## UNIVERSITY <br> 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 $350 \times 350$ 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.. [GaussSeidel, ILU, ...]

## Background: Incomplete LU (ILU) preconditioners

## ILU: $\quad A \approx L U$

Simplest Example: ILU(0) $\rightarrow$




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

$$
P A P^{T}=\left(\begin{array}{ll}
B & F \\
E & C
\end{array}\right)=
$$

> Block factorize:


$$
\left(\begin{array}{ll}
B & F \\
E & C
\end{array}\right)=\left(\begin{array}{cc}
L & 0 \\
E U^{-1} & I
\end{array}\right)\left(\begin{array}{cc}
U & L^{-1} F \\
0 & S
\end{array}\right)
$$

$>\boldsymbol{S}=\boldsymbol{C}-\boldsymbol{E} \boldsymbol{B}^{-1} \boldsymbol{F}=$ Schur complement + dropping to reduce fill
$>$ Next step: treat the Schur complement recursively

## Algebraic Recursive Multilevel Solver (ARMS)

## Level l Factorization:

$$
\left(\begin{array}{ll}
\boldsymbol{B}_{l} & \boldsymbol{F}_{l} \\
\boldsymbol{E}_{l} & \boldsymbol{C}_{l}
\end{array}\right) \approx\left(\begin{array}{cc}
\boldsymbol{L}_{l} & \mathbf{0} \\
\boldsymbol{E}_{l} \boldsymbol{U}_{l}^{-1} & \boldsymbol{I}
\end{array}\right)\left(\begin{array}{cc}
\boldsymbol{I} & \mathbf{0} \\
\mathbf{0} & \boldsymbol{A}_{l+1}
\end{array}\right)\left(\begin{array}{cc}
\boldsymbol{U}_{l} & \boldsymbol{L}_{l}^{-1} \boldsymbol{F}_{l} \\
\mathbf{0} & \boldsymbol{I}
\end{array}\right)
$$

> Perform above block factorization recursively on $\boldsymbol{A}_{l+1}$
$>$ Blocks in $\boldsymbol{B}_{l}$ 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]
- 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 $\boldsymbol{B}$ block
$>$ Permute rows * and * columns of $\boldsymbol{A}$. Use two permutations $\boldsymbol{P}$ (rows) and $\boldsymbol{Q}$ (columns) to transform $\boldsymbol{A}$ into

$$
\boldsymbol{P} A Q^{T}=\left(\begin{array}{ll}
\boldsymbol{B} & \boldsymbol{F} \\
\boldsymbol{E} & \boldsymbol{C}
\end{array}\right)
$$

$P, Q$ is a pair of permutations (rows, columns) selected so that the $\boldsymbol{B}$ 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'

$$
\boldsymbol{P}_{l} A_{l} Q_{l}^{T}=\left(\begin{array}{cc}
\boldsymbol{B}_{l} & \boldsymbol{F}_{l} \\
\boldsymbol{E}_{l} & \boldsymbol{C}_{l}
\end{array}\right) \approx\left(\begin{array}{cc}
\boldsymbol{L}_{l} & 0 \\
\boldsymbol{E}_{l} \boldsymbol{U}_{l}^{-1} & \boldsymbol{I}
\end{array}\right) \times\left(\begin{array}{cc}
\boldsymbol{U}_{l} & \boldsymbol{L}_{l}^{-1} \boldsymbol{F}_{l} \\
\mathbf{0} & \boldsymbol{A}_{l+1}
\end{array}\right)
$$

where

$$
\begin{aligned}
B_{l} & \approx L_{l} U_{l} \\
A_{l+1} & \approx C_{l}-\left(E_{l} U_{l}^{-1}\right)\left(L_{l}^{-1} F_{l}\right)
\end{aligned}
$$

