

Preconditioning symmetric and highly indefinite problems

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Indefinite Preconditioning



- Applications Problems
- Advances using matchings
- Advanced Symmetric Incomplete Factorizations
 - Shifted systems
 - Numerical results





Applications Problems

- Advances using matchings
- 3 Advanced Symmetric Incomplete Factorizations
- 4 Shifted systems
- 5 Numerical results
- Conclusions



(-1)

Model describes electronic transport properties of disordered quantum systems

Discretization approach: periodic uniform grid in a 3D cube

- symmetric eigenvalue problem $Ax = \lambda x$ in 3D
- λ quantum mechanical energy levels
- x quantum mechanical wave functions

$$arepsilon_{ijk} x_{ijk} - \sum_{|p-i|=1, |q-j|=1, |r-j|=1} x_{pqr} = \lambda x_{ijk}$$

$$arepsilon_{\textit{ijk}} \in [-\omega/2, \omega/2]$$
 i.i.d.

- ω refers to the disorder strength
- $\omega \approx \omega_c = 16.5$ critical behaviour
- $\omega \ll \omega_c \rightarrow$ wave function is fluctuating from site to site
- $\omega \gg \omega_c \rightarrow$ wave function is localized



wave function distribution

$$\omega = 14.5$$
 $\omega = 16.5$ $\omega = 18.5$





Challenges

- physically sensible resultats require large scale simulation, $n = m^3$ (e.g. m = 100, 200, ...)
- physically interesting: eigenvectors at $\lambda = 0$ where $\omega = \omega_c$
- solution approach based on preconditioned eigenvalue solver (Jacobi-Davidson)
- A is symmetric and highly indefinite



• a symmetry-preserving preconditioner for A is desirable



Helmholtz equations

$$-\Delta u - k^{2}u = b \text{ in } \Omega$$

$$k = \frac{2\pi f}{c}, \quad f \text{ frequency, } c \text{ speed of sound}$$

Boundary conditions:

- $\begin{array}{ll} u = g_1 \text{ on } \Gamma_1, & \frac{\partial u}{\partial \nu} = g_2 \text{ on } \Gamma_2, & \frac{\partial u}{\partial \nu} + iku = 0 \text{ on } \Gamma_3. \\ \text{Dirichlet} & \text{Neumann} & \text{Sommerfeld} \end{array}$
- Complex symmetric (Sommerfeld radiation b.c.!)
- Highly indefinite, discretization with mesh size h requires

$$kh \leqslant \frac{2\pi}{L}$$

to have L grid points per wave length.



3D Seismic Imaging Problem



- Helmholtz equation in a cube
- point source in the middle of the upper boundary
- Sommerfeld b.c.
- irregular velocity distribution



Time-harmonic Maxwell equations

First order formulation

$$(+i\omega\varepsilon \mathbf{E} - \operatorname{curl}(\mathbf{H}) = -\sigma \mathbf{E} - J_{\mathbf{E}},$$

 $(-i\omega\mu\mathbf{H} - \operatorname{curl}(\mathbf{E}) = 0,$

- boundary conditions on $\partial \Omega = \Gamma_a \cup \Gamma_m$
- perfect electric conductor condition $\boldsymbol{n} \times \boldsymbol{E} = 0$ on Γ_m
- Silver-Müller absorbing condition $\mathcal{L}(\boldsymbol{E}, \boldsymbol{H}) = \mathcal{L}(\boldsymbol{E}^{inc}, \boldsymbol{H}^{inc})$ on Γ_a
- discretization leads to complex-symmetric system Ax = b, where

$$A = \mathbf{i}\omega \begin{pmatrix} M_{\varepsilon} & 0\\ 0 & -M_{\mu} \end{pmatrix} + \begin{pmatrix} C_{11} + M_{\sigma} & -C_{12}\\ -C_{12}^{\tau} & -C_{22} \end{pmatrix}$$



