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Multilevel preconditioning techniques with applications

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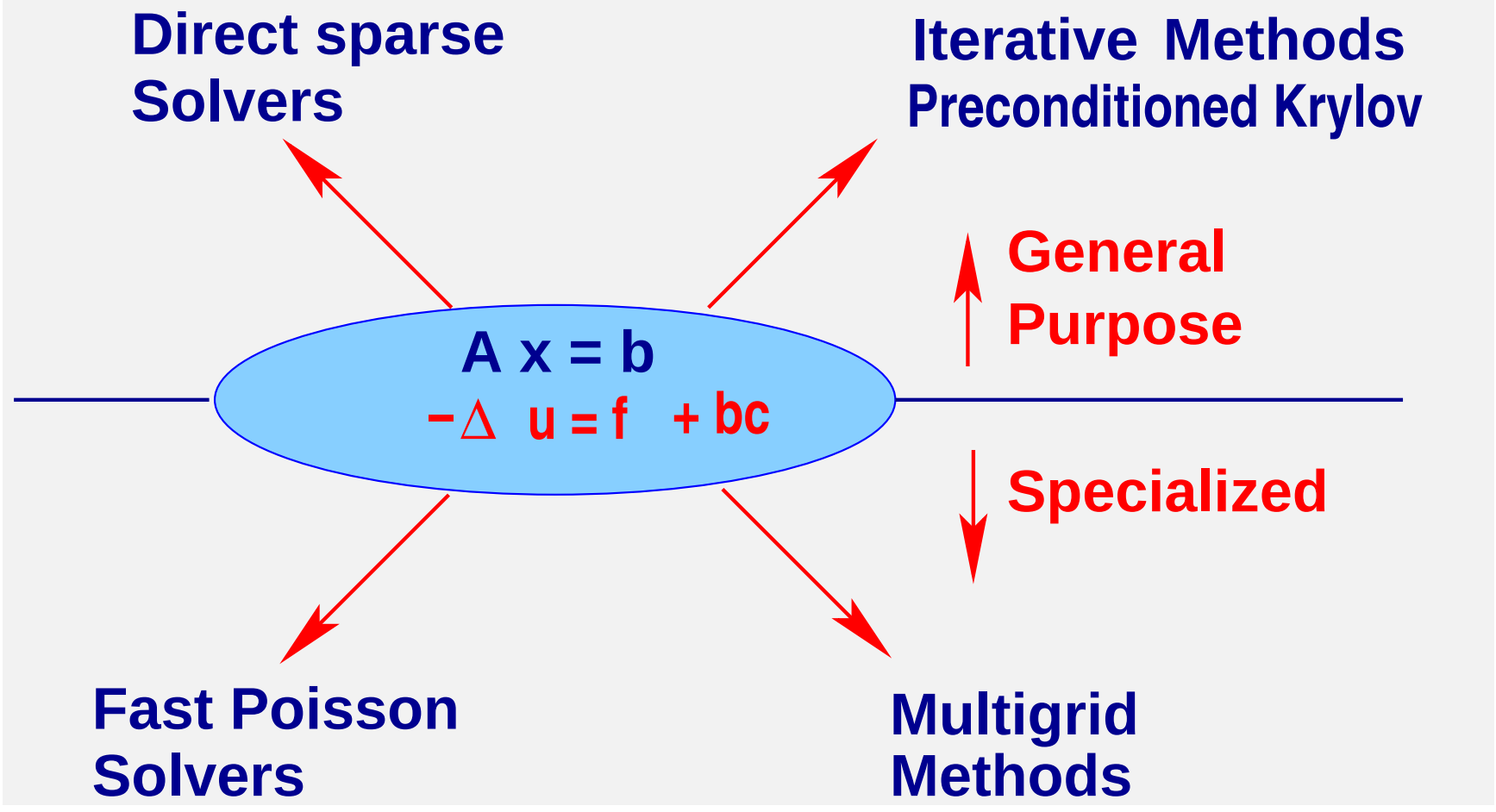
Introduction: Linear System Solvers



A few observations

- Problems are getting harder for Sparse Direct methods (more 3-D models, much bigger problems,..)
- Problems are also getting difficult for iterative methods Cause: more complex models - away from Poisson
- Researchers on both camps are learning each other's tricks to develop preconditioners.
- Much of recent work on solvers has focussed on:

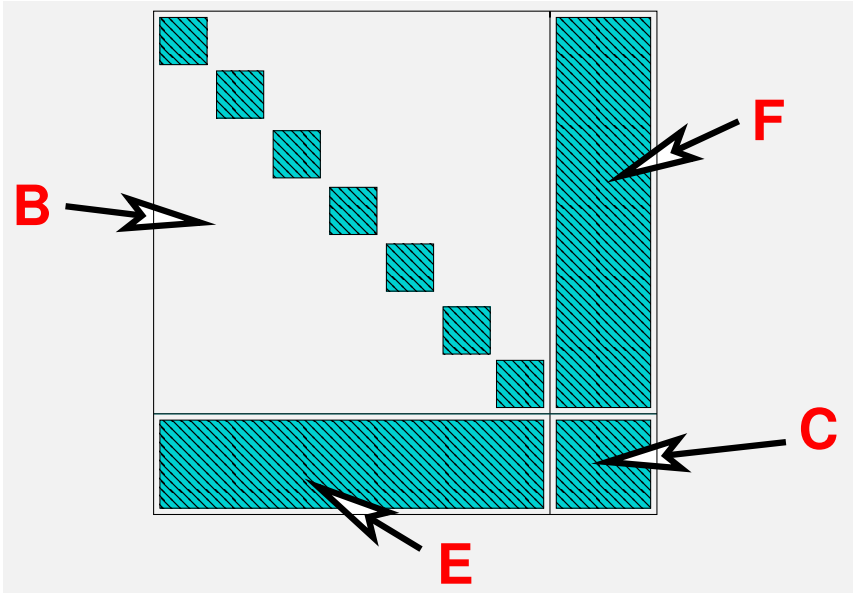
(1) Parallel implementation – scalable performance

(2) Improving Robustness, developing more general preconditioners

Algebraic Recursive Multilevel Solver (ARMS)

- Reorder matrix using 'group-independent sets'. Result

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



- Block factorize:

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

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

- Next step: treat the Schur complement recursively

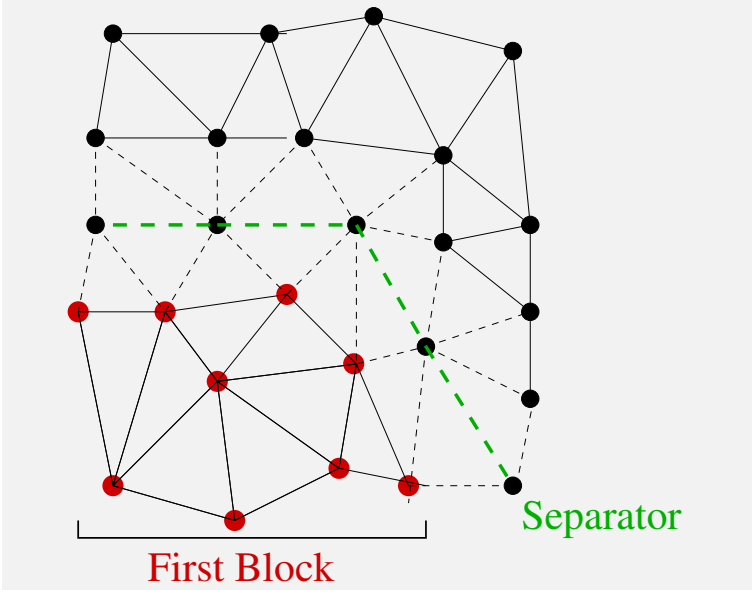
Algebraic Recursive Multilevel Solver (ARMS)

Level l Factorization:

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

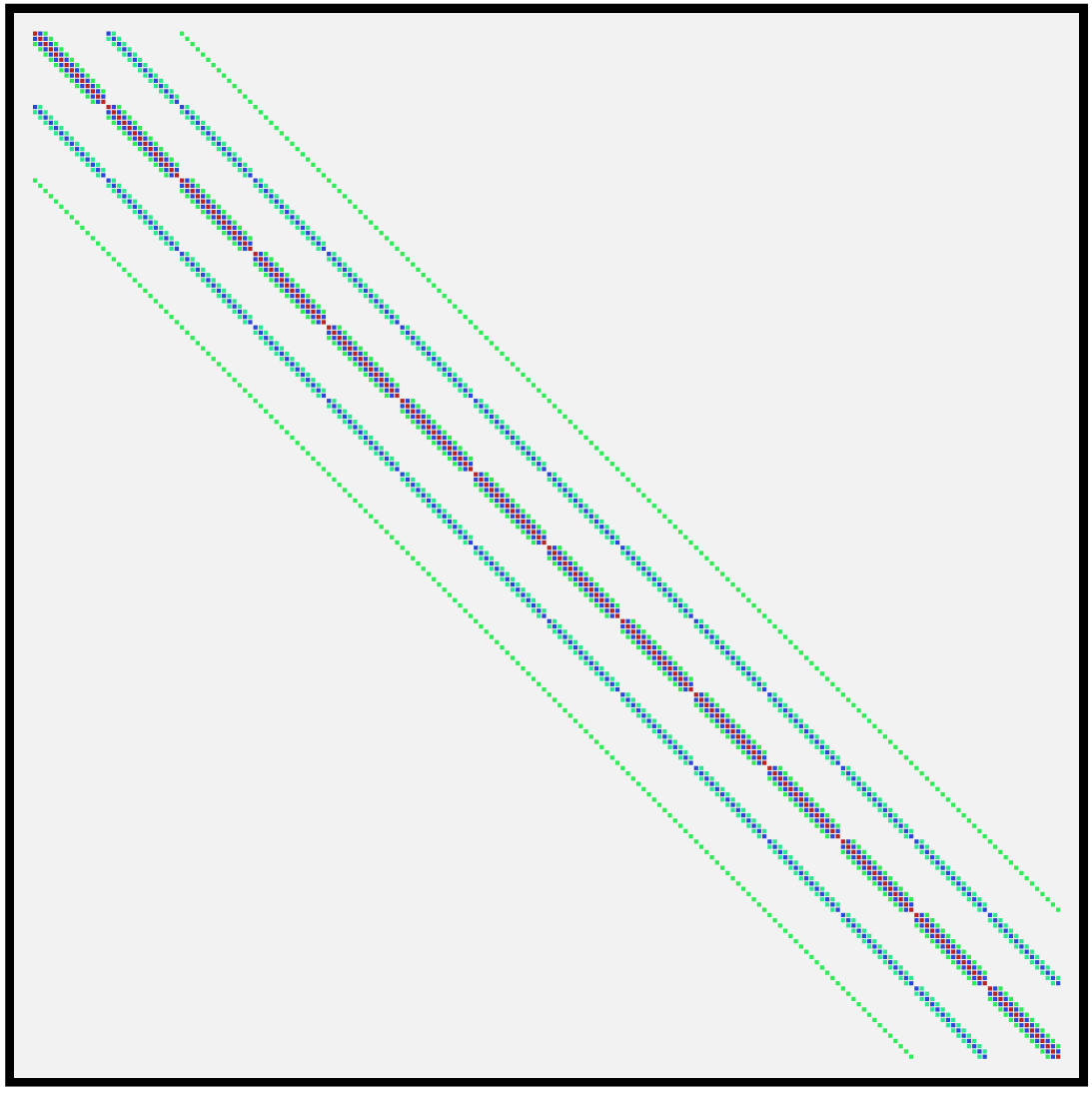
- L-solve $\sim$ restriction; U-solve $\sim$ prolongation.
- Perform above block factorization recursively on A_{l+1}
- Blocks in B_l treated as sparse. Can be large or small.
- Algorithm is fully recursive
- Stability criterion in block independent sets algorithm

