BeBOP:
Berkeley Benchmarking and Optimization

Automatic Performance Tuning of Numerical Kernels

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Support from DOE SciDAC, NSF, Intel

Performance Tuning Participants

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- Researchers
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- PhD Students
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Outline

- Motivation, History, Related work
- Tuning Sparse Matrix Operations
- Results on Sun Ultra 1/170
- Recent results on P4
- Recent results on Itanium
- Some (non SciDAC) Target Applications
  - SUGAR – a MEMS CAD system
  - Information Retrieval
- Future Work

Motivation
History
Related Work

Conventional Performance Tuning

- Motivation: performance of many applications dominated by a few kernels
- Vendor or user hand tunes kernels
- Drawbacks:
  - Very time consuming and tedious work
  - Even with intimate knowledge of architecture and compiler, performance hard to predict
  - Growing list of kernels to tune
    - Example: New BLAS Standard
  - Must be redone for every architecture, compiler
  - Compiler technology often lags architecture
  - Not just a compiler problem:
    - Best algorithm may depend on input, so some tuning at run-time.
    - Not all algorithms semantically or mathematically equivalent

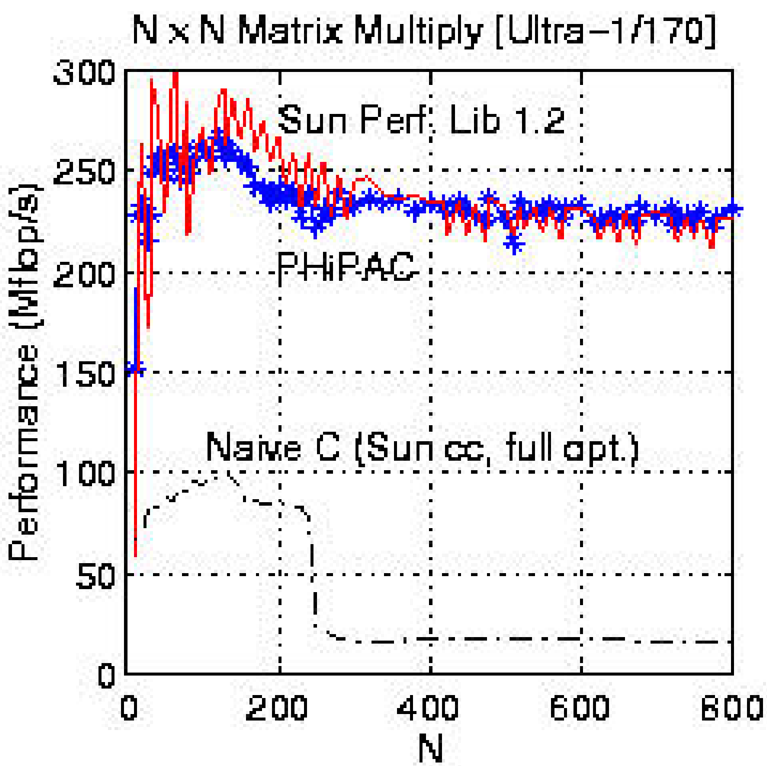
Automatic Performance Tuning

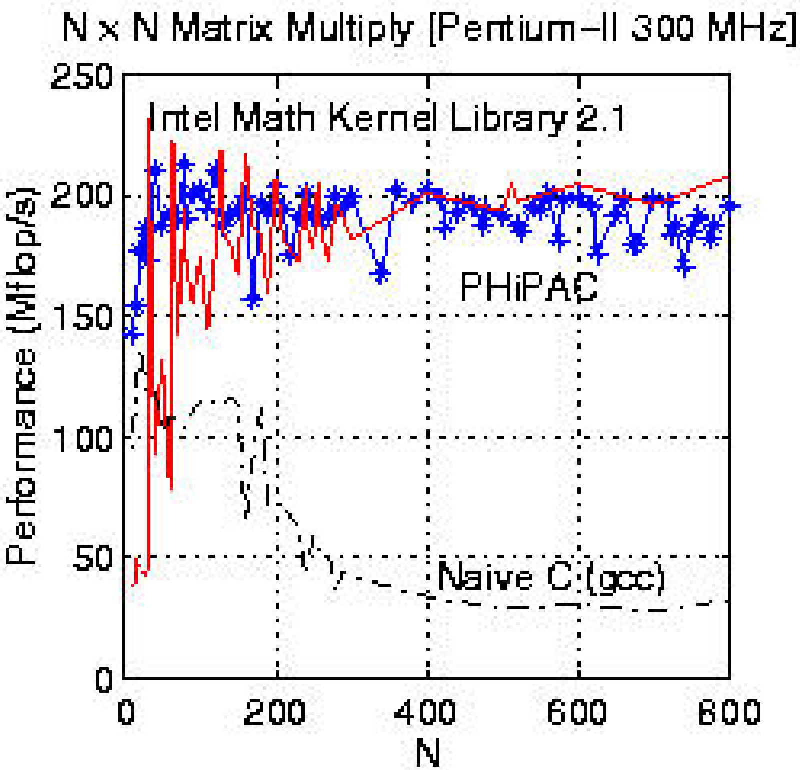
- Approach: for each kernel
  1. Identify and generate a space of algorithms
  2. Search for the fastest one, by running them
- What is a space of algorithms?
  - Depending on kernel and input, may vary
    - instruction mix and order
    - memory access patterns
    - data structures
    - mathematical formulation
- When do we search?
  - Once per kernel and architecture
  - At compile time
  - At run time
  - All of the above

Some Automatic Tuning Projects

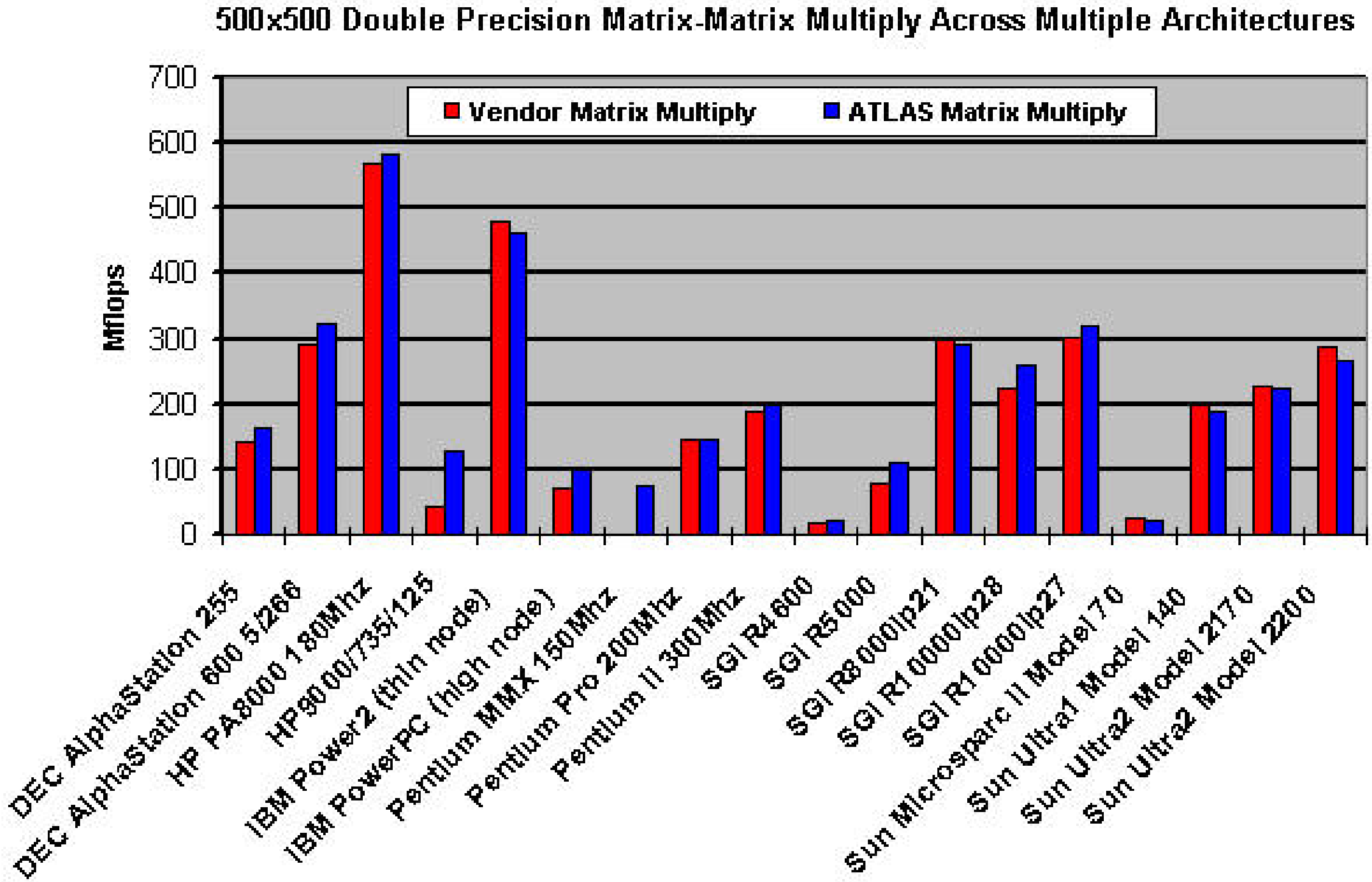
- PHIPAC (www.icsi.berkeley.edu/~bilmes/phipac) (Bilmes,Asanovic,Vuduc,Demmel)
- ATLAS (www.netlib.org/atlas) (Dongarra, Whaley; in Matlab)
- XBLAS (www.nersc.gov/~xiaoye/XBLAS) (Demmel, X. Li)
- Sparsity (www.cs.berkeley.edu/~yelick/sparsity) (Yelick, Im)
- FFTs and Signal Processing
  - FFTW (www.fftw.org)
    - Won 1999 Wilkinson Prize for Numerical Software
  - SPIRAL (www.ece.cmu.edu/~spiral)
    - Extensions to other transforms, DSPs
  - UHFFT
    - Extensions to higher dimension, parallelism
- Special session at ICCS 2001
  - Organized by Yelick and Demmel
  - www.ucalgary.ca/iccs
  - Proceedings available
  - Pointers to other automatic tuning projects at
    - www.cs.berkeley.edu/~yelick/iccs-tune

Tuning pays off – PHIPAC (Bilmes, Asanovic, Vuduc, Demmel)





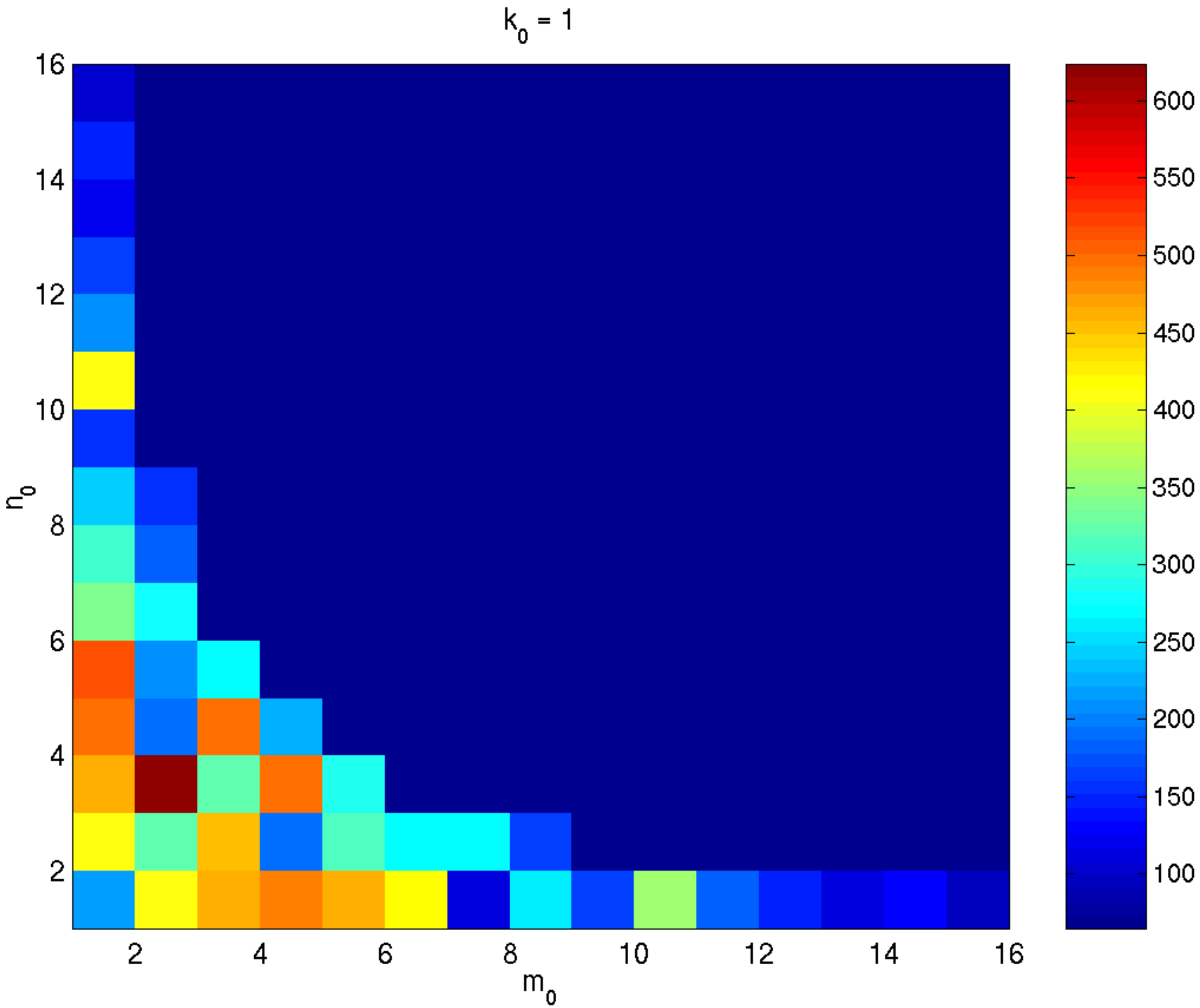
Tuning pays off – ATLAS (Dongarra, Whaley)



Extends applicability of PHIPAC

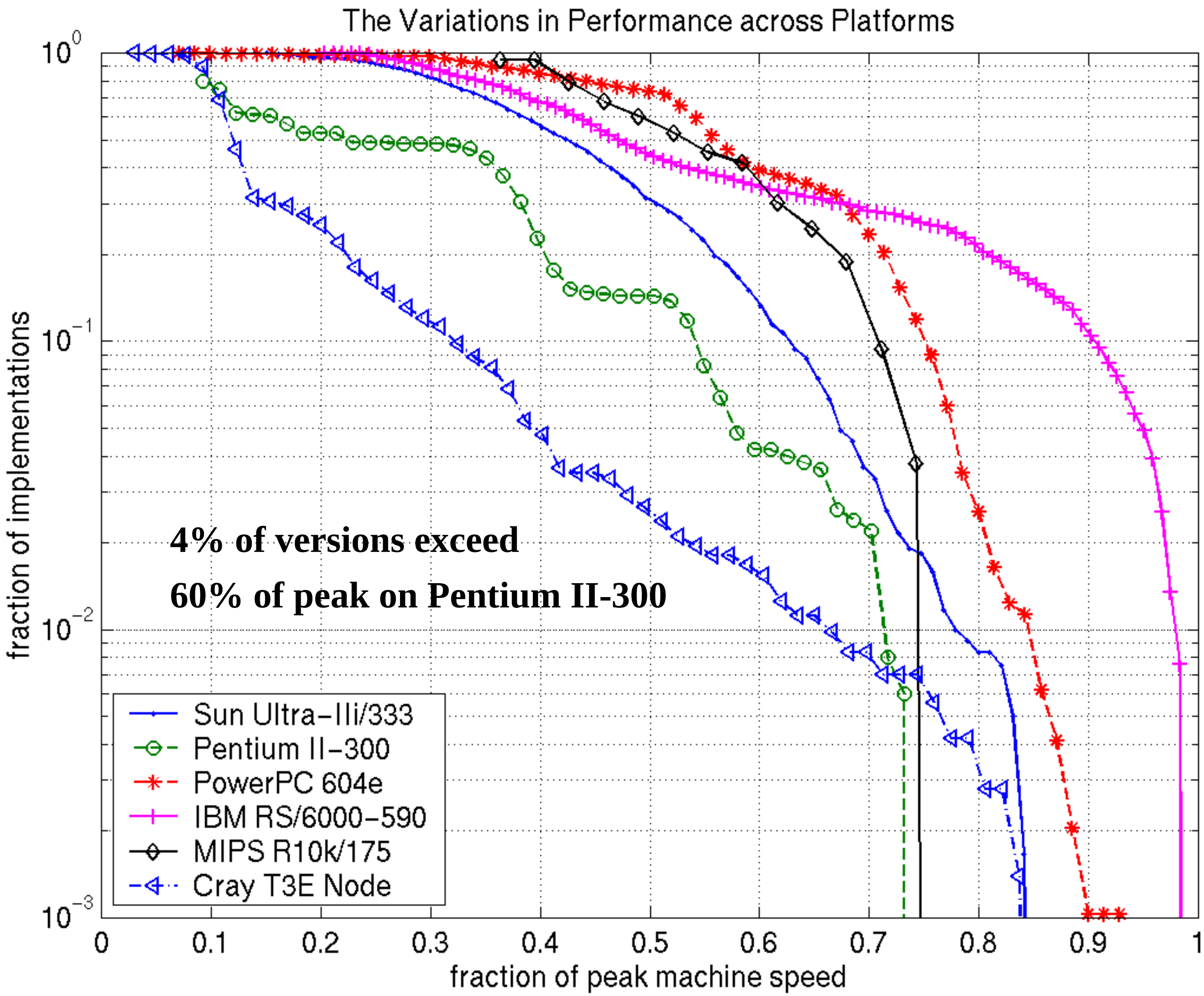
Incorporated in Matlab (with rest of LAPACK)

Search for optimal register tile sizes on Sun Ultra 10

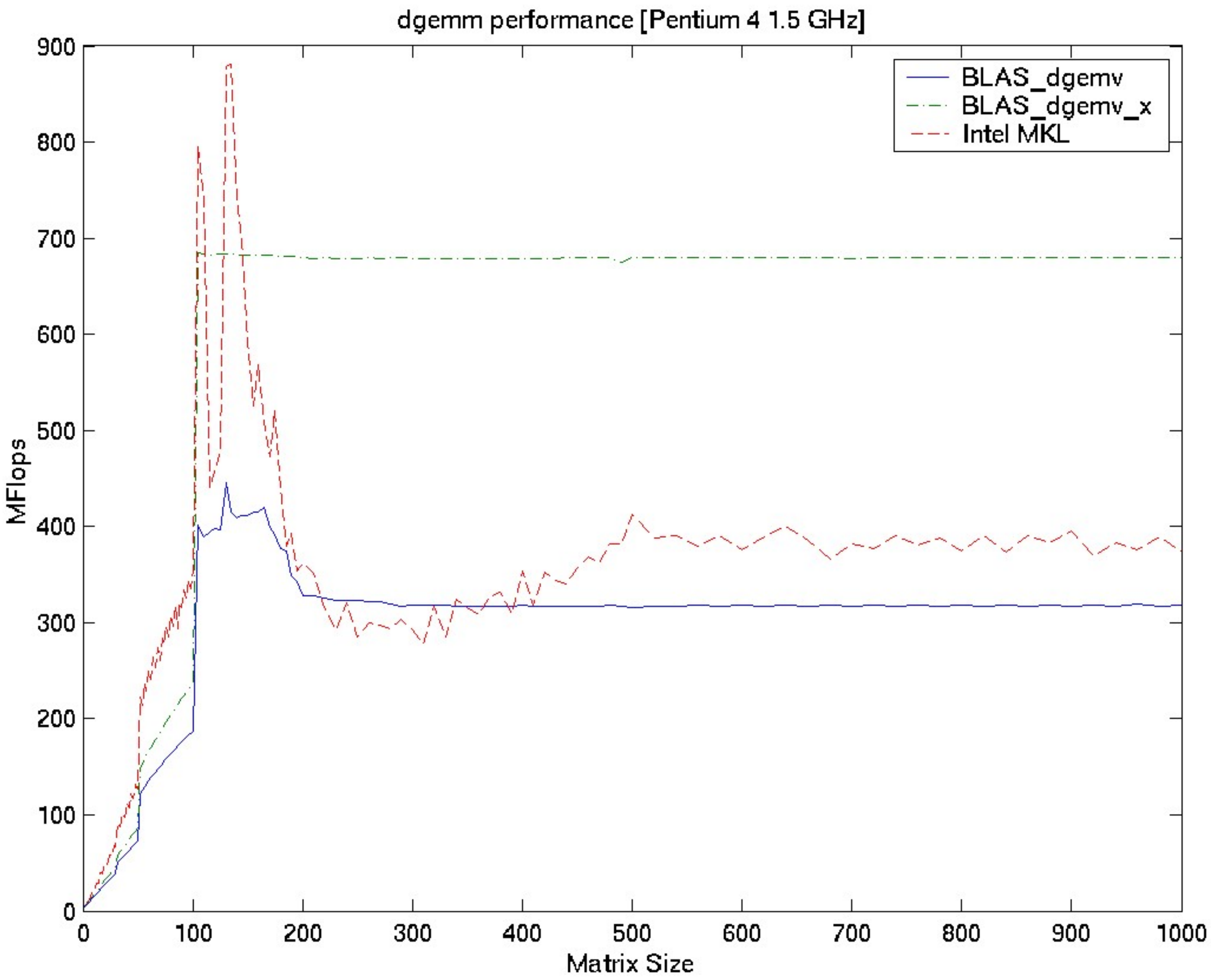


16 registers, but 2-by-3 tile size fastest

Search for Optimal L0 block size in dense matmul



High precision dense mat-vec multiply (XBLAS)



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 $|s(1)| \geq |s(2)| \geq \cdots \geq |s(n)|$
    - 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 $n \leq 2^{F-f} + 1$, then error $\leq$ 1.5 ulps
    - If $n = 2^{F-f} + 2$, then error $\leq 2^{2f-F}$ ulps (can be >> 1)
    - If $n \geq 2^{F-f} + 3$, then error can be arbitrary ($S \neq 0$ but sum = 0)
  - Examples
    - s(i) double (f=53), SUM double extended (F=64)
      - accurate if $n \leq 2^{11} + 1 = 2049$
    - 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) $\Rightarrow$
      - accurate if $n \leq 2^{16} + 1 = 65537$

Tuning Sparse Matrix Computations

Tuning Sparse matrix-vector multiply

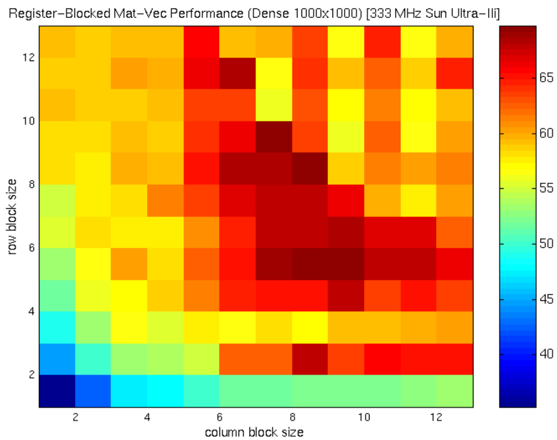
- Sparsity
  - Optimizes y = A*x for a particular sparse A
- Im and Yelick
- Algorithm space
  - Different code organization, instruction mixes
  - Different register blockings (change data structure and fill of A)
  - Different cache blocking
  - Different number of columns of x
  - Different matrix orderings
- Software and papers available
  - www.cs.berkeley.edu/~yelick/sparsity

How Sparsity tunes y = A*x

- Register Blocking
  - Store matrix as dense r x c blocks
  - Precompute performance in **Mflops** of dense A*x for various register block sizes r x c
  - Given A, sample it to estimate **Fill** if A blocked for varying r x c
  - Choose r x c to minimize estimated running time **Fill/Mflops**
    - Store explicit zeros in dense r x c blocks, unroll
- Cache Blocking
  - Useful when source vector x enormous
  - Store matrix as sparse 2^k x 2^l blocks
  - Search over 2^k x 2^l cache blocks to find fastest

Register-Blocked Performance of SPMV on Dense Matrices (up to 12x12)

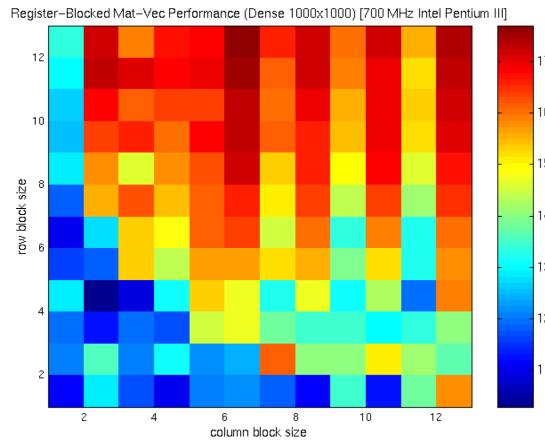
333 MHz Sun Ultra IIi



70 Mflops

35 Mflops

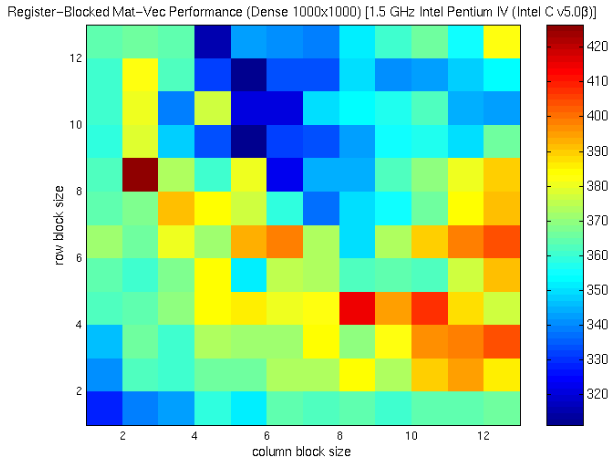
800 MHz Pentium III



175 Mflops

105 Mflops

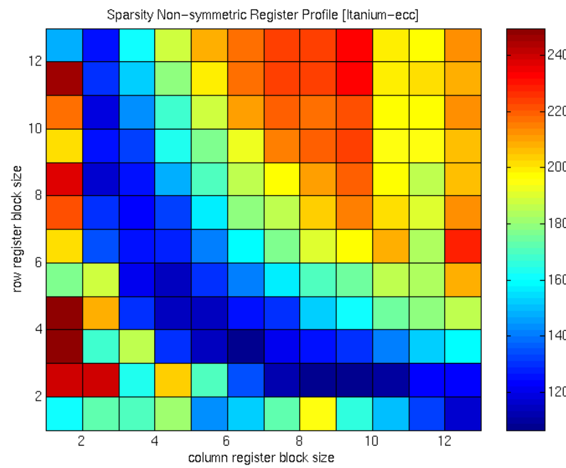
1.5 GHz Pentium 4



425 Mflops

310 Mflops

800 MHz Itanium



250 Mflops

110 Mflops

Which other sparse operations can we tune?

