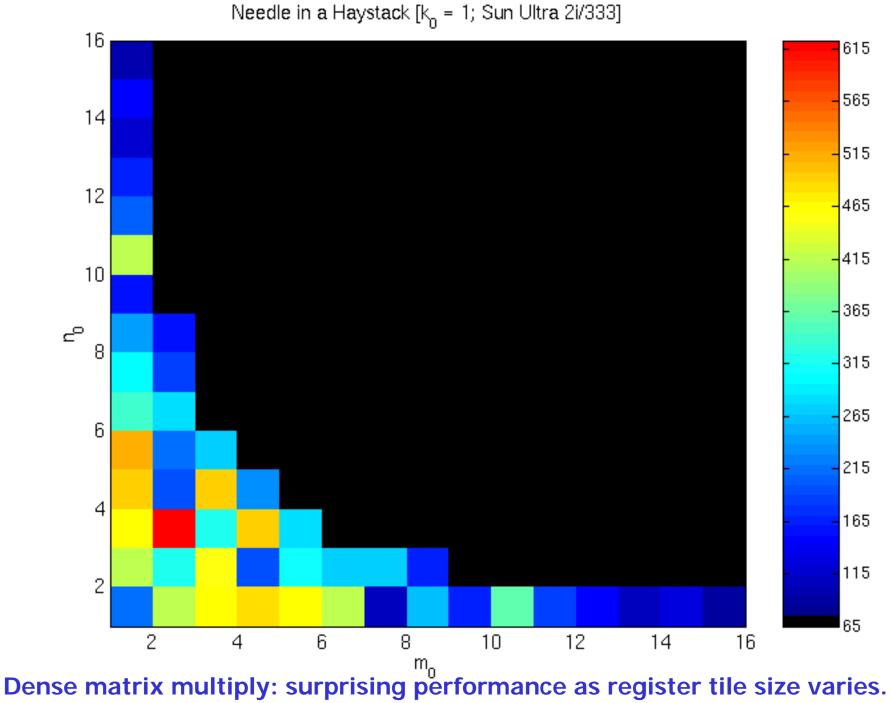


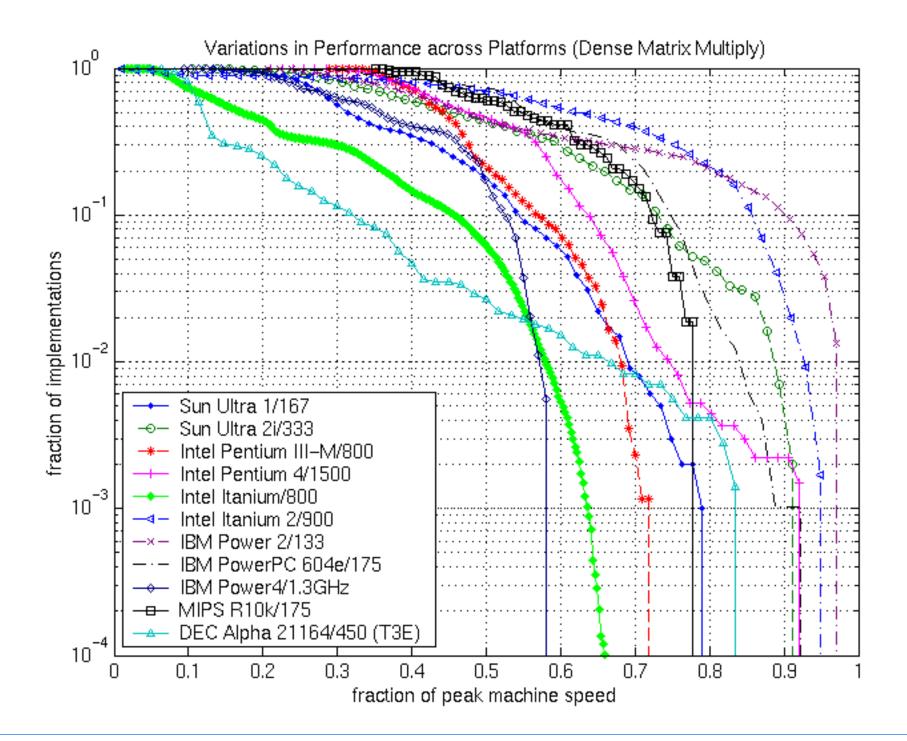


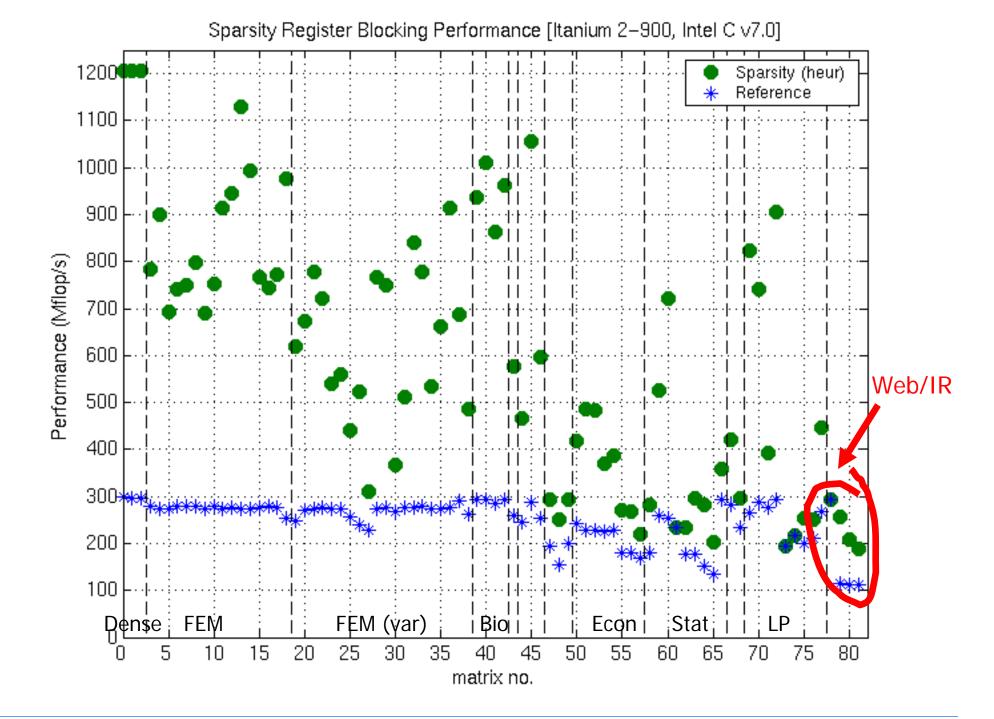


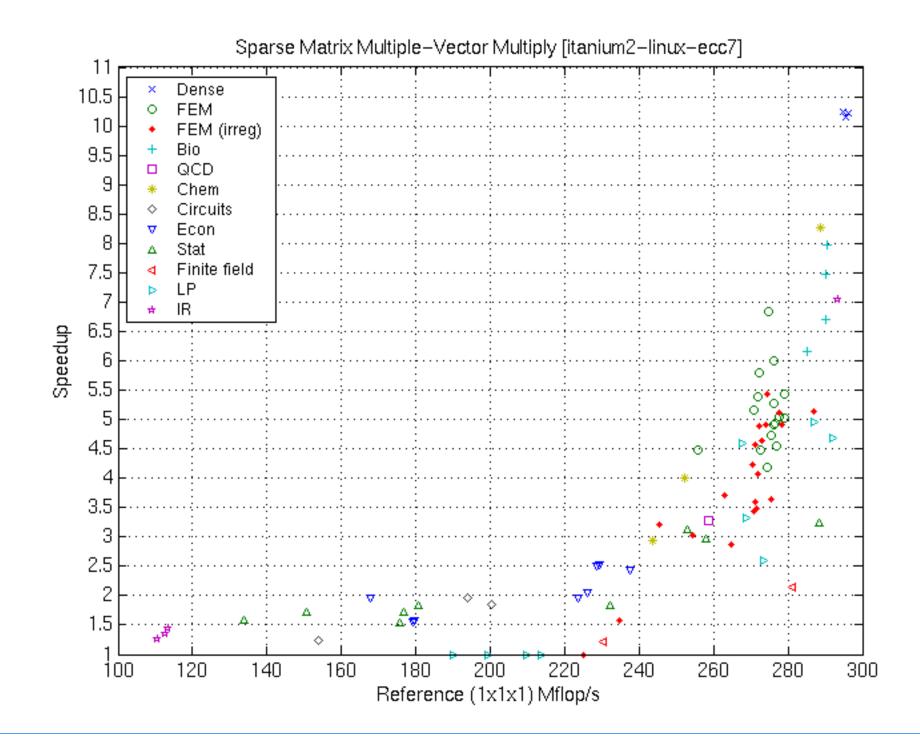
#### Dense Tuning is Hard, Too

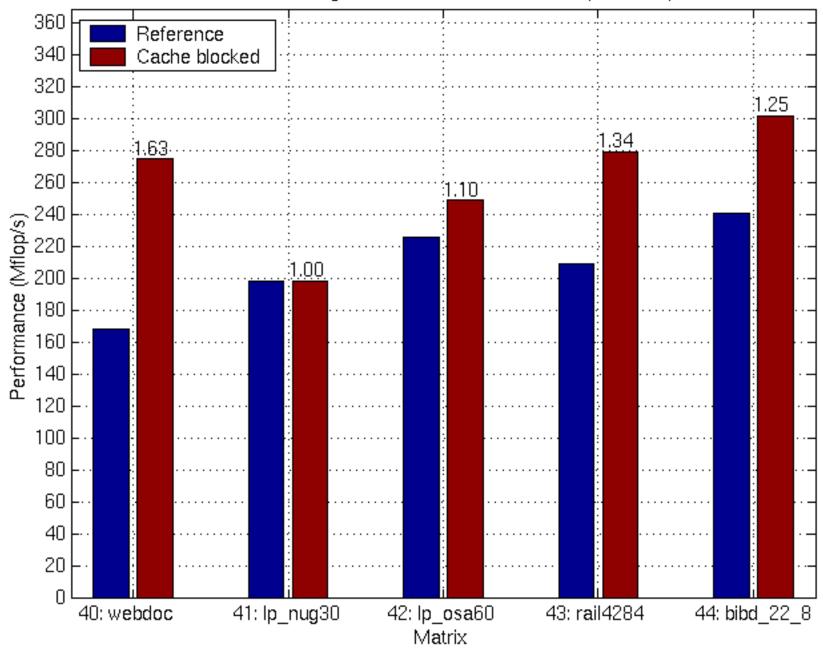
Even dense matrix multiply can be notoriously difficult to tune