Group Independent Set reordering

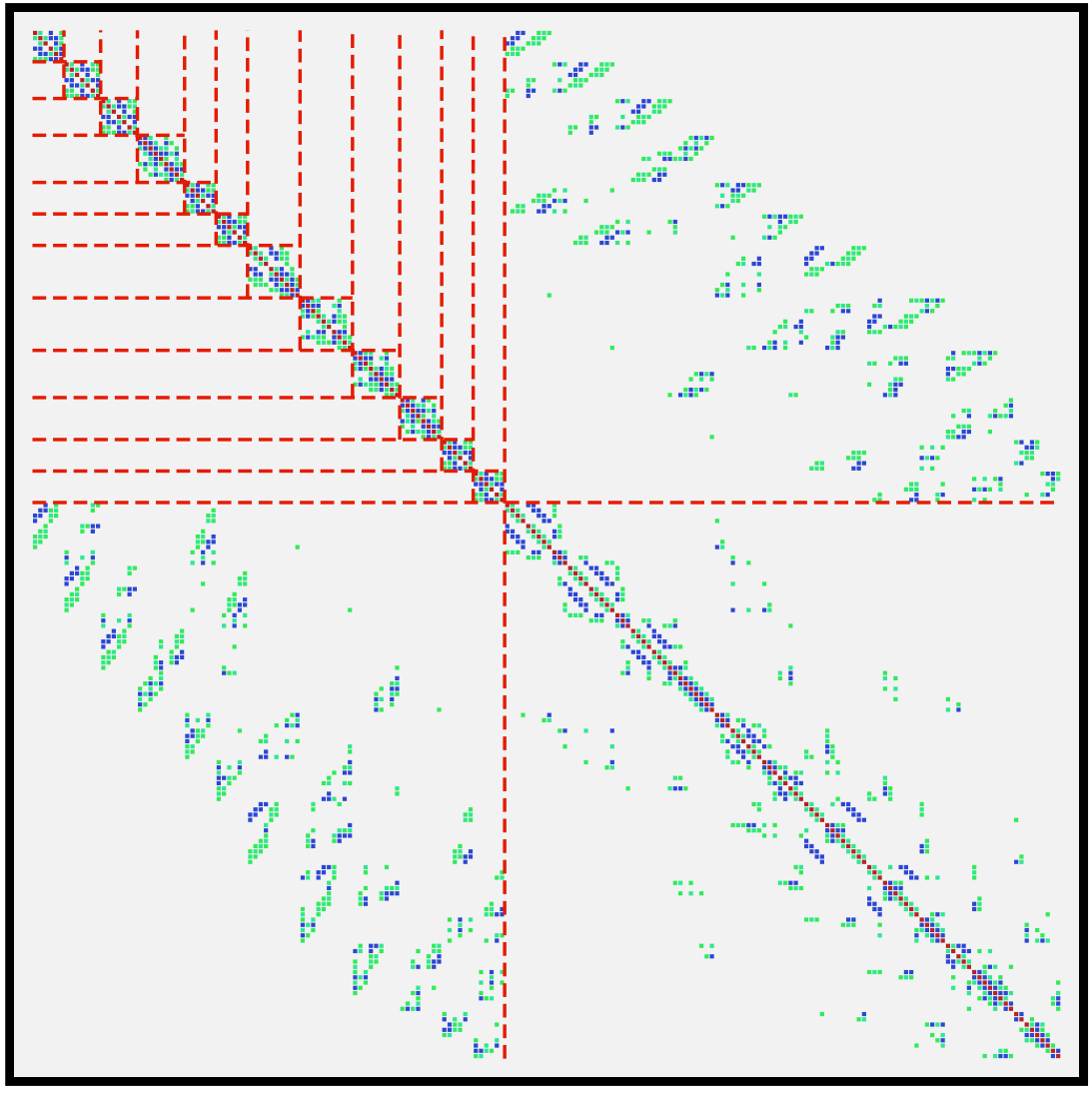


Simple strategy: Level taversal until there are enough points to form a block. Reverse ordering. Start new block from non-visited node. Continue until all points are visited. Add criterion for rejecting "not sufficiently diagonally dominant rows."

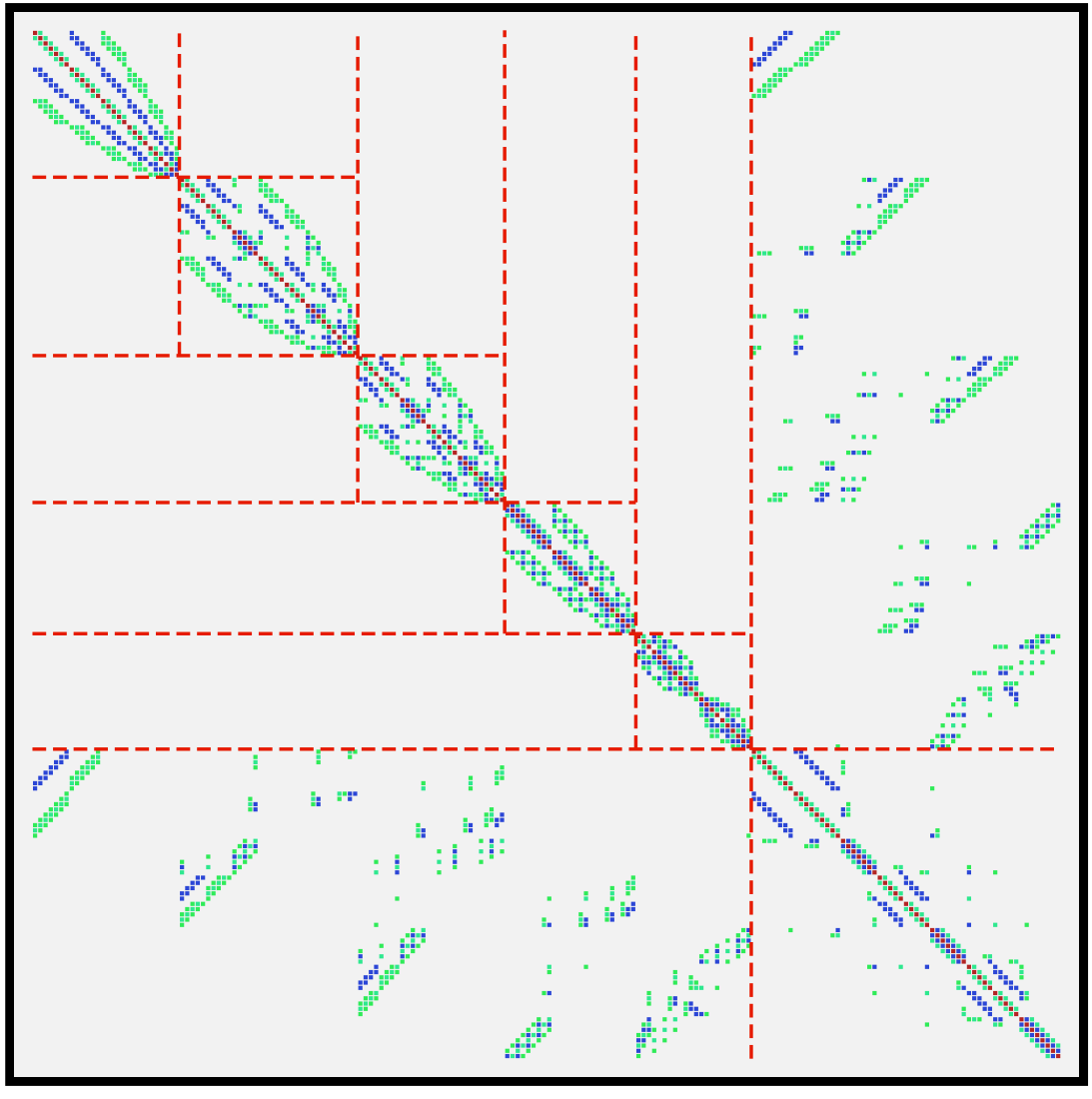
Original matrix



Block size of 6



Block size of 20



Related ideas

➤ See *Y. Notay*, Algebraic Multigrid and algebraic multilevel techniques, a theoretical comparison, NLAA, 2005.

➤ Some of these ideas are related to work by Axelsson and co-workers [e.g., AMLI] – see Axelsson's book

➤ Work by Bank & Wagner on MLILU quite similar to ARMS – but uses AMG framework: [*R. E. Bank and C. Wagner*, Multilevel ILU decomposition, Numer. Mat. (1999)]

➤ Main difference with AMG framework: block ILU-type factorization to obtain Coarse-level operator. + use of relaxation.

➤ In AMG $\boldsymbol{S = P^T A P}$ with $\boldsymbol{P}$ of size $\boldsymbol{(n_F + n_C) \times n_C}$

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 $\longrightarrow$ 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

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

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

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

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 B is of dimension 1 $\longrightarrow$ 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

$$p_i \neq p_j, \text{ for } i \neq j \qquad q_i \neq q_j, \text{ for } i \neq j$$

➤ When $n_M = n \longrightarrow$ (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.

