## ,Numerical Linear Algebra

Preconditioning techniques
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Many issues related to iterative solution of linear systems of equations are contradictory:

■ numerical efficiency vs computational efficiency
■ numerical efficiency vs parallelization
-


## Example 1: Multiphace flow simulation (2D)

| DOF | Block preconditioner |  |  | Direct solver (MUMPS) |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | N1/N2 | time(s) | MB | N1 | time(s) | M $B$ |
| 131072 | 4/10 | 16.98 | 185 | 3 | 7.2 | 352 |
| 528392 | 4/10 | 72.61 | 646 | 3 | 53.4 | 1409 |
| 1176578 | 4/10 | 170 | 1429 | 3 | 193.75 | 3126 |
| 2097152 | 4/10 | 306.05 | 2587 | Out of memory |  |  |

$$
\begin{array}{cc}
72.61 / 16.98=4.28 & 53.4 / 7.2=7.4 \\
170 / 72.61=2.34 & 193.75 / 53.4=3.62 \\
306.05 / 170=1.8 & ?
\end{array}
$$

Scalability of sparse direct solvers, cont

Example 2: Linear elasticity, 2D

|  | Assembly time (s) |  | Solution time (s) |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| N | Abaqus | Iterative | Abaqus | Iterative |  |
|  |  |  |  | time | iterations |
| 2D |  |  |  |  |  |
| 6043 | 1 | 0.2178 | 1.098 | 1.02 (0.4863) | $13(1,1)$ |
| 23603 | 3.326 | 0.8857 | 4.718 | 4.225 (1.995) | $12(1,1)$ |
| 93283 | 13.02 | 3.978 | 18.05 | 19.38 (9.813) | $11(2,1)$ |
| 370883 | 50.54 | 17.71 | 72.98 | 89.34 (49.43) | $11(2,1)$ |
| 1479043 | 269.1 | 77.7 | 317.5 | 431.8 (257.6) | $12(2,1)$ |
| 4.29694 .1422 |  |  |  |  |  |
|  |  | 3.8258 | 4.5870 |  |  |
|  |  | 4.0432 | 4.6099 |  |  |

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Example, what are we after?

| $\varepsilon \downarrow h \rightarrow$ | $2^{-4}(289)$ | $2^{-5}(1089)$ | $2^{-6}(4225)$ | $2^{-7}(16641)$ | $2^{-8}(66049)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\beta=10^{-6}$ |  |  |  |  |  |
| $10^{-2}$ | $\mathbf{3 ( 8 )}$ | $\mathbf{4 ( 1 1 )}$ | $\mathbf{3 ( 1 3 )}$ | $\mathbf{4 ( 1 4 )}$ | $\mathbf{4 ( 1 1 )}$ |
|  | 0.03 | 0.1 | 0.212 | 1.185 | 4.442 |
| $10^{-4}$ | $\mathbf{3 ( 1 0 )}$ | $\mathbf{4 ( 1 7 )}$ | $\mathbf{5 ( 1 6 )}$ | $\mathbf{5 ( 1 5 )}$ | $\mathbf{6 ( 1 1 )}$ |
|  | 0.033 | 0.128 | 0.436 | 1.669 | 9.431 |
| $10^{-6}$ | $\mathbf{3 ( 1 2 )}$ | $\mathbf{4 ( 2 3 )}$ | $\mathbf{4 ( 2 6 )}$ | $\mathbf{4 ( 2 9 )}$ | $\mathbf{7 ( 2 0 )}$ |
|  | 0.037 | 0.154 | 0.721 | 3.745 | 23.053 |
| $10^{-8}$ | $\mathbf{3 ( 1 4 )}$ | $\mathbf{4 ( 2 8 )}$ | $\mathbf{4 ( 3 3 )}$ | $\mathbf{4 ( 3 8 )}$ | $\mathbf{6 ( 2 6 )}$ |
|  | 0.04 | 0.18 | 0.607 | 2.729 | 28.763 |
| $10^{-10}$ | $\mathbf{3 ( 1 7 )}$ | $\mathbf{4 ( 3 3 )}$ | $\mathbf{4 ( 3 9 )}$ | $\mathbf{4 ( 4 6 )}$ | $\mathbf{6 ( 3 1 )}$ |
|  | 0.043 | 0.208 | 0.723 | 3.328 | 16.242 |

Table 1: Performance of a nonlinear solver

Example 2: Linear elasticity, 3D

| Assembly time (s) |  |  |  |  | Solution time (s) |  |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| N | Abaqus | Iterative | Abaqus | Iterative |  |  |
|  | 2 D |  |  |  |  |  |
| 6043 | 1 | 0.2178 | 1.098 | $1.02(0.4863)$ | $13(1,1)$ |  |
| 23603 | 3.326 | 0.8857 | 4.718 | $4.225(1.995)$ | $12(1,1)$ |  |
| 93283 | 13.02 | 3.978 | 18.05 | $19.38(9.813)$ | $11(2,1)$ |  |
| 370883 | 50.54 | 17.71 | 72.98 | $89.34(49.43)$ | $11(2,1)$ |  |
| 1479043 | 269.1 | 77.7 | 317.5 | $431.8(257.6)$ | $12(2,1)$ |  |
| 3 D |  |  |  |  |  |  |
| 12512 | 1.525 | 1.899 | 3.049 | $8.009(3.465)$ | $12(2,1)$ |  |
| 89700 | 14.09 | 8.756 | 43.29 | $63.34(33.08)$ | $13(2,1)$ |  |
| 678116 | 110.3 | 65.8 | 1347 | $749.3(506.8)$ | $15(4,1)$ |  |

Hybrid solvers
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Table 2: Performance of a nonlinear solver


## Requirements:

## ■ Numerical efficiency

-The condition number $\varkappa\left(C^{-1} A\right)$ should be as small as possible and independent of problem, discretization and method parameters.
Wishes: $\varkappa\left(C^{-1} A\right)=O(1)$
Eigenvalues clusteres in small intervals on the real axes or in a few tight clusters, well separated from the origin.

