OF MINNESOTA TWIN CITIES

Multilevel preconditioning techniques with applications

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Introduction: Linear System Solvers



Long standing debate: direct vs. iterative

- Starting in the 1970's: huge progress of sparse direct solvers
- Iterative methods much older not designed for 'general systems'. Big push in the 1980s with help from 'preconditioning'
- ► General consensus now: Direct methods do well for 2-D problems and some specific applications [e.g., structures, ...]
- Usually too expensive for realistic 3-D problems
- Huge difference between 2-D and 3-D case
- > \rightarrow Do the test: Two Laplacean matrices of same dimension n = 122, 500.

First: on a 350×350 grid (2D);

Second: on a $50 \times 50 \times 49$ grid (3D)

Pattern of similar [much smaller] coefficient matrices



Background: Preconditioned iterative solvers

Two ingredients:

An accelerator: Conjugate gradient, BiCG, GMRES, BICGSTAB,... ['Krylov subspace methods']
A preconditioner: makes the system easier to solve by accelerator, e.g. Incomplete LU factorizations; SOR/SSOR; Multigrid, ...

One viewpoint:

Goal of accelerator: find best combination of basic iterates

► Goal of preconditioner: generate good basic iterates.. [Gauss-Seidel, ILU, ...]

Background: Incomplete LU (ILU) preconditioners



Common difficulties of ILUs: Often fail for indefinite problems Not too good for highly parallel environments

Past work: Algebraic Recursive Multilevel Solver (ARMS)

Reorder matrix using 'group-independent sets'. Result

$$PAP^T = \begin{pmatrix} B & F \\ E & C \end{pmatrix} =$$

Block factorize:



$$egin{pmatrix} m{B} & m{F} \\ m{E} & m{C} \end{pmatrix} \;=\; egin{pmatrix} m{L} & m{0} \\ m{E}m{U^{-1}} & m{I} \end{pmatrix} \; egin{pmatrix} m{U} & m{L^{-1}F} \\ m{0} & m{S} \end{pmatrix}$$

> $S = C - EB^{-1}F$ = Schur complement + dropping to reduce fill

Next step: treat the Schur complement recursively

Algebraic Recursive Multilevel Solver (ARMS)

Level *l* Factorization:

$$\begin{pmatrix} B_l & F_l \\ E_l & C_l \end{pmatrix} \approx \begin{pmatrix} L_l & 0 \\ E_l U_l^{-1} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & A_{l+1} \end{pmatrix} \begin{pmatrix} U_l & L_l^{-1} F_l \\ 0 & I \end{pmatrix}$$

> Perform above block factorization recursively on A_{l+1}

- > Blocks in B_l treated as sparse. Can be large or small.
- Algorithm is fully recursive
- > L-solve \sim restriction; U-solve \sim prolongation.
- Stability criterion in block independent sets algorithm
- ► A few similar ideas in the literature: Y. Notay '05, AMLI work (Axelson et al. 2000's), MLILU (Bank Wagner '99), ...

Group Independent Set reordering



Simple strategy: Level taversal until there are enough points to form a block. Reverse ordering. Start new block from non-visited node. Continue until all points are visited. Add criterion for rejecting "not sufficiently diagonally dominant rows."

Original matrix



Block size of 20



NONSYMMETRIC REORDERINGS

Enhancing robustness: One-sided permutations

Very useful techniques for matrices with extremely poor structure. Not as helpful in other cases.

Previous work:

- Benzi, Haws, Tuma '99 [compare various permutation algorithms in context of ILU]
- Duff '81 [Propose max. transversal algorithms. Basis of many other methods. Also Hopcroft & Karp '73, Duff '88]
- \bullet Olchowsky and Neumaier '96 maximize the product of diagonal entries \rightarrow LP problem
- Duff, Koster, '99 [propose various permutation algorithms. Also discuss preconditioners] Provide MC64

Two-sided permutations with diagonal dominance

Idea: ARMS + exploit nonsymmetric permutations

- > No particular structure or assumptions for B block
- > Permute rows * and * columns of A. Use two permutations P (rows) and Q (columns) to transform A into

$$PAQ^T = \begin{pmatrix} B & F \\ E & C \end{pmatrix}$$

P, Q is a pair of permutations (rows, columns) selected so that the B block has the 'most diagonally dominant' rows (after nonsym perm) and few nonzero elements (to reduce fill-in).