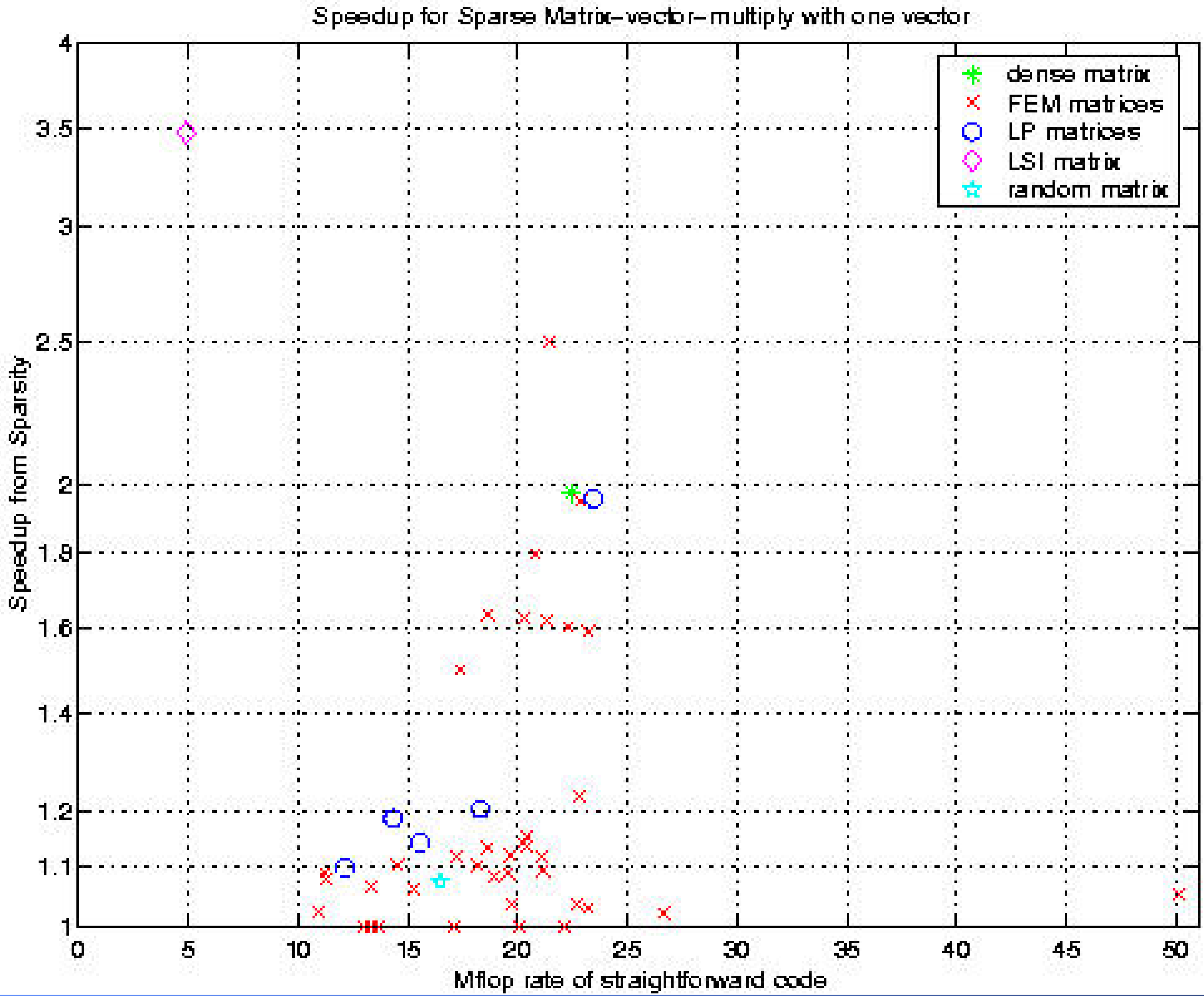
- General matrix-vector multiply $A*x$
  - Possibly many vectors x
- Symmetric matrix-vector multiply $A*x$
- Solve a triangular system of equations $T^{-1}*x$
- $y = A^T*A*x$
  - Kernel of Information Retrieval via LSI (SVD)
  - Same number of memory references as $A*x$
    - $y = \sum_i (A(i,:))^T * (A(i,:) * x)$
- Future work
  - A^2*x, A^k*x
    - Kernel of Information Retrieval used by Google
    - Includes Jacobi, SOR, …
    - Changes calling algorithm
  - A^T*M*A
    - Matrix triple product
    - Used in multigrid solver
  - What does SciDAC need?

Test Matrices

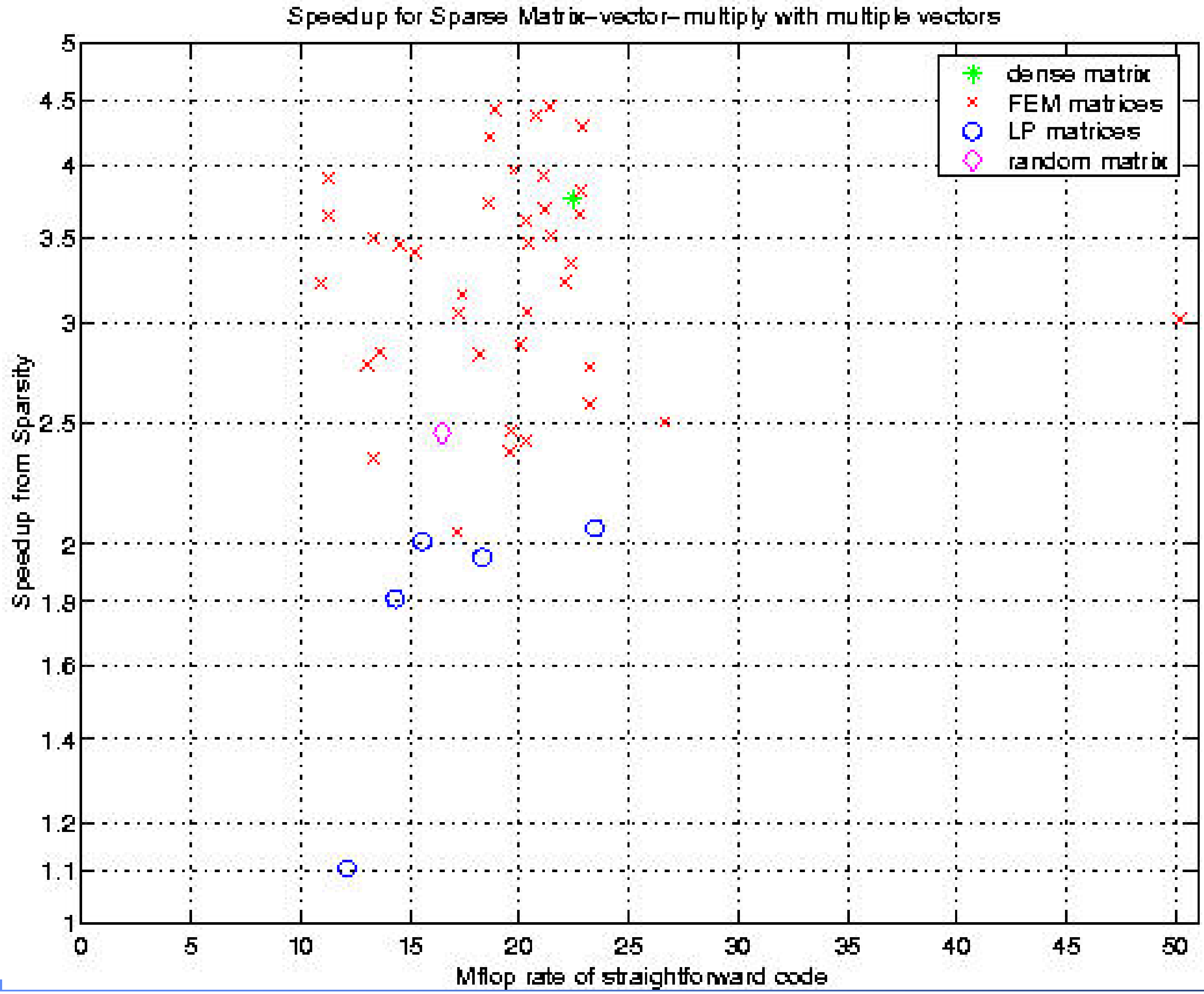
- General Sparse Matrices
  - Up to n=76K, nnz = 3.21M
  - From many application areas
  - 1 – Dense
  - 2 to 17 - FEM
  - 18 to 39 - assorted
  - 41 to 44 – linear programming
  - 45 - LSI
- Symmetric Matrices
  - Subset of General Matrices
  - 1 – Dense
  - 2 to 8 - FEM
  - 9 to 13 - assorted
- Lower Triangular Matrices
  - Obtained by running SuperLU on subset of General Sparse Matrices
  - 1 – Dense
  - 2 – 13 – FEM
- Details on test matrices at end of talk

Results on Sun Ultra 1/170

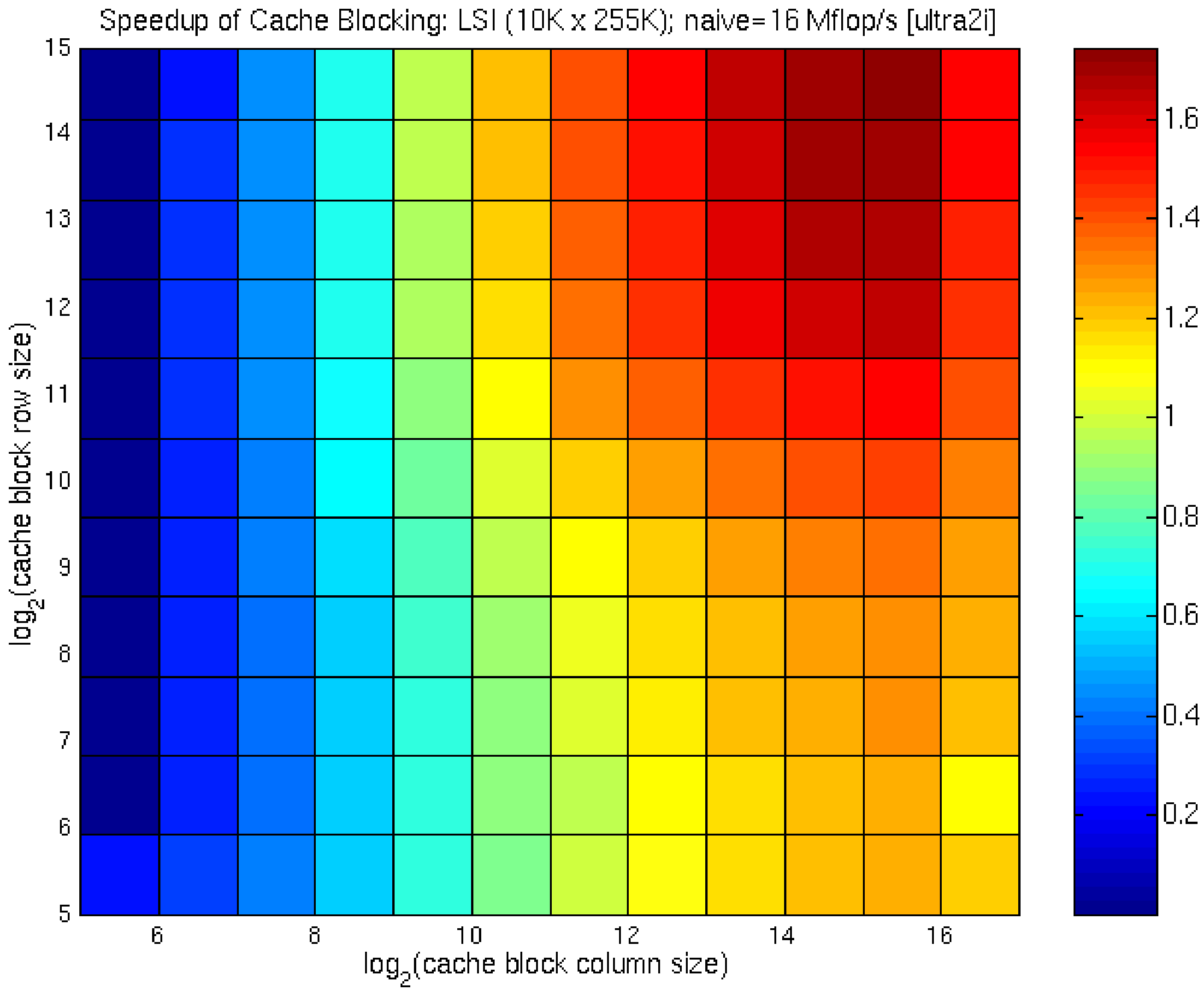
Speedups on SPMV from Sparsity on Sun Ultra 1/170 – 1 RHS



Speedups on SPMV from Sparsity on Sun Ultra 1/170 – 9 RHS

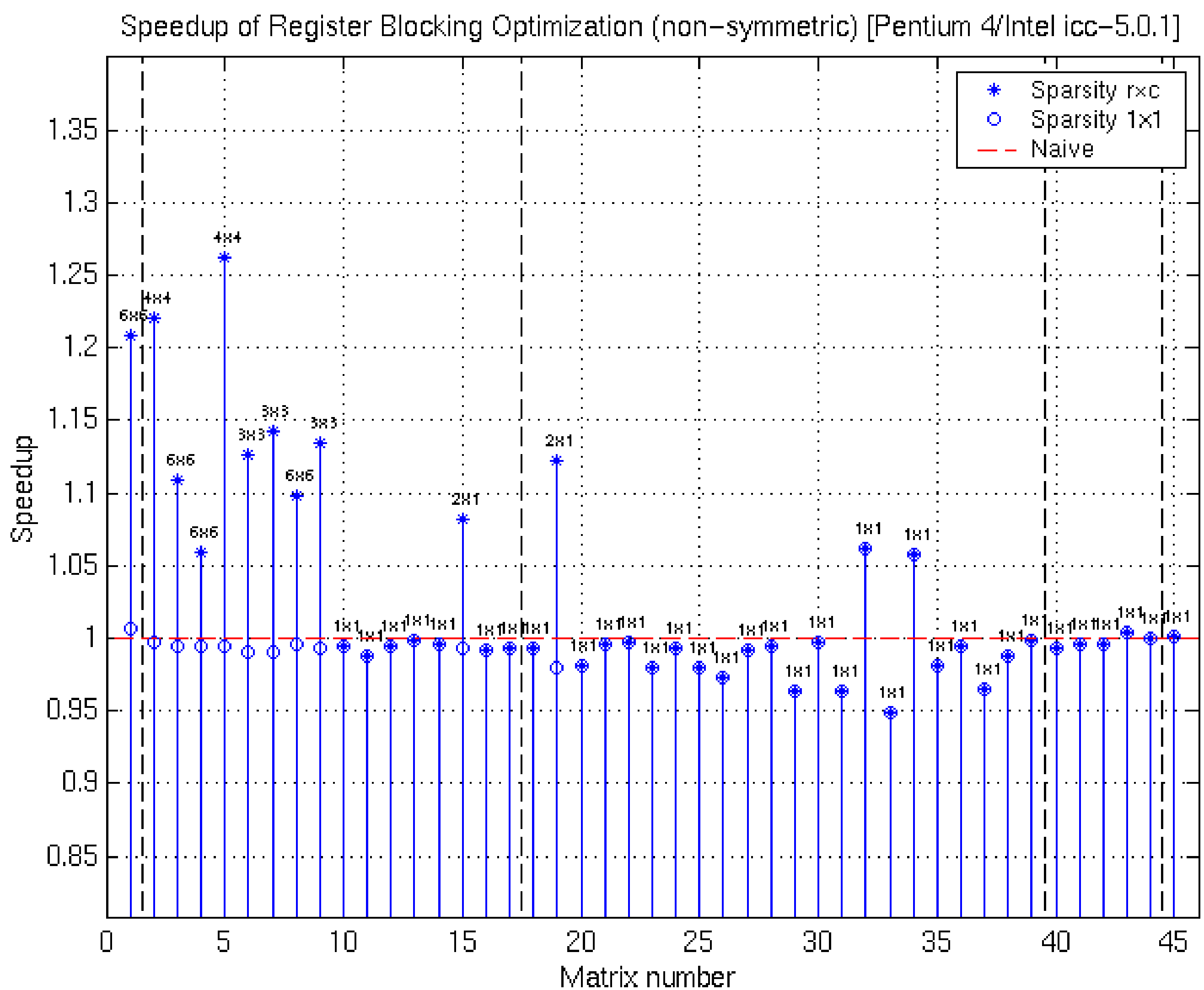


Speed up from Cache Blocking on LSI matrix on Sun Ultra

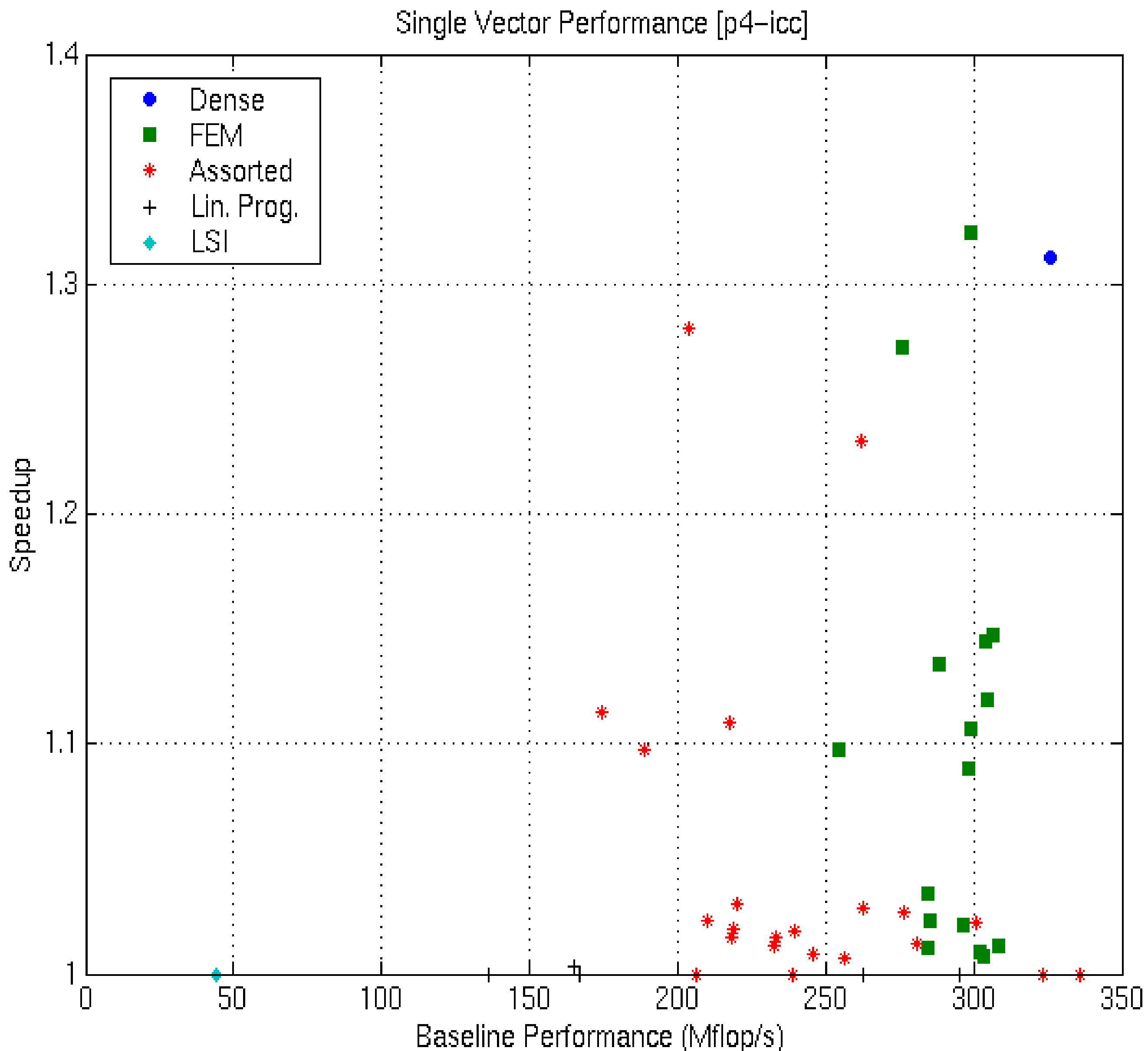


Recent Results
on P4 using icc and gcc

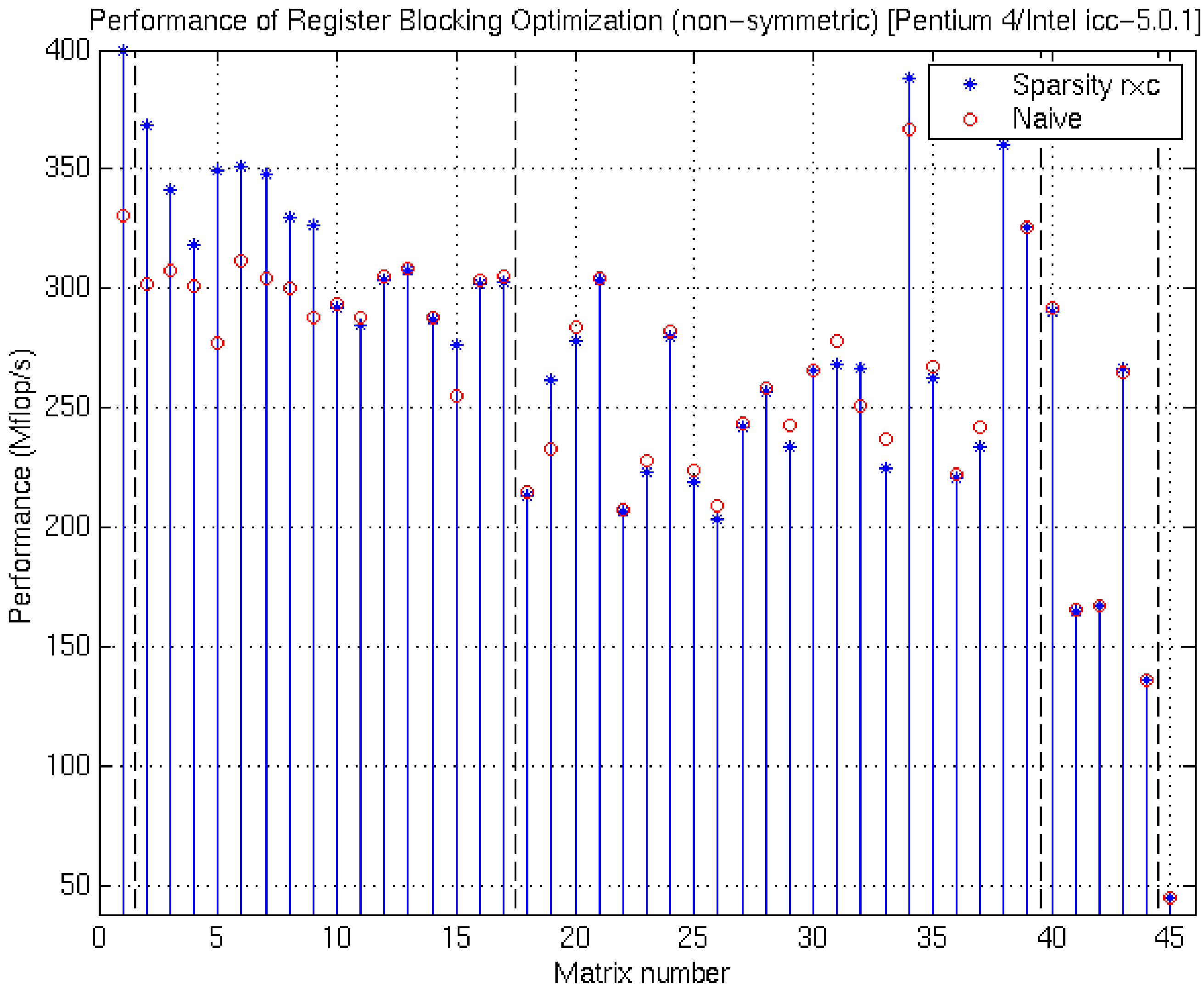
Speedup of SPMV from Sparsity on P4/icc-5.0.1



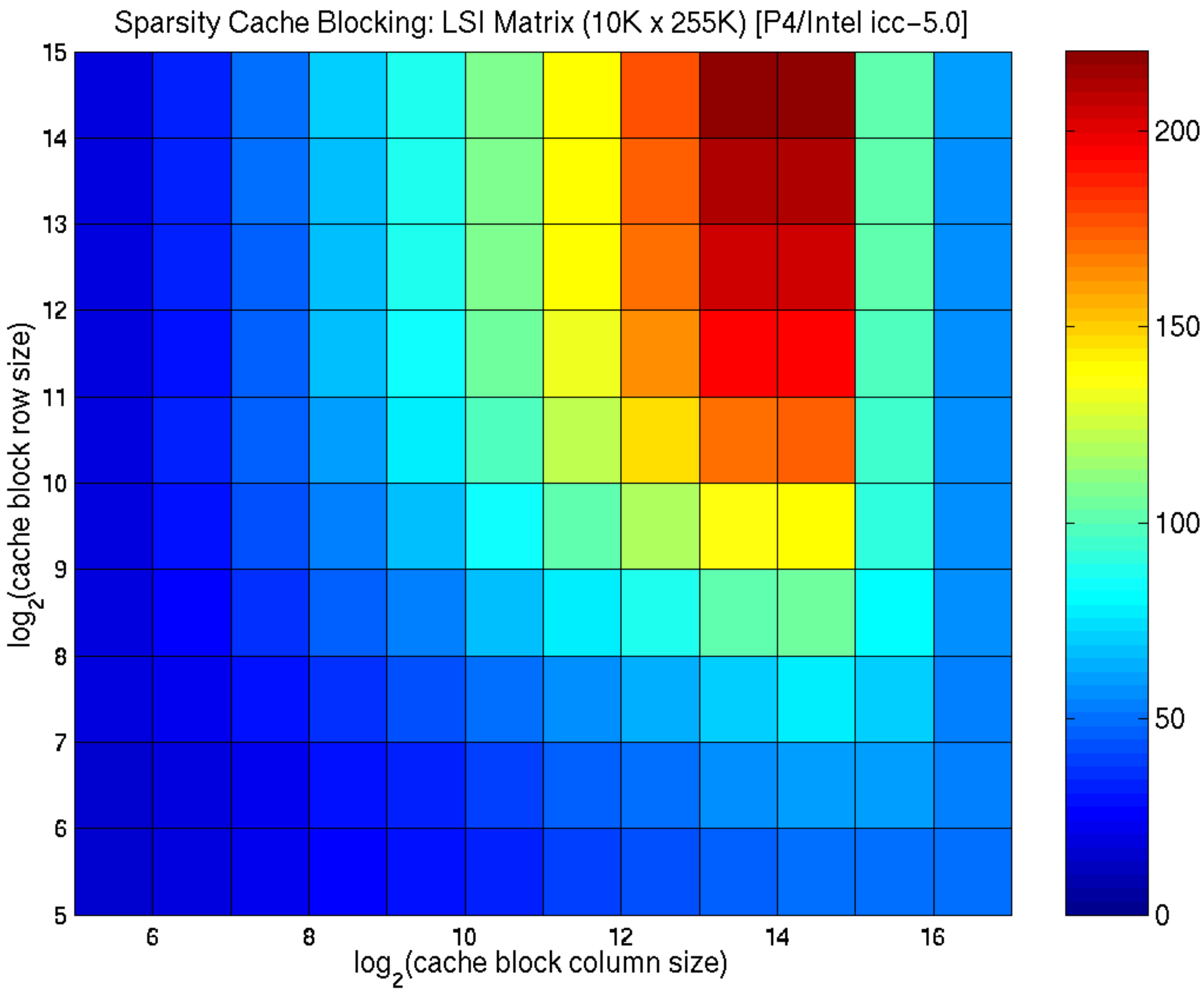
Single vector speedups on P4 by matrix type – best r x c



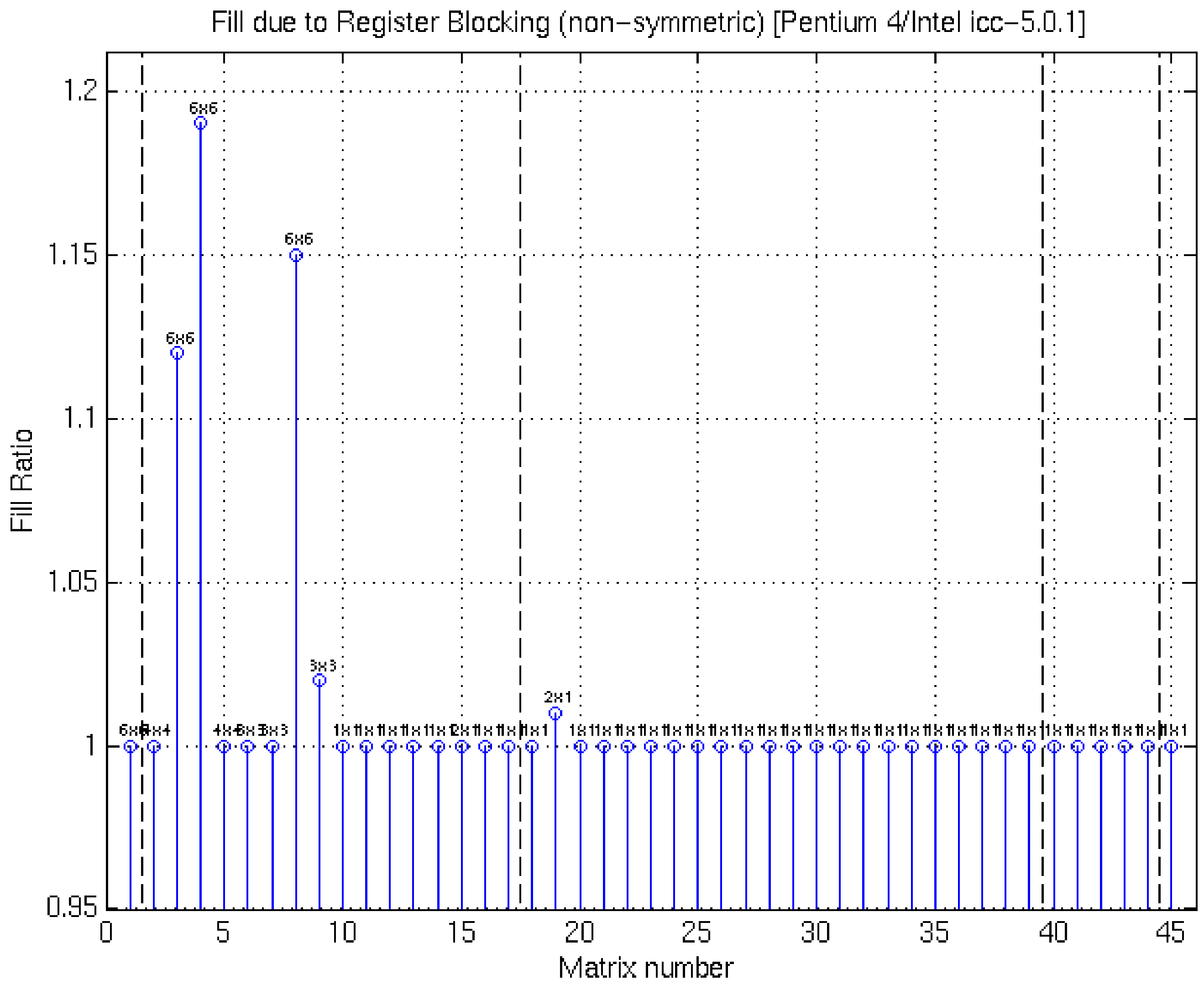
Performance of SPMV from Sparsity on P4/icc-5.0.1