Applications Problems

Advances using matchings

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Example





Example



Associated graph



Example



- Associated graph
- (Perfect) matching. (At most) one edge for each row/column



Example



• (Perfect) matching. (At most) one edge for each row/column



Example



Associated permutation



Example



Permuted matrix



Maximum Weight Matchings

Find matching such that $\prod_{i=1}^{n} |a_{\pi(i),i}|$ is maximized

• reformulation: minimize
$$\sum_{i=1}^{n} |c_{\pi(i),i}|$$
, where
 $c_{ij} = \begin{cases} \max_{j} |a_{ij}| - \log |a_{ij}| & a_{ij} \neq 0 \\ \infty & \text{otherwise} \end{cases}$

 known linear-sum assignment problem, can be solved by sparse variant of Kuhn-Munkres algorithm

• dense case [Olschowka,Neumeier'96], sparse case [Duff,Koster'99]



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 known linear-sum assignment problem, can be solved by sparse variant of Kuhn-Munkres algorithm

- solution leads to two vectors $(u_i)_i$, $(v_j)_j$ such that
 - $u_i + u_j \leq c_{ij}$ and if (i, j) are part of the matching $u_i + u_j = c_{ij}$
 - diagonal scalings D_r = dgl (e^{u_i})_i, D_c = dgl (e^{v_i} / max_k |a_{jk}|)_j

• dense case [Olschowka,Neumeier'96], sparse case [Duff,Koster'99]



Find matching such that $\prod_{i=1}^{n} |a_{\pi(i),i}|$ is maximized

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• solution leads to two vectors $(u_i)_i$, $(v_j)_j$ such that

• $u_i + u_j \leq c_{ij}$ and if (i, j) are part of the matching $u_i + u_j = c_{ij}$

- diagonal scalings D_r = dgl (e^{u_i})_i, D_c = dgl (e^{v_i} / max_k |a_{jk}|)_j
- yields permutation Π and diagonal scalings D_r and D_c .

 $A \rightarrow \Pi^{\top} D_r A D_c$ such that $|a_{ii}| = 1, |a_{ij}| \leq 1$ for all i, j

• dense case [Olschowka,Neumeier'96], sparse case [Duff,Koster'99]

Technische

Universität Braunschweig



To download ILUPACK, visit http://ilupack.tu-bs.de

```
≫ % add ILUPACK MEX interface drivers
>> addpath 'ilupack/'
≫ % load sample matrix
\gg load west0479; A=west0479;
≫ % display matrix
\gg figure(1); spy(A)
>> % reorder and rescale matrix using maximum weight matchings
>> [pl,pr,Dl,Dr]=mwm(A); M=Dl*A(pl,pr)*Dr;
>> % show improved block diagonal part
>> full(M(1:10,1:10))
>> % display reordered matrix
\gg figure (2); spy (M)
>> % maxmimum weight matching + Metis nested dissection
>> [pl,pr,Dl,Dr]=mwmmetisn(A); M=Dl*A(pl,pr)*Dr;
≫ figure(3); spy(M)
```



Symmetric matchings [Duff,Gilbert'02], [Duff,Pralet'04]





Symmetric matchings [Duff,Gilbert'02], [Duff,Pralet'04]

Decompose permutation as product of cycles





Basic Idea of Symmetric Matchings

Symmetric matchings [Duff,Gilbert'02], [Duff,Pralet'04]

- Decompose permutation as product of cycles
- each cycle is associated with a diagonal block, pivots stay there





Symmetric matchings [Duff,Gilbert'02], [Duff,Pralet'04]

- Decompose permutation as product of cycles
- each cycle is associated with a diagonal block, pivots stay there
- pivots stay inside if related SYMMETRIC permutation is applied





Basic Idea of Symmetric Matchings

- break up cycles into pairs of 2-cycles and group them together
 - various strategies of breaking up the cycles [Duff,Gilbert'02],[Duff,Pralet'04],[Schenk,Hagemann'04]
 - long cycles rarely show up in practice [Duff,Pralet'04]
- Scaling replaced by symmetric scaling $D = (D_c D_r)^{1/2}$ ensures that entries are still at most 1 in modulus

Example







Original matrix





1. step. Apply symmetric maximum weight matching





2. step. Compress 2 \times 2 blocks





3. step. Reorder the system with some reordering (AMD, METIS, RCM,...)