Multilevel framework

At the *l*-th level reorder matrix as shown above and then carry out the block factorization 'approximately'

$$P_l A_l Q_l^T = \begin{pmatrix} B_l & F_l \\ E_l & C_l \end{pmatrix} \approx \begin{pmatrix} L_l & 0 \\ E_l U_l^{-1} & I \end{pmatrix} \times \begin{pmatrix} U_l & L_l^{-1} F_l \\ 0 & A_{l+1} \end{pmatrix},$$

where

$$egin{aligned} B_l &pprox L_l U_l\ A_{l+1} &pprox C_l - (E_l U_l^{-1}) (L_l^{-1} F_l) \ . \end{aligned}$$

> As before the matrices $E_l U_l^{-1}$, $L_l^{-1} F_l$ or their approximations

$$G_l pprox E_l U_l^{-1} , \qquad W_l pprox L_l^{-1} F_l$$

need not be saved.

Interpretation in terms of complete pivoting

Rationale: Critical to have an accurate and well-conditioned *B* block [Bollhöfer, Bollhöfer-YS'04]

> Case when B is of dimension 1 \rightarrow a form of complete pivoting ILU. Procedure \sim block complete pivoting ILU

Matching sets:define B block. \mathcal{M} is a set of n_M pairs (p_i, q_i) where $n_M \leq n$ with $1 \leq p_i, q_i \leq n$ for $i = 1, \ldots, n_M$ and

 $p_i
eq p_j, ext{ for } i
eq j \qquad q_i
eq q_j, ext{ for } i
eq j$

> When $n_M = n \rightarrow$ (full) permutation pair (P, Q). A partial matching set can be easily completed into a full pair (P, Q) by a greedy approach.

Matching - preselection

Algorithm to find permutation consists of 3 phases.

(1) **Preselection:** to filter out poor rows (dd. criterion) and sort the selected rows.

(2) Matching: scan candidate entries in order given by preselection and accept them into the \mathcal{M} set, or reject them.

(3) Complete the matching set: into a complete pair of

permutations (greedy algorithm)

► Let
$$j(i) = \operatorname{argmax}_j |a_{ij}|$$
.

> Use the ratio $\gamma_i = rac{|a_{i,j(i)}|}{\|a_{i,:}\|_1}$ as a measure of diag. domin. of row i

Matching: Greedy algorithm

- > Simple algorithm: scan pairs (i_k, j_k) in the given order.
- > If i_k and j_k not already assigned, assign them to \mathcal{M} .



COMPLEX SHIFTING

Use of complex shifts

Several papers promoted the use of complex shifts [or very similar approaches] for Helmholtz

[1] X. Antoine – Private comm.

[2] Y.A. Erlangga, C.W. Oosterlee and C. Vuik, SIAM J. Sci. Comput., 27, pp. 1471-1492, 2006

[3] M. B. van Gijzen, Y. A. Erlangga, and C. Vuik, SIAM J. Sci. Comput., Vol. 29, pp. 1942-1958, 2007

[4] M. Magolu Monga Made, R. Beauwens, and G. Warzée, Comm. in Numer. Meth. in Engin., 16(11) (2000), pp. 801-817.

** Joint work with Daniel Osei-Kuffuor

> Illustration with an experiment: finite difference discretization of $-\Delta$ on a 25×20 grid.

- > Add a negative shift of -1 to resulting matrix.
- > Do an ILU factorization of A and plot eigs of $L^{-1}AU^{-1}$.
- Used LUINC from matlab no-pivoting and threshold = 0.1.