- Computational efficiency
- The construction of $C$ should be computationally cheap
-The solution of systems with $C$ should be much cheaper (easier) than with $A$
■ Papallel efficiency
$\square$ Both the construction and the solution with the preconditioner should be parallelizable

Clearly the goals are contradicting

Types of preconditioners

Left preconditioning $A \mathbf{x}=\mathbf{b} \Longrightarrow C^{-1} A \mathbf{x}=C^{-1} \mathbf{b}$
$\operatorname{eig}(X Y)=e i g(Y X)$ up to some zero eigenvalues
■Right Preconditioning $A \mathbf{x}=\mathbf{b} \Longrightarrow A C^{-1} \mathbf{y}=\mathbf{b}, \mathbf{x}=C^{-1} \mathbf{y}$
■ymmetric preconditioning

$$
A \mathbf{x}=\mathbf{b} \Longrightarrow C_{1}^{-1} A C_{2}^{-1} \mathbf{y}=C_{1}^{-1} \mathbf{b}, \mathbf{x}=C_{2}^{-1} \mathbf{y}
$$

$\square$ Approximate inverse (multiplicative preconditioning)
$C \approx A^{-1}$. Then no solution but only multiplication with $C$ occur
■ Implicitly defined preconditioners $\left[C^{-1}\right] A \mathbf{x}=\left[C^{-1}\right] \mathbf{b}$
■ Variable (nonlinear) preconditioners $C$ changes from one iteration to another or a number of times through the iterative process. Flexible GMRES, GCG, GCR

- Inner-outer iterations (inner stopping tolerance)


## Types of preconditioners

'Given-the-matrix' - only the matrix is given and the origin of the problem is no known or is not to be used during the solution process Very general, thus, expected to be less numerically efficient.

■'Given-the-problem' - we are in a position to use knowledge about the mesh discretization technique, the origin of the problem (the PDE, for instance)


Examples:
Linear elasticity (Korn's inequality)
Navier-Stokes

Include preconditioning: $C^{-1} A \mathbf{x}=C^{-1} \mathbf{b}$

| Unpreconditioned CG | Preconditioned CG |
| :---: | :---: |
| $x=x 0$ | $\mathrm{x}=\mathrm{x} 0$ |
| $r=A^{*} x-b$ | $r=A^{*} x-b ; C^{*} h=r$ |
| delta0 $=(r, r)$ | delta0 $=(r, h)$ |
| $\mathrm{g}=-\mathrm{r}$ | $\mathrm{g}=-\mathrm{h}$ |
| Repeat: $\mathrm{h}=\mathrm{A}^{*} \mathrm{~g}$ | Repeat: $\mathrm{h}=\mathrm{A}^{*} \mathrm{~g}$ |
| tau $=$ delta0/(g, h$)$ | tau $=$ delta0/(g,h) |
| $x=x+\tan ^{*} \mathrm{~g}$ | $\mathrm{x}=\mathrm{x}+\tan ^{*} \mathrm{~g}$ |
| $r=r+t a u^{*} h$ | $r=r+t a u^{*}{ }^{\text {c }}$ C*h $^{*}=r$ |
| delta1 $=(\mathrm{r}, \mathrm{r})$ | delta1 = (r,h) |
| if delta1 <= eps, stop | if delta1 <= eps, stop |
| beta $=$ delta $1 /$ delta0 | beta $=$ delta $1 /$ delta0 |
| $g=-r+$ beta* $^{*} \mathrm{~g}$ | $\mathrm{g}=-\mathrm{h}+$ beta* $^{\text {a }}$ |

Start with LU factorization $A(m, n)$
for $k=1,2 \cdots m-1$
$d=1 / a_{k k}^{(k)}$
for $i=k+1, \cdots m$
$\ell_{i k}^{(k)}=-a_{i k}^{(k)} d$
for $j=k+1, \cdots n$
$a_{i j}^{(k+1)}=a_{i j}^{(k)}+\ell_{i k} a_{k j}^{(k)}$
end
end
end

The operational count for the LU factorization can be obtained by integrating the loops:

$$
\text { Flops }{ }_{L U}=\int_{1}^{m-1} \int_{k}^{m} \int_{k}^{n} d_{j} d_{i} d_{k} \approx n^{3} / 3(m=n)
$$



The block version offers possibility to use BLAS3.

## Incomplete LU factorization $A(n, n)$

```
for k=1,2\cdotsm-1
        d=1/\mp@subsup{a}{kk}{(k)}
    for i=k+1,\cdotsm
        \ell (k)}=-\mp@subsup{a}{ik}{(k)}
        for j=k+1,\cdotsn
            a}\mp@subsup{i}{}{(k+1)}=\mp@subsup{a}{ij}{(k)}+\mp@subsup{\ell}{ik}{}\mp@subsup{a}{kj}{(k)
            when some condition holds true, drop }\mp@subsup{a}{ij}{(k+1)
            end
    end
end
```


## Most often used conditions:

- $a_{i j}^{(k)}$ too small compared to some (relative) value
- $a_{i j}^{(k)}$ does not belong to a chosen sparsity pattern

Loss of information.

## Incomplete Factorization Preconditioners

How much ILU can improve the convergence of an iterative process?
Example: 2D, Discrete Laplace operator L(spd).
$\lambda_{\min }(A)=h^{2}, \lambda_{\max }(A)=O(1), \varkappa(L)=\lambda_{\max }(A) / \lambda_{\min }(A)=O\left(h^{-2}\right)$.
The convergence estimate for the CG method is:

$$
\begin{aligned}
\left\|\mathbf{e}^{\mathbf{k}}\right\|_{L} & \leq 2\left[\frac{\varkappa(L)+1}{\varkappa(L)-1}\right]^{k}\left\|\mathbf{e}^{\mathbf{0}}\right\|_{L} \\
k & >\frac{1}{2} \sqrt{\varkappa} \ln \left(\frac{2}{\varepsilon}\right)
\end{aligned}
$$

$\Rightarrow k=O\left(h^{-1}\right)$.
Let $C=L L^{T}$, where $L$ is some ILU-obtained approximation of the exact Cholesky factor of $L$. Then

$$
\varkappa\left(C^{-1} L\right)=O\left(h^{-1}\right) .
$$

Thus, only the constant is improved!