$>$ As before the matrices $\boldsymbol{E}_{l} \boldsymbol{U}_{l}^{-1}, \boldsymbol{L}_{l}^{-1} \boldsymbol{F}_{l}$ or their approximations

$$
G_{l} \approx E_{l} U_{l}^{-1}, \quad W_{l} \approx L_{l}^{-1} F_{l}
$$

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 $\boldsymbol{B}$ 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

$$
p_{i} \neq p_{j}, \text { for } i \neq j \quad q_{i} \neq q_{j}, \text { for } i \neq j
$$

$>$ 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 $j(i)=\operatorname{argmax}_{j}\left|a_{i j}\right|$.
$>$ Use the ratio $\quad \gamma_{i}=\frac{\left|a_{i, j i}\right|}{\left\|a_{i, i}\right\|_{1}}$ as a measure of diag. domin. of row $i$

## Matching: Greedy algorithm

$>$ Simple algorithm: scan pairs $\left(i_{k}, j_{k}\right)$ in the given order.
$>$ If $i_{k}$ and $j_{k}$ not already assigned, assign them to $\mathcal{M}$.


Matrix after preselection


Matrix after Matching perm.

## 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 $25 \times 20$ grid.
$>$ Add a negative shift of -1 to resulting matrix.
$>$ Do an ILU factorization of $\boldsymbol{A}$ and plot eigs of $\boldsymbol{L}^{-1} \boldsymbol{A} \boldsymbol{U}^{-1}$.
$>$ Used LUINC from matlab-no-pivoting and threshold $=0.1$.

## > Terrible spectrum:


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


## Explanation

## Question:

What if we do an exact factorization [droptol = 0]?
$>\quad \Lambda\left(L^{-1} A U^{-1}\right)=$ $\Lambda\left[(A+\alpha i I)^{-1} A\right]$
$>\Lambda=\left\{\frac{\lambda_{j}}{\lambda_{j}+i \alpha}\right\}$
> Located on a circle with a cluster at one.
> 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 $\Omega_{e}$ of $\mathbb{R}^{d}$

$$
\left\{\begin{aligned}
\Delta u+k^{2} u & =f \quad \text { in } \Omega \\
u & =-u_{i n c} \text { on } \Gamma \\
\text { or } \frac{\partial u}{\partial n} & =-\frac{\partial u_{\text {inc }}}{\partial n} \text { on } \Gamma \\
\lim _{r \rightarrow \infty} r^{(d-1) / 2}\left(\frac{\partial u}{\partial \vec{n}}-i k u\right) & =0 \quad \text { Sommerfeld cond. }
\end{aligned}\right.
$$

where: $\boldsymbol{u}$ the wave diffracted by $\Gamma, f=$ source function = zero outside domain
> Issue: non-reflective boundary conditions when making the domain finite.
$>$ Artificial boundary $\Gamma_{a r t}$ 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 $r_{0}=0.5 \mathrm{~m}$. Incident plane wave with a wavelength $\lambda$; propagates along the $x$-axis. 2nd order Bayliss-Turkel boundary conditions used on $\Gamma_{a r t}$, located at a distance $2 r_{0}$ from obstacle. Discretization: isoparametric elements with 4 nodes. Analytic solution known.


## Comparisons

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


ARMS \& shifted variants


ILUT \& shifted variants
> Wavenumber varied - tests with ILUT

| Preconditioner | $k$ | $\frac{\lambda}{h}$ | Iters. | Fill Factor | $\left\\|(L U)^{-1} e\right\\|_{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ILUT (no shift) | $4 \pi$ | 60 | 134 | 2.32 | $3.65 e+03$ |
|  | $8 \pi$ | 30 | 263 | 2.25 | $1.23 \mathrm{e}+04$ |
|  | $16 \pi$ | 15 | - | - | - |
|  | $24 \pi$ | 10 | - | - | - |
|  | $4 \pi$ | 60 | 267 | 2.24 | $2.29 e+03$ |
|  | $8 \pi$ | 30 | 255 | 2.23 | $4.73 \mathrm{e}+03$ |
|  | $16 \pi$ | 15 | 101 | 3.14 | $6.60 \mathrm{e}+02$ |
|  | $24 \pi$ | 10 | 100 | 3.92 | $2.89 e+02$ |
| ILUT ( $\boldsymbol{\tau}$-based) $)$ |  |  |  |  |  |
|  | $4 \pi$ | 60 | 132 | 2.31 | $2.98 e+03$ |
|  | $8 \pi$ | 30 | 195 | 2.19 | $4.12 e+03$ |
|  | $16 \pi$ | 15 | 75 | 3.11 | $7.46 e+02$ |
|  | $24 \pi$ | 10 | 86 | 3.85 | $2.73 \mathrm{e}+02$ |