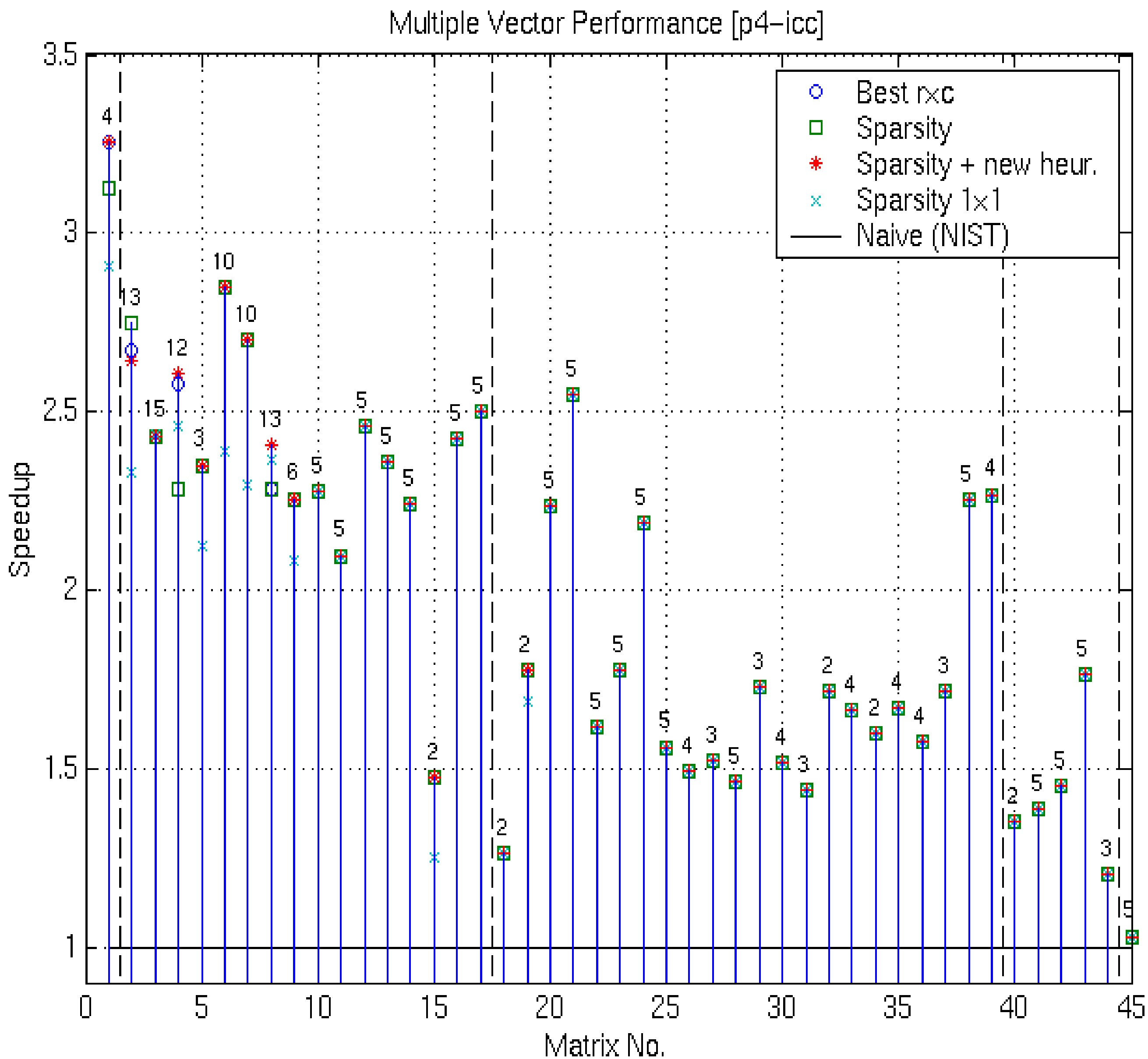
Sparsity cache blocking results on P4 for LSI



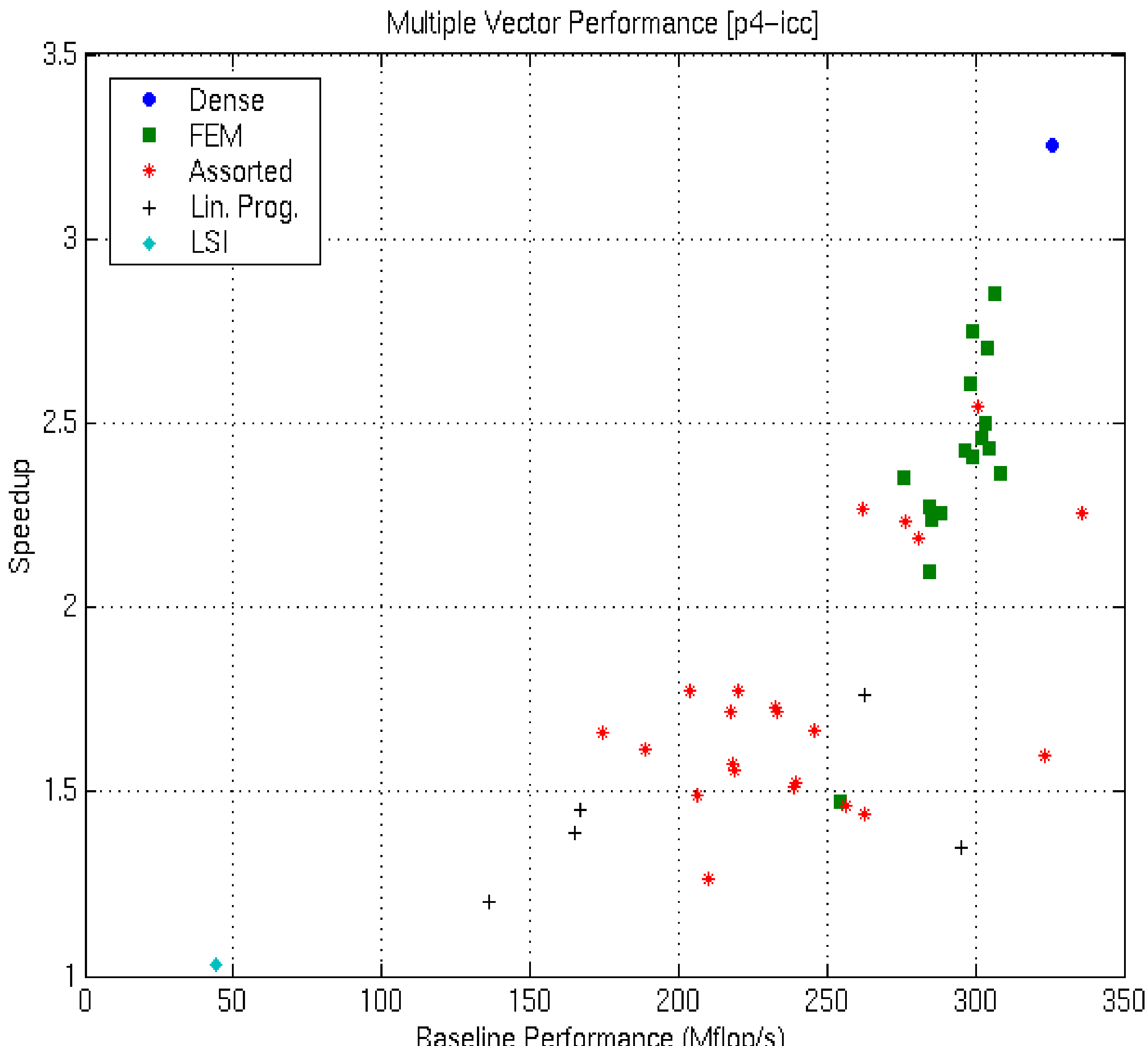
Fill for SPMV from Sparsity on P4/icc-5.0.1



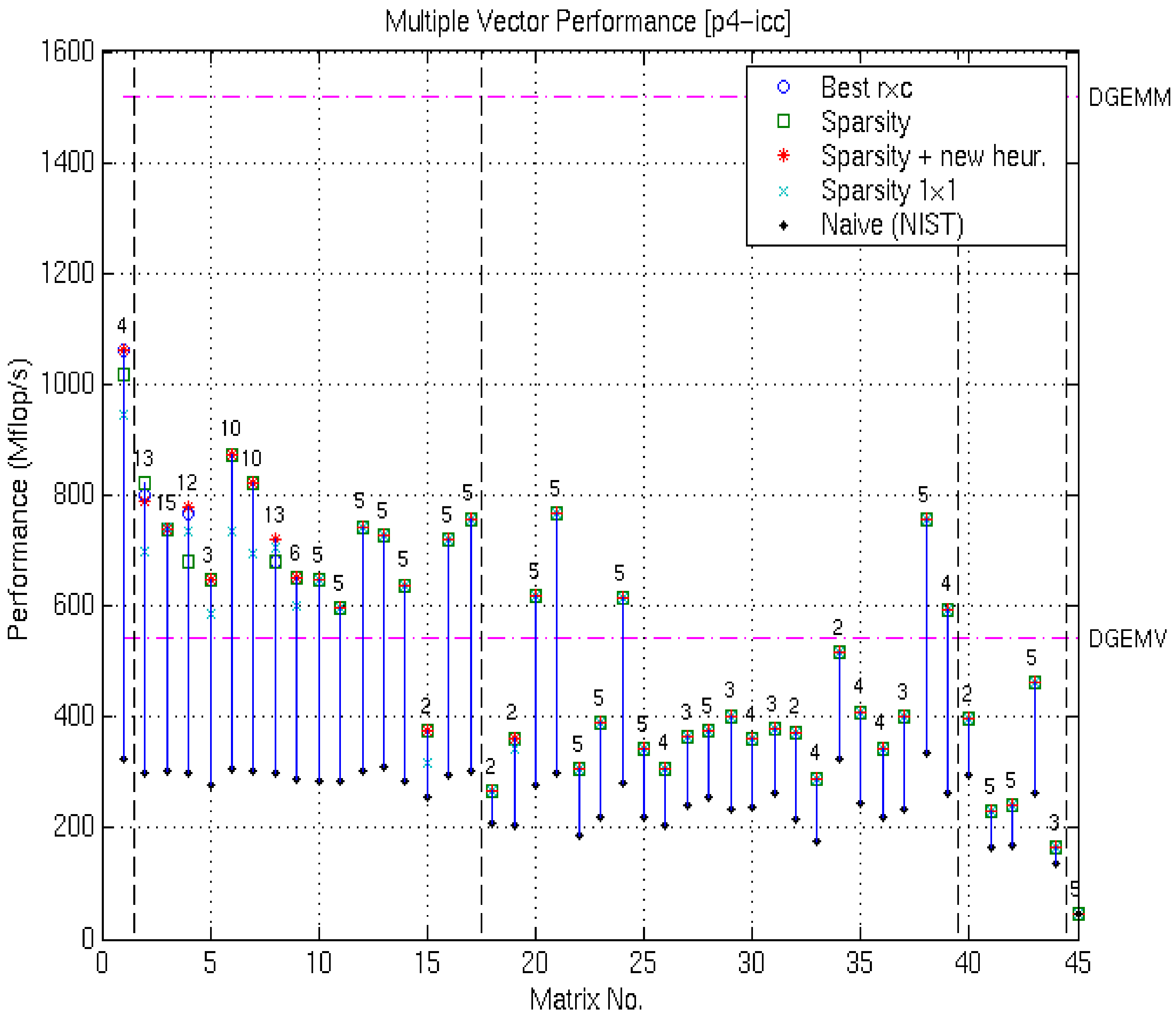
Multiple vector speedups on P4



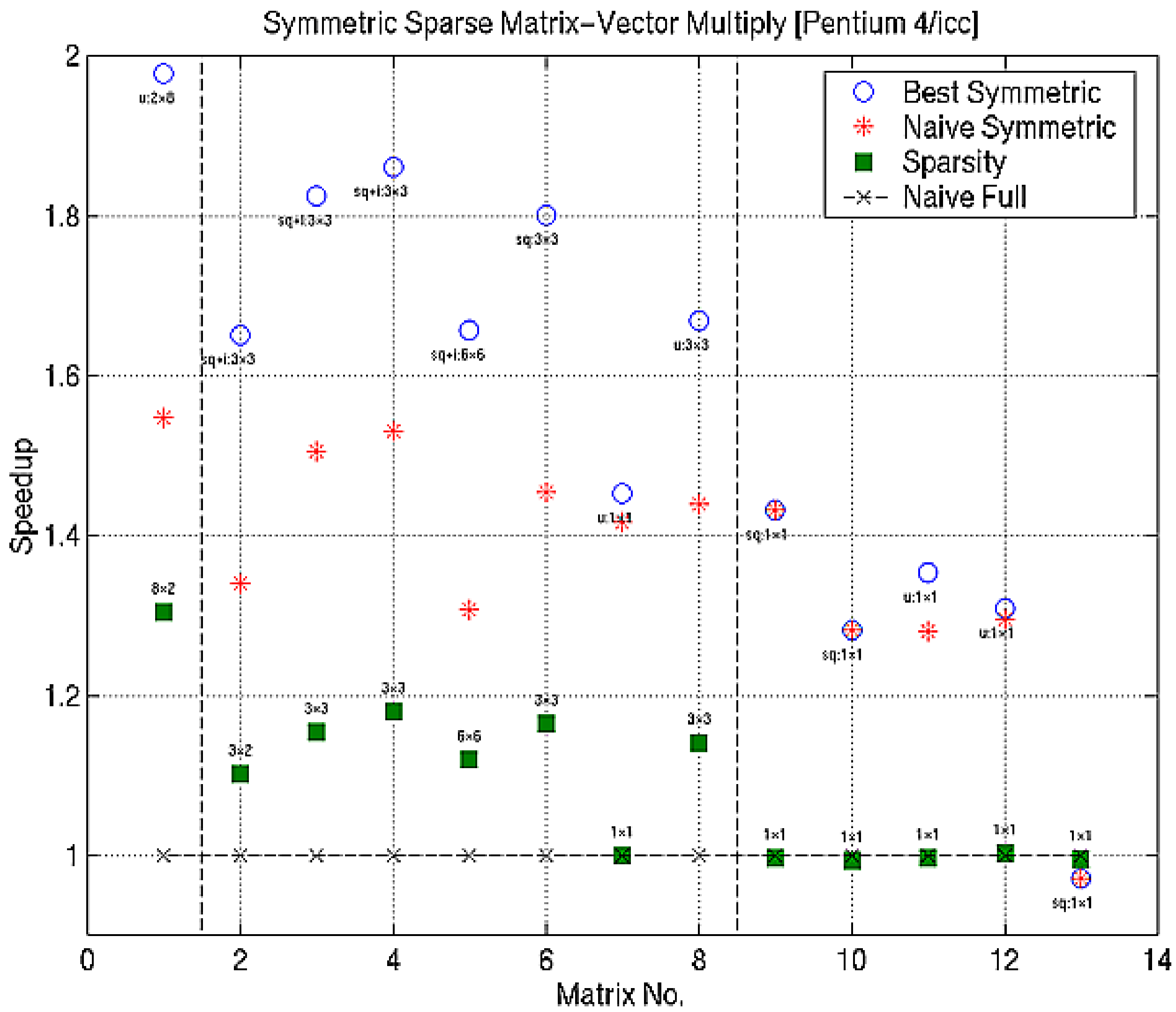
Multiple vector speedups on P4 – by matrix type



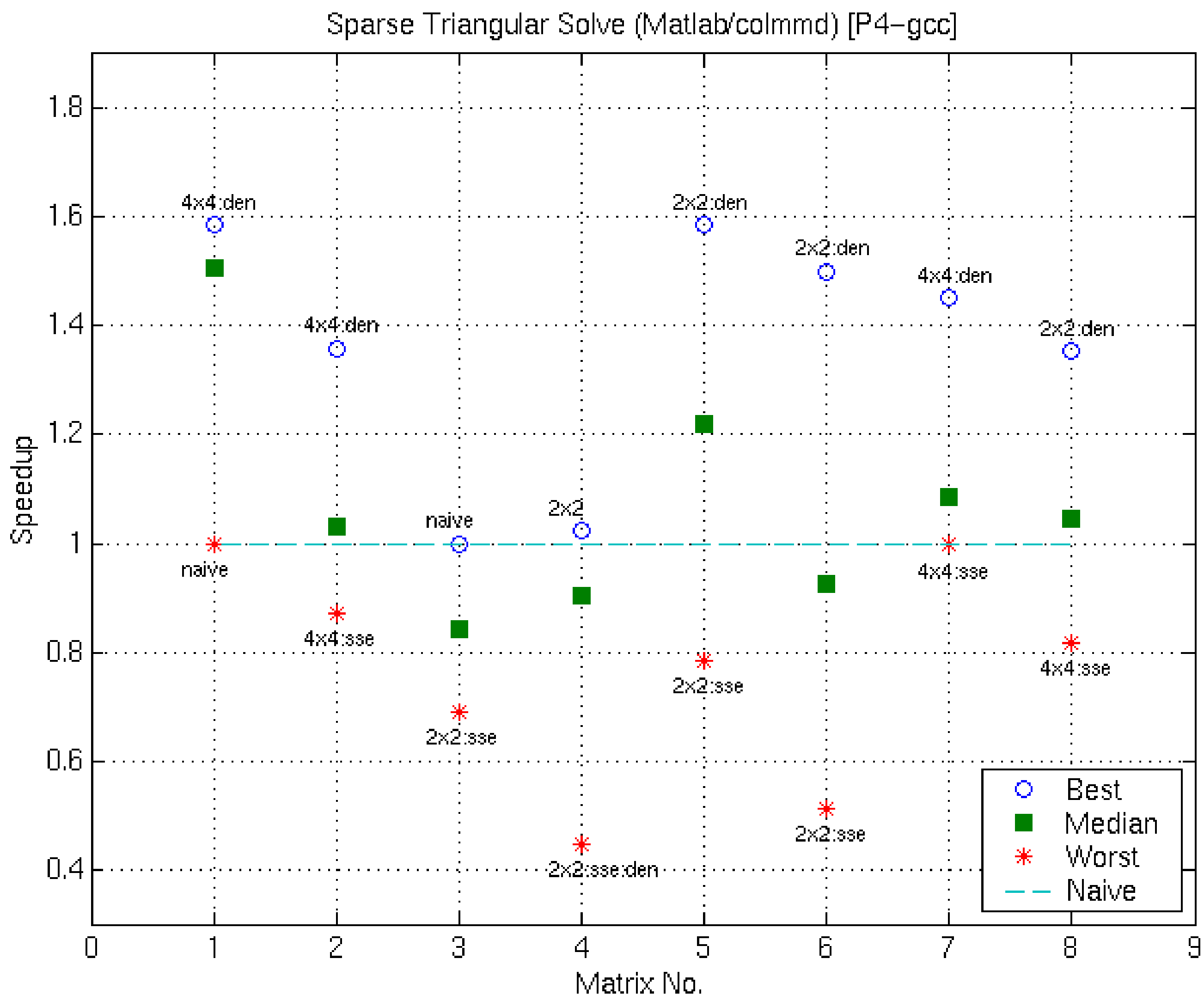
Multiple Vector Performance on P4



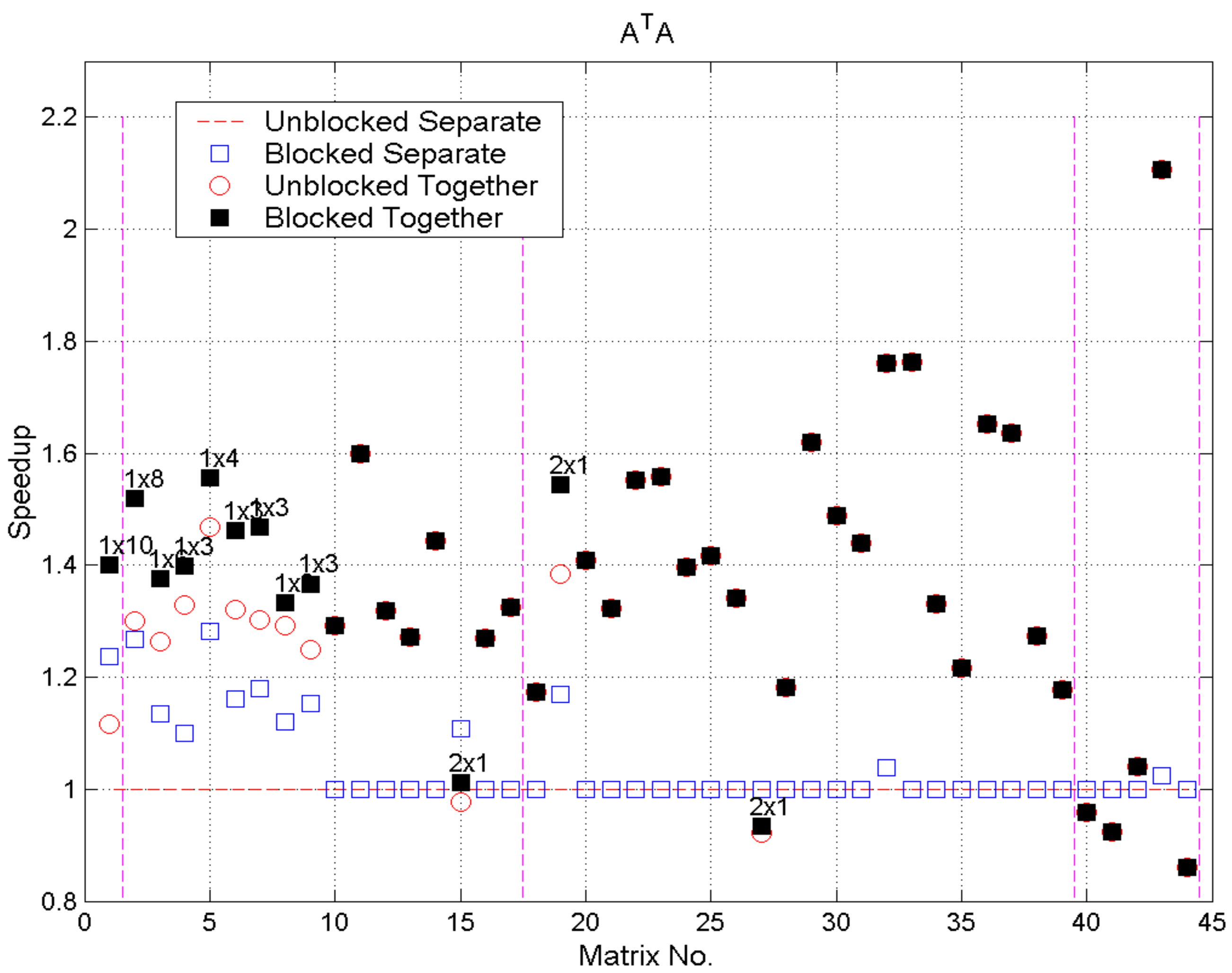
Symmetric Sparse Matrix-Vector Multiply on P4 (vs naïve full = 1)



Sparse Triangular Solve (Matlab's colmmd ordering) on P4

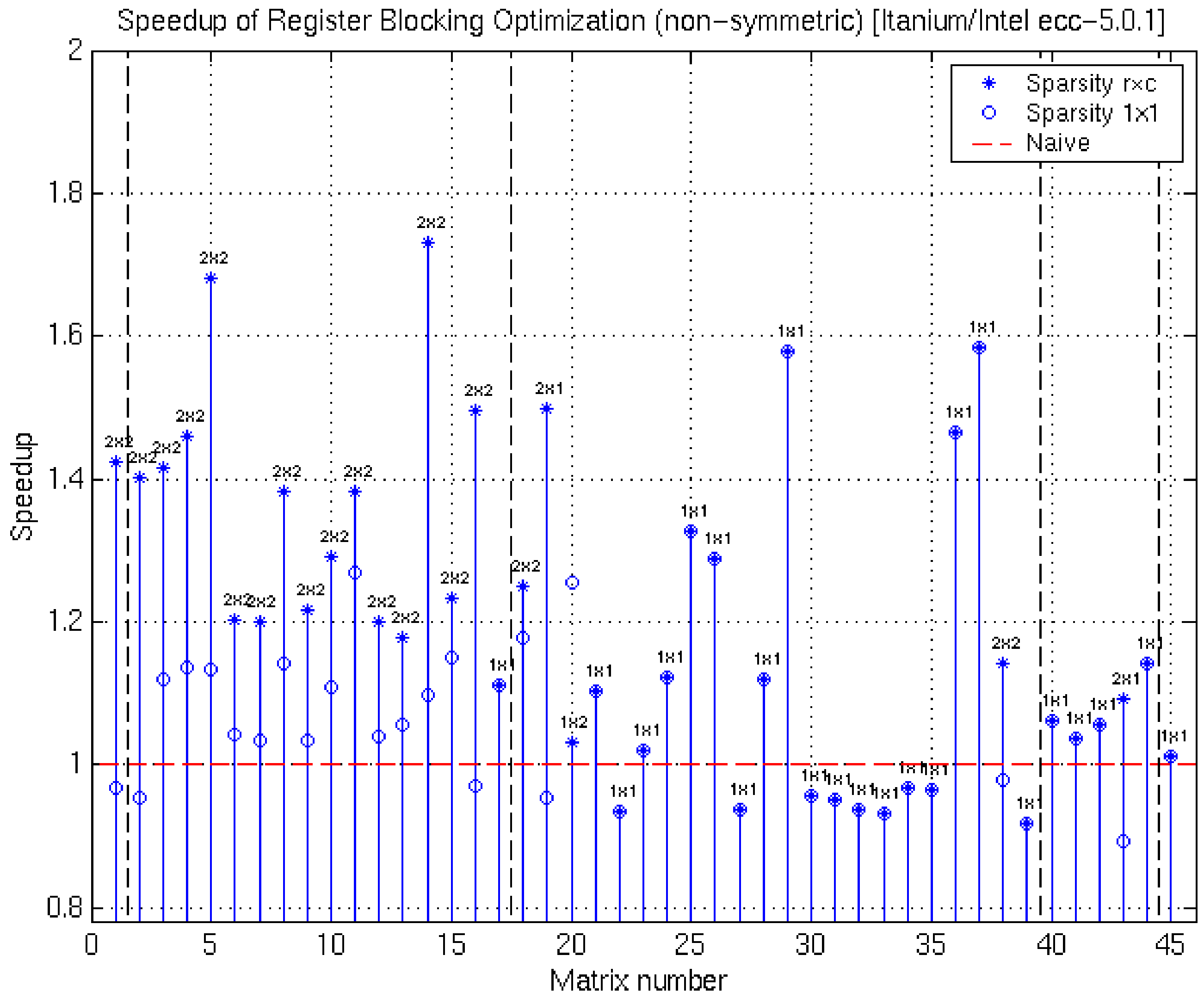


A^T*A on P4 (Accesses A only once)