## Incomplete Factorization Preconditioners, cont.

RILU (Relaxed ILU)
Instead of dropping $a_{i j}^{(k+1)}$, let $a_{k+1, k+1}^{(k+1)}=a_{k+1, k+1}^{(k+1)}+\omega a_{i j}^{(k+1)}$
Implemented in IFPACK (part of Trilinos, Sandia Nat. Lab.)
User manual: For most situations, RelaxValue should be set to zero.

- For certain kinds of problems, e.g., reservoir modeling, there is a conservation principle involved such that any operator should obey a zero row-sum property. MILU was designed for these cases and you should set the RelaxValue to 1.
- For other situations, setting Relax Value to some nonzero value may improve the stability of factorization, and can be used if the computed ILU factors are poorly conditioned.

■ ILU, based on apriori chosen spartity pattern (ILU(0)): the nonzero pattern of $L$ and $U$ coincides with that of the lower/upper part of $A$
ILUT: Threshhold-based ILU
Reference: Yousef Saad, A dual threshold incomplete LU factorization, Numerical Linear Algebra with Applications, 1 (1994), 387-402.
■ ILUTP: Threshhold\&Permutation-based ILU, available in Matlab.

## ILU(p)

For all nonzero elements $a_{i j}$ define $u_{i j}=a_{i j}, \operatorname{lev}\left(u_{i j}\right)=0$
For $i=2, \cdots, n$ do
For $k=1, \cdots, k-1$ and if $u_{i j} \neq 0$ do
Compute $l_{i k}=u_{i k} / u_{k k}$, set $\operatorname{lev}\left(l_{i k}\right)=\operatorname{lev}\left(u_{i k}\right)$
Compute $u_{i *}=u_{i *}-l_{i k} u_{k *}$
Update the levels of $u_{i *}$ as follows

$$
\operatorname{level}\left(f_{i j}\right)=\operatorname{level}\left(\left(_{i j}\right)+\operatorname{level}\left(u_{k j}\right)+1\right.
$$

Replace any element in row $i$ with $\operatorname{lev}\left(u_{i j}\right)>p$ by zero.

## EndFor

EndFor

## ILU preconditioners, cont.

```
ILUT (Generic ILU with threshhold), Y. Saad, 1994
row(1:n) = 0
do i=2:n
    row(1:n) = a(i,1:n) % sparse copy
    for k=1:i-1 and where row(k) is nonzero, do
            row(k)=row(k)/a(kk)
            apply a dropping rule to row(k)
            if row(k)\not=0
                row(k+1,n)=row(k+1,n)-row(k)*u(k,k+1:n) % sparse update
            endif
        enddo
    apply a dropping rule to row(1:n)
    l(i,1:i-1)=row(1:i-1) % sparse copy
    u(i,i:n) = row(i:n) % sparse copy
    row(1:n) = 0
    enddo
15 enddo
```


## Block ILU preconditioners

## BILUT Block-ILUT

General design of the solver: CUDA, SIMT (Single Instruction Multiple threads)

1. CRS sparse format
2. Reorder using RCM (Recursive Cuthill-McKee)
3. Use Metis to generate a balanced partitioning; reorder and repartition after long time intervals
4. FGMRES with some preconditioner per timestep.

Reference: H. Sudan, H. Klie, R. Li and Y. Saad, High Performance Manycore Solvers for Reservoir Simulation
European Association of Geoscientists \& Engineers Conference Proceedings, ECMOR
XII - 12th European Conference on the Mathematics of Oil Recovery, Sep 2010
cp-163-00042 ISBN: 978-90-73781-89-4
DOI: https://doi.org/10.3997/2214-4609.20144961

Block ILU preconditioners, cont.

Attractive: $D$-diagonal.
How do we obtain a permutation, such that we get $D-$
diagonal?
Use multicoloring algorithm:
For $1=1: n$
Set color(i)=0
endfor
For $1=1: n$
Set color( i$)=\min (k>0: k \neq \operatorname{color}(\mathrm{j})$ for $j \in \operatorname{Adj}(i)$
endfor
where $\operatorname{Adj}(i)=\left\{j \neq i: a_{i j} \neq 0\right\}$.
$\square L D L^{T}$ and $L D U$ preconditioners
$\square$ Let $A=D_{A}-L_{A}-U_{A}$.
Symmetric Gauss-Seidel preconditioner: $C=\left(D_{A}-L_{A}\right) D_{A}^{-1}\left(D_{A}-U_{A}\right)$ Note:

$$
C=\left(D_{A}-L_{A}\right) D_{A}^{-1}\left(D_{A}-U_{A}\right)=D_{A}-L_{A}-U_{A}+L D_{A}^{-1} U=A+L D_{A}^{-1} U
$$

$$
\begin{aligned}
A=L U & =\left[\begin{array}{cccc}
I_{1} & 0 & \cdots & 0 \\
L_{2,1} & I_{2} & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots \\
L_{n, 1} & L_{n, 2} & \cdots & I_{n}
\end{array}\right]\left[\begin{array}{cccc}
D_{1} & U_{1,2} & \cdots & U_{1, n} \\
0 & D_{2} & \cdots & U_{2, n} \\
\vdots & \vdots & \cdots & \vdots \\
0 & 0 & \cdots & D_{n}
\end{array}\right] \\
\mathbf{y}_{i}=\mathbf{y}_{i}-\sum_{j=1}^{i-1} L_{j i} \mathbf{y}_{j} & \mathbf{x}_{i}=D_{i}^{-1}\left(\mathbf{y}_{i}-\sum_{j=i+1}^{n} U_{i j} \mathbf{x}_{j}\right)
\end{aligned}
$$