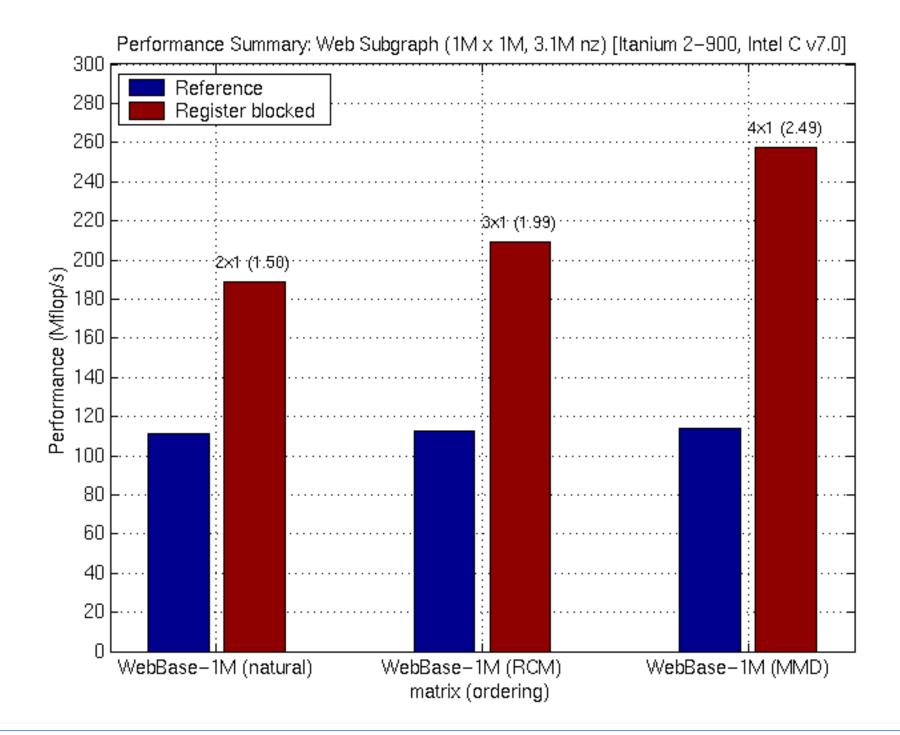


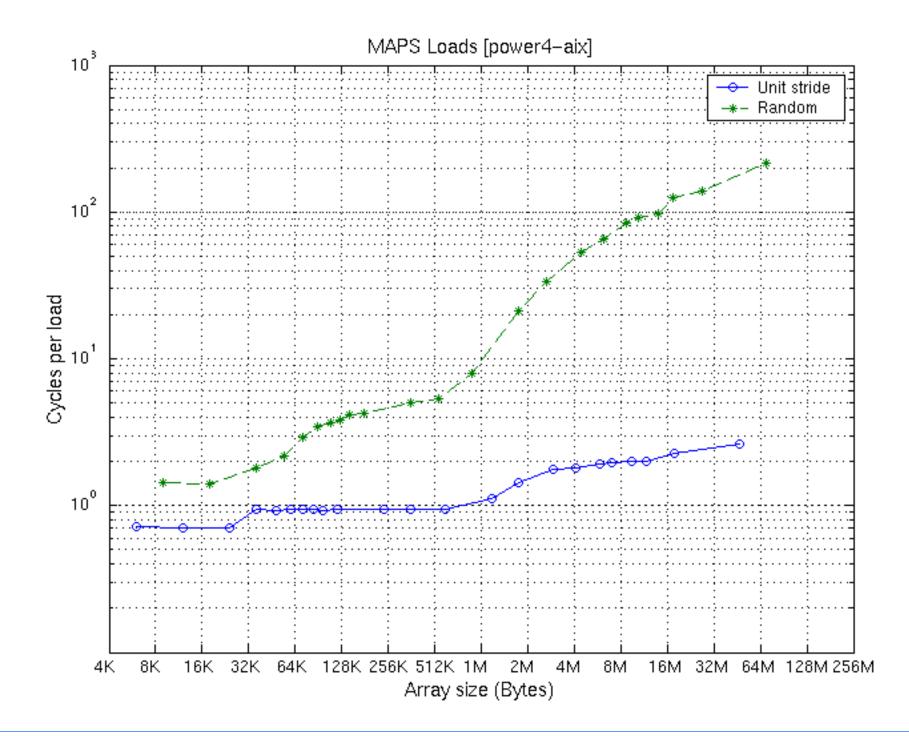
Cache Blocking Performance: Intel Itanium 2 (900 MHz)

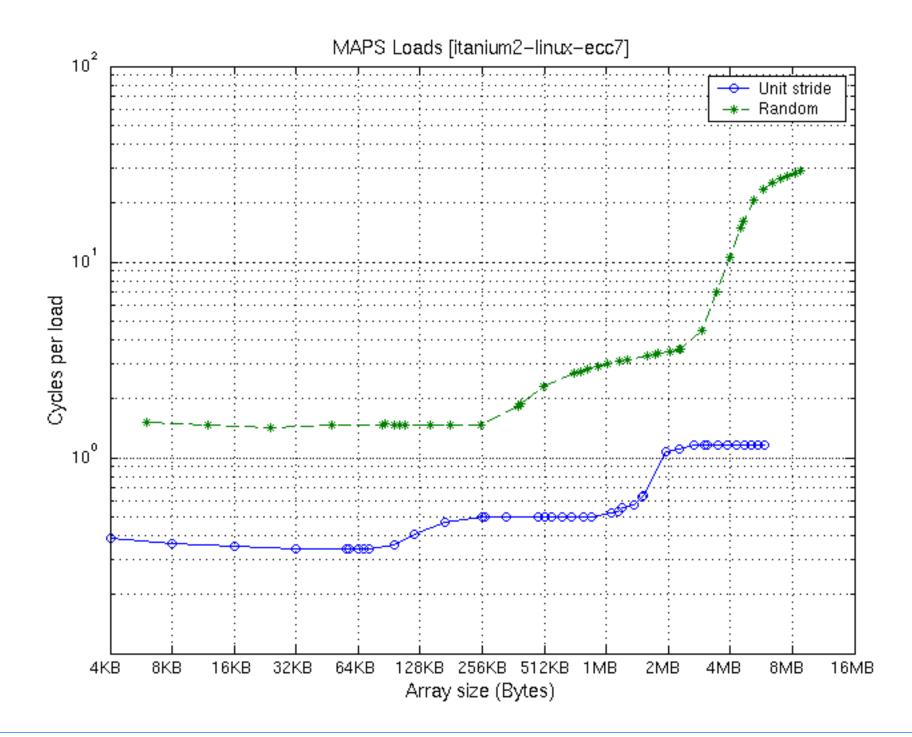


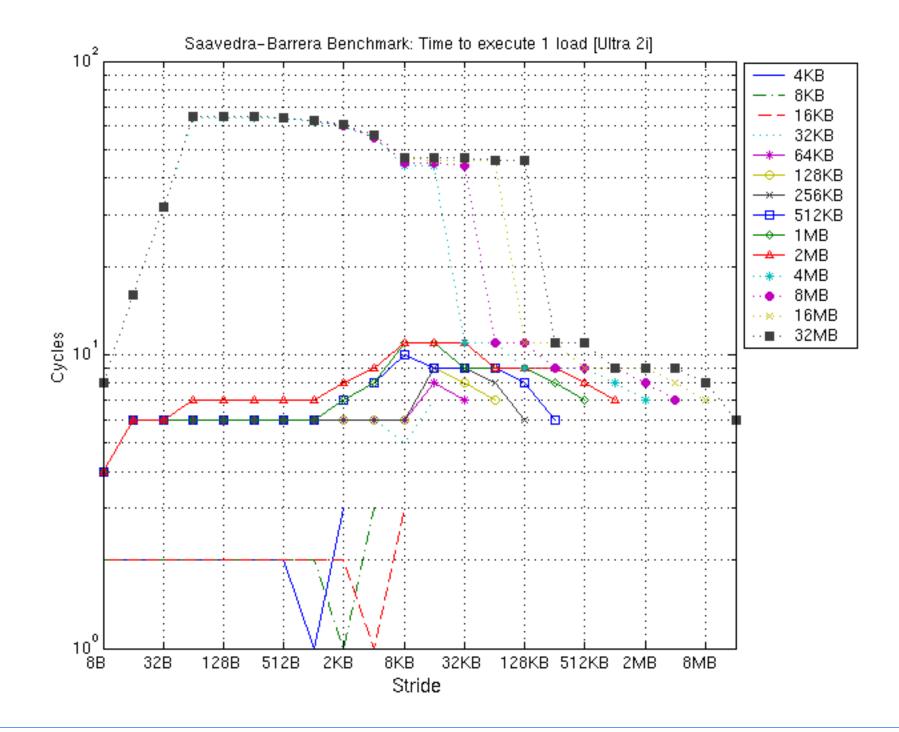
## What about the Google Matrix?

