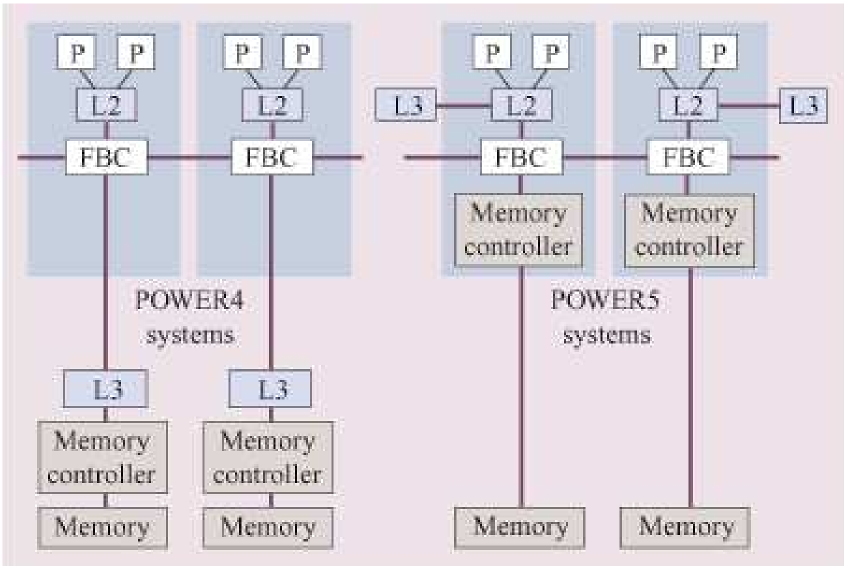
Scalable Preconditioning Techniques Based on Weighted Bandwidth Reduction

Background

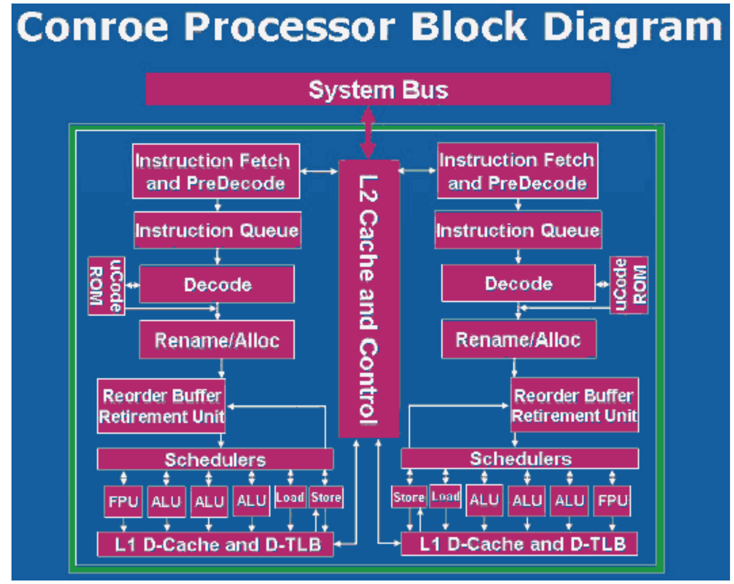
- Emerging architectures increasingly rely on parallelism (chip-level and system-level) for performance.
- Concurrency and localization play critical roles in overall performance of programs.
- Chip multiprocessors (multicore, multiscalar, cell-type) put increasing pressure on the memory subsystem.
- Algorithms and programs for such platforms must explicitly account for concurrency and memory references as primary metrics (as opposed to FLOP counts).

Conventional Architectures

IBM Power 5

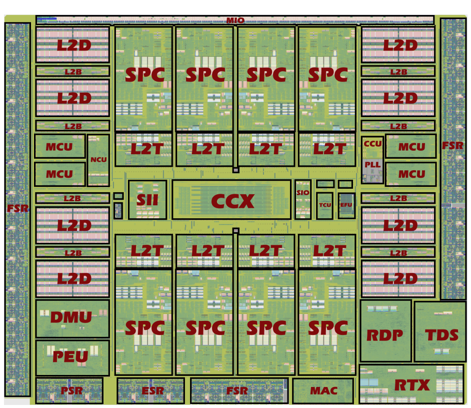


Intel/Conroe



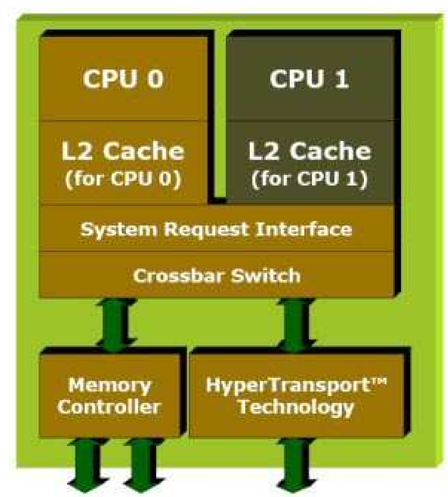
Sun Niagara 2

Niagara-2 Chip Overview



- 8 Sparc cores, 8 threads each
- Shared 4MB L2, 8-banks, 16-way associative
- Four dual-channel FBDIMM memory controllers
- Two 10/1 Gb Enet ports w/onboard packet classification and filtering
- One PCI-E x8 1.0 port
- 711 signal I/O, 1831 total

AMD Opteron



AMD Athlon™ 64 X2
Dual-Core Processor Design

Implications for Sparse Linear System Solvers

- Maximal use of dense kernels in sparse solvers.
- Develop methods that optimize concurrency – iterative methods with preconditioners that have dense kernels.
- A natural candidate for such a preconditioner is a banded matrix.

Banded Preconditioners for Iterative Methods

- Derive banded approximations to the matrix, which can act as good preconditioners.

- Bands must be narrow and capture much of the matrix norm.

- Use banded solvers with high FLOP counts and concurrency.

Key questions:

- How do we derive such narrow-banded preconditioners (non-symmetric permutations)?

- Can such simple preconditioners be competitive against traditional preconditioners in terms of iteration counts, FLOPS, FLOP counts, and parallelism?

Contributions and Results

- Banded preconditioners (with suitable reordering) can significantly outperform ILU preconditioners in terms of iteration counts, FLOP counts, as well as concurrency for large classes of matrices!

- Reordering schemes based on weighted spectral methods are highly effective in deriving narrow banded preconditioners.

- The overhead of such reordering schemes is easily offset by the lower solution cost for the system.

- A number of banded solvers (LAPACK, Spike) can be used for the inner solve.

Bandwidth Reduction

- Traditional algorithms (*e.g.*, Cuthill-McKee (Cuthill & McKee, 1969), Spectral reordering (Barnard *et al.*, 1995)) are aimed at minimizing the bandwidth

$$BW(A) = \max_{i,j:A(i,j)>0} |i - j|$$

- Heavy (high-magnitude) nonzeros that are distant from the diagonal may significantly degrade the performance (convergence rate)
  - Particularly, for ill conditioned matrices.