## Power(q)-pattern Method, Dimitar Lukarski

## Building of power $(q)$-pattern - ILU $(p, q)$

■ Perform multi-coloring analysis for $|A|^{q}$ and obtain - corresponding permutation $\pi$
the number of colors $B$ and local block sizes $b_{i}$
■ Permute $A_{\pi}:=\pi A \pi^{-1}$
■ Apply a modified ILU $(p)$ factorization to $A$
Central result: For $q=p+1$ the diagonal blocks of $L$ and $U$ becone diagona themselves. No fill-ins here!
p - fill-in levels
q-describes the degree of parallelism
D. Lukarski, J.-P- Weiss, Enhanced Parallel ILU(p)-based Preconditioners for Multi-core CPUs and GPUs - The Power(q)-pattern Method, January 2011, DOI:
10.11588/emclpp.2011.08.11690

■ LU sweeps, solve in parallel $L U z=r$

- Re-formulate into a block-form
- Use fine-grained parallelism on the block level

■ Parallelism $=N /$ Num blocks

$$
\begin{aligned}
x_{i} & :=D_{L i}^{-1}\left(r_{i}-\sum_{j=1}^{i-1} L_{i, j} x_{j}\right) \\
z_{i} & :=D_{U i}^{-1}\left(x_{i}-\sum_{j=1}^{B-i} U_{i, j} z_{i+j}\right)
\end{aligned}
$$

$\operatorname{ILU}(p, q)$ constructs $D_{L i}^{-1}$ and $D_{U i}^{-1}$ to be with diagonal elements only
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Block-tridiagonal matrices, cont.

When the subdomains are ordered lexicographically from left to right, a domain $\Omega_{i}$ becomes coupled only to its pre- and postdecessors $\Omega_{i-1}$ and $\Omega_{i+1}$, respectively and the corresponding matrix takes the form of a block tridiagonal matrix
$A=\operatorname{tridiag}\left(A_{i, i-1}, A_{i, i}, A_{i, i+1}\right)$, or

$$
A=\left[\begin{array}{cccc}
A_{11} & A_{12} & & 0 \\
A_{21} & A_{22} & A_{23} & \\
& \ddots & \ddots & \ddots \\
0 & & A_{n, n-1} & A_{n, n}
\end{array}\right]
$$

For definiteness we let the boundary meshline $\bar{\Omega}_{i} \cap \bar{\Omega}_{i+1}$ belong to $\Omega_{i}$.
In order to preserve the sparsity pattern we shall factor $A$ without use of permutations.
Naturally, the lines of intersection do not have to be straight.


Examples of subdomain decompositions
Paper:
Modification and compensation strategies for threshold-based incomplete factorizations
S. MacLachlan, D. Osei-Kuffuor, Yousef Saad

| Examples of ILU performance (numerical) |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $d t$ | Precond.with $\widehat{A}_{0}$ |  | ILU |  |
|  | N1/N2 | time(s) | N1/N2 | time(s) |
| $h$ | 4/10 | 14.58 |  |  |
| $h / 4$ | 4/10 | 16.98 | no conv | rgence |
| $h / 5$ | 4/10 | 16.77 |  |  |
| $h / 10$ | 4/10 | 14.67 | 4/42 | 23.66 |
| $h / 20$ | 4/10 | 14.62 | 4/13 | 13.23 |
| $h / 40$ | 4/10 | 14.11 | 4/10 | 10.55 |

Multiphace flow with convection: Two preconditioners: Run time and number of iterations, $P e=1000$


Problem 2: Two preconditioners: run time and number of iterations, $P e=1$.

## PROS:

■ Very general, no additional knowledge of the problem is required

- Relatively easy to implement
- Available in the software packages

CONS:
■ Method parameters to tune; nonlinear behaviour wrt to $\tau$
■ Not very nummerically efficient (may not converge)

- Problem-dependent behavious
- Relatively less degrees of parallelism

Time to solve the Poisson model problem on a regular grid with $N$ points

| Solver | 1 D | 2 D | 3 D |
| :--- | :---: | :---: | :---: |
| Sparse Choleski | $O(N)$ | $O\left(N^{1.5}\right)$ | $O\left(N^{2}\right)$ |
| Unprecond. CG | $O\left(N^{2}\right)$ | $O\left(N^{1.5}\right)$ | $O\left(N^{1.33}\right)$ |
| IC-precond. CG | $O\left(N^{1.5}\right)$ | $O\left(N^{1.25}\right)$ | $O\left(N^{1.17}\right)$ |
| Multigrid | $O(N)$ | $O(N)$ | $O(N)$ |

## Approximate inverse preconditioning

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- Thomas Huckle,

Modified Sparse Approximate Inverses
http://www5.in.tum.de/wiki/index.php/MSPAI Factorized Sparse Approximate Inverses
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## -

## Approximate inverses: Explicit Methods

Given a sparse matrix $A=\left[a_{i j}\right] \in^{n \times n}$.
Let $S$ be a sparsity pattern. We want to compute $G \in \mathcal{S}$, such that

$$
(G A)_{i j}=\delta_{i j},(i, j) \in \mathcal{S}
$$

i.e.

$$
\sum_{k:(i, k) \in S} g_{i k} a_{k j}=\delta_{i j},(i, j) \in \mathcal{S}
$$

Some observations
$\oplus \quad$ the elements in the $i$ th row of $G$ can be computed independently;
$\ominus \quad$ even if $A$ is symmetric, $G$ is not necessarily symmetric, because $g_{i j}$ and $g_{j i}$ are, in general, not equal.