> Wavenumber varied - tests with ARMS

| Preconditioner | $k$ | $\frac{\lambda}{h}$ | Iters. | Fill Factor | $\left\\|(\boldsymbol{L U})^{-1} e\right\\|_{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ARMS (no shift) | $4 \pi$ | $\mathbf{6 0}$ | $\mathbf{1 2 0}$ | 3.50 | $7.48 e+03$ |
|  | $\mathbf{8 \pi}$ | $\mathbf{3 0}$ | $\mathbf{1 6 9}$ | 4.03 | $1.66 \mathrm{e}+04$ |
|  | $\mathbf{1 6 \pi}$ | $\mathbf{1 5}$ | $\mathbf{2 8 2}$ | 4.50 | $2.44 \mathrm{e}+03$ |
|  | $\mathbf{2 4 \pi}$ | $\mathbf{1 0}$ | - | - | - |
|  | $\mathbf{4 \pi}$ | $\mathbf{6 0}$ | 411 | 3.83 | $5.12 e+02$ |
|  | $8 \pi$ | $\mathbf{3 0}$ | $\mathbf{3 1 1}$ | 4.37 | $5.67 \mathrm{e}+02$ |
|  | $\mathbf{1 6 \pi}$ | $\mathbf{1 5}$ | $\mathbf{1 8 7}$ | 4.71 | $3.92 \mathrm{e}+02$ |
|  | $\mathbf{2 4 \pi}$ | $\mathbf{1 0}$ | $\mathbf{1 8 5}$ | 3.00 | $2.54 \mathrm{e}+02$ |
|  | $4 \pi$ | $\mathbf{6 0}$ | $\mathbf{1 0 6}$ | 3.45 | $7.56 e+03$ |
| ARMS $(\boldsymbol{\tau}$-based) $)$ | $8 \pi$ | $\mathbf{3 0}$ | 79 | 3.84 | $6.41 \mathrm{e}+03$ |
|  | $\mathbf{1 6 \pi}$ | $\mathbf{1 5}$ | 39 | 3.95 | $1.26 \mathrm{e}+03$ |
|  | $\mathbf{2 4 \pi}$ | $\mathbf{1 0}$ | $\mathbf{9 4}$ | 3.02 | $4.71 \mathrm{e}+02$ |

## 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

## Tesla C1060

** Joint work with Ruipeng Li

## 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 : $2 \times(8 \mathrm{SMXs}) \rightarrow 2 \times 1,536$ cores, 8 GB Mem.; Peak: $\approx 4.6$ TFLOPS]


## The CUDA environment: The big picture

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

## Typical program:

1. Generate data on CPU
2. Allocate memory on GPU cudaMalloc(...)
3. Send data Host $\rightarrow$ GPU cudaMemcpy (...)
4. Execute GPU 'kernel':
kernel $\lll$ (...) $\ggg>$ (..)
5. Copy data GPU $\rightarrow$ CPU
cudaMemcpy (...)