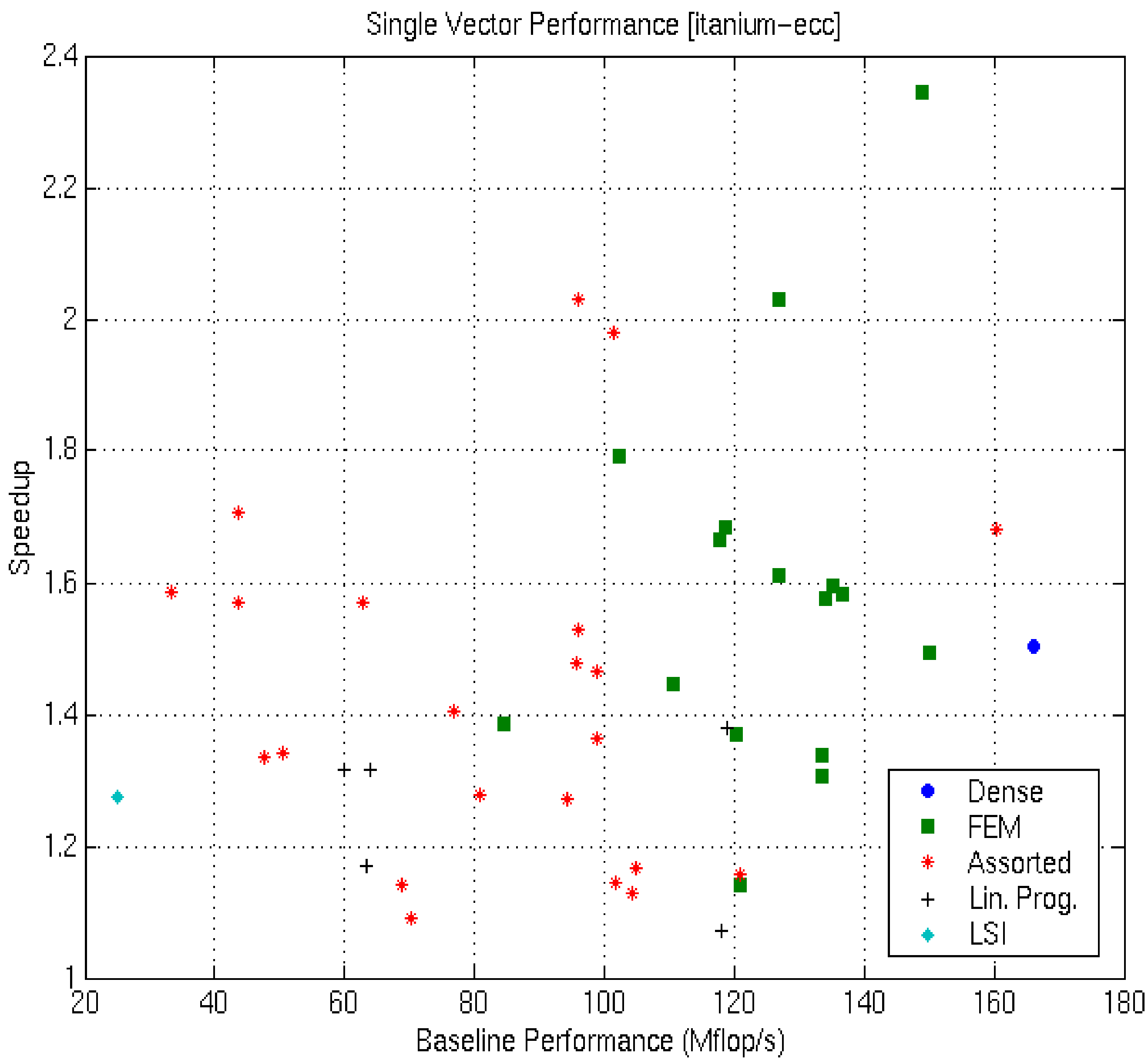


Preliminary Results on Itanium using ecc

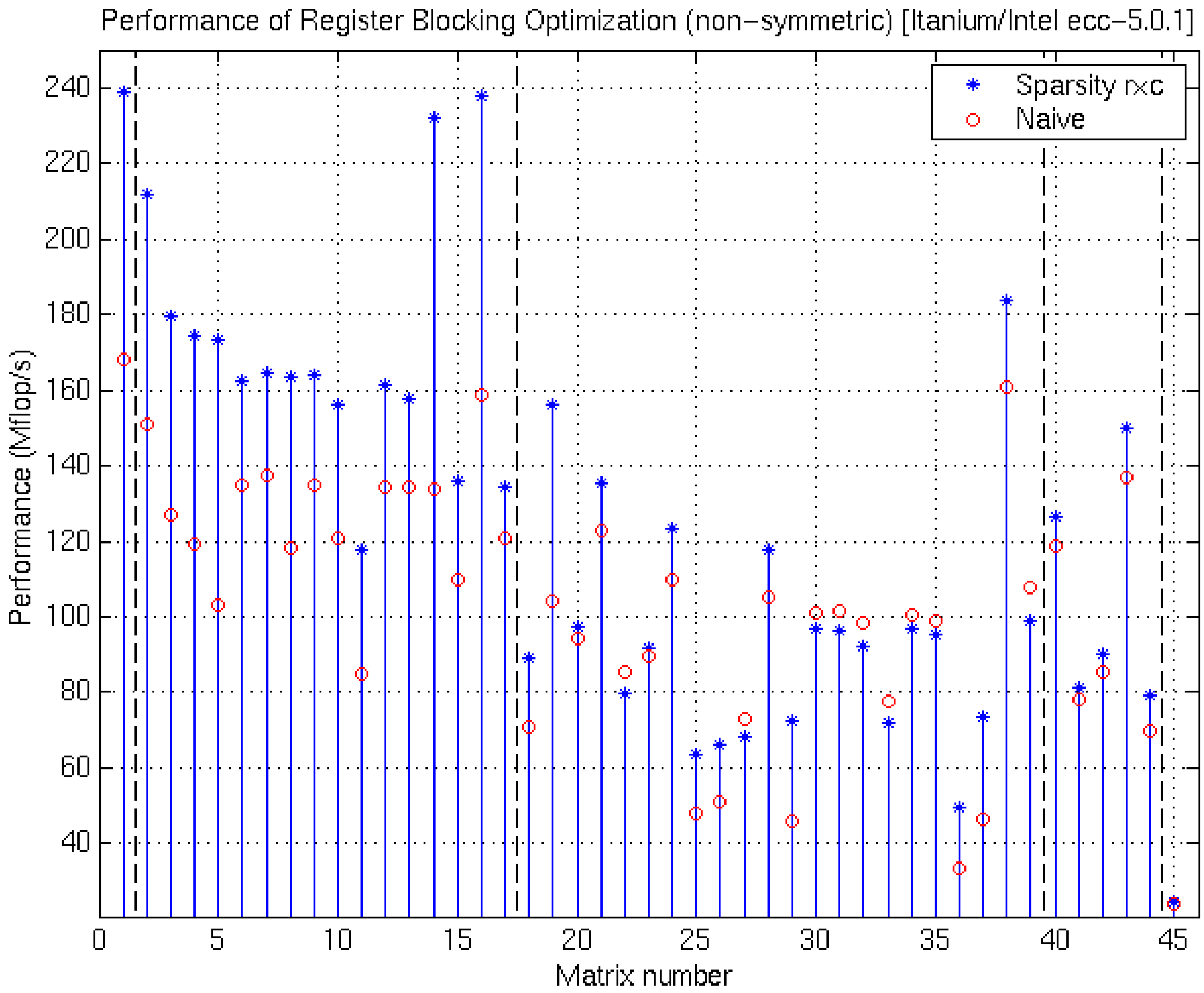
Speedup of SPMV from Sparsity on Itanium/ecc-5.0.1



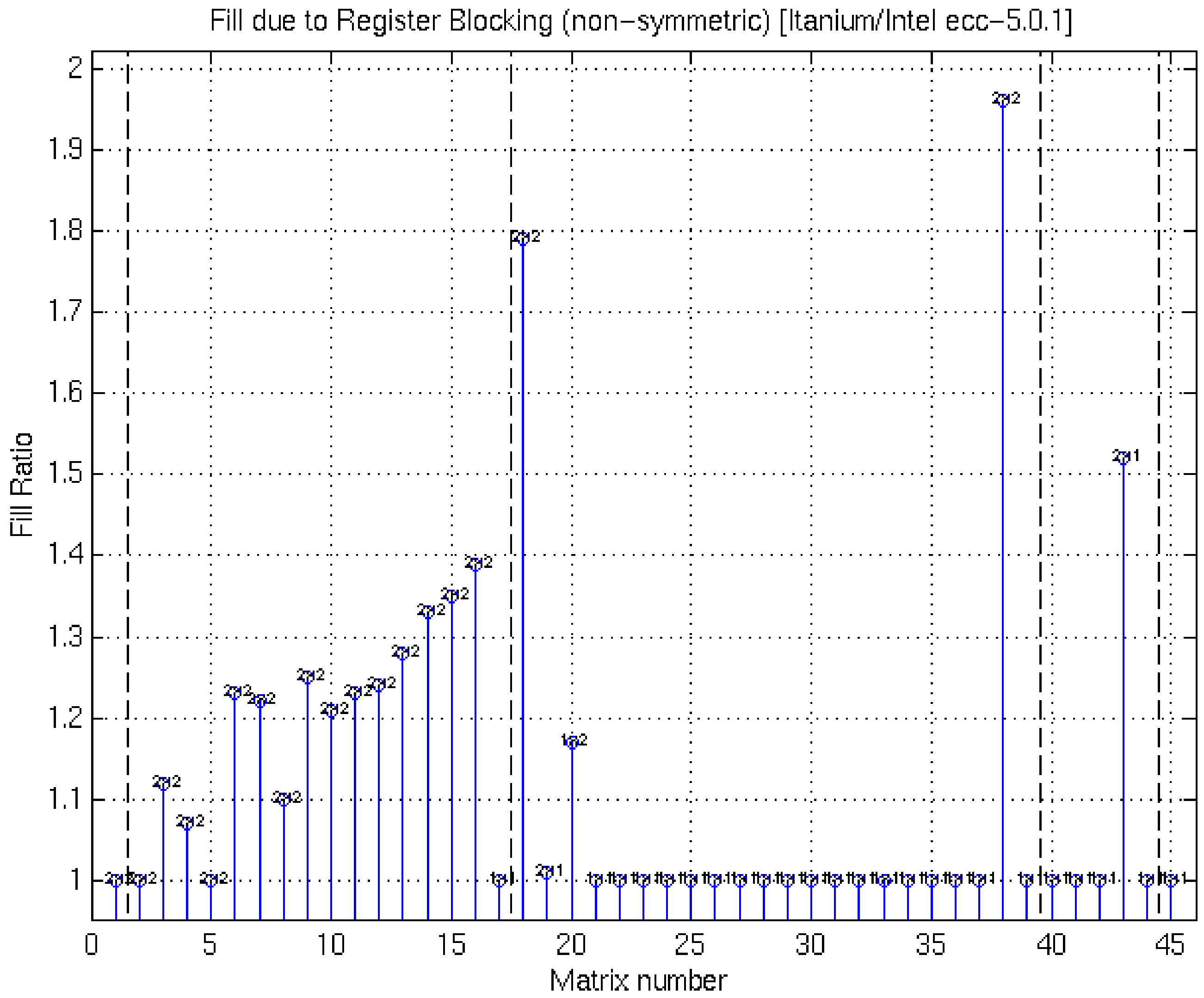
Single vector speedups on Itanium by matrix type



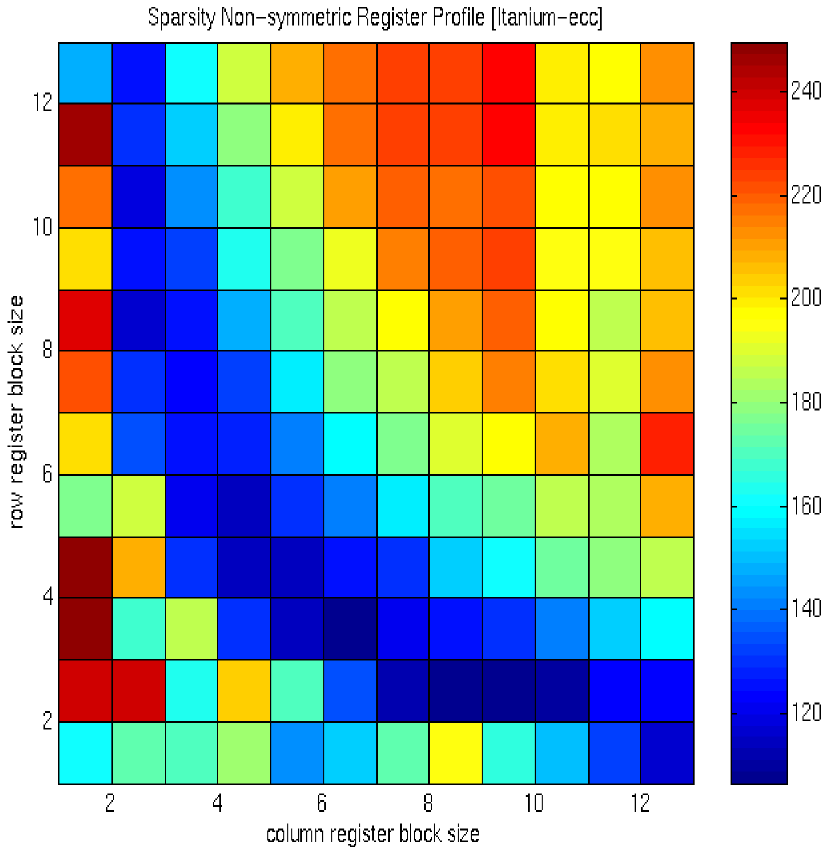
Raw Performance of SPMV from Sparsity on Itanium



Fill for SPMV from Sparsity on Itanium

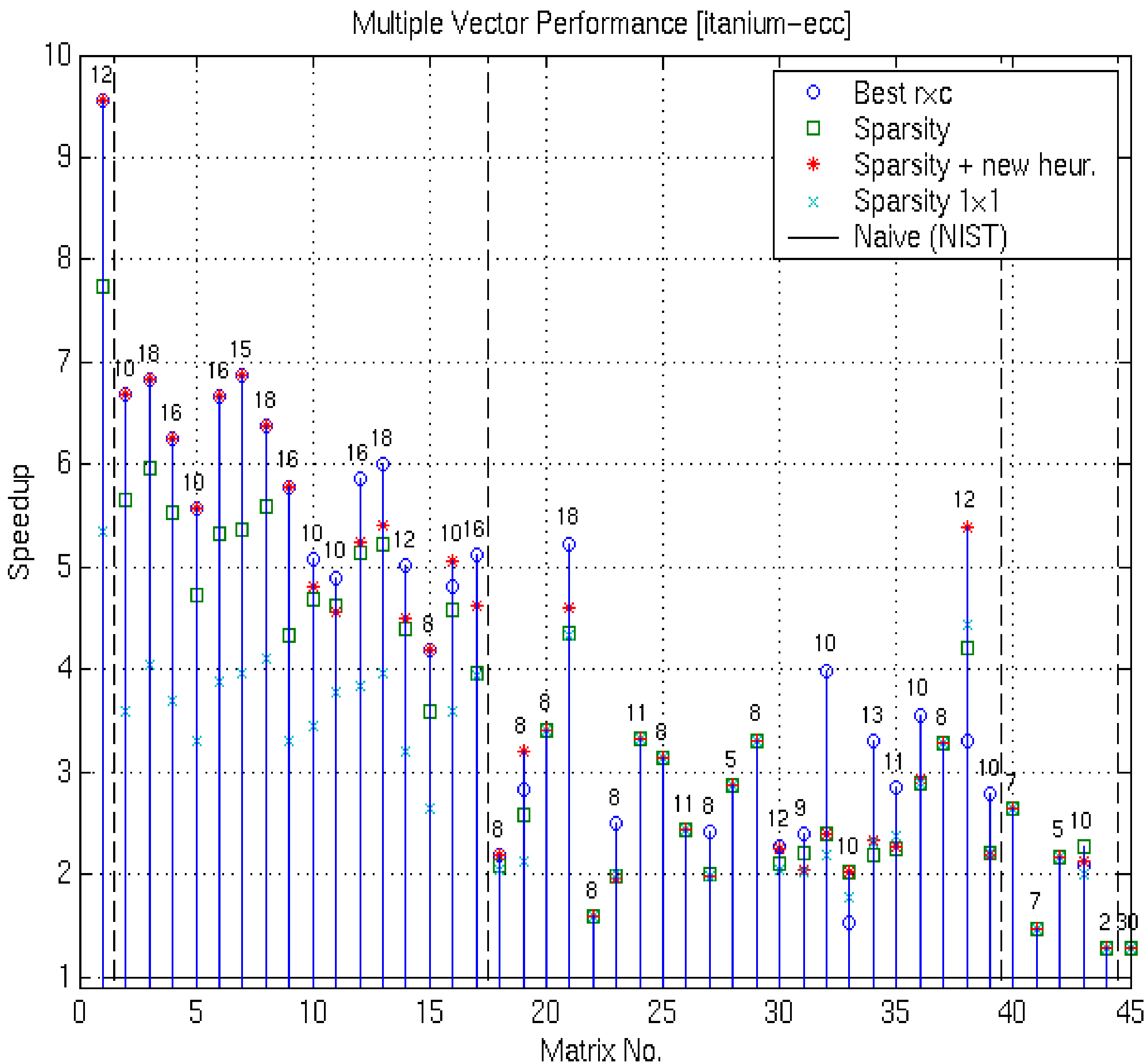


Improvements to register block size selection

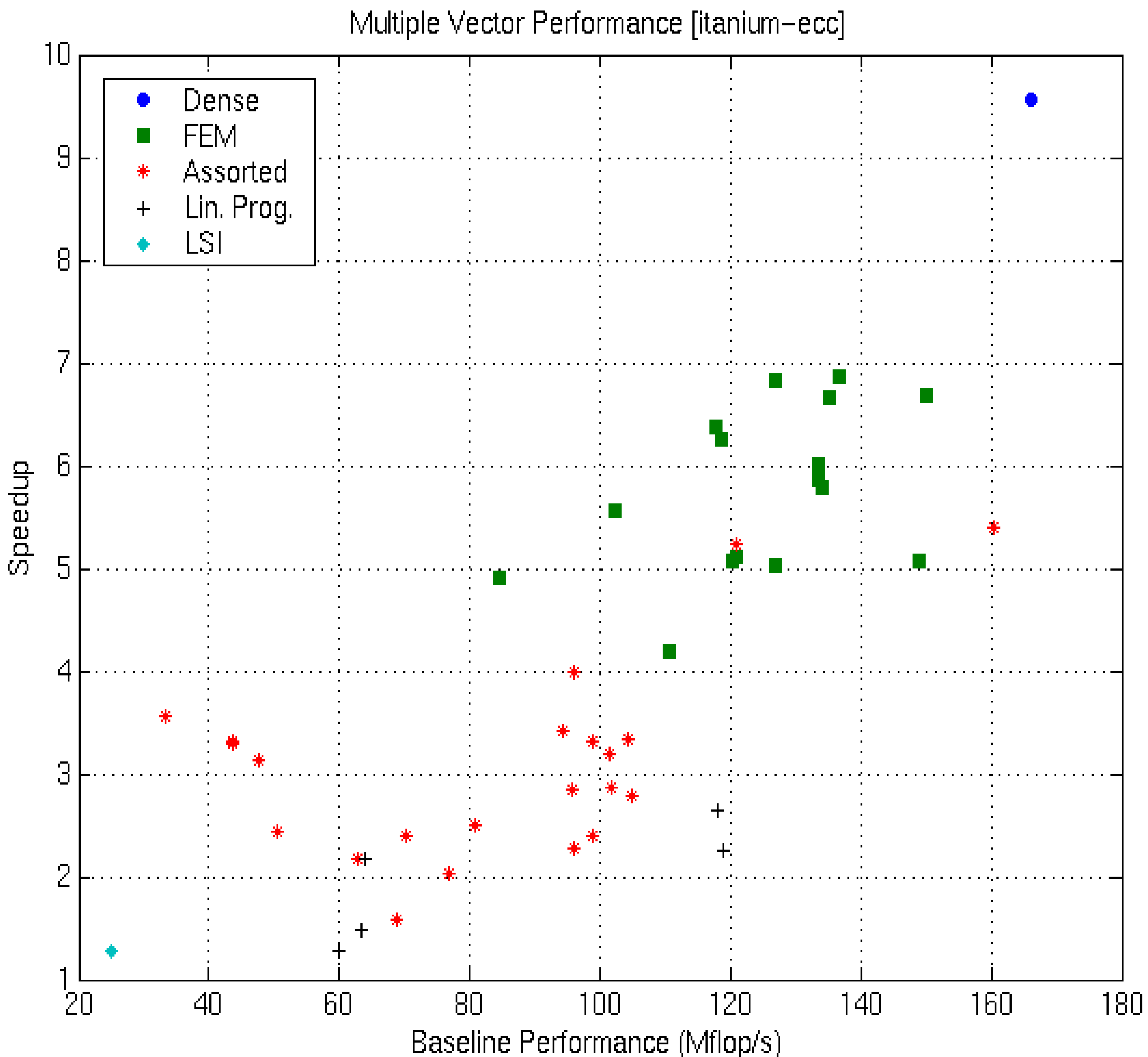


- Initial heuristic to determine best r x c block biased to diagonal of performance plot
- Didn't matter on Sun, does on P4 and Itanium since performance so "nondiagonally dominant"
- Matrix 8:
  - Chose 2x2 (164 Mflops)
  - Better: 3x1 (196 Mflops)
- Matrix 9:
  - Chose 2x2 (164 Mflops)
  - Better: 3x1 (213 Mflops)

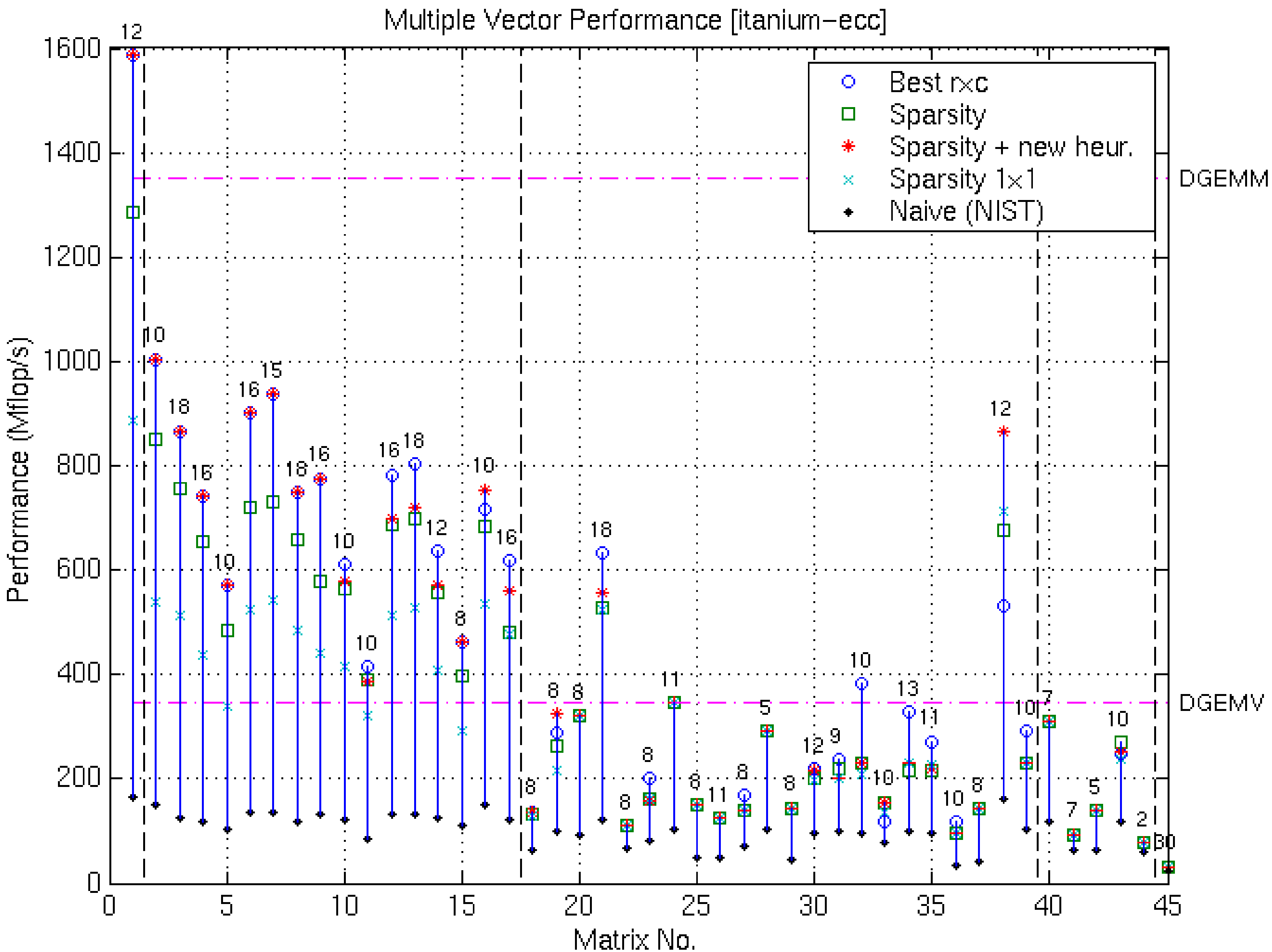
Multiple vector speedups on Itanium



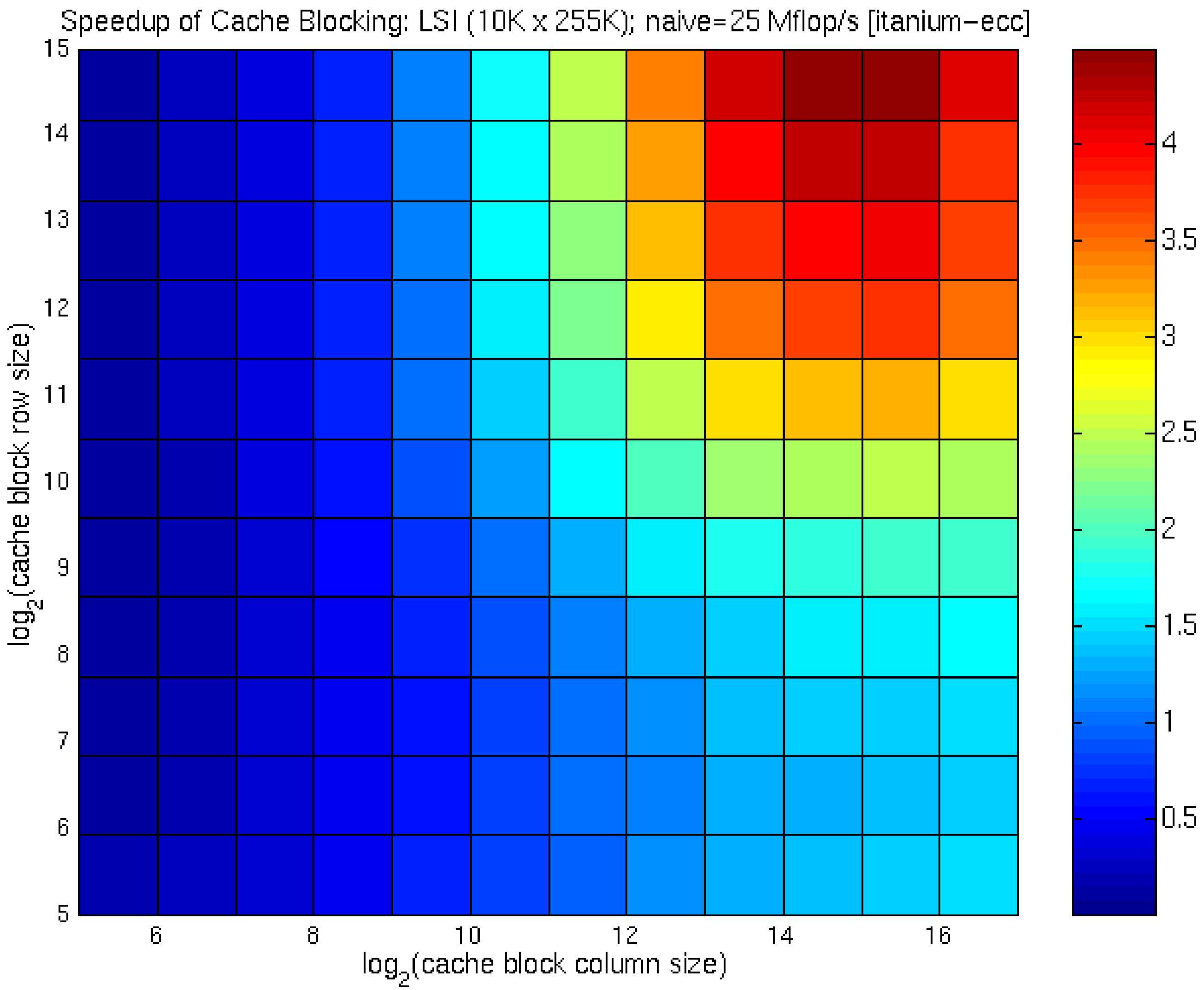
Multiple vector speedups on Itanium – by matrix type