Accounting for Heavy Entries

- We generalize the definition of bandwith
- For given b, we define bandweight as

$$w_b(A) = \sum_{i,j:|i-j|<b} |A(i,j)|$$

- Then, for given α, we define α-bandwidth as the smallest bandwidth that encapsulates an α fraction of total matrix weight

$$BW_\alpha(A) = \min b \text{ such that } w_b(A) \geq \alpha \times \sum_{i,j} |A(i,j)|$$

  - Observe that this is a generalization of bandwidth, such that $BW_1(A) = BW(A)$

Spectral Ordering

- Commonly used in graph-theoretic applications and matrix algorithms

- Find x that minimizes

$$\sum_{i,j:A(i,j)>0} (x(i) - x(j))^2$$

  - Reorder rows and columns of A accordingly

- The eigenvector that corresponds to the smallest non-zero eigenvalue of the Laplacian

$$\begin{aligned} L(i,j) &= -1 && \textbf{if } i \neq j \wedge A(i,j) > 0 \\ L(i,i) &= |\{j : A(i,j) > 0\}|, \end{aligned}$$

  a.k.a, Fiedler vector, minimizes this cost function (Fiedler, 1973)

  - Can be computed effectively using iterative techniques (*e.g.*, CG (Kruyt, 1995))

Weighted Spectral Ordering

- Fiedler's result generalizes to weighted graphs (matrices) as well
- Define Weighted Laplacian as

$$\begin{aligned} \bar{L}(i,j) &= -|A(i,j)| \qquad\qquad \textbf{if } i \neq j \\ \bar{L}(i,i) &= \textstyle\sum_j |A(i,j)| \end{aligned}$$

- The eigenvector that corresponds to the smallest non-zero eigenvalue of the weighted Laplacian minimizes

$$x^T \bar{L} x = \sum_{i,j} |A(i,j)|(x(i) - x(j))^2,$$

- Observe that $x^T L x$ is closely related to $\sum_{i,j} |A(i,j)| - w_b(A)$, with proper quantization

Weighted Bandwidth Reduction

- For large enough α, use Weighted Spectral Ordering as a heuristic to minimize α-bandwidth
  - Find $\hat{x}$, the eigenvector corresponding to smallest non-zero eigenvalue of $\bar{L}$
  - Find permutation $\Pi = \{i_1, i_2, ..., i_n :$ if $j < k,\ x(i_j) < x(i_k)\}$
  - Reorder rows and columns of A accordingly to obtain $\bar{A} = A(\Pi, \Pi)$

- Observe that the heavy entries of the reordered matrix, $\bar{A}$ are close to its diagonal, *i.e.*, $\bar{A}$ has a smaller α-bandwidth compared to A

- Drop all entries that are outside α-bandwidth of $\bar{A}$

$$\tilde{A} = \{\tilde{A}(i,j) : \tilde{A}(i,j) = \bar{A}(i,j) \text{ if } |i-j| \leq BW_\alpha(\bar{A}),\ 0 \text{ else}\}$$

- Use $\tilde{A}$ as a banded preconditioner to solve the system A

Experimental Results

- Matrices gathered from UF Sparse Matrix Collection
  - All software is implemented in Fortran
  - Sequential timings were done on a clovertown machine
  - BICGSTAB is used as the iterative solver
  - All matrices are first reordered using MC64, to move heaviest entries to the diagonal

Experimental Results

- Application of Weighted Spectral Ordering (WSO)
  - Reorder $|A| + |A^T|$ using MC73
  - Find the bandwidth that encapsulates 99% of overall matrix norm ($\alpha = 0.99$)
  - Drop entries that fall out of this bandwidth to obtain the Weighted Spectral Preconditioner

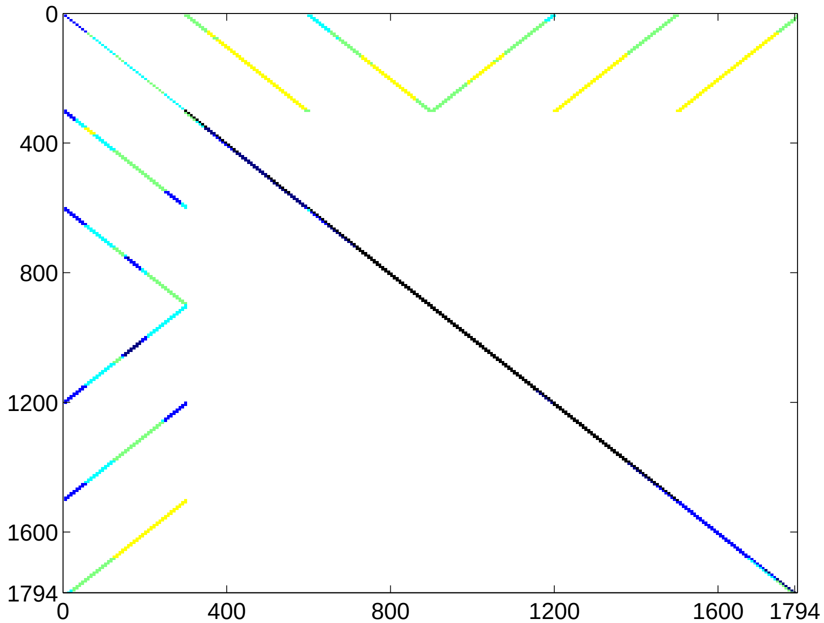
Experimental Results

- Comparison with no preconditioner and ILU
  - ILUT (Saad, 1994) is used as a basis for comparison.
  - Fill-in is set to match the storage required for dense storage of WSO's required bandwidth (ILUBW)
  - Drop tolerance is set to 10^{-1} (ILU1), 10^{-3} (ILU3)

epb0 Matrix

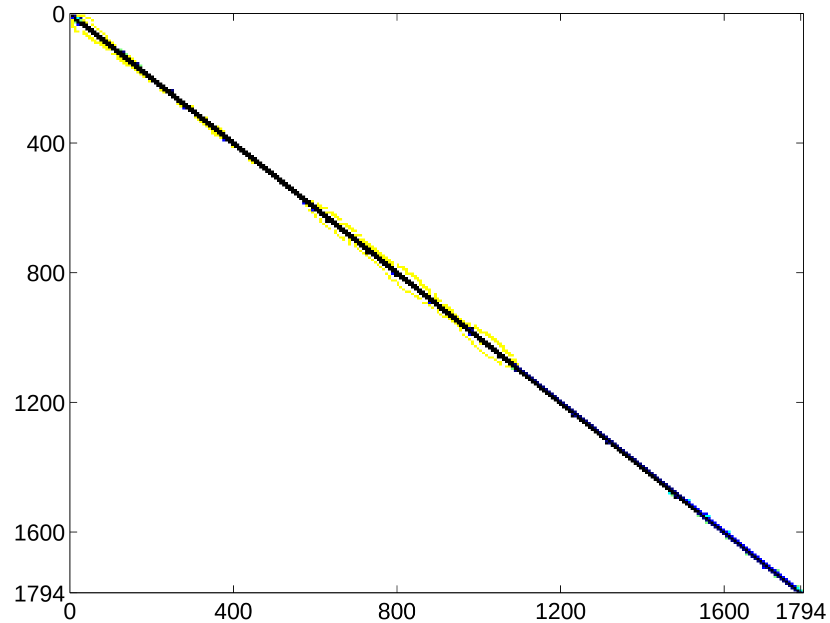
- Plate-fin heat exchanger w/ simple model
  - 1794×1794, 7764 non-zeros