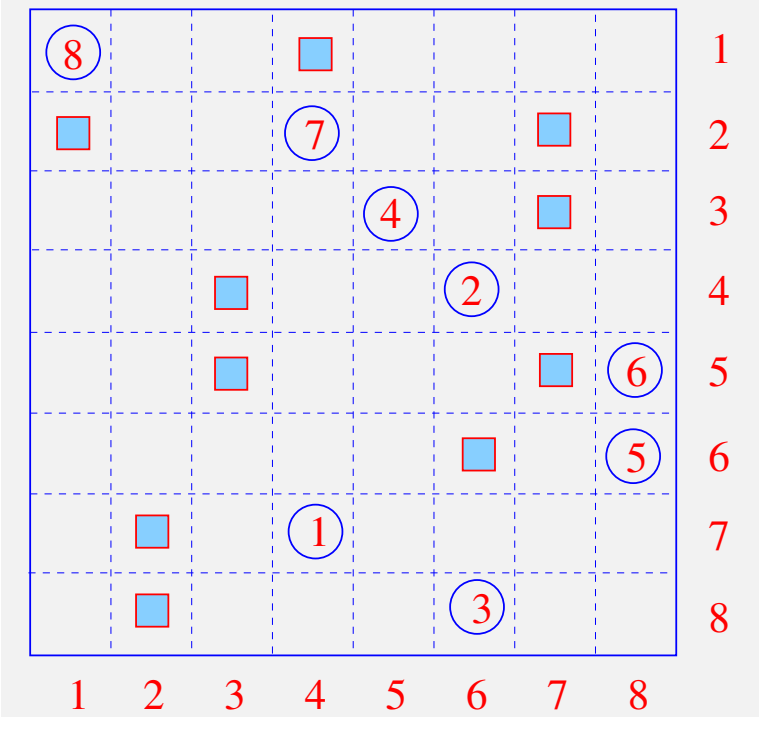
(2) Matching: scan candidate entries in order given by preselection and accept them into the $\mathfrak{M}$ set, or reject them.

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

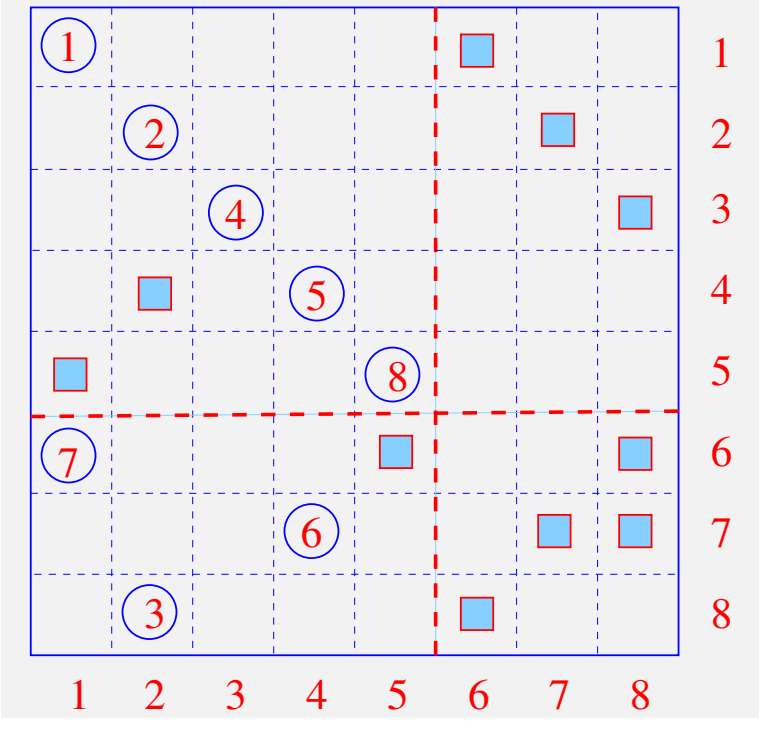
- Let $j(i) = \mathbf{argmax}_j |a_{ij}|$.
- Use the ratio $\gamma_i = \frac{|a_{i,j(i)}|}{\|a_{i,:}\|_1}$ as a measure of diag. domin. of row i

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 $\mathcal{M}$.



Matrix after preselection



Matrix after Matching perm.

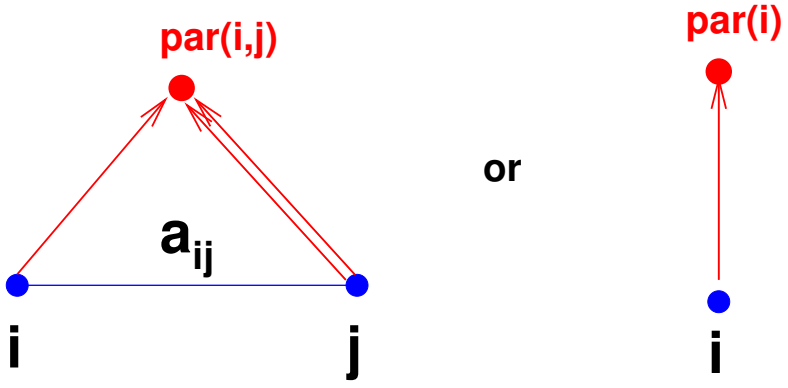
MATLAB DEMO

COARSENING

Divide and conquer and coarsening (work in progress)

➤ Want to mix ideas from AMG with purely algebraic strategies based on graph coarsening

First step: Coarsen. We use matching: coalesce two nodes into one 'coarse' node

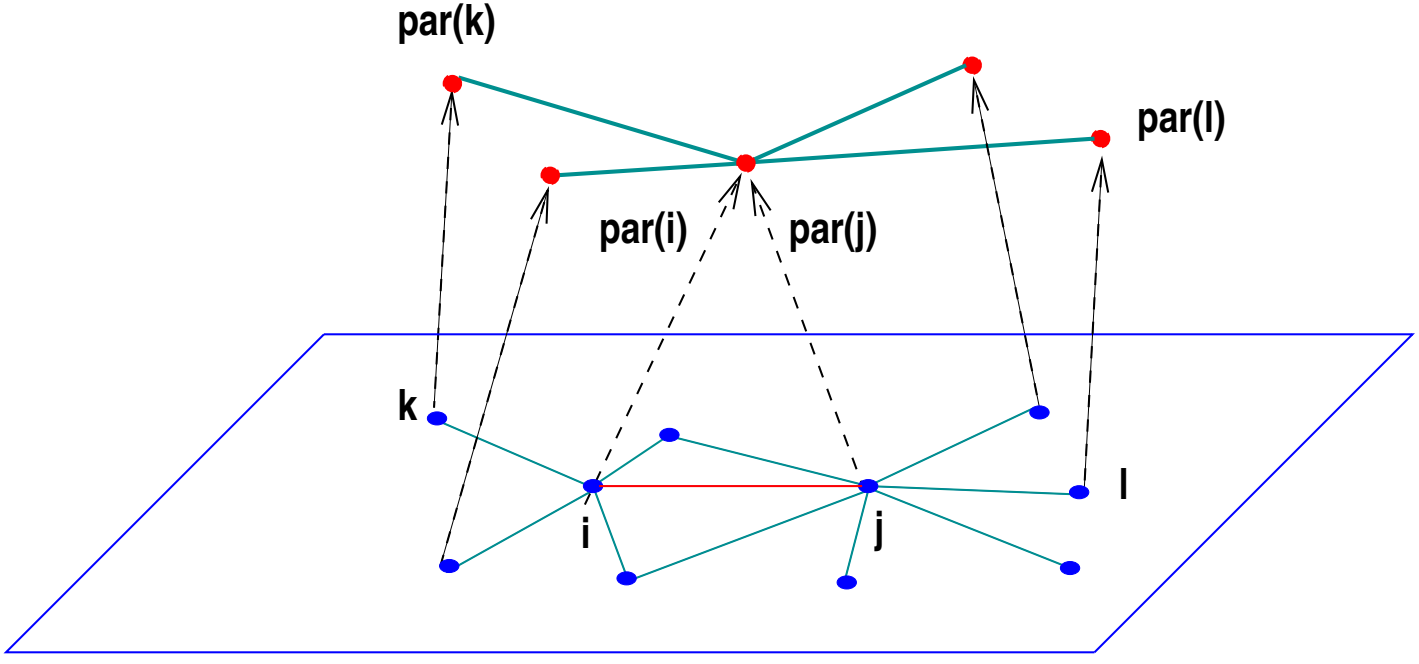


Second step: Get graph (+ weights) for the coarse nodes - One way to define Adj$[par(i,j)]$:

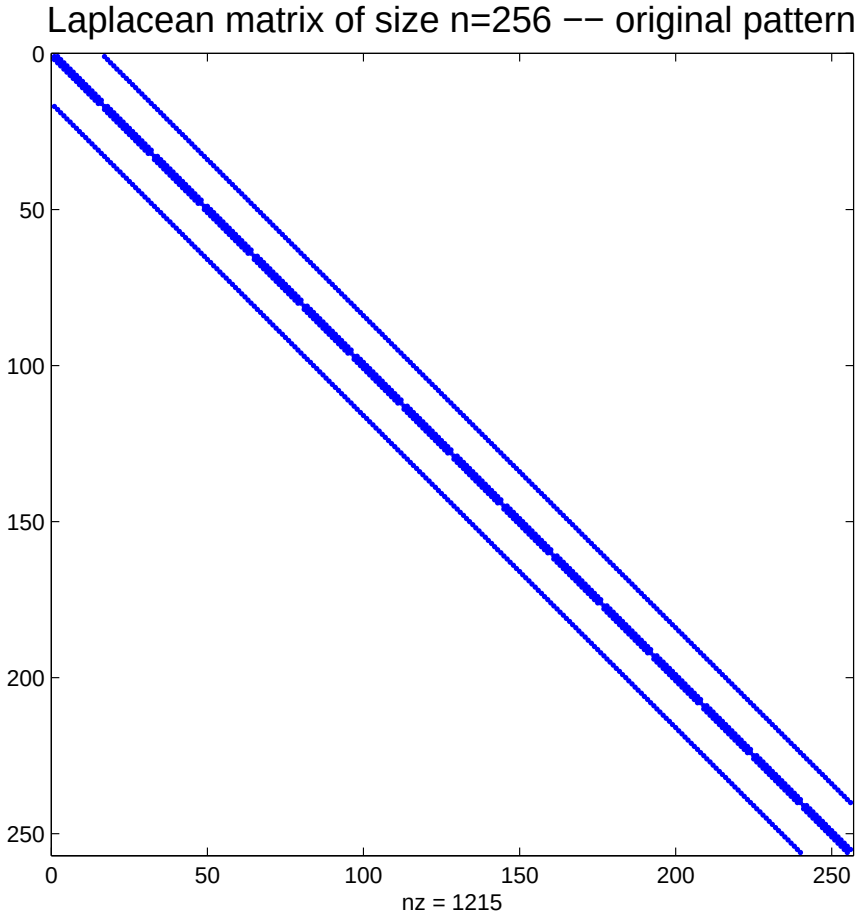
$$\{par(i,k)\ k \in Adj(i)\} \bigcup \{par(j,k)\ k \in Adj(j)\}$$