> Now plot eigs of $L^{-1}AU^{-1}$ where L, U are inc. LU factors of B = A + 0.25 * i



Explanation

Question:What if we do an exact
factorization [droptol = 0]? $\land (L^{-1}AU^{-1}) =$ $\land (L^{-1}AU^{-1}) =$ $\land [(A + \alpha iI)^{-1}A]$ $\land = \left\{ \frac{\lambda_j}{\lambda_j + i\alpha} \right\}$ \land Located on a circle –
with a cluster at one. \checkmark Figure shows situation
on the same example



Application to the Helmholtz equation

Started from collaboration with Riyad Kechroud, Azzeddine Soulaimani (ETS, Montreal), and Shiv Gowda: [Math. Comput. Simul., vol. 65., pp 303–321 (2004)]

Problem is set in the open domain Ω_e of \mathbb{R}^d

$$egin{array}{rcl} \Delta u+k^2u&=&f& ext{in}&\Omega\ u&=-u_{inc}& ext{on}&\Gamma\ or&rac{\partial u}{\partial n}=-rac{\partial u_{inc}}{\partial n}& ext{on}&\Gamma \end{array}$$

 $\lim_{r o\infty}r^{(d-1)/2}\,\left(rac{\partial u}{\partialec n}-iku
ight)=0$ Sommerfeld cond.

where: u the wave diffracted by Γ , f = source function = zero outside domain

Issue: non-reflective boundary conditions when making the domain finite.

- > Artificial boundary Γ_{art} added Need non-absorbing BCs.
- ► For high frequencies, linear systems become very 'indefinite' – [eigenvalues on both sides of the imaginary axis]
- Not very good for iterative methods

Application to the Helmholtz equation

Test Problem Soft obstacle = disk of radius $r_0 = 0.5m$. Incident plane wave with a wavelength λ ; propagates along the x-axis. 2nd order Bayliss-Turkel boundary conditions used on Γ_{art} , located at a distance $2r_0$ from obstacle. Discretization: isoparametric elements with 4 nodes. Analytic solution known.



Comparisons

▶ Test problem just seen. Mesh size $1/h = 160 \rightarrow n = 28,980, nnz = 260,280$



> Wavenumber varied - tests with ILUT

Preconditioner	k	$\frac{\lambda}{h}$	Iters.	Fill Factor	$ (LU)^{-1}e _2$
	4π	60	134	2.32	3.65e + 03
	8π	30	263	2.25	1.23e+04
	16π	15		-	-
	24π	10		-	-
	4π	60	267	2.24	2.29e + 03
	8π	30	255	2.23	4.73e+03
ILUT (uu-baseu)	16π	15	101	3.14	6.60e+02
	24π	10	100	3.92	2.89e+02
	4π	60	132	2.31	2.98e + 03
	8π	30	195	2.19	4.12e+03
ILUT ($ au$ -based)	16π	15	75	3.11	7.46e+02
	24π	10	86	3.85	2.73e+02

Wavenumber varied - tests with ARMS

Preconditioner	k	$\frac{\lambda}{h}$	Iters.	Fill Factor	$ (LU)^{-1}e _2$
	4π	60	120	3.50	7.48e + 03
ADMS (no chift)	8π	30	169	4.03	1.66e+04
	16π	15	282	4.50	2.44e+03
	24π	10		-	-
	4π	60	411	3.83	5.12e + 02
APMS (dd bacad)	8π	30	311	4.37	5.67e+02
Anivis (uu-baseu)	16π	15	187	4.71	3.92e+02
	24π	10	185	3.00	2.54e+02
	4π	60	106	3.45	7.56e + 03
ARMS ($ au$ -based)	8π	30	79	3.84	6.41e+03
	16π	15	39	3.95	1.26e+03
	24π	10	94	3.02	4.71e+02

SPARSE MATRIX COMPUTATIONS ON GPUS

Sparse matrix computations with GPUs **

GPUs Currently a very popular approach to: inexpensive supercomputing

> Can buy \sim one Teraflop peak power for around a little more tham \$1,000



** Joint work with Ruipeng Li

Tesla C1060

Tesla C 1060:



- * 240 cores
- * 4 GB memory
- * Peak rate: 930 GFLOPS [single]
- * Clock rate: 1.3 Ghz
- * 'Compute Capability': 1.3 [allows double precision]

Next: Fermi [48 cores/SM]— followed by [very recently]:

Kepler [note: 6 GHz (!), 192 cores/SMX, 4 SMXs in a GPC]

▶ Tesla K10 : 2 × (8 SMXs) \rightarrow 2 × 1,536 cores, 8GB Mem.; Peak: ≈ 4.6 TFLOPS]