Original Matrix



Bandwidth: 3587

Reordered Matrix

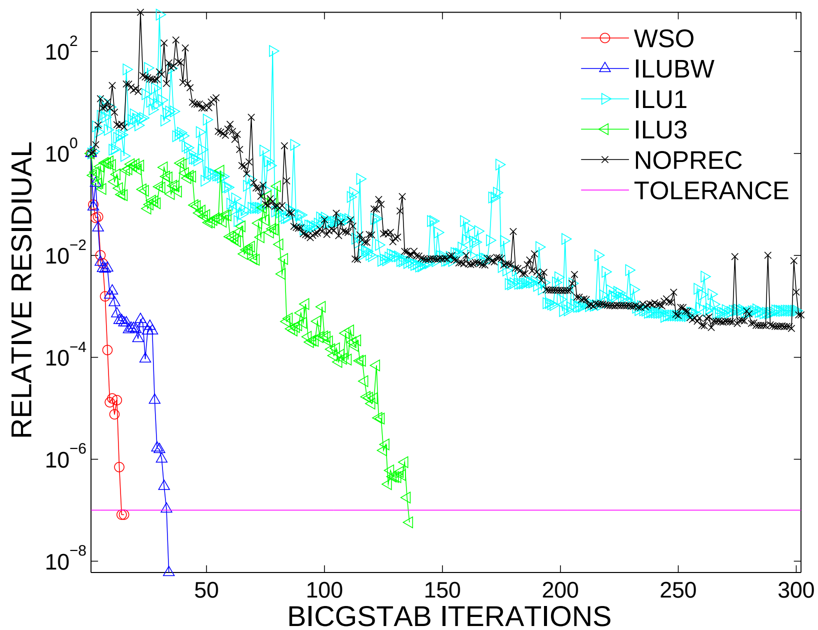


Bandwidth: 76

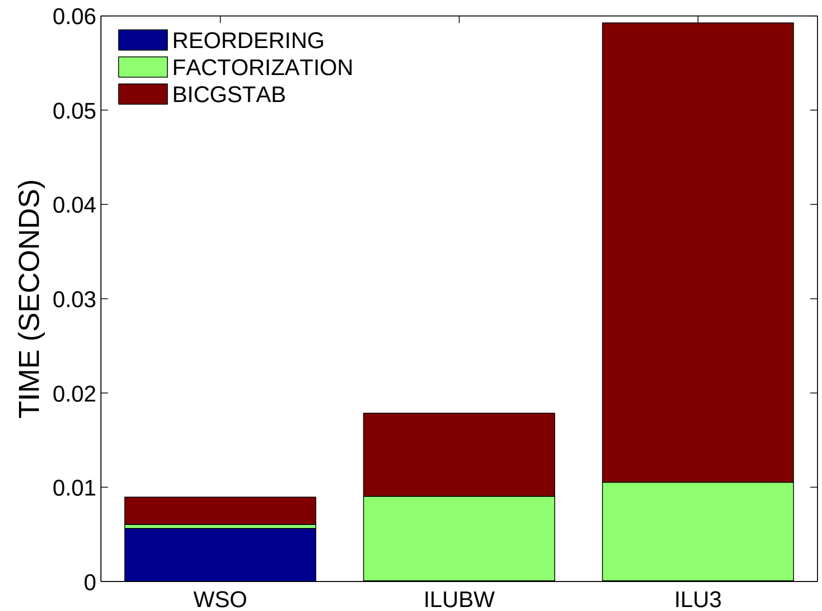
99% of matrix norm lies within a bandwidth of 19 after WSO

epb0 Results

Residual Plot



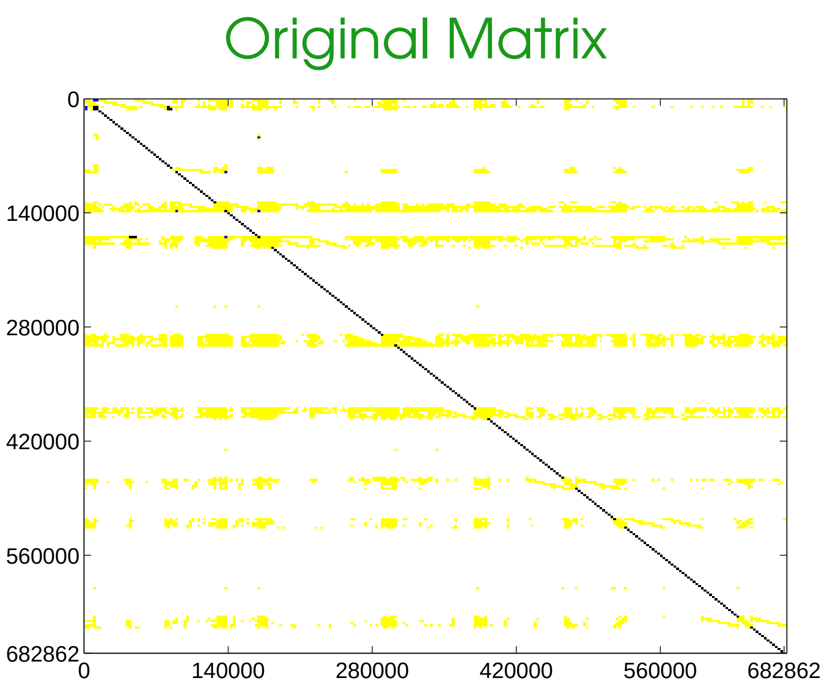
Runtime Performance



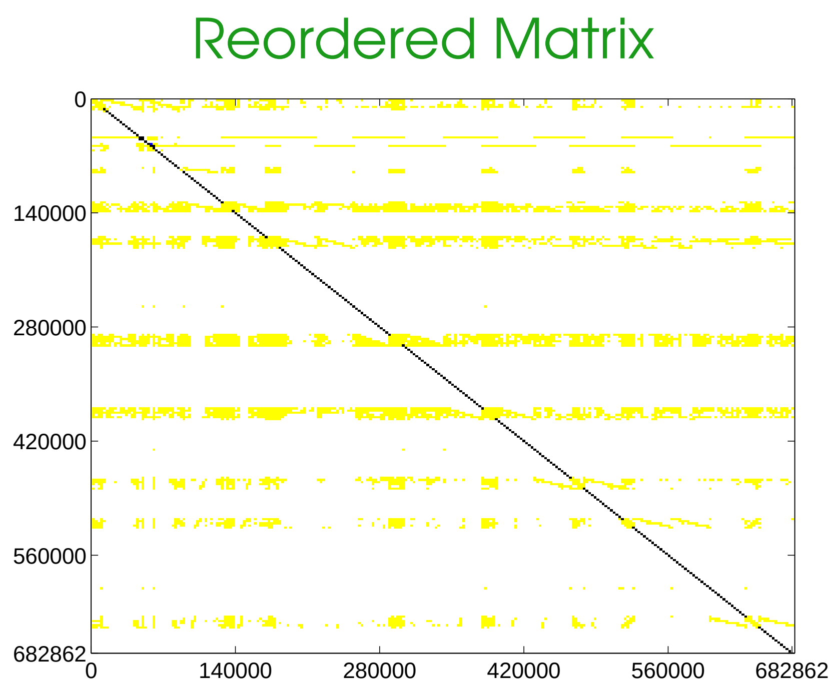
- BICGSTAB converges in 14 iterations with WSO preconditioner
  - No convergence after 300 iterations with no preconditioner or ILU with drop tolerance 10^{-1}