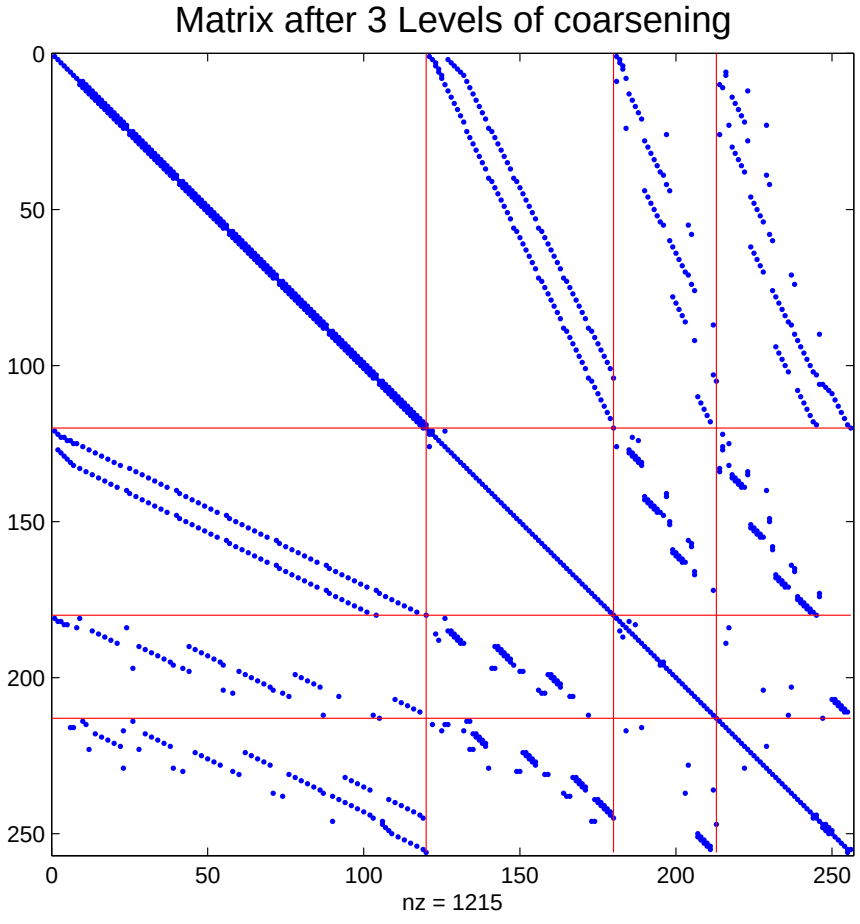
Third step: Repeat

Illustration of the coarsening step



Example 1: A simple 16×16 mesh ($n = 256$).



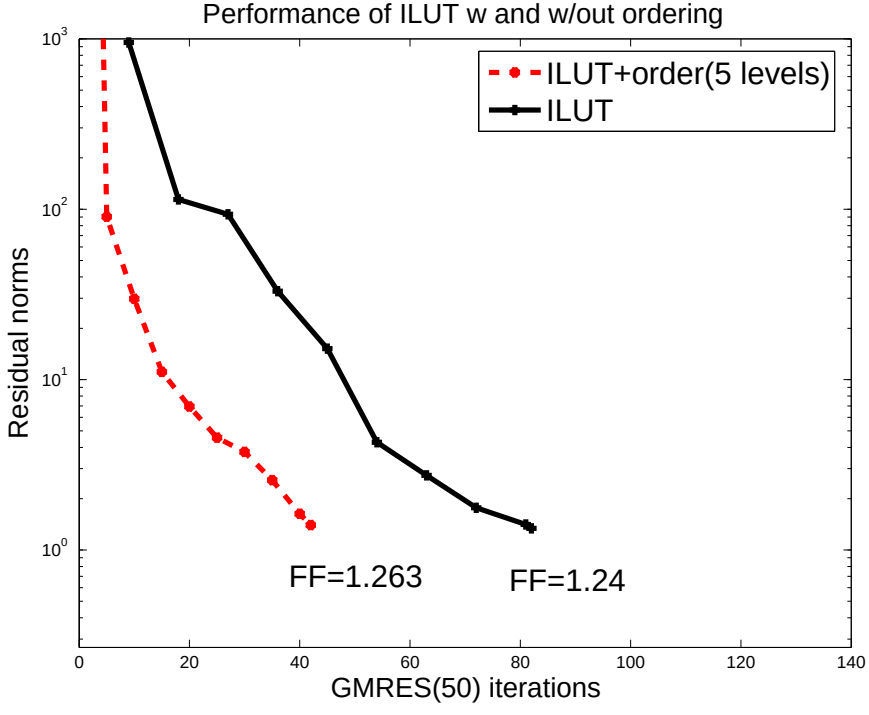


First idea: use ILU on the reordered matrix

- For example: use ILUT

Illustration: Matrix Raj1 from the Florida collection

- Size $n = 263,743$. $Nnz = 1,302,464$ nonzero entries
- Matrix is nearly singular – poorly conditioned. Iterate to reduce residual by 10^{10}.



- Reordering appears to be quite good for ILU.

Saving memory with Pruned ILU

- Let $A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = \begin{pmatrix} I & 0 \\ EB^{-1} & I \end{pmatrix} \begin{pmatrix} B & F \\ 0 & S \end{pmatrix}$;
- $S = C - EB^{-1}F$ = Schur complement

Solve:

$$\begin{pmatrix} I & 0 \\ EB^{-1} & I \end{pmatrix} \begin{pmatrix} B & F \\ 0 & S \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = ..$$

1) $w_1 = B^{-1} b_1$
2) $w_2 = b_2 - E * w_1$
3) $x_2 = S^{-1} w_2$
4) $w_1 = b_1 - F * x_2$
5) $x_1 = B^{-1} w_1$

- Known result: LU factorization of S == trace of LU factorization of A.
- Idea: exploit recursivity for B-solves - keep only the block-diagonals from ILU..

From L U =

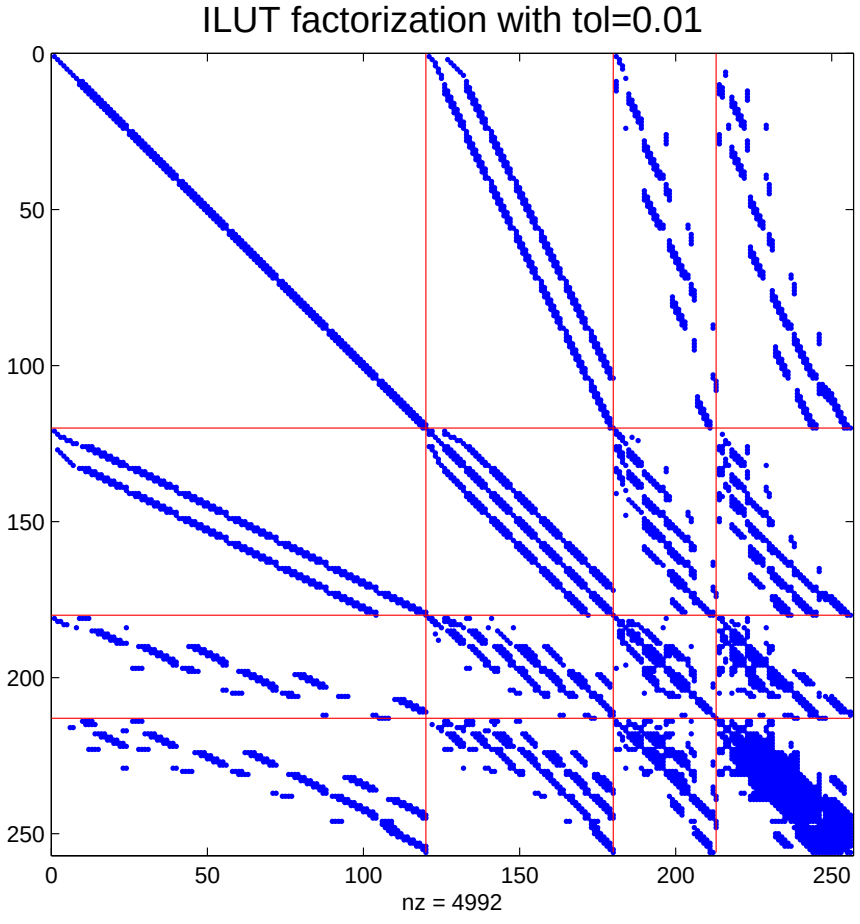
$$\left[\begin{array}{c|c|c} B_1 & B_1^{-1}F_1 & B_2^{-1}F_2 \\ \hline E_1B_1^{-1} & S_1 & \\ \hline \multicolumn{2}{c|}{E_2B_2^{-1}} & S_2 \end{array}\right]$$

Keep only

$$\left[\begin{array}{c|c|c} B_1 & & \\ \hline & S_1 & \\ \hline & & S_2 \end{array}\right]$$

- Big savings in memory
- Additional computational cost
- Expensive for more than a few levels (2 or 3)..

Example : A simple 16×16 mesh ($n = 256$).