The CUDA environment: The big picture

A host (CPU) and an attached device (GPU)

Typical program:



Sparse matrix computations on GPUs

Main issue in using GPUs for sparse computations:

• Huge performance degradation due to 'irregular sparsity'

	Matrix -name	N	NNZ		
Matrices:	FEM/Cantilever	62,451	4,007,383		
	Boeing/pwtk	217,918	11,634,424		

Performance of Mat-Vecs on NVIDIA Tesla C1060

	Sing	gle Pr	ecision	Double Precision				
Matrix	CSR	JAD	DIA	CSR	JAD	DIA		
FEM/Cantilever	9.4	10.8	25.7	7.5	5.0	13.4		
Boeing/pwtk	8.9	16.6	29.5	7.2	10.4	14.5		

Sparse Forward/Backward Sweeps

Next major ingredient of precond. Krylov subs. methods

ILU preconditioning operations require L/U solves: $x \leftarrow U^{-1}L^{-1}x$ Sequential outer loop.

for i=1:n for j=ia(i):ia(i+1) $x(i) = x(i) - a(j)^*x(ja(j))$ end end

Parallelism can be achieved with level scheduling:

- Group unknowns into levels
- Compute unknowns x(i) of same level simultaneously
- $ullet 1 \leq nlev \leq n$

ILU: Sparse Forward/Backward Sweeps

• Very poor performance [relative to CPU]

Matrix	N	CPU	GPL		
IVIALITA	IN	<u>M</u> flops	#lev	<u>M</u> flops	ble
Boeing/bcsstk36	23,052	627	4,457	43	era
FEM/Cantilever	62,451	653	2,397	168	nis
COP/CASEYK	696,665	394	273	142	
COP/CASEKU	208,340	373	272	115	rec

GPU Sparse Triangular Solve with Level Scheduling

- Very poor performance when #levs is large
- A few things can be done to reduce the # levels but perf. will remain poor

So...

Either GPUs must go...

or ILUs must go...

Alternatives to ILU preconditioners

What would be a good alternative?

Wish-list:

- A preconditioner requiring few 'irregular' computations
- Something that trades volume of computations for speed
- If possible something that is robust for indefinite case
- Good candidate:
- Multilevel Low-Rank (MLR) approximate inverse preconditioners

Related work:

• Work on HSS matrices [e.g., JIANLIN XIA, SHIVKUMAR CHAN-DRASEKARAN, MING GU, AND XIAOYE S. LI, *Fast algorithms for hierarchically semiseparable matrices*, Numerical Linear Algebra with Applications, 17 (2010), pp. 953–976.]

- Work on H-matrices [Hackbusch, ...]
- Work on 'balanced incomplete factorizations' (R. Bru et al.)
- Work on "sweeping preconditioners" by Engquist and Ying.
- Work on computing the diagonal of a matrix inverse [Jok Tang and YS (2010) ..]

Low-rank Multilevel Approximations

Starting point: symmetric matrix derived from a 5-point discretization of a 2-D Pb on $n_x \times n_y$ grid



Corresponding splitting on FD mesh:



 \blacktriangleright $A_{11} \in \mathbb{R}^{m imes m}$, $A_{22} \in \mathbb{R}^{(n-m) imes (n-m)}$

In the simplest case second matrix is:



Above splitting can be rewritten as

$$A = \underbrace{(A + EE^T)}_B - EE^T$$

Note: $B_1 := A_{11} + E_1 E_1^T$, $B_2 := A_{22} + E_2 E_2^T$.

Shermann-Morrison formula:

$$A^{-1} = B^{-1} + B^{-1}E(\overbrace{I - E^{T}B^{-1}E}^{X})^{-1}E^{T}B^{-1}$$

$$A^{-1} = B^{-1} + (B^{-1}E)X^{-1}(B^{-1}E)^{T}$$
$$X = I - E^{T}B^{-1}E$$

$$\blacktriangleright$$
 Note: $E \in \mathbb{R}^{n imes n_x}$, $X \in \mathbb{R}^{n_x imes n_x}$

> n_x = number of points in separator [$O(n^{1/2})$ for 2-D mesh, $O(n^{2/3})$ for 3-D mesh]