## Example:

## Choose $\mathcal{S}$ to be the tridiagonal part of $A$,

$\mathcal{S}=\left\{(1,1),(1,2),\{(i, i-1),(i, i),(i, i+1)\}_{i=1}^{n},(n, n-1),(n, n)\right\}$.
Then, when computing the $i$ th row of $G$ we need only the entries of the matrix
$A$, namely,

$$
A^{i}=\left[\begin{array}{ccc}
a_{i-1, i-1} & a_{i-1, i} & a_{i-1, i+1} \\
a_{i, i-1} & a_{i, i} & a_{i, i+1} \\
a_{i+1, i-1} & a_{i+1, i} & a_{i+1, i+1}
\end{array}\right]
$$

Given $A \in R^{n \times n}$ and $\mathcal{S}$
for $i=1$ :n,
Extract from $A$ the small matrix $A^{i}$, needed to compute
the entries of $G(i,:)$
Solve with $A^{i}$
Store row $G(i,:)$
end
We want to find $G$ with the same sparsity pattern as $A$, i.e.,

$$
\begin{array}{r}
A=\left[\begin{array}{cccc}
2 & -1 & 0 & 0 \\
-1 & 3 & -2 & 0 \\
0 & -2 & 4 & -1 \\
0 & 0 & -1 & 2
\end{array}\right] \quad G=\left[\begin{array}{cccc}
g_{11} & g_{12} & 0 & 0 \\
g_{21} & g_{22} & g_{23} & 0 \\
0 & g_{32} & g_{33} & g_{34} \\
0 & 0 & g_{43} & g_{44}
\end{array}\right] \\
G(1,:): \begin{array}{r}
2 g_{21}-g_{22}
\end{array}=0 \\
2 g_{11}-g_{12}=1 \\
-g_{11}+3 g_{12}=0
\end{array} \quad G(2,:): \begin{array}{r}
-g_{21}+3 g_{22}-2 g_{23}
\end{array}=1
$$

Example, cont.

$$
A^{-1}=\frac{1}{19}\left[\begin{array}{cccc}
13 & 7 & 4 & 2 \\
7 & 14 & 8 & 4 \\
4 & 8 & 10 & 5 \\
2 & 4 & 5 & 12
\end{array}\right]
$$

$$
G=\left[\begin{array}{cccc}
\frac{3}{5} & \frac{1}{5} & 0 & 0 \\
\frac{1}{3} & \frac{2}{3} & \frac{1}{3} & 0 \\
0 & \frac{4}{13} & \frac{6}{13} & \frac{3}{13} \\
0 & 0 & \frac{1}{7} & \frac{4}{7}
\end{array}\right] \quad G A=\left[\begin{array}{cccc}
1 & 0 & -0.40 & 0 \\
0 & 1 & 0 & -0.33 \\
-0.31 & 0 & 1 & 0 \\
0 & -0.28 & 0 & 1
\end{array}\right]
$$

Example, cont.

Note: the second row of $G$ is the second row of the matrix

$$
B=\left[\begin{array}{cccc}
2 & -1 & 0 & 0 \\
-1 & 3 & -2 & 0 \\
0 & -2 & 4 & 0 \\
0 & 0 & 0 & 1
\end{array}\right]^{-1}, G B=\left[\begin{array}{cccc}
1 & 0 & -0.4 & 0 \\
0 & 1 & 0 & 0 \\
-0.31 & 0 & 1.2308 & 0.4615 \\
0 & -0.2857 & 0.5714 & 1.1429
\end{array}\right]
$$

However, if we compute $A G$ then

$$
A G=\left[\begin{array}{cccc}
0.8667 & -0.2667 & -0.3333 & 0 \\
0.4000 & 1.1846 & 0.0769 & -0.4615 \\
-0.6667 & -0.1026 & 1.0366 & 0.3516 \\
0 & -0.3077 & -0.1758 & 0.9121
\end{array}\right]
$$

i.e., the matrix $G$ is computed as a left-side approximate inverse of $A$ and as such is somewhat less accurate than as a right-side approximate inverse

The drawback of the above method is that
in general even if $A$ is symmetric, $G$ is not!

## Let $A$ be in a factored form.

Suppose $A=L D^{-1} U$ is a triangular matrix factorization of $A$. If $A$ is a band matrix then $L$ and $U$ are also band matrices.
Let $L=I-\widetilde{L} ; U=I-\widetilde{U}$, where $\widetilde{L}$ and $\widetilde{U}$ are strictly lower and upper triangular matrices correspondingly.

Lemma 1 Using the above notations it can be shown that
(i) $A^{-1}=D L^{-1}+\widetilde{U} A^{-1}$,
(ii) $A^{-1}=U^{-1} D+A^{-1} \widetilde{L}$.

Proof

$$
\begin{gathered}
A=L D^{-1} U \Longrightarrow A^{-1}=U^{-1} D L^{-1} \\
\Longrightarrow(I-\widetilde{U}) A^{-1}=D L^{-1} \Longrightarrow A^{-1}=D L^{-1}+\widetilde{U} A^{-1} .
\end{gathered}
$$

Also

$$
A^{-1}(I-\widetilde{L})=U^{-1} D \Longrightarrow A^{-1}=U^{-1} D+A^{-1} \widetilde{L}
$$


is indefinite.
endfor
endfor
$q$ is the bandwidth.
for $r=n, n-1, \cdots, 1$
for $r=n, n-1, \cdots, 1$
$\left(A^{-1}\right)_{r, r}=D_{r, r}+\sum_{s=1}^{\min (q, n-r)} \widetilde{U}_{r, r+s}\left(A^{-1}\right)_{r+s, r}$
for $k=1,2, \cdots, q$
$\left(A^{-1}\right)_{r-k, r}=\sum_{s=1}^{\min (q, n-r+k)} \widetilde{U}_{r-k, r-k+s}\left(A^{-1}\right)_{r-k+s, r} \leadsto(i)$
$\left(A^{-1}\right)_{r, r-k}=\sum_{t=1}^{\min (q, n-r+k)}\left(A^{-1}\right)_{r, r-k+t} \widetilde{L}_{r-k+t, r-k} \leadsto(i i)$
endfor
endfor

A general framework for computing approximate inverses


Let a sparsity pattern $\mathcal{S}$ be given. Consider the functional

$$
F_{W}(G)=\|I-G A\|_{W}^{2}=\operatorname{tr}(I-G A) W(I-G A)^{T}
$$

where the weight matrix $W$ is spd If $W \equiv I$ then $\|I-G A\|_{I}$ is the Frobenius norm of $I-G A$.