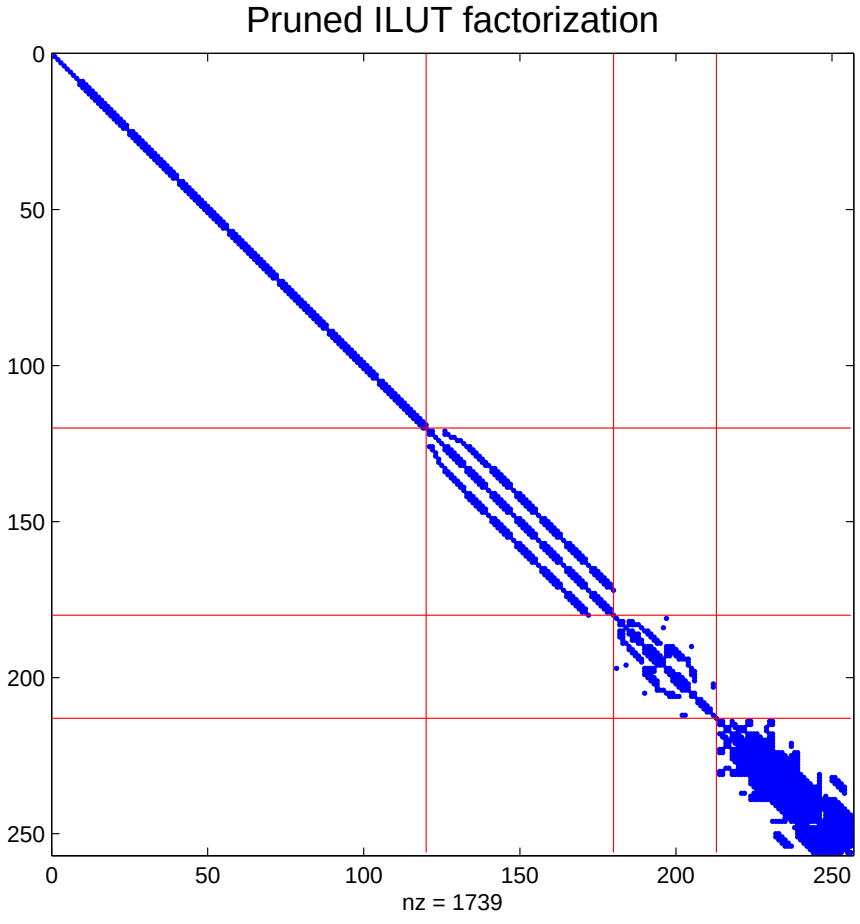
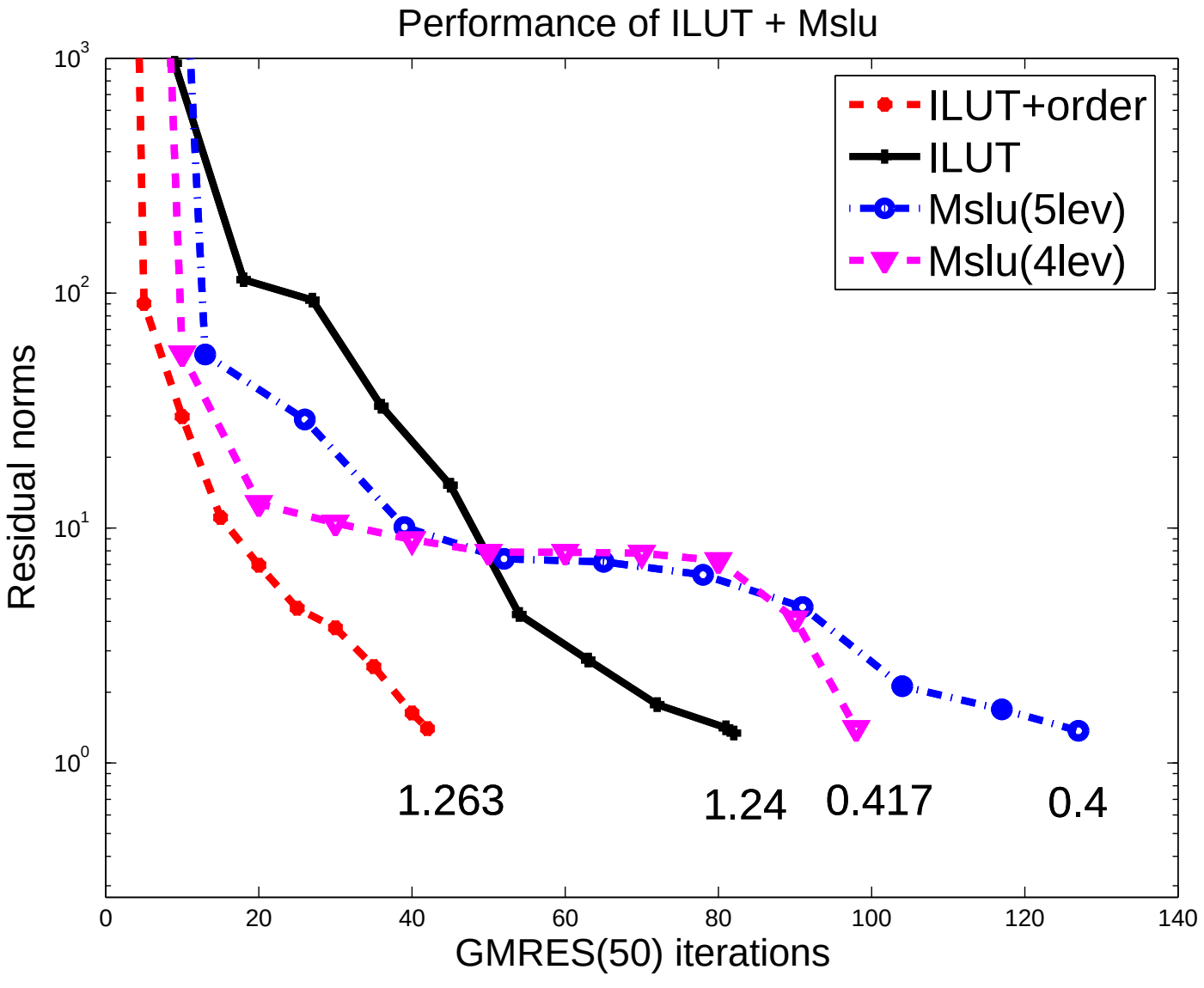


Illustration: Back to Raj1 matrix from the Florida collection



HELMHOLTZ

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 $\mathbb{R}^d$

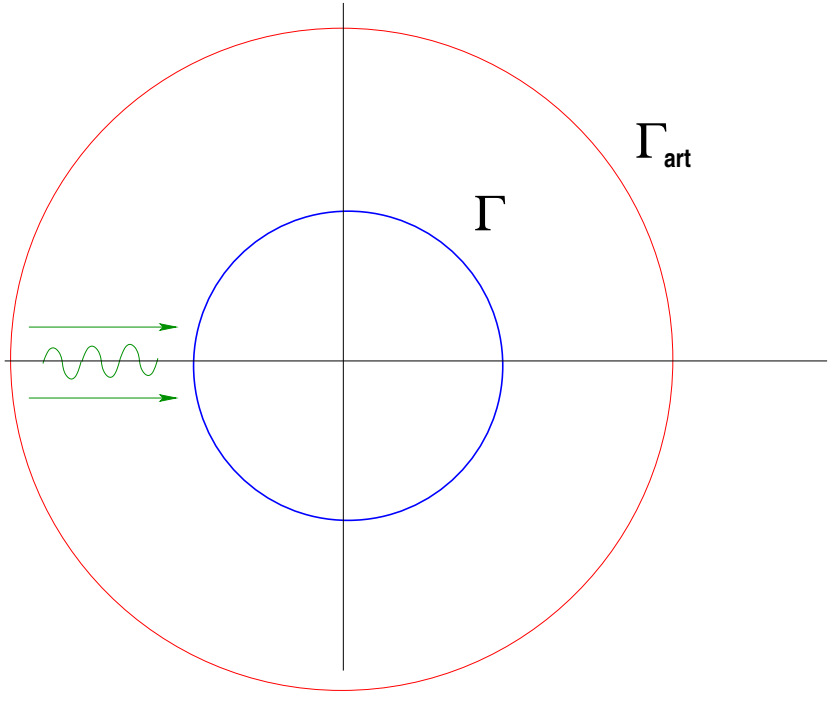
$$\begin{cases} \Delta u + k^2 u = f \quad \text{in} \quad \Omega \\ u = -u_{inc} \quad \text{on} \quad \Gamma \\ or \ \frac{\partial u}{\partial n} = -\frac{\partial u_{inc}}{\partial n} \quad \text{on} \quad \Gamma \\ \\ lim_{r\to\infty} \ r^{(d-1)/2} \ \left(\frac{\partial u}{\partial \vec{n}} - iku\right) = 0 \quad \text{Sommerfeld cond.} \end{cases}$$

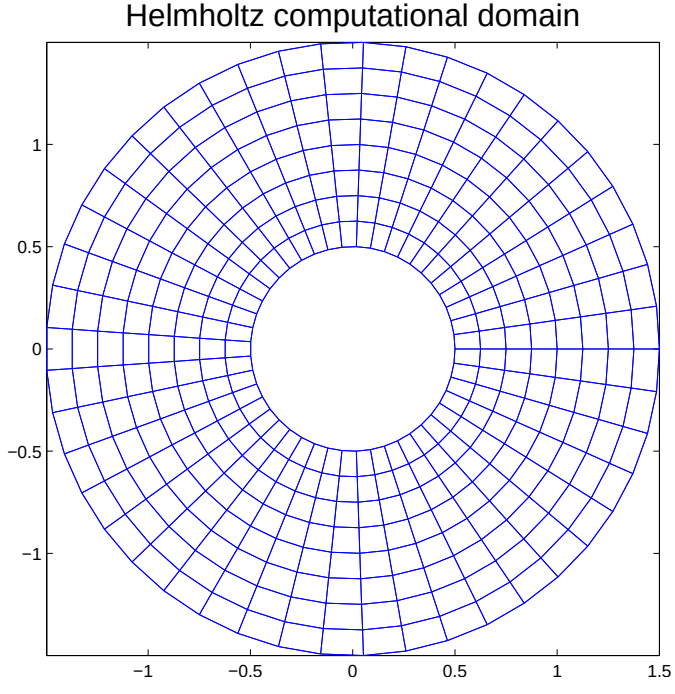
where: u the wave diffracted by Γ, f = source function = zero outside domain

- 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.





Use of complex shifts

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

[1] X. Antoine – Private comm.

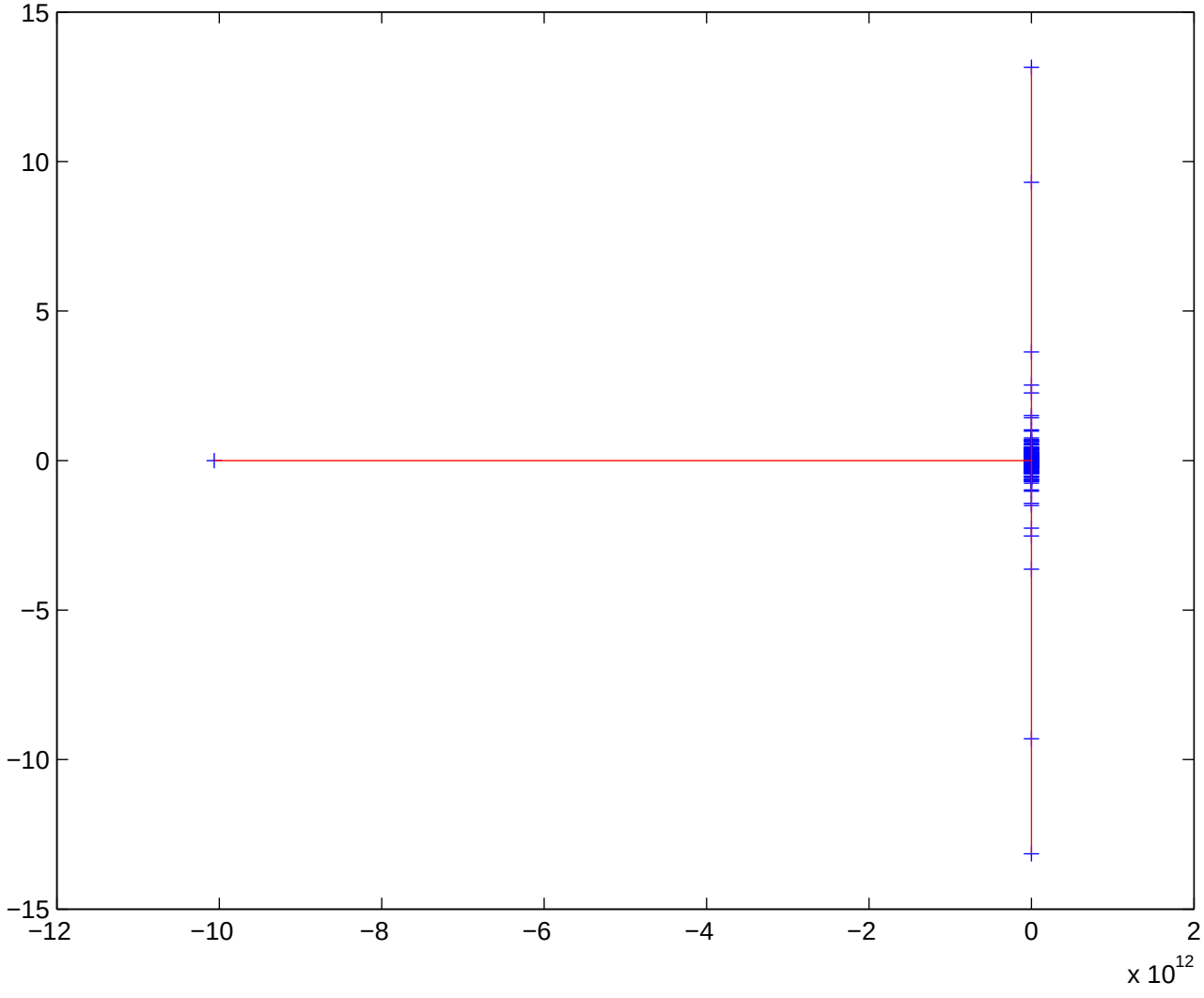
[2] Y.A. Erlangga, C.W. Oosterlee and C. Vuik, SIAM J. Sci. Comput.,27, pp. 1471-1492, 2006