• Use in a recursive framework

• Similar idea was used for computing the diagonal of the inverse [J. Tang YS '10]

First thought : approximate X and exploit recursivity $B^{-1}[v + E\tilde{X}^{-1}E^{T}B^{-1}v].$

However wont work : cost explodes with # levels

> Alternative: lowrank approx. for $B^{-1}E$

$$B^{-1}E pprox U_k V_k^T, egin{array}{c} U_k \in \mathbb{R}^{n imes k}, \ V_k \in \mathbb{R}^{n_x imes k}, \ V_k \in \mathbb{R}^{n_x imes k}, \end{array}$$

. . 1

Multilevel Low-Rank (MLR) algorithm

> Method: Use lowrank approx. for $B^{-1}E$

$$B^{-1}E pprox U_k V_k^T, egin{array}{c} U_k \in \mathbb{R}^{n imes k}, \ V_k \in \mathbb{R}^{n_x imes k}, \end{array}$$

Replace $B^{-1}E$ by $U_kV_k^T$ in $X = I - (E^TB^{-1})E$: $X \approx G_k = I - V_kU_k^TE, \quad (\in \mathbb{R}^{n_x \times n_x}) \quad \text{Leads to } \dots$

$$P^{\text{reconditionel}} M^{-1} = B^{-1} + U_k H_k U_k^T, \quad H_k = V_k^T G_k^{-1} V_k$$

$$\text{Use recursivity}$$

► We can show :

$$egin{array}{ll} H_k = (I - U_k^T E V_k)^{-1} & ext{and} \ H_k^T = H_k & \end{array}$$

Recursive multilevel framework

•
$$A_i = B_i + E_i E_i^T$$
, $B_i \equiv \begin{pmatrix} B_{i_1} \\ B_{i_2} \end{pmatrix}$.

- Next level, set $A_{i_1}\equiv B_{i_1}$ and $A_{i_2}\equiv B_{i_2}$
- Repeat on A_{i_1}, A_{i_2}
- Last level, factor A_i (IC, ILU)
- Binary tree structure:



Generalization: Domain Decomposition framework

Domain partitioned into 2 domains with an edge separator



Matrix can be permuted to:

$$PAP^T = egin{pmatrix} \hat{B}_1 & \hat{F}_1 & \ \hat{F}_1^T & C_1 & -X \ \hline & \hat{B}_2 & \hat{F}_2 \ & -X^T & \hat{F}_2^T & C_2 \ \end{pmatrix}$$

Interface nodes in each domain are listed last.

Each matrix \hat{B}_i is of size $n_i \times n_i$ (interior var.) and the matrix C_i is of size $m_i \times m_i$ (interface var.)

Let:
$$E_{\alpha} = \begin{pmatrix} 0 \\ \alpha I \\ 0 \\ \frac{X^T}{\alpha} \end{pmatrix}$$
 then we have:

$$egin{aligned} m{P}m{A}m{P}^T &= egin{pmatrix} m{B}_1 \ & m{B}_2 \end{pmatrix} - m{E}m{E}^T & ext{with} & m{B}_i &= egin{pmatrix} m{\hat{B}}_i & m{\hat{F}}_1 \ m{\hat{F}}_i^T & m{C}_i + m{D}_i \end{pmatrix} \ & ext{and} & egin{pmatrix} m{D}_1 &= m{lpha}^2m{I} \ m{D}_2 &= m{rac{1}{lpha^2}}X^TX \end{aligned}$$

- > α used for balancing
- > Better results when using diagonals instead of αI

EXPERIMENTS

Experimental setting

- Hardware: Intel Xeon X5675 processor (12 MB Cache, 3.06 GHz, 6-core)
- C/C++; Intel Math Kernel Library (MKL, version 10.2)
- ullet Stop when: $\|r_i\| \leq 10^{-8} \|r_0\|\,$ or its exceeds 500
- Model Problems in 2-D/3-D:

$$-\Delta u - cu = g ext{ in } \Omega ext{ + B.C.}$$

- ullet 2-D: $g(x,y)=-\left(x^2+y^2+c
 ight)e^{xy};\quad \Omega=\left(0,1
 ight)^3.$
- 3-D: $g(x,y,z) = -6 c \left(x^2 + y^2 + z^2\right); \quad \Omega = \left(0,1\right)^3.$
- F.D. Differences discret.