ASIC_680k Matrix

- Sandia, Xyce circuit simulation matrix (stripped)
  - 682862×682862, 2638997 non-zeros



Bandwidth: 1328578

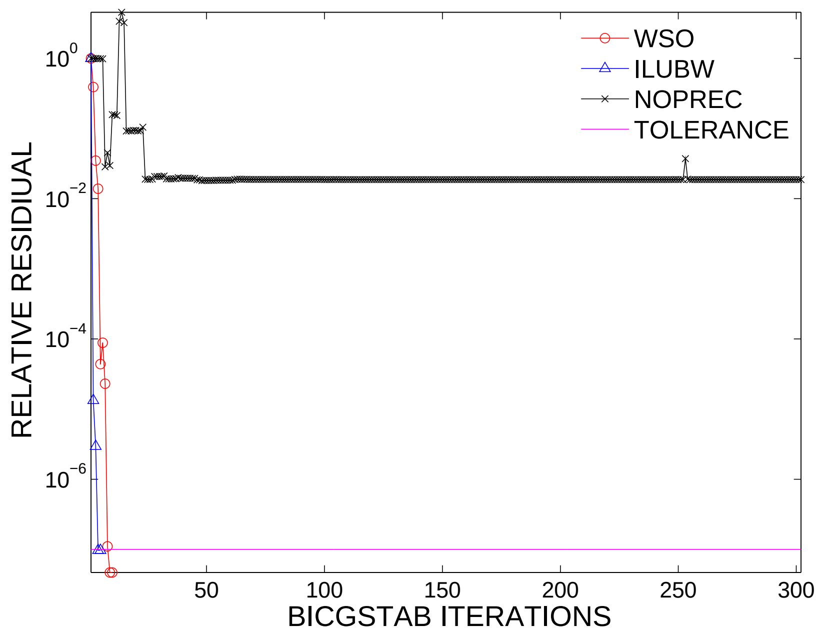


Bandwidth: 1328726

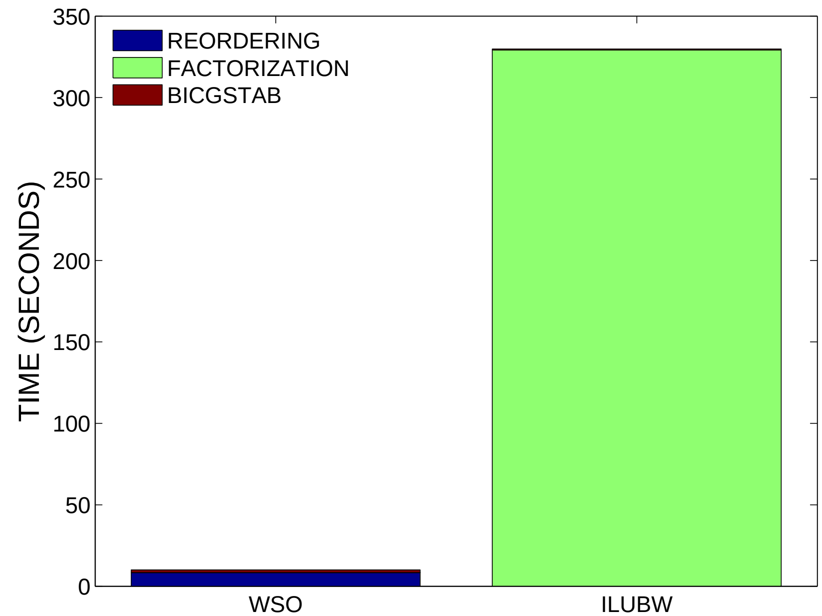
99% of matrix norm lies within a bandwidth of 5 after WSO

ASIC_680k Results

Residual Plot



Runtime Performance

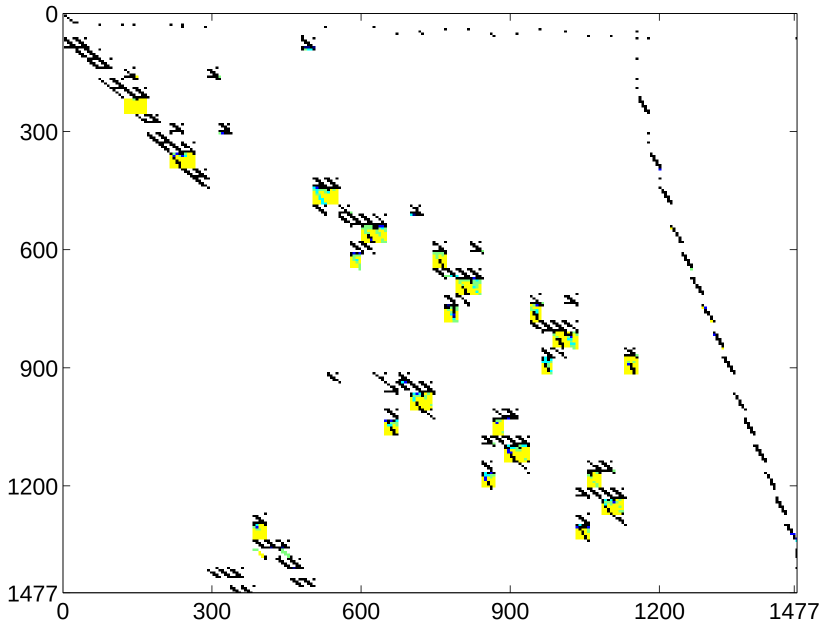


- BICGSTAB converges in 9 iterations with WSO preconditioner
  - ILU with fill-in equivalent to bandwith of WSO preconditioner converges faster (4 iterations), but factorization takes too much time
  - ILU factorization unsucessful for drop tolerance 10^{-1},10^{-3}
  - No convergence after 300 iterations with no preconditioner

lhr01 Matrix

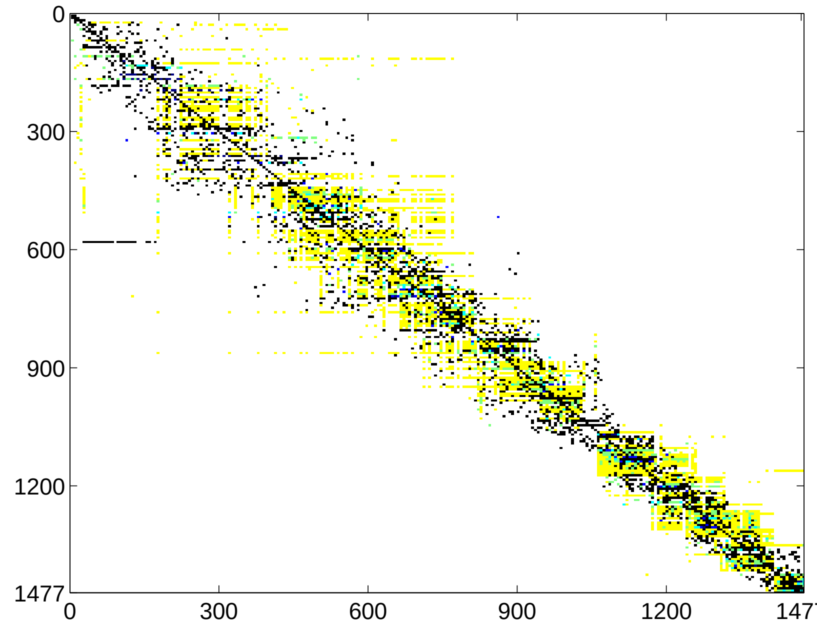
- Light hydrocarbon recovery
  - 14777×14777, 18427 non-zeros