4. step. Expand 2×2 blocks



- >> % create Anderson model matrix \gg m=50; w=0.1; A=anderson(m,w); \gg % reorder and rescale matrix using symmetric maximum weight ≫ % matchings + RCM \gg [p,D]=symmwmrcm(A); >> % show improved block diagonal part >> M=D*A(p,p)*D; full(M(1:10,1:10)) >> % display reordered matrix \gg figure(1); spy(A(p,p)) \gg % compare with the scalar variant by adding a diagonal shift >> [p,D]=symmwmrcm(A+5*norm(A,1)*speye(m^3)); \gg figure(2); spy(A(p,p)) >> % reorder and rescale now with Metis nested dissection >> [p,D]=symmwmmetisn(A);figure(1);spy(A(p,p)) >> [p,D]=symmwmmetisn(A+5*norm(A,1)*speye(m^3));
- \gg figure(2); spy(A(p,p))



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 $A \to \Pi^\top DAD\Pi$



$\textbf{A} \rightarrow \boldsymbol{\Pi}^\top \textbf{D} \textbf{A} \textbf{D} \boldsymbol{\Pi}$

• Select 1 \times 1 and 2 \times 2 block diagonal pivots



 $A \to \Pi^{\top} DAD\Pi$

- Select 1 \times 1 and 2 \times 2 block diagonal pivots
- postpone updates if "small" pivots occur

$$A \longrightarrow \left(\begin{array}{cc} A_{\mathcal{F}\mathcal{F}} & A_{\mathcal{F}\mathcal{C}} \\ A_{\mathcal{C}\mathcal{F}} & A_{\mathcal{C}\mathcal{C}} \end{array} \right)$$



 $A \to \Pi^{\top} DAD\Pi$

- Select 1 \times 1 and 2 \times 2 block diagonal pivots
- postpone updates if "small" pivots occur

$$\mathsf{A} \longrightarrow \left(\begin{array}{cc} \mathsf{A}_{\mathcal{F}\mathcal{F}} & \mathsf{A}_{\mathcal{F}\mathcal{C}} \\ \mathsf{A}_{\mathcal{C}\mathcal{F}} & \mathsf{A}_{\mathcal{C}\mathcal{C}} \end{array} \right)$$

approximate block decomposition

$$\begin{pmatrix} A_{\mathcal{F}\mathcal{F}} & A_{\mathcal{F}\mathcal{C}} \\ A_{\mathcal{C}\mathcal{F}} & A_{\mathcal{C}\mathcal{C}} \end{pmatrix} = \begin{pmatrix} L_{\mathcal{F}\mathcal{F}} & 0 \\ L_{\mathcal{C}\mathcal{F}} & I \end{pmatrix} \begin{pmatrix} D_{\mathcal{F}\mathcal{F}} & 0 \\ 0 & S_{\mathcal{C}\mathcal{C}} \end{pmatrix} \begin{pmatrix} L_{\mathcal{F}\mathcal{F}}^{\top} & L_{\mathcal{C}\mathcal{F}}^{\top} \\ 0 & I \end{pmatrix} + E$$

$$\underbrace{\left(\bigsqcup_{L} & \bigcup_{L} & \bigcup_{L}$$



 $A \to \Pi^{\top} DAD\Pi$

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$$\underbrace{\left(\bigsqcup_{L} \right)}_{L} \underbrace{\left(\bigsqcup_{L} \right)}_{L} \underbrace{\left(\bigsqcup_{L} \right)}_{D} \underbrace{\left(\bigsqcup_{L} \right)}_{L^{\top}} \underbrace{\left(\bigsqcup_{L} \right)}_{L^{$$

Multilevel approach: analogous principle recursively applied to S_{CC} , i.e., repeat

- matching and reordering
- postpone "bad" pivots while computing ILU

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Indefinite Preconditioning



Matchings and Multilevel ILU

Several codes using unsymmetric/symmetric matchings, e.g.,

- PARDISO [Schenk, Gärtner]
- MUMPS [Amestoy et al.]
- HSL library [Duff, Scott, Reid, ...]
- ILUPACK [Bo. et al.]