Multiple Vector Performance on Itanium



Speed up from Cache Blocking on LSI matrix on Itanium



Applications of Performance Tuning (non SciDAC)

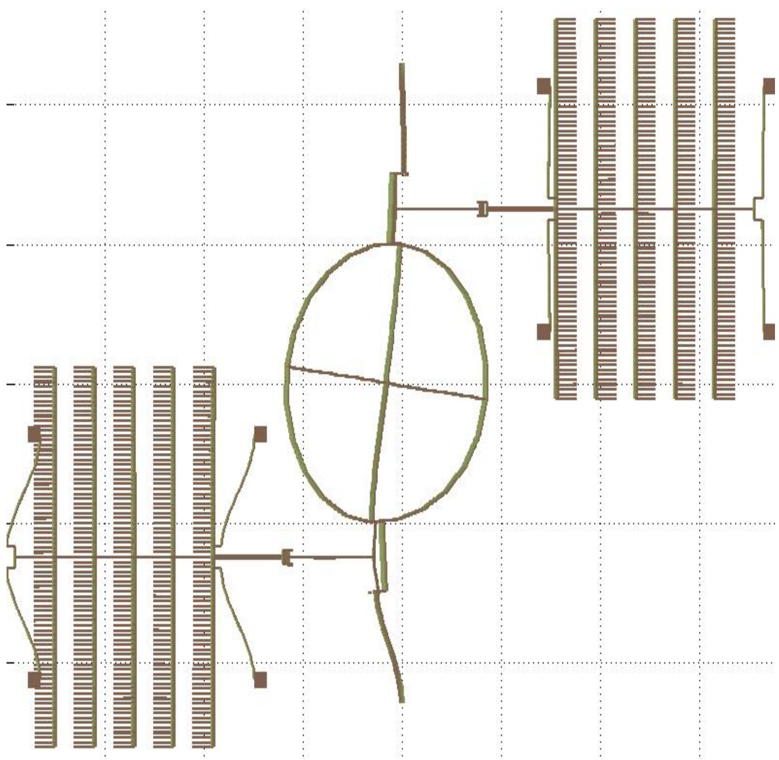
SUGAR – A CAD Tool for MEMS

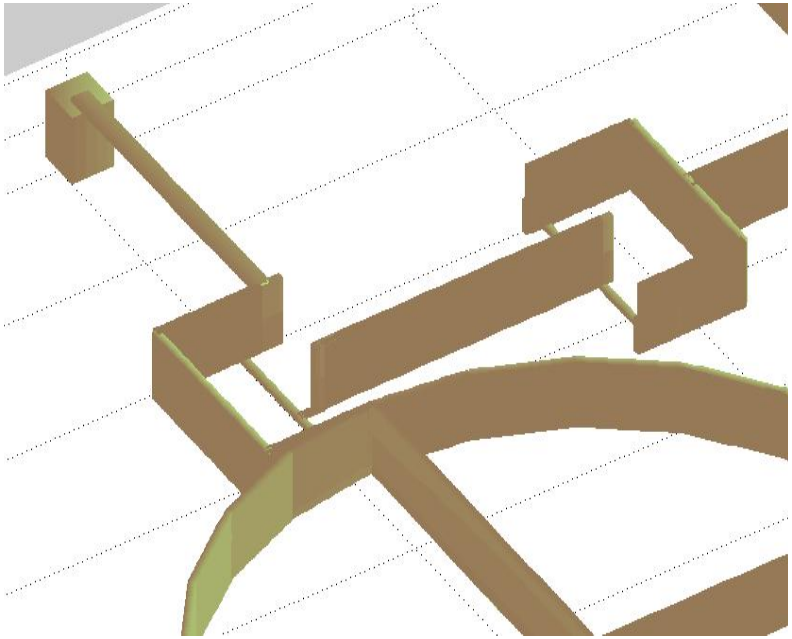
Applications to SUGAR – a tool for MEMS CAD

- Demmel, Bai, Pister, Govindjee, Agogino, Gu, …
- Input: description of MicroElectroMechanical System (as netlist)
- Output:
  - **DC, steady state, modal, transient analyses to assess behavior**
  - **CIF for fabrication**
- Simulation capabilities
  - **Beams and plates (linear, nonlinear, prestressed,…)**
  - **Electrostatic forces, circuits**
  - **Thermal expansion, Couette damping**
- Availability
  - **Matlab**
    - Publicly available
    - www-bsac.eecs.berkeley.edu/~cfm
    - 249 registered users, many unregistered
  - **Web service – M & MEMS**
    - Runs on Millennium
    - sugar.millennium.berkeley.edu
    - Now in use in EE 245 at UCB…96 users
- Lots of new features being added, including interface to measurements

Micromirror (Last, Pister)

- Laterally actuated torsionally suspended micromirror
- Over 10K dof, 100 line netlist (using subnets)
- DC and frequency analysis
- All algorithms reduce to previous kernels





Applications of Performance Tuning

Information Retrieval

Information Retrieval

- Jordan
- Collaboration with Intel team building probabilistic graphical models
- Better alternatives to LSI for document modeling and search
- Latent Dirichlet Allocation (LDA)
  - Model documents as union of themes, each with own word distribution
  - Maximum likelihood fit to find themes in set of documents, classify them
  - Computational bottleneck is solution of enormous linear systems
  - One of largest Millennium users
- Identifying influential documents
  - Given hyperlink patterns of documents, which are most influential?
  - Basis of Google (eigenvector of link matrix → sparse matrix vector multiply)
  - Applying Markov chain and perturbation theory to assess reliability
- Kernel ICA
  - Estimate set of sources s and mixing matrix A from samples x = A*s
  - New way to sample such that sources are as independent as possible
  - Again reduces to linear algebra kernels…

More on Kernel ICA

- Algorithm 1
  - nonlinear eigenvalue problem, reduces to a sequence of many
  - very large generalized spd eigenproblems $A - \lambda B$
    - Block structured, A dense, B block diagonal
    - Only smallest nonzero eigenvalue needed
  - Sparse eigensolver (currently ARPACK/eigs)
    - Use Incomplete Cholesky (IC) to get low rank approximzation to dense subblocks comprising A and B
    - Use Complete (=Diagonal) Pivoting but take only 20 << n steps
    - Cost is O(n)
      - Evaluating matrix entries (exponentials) could be bottleneck
      - Need fast, low precision exponential
- Algorithm 2
  - Like Algorithm 1, but find all eigenvalues/vectors of $A - \lambda B$
  - Use Holy Grail

Future Work

- SciDAC
  - Evaluate on SciDAC applications
  - Determine interfaces for integration into SciDAC applications
- Further exploit Itanium, other architectures
  - 128 (82-bit) floating point registers
    - 9 HW formats: 24/8(v), 24/15, 24/17, 53/11, 53/15, 53/17, 64/15, 64/17
    - Many fewer load/store instructions
  - fused multiply-add instruction
  - predicated instructions
  - rotating registers for software pipelining
  - prefetch instructions
  - three levels of cache
- Tune current and wider set of kernels
  - Improve heuristics, eg choice of r x c
- Further automate performance tuning (NSF)
  - Generation of algorithm space generators

Background on Test Matrices

Sparse Matrix Benchmark Suite (1/3)

#	Matrix Name	Problem Domain	Dimension	No. Non-zeros
1	dense	Dense matrix	1,000	1.00 M
2	raefsky3	Fluid structure interaction	21,200	1.49 M
3	inaccura	Accuracy problem	16,146	1.02 M
4	bcsstk35*	Stiff matrix automobile frame	30,237	1.45 M
5	venkat01	Flow simulation	62,424	1.72 M
6	crystk02*	FEM crystal free-vibration	13,965	969 k
7	crystk03*	FEM crystal free-vibration	24,696	1.75 M
8	nasasrb*	Shuttle rocket booster	54,870	2.68 M
9	3dtube*	3-D pressure tube	45,330	3.21 M
10	ct20stif*	CT20 engine block	52,329	2.70 M
11	bai	Airfoil eigenvalue calculation	23,560	484 k
12	raefsky4	Buckling problem	19,779	1.33 M
13	ex11	3-D steady flow problem	16,214	1.10 M
14	rdist1	Chemical process simulation	4,134	94.4 k
15	vavasis3	2-D PDE problem	41,092	1.68 M

Note: * indicates a symmetric matrix.

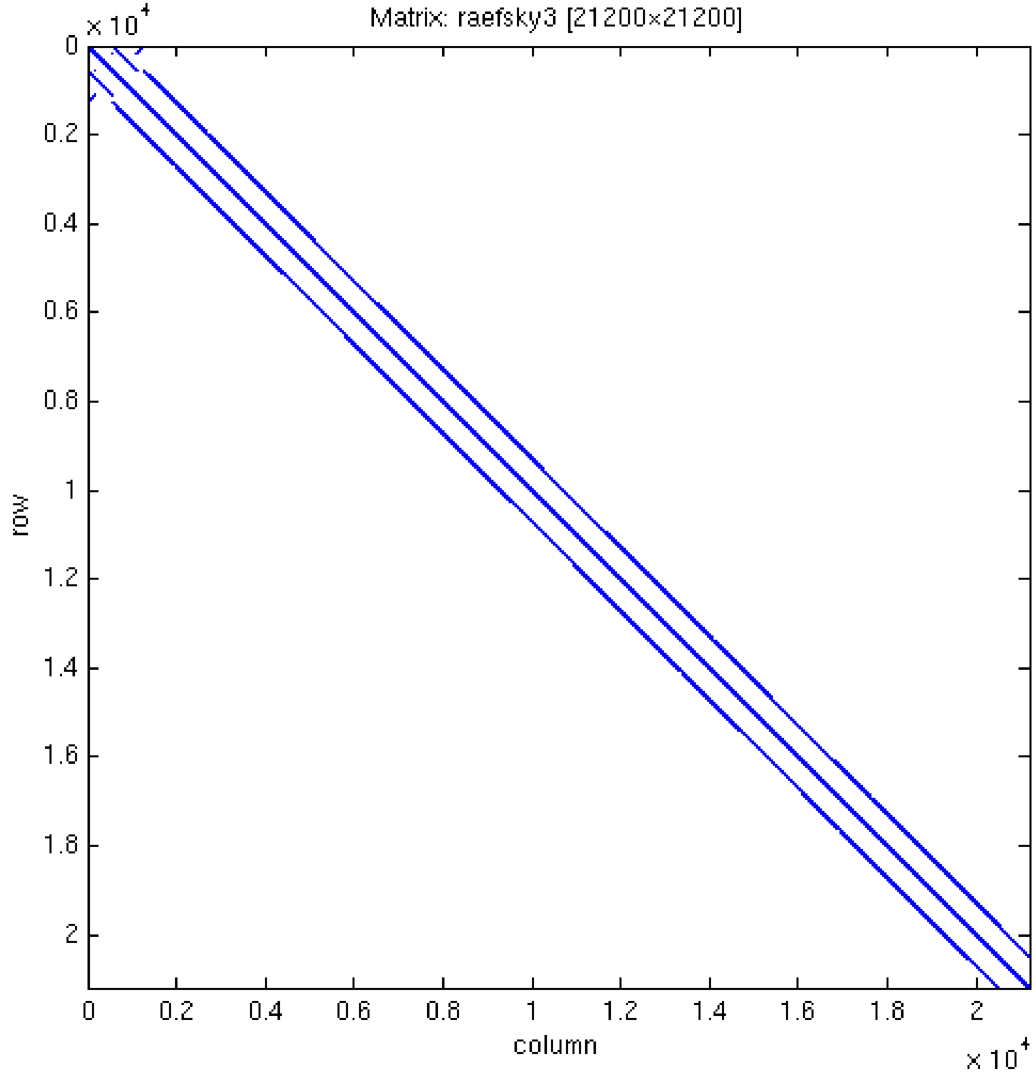
Sparse Matrix Benchmark Suite (2/3)

#	Matrix Name	Problem Domain	Dimension	No. Non-zeros
16	orani678	Economic modeling	2,529	90.2 k
17	rim	FEM fluid mechanics problem	22,560	1.01 M
18	memplus	Circuit simulation	17,758	126 k
19	gemat11	Power flow	4,929	33.1 k
20	lhr10	Chemical process simulation	10,672	233 k
21	goodwin*	Fluid mechanics problem	7,320	325 k
22	bayer02	Chemical process simulation	13,935	63.7 k
23	bayer10	Chemical process simulation	13,436	94.9 k
24	coater2	Simulation of coating flows	9,540	207 k
25	finan512*	Financial portfolio optimization	74,752	597 k
26	onetone2	Harmonic balance method	36,057	228 k
27	pwt*	Structural engineering	36,519	326 k
28	vibrobox*	Vibroacoustics	12,328	343 k
29	wang4	Semiconductor device simulation	26,068	177 k
30	lnsp3937	Fluid flow modeling	3,937	25.4 k

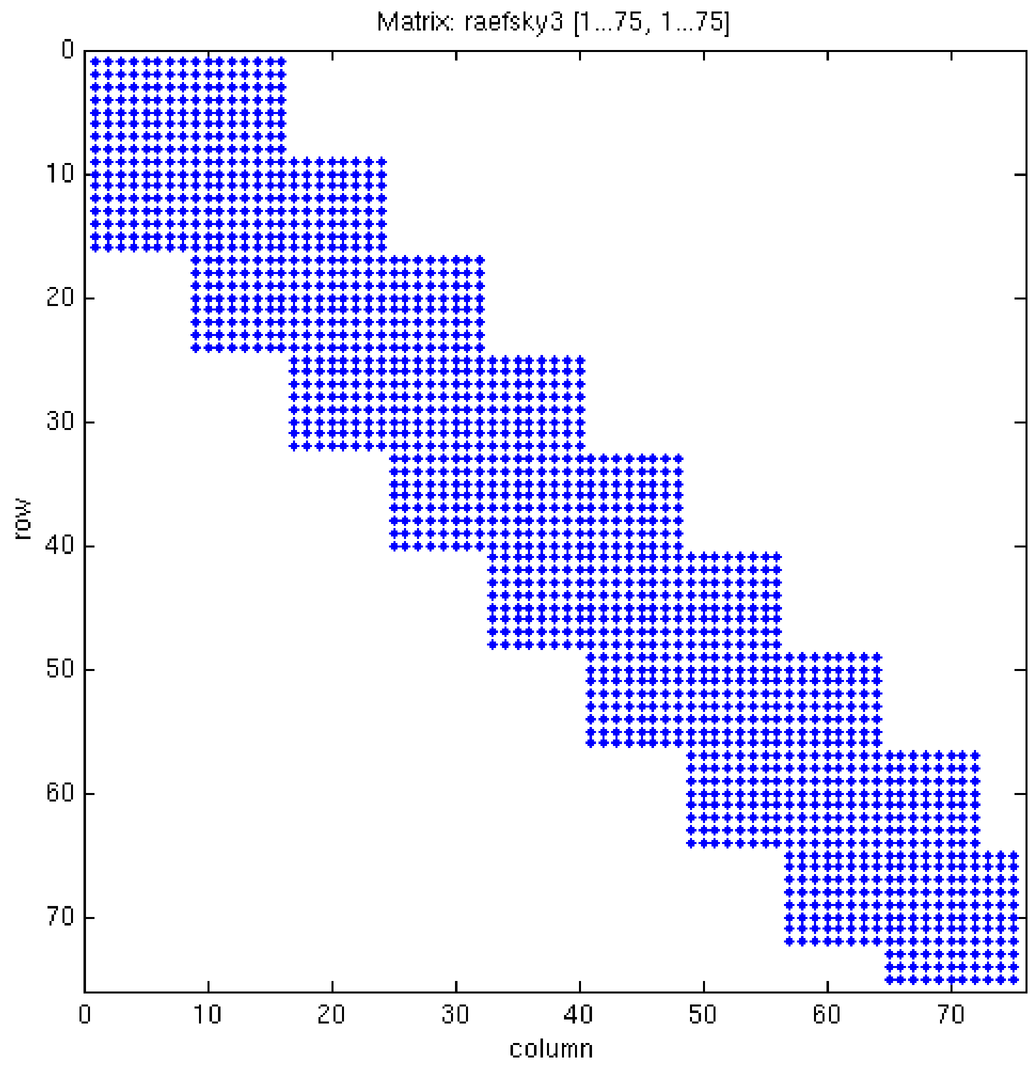
Sparse Matrix Benchmark Suite (3/3)

#	Matrix Name	Problem Domain	Dimensions	No. Non-zeros
31	lns3937	Fluid flow modeling	3,937	25.4 k
32	sherman5	Oil reservoir modeling	3,312	20.8 k
33	sherman3	Oil reservoir modeling	5,005	20.0 k
34	orsreg1	Oil reservoir modeling	2,205	14.1 k
35	saylr4	Oil reservoir modeling	3,564	22.3 k
36	shyy161	Viscous flow calculation	76,480	330 k
37	wang3	Semiconductor device simulation	26,064	177 k
38	mcfe	Astrophysics	765	24.4 k
39	jpwh991	Circuit physics problem	991	6,027
40	gupta1*	Linear programming	31,802	2.16 M
41	lpcreb	Linear programming	9,648 x 77,137	261 k
42	lpcred	Linear programming	8,926 x 73,948	247 k
43	lpfit2p	Linear programming	3,000 x 13,525	50.3 k
44	lpnug20	Linear programming	15,240 x 72,600	305 k
45	lsi	Latent semantic indexing	10 k x 255 k	3.7 M

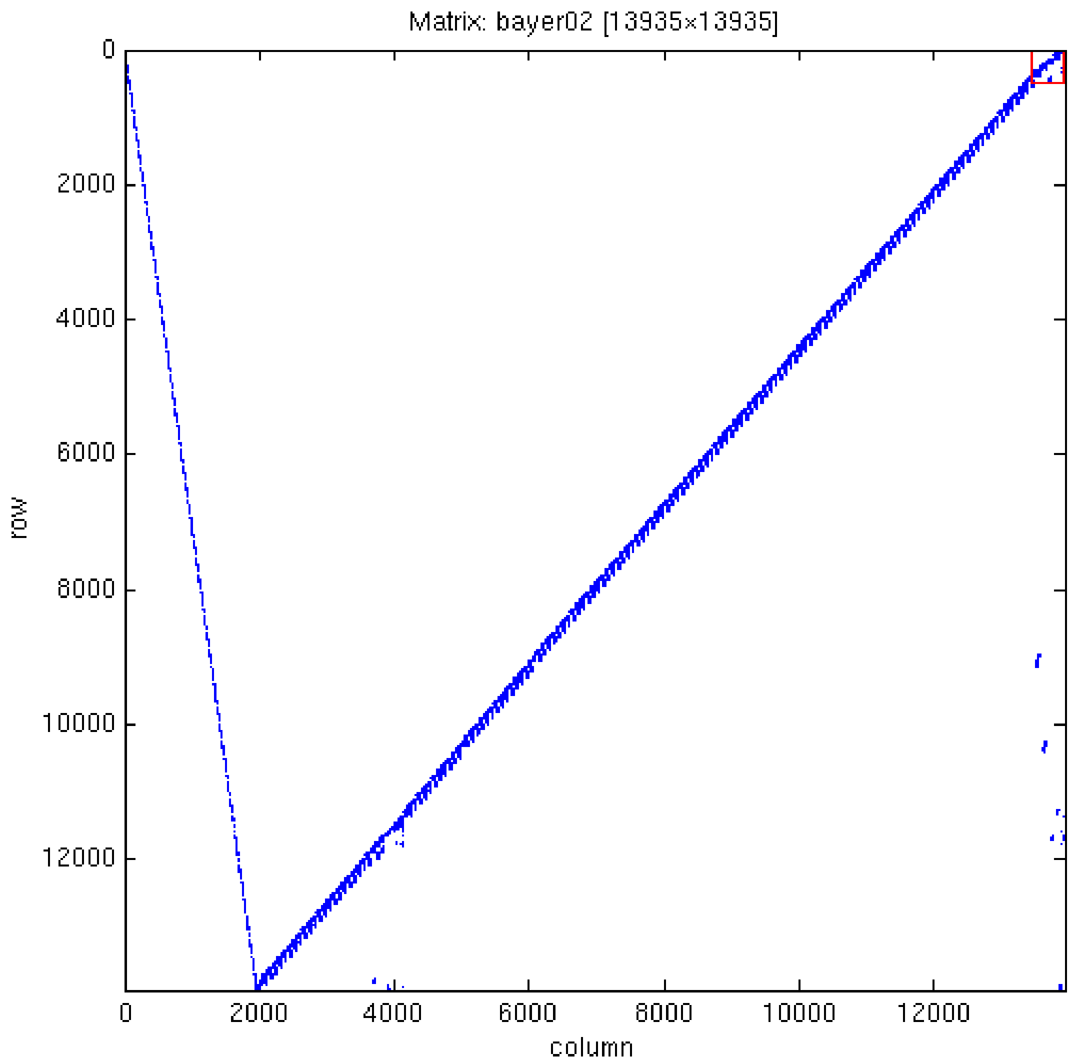
Matrix #2 - raefsky3 (FEM/Fluids)



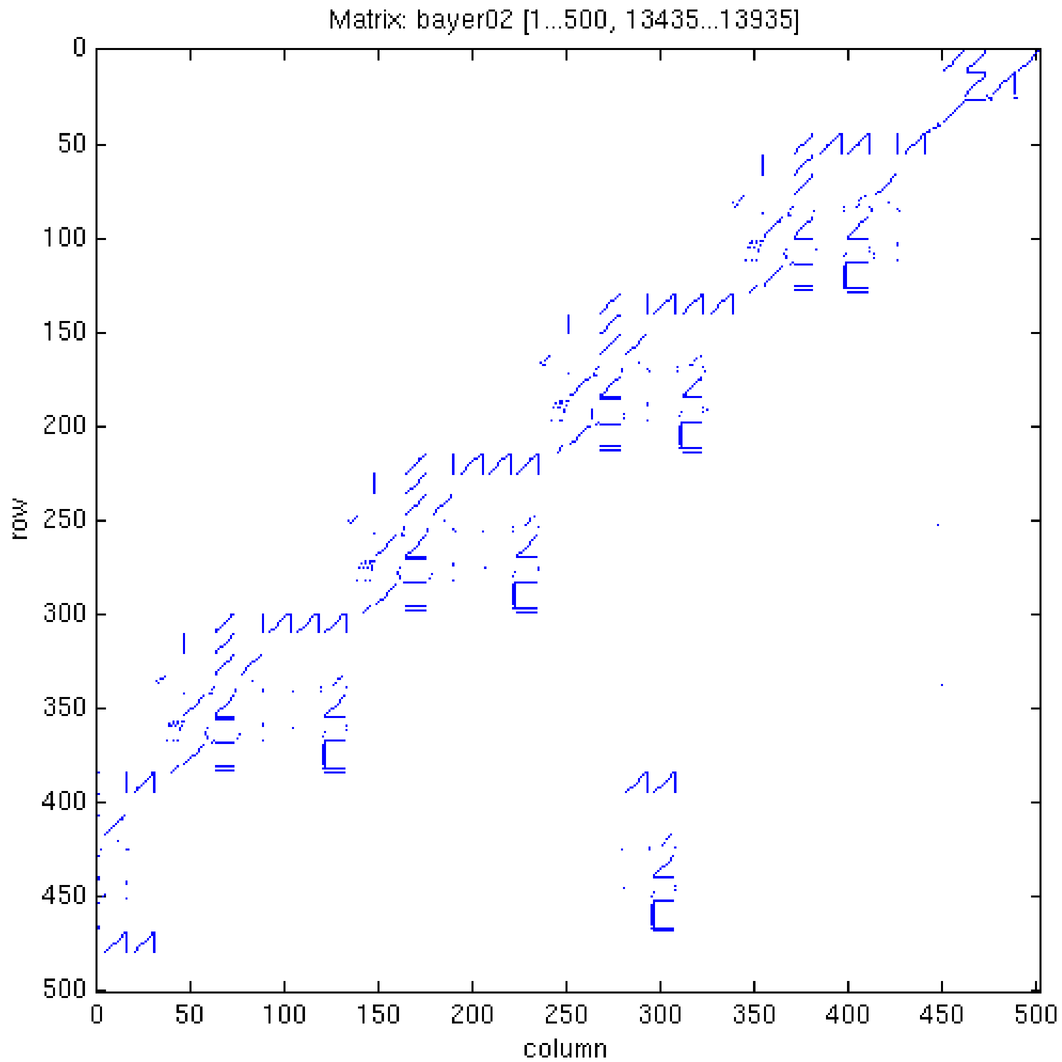
Matrix #2 (cont'd) – raefsky3 (FEM/Fluids)



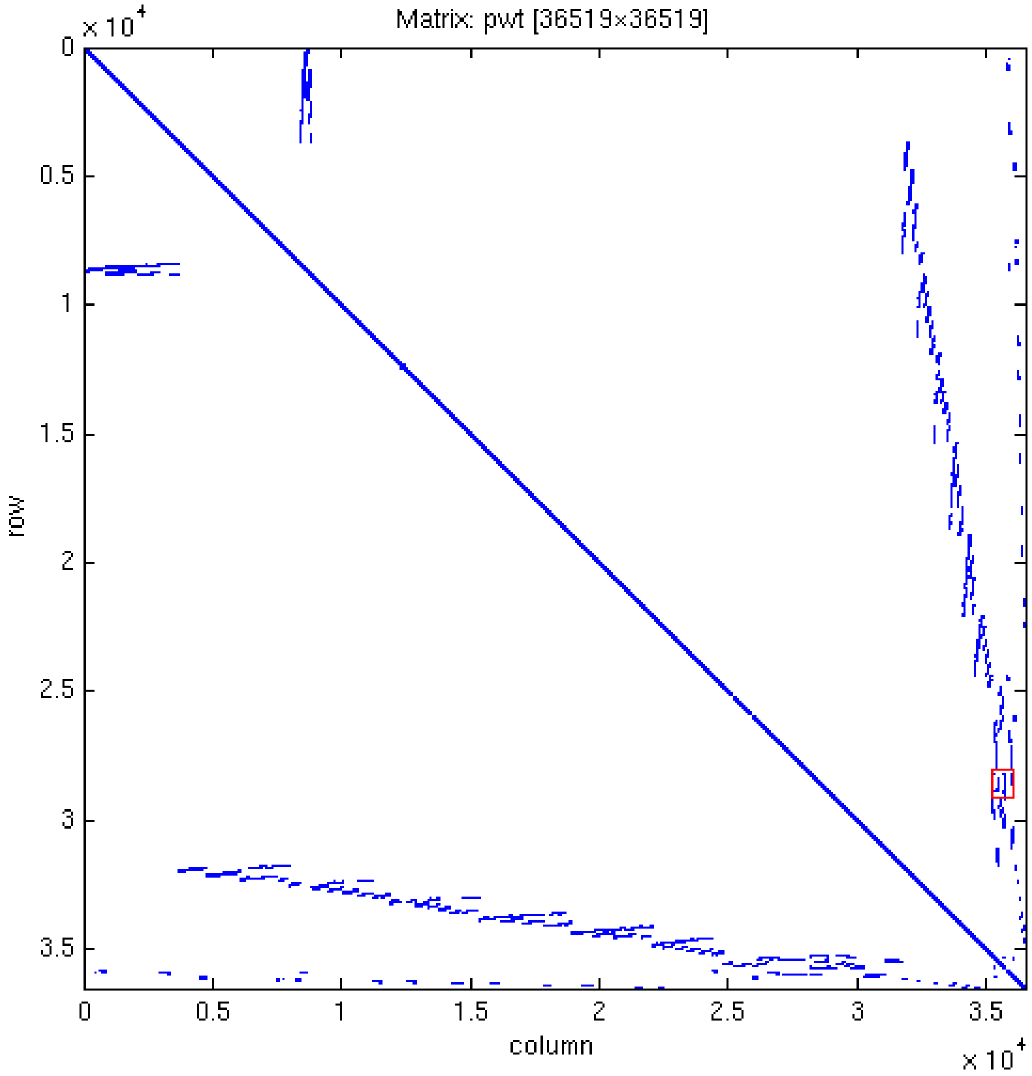
Matrix #22 - bayer02 (chemical process simulation)