Original Matrix



Bandwidth: 2537

Reordered Matrix

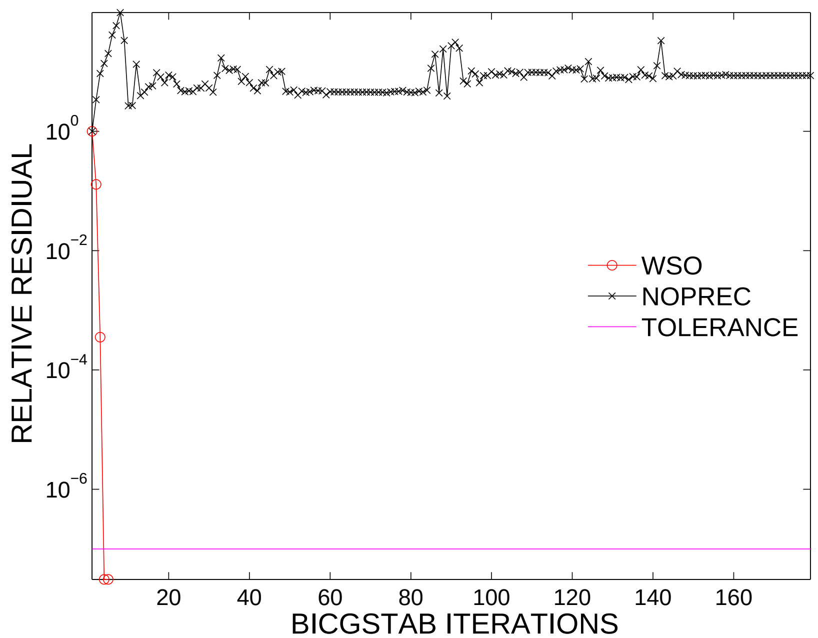


Bandwidth: 1341

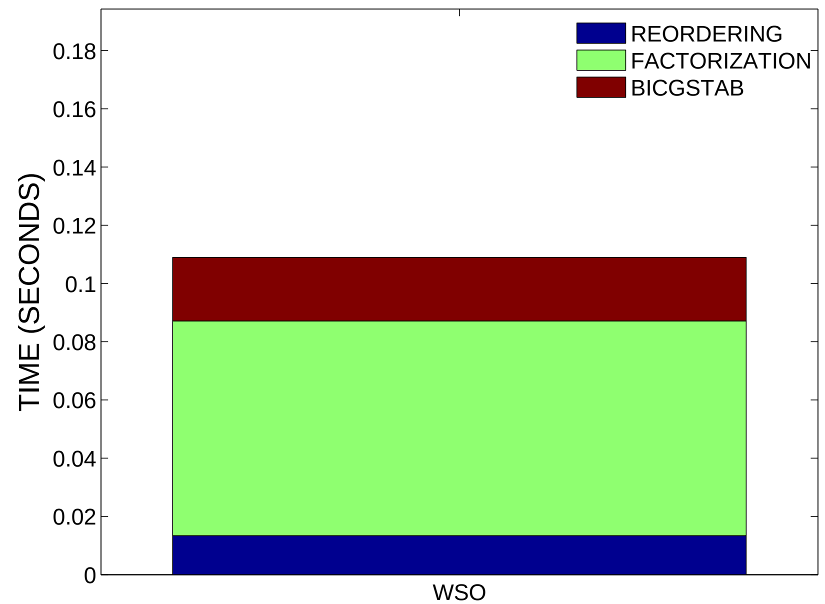
99% of matrix norm lies within a bandwidth of 601 after WSO

lhr01 Results

Residual Plot



Runtime Performance

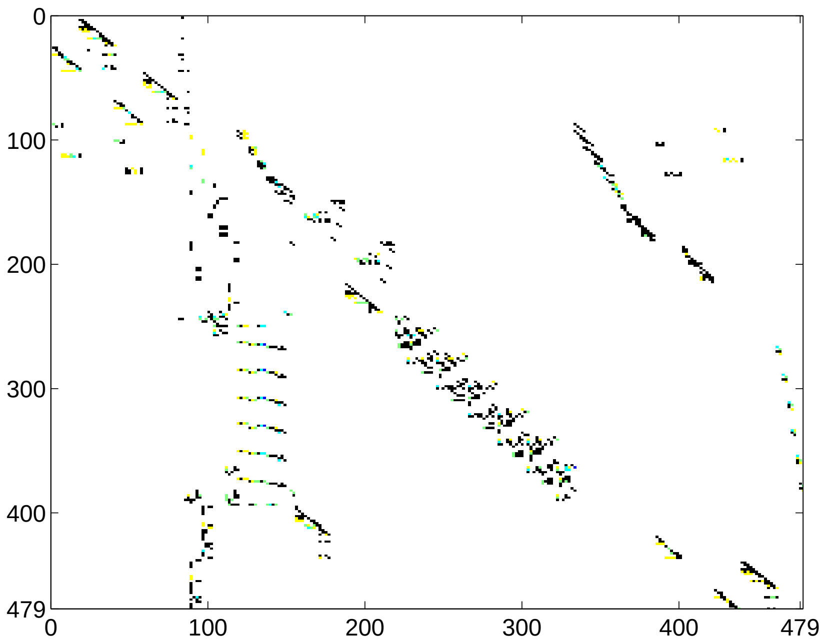


- BICGSTAB converges in only 4 iterations with WSO preconditioner!
  - No convergence with no preconditioner in 300 iterations
  - ILU factorization unsucessful for all variants

west0479 Matrix

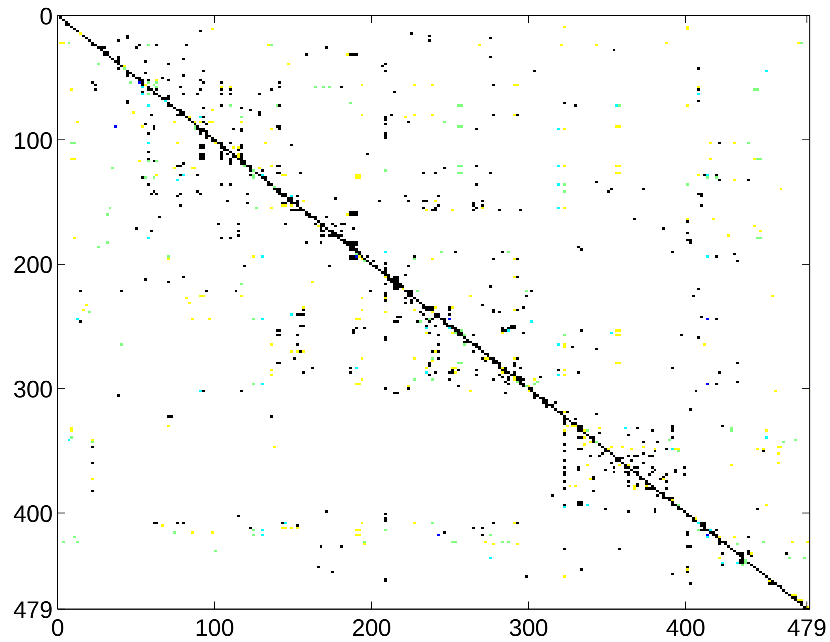
- U8 stage column section, all sections rigorous (chemical engineering)
  - 479×479, 1888 non-zeros
  - Known as a horror matrix