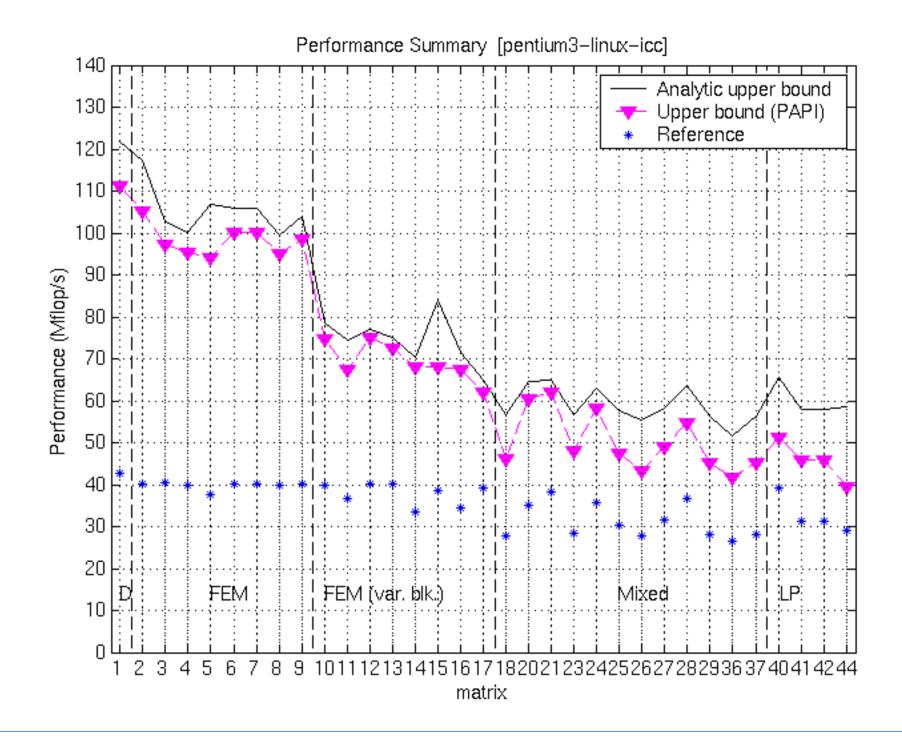
- Google approach
  - Approx. once a month: rank all pages using connectivity structure
    - Find dominant eigenvector of a matrix
  - At query-time: return list of pages ordered by rank
- Matrix:  $A = \alpha G + (1-\alpha)(1/n)uu^T$ 
  - Markov model: Surfer follows link with probability  $\alpha,$  jumps to a random page with probability 1- $\alpha$
  - G is n x n connectivity matrix [n  $\approx$  3 billion]
    - g<sub>ij</sub> is non-zero if page i links to page j
    - Normalized so each column sums to 1
    - Very sparse: about 7-8 non-zeros per row (power law dist.)
  - u is a vector of all 1 values
  - Steady-state probability  $x_i$  of landing on page i is solution to x = Ax
- Approximate x by power method:  $x = A^k x_0$ 
  - In practice,  $k \approx 25$