Clearly $F_{W}(G) \geq 0$. If $G=A^{-1}$ then $F_{W}(G)=0$. Hence, we want to compute the entries of $G$ in order to minimize $F_{W}(G)$, i.e. to find $\hat{G} \in S$, such that

$$
\|I-\hat{G} A\|_{W} \leq\|I-G A\|_{W}, \forall G \in S
$$

The following properties of $\operatorname{tr}(\cdot)$ will be used:

$$
\operatorname{tr} A=\operatorname{tr} A^{T}, \operatorname{tr}(A+B)=\operatorname{tr} A+\operatorname{tr} B
$$

$$
\begin{align*}
F_{W}(G) & =\operatorname{tr}(I-G A) W(I-G A)^{T} \\
& =\operatorname{tr}\left(W-G A W-W(G A)^{T}+G A W(G A)^{T}\right)  \tag{1}\\
& =\operatorname{tr} W-\operatorname{tr} G A W-\operatorname{tr}(G A W)^{T}+\operatorname{tr} G A W A^{T} G^{T} .
\end{align*}
$$

Minimize $F_{W}$ w.r.t. $G$, consider the entries $g_{i, j}$ as variables. The necessary condition for a minimizing point are

$$
\begin{equation*}
\frac{\partial F_{W}(G)}{\partial g_{i j}}=0,(i, j) \in \mathcal{S} \tag{2}
\end{equation*}
$$

From (1) and (2) we get $-2\left(W A^{T}\right)_{i j}+2\left(G A W A^{T}\right)_{i j}=0$, or

$$
\begin{equation*}
\left(G A W A^{T}\right)_{i j}=\left(W A^{T}\right)_{i j},(i, j) \in \mathcal{S} \tag{3}
\end{equation*}
$$

The equations (3) may or may not have a solution, depending on the particular matrix $A$ and the choice of $\mathcal{S}$ and $W$.
$■$ Step 1: Let $\widetilde{A}$ be $A$ with deleted small entries, i.e. $\widetilde{A} \in \mathcal{S}_{3}$.

- Step 2: Compute $\widetilde{G}:(\widetilde{G} A)_{i j}=\delta_{i j},(i, j) \in S_{3}$.
- Step 3: Find $G=\bar{G}+D$, where $\bar{G}=\frac{1}{2}\left(\widetilde{G}+\widetilde{G}^{T}\right)$ and $D$ is diagonal, computed from the following imposed condition on $G$, i.e.

$$
G A \mathbf{e}=\mathbf{e},
$$

and $\mathrm{e}=(1,1, \cdots, 1)^{T}$.
The diagonal compensation technique prescribes the spd property of $A$.

The methods described till now do not guarantee that $G$ will be such a matrix.
We want now to compute an spd approximate inverse of an spd matrix.
Let $\mathcal{S}$ be a symmetric sparsity pattern. We seek $G$ of the form

$$
G=L_{G}^{T} L_{G}, L_{G} \in \mathcal{S}_{L}
$$

Clearly $G$ will be spd
Theorem 1 A matrix $G$ of the form $G=L_{G}^{T} L_{G}$ which is an spd approximation of $A^{-1}$ can be computed from the following relation:

$$
\begin{equation*}
\min _{X \in \mathcal{S}_{L}} \frac{\frac{1}{n} \operatorname{tr} X A X^{T}}{\left(\operatorname{det}\left(X A X^{T}\right)\right)^{\frac{1}{n}}}=\frac{\frac{1}{n} \operatorname{tr} L_{G} A L_{G}^{T}}{\left(\operatorname{det}\left(L_{G} A L_{G}^{T}\right)\right)^{\frac{1}{n}}} \tag{4}
\end{equation*}
$$

Thus, we minimize Expression_A computing

$$
\begin{equation*}
d_{i}=\frac{1}{\left((I-\widetilde{X}) A(I-\widetilde{X})^{T}\right)_{i i}^{\frac{1}{2}}} \tag{7}
\end{equation*}
$$

Let $\widetilde{L}_{G}$ be the solution of (7). Note that it is strictly lower triangular. Let the entries $d_{i}$ of $D$ are computed from the relations (7), where instead of $\widetilde{X} \widetilde{L}_{G}$ is used. Then the matrix $L_{G}^{T} L_{G}$, where $L_{G}=D\left(I-\widetilde{L}_{G}\right)$, will be the searched approximation of $A^{-1}$ :

- $\left(L_{G} A L_{G}^{T}\right)_{i i}=1$ by construction;
- The equality (4) gives a measure of the quality of the approximate inverse constructed (the K-condition number (Igor Kaporin).

Let $A=\operatorname{tridiag}(-1,4,-1)$. Find $L_{G}^{T} L_{G}$ - an approximate inverse of $A$, where $L_{G}$ is bidiagonal. Thus, $\mathcal{S}_{\widetilde{L}}=\left\{\{(i-1, i)\}_{i=2}^{n}\right\}$.
First we compute a strictly lower bidiagonal matrix $\widetilde{L}$ from the condition

$$
(\widetilde{L} A)_{i, j}=(A)_{i, j}, i, j \in \mathcal{S}_{\widetilde{L}}
$$

which gives us

$$
\widetilde{L}=\left[\begin{array}{cccccc}
0 & & & & & \\
\frac{1}{4} & 0 & & & & \\
& \frac{1}{4} & 0 & & & \\
& & & \ddots & & \\
& & & \frac{1}{4} & 0 & \\
& & & & \frac{1}{4} & 0
\end{array}\right]
$$

Then $d_{i}$ are found to be

$$
d_{1}=\frac{1}{2}, d_{i}=\frac{2}{\sqrt{15}}, i=1,2, \cdots, n
$$



## Extensions

■ When minimizing $\|I-A G\|_{F}$, minimize the 2-norm of each column separately, $\left\|\mathbf{e}_{k}-A \mathbf{g}_{k}\right\|_{F}, k=1, \cdots, n$

- use adaptive $\mathcal{S}$ (much more expensive)

■ used the sparsity pattern of powers of $A$

- Modified SPAI: combines
- Frobenius norm minimization
- MILU
- vector probing

MSPAI
Consider the formulation:

$$
\min _{G}\|C G-B\|_{F}=\min _{G}\left\|\left[\begin{array}{c}
C \\
\rho \mathbf{e}^{T} C
\end{array}\right] G-\left[\begin{array}{c}
B_{0} \\
\rho \mathbf{e}^{T} B_{0}
\end{array}\right]\right\|_{F}
$$