Original Matrix



Bandwidth: 726

Reordered Matrix

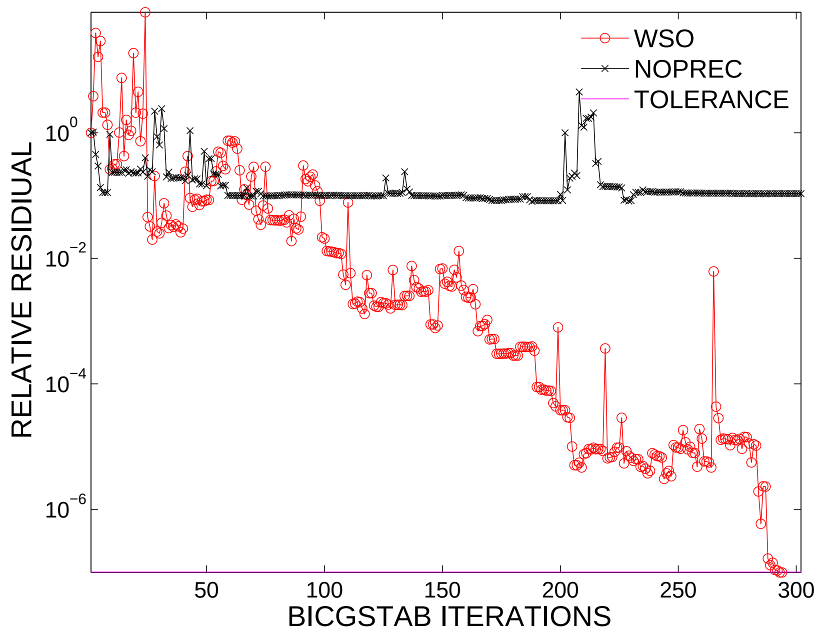


Bandwidth: 872

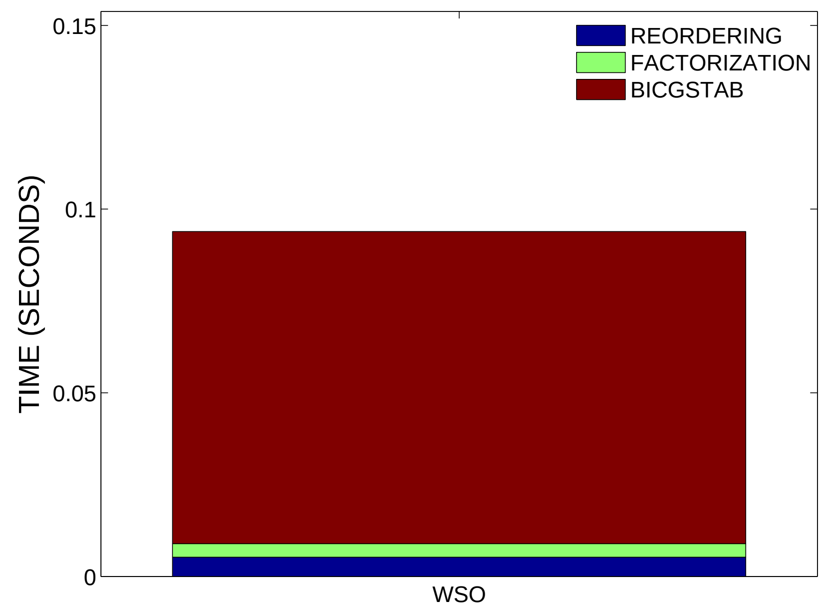
99% of matrix norm lies within a bandwidth of 221 after WSO

west0479 Results

Residual Plot



Runtime Performance

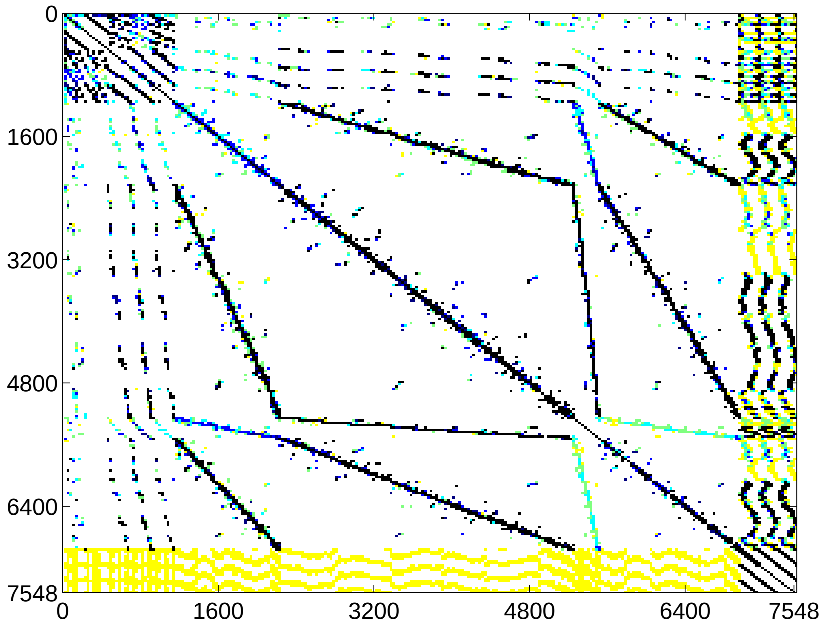


- BICGSTAB converges in 293 iterations with WSO preconditioner
  - No convergence with no preconditioner in 300 iterations
  - ILU factorization unsucessful for all variants

fp Matrix

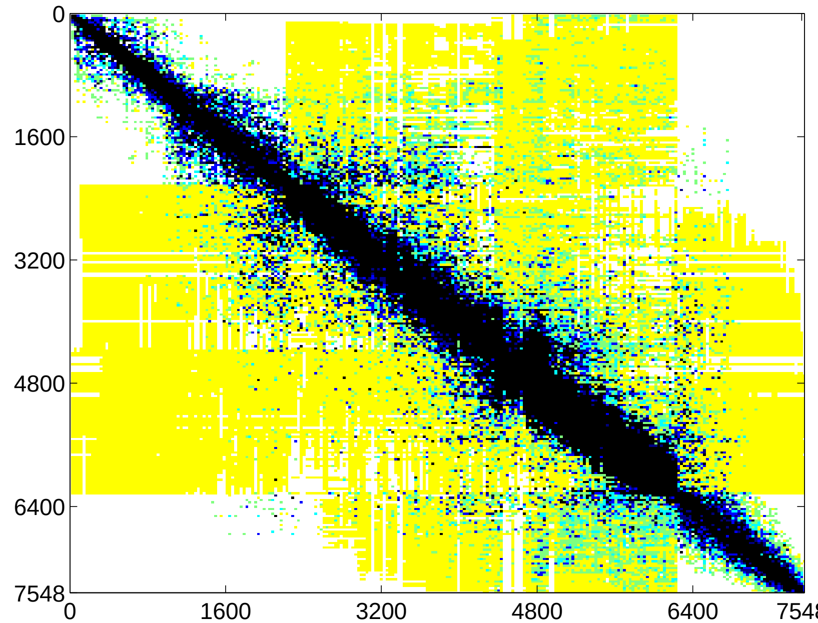
- 2-D Fokker Planck equation, electron dynamics in external field
  - 7548×7548, 834222 non-zeros