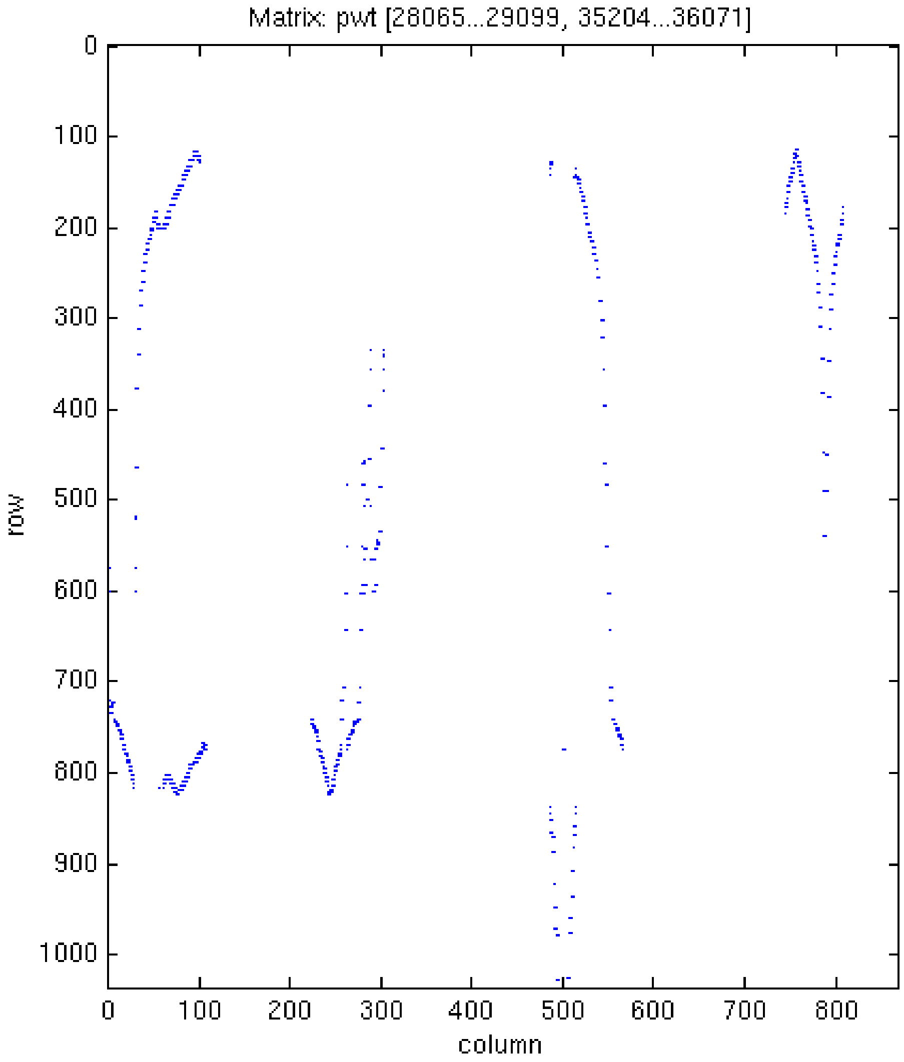
Matrix #22 (cont'd)- bayer02 (chemical process simulation)



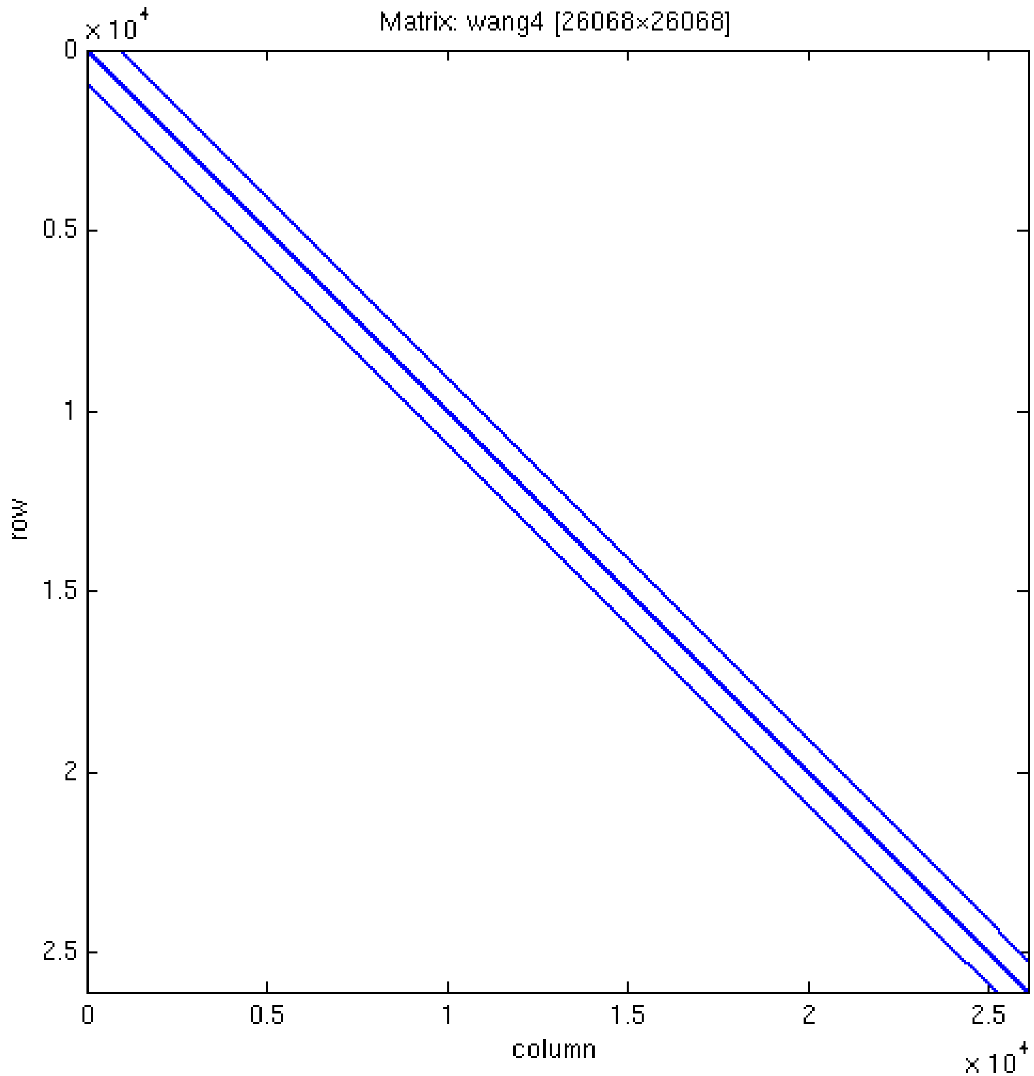
Matrix #27 - pwt (structural engineering)



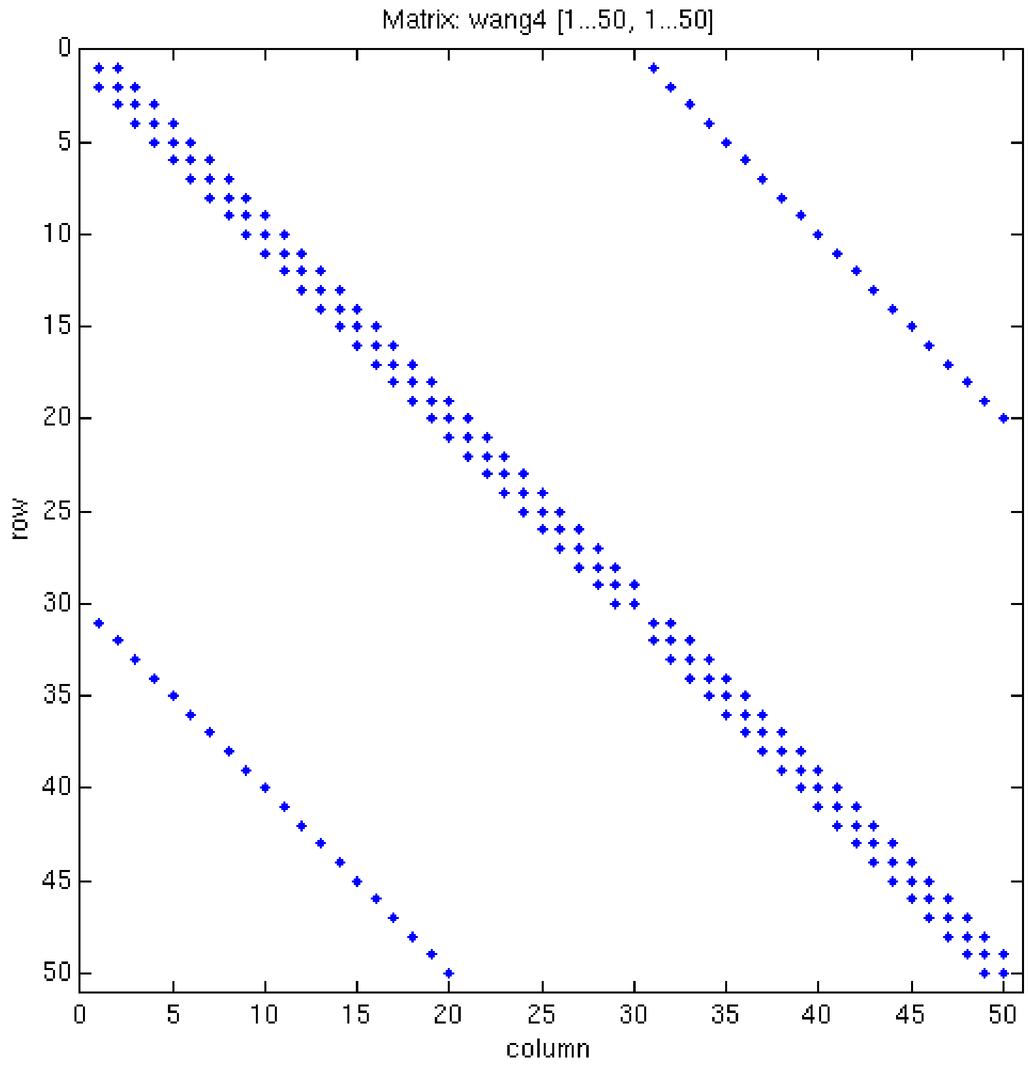
Matrix #27 (cont'd)- pwt (structural engineering)



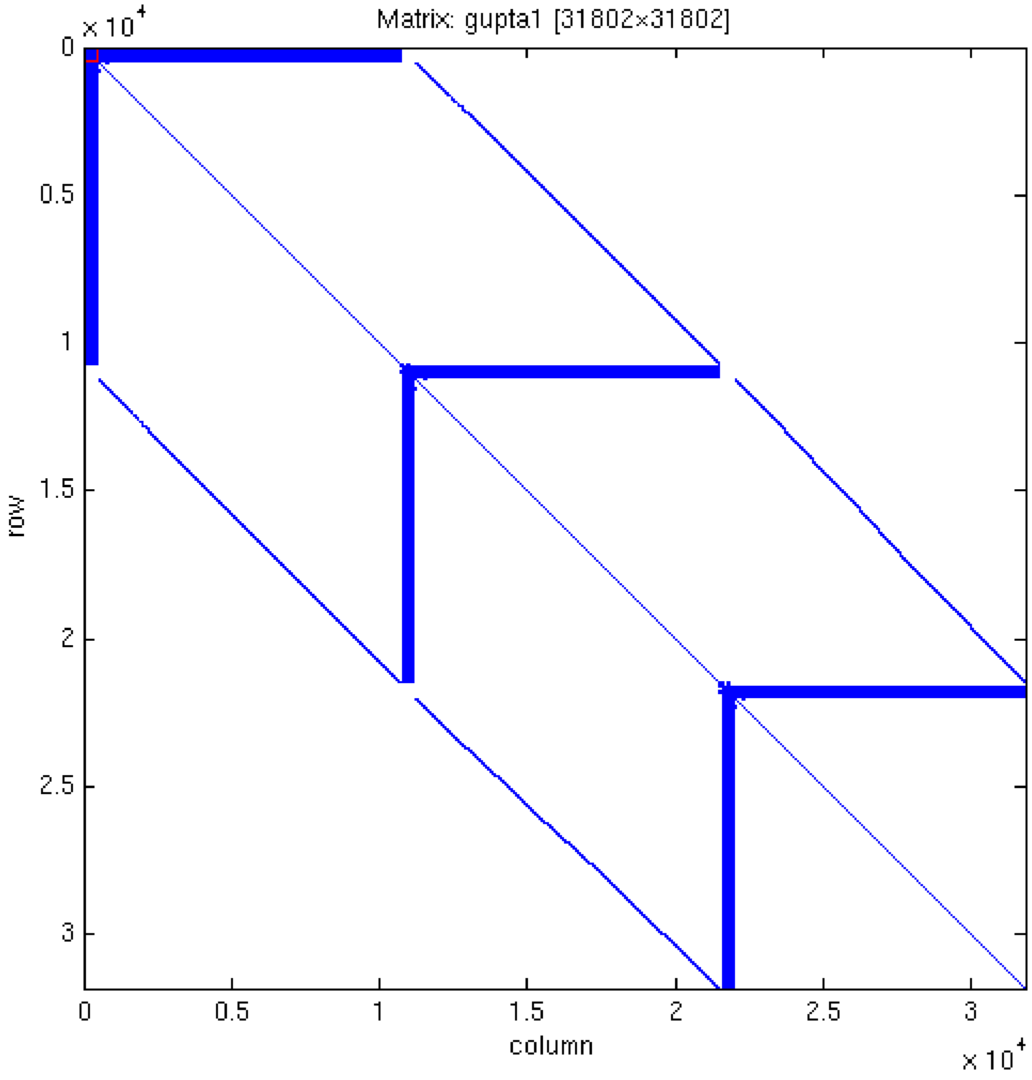
Matrix #29 – wang4 (semiconductor device simulation)



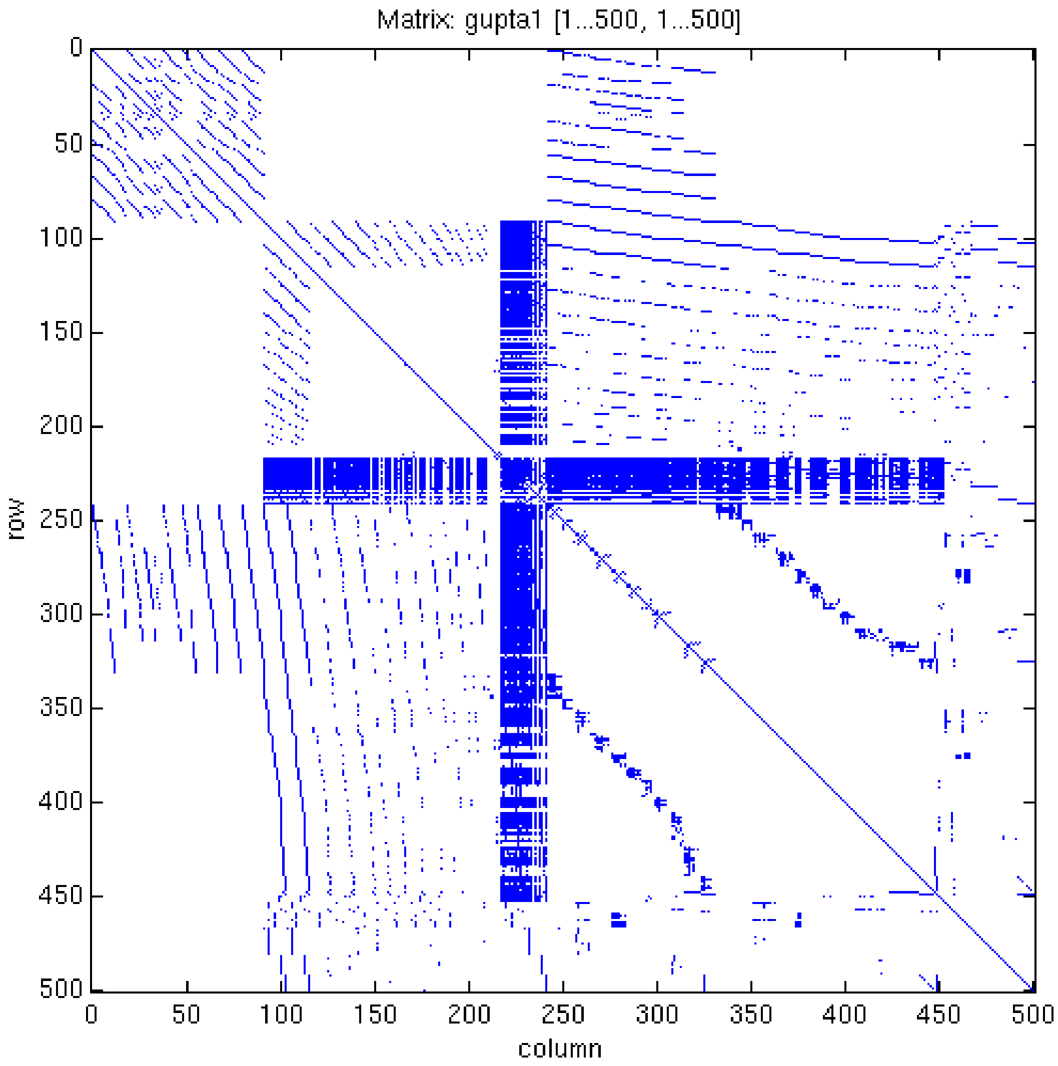
Matrix #29 (cont'd)-wang4 (seminconductor device sim.)



Matrix #40 – gupta1 (linear programming)



Matrix #40 (cont'd) – gupta1 (linear programming)



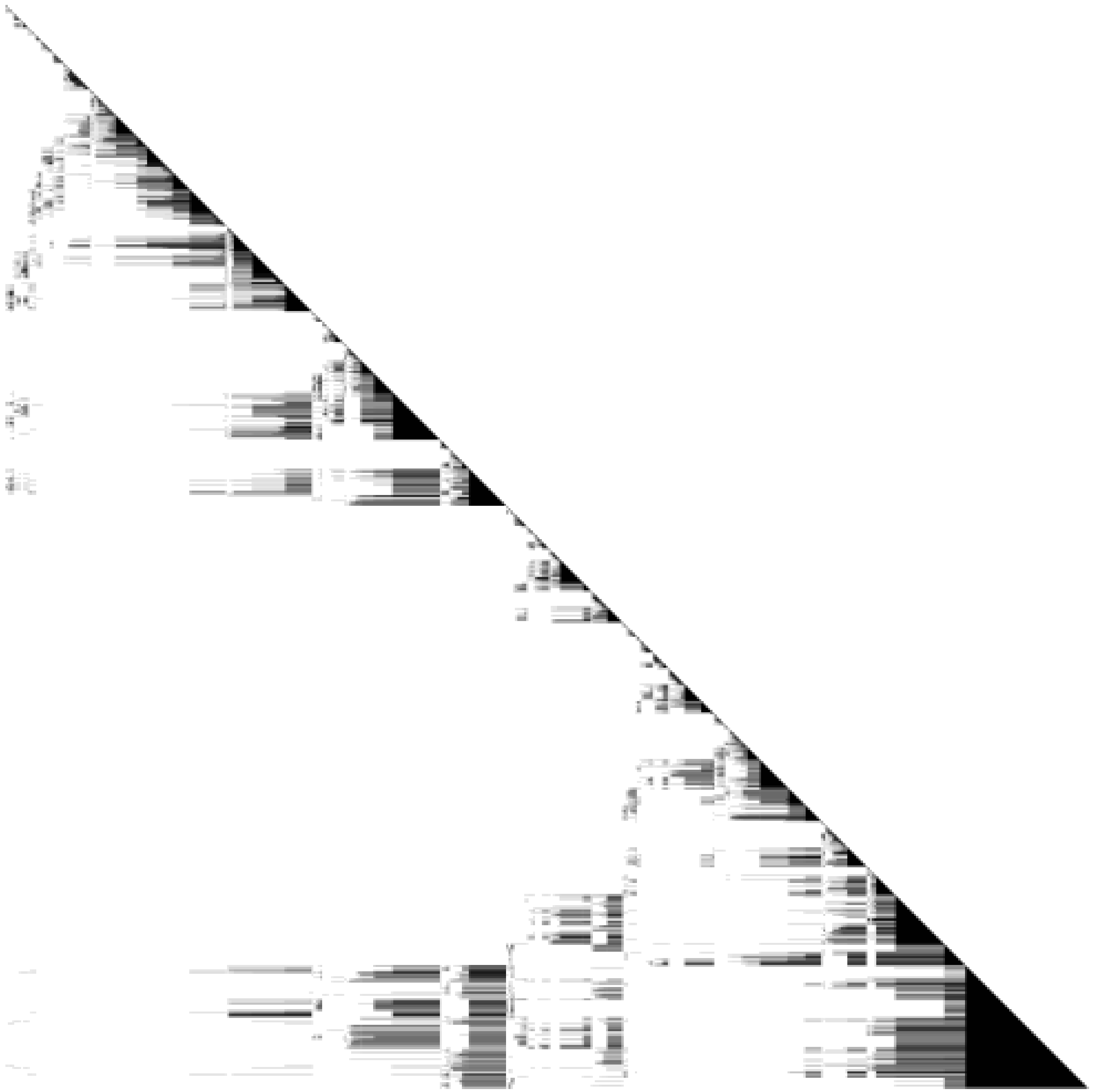
Symmetric Matrix Benchmark Suite

#	Matrix Name	Problem Domain	Dimension	No. Non-zeros
1	dense	Dense matrix	1,000	1.00 M
2	bcsstk35	Stiff matrix automobile frame	30,237	1.45 M
3	crystk02	FEM crystal free vibration	13,965	969 k
4	crystk03	FEM crystal free vibration	24,696	1.75 M
5	nasasrb	Shuttle rocket booster	54,870	2.68 M
6	3dtube	3-D pressure tube	45,330	3.21 M
7	ct20stif	CT20 engine block	52,329	2.70 M
8	gearbox	Aircraft flap actuator	153,746	9.08 M
9	cfd2	Pressure matrix	123,440	3.09 M
10	finan512	Financial portfolio optimization	74,752	596 k
11	pwt	Structural engineering	36,519	326 k
12	vibrobox	Vibroacoustic problem	12,328	343 k
13	gupta1	Linear programming	31,802	2.16 M

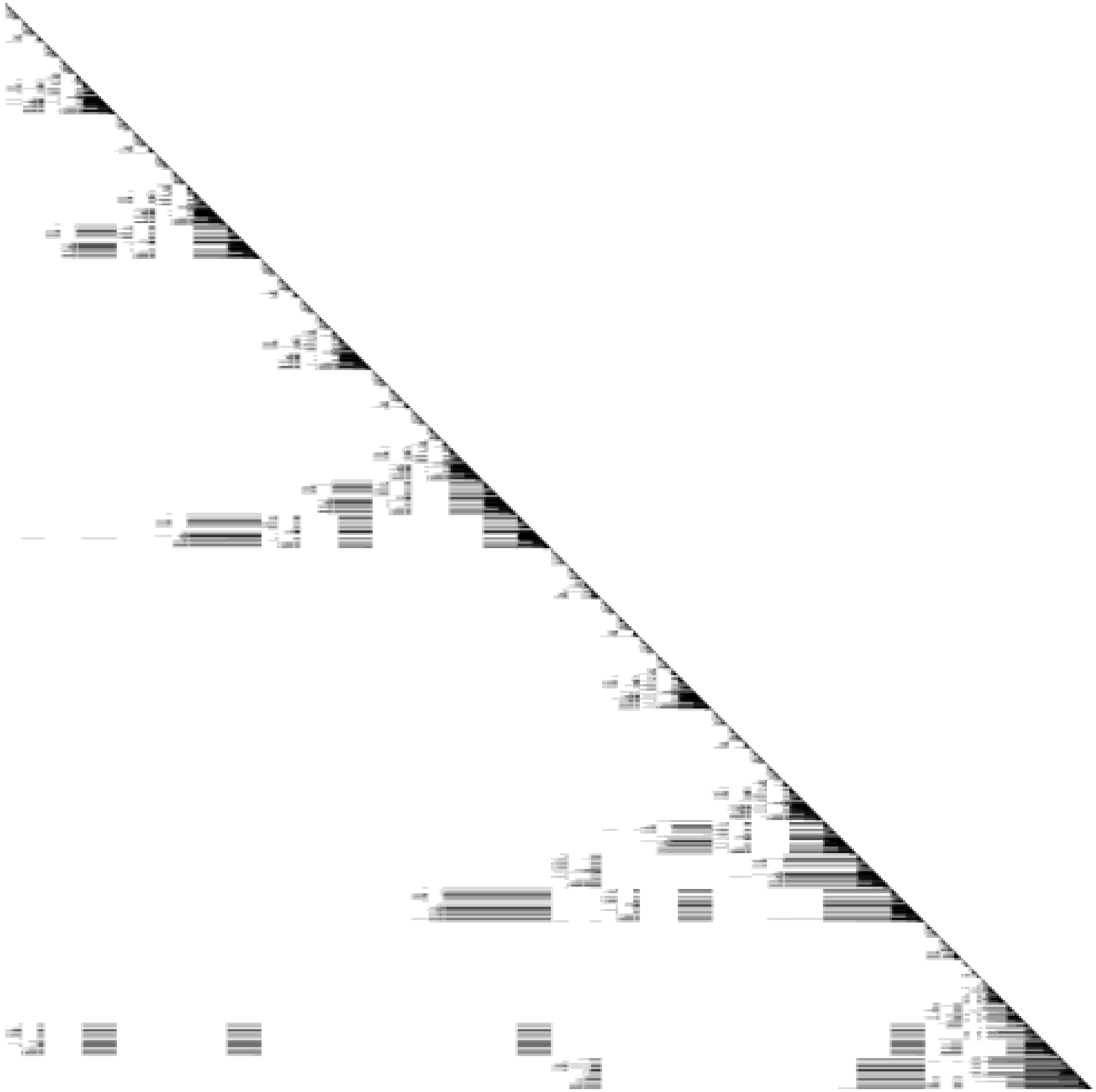
Lower Triangular Matrix Benchmark Suite

#	Matrix Name	Problem Domain	Dimension	No. of non-zeros
1	dense	Dense matrix	1,000	500 k
2	ex11	3-D Fluid Flow	16,214	9.8 M
3	goodwin	Fluid Mechanics, FEM	7,320	984 k
4	lhr10	Chemical process simulation	10,672	369 k
5	memplus	Memory circuit simulation	17,758	2.0 M
6	orani678	Finance	2,529	134 k
7	raefsky4	Structural modeling	19,779	12.6 M
8	wang4	Semiconductor device simulation, FEM	26,068	15.1 M

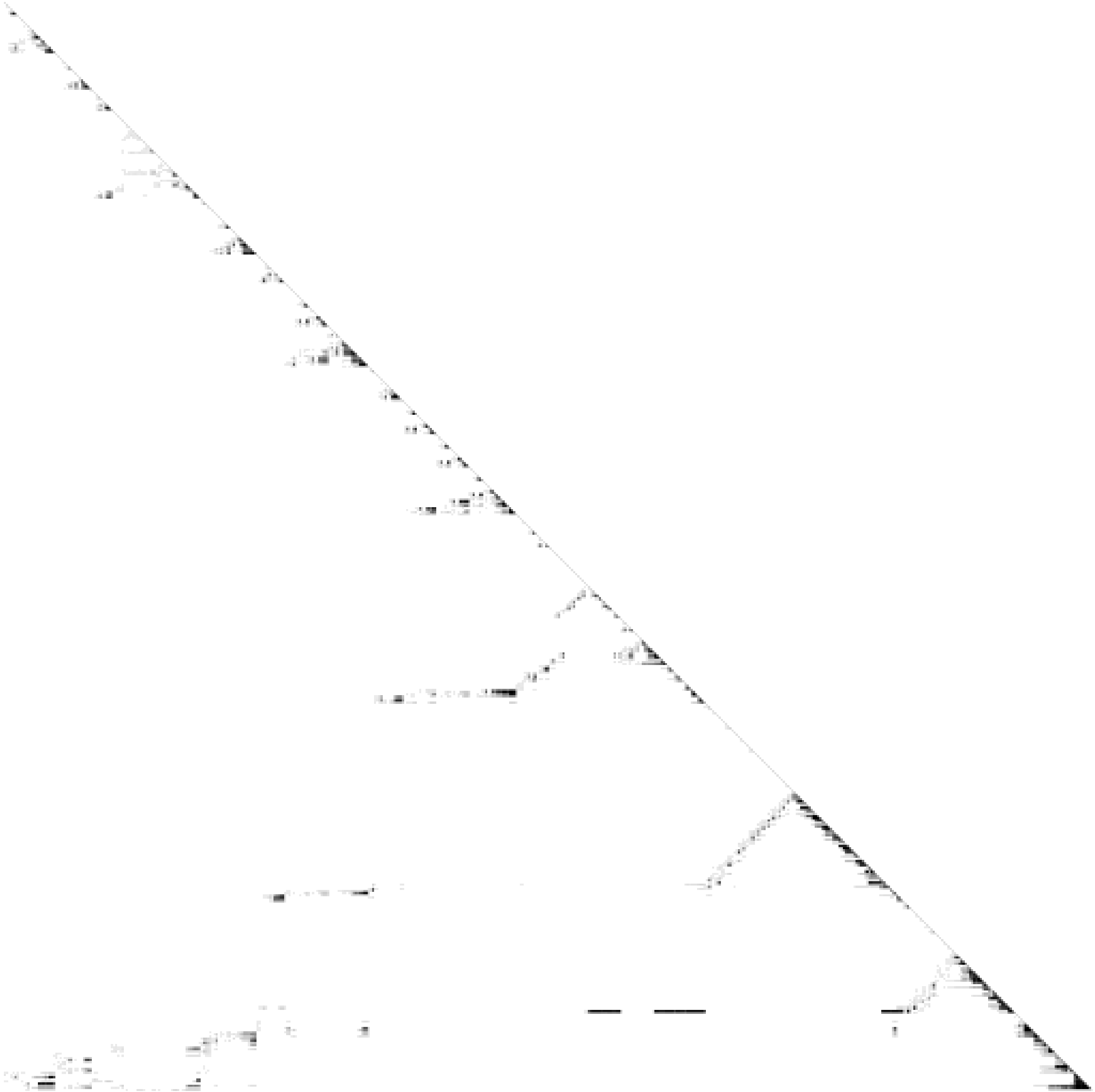
Lower triangular factor: Matrix #2 – ex11