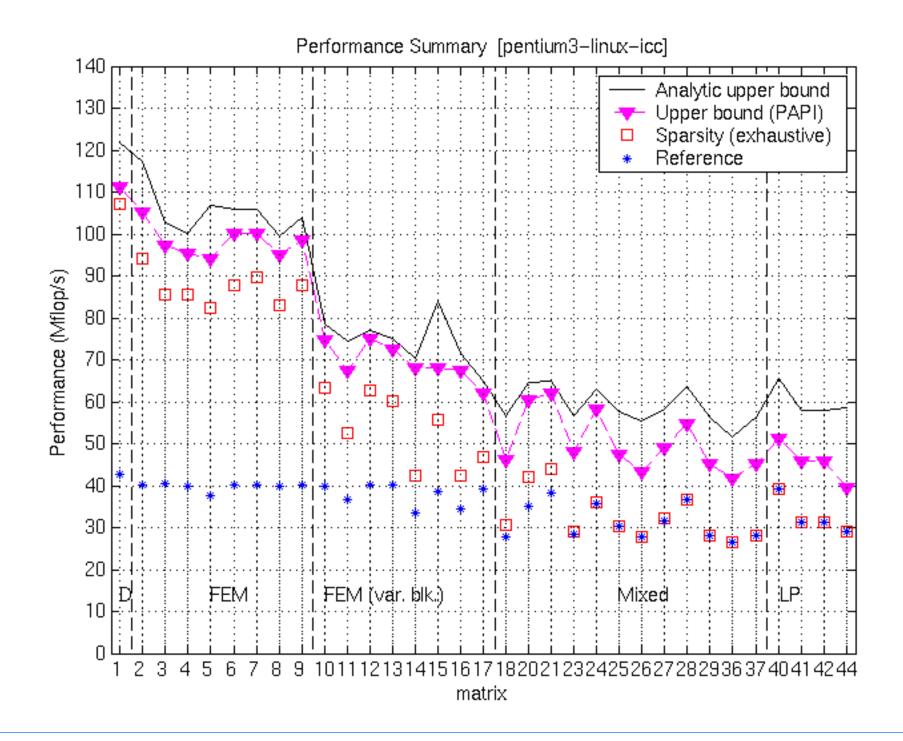


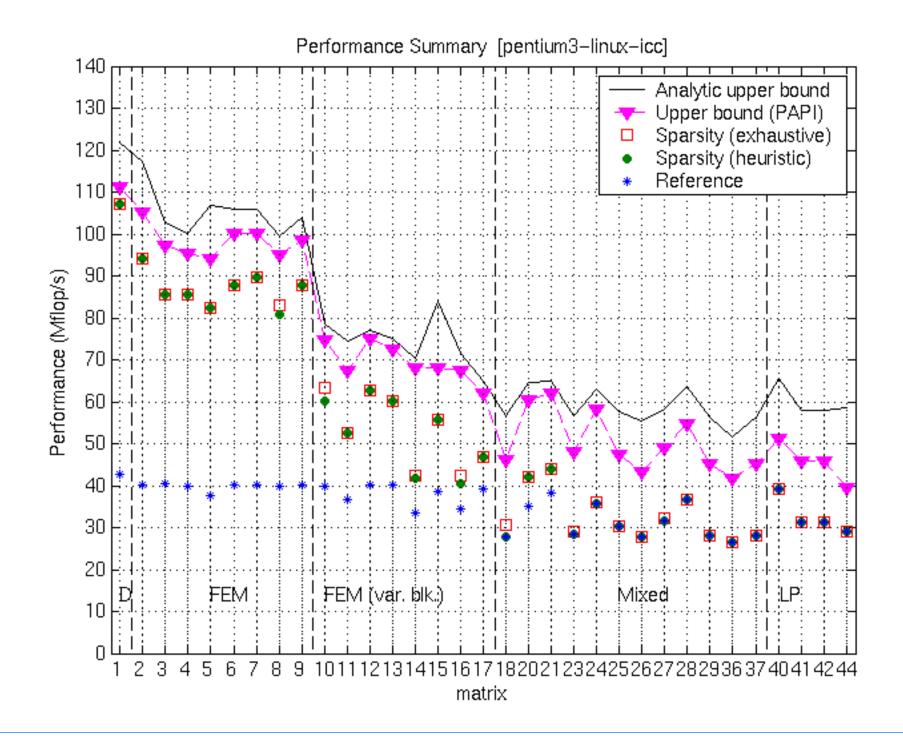


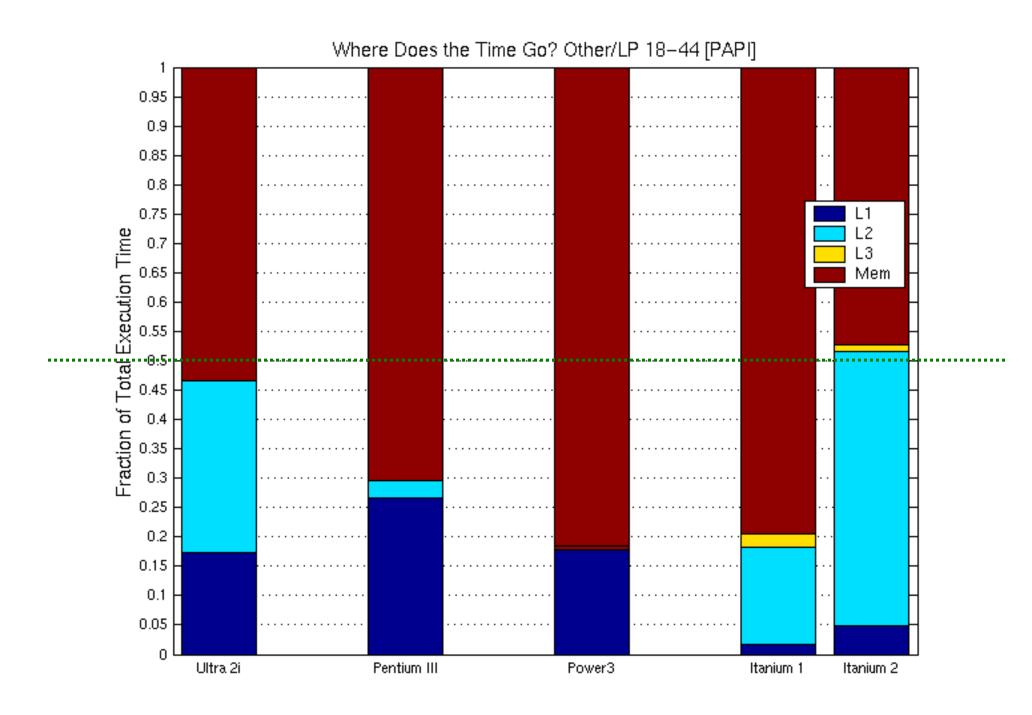


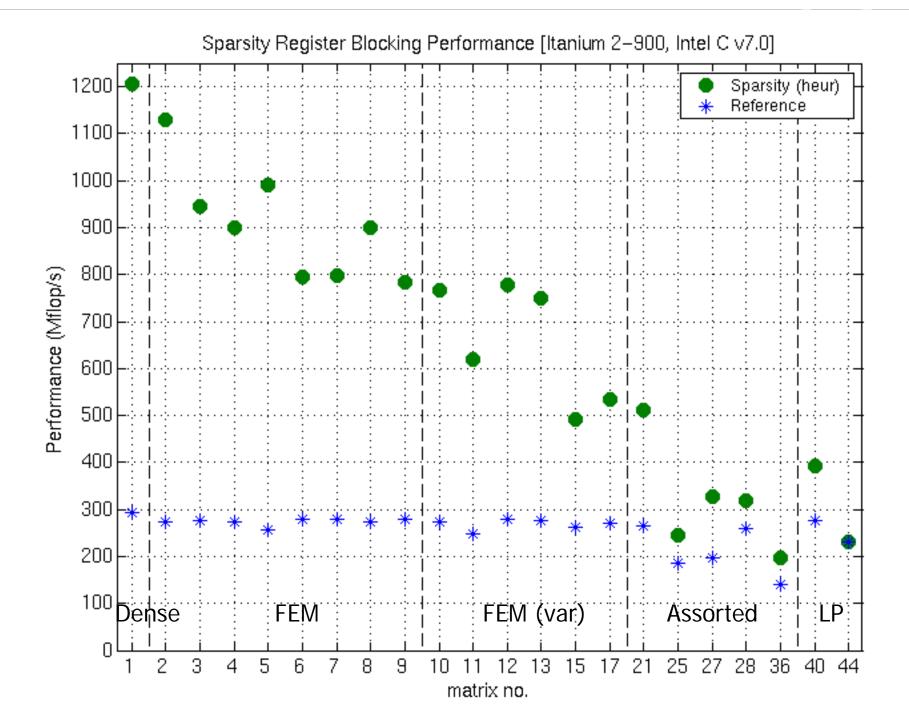












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### Tuning Sparse Triangular Solve (SpTS)

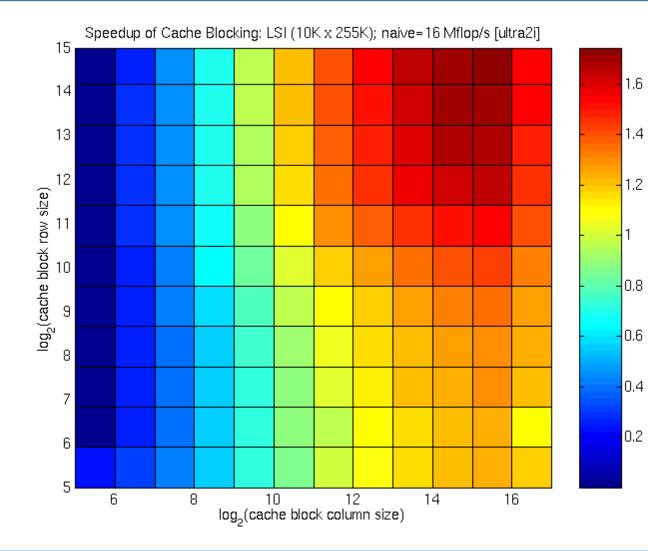
- Compute x=L<sup>-1</sup>\*b where L sparse lower triangular, x & b dense
- L from sparse LU has rich dense substructure
  - Dense trailing triangle can account for 20—90% of matrix non-zeros
- SpTS optimizations
  - Split into sparse trapezoid and dense trailing triangle
  - Use tuned dense BLAS (DTRSV) on dense triangle
  - Use Sparsity register blocking on sparse part
- Tuning parameters
  - Size of dense trailing triangle
  - Register block size

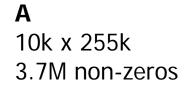


### **Sparse Kernels and Optimizations**

- Kernels
  - Sparse matrix-vector multiply (SpMV): y=A\*x
  - Sparse triangular solve (SpTS):  $x=T^{-1}*b$
  - $y = AA^T * x, y = A^T A^* x$
  - Powers ( $y=A^{k*x}$ ), sparse triple-product ( $R^*A^*R^T$ ), ...
- Optimization techniques (implementation space)
  - Register blocking
  - Cache blocking
  - Multiple dense vectors (x)
  - A has special structure (e.g., symmetric, banded, ...)
  - Hybrid data structures (*e.g.,* splitting, switch-to-dense, ...)
  - Matrix reordering
- How and when do we search?
  - Off-line: Benchmark implementations
  - Run-time: Estimate matrix properties, evaluate performance models based on benchmark data

## Cache Blocked SpMV on LSI Matrix: Ultra 2i



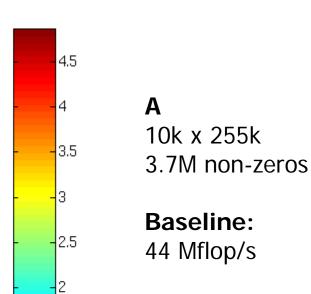


Baseline: 16 Mflop/s

Best block size & performance: 16k x 64k 28 Mflop/s

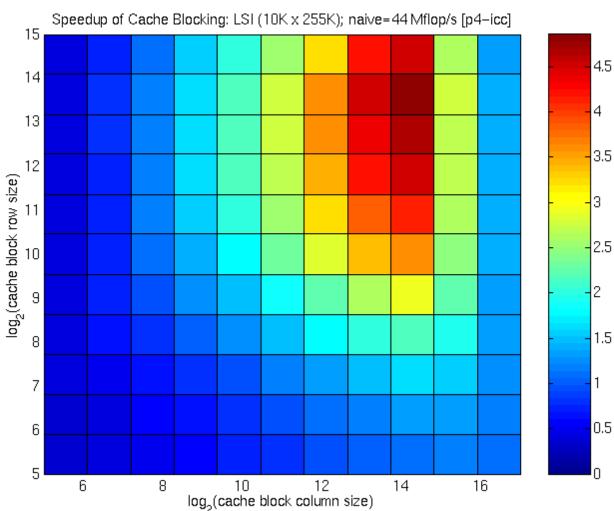
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## Cache Blocking on LSI Matrix: Pentium 4

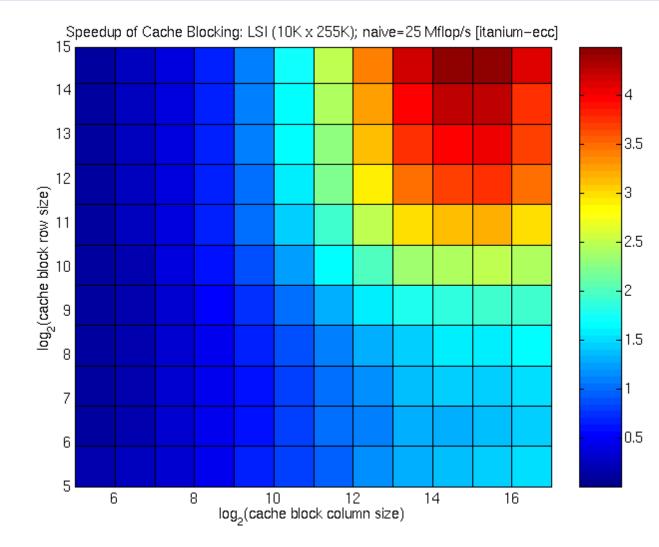


Ο

Best block size & performance: 16k x 16k 210 Mflop/s



### Cache Blocked SpMV on LSI Matrix: Itanium



A 10k x 255k 3.7M non-zeros

**Baseline:** 25 Mflop/s

Best block size & performance: 16k x 32k 72 Mflop/s

### Cache Blocked SpMV on LSI Matrix: Itanium 2

Cache Blocking Performance (Mflop/s) -- LSI Matrix (10k x 255k) [Itanium 2-900, Intel C v7.0] 14.5 274 264 14 1.02 1.59 1.63 1.58 1.28 1.00 1.48 254 13.5 244 13 1.01 1.28 1.47 1.58 1.60 1.56 1.00 234 log<sub>2</sub>(row block size) 12.5 11.5 224 1.01 1.26 1.46 1.56 1.58 1.53 1.00 214 204 11 1.00 1.25 1.44 1.54 1.56 1.48 1.00 194 10.5 184 10 .97 1.21 1.38 1.47 1.49 1.40 1.00 174 164 13 15 12 14 16 17 18 log\_(column block size)

**A** 10k x 255k 3.7M non-zeros **Baseline:** 170 Mflop/s

> Best block size & performance: 16k x 65k 275 Mflop/s

#### **Summary and Questions**

- Need to understand matrix structure and machine
  - BeBOP: suite of techniques to deal with different sparse structures and architectures
- Google matrix problem
  - Established techniques within an iteration
  - Ideas for inter-iteration optimizations
  - Mathematical structure of problem may help
- Questions
  - Structure of G?
  - What are the computational bottlenecks?
  - Enabling future computations?
    - E.g., topic-sensitive PageRank → multiple vector version [Haveliwala '02]
  - See www.cs.berkeley.edu/~richie/bebop/intel/google for more info, including more complete Itanium 2 results.