Many approaches to multilevel ILU, e.g.,

- (p)ARMS [Saad et al.]
- MRILU [Wubs et al.]
- ILUPACK [Bo. et al.]

Common believe

$$A \to \left(\begin{array}{cc} A_{\mathcal{FF}} & A_{\mathcal{FC}} \\ A_{\mathcal{CF}} & A_{\mathcal{CC}} \end{array}\right)$$

such that $A_{\mathcal{FF}}$ is easy to factorize, (independent sets, (block) diagonal dominance, ...)



Block diagonal dominance

Example Anderson model

Rows that satisfy $\sum_{j:j \neq i} |a_{ij}| / |a_{ii}| \le 0.9$: ω 14.0 $\omega_c = 16.5$ 21.0

% 4.8% 19.2% 36.5%

Now scratch out one out of seven rows/columns to make $A_{\mathcal{FF}}$ more diagonally dominant.

Rows of A_{FF} that satisfy $\sum_{i:i\neq i} |a_{ij}|/|a_{ii}| \leq 0.9$:

 ω 14.0 $\omega_c = 16.5$ 21.0 % 20.6% 32.7% 47.1%



Block diagonal dominance

Example Anderson model

Rows that satisfy $\sum_{j:j \neq i} |a_{ij}| / |a_{ij}| \leqslant 0.9$: ω 14.0 $\omega_c = 16.5$ 21.0 $\omega = 10.0^{\circ}$ 26 5%

% 4.8% 19.2% 36.5%

Now scratch out one out of seven rows/columns to make $A_{\mathcal{F}\mathcal{F}}$ more diagonally dominant.

Rows of A_{FF} that satisfy $\sum_{i:i\neq i} |a_{ij}|/|a_{ii}| \leq 0.9$:

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Remark. For Helmholtz we could similarly scratch out some rows/columns



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 ω 14.0 $\omega_c = 16.5$ 21.0 % 20.6% 32.7% 47.1%

Remark. For Helmholtz we could similarly scratch out some rows/columns

Warning

There is no guarantee that the (approximate) Schur complement will have a similar diagonal dominance structure!



• Suppose that $A = A^T$, $A = LDL^T$ and

$$\sum_{i:i\neq j} \left| A_{ij} A_{jj}^{-1} \right| \leqslant \frac{\kappa - 1}{\kappa} \Longrightarrow \| L^{-1} \|_1 \leqslant \kappa.$$

- Idea! Instead of constructing some block diagonal dominant block A_{FF}, directly construct L such that ||L⁻¹|| ≤ κ.
- $||L^{-1}||$ can be efficiently estimated [Cline,Moler,Stewart,Wilkinson'77]