Original Matrix



Bandwidth: 15086

Reordered Matrix

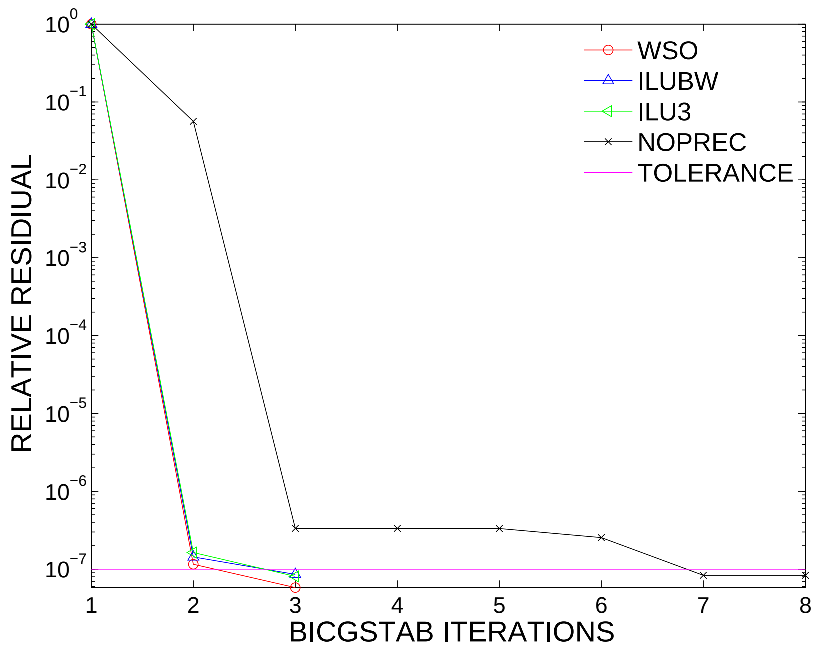


Bandwidth: 12368

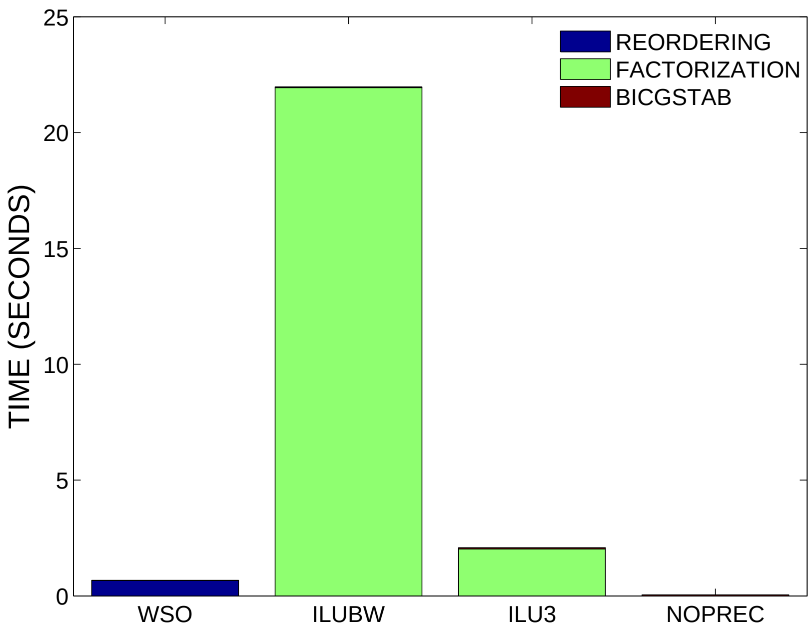
99% of matrix norm lies within a bandwidth of 5 after WSO

fp Results

Residual Plot



Runtime Performance

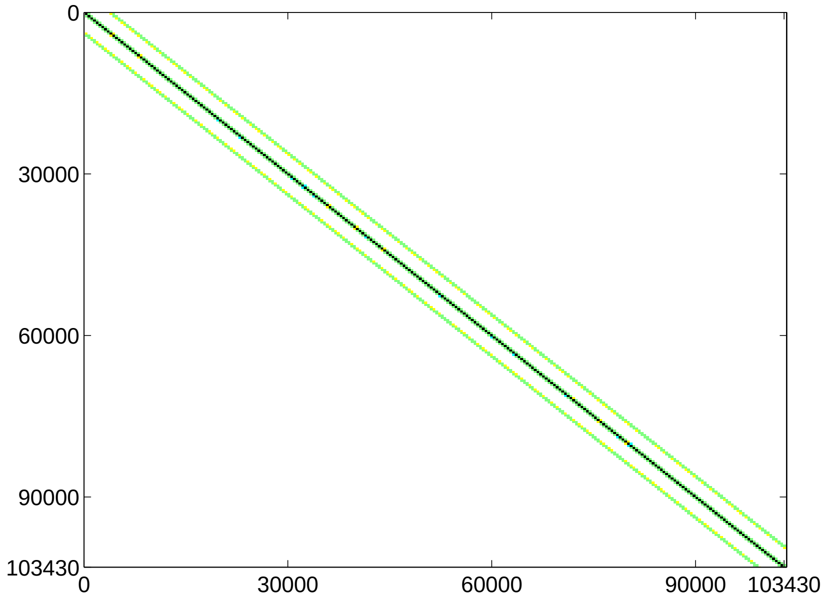


- BICGSTAB converges in 2 iterations with WSO preconditioner, as well as ILU with 10^{-3} drop tolerance, 2 fill-in
  - Convergence in 7 iterations with no preconditioner
  - Reordering, factorization take too much time as compared to preconditioner savings