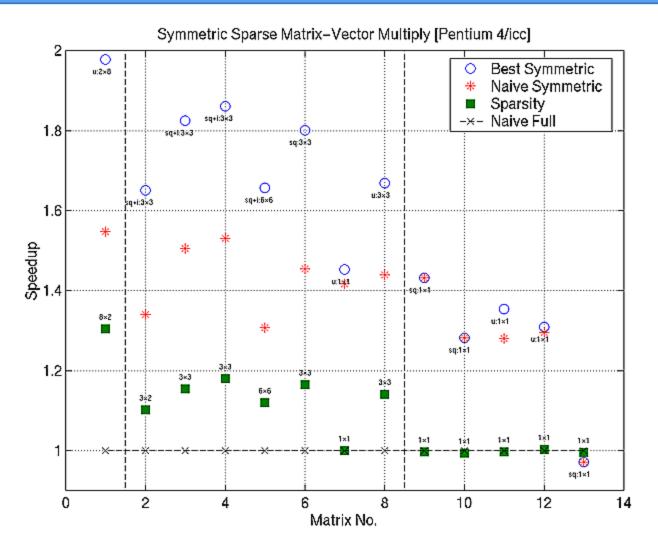


# **Exploiting Matrix Structure**

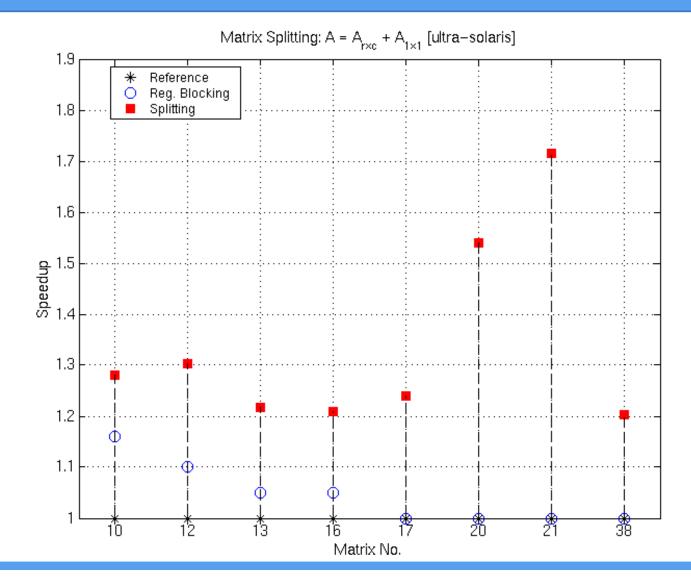
- Symmetry (numerical or structural)
  - Reuse matrix entries
  - Can combine with register blocking, multiple vectors, ...
- Matrix splitting
  - Split the matrix, e.g., into r x c and 1 x 1
  - No fill overhead
- Large matrices with random structure
  - E.g., Latent Semantic Indexing (LSI) matrices
  - Technique: cache blocking
    - Store matrix as 2<sup>i</sup> x 2<sup>j</sup> sparse submatrices
    - Effective when *x* vector is large
    - Currently, search to find fastest size



#### Symmetric SpMV Performance: Pentium 4



#### SpMV with Split Matrices: Ultra 2i



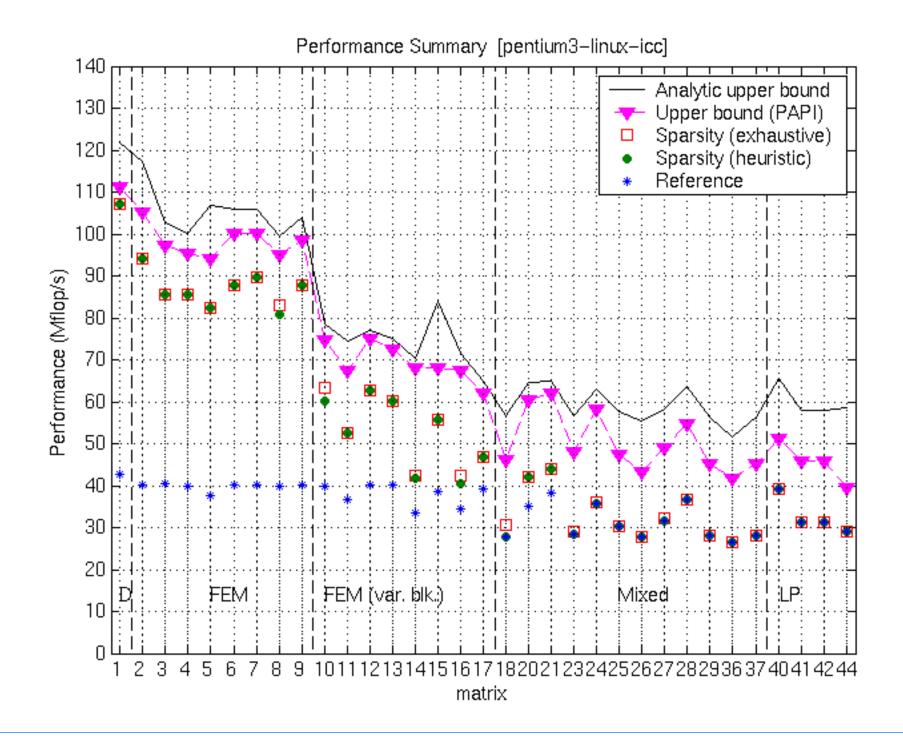
### Cache Blocking on Random Matrices: Itanium

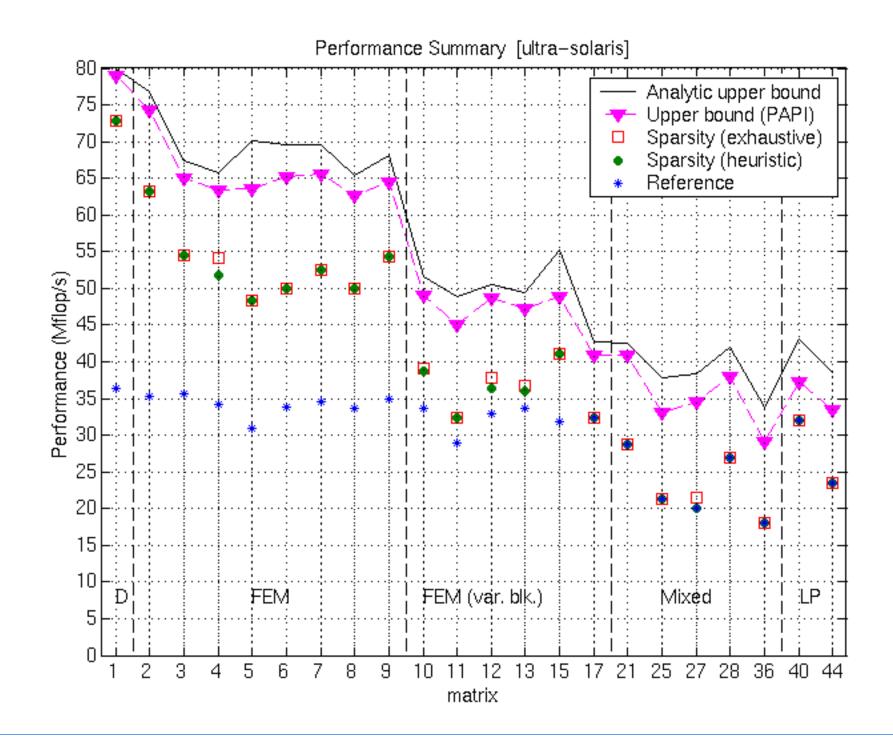
Z=0.015936; ref = 172.4 MFLOPS Z=0.126777 ; ref = 127.2 MFLOPS 5 5 1.1 0.9 4 4 1 rows[2<sup>R</sup> \* 1K] 5 5 0.8 rows [2<sup>R +</sup> 1k] 0.9 3 0.7 Speedup on four banded 0.8 2 random matrices. 0.6 0.7 0.5 1 1 0.6 0.4 0.5 0 0 0 2 4 6 8 0 2 4 6 8 cols  $[2^{C} \star 1k]$  $cols [2^{C} * 1k]$ Z=0.360000 ; ref = 79.6 MFLOPS Z=1.000000 ; ref = 43.5 MFLOPS 5 5 2.5 1.4 4 4 rows (2<sup>R</sup> \* 1 k) 5 5 5 2 rows [2<sup>R</sup> \* 1 k] 1.2 3 1.5 2 1 1 0.8 1 1 0 0 2 6 2 0 4 8 0 4 6 8 cols  $[2^{C} \star 1k]$  $cols [2^{C} * 1k]$ 