$\rho=0, C_{0}=A, B_{0}=I$ - the original form
$C_{0}=I, B_{0}=A$ - explicit approximation of $A$
$\rho=[1,1, \cdots, 1]$ - MILU
Improve existing approximations:

$$
\min _{U}\left\|\left[\begin{array}{c}
L \\
\rho \mathbf{e}^{T} L
\end{array}\right] U-\left[\begin{array}{c}
A \\
\rho \mathbf{e}^{T} A
\end{array}\right]\right\|_{F}
$$


with $R_{k}$ being the Boolean matrices which prescribe the local-to-global correspondence of the numbered degrees of freedom.
Is this of interest?

$$
B^{-1}=\sum_{k=1}^{M} R_{k}^{T} A_{k}^{-1} R_{k}
$$

$B^{-1}$ and $A^{-1}$ are spectrally equivalent, namely, for some $0<\alpha_{1}<\alpha_{2}$ there holds

$$
\alpha_{1} A_{11}^{-1} \leq B_{11}^{-1} \leq \alpha_{2} A_{11}^{-1}
$$



The approximate inverse (mesh (AI))
Numerical Linear Alsebra - p. 6992


The exact inverse matrix (mesh (inv (A) ))
Numerical Linear Algebra - p. 70/92


The difference (mesh (inv (A) -AI))

FEM-SPAI


The product with $A$ (mesh (AI*A))

FEM-SPAI: Scalability figures: Constant problem size

| \#proc | $n_{\text {fine }}$ | $t_{B_{11}^{-1} / t_{A}}$ | $t_{\text {repl }}[\mathrm{s}]$ | $t_{\text {solution }}[\mathrm{s}]$ | $\#$ iter |
| :--- | ---: | ---: | ---: | ---: | ---: |
| 4 | 197129 | 0.005 | 0.28 | 7.01 | 5 |
| 16 | 49408 | 0.180 | 0.07 | 0.29 | 5 |
| 64 | 12416 | 0.098 | 0.02 | 0.03 | 5 |
| Problem size: 787456 |  |  |  |  |  |
| Solution method: PCG |  |  |  |  |  |
| Relative stopping criterium: $<10^{-6}$ |  |  |  |  |  |

FEM-SPAI: Scalability figures: Constant load per processor

| $\#$ proc | $t_{B_{1}^{-1} / t_{A}}$ | $t_{\text {repl }}[\mathbf{s}]$ | $t_{\text {solution }}[\mathbf{s}]$ | $\#$ iter |
| :--- | ---: | ---: | ---: | ---: |
| 1 | 0.0050 | - | 0.17 | 5 |
| 4 | 0.0032 | 0.28 | 7.01 | 5 |
| 16 | 0.0035 | 0.24 | 4.55 | 5 |
| 64 | 0.0040 | 0.23 | 12.43 | 5 |

Local number of degrees of freedom: 197129
Solution method: PCG
Relative stopping criterium: $<10^{-6}$

Many different interpretations within the PDE community:
■ Parallel computing: data decomposition (independent of numerical method)
■ Asymptotic analysis: separation of physical domain into regions with possibly different models

- Preconditioning methods: solution of a large linear system arising from the discretization of the PDE on the whole domain by DDM as a solver or a preconditioner:
- Overlapping domain decomposition

■ Non-overlapping domain decomposition

## Domain decomposition:

Domain decomposition - decomposition of the spatial domain into several subdomains. Search the global true solution through (iteratively) solving subproblems while enforcing suitable continuity requirements between neighbor subdomains.

■ Flexible - localized treatment of complex and irregular geometries, singularities etc.

- Efficient - often optimal convergence rate

■ Easy to parallelize (coarse grain parallelization)

Matrix form of Alternating Schwarz

Decompose $A$ as $A_{i} A_{\partial \Omega_{i} \backslash \Gamma_{i}} A_{\Gamma_{i}}$.
Let $I_{\Omega_{i} \rightarrow \Gamma_{j}}$ be the discrete operator that interpolates the nodes in the interior of $\Omega_{i}$ to $\Gamma_{j}$. Then:

$$
\begin{aligned}
& A_{\Omega_{1}} \mathbf{u}_{\Omega_{1}}^{k}=\mathbf{f}_{1}-A_{\Gamma_{1}} I_{\Omega_{2} \rightarrow \Gamma_{1}} \mathbf{u}_{\Omega_{2}}^{k-1} \\
& A_{\Omega_{2}} \mathbf{u}_{\Omega_{2}}^{k}=\mathbf{f}_{2}-A_{\Gamma_{2}} I_{\Omega_{1} \rightarrow \Gamma_{2}} \mathbf{u}_{\Omega_{1}}^{k}
\end{aligned}
$$

Gauss-Seidel method for the system

$$
\left[\begin{array}{cc}
A_{\Omega_{1}} & A_{\Gamma_{1}} I_{\Omega_{2} \rightarrow \Gamma_{1}} \\
A_{\Gamma_{2}} I_{\Omega_{1} \rightarrow \Gamma_{2}} & A_{\Omega_{2}}
\end{array}\right]\left[\begin{array}{l}
\mathbf{u}_{\Omega_{1}} \\
\mathbf{u}_{\Omega_{2}}
\end{array}\right]=\left[\begin{array}{l}
\mathbf{f}_{1} \\
\mathbf{f}_{2}
\end{array}\right]
$$

$$
A \mathbf{u}=\mathbf{f}
$$




Rearrange as a simple iteration:

$$
\begin{aligned}
& \mathbf{u}_{\Omega_{1}}^{k}=\mathbf{u}_{\Omega_{1}}^{k-1}+A_{\Omega_{1}}^{-1}\left(\mathbf{f}_{1}-A_{\Omega_{1}} \mathbf{u}_{\Omega_{1}}^{k-1}-A_{\Gamma_{1}} I_{\Omega_{2} \rightarrow \Gamma_{1}} \mathbf{u}_{\Omega_{2}}^{k-1}\right) \\
& \mathbf{u}_{\Omega_{2}}^{k}=\mathbf{u}_{\Omega_{2}}^{k-1}+A_{\Omega_{2}}^{-1}\left(\mathbf{f}_{2}-A_{\Omega_{2}} \mathbf{u}_{\Omega_{2}}^{k-1}-A_{\Gamma_{1}} I_{\Omega_{1} \rightarrow \Gamma_{2}} \mathbf{u}_{\Omega_{2}}^{k}\right)
\end{aligned}
$$