[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.

- 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.

Terrible spectrum:

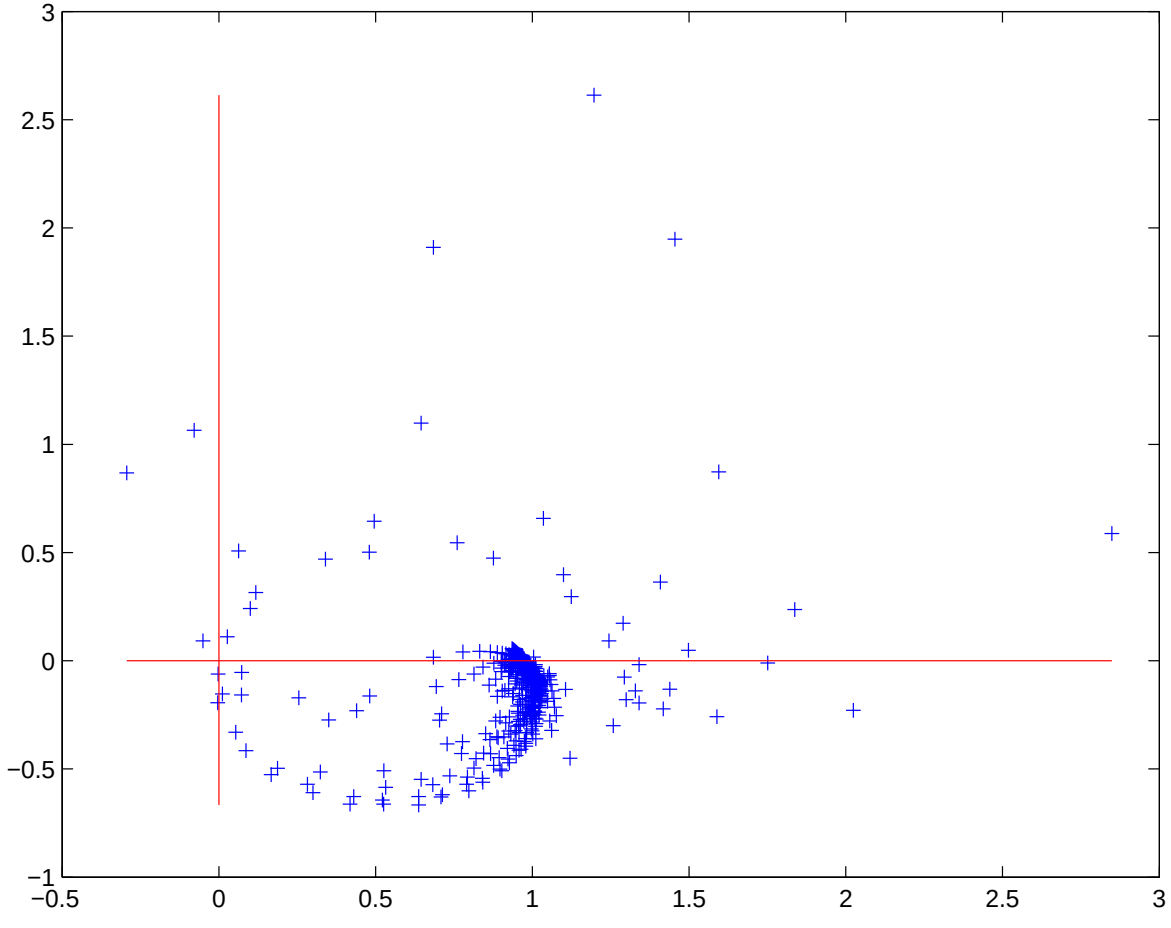


➤ Now plot eigs of $L^{-1}AU^{-1}$ where L, U are inc. LU factors of $B = A + 0.25 * i$

➤ Much better! Observed by many [PDE viewpoint]

Idea:

Adapt technique to ILU:
Add complex shifts before ILU

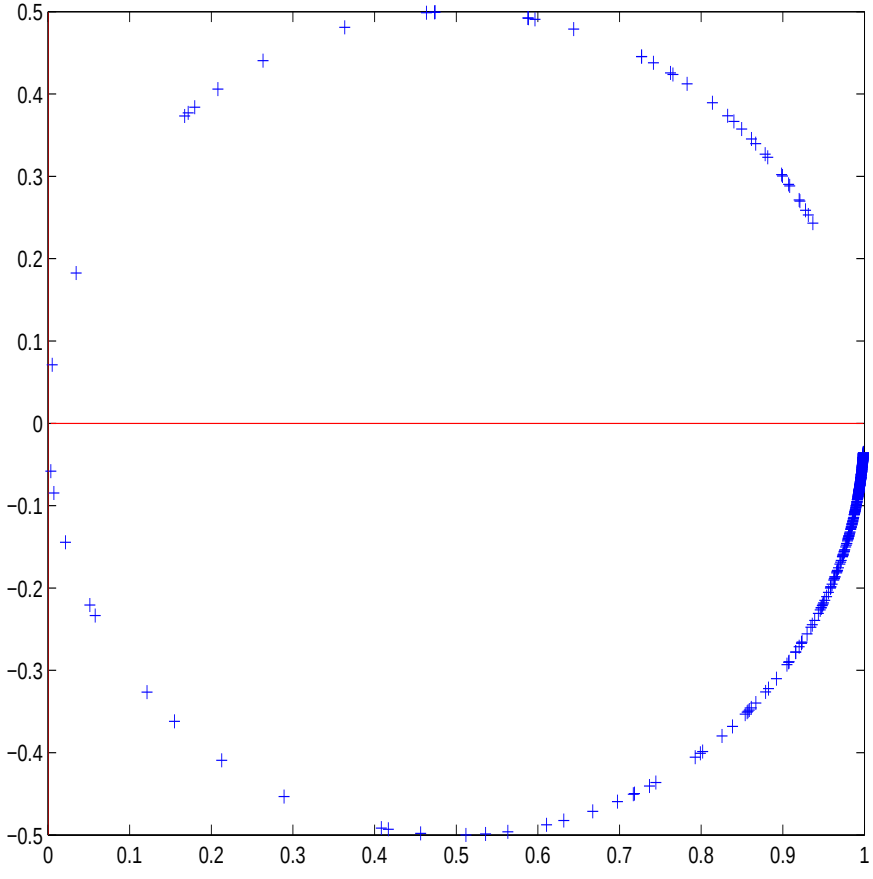


Explanation

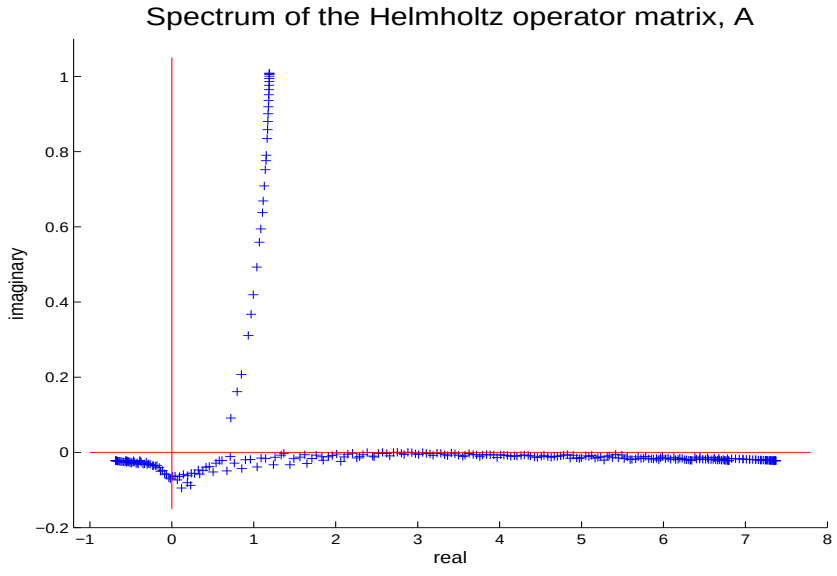
Question:

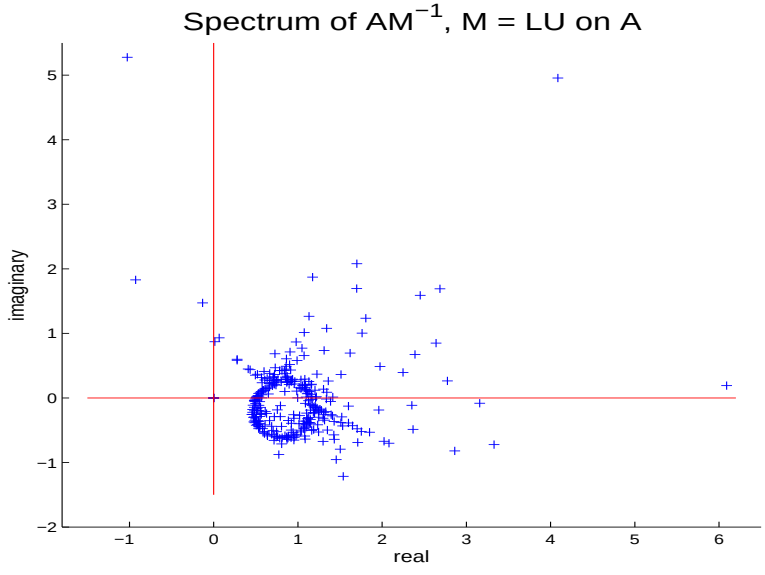
What if we do an exact factorization [droptol = 0]?