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```
>> % create Anderson model matrix
\gg m=50; w=16.5; A=anderson(m,w);
\gg % init parameters to their default values
≫ options=AMGinit(A)
>> % factorize A using multilevel ILU and inverse-based pivoting
≫ tic; [P, options]=AMGfactor (A, options); toc
\gg % display reordered matrix
>> figure(1);AMGspy(P); figure(2);AMGspy(A,P);
\gg % fill-in of the preconditioner
≫ AMGnnz(P)/nnz(A)
≫ P
\gg % iterative solution
>> tic; [x, options] = AMGsolver(A, P, options, A*ones(m^3, 1)); toc
≫ options.niter
>> % remove preconditioner
\gg P=AMGdelete(P)
```



• Original background [Bo., Saad'06]. Error introduced by ILU

A = LDU + E,

preconditioning requires small "inverse error"

$$L^{-1}AU^{-1} = D + L^{-1}EU^{-1} \equiv D + F.$$

D is not taken into account, but a major approach to bound the error.

- Also connections to factored approximate inverses were one root.
- More recently, observations indicated that a tight κ such as κ = 3 (Anderson) let the inverse-based pivoting process act like a coarsening strategy.



Inverse-based coarsening in the Helmholtz case

$$-\Delta u - k^2 u = b$$





Inverse-based coarsening in the Helmholtz case

-k = 200





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Indefinite Preconditioning



$$A^{-1} \approx \underbrace{L^{-T}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa}$$



$$A^{-1} \approx \underbrace{L^{-T}_{\approx\kappa} D^{-1} \underbrace{L^{-1}_{\approx\kappa}}_{\approx\kappa} D^{T}_{\mathcal{FF}} L^{T}_{\mathcal{FF}} D^{-1} = \begin{pmatrix} (L_{\mathcal{FF}} D_{\mathcal{FF}} L^{T}_{\mathcal{FF}})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -L^{-T}_{\mathcal{FF}} L^{T}_{\mathcal{CF}} \\ I \end{pmatrix}}_{I_{h}} S^{-1}_{\mathcal{CC}} \underbrace{\begin{pmatrix} -L_{\mathcal{CF}} L^{-1}_{\mathcal{FF}} & I \end{pmatrix}}_{I_{h}^{T}} D^{-1}_{\mathcal{CF}}$$



$$A^{-1} \approx \underbrace{L^{-T}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa}$$
$$= \begin{pmatrix} (L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{T})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -L_{\mathcal{F}\mathcal{F}}^{-T} L_{\mathcal{C}\mathcal{F}}^{T} \\ I \end{pmatrix}}_{l_{h}} S^{-1}_{\mathcal{C}\mathcal{C}} \underbrace{\begin{pmatrix} -L_{\mathcal{C}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{-1} & I \end{pmatrix}}_{l_{h}^{T}}$$

 $Ax = \varepsilon x$



$$A^{-1} \approx \underbrace{L^{-I}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa}$$
$$= \begin{pmatrix} (L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{\mathsf{T}})^{-1} & 0\\ 0 & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -L_{\mathcal{F}\mathcal{F}}^{\mathsf{T}} L_{\mathcal{C}\mathcal{F}}^{\mathsf{T}}\\ I \end{pmatrix}}_{l_{h}} S_{\mathcal{C}\mathcal{C}}^{-1} \underbrace{\begin{pmatrix} -L_{\mathcal{C}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{-1} & I \end{pmatrix}}_{l_{h}^{\mathsf{T}}}$$

$$Ax = \varepsilon x$$