Lower triangular factor: Matrix #3 - goodwin

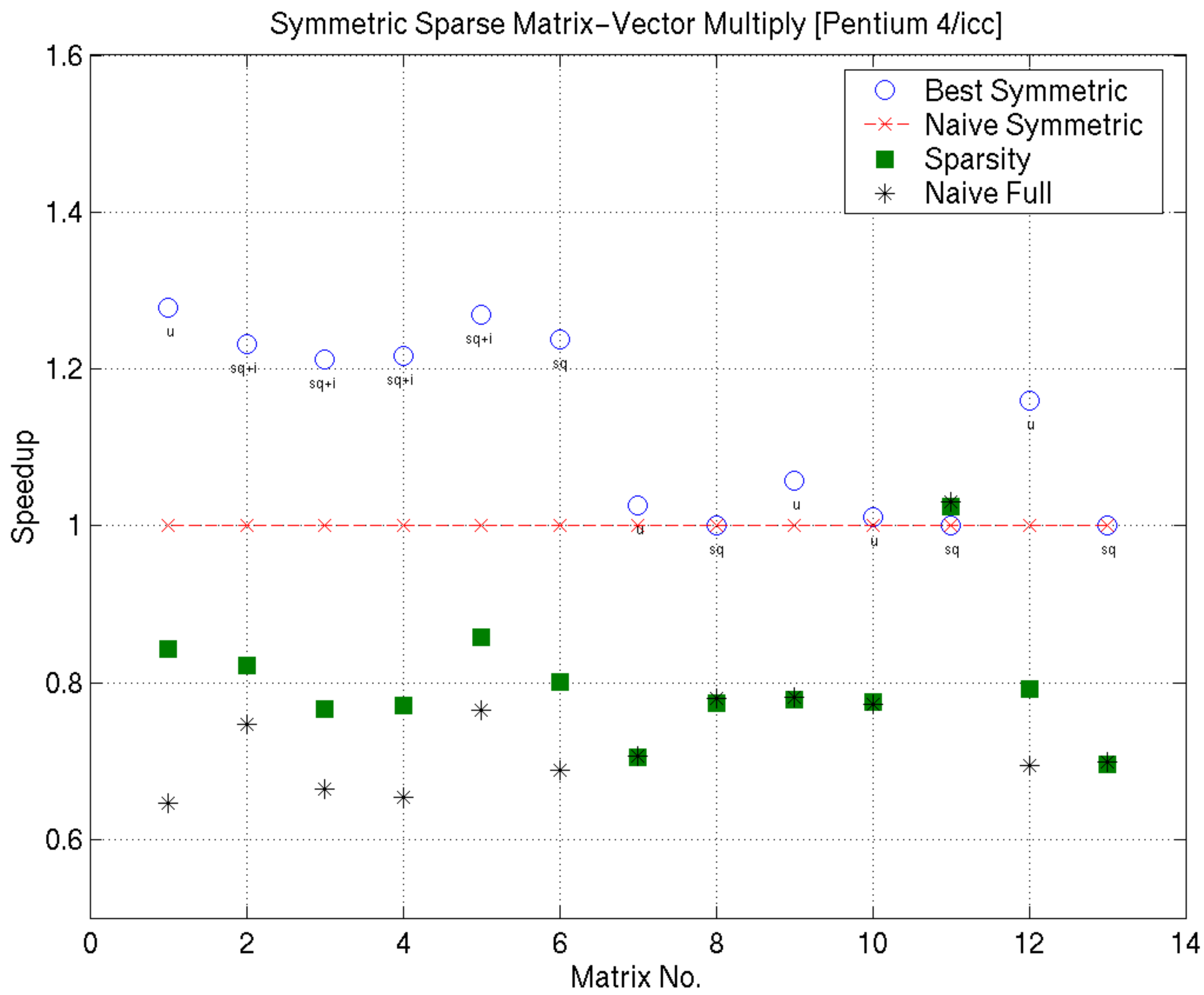


Lower triangular factor: Matrix #4 – lhr10

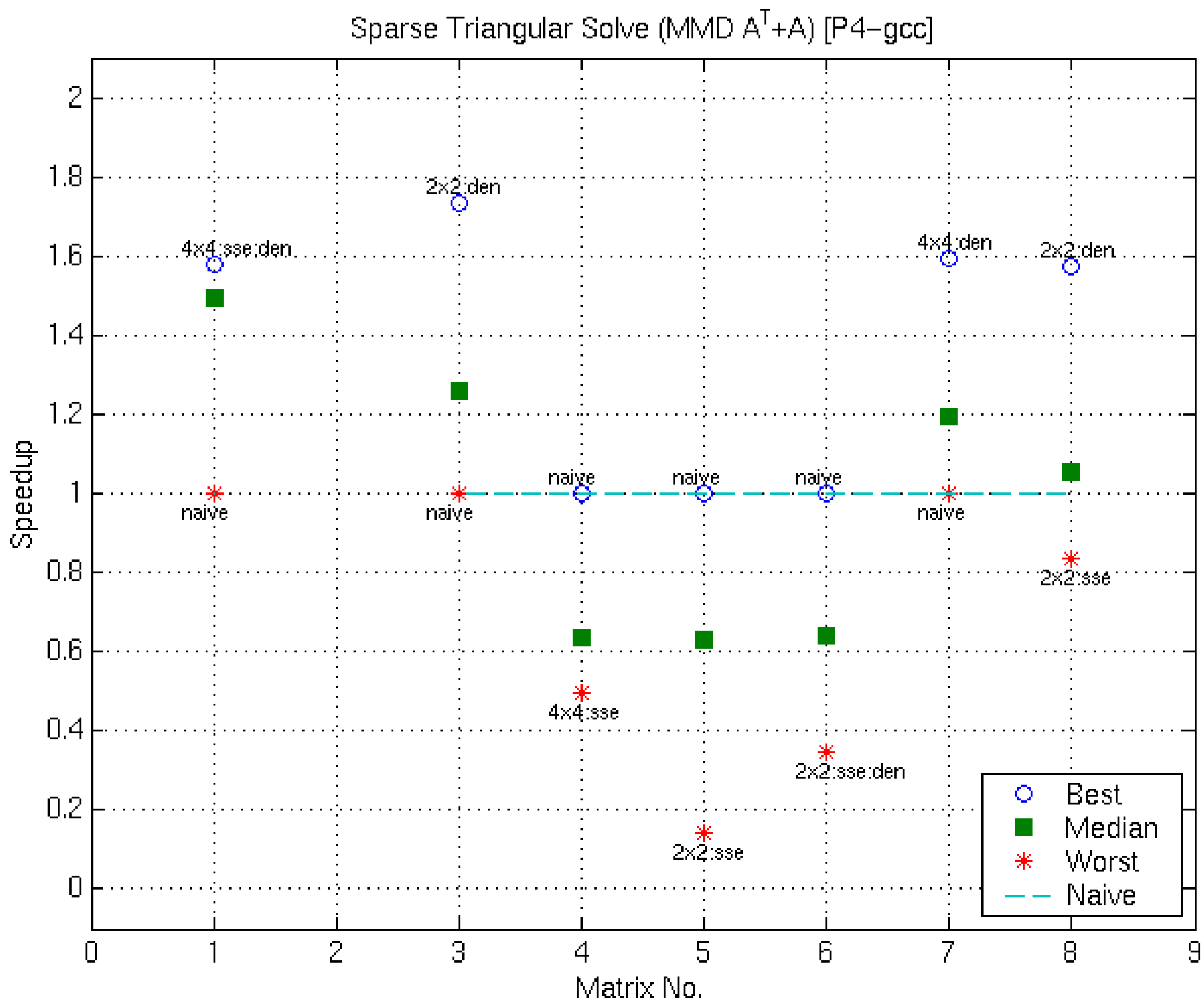


Extra Slides

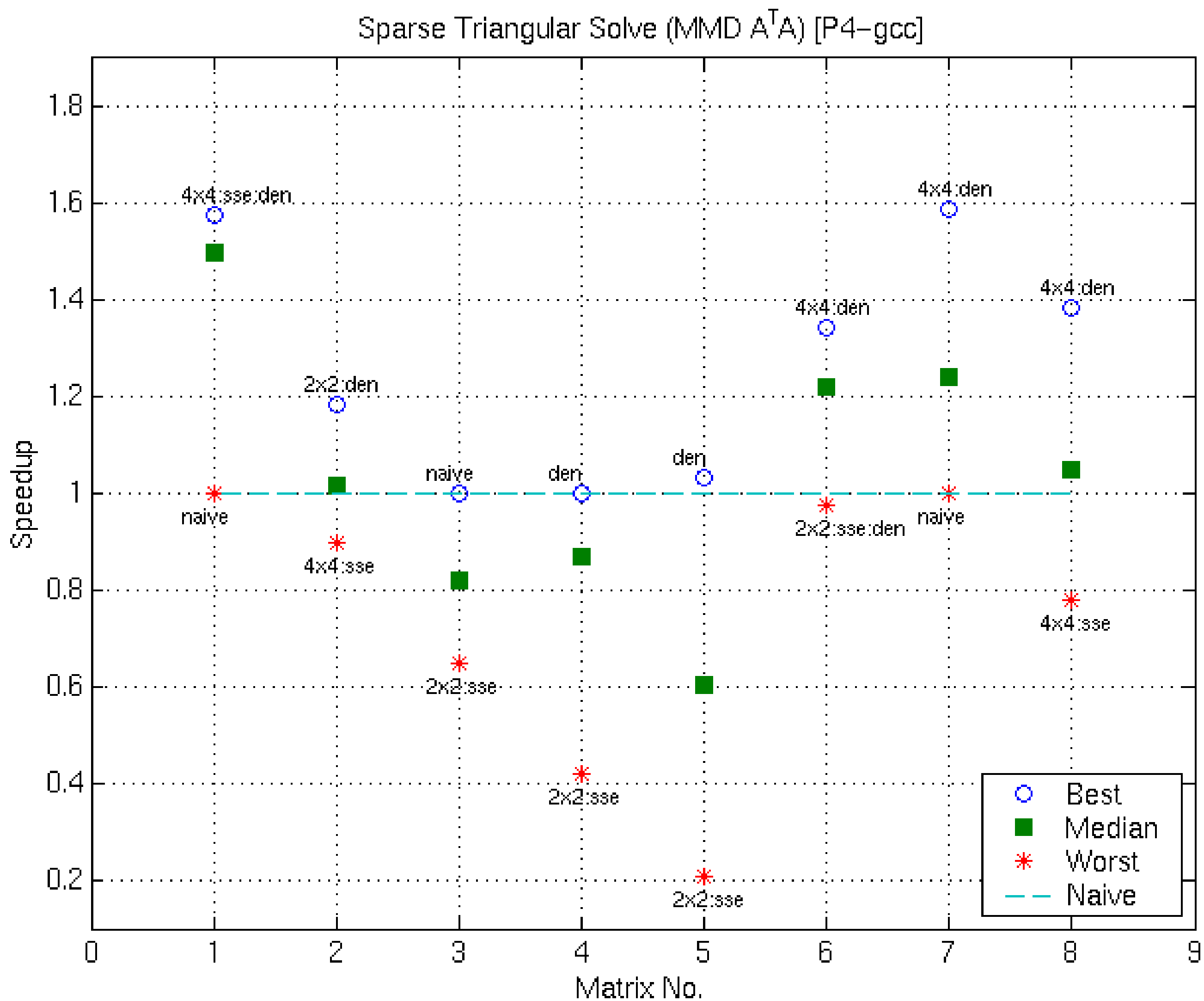
Symmetric Sparse Matrix-Vector Multiply on P4 (vs naïve symmetric = 1)



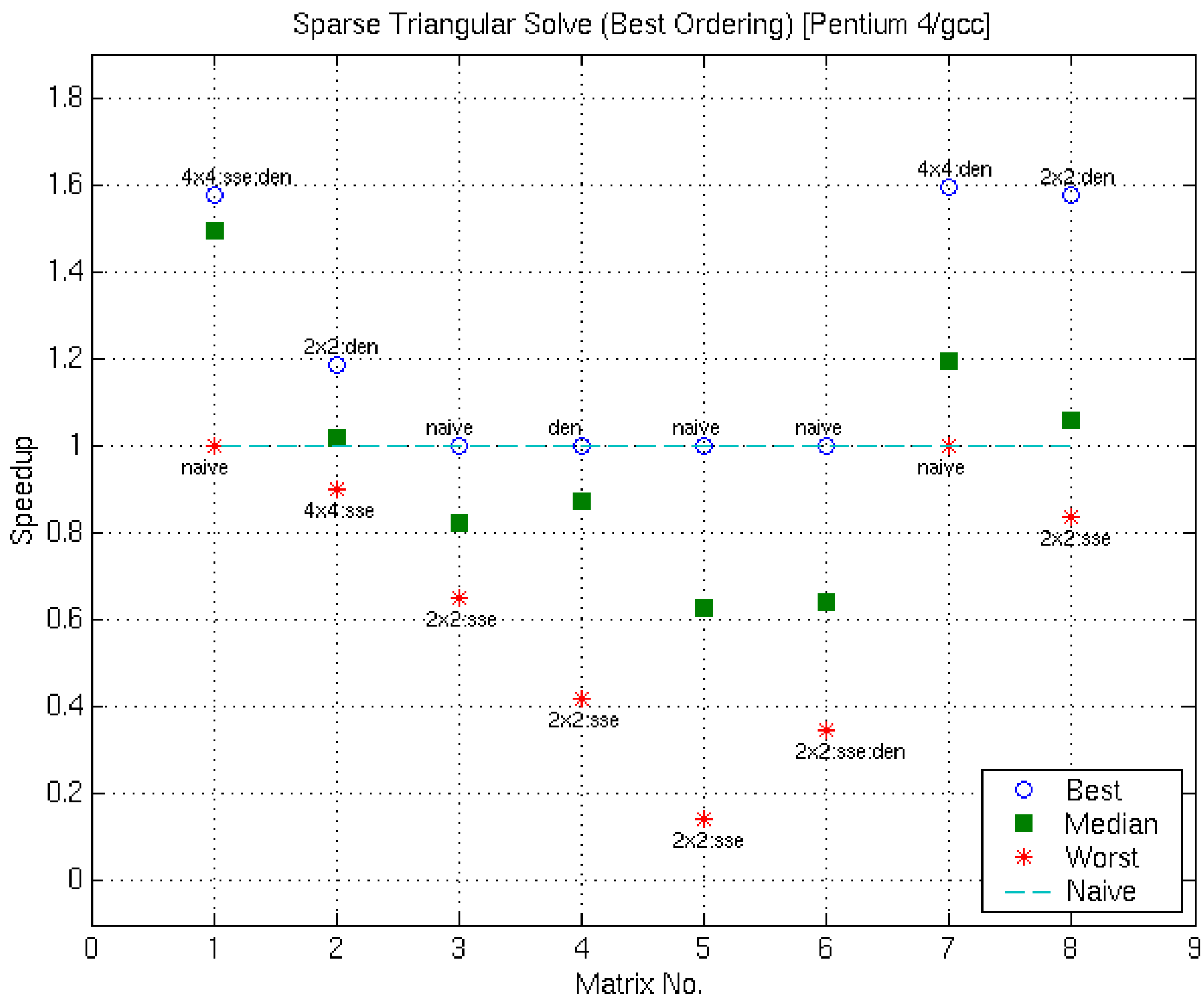
Sparse Triangular Solve (mmd on A^T+A ordering) on P4



Sparse Triangular Solve (mmd on A^T*A ordering) on P4

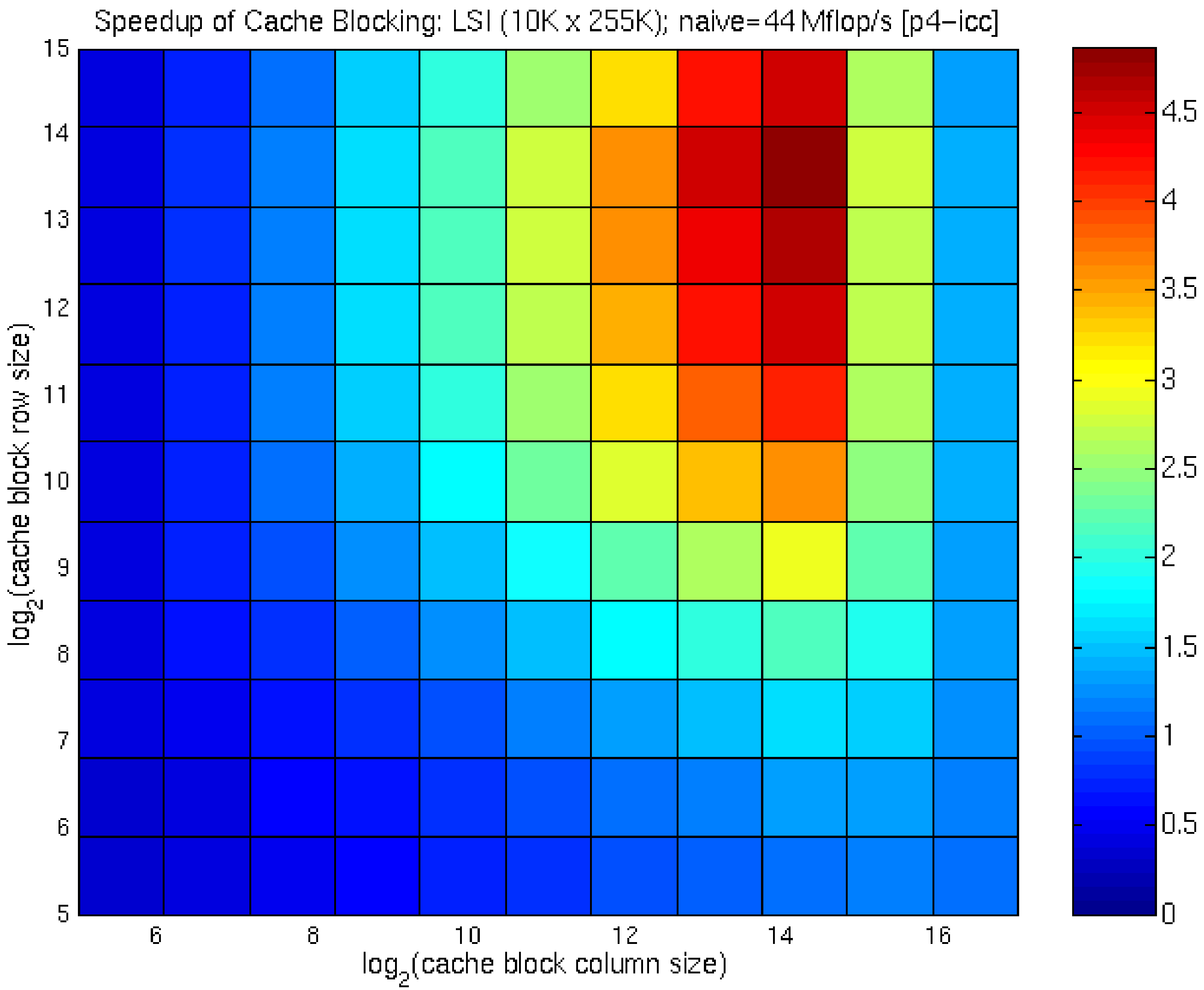


Sparse Triangular Solve (best of 3 orderings) on P4

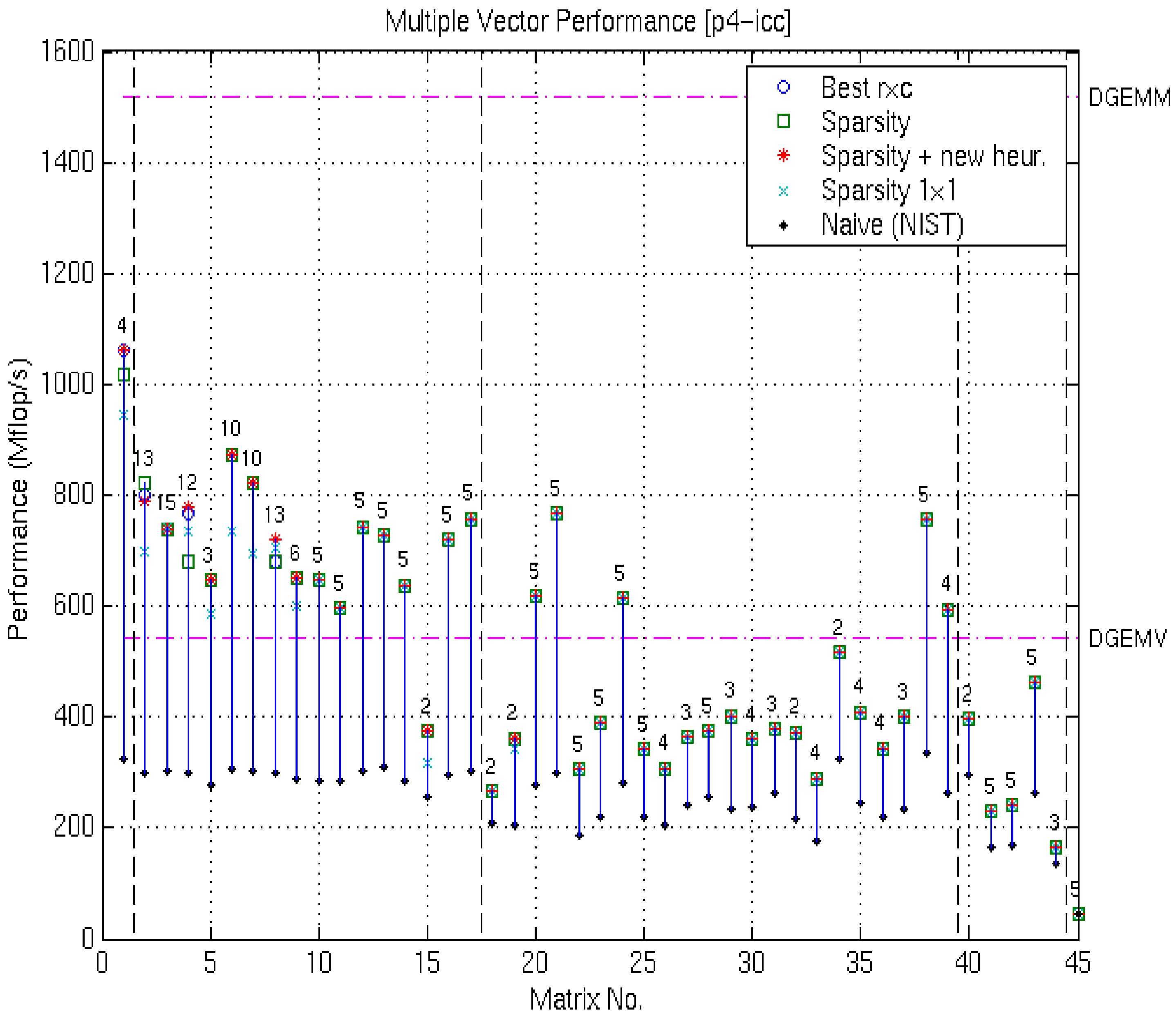


New slides from Rich

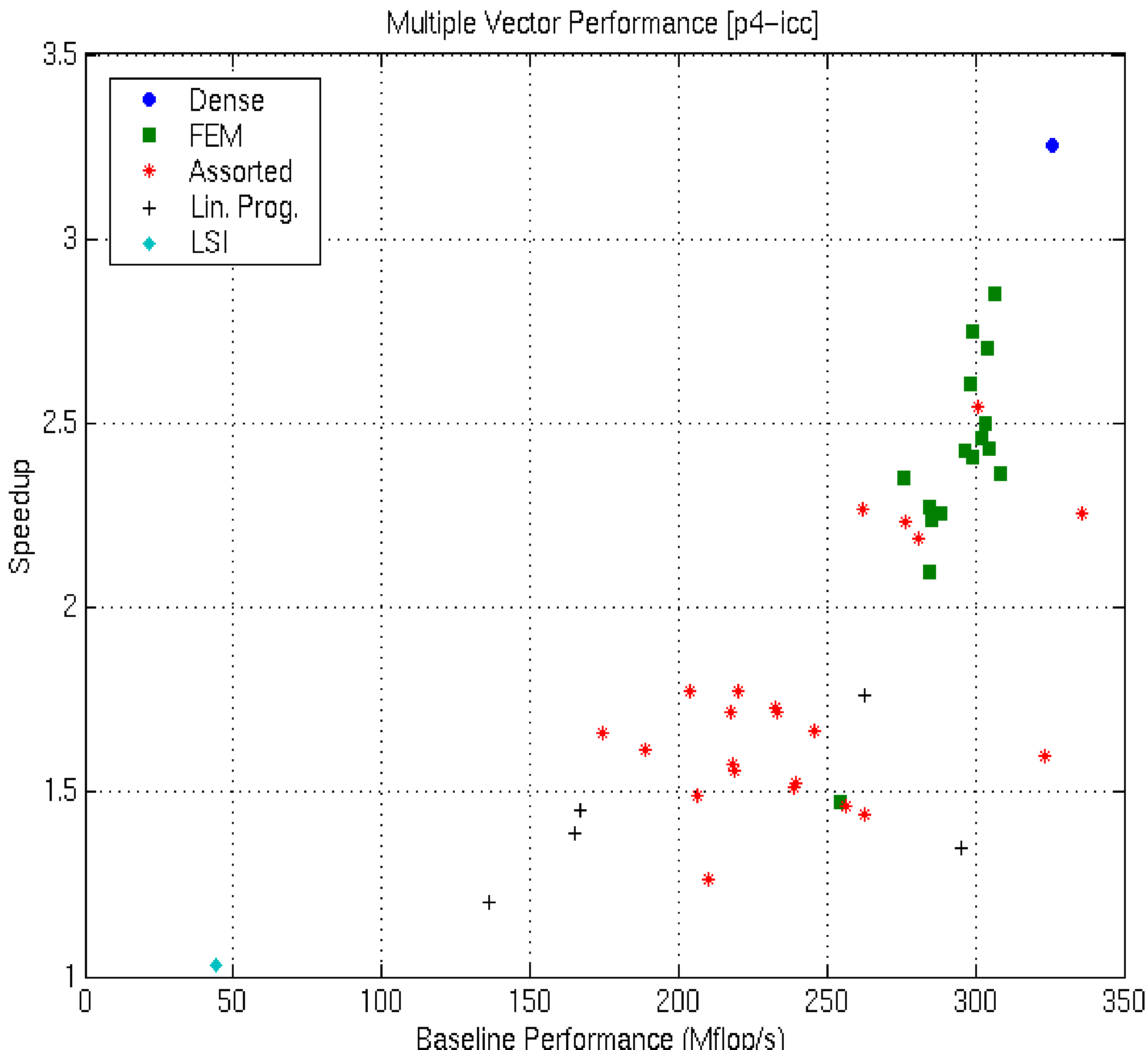
Speed up from Cache Blocking on LSI matrix on P4