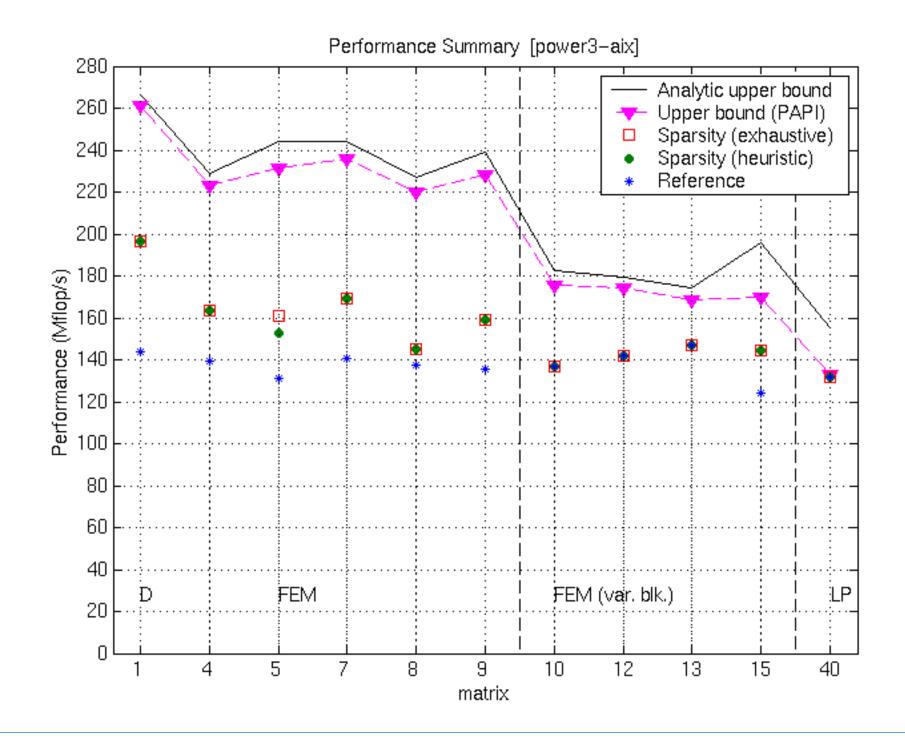


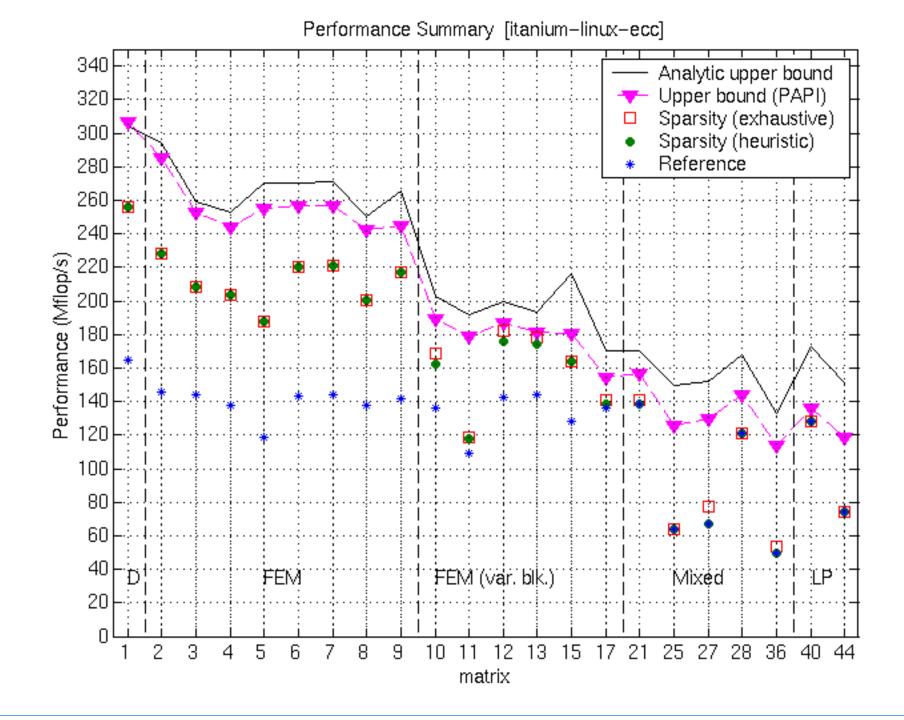
### **Sparse Kernels and Optimizations**

- Kernels
  - Sparse matrix-vector multiply (SpMV): y=A\*x
  - Sparse triangular solve (SpTS):  $x=T^{-1}*b$
  - $y = AA^T * x, y = A^T A^* x$
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  - Cache blocking
  - Multiple dense vectors (x)
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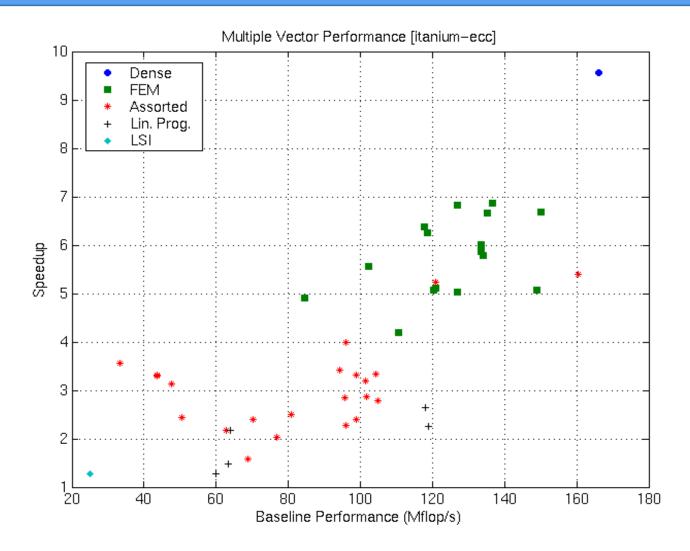




## **Possible Optimization Techniques**

- Within an iteration, *i.e.*, computing (G+uu<sup>T</sup>)\*x once
  - Cache block G\*x
    - On linear programming matrices and matrices with random structure (*e.g.*, LSI), 1.5—4x speedups
    - Best block size is matrix and machine dependent
  - Reordering and/or splitting of G to separate dense structure (rows, columns, blocks)
- Between iterations, *e.g.*, (G+uu<sup>T</sup>)<sup>2</sup>x
  - $(G+uu^T)^2 x = G^2 x + (Gu)u^T x + u(u^T G)x + u(u^T u)u^T x$ 
    - Compute Gu, u<sup>T</sup>G, u<sup>T</sup>u once for all iterations
    - G<sup>2</sup>x: Inter-iteration tiling to read G only once

#### Multiple Vector Performance: Itanium

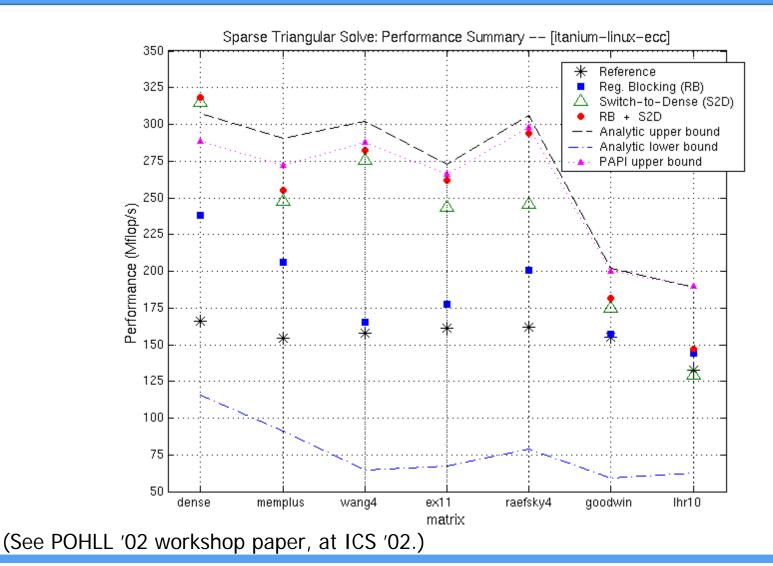




## **Sparse Kernels and Optimizations**

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#### SpTS Performance: Itanium





## **Sparse Kernels and Optimizations**

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  - Sparse matrix-vector multiply (SpMV): y=A\*x
  - Sparse triangular solve (SpTS):  $x=T^{-1}*b$
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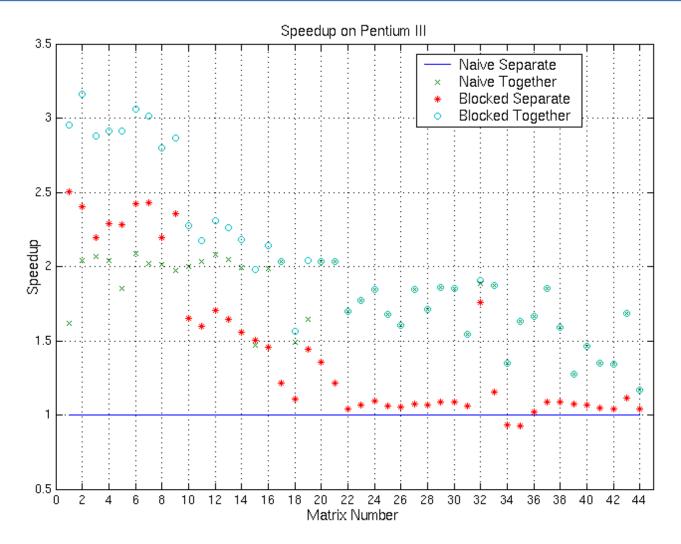
## Optimizing AA<sup>T</sup>\*x

- Kernel:  $y = AA^T * x$ , where A is sparse, x & y dense
  - Arises in linear programming, computation of SVD
  - Conventional implementation: compute  $z=A^T*x$ , y=A\*z
- Elements of A can be reused:

$$y = (a_1 \Lambda \ a_n) \begin{pmatrix} a_1^T \\ M \\ a_n^T \end{pmatrix} x = \sum_{k=1}^n a_k (a_k^T x)$$

• When  $a_k$  represent blocks of columns, can apply register blocking.