$$\frac{1}{\varepsilon} x = A^{-1} x \approx \left(\begin{array}{c} \underbrace{(L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{\mathsf{T}})^{-1}}_{\approx C} & 0 \\ 0 & 0 \end{array} \right) x + \underbrace{I_h}_{\approx \kappa} S_{\mathcal{C}\mathcal{C}}^{-1} \underbrace{I_h^{\mathsf{T}}}_{\approx \kappa} x$$



$$A^{-1} \approx \underbrace{L^{-T}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa}$$
$$= \begin{pmatrix} (L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{\mathsf{T}})^{-1} & 0\\ 0 & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -L^{-T}_{\mathcal{F}\mathcal{F}} L_{\mathcal{C}\mathcal{F}}^{\mathsf{T}}\\ I \end{pmatrix}}_{I_h} S^{-1}_{\mathcal{C}\mathcal{C}} \underbrace{\begin{pmatrix} -L_{\mathcal{C}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{-1} & I \end{pmatrix}}_{I_h^{\mathsf{T}}}$$

$$Ax = \varepsilon x$$

$$\frac{1}{\varepsilon} x = A^{-1} x \approx \left(\begin{array}{c} (\underline{L_{\mathcal{F}\mathcal{F}}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{\mathsf{T}})^{-1} & 0 \\ \approx C & 0 \end{array} \right) x + \underbrace{I_h}_{\approx \kappa} \underbrace{S_{\mathcal{C}\mathcal{C}}^{-1}}_{\mathsf{LARGE}} \underbrace{I_h^{\mathsf{T}}}_{\approx \kappa} x$$

 \Rightarrow by inverse-based coarsening $S_{\mathcal{CC}}$ captures the eigenvalues with small modulus



Theorem (Bo., Grote, Schenk'08)

Let A be a nonsingular, real, symmetric. Under some moderate assumptions [...] we have that all small positive eigenvalues μ_j of S_c satisfy

$$\lambda_j \leqslant \mu_j \lessapprox \kappa^2 \lambda_j,$$

where λ_j are their counter parts w.r.t. A.

A similar result holds for the largest negative eigenvalues close to 0.

Remark. This result does not apply dropping.



Analogy to Multigrid Methods Eigenvalues of coarse grid systems

$$-\Delta u - k^2 u = f$$
 in $\Omega = [0, 1]^2, k = 50, N = 80 = [5k/\pi]$

Standard "Geometric" Multigrid, Eigenvalue Distribution

Level	Ν	size	negative ev.	positive ev.
1	80	6'400	187	6213
2	40	1'600	205	1395
3	20	400	313	87
4	10	100	100	0

Algebraic Multilevel ILU, Eigenvalue Distribution

Level	size	negative ev.	positive ev.
1	6'400	187	6213
2	2'276	187	2089
3	1'284	190	1094
4	801	164	637
5	350	_	_

• For standard multigrid, eigenvalues cross the origin while coarsening

• For drop tolerance $\tau = 0$, this cannot happen to the algebraic multilevel ILU

• Experiment uses
$$au = 10^{-3}$$

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Shifted Systems

• To improve the diagonal dominance of A we could introduce imaginary shifts

 $A \rightarrow A + i\beta I$, for some $\beta > 0$.

- systems change from real symmetric to complex symmetric
- Helmholtz case

$$A-k^2M\to A-(1-\mathbf{i}\beta)k^2M.$$

- [Magolu '01] was among the first people to use shifts for ILUs to prevent large fill
- [Erlangga, Vuik, Oosterlee'04,'06] successfully use shifts to set up multigrid for the shifted system and apply it to the original system
- [van Gijzen, Erlangga, Vuik'07] show that the eigenvalues of

$$(A - (1 - \beta i)k^2M)^{-1}(A - k^2M)$$

are located on a disc around $z = \frac{1}{2}$ with radius $r = \frac{1}{2}$ in the complex plane.



Eigenvalues of the preconditioned system