Symmetric indefinite cases

- c > 0 in $-\Delta u cu$; i.e., $-\Delta$ shifted by -sI.
- \bullet 2D case: s=0.01, 3D case: s=0.05
- MLR + GMRES(40) compared to ILDLT + GMRES(40)
- 2-D problems: #lev= 4, rank= 5, 7, 7
- 3-D problems: #lev= 5, rank= 5, 7, 7
- ILDLT failed for most cases
- Difficulties in MLR: #lev cannot be large, [no convergence]
- inefficient factorization at the last level (memory, CPU time)

Grid	IL	DLT-GN	/ RE	S	MLR-GMRES				
	fill	p-t	its	i-t	fill	p-t	its	i-t	
256^{2}	6.5	0.16	F		6.0	0.39	84	0.30	
512^{2}	8.4	1.25	F		8.2	2.24	246	6.03	
1024^{2}	10.3	10.09	F		9.0	15.05	F		
$32^2 imes 64$	5.6	0.25	61	0.38	5.4	0.98	62	0.22	
64 ³	7.0	1.33	F		6.6	6.43	224	5.43	
128^{3}	8.8	15.35	F		6.5	28.08	F		

General symmetric matrices - Test matrices

MATRIX	Ν	NNZ	SPD	DESCRIPTION
Andrews/Andrews	60,000	760,154	yes	computer graphics pb.
Williams/cant	62,451	4,007,383	yes	FEM cantilever
UTEP/Dubcova2	65,025	1,030,225	yes	2-D/3-D PDE pb.
Rothberg/cfd1	70,656	1,825,580	yes	CFD pb.
Schmid/thermal1	82,654	574,458	yes	thermal pb.
Rothberg/cfd2	123,440	3,085,406	yes	CFD pb.
Schmid/thermal2	1,228,045	8,580,313	yes	thermal pb.
Cote/vibrobox	12,328	301,700	no	vibroacoustic pb.
Cunningham/qa8fk	66,127	1,660,579	no	3-D acoustics pb.
Koutsovasilis/F2	71,505	5,294,285	no	structural pb.

Generalization of MLR via DD

- **DD:** PartGraphRecursive **from METIS**
- balancing with diagonals
- higher ranks used in two problems (cant and vibrobox)
- Show SPD cases first then non-SPD

MATRIX	ICT/ILDLT					MLR-CG/GMRES						
	fill	p-t	its	i-t	k	lev	fill	p-t	its	i-t		
Andrews	2.6	0.44	32	0.16	2	6	2.3	1.38	27	0.08		
cant	4.3	2.47	F	19.01	10	5	4.3	7.89	253	5.30		
Dubcova2	1.4	0.14	42	0.21	4	4	1.5	0.60	47	0.09		
cfd1	2.8	0.56	314	3.42	5	5	2.3	3.61	244	1.45		
thermal1	3.1	0.15	108	0.51	2	5	3.2	0.69	109	0.33		
cfd2	3.6	1.14	F	12.27	5	4	3.1	4.70	312	4.70		
thermal2	5.3	4.11	148	20.45	5	5	5.4	15.15	178	14.96		

MATRIX	ICT/ILDLT					MLR-CG/GMRES					
	fill	p-t	its	i-t	k	lev	fill	p-t	its	i-t	
vibrobox	3.3	0.19	F	1.06	10	4	3.0	0.45	183	0.22	
qa8fk	1.8	0.58	56	0.60	2	8	1.6	2.33	75	0.36	
F2	2.3	1.37	F	13.94	5	5	2.5	4.17	371	7.29	

Conclusion

General rule: ILU-based preconditioners not meant to replace tailored preconditioners. Can be very useful as parts of other techniques.

Robustness can be improved with nonsymmetric permutations and the inclusion of complex shifting strategies

► GPUs for irregular sparse matrix computations: Much remains to be done both in hardware and in algorithms/software. In general, some of the old methods will see a come-back

More interestingly: new methods such as low-rank approximation methods will be developed