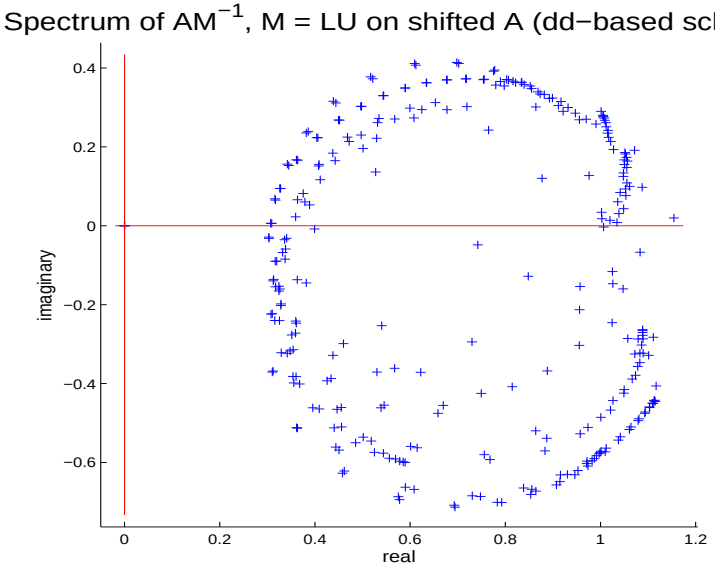
- $\Lambda(L^{-1}AU^{-1}) = \Lambda[(A+\alpha iI)^{-1}A]$
- $\Lambda = \left\{\frac{\lambda_j}{\lambda_j+i\alpha}\right\}$
- Located on a circle – with a cluster at one.
- Figure shows situation on the same example

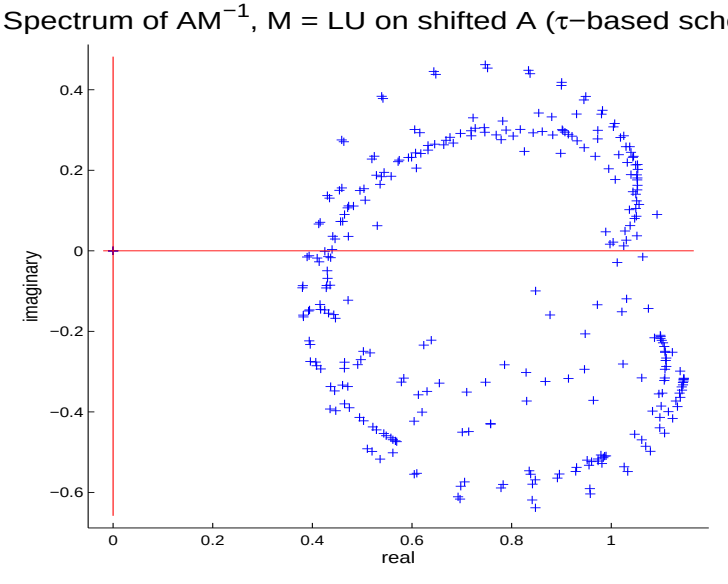


- Next figures approximate spectra for previous (real) example


Spectrum of the Helmholtz operator matrix, A
imaginary
real

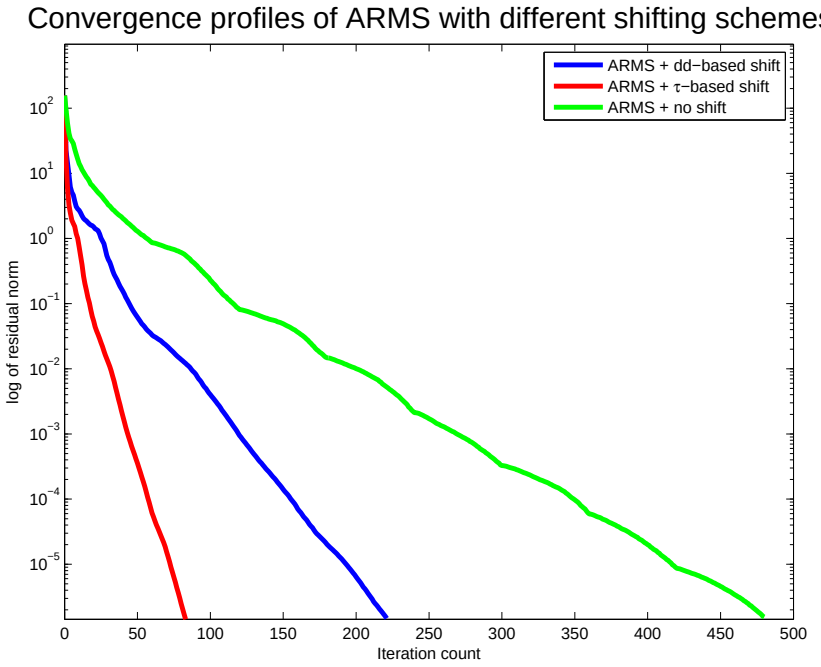

Spectrum of AM^{-1}, M = LU on A
imaginary
real

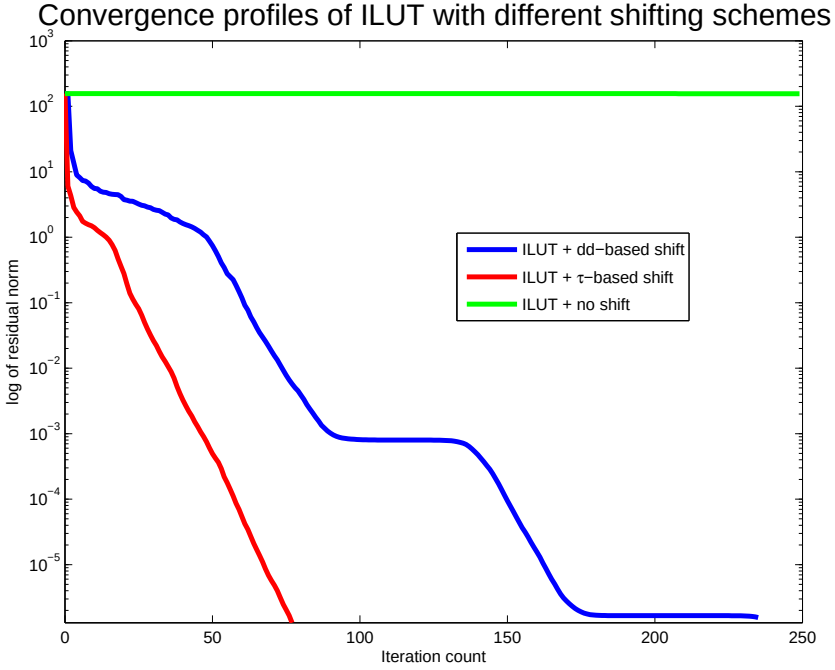

Spectrum of AM^{-1}, M = LU on shifted A (dd−based scheme)
imaginary
real


Spectrum of AM^{-1}, M = LU on shifted A (τ−based scheme)
imaginary
real

Recent comparisons

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





ARMS & shifted variants

ILUT & shifted variants

** Joint work with Daniel Osei-Kuffuor

Wavenumber varied - tests with ILUT

Preconditioner	k	$\frac{\lambda}{h}$	**Iters.**	**Fill Factor**	$\|\|(LU)^{-1}e\|\|_2$
ILUT (no shift)	4π	60	134	2.32	$3.65e+03$
	8π	30	263	2.25	1.23e+04
	16π	15	—	-	-
	24π	10	—	-	-
ILUT (dd-based)	4π	60	267	2.24	$2.29e+03$
	8π	30	255	2.23	4.73e+03
	16π	15	101	3.14	6.60e+02
	24π	10	100	3.92	2.89e+02
ILUT (τ-based)	4π	60	132	2.31	$2.98e+03$
	8π	30	195	2.19	4.12e+03
	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	$\|\|(LU)^{-1}e\|\|_2$
ARMS (no shift)	4π	60	120	3.50	$7.48e+03$
	8π	30	169	4.03	1.66e+04
	16π	15	282	4.50	2.44e+03
	24π	10	—	-	-
ARMS (dd-based)	4π	60	411	3.83	$5.12e+02$
	8π	30	311	4.37	5.67e+02
	16π	15	187	4.71	3.92e+02
	24π	10	185	3.00	2.54e+02
ARMS (τ-based)	4π	60	106	3.45	$7.56e+03$
	8π	30	79	3.84	6.41e+03
	16π	15	39	3.95	1.26e+03
	24π	10	94	3.02	4.71e+02

DIAGONAL ESTIMATORS

*Application: Computing Diag[Inv[A]] ***

➤ Many problems lead to the computation of Diag[Inv[A]] or (easier) Trace[Inv[A]]

Examples:

➤ In Density Functional Theory (DFT): charge density is nothing but $Diag[f(H)]$, where f = step function. Approximating f by a rational function leads to evaluating Diag[Inv[A]]

➤ In Stastistics: $Trace[Inv[A]]$ is stochastically estimated to get parameters in Cross-Validation techniques. [Huntchinson '90]

** Joint work with J. Tang

- In Dynamic Mean Field Theory (DMFT), we look for the diagonal of "Green's function" to solve Dyson's equation.. [see J. Freericks 2005]
- In uncertainty quantification, the diagonal of the inverse of a covariance matrix is needed [Bekas, Curioni, Fedulova '09]
- Stochastic estimations of Trace(f(A)) extensively used by quantum chemists to estimate Density of States[1]

1.Ref: H. Röder, R. N. Silver, D. A. Drabold, J. J. Dong, Phys. Rev. B. 55, 15392 (1997)

Stochastic Estimator

Notation:

- A = original matrix, $B = A^{-1}$.
- $\delta(B) = \text{diag}(B)$ [matlab notation]
- $\mathcal{D}(B)$ = diagonal matrix with diagonal $\delta(B)$
- $\odot$ and $\oslash$: Elementwise multiplication and division of vectors
- $\{v_j\}$: Sequence of s random vectors

Result:

$$\delta(B) \approx \left[\sum_{j=1}^{s} v_j \odot Bv_j\right] \oslash \left[\sum_{j=1}^{s} v_j \odot v_j\right]$$

Refs: C. Bekas , E. Kokiopoulou & YS ('05), Recent: C. Bekas, A. Curioni, I. Fedulova '09.