```
>> % create 3D Helmholtz matrix with zero b.c.
>> k=50; L=5; [A,m]=helmholtz(k,L); size(A,1)
\gg % shift matrix with a complex shift
M=A+sqrt (-1) *0.1*k^2*speye (m^3);
\gg % init parameters to their default values
>> options=AMGinit(M); options.maxit=1000
>> % factorize shifted matrix M using multilevel ILU
≫ tic; [P, options]=AMGfactor (M, options); toc
>> AMGnnz(P)/nnz(A), length(P), P(1), AMGspy(P)
\gg % iterative solution
>> tic;[x,options]=AMGsolver(A,P,options,A*ones(m<sup>3</sup>,1));toc
\gg options.niter
>> % remove preconditioner
```

 \gg P=AMGdelete(P)



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- system A is real or complex symmetric
- preconditioner *P* is also real (resp. complex) symmetric.
- The simplified QMR method [Freund, Jarre'99] is a quasi-minimum residual method
- formally a two-sided Lanczos method with a special left initial guess
- sQMR can make use of symmetry
- one step sQMR is almost as cheap as one step of CG (i.e., only one mat-vec, one prec step)



 $n = m^3$, m = 100, 130, 160, 190. $\omega = \omega_c = 16.5$.

Compute 5 eigenvalues and associated eigenvectors closest to $\lambda = 0$.

	time			
size $n = m^3$	10 ⁶	$2\cdot 10^6$	$4\cdot 10^{6}$	$7\cdot 10^{6}$
Cullum–Willoughby Lanczos	71 : 04	_	_	_



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Cullum–Willoughby Lanczos	71 : 04	_	_	_
ARPACK + PARDISO	5 : 37	—		_



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size $n = m^3$	10 ⁶	$2\cdot 10^6$	$4\cdot 10^{6}$	7 · 10 ⁶
Cullum–Willoughby Lanczos	71 : 04	—	_	_
ARPACK + PARDISO	5 : 37	—	—	—
ARPACK + ILUPACK	0 : 45	5 : 46	13 : 58	_



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Compute 5 eigenvalues and associated eigenvectors closest to $\lambda = 0$.

	time			
size $n = m^3$	10 ⁶	$2\cdot 10^6$	$4\cdot 10^{6}$	$7\cdot 10^{6}$
Cullum–Willoughby Lanczos	71 : 04	—	—	—
ARPACK + PARDISO	5 : 37	_	—	—
ARPACK + ILUPACK	0:45	5 : 46	13 : 58	—
Jacobi–Davidson + ILUPACK	0 : 18	1:01	5 : 03	9:06

results from [Schenk,Bo.,Römer'05,'08]



 $n = m^3$, m = 100, 130, 160, 190. $\omega = \omega_c = 16.5$.

Compute 5 eigenvalues and associated eigenvectors closest to $\lambda = 0$.

	memory [GB]			
size $n = m^3$	10 ⁶	$2\cdot 10^6$	$4\cdot 10^{6}$	7 · 10 ⁶
Cullum–Willoughby Lanczos	0.3	—	—	—
ARPACK + PARDISO	14.3	—	_	—
ARPACK + ILUPACK	1.4	3.0	5.8	_
Jacobi–Davidson + ILUPACK	1.4	3.0	5.8	9.6

results from [Schenk,Bo.,Römer'05,'08]



3D seismic imaging problem

- Helmholtz equation $-\Delta u (1 i\alpha)k^2 u = b$ in 3D ($20km \times 20km \times 4km$)
- inverse-based multilevel ILU applied to shifted system $A + i \cdot 0.1k^2I$



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Example

freq.	grid		Multilevel ILU		
[Hz]	points	damping α	iteration (secs)		
		0.0	17 (25)		
2.5	$101 \times 101 \times 24$	0.025	14 (22)		
		0.050	12 (15)		
5	201 × 201 × 48	0.0	35 (410)		
		0.025	21 (321)		
		0.050	17 (268)		
10		0.0	78 (4,243)		
	401 imes 401 imes 94	0.025	54 (3,188)		
		0.050	30 (1,602)		

results from [Bo.,Grote,Schenk'09]



• add artificial conductivity for **E** and similar contribution for **H** such that the reduced second order system refers to a shifted Helmholtz equation

$$\begin{pmatrix} +i\omega\varepsilon \mathbf{E} - \operatorname{curl}(\mathbf{H}) &= -\beta_{\mathbf{E}}\omega\varepsilon \mathbf{E}, \\ -i\omega\mu \mathbf{H} - \operatorname{curl}(\mathbf{E}) &= +\beta_{\mathbf{H}}\omega\mu \mathbf{H}, \end{pmatrix}$$

Reduced second order system

$$\rightarrow \left\{ \begin{array}{l} -(1-\beta_{\mathsf{E}}\beta_{\mathsf{H}}-(\beta_{\mathsf{E}}+\beta_{\mathsf{H}})\mathbf{i})\omega^{2}\mathsf{div}(\varepsilon \mathsf{grad})\varphi,\\ \left(-(1-\beta_{\mathsf{E}}\beta_{\mathsf{H}}-(\beta_{\mathsf{E}}+\beta_{\mathsf{H}})\mathbf{i})\omega^{2}\varepsilon-\mathsf{div}(\frac{1}{\mu}\mathsf{grad})\right)\mathsf{U} \end{array} \right.$$

Essentially reduces to a Helmholtz equation



Applications Problems

- 2 Advances using matchings
- 3 Advanced Symmetric Incomplete Factorizations
- 4 Shifted systems
- Numerical results





- structure-preserving ILU-type methods for indefinite systems
- combinatorial approach using maximum weight matchings to improve block diagonal pivots
- multilevel and inverse-based approach to deal with small pivots
- Software
 - ILUPACK, multilevel preconditioning package and solvers for various type of problems.
 To download *ILUPACK*, visit http://ilupack.tu-bs.de
 - JADAMILU, Jacobi-Davidson eigenvalue solver for generalized symmetric / Hermitian eigenvalue problems including ILUPACK's preconditioner. To download JADAMILU, visit http://homepages.ulb.ac.be/~jadamilu/