## Sparse matrix computations on GPUs

Main issue in using GPUs for sparse computations:

- Huge performance degradation due to 'irregular sparsity'
> Matrices:

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

> Performance of Mat-Vecs on NVIDIA Tesla C1060

|  | Single Precision |  |  | 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

$$
\begin{aligned}
& \text { for } i=1: n \\
& \quad \text { for } j=i a(i): i a(i+1) \\
& \qquad x(i)=x(i)-a(j)^{*} x(j a(j))
\end{aligned}
$$

ILU preconditioning operations require L/U solves: $\boldsymbol{x} \leftarrow \boldsymbol{U}^{-1} L^{-1} \boldsymbol{x}$
$>$ Sequential outer loop.
end
end
> Parallelism can be achieved with level scheduling:

- Group unknowns into levels
- Compute unknowns $x(i)$ of same level simultaneously
- $1 \leq n l e v \leq n$


## ILU: Sparse Forward/Backward Sweeps

- Very poor performance [relative to CPU]

| Matrix | N | CPU Mflops | GPU-Lev |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | \#lev | Mflops |
| Boeing/bcsstk36 | 23,052 | 627 | 4,457 | 43 |
| FEM/Cantilever | 62,451 | 653 | 2,397 | 168 |
| COP/CASEYK | 696,665 | 394 | 273 | 142 |
| COP/CASEKU | 208,340 | 373 | 272 | 115 |

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 Chandrasekaran, 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 $\boldsymbol{n}_{\boldsymbol{x}} \times \boldsymbol{n}_{\boldsymbol{y}}$ grid

$$
\left.\begin{array}{l}
A=\left(\begin{array}{cccc|ccc}
\boldsymbol{A}_{1} & \boldsymbol{D}_{2} & & & \\
\boldsymbol{D}_{2} & \boldsymbol{A}_{2} & \boldsymbol{D}_{3} & & & & \\
& \ddots & \cdots & \cdots & & & \\
& & \boldsymbol{D}_{\alpha} & \boldsymbol{A}_{\alpha} & \boldsymbol{D}_{\alpha+1} & & \\
\hline & & & \boldsymbol{D}_{\alpha+1} & \boldsymbol{A}_{\alpha+1} & \cdots & \\
& & & & \cdots & \cdots & \cdots \\
& & & & & \boldsymbol{D}_{n_{y}} & \boldsymbol{A}_{n_{y}}
\end{array}\right) \\
A=\left(\begin{array}{ll}
\boldsymbol{A}_{11} & \boldsymbol{A}_{12} \\
\boldsymbol{A}_{21} & \boldsymbol{A}_{22}
\end{array}\right) \equiv\left(\begin{array}{ll}
\boldsymbol{A}_{11} & \\
& \boldsymbol{A}_{22}
\end{array}\right)+\left(\right.
\end{array}\right)
$$

## Corresponding splitting on FD mesh:


$>\boldsymbol{A}_{11} \in \mathbb{R}^{m \times m}, \boldsymbol{A}_{22} \in \mathbb{R}^{(n-m) \times(n-m)}$
$>$ In the simplest case second matrix is:

$$
\begin{aligned}
& \left(\begin{array}{ll}
\boldsymbol{A}_{11} & \boldsymbol{A}_{12} \\
\boldsymbol{A}_{21} & \boldsymbol{A}_{22}
\end{array}\right)=\left(\begin{array}{ll}
\boldsymbol{A}_{11} & \\
& \boldsymbol{A}_{22}
\end{array}\right)+\begin{array}{|c|c|}
\hline-1 \\
& \\
& \\
&
\end{array} \\
& >\text { Write 2nd } \\
& \text { matrix as: } \\
& \mathbf{E}^{\mathbf{\top}}=\square \mathbf{I} \text { I }
\end{aligned}
$$

- Above splitting can be rewritten as

$$
\boldsymbol{A}=\underbrace{\left(\boldsymbol{A}+\boldsymbol{E} \boldsymbol{E}^{T}\right)}_{B}-\boldsymbol{E} \boldsymbol{E}^{T}
$$

$$
\begin{gathered}
A=\boldsymbol{B}-\boldsymbol{E} \boldsymbol{E}^{T} \\
B:=\left(\begin{array}{cc}
\boldsymbol{B}_{1} & \\
& \boldsymbol{B}_{2}
\end{array}\right) \in \mathbb{R}^{n \times n}, \quad \boldsymbol{E}:=\binom{\boldsymbol{E}_{1}}{\boldsymbol{E}_{2}} \in \mathbb{R}^{n \times n_{x}}
\end{gathered}
$$