Additive and multiplicative Schwarz methods:

$$
\begin{aligned}
& \mathbf{u}_{\Omega_{1}}^{k}=\mathbf{u}_{\Omega_{1}}^{k-1}+A_{\Omega_{1}}^{-1}\left(\mathbf{f}_{1}-A_{\Omega_{1}} \mathbf{u}_{\Omega_{1}}^{k-1}-A_{\Omega \backslash \bar{\Omega}_{1}} \mathbf{u}_{\Omega \backslash \bar{\Omega}_{1}}^{k-1}\right) \\
& \mathbf{u}_{\Omega_{2}}^{k}=\mathbf{u}_{\Omega_{2}}^{k-1}+A_{\Omega_{2}}^{-1}\left(\mathbf{f}_{2}-A_{\Omega_{2}} \mathbf{u}_{\Omega_{2}}^{k-1}-A_{\Omega \backslash \bar{\Omega}_{2}} \mathbf{u}_{\Omega \backslash \overline{\Omega_{2}}}^{k-1}\right)
\end{aligned}
$$

$$
\Uparrow
$$

$$
\mathbf{u}_{\Omega \backslash \bar{\Omega}_{2}}^{k}
$$

$$
\begin{aligned}
& \mathbf{u}^{k+1 / 2}=\mathbf{u}^{k}+\left[\begin{array}{cc}
A_{\Omega_{1}}^{-1} & 0 \\
0 & 0
\end{array}\right]\left(\mathbf{f}-A \mathbf{u}^{k}\right) \\
& \mathbf{u}^{k+1}=\mathbf{u}^{k+1 / 2}+\left[\begin{array}{cc}
0 & 0 \\
0 & A_{\Omega_{2}}^{-1}
\end{array}\right]\left(\mathbf{f}-A \mathbf{u}^{k+1 / 2}\right)
\end{aligned}
$$

Final form, many subdomains

$$
\begin{gathered}
\mathbf{u}^{k+1}=\mathbf{u}^{k}+\sum_{i=1}^{p} B_{i}\left(\mathbf{f}-A \mathbf{u}^{k}\right) \\
\mathbf{u}^{k+1 / p}=\mathbf{u}^{k}+B_{1}\left(\mathbf{f}-A \mathbf{u}^{k}\right) \\
\mathbf{u}^{k+2 / p}=\mathbf{u}^{k+1 / p}+B_{2}\left(\mathbf{f}-A \mathbf{u}^{k+1 / p}\right) \\
\vdots \\
\mathbf{u}^{k+1}=\mathbf{u}^{k+(p-1) / p}+B_{p}\left(\mathbf{f}-A \mathbf{u}^{k+(p-1) / p}\right) \\
\mathbf{u}^{k+1}=\mathbf{u}^{k}+\left(I-\left(I-B_{p} A\left(\cdots\left(I-B_{A}\right)\right)\right)\right) A^{-1}\left(\mathbf{f}-A \mathbf{u}^{k}\right)
\end{gathered}
$$

Denote: $\mathbf{u}_{\Omega_{1}}=R_{1} \mathbf{u}=\left[\begin{array}{ll}I & 0\end{array}\right]\left[\begin{array}{c}\mathbf{u}_{\Omega_{1}} \\ \mathbf{u}_{\Omega \backslash \Omega_{1}}\end{array}\right]$
$\mathbf{u}_{\Omega_{2}}=R_{2} \mathbf{u}=\left[\begin{array}{ll}0 & I\end{array}\right]\left[\begin{array}{c}\mathbf{u}_{\Omega \backslash \Omega_{2}} \\ \mathbf{u}_{\Omega_{2}}\end{array}\right]$
Then $A_{\Omega_{i}}=R_{i} A R_{i}^{T}$; let $B_{i}=R_{i}^{T}\left(R_{i} A R_{i}^{T}\right)^{-1} R_{i}$.

$$
\begin{aligned}
& \mathbf{u}^{k+1}=\mathbf{u}^{k}+\left(B_{1}+B_{2}-B_{2} A B_{1}\right)\left(\mathbf{f}-A \mathbf{u}^{k}\right) \\
& \mathbf{u}^{k+1}=\mathbf{u}^{k}+\left(B_{1}+B_{2}\right)\left(\mathbf{f}-A \mathbf{u}^{k}\right)
\end{aligned}
$$

## Problem:

Too slow Convergence deteriorates as $p$ increases ( $H$ decreases).
Reason: The only global communication of information between subdomains are through overlapping regions. Too slow!
How to speed up? Coarse grid correction.

$$
\mathbf{u}^{\text {fine }}=\mathbf{u}^{\text {fine }}+R^{T} A_{C}^{-1} R\left(\mathbf{f}-A \mathbf{u}^{\text {fine }}\right)
$$

Two-level additive Schwarz method:

$$
\mathbf{u}^{k+1}=\mathbf{u}^{k}+\left(R^{T} A_{C}^{-1} R+\sum_{i=1}^{p} R^{T} A_{i}^{-} R\right) \mathbf{r}^{k}
$$

## Summarizing DD:

- multiplicative is faster than additive

■ overlapping or nonoverlapping; large overlap is better for convergence

- deteorating convergence when increasing the number of subdomains (if implemented straightforwardly)
■ stabilization with a coarse grid corrrection, nearly optimal convergence
- used as a preconditiner

■ used in a Multigrid setting as a smoother
■ attractive for parallel computations (FETI, BETI, ...)



Results with solver only one AMG iteration and tolerance $1 e-7$


Results with solver only one AMG iteration and tolerance $1 e-12$


Results with inner solver and tolerance $1 e-12$