## Optimized AA<sup>T</sup>\*x Performance: Pentium III





## **Current Directions**

#### Applying new optimizations

- Other split data structures (variable block, diagonal, ...)
- Matrix reordering to create block structure
- Structural symmetry
- New kernels (triple product *RAR<sup>T</sup>*, powers *A<sup>k</sup>*, …)
- Tuning parameter selection
- Building an automatically tuned sparse matrix library
  - Extending the Sparse BLAS
  - Leverage existing sparse compilers as code generation infrastructure
  - More thoughts on this topic tomorrow



## **Related Work**

- Automatic performance tuning systems
  - PHiPAC [Bilmes, et al., '97], ATLAS [Whaley & Dongarra '98]
  - FFTW [Frigo & Johnson '98], SPIRAL [Pueschel, *et al.*, '00], UHFFT [Mirkovic and Johnsson '00]
  - MPI collective operations [Vadhiyar & Dongarra '01]
- Code generation
  - FLAME [Gunnels & van de Geijn, '01]
  - Sparse compilers: [Bik '99], Bernoulli [Pingali, et al., '97]
  - Generic programming: Blitz++ [Veldhuizen '98], MTL [Siek & Lumsdaine '98], GMCL [Czarnecki, *et al.* '98], …
- Sparse performance modeling
  - [Temam & Jalby '92], [White & Saddayappan '97], [Navarro, et al., '96], [Heras, et al., '99], [Fraguela, et al., '99], ...



## More Related Work

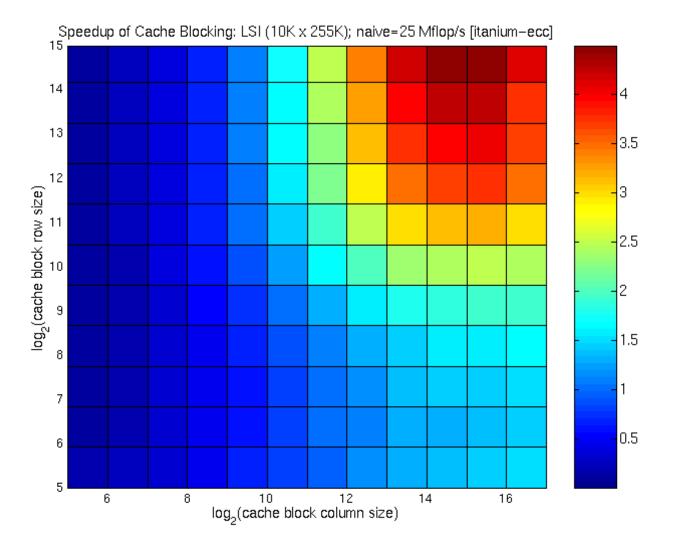
- Compiler analysis, models
  - CROPS [Carter, Ferrante, *et al.*]; Serial sparse tiling [Strout '01]
  - TUNE [Chatterjee, et al.]
  - Iterative compilation [O'Boyle, et al., '98]
  - Broadway compiler [Guyer & Lin, '99]
  - [Brewer '95], ADAPT [Voss '00]
- Sparse BLAS interfaces
  - BLAST Forum (Chapter 3)
  - NIST Sparse BLAS [Remington & Pozo '94]; SparseLib++
  - SPARSKIT [Saad '94]
  - Parallel Sparse BLAS [Fillipone, et al. '96]



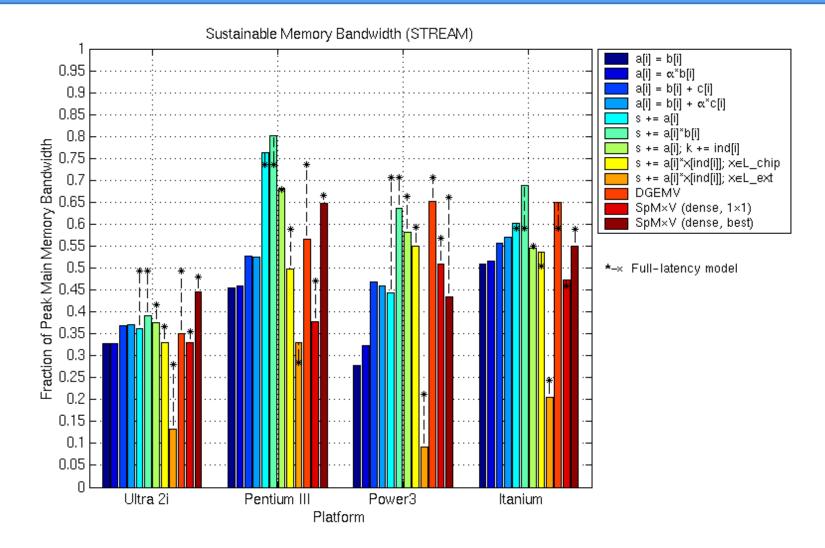
# Context: Creating High-Performance Libraries

- Application performance dominated by a few computational kernels
- Today: Kernels hand-tuned by vendor or user
- Performance tuning challenges
  - Performance is a complicated function of kernel, architecture, compiler, and workload
  - Tedious and time-consuming
- Successful automated approaches
  - Dense linear algebra: ATLAS/PHiPAC
  - Signal processing: FFTW/SPIRAL/UHFFT

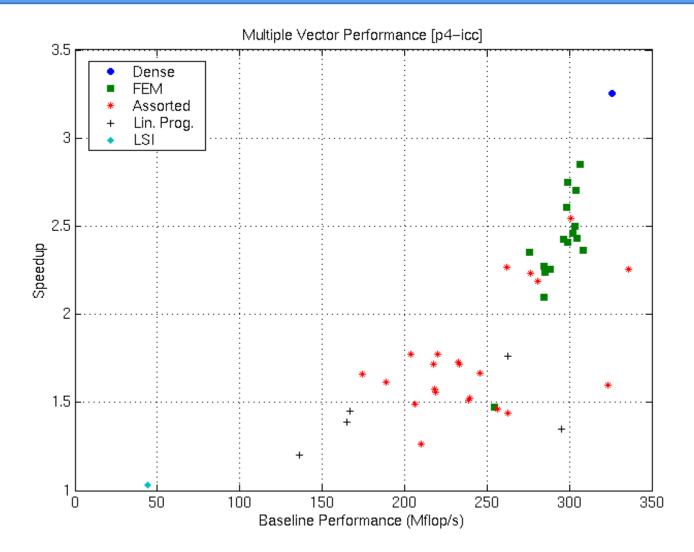
#### Cache Blocked SpMV on LSI Matrix: Itanium



### Sustainable Memory Bandwidth

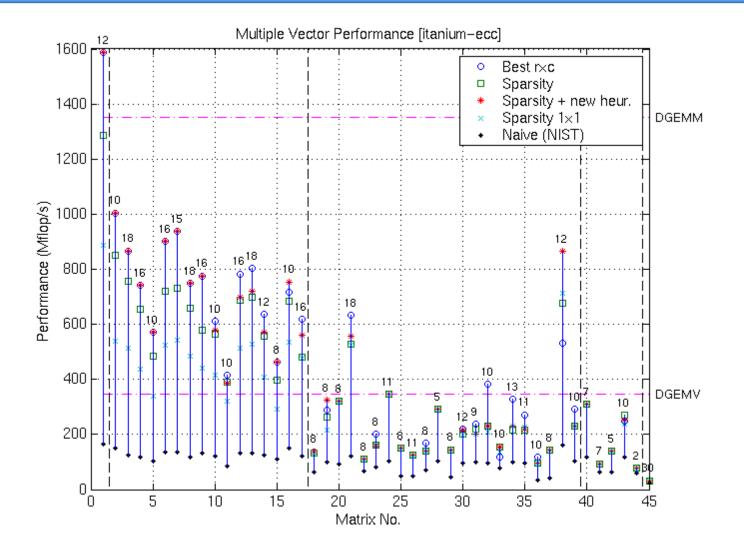


#### Multiple Vector Performance: Pentium 4

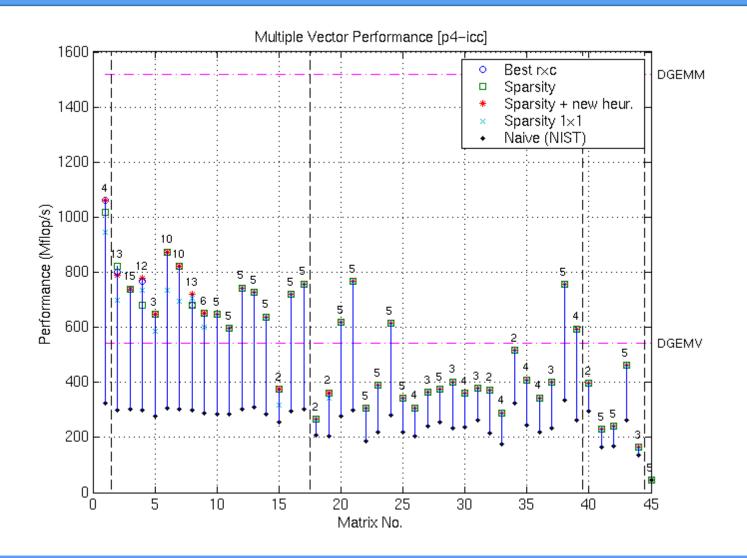


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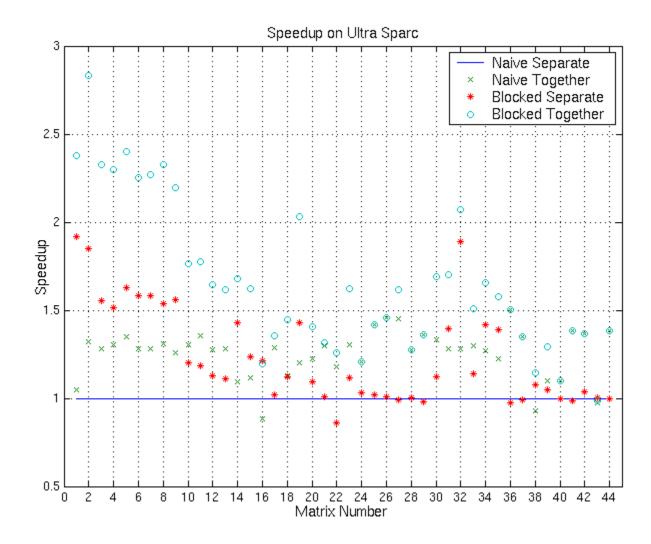
#### **Multiple Vector Performance: Itanium**