Note: $B_{1}:=A_{11}+E_{1} E_{1}^{T}, \quad B_{2}:=A_{22}+E_{2} E_{2}^{T}$.
> Shermann-Morrison formula:

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

$$
\begin{aligned}
A^{-1} & =B^{-1}+\left(B^{-1} E\right) X^{-1}\left(B^{-1} E\right)^{T} \\
\boldsymbol{X} & =\boldsymbol{I}-\boldsymbol{E}^{T} \boldsymbol{B}^{-1} \boldsymbol{E}
\end{aligned}
$$

$>$ Note: $\boldsymbol{E} \in \mathbb{R}^{n \times n_{x}}, \boldsymbol{X} \in \mathbb{R}^{n_{x} \times n_{x}}$
$>\boldsymbol{n}_{x}=$ number of points in separator $\left[O\left(\boldsymbol{n}^{1 / 2}\right)\right.$ for 2-D mesh, $O\left(n^{2 / 3}\right)$ 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 $\boldsymbol{X}$ and exploit recursivity

$$
B^{-1}\left[v+\boldsymbol{E} \tilde{\boldsymbol{X}}^{-1} \boldsymbol{E}^{T} B^{-1} \boldsymbol{v}\right] .
$$

> However wont work: cost explodes with \# levels
> Alternative: lowrank approx. for $\boldsymbol{B}^{-1} \boldsymbol{E}$

$$
\begin{array}{ll}
B^{-1} \boldsymbol{E} \approx \boldsymbol{U}_{k} \boldsymbol{V}_{k}^{T}, \quad \begin{array}{l}
U_{k} \in \mathbb{R}^{n \times k}, \\
V_{k} \in \mathbb{R}^{n_{x} \times k}
\end{array},
\end{array}
$$

## Multilevel Low-Rank (MLR) algorithm

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

$$
\boldsymbol{B}^{-1} \boldsymbol{E} \approx \boldsymbol{U}_{k} \boldsymbol{V}_{k}^{T}
$$

$$
\begin{aligned}
& \boldsymbol{U}_{k} \in \mathbb{R}^{n \times k} \\
& \boldsymbol{V}_{k} \in \mathbb{R}^{n_{x} \times k}
\end{aligned}
$$

$>$ Replace $\boldsymbol{B}^{-1} \boldsymbol{E}$ by $\boldsymbol{U}_{k} \boldsymbol{V}_{k}^{T}$ in $\boldsymbol{X}=\boldsymbol{I}-\left(\boldsymbol{E}^{T} \boldsymbol{B}^{-1}\right) \boldsymbol{E}$ :

$$
\boldsymbol{X} \approx \boldsymbol{G}_{k}=\boldsymbol{I}-\boldsymbol{V}_{k} \boldsymbol{U}_{k}^{T} \boldsymbol{E}, \quad\left(\in \mathbb{R}^{n_{x} \times n_{x}}\right) \quad \text { Leads to } \ldots
$$



$$
\begin{gathered}
M^{-1}=B^{-1}+U_{k} H_{k} U_{k}^{T}, \quad H_{k}=V_{k}^{T} G_{k}^{-1} V_{k} \\
\text { Use recursivity }
\end{gathered}
$$

We can show :

$$
\begin{aligned}
& \boldsymbol{H}_{k}=\left(\boldsymbol{I}-\boldsymbol{U}_{k}^{T} \boldsymbol{E} V_{k}\right)^{-1} \quad \text { and } \\
& \boldsymbol{H}_{k}^{T}=\boldsymbol{H}_{k}
\end{aligned}
$$