matrix_9 Matrix

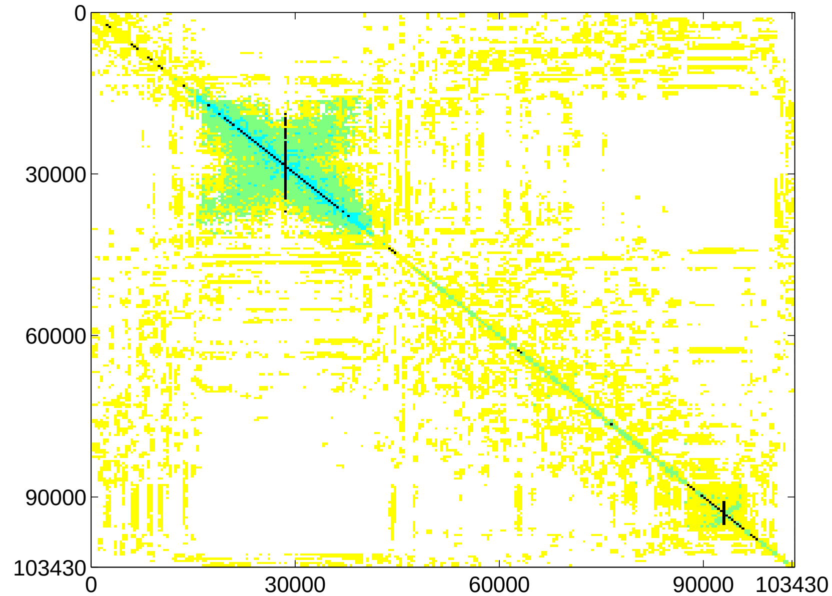
- Semiconductor device problem
  - 103430×103430, 1205518 non-zeros

Original Matrix



Bandwidth: 107410

Reordered Matrix

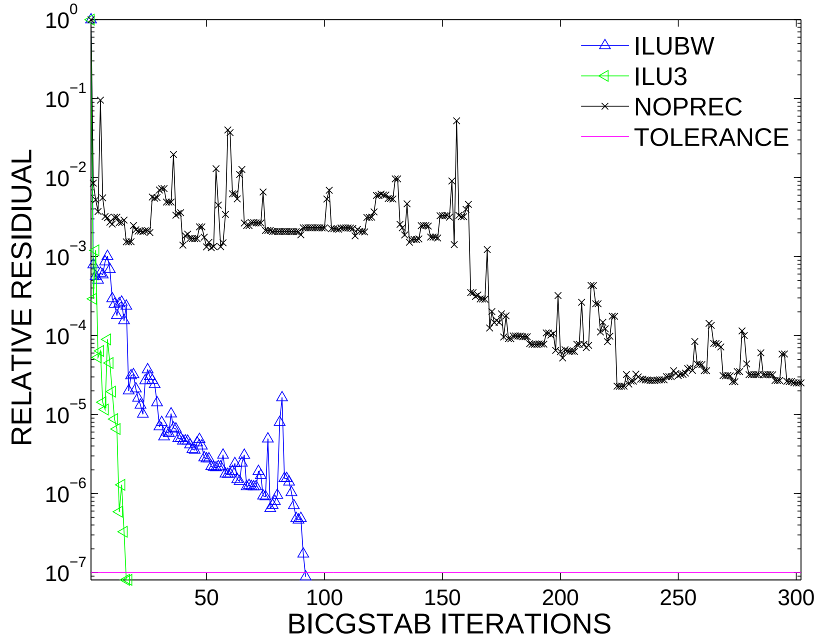


Bandwidth: 198951

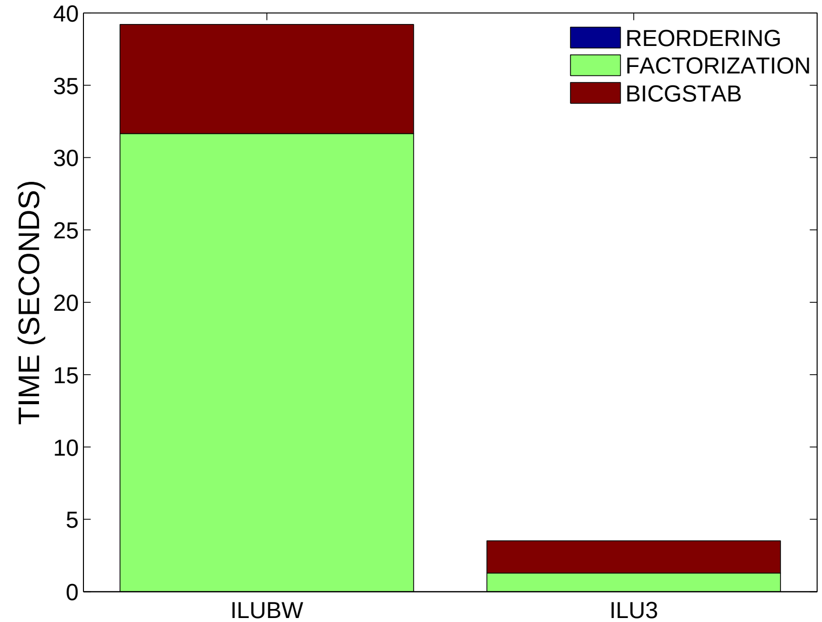
99% of matrix norm lies within a bandwidth of 10673 after WSO

fp Results

Residual Plot



Runtime Performance



- BICGSTAB runs out of memory with WSO preconditioner
  - BICGSTAB does not converge with no preconditioner
  - ILU with 10^{-3} fill-in tolerance converges in 16 iterations

Summary

	Preconditioner				
Matrix	None	ILUBW	ILU1	ILU3	WSO
epb0	> 0.019	0.018	> 0.029	0.059	0.009
	> 300	33	> 300	135	14
ASIC_680k	> 38.2	329.8	∞	∞	10.1
	> 300	4	∞	∞	9
lhr01	> 0.02	∞	∞	∞	0.11
	> 300	∞	∞	∞	4
west0479	> 0.009	∞	∞	∞	0.094
	> 300	∞	∞	∞	293
fp	0.05	21.97	∞	2.09	0.68
	7	2	∞	2	2
matrix_9	> 8.2	39.2	∞	3.5	∞
	> 300	91	∞	16	∞

Total runtime (reordering+factorization+bicgstab) is reported in seconds.

Number of iterations are reported on the row below.

Banded Preconditioners: Parallel Performance

Processors	bstd1.3M	astd650K
2	1	1
4	1.83	1.75
8	3.38	3.27
16	6.30	6.04
32	12.44	11.04
64	22.78	20.08
128	39.91	34.85

Scaling characteristics of banded preconditioned BiCG solver.

Concluding Remarks

- Banded preconditioners with suitable reordering techniques can be very powerful for diverse classes of applications.
- Banded preconditioners typically yield much better CPU performance and parallel performance.
- Due to memory reuse associated with dense kernels, they are well-suited to conventional chip multiprocessor architectures.

References

(1) E. Cuthill and J. McKee. Reducing the bandwidth of sparse symmetric matrices. In *In Proc. 24th Nat. Conf. ACM*, pages 157–172, 1969.

(2) M. Fiedler. Algebraic connectivity of graphs. *Czechoslovak Mathematical Journal*, 1973.

(3) Y. Saad. I ILUT: A dual threshold incomplete ILU factorization. *Numerical Linear Algebra with Applications*, 1:387–402, 1994.

(4) S. T. Barnard, A. Pothen, and H. Simon. A spectral algorithm for envelope reduction of sparse matrices. *Numerical Linear Algebra with Applications*, 2(4):317–334, 1995.

(5) N. P. Kruyt. A conjugate gradient method for the spectral partitioning of graphs. *Parallel Computing*, 22(11):1493–1502, 1996.