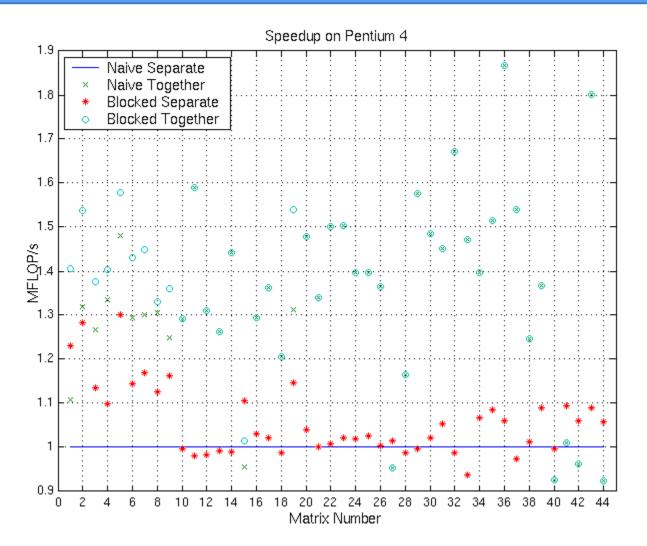
#### Multiple Vector Performance: Pentium 4



## Optimized $AA^T * x$ Performance: Ultra 2i

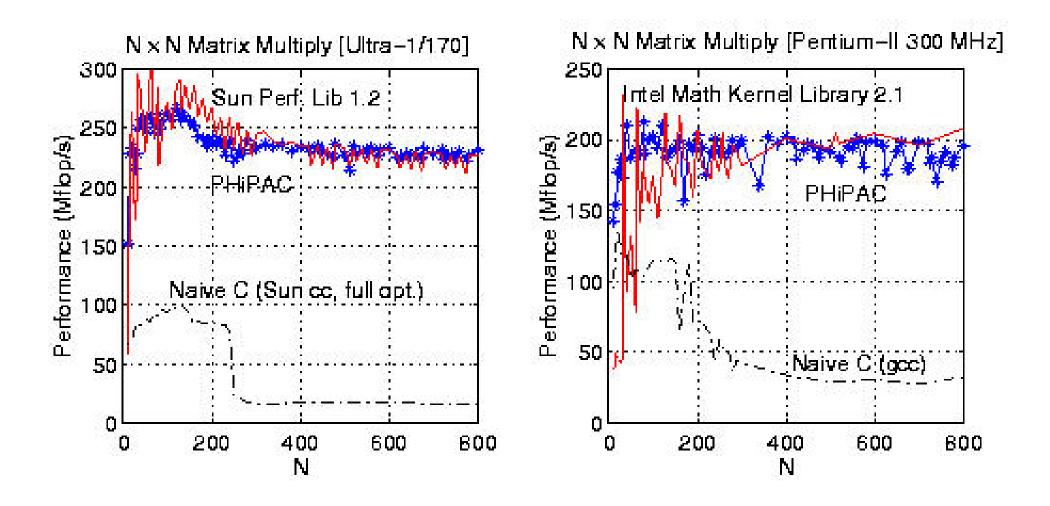


## Optimized AA<sup>T</sup>\*x Performance: Pentium 4





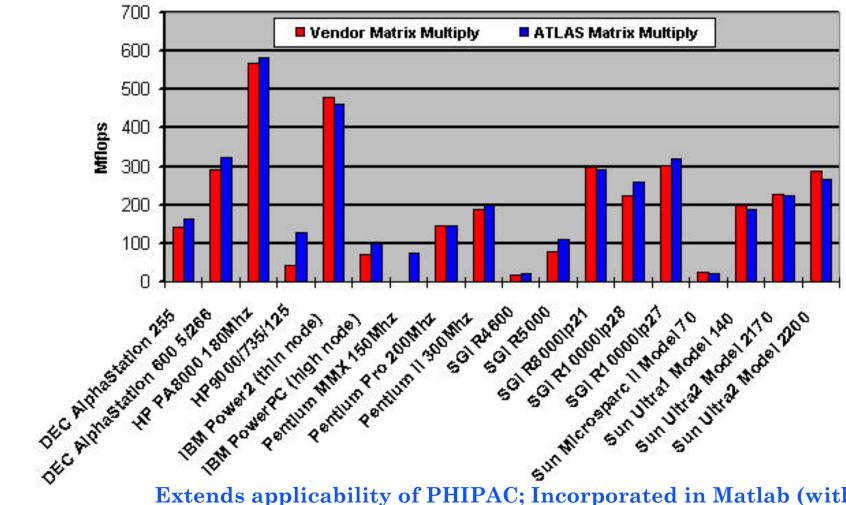
## Tuning Pays Off—PHiPAC



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## Tuning pays off – ATLAS

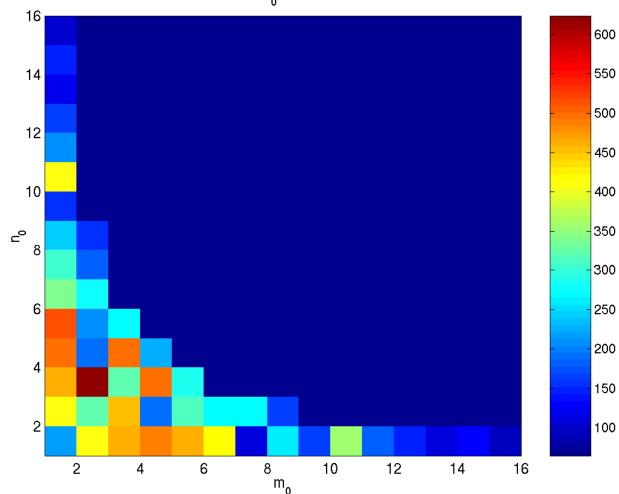
500x500 Double Precision Matrix-Matrix Multiply Across Multiple Architectures



Extends applicability of PHIPAC; Incorporated in Matlab (with rest

## Register Tile Sizes (Dense Matrix Multiply)





#### k<sub>0</sub> = 1

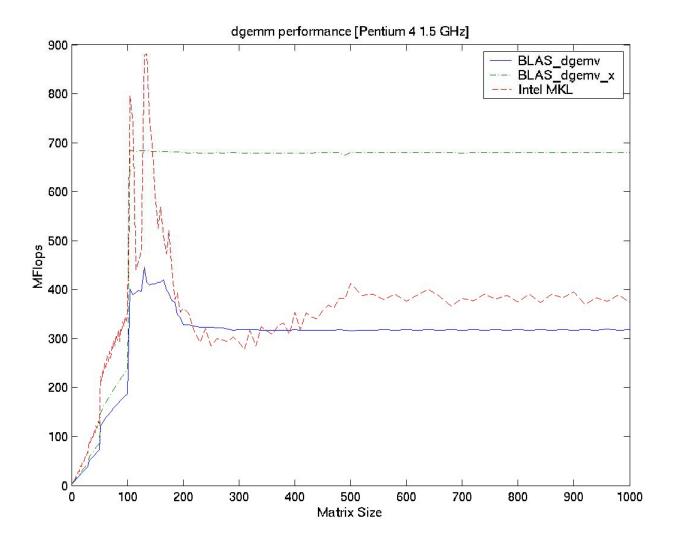
#### 333 MHz Sun Ultra 2i

2-D slice of 3-D space; implementations colorcoded by performance in Mflop/s

## 16 registers, but 2-by-3 tile size fastest



#### High Precision GEMV (XBLAS)



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# High Precision Algorithms (XBLAS)

- Double-double (High precision word represented as pair of doubles)
  - Many variations on these algorithms; we currently use Bailey's
- Exploiting Extra-wide Registers
  - Suppose s(1), ..., s(n) have f-bit fractions, SUM has F>f bit fraction
  - Consider following algorithm for  $S = \Sigma_{i=1,n} s(i)$ 
    - Sort so that  $|s(1)| \ge |s(2)| \ge \cdots \ge |s(n)|$
    - SUM = 0, for i = 1 to n SUM = SUM + s(i), end for, sum = SUM
  - Theorem (D., Hida) Suppose F<2f (less than double precision)
    - If  $n \le 2^{\mathbf{F} \cdot \mathbf{f}} + 1$ , then error  $\le 1.5$  ulps
    - If  $n = 2^{F-f} + 2$ , then error  $\leq 2^{2f-F}$  ulps (can be >> 1)
    - If  $n \ge 2^{F-f} + 3$ , then error can be arbitrary (S  $\neq 0$  but sum = 0)
  - Examples
    - s(i) double (f=53), SUM double extended (F=64)
      - accurate if  $n \le 2^{11} + 1 = 2049$
    - Dot product of single precision x(i) and y(i)
      - s(i) = x(i)\*y(i) (f=2\*24=48), SUM double extended (F=64) ⇒
      - accurate if  $n \le 2^{16} + 1 = 65537$