## Recursive multilevel framework

- $\boldsymbol{A}_{i}=\boldsymbol{B}_{i}+\boldsymbol{E}_{i} \boldsymbol{E}_{i}^{T}, \boldsymbol{B}_{i} \equiv\left(\begin{array}{lll}\boldsymbol{B}_{i_{1}} & \\ & \boldsymbol{B}_{i_{2}}\end{array}\right)$.
- Next level, set $\boldsymbol{A}_{i_{1}} \equiv \boldsymbol{B}_{i_{1}}$ and $\boldsymbol{A}_{i_{2}} \equiv \boldsymbol{B}_{i_{2}}$
- Repeat on $\boldsymbol{A}_{i_{1}}, \boldsymbol{A}_{i_{2}}$
- Last level, factor $\boldsymbol{A}_{i}$ (IC, ILU)
- Binary tree structure:



## Generalization: Domain Decomposition framework

Domain partitioned into 2 domains with an edge separator

> Matrix can be permuted to:

$$
P A P^{T}=\left(\begin{array}{cc|cc}
\hat{B}_{1} & \hat{F}_{1} & & \\
\hat{F}_{1}^{T} & C_{1} & & -X \\
\hline & & \hat{B}_{2} & \hat{F}_{2} \\
& -X^{T} & \hat{F}_{2}^{T} & C_{2}
\end{array}\right)
$$

$>$ 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.)

$$
\text { Let: } \quad \boldsymbol{E}_{\alpha}=\left(\begin{array}{c}
0 \\
\alpha I \\
0 \\
\frac{X^{T}}{\alpha}
\end{array}\right) \quad \text { then we have: }
$$

$$
\begin{gathered}
\boldsymbol{P A} A P^{T}=\left(\begin{array}{ll}
B_{1} & \\
& B_{2}
\end{array}\right)-\boldsymbol{E} \boldsymbol{E}^{T} \quad \text { with } \quad \boldsymbol{B}_{i}=\left(\begin{array}{cc}
\hat{\boldsymbol{B}}_{i} & \hat{\boldsymbol{F}}_{1} \\
\hat{\boldsymbol{F}}_{i}^{T} & C_{i}+D_{i}
\end{array}\right) \\
\text { and }\left\{\begin{array}{l}
D_{1}=\alpha^{2} \boldsymbol{I} \\
D_{2}=\frac{1}{\alpha^{2}} \boldsymbol{X}^{T} \boldsymbol{X}
\end{array}\right.
\end{gathered}
$$

$>\alpha$ used for balancing
> Better results when using diagonals instead of $\alpha I$

## 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)
- Stop when: $\left\|r_{i}\right\| \leq 10^{-8}\left\|r_{0}\right\|$ or its exceeds 500
- Model Problems in 2-D/3-D:

$$
-\Delta u-c u=g \text { in } \Omega \quad+\text { В.С. }
$$

-2-D: $g(x, y)=-\left(x^{2}+y^{2}+c\right) e^{x y} ; \quad \Omega=(0,1)^{3}$.

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


## Symmetric indefinite cases

- $c>0$ in $-\Delta u-c u$; i.e., $-\Delta$ shifted by $-s I$.
- 2D case: $s=0.01$, 3D case: $s=0.05$
- MLR + GMRES(40) compared to ILDLT + GMRES(40)
- 2-D problems: $\# \mathrm{lev}=4$, 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 | ILDLT-GMRES |  |  |  | MLR-GMRES |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | fill |  |  | i-t | fill |  |  | 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 |  |
| $32^{2} \times 64$ | 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 | N | NNZ | SPD $\quad$ 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 | $k$ | 元 | fill | p-t | its | i-t |  |
|  | 2.6 | 0.44 | 32 | 0.16 | 2 | 6 | 2.3 | 1.38 | 27 | 0.08 |  |
|  | 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 |  |


|  | ICT/ILDLT |  |  |  |  | MLR-CG/GMRES |  |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| MATRIX | fill | p-t | its | i-t | $k$ | d | 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