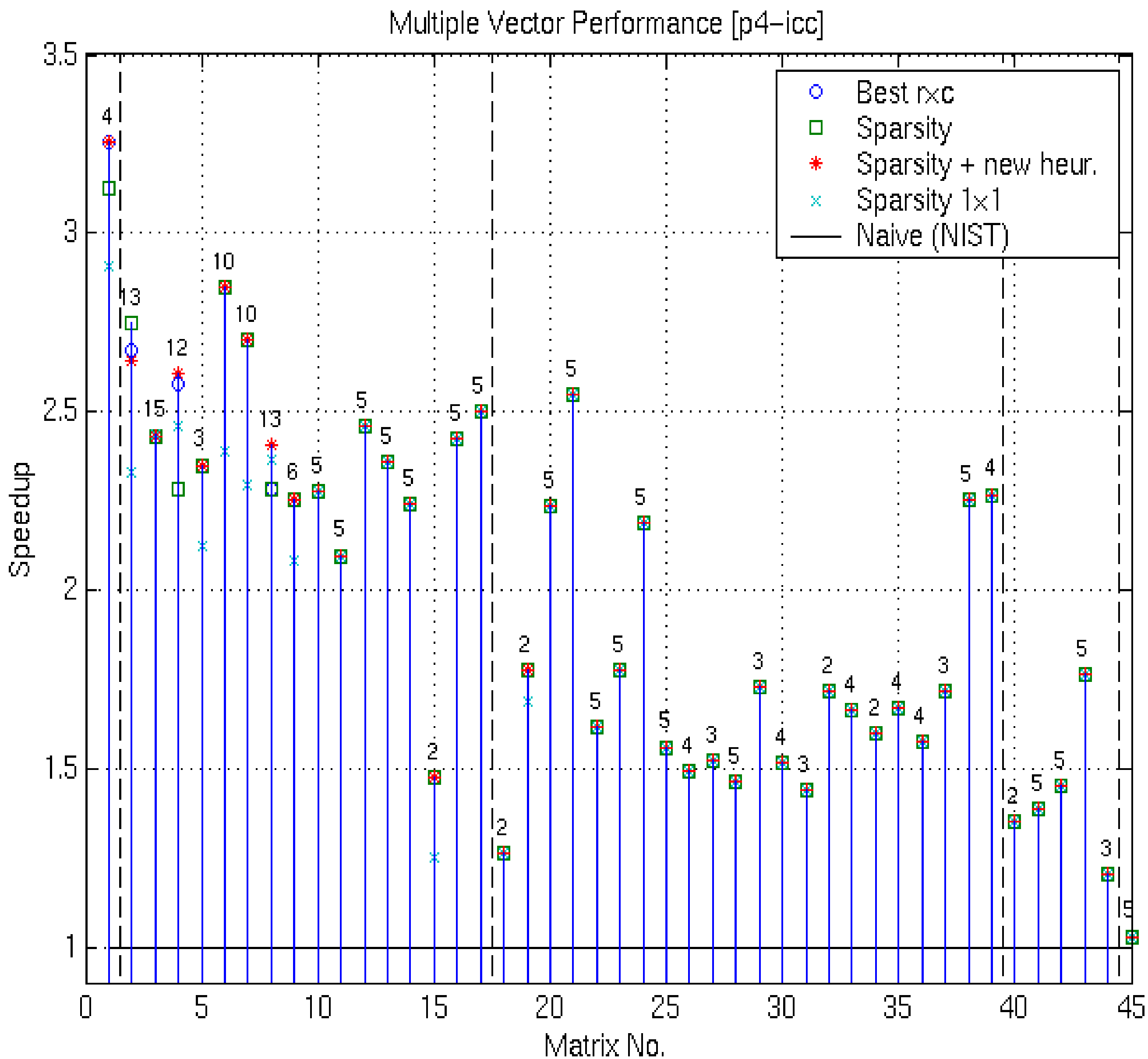
Multiple Vector Performance on P4



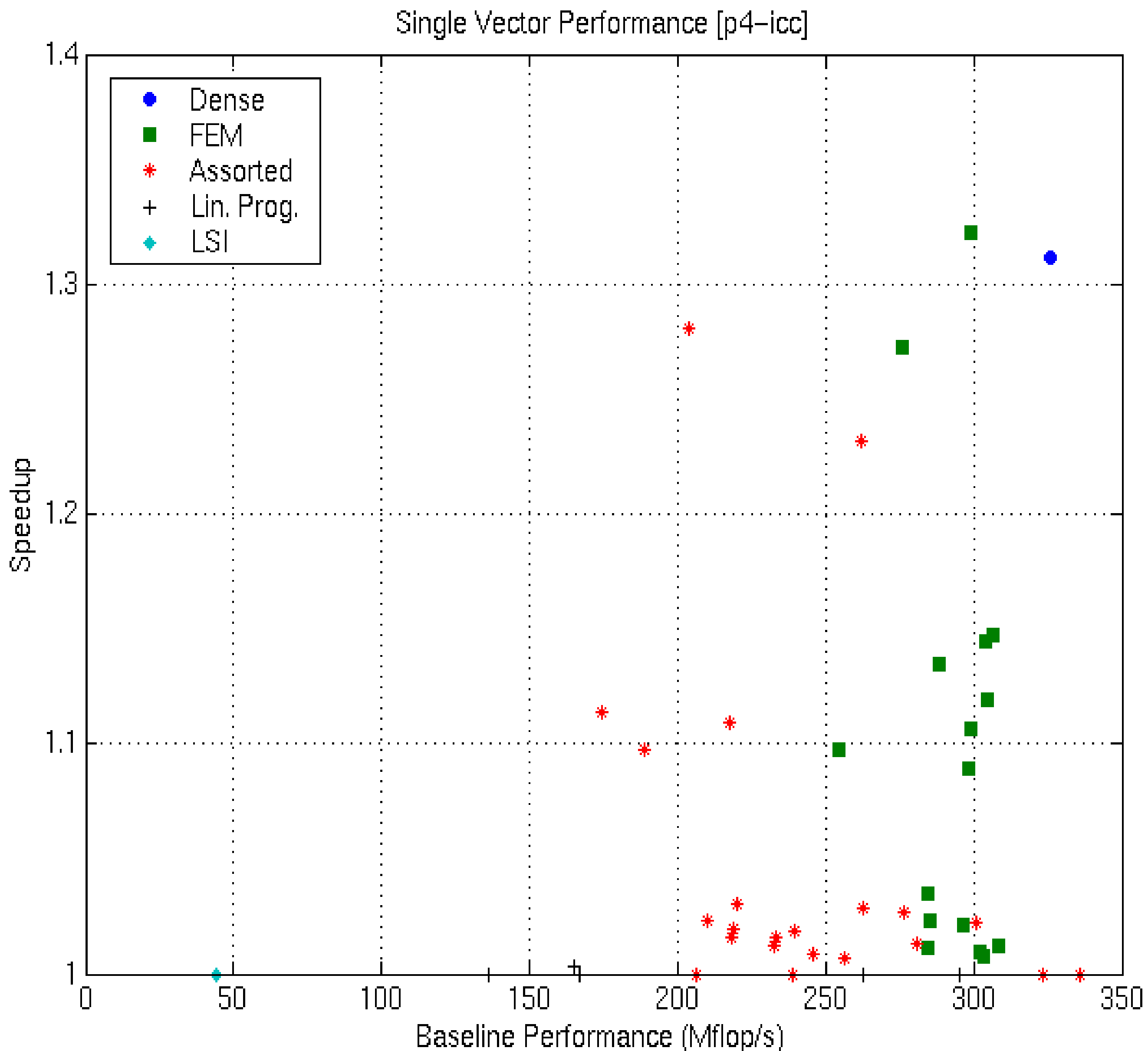
Multiple vector performance on P4 – by matrix type



Multiple vector speedups on P4



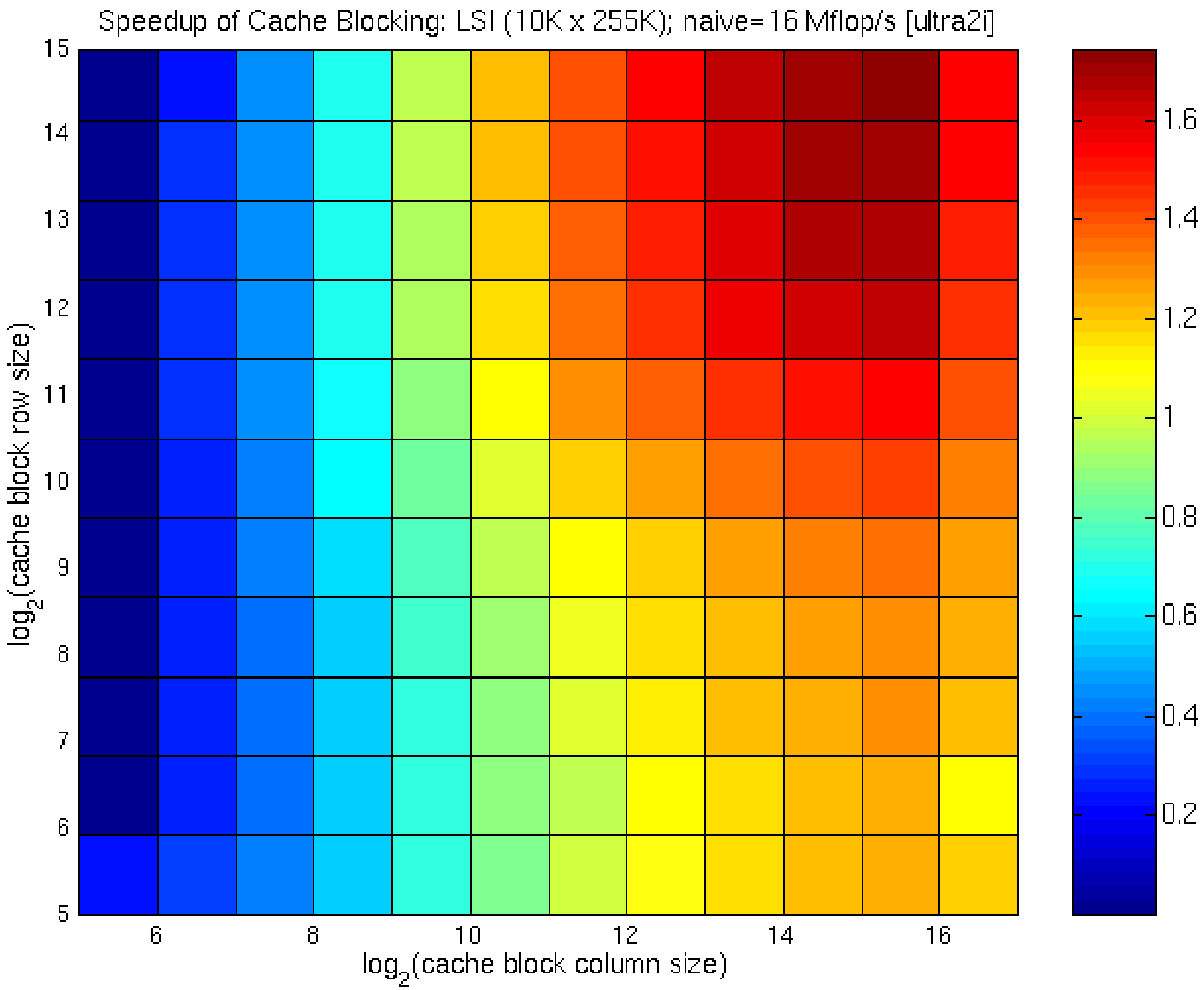
Single vector speedups on P4 by matrix type



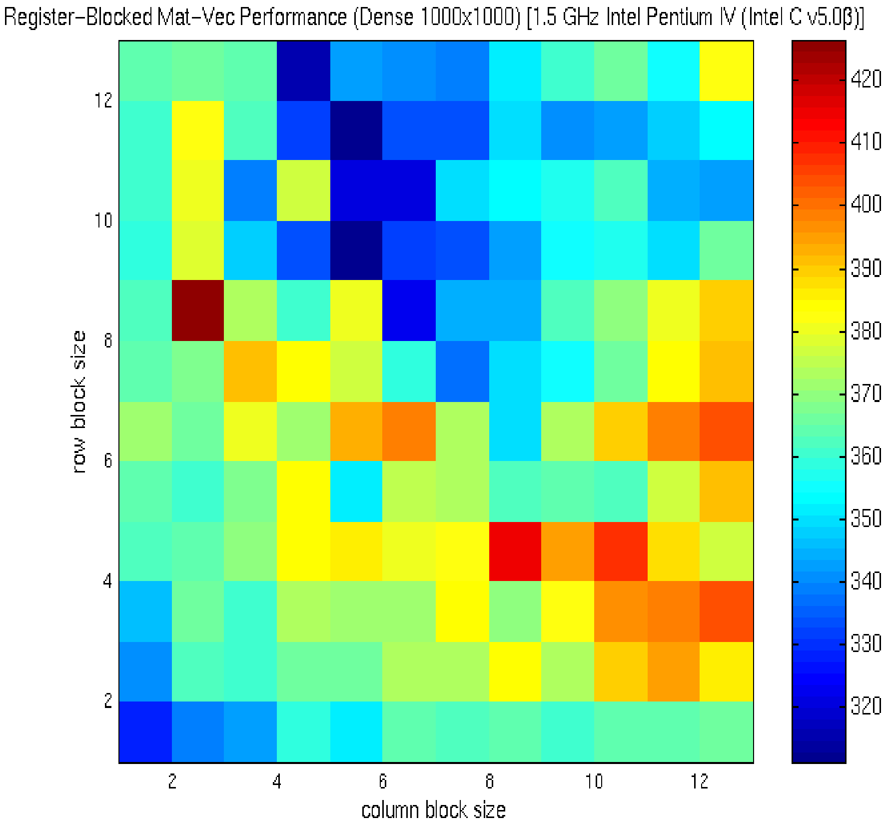
Performance Tuning

- Motivation: performance of many applications dominated by a few kernels
- MEMS CAD → Nonlinear ODEs → Nonlinear equations → Linear equations → Matrix multiply
  - Matrix-by-matrix or matrix-by-vector
  - Dense or Sparse
- Information retrieval by LSI → Compress term-document matrix → … → Sparse mat-vec multiply
- Information retrieval by LDA → Maximum likelihood estimation → … → Solve linear systems
- Many other examples (not all linear algebra)

Speed up from Cache Blocking on LSI matrix on Sun Ultra



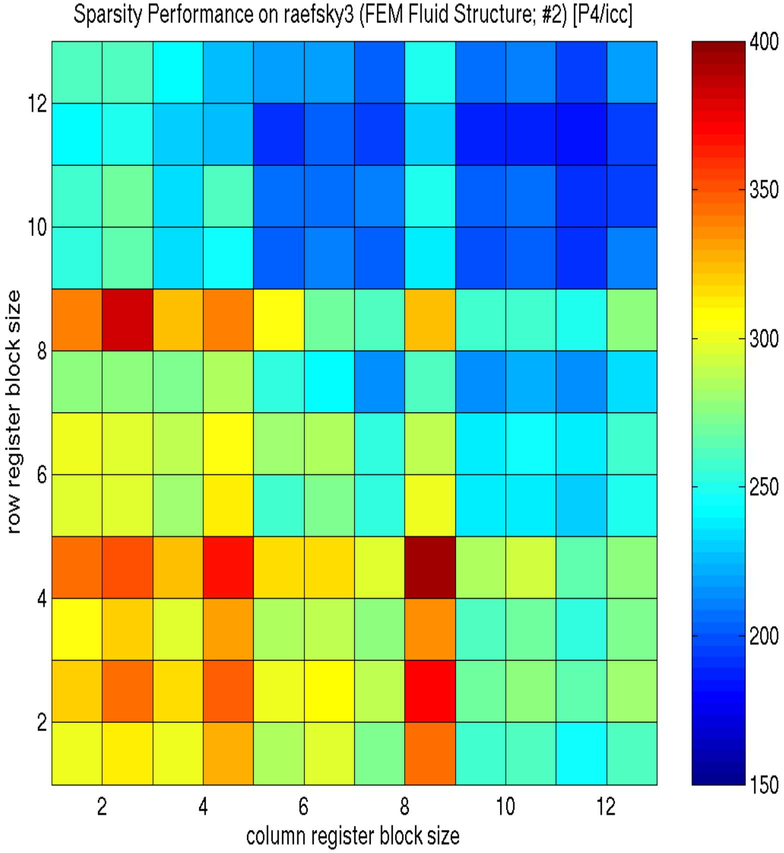
Possible Improvements



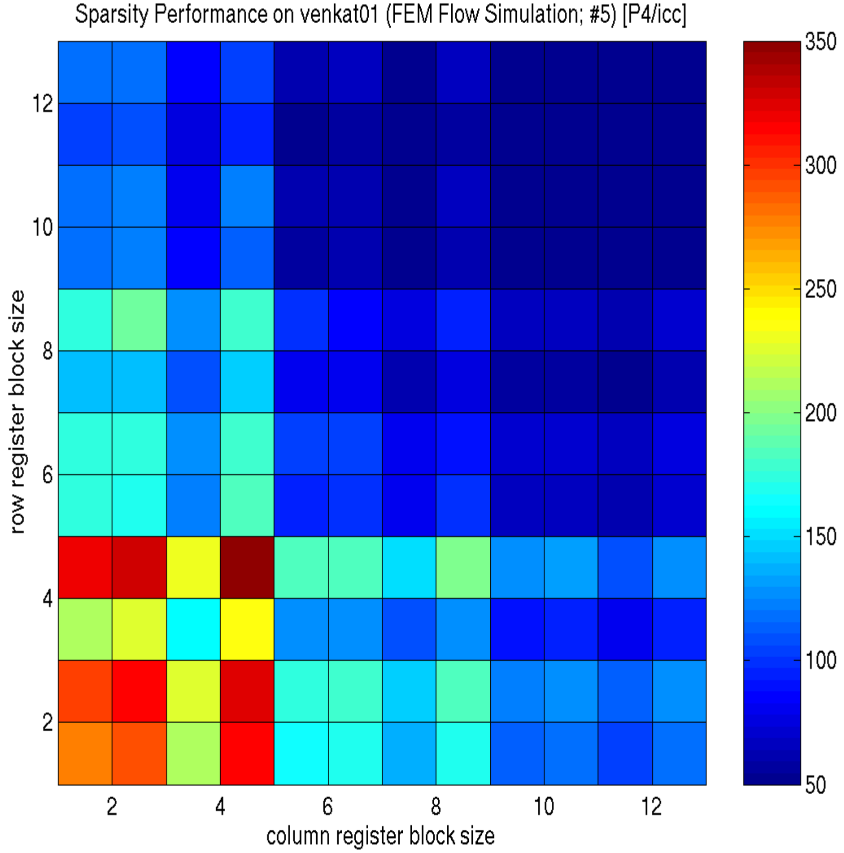
- Doesn't work as well as on Sun Ultra 1/170; Why?
- Current heuristic to determine best r x c block biased to diagonal of performance plot
- Didn't matter on Sun, does on P4 and Itanium since performance so "nondiagonally dominant"

Sparsity reg blocking results on P4 for FEM/fluids matrices

Matrix #2 (150 Mflops to 400 Mflops)



Matrix #5 (50 Mflops to 350 Mflops)



Possible collaborations with Intel

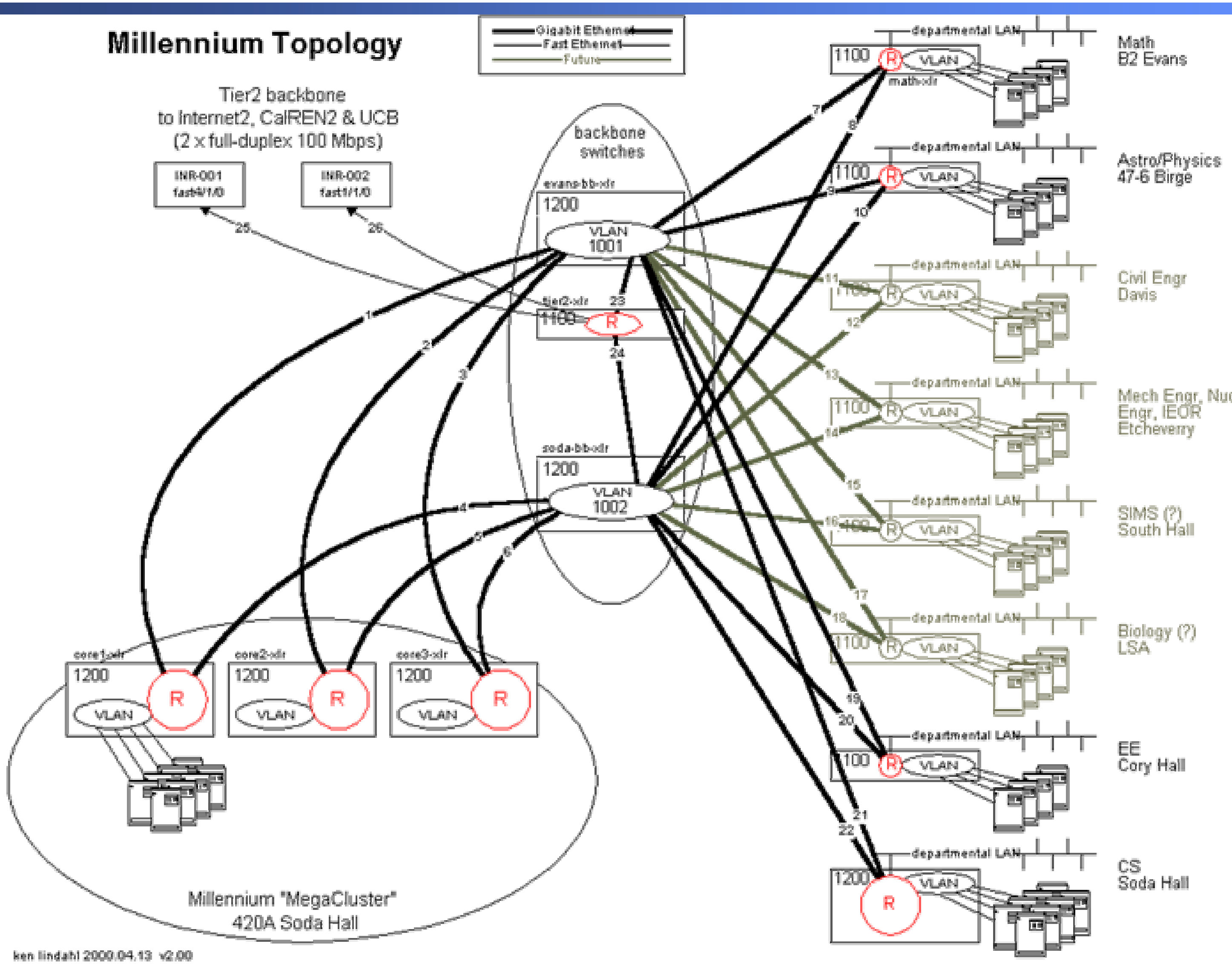
- Getting right tools
- Getting faster, less accurate transcendental functions
- Provide feedback on tools
- Provide tuned kernels, benchmarks, IR apps
- Provide system for tuning future kernels
  - To provide users
  - To evaluate architectural designs

Millennium

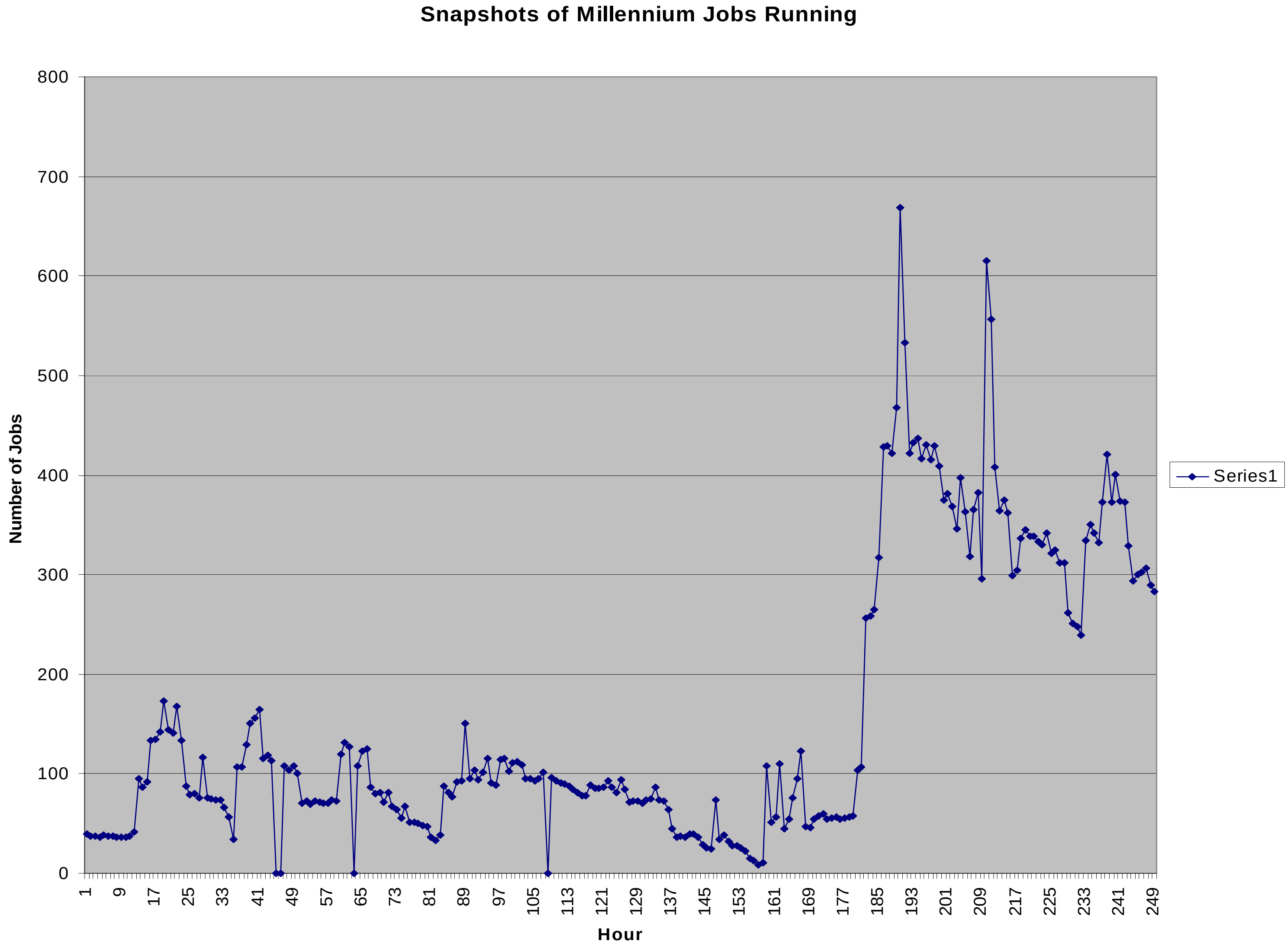
Millennium

- Cluster of clusters at UC Berkeley
  - 309 CPU cluster in Soda Hall
  - Smaller clusters across campus
- Made possible by Intel equipment grant
- Significant other support
  - NSF, Sun, Microsoft, Nortel, campus
- www.millennium.berkeley.edu

Millennium Topology



Millennium Usage Oct 1 – 11, 2001



100% utilization for last few days
About half the jobs are parallel

Usage highlights

- AMANDA
  - Antarctic Muon And Neutrino Detector Array
  - amanda.berkeley.edu
  - 128 scientists from 15 universities and institutes in the U.S. and Europe.
- TEMPEST
  - EUV lithography simulations via 3D electromagnetic scattering
  - cuervo.eecs.berkeley.edu/Volcano/
  - study the defect printability on multilayer masks
- Titanium
  - High performance Java dialect for scientific computing
  - www.cs.berkeley.edu/projects/titanium
  - Implementation of shared address space, and use of SSE2
- Digital Library Project
  - Large database of images
  - elib.cs.berkeley.edu/
  - Used to run spectral image segmentation algorithm for clustering, search on images

Usage highlights (continued)

- CS 267
  - Graduate class in parallel computing, 33 enrolled
  - www.cs.berkeley.edu/~dbindel/cs267ta
  - Homework
- Disaster Response
  - Help find people after Sept 11, set up immediately afterwards
  - safe.millennium.berkeley.edu
  - 48K reports in database, linked to other survivor databases
- MEMS CAD (MicroElectroMechanical Systems Computer Aided Design)
  - Tool to help design MEMS systems
  - Used this semester in EE 245, 93 enrolled
  - sugar.millennium.berkeley.edu
  - More later in talk
- Information Retrieval
  - Development of faster information retrieval algorithms
  - www.cs.berkeley.edu/~jordan
  - More later in talk
- Many applications are part of CITRIS