➤ Let $V_s = [v_1, v_2, \ldots, v_s]$. Then, alternative expression:

$$\mathcal{D}(B) \approx \mathcal{D}(BV_sV_s^\top)\mathcal{D}^{-1}(V_sV_s^\top)$$

Question: When is this result exact?

Main Proposition

- Let $V_s \in \mathbb{R}^{n\times n}$ with rows $\{v_{j,:}\}$; and $B \in \mathbb{C}^{n\times n}$ with elements $\{b_{jk}\}$
- Assume that: $\langle v_{j,:}, v_{k,:}\rangle = 0$, $\forall j \neq k$, s.t. $b_{jk} \neq 0$

Then:

$$\mathcal{D}(B) = \mathcal{D}(BV_sV_s^\top)\mathcal{D}^{-1}(V_sV_s^\top)$$

➤ Approximation to b_{ij} exact when rows i and j of V_s are $\perp$

Probing

Goal: Find V_s such that (1) s is small and (2) V_s satisfies Proposition (rows i & j orthgonoal for any nonzero b_{ij})

Difficulty: Can work only for sparse matrices but $B = A^{-1}$ is usually dense

- B can sometimes be approximated by a sparse matrix.
- Consider for some ϵ : $$(B_\epsilon)_{ij} = \begin{cases} b_{ij}, & |b_{ij}| > \epsilon \\ 0, & |b_{ij}| \leq \epsilon \end{cases}$$
- B_ϵ will be sparse under certain conditions, e.g., when A is diagonally dominant
- In what follows we assume B_ϵ is sparse and set $B := B_\epsilon$.
- Pattern will be required by standard probing methods.

Generic Probing Algorithm

ALGORITHM : 1. *Probing*

Input: A, s

Output: Matrix $\mathcal{D}(B)$

Determine $V_s := [v_1, v_2, \ldots, v_s]$

for $j \leftarrow 1$ **to** s

  Solve $Ax_j = v_j$

end

Construct $X_s := [x_1, x_2, \ldots, x_s]$

Compute $\mathcal{D}(B) := \mathcal{D}\left(X_s V_s^\top\right) \mathcal{D}^{-1}(V_s V_s^\top)$

➤ Note: rows of V_s are typically scaled to have unit 2-norm =1., so $\mathcal{D}^{-1}(V_s V_s^\top) = I$.

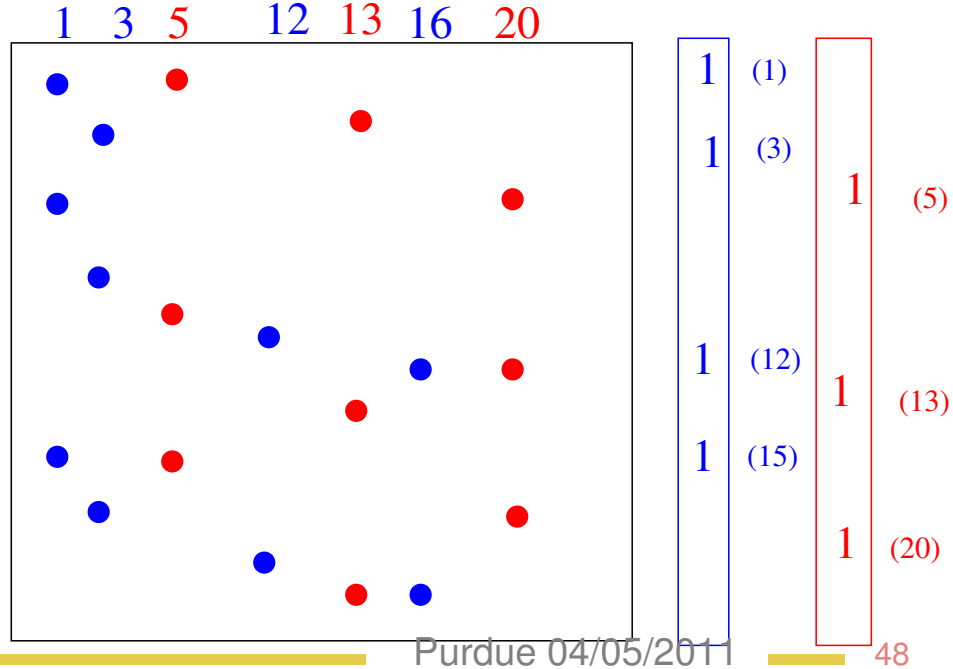
Standard probing (e.g. to compute a Jacobian)

➤ Several names for same method: “probing”; “CPR”, “Sparse Jacobian estimators”,..

Basis of the method: can compute Jacobian if a coloring of the columns is known so that no two columns in the same color overlap.

All entries of same color can be computed with one mat-vec.

Example: For all blue entries multiply B by the blue vector on right.



What about Diag(inv(A))?

- Define v_i - probing vector associated with color i:

$$[v_i]_k = \begin{cases} 1 \text{ if } color(k) == i \\ 0 \text{ otherwise} \end{cases}$$

- Will satisfy requirement of Proposition.... but
- ... this coloring is not what is needed! [It is an overkill]

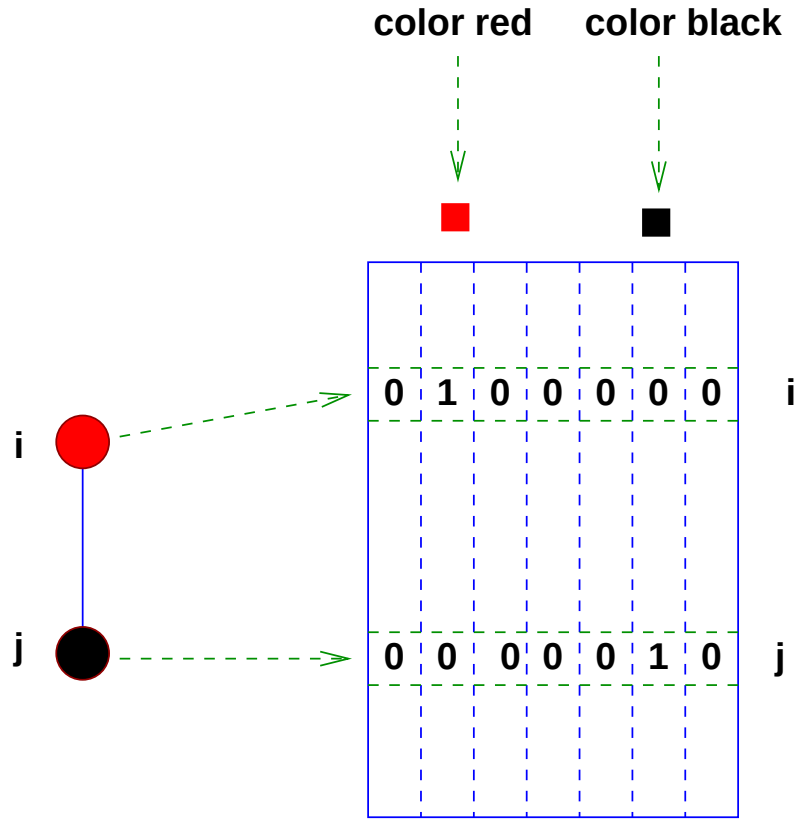
Alternative:

- Color the graph of B in the standard graph coloring algorithm [Adjacency graph, not graph of column-overlaps]

Result: Graph coloring yields a valid set of probing vectors for $\mathcal{D}(B)$.

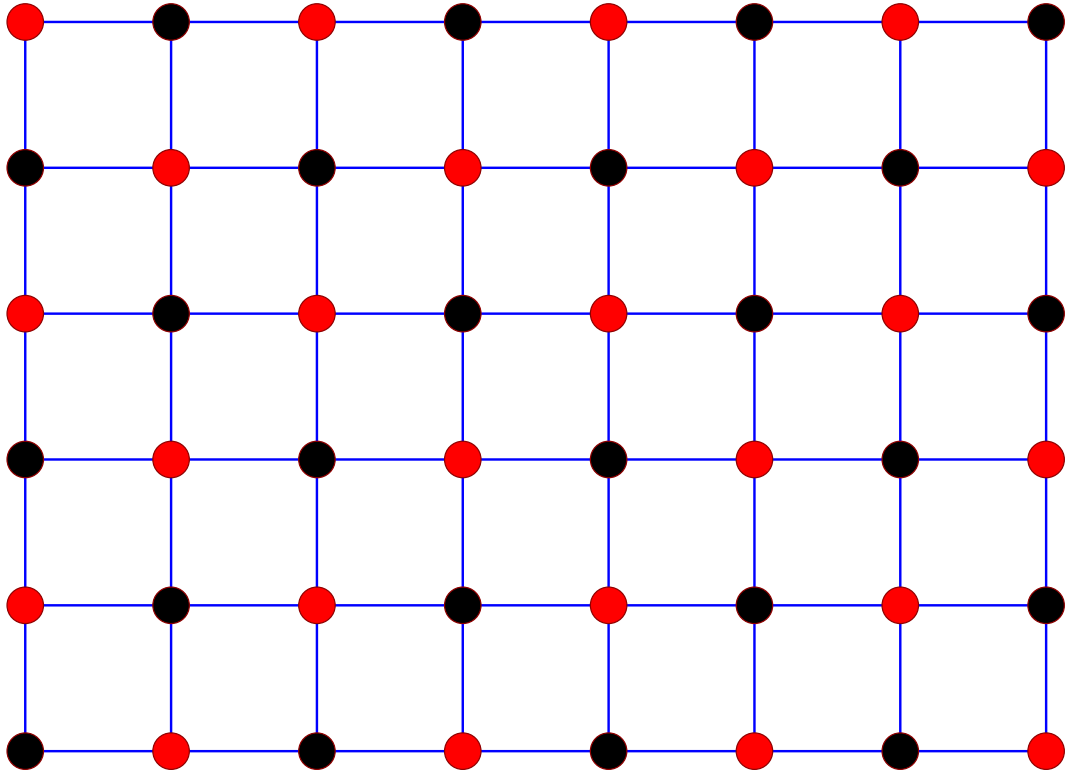
Proof:

- Column v_c: one for each node i whose color is c, zero elsewhere.
- Row i of V_s: has a '1' in column c, where $c = color(i)$, zero elsewhere.



- If $b_{ij} \neq 0$ then in matrix V_s:
  - i-th row has a '1' in column $color(i)$, '0' elsewhere.
  - j-th row has a '1' in column $color(j)$, '0' elsewhere.
- The 2 rows are orthogonal.

Example:



- Two colors required for this graph $\longrightarrow$ two probing vectors
- Standard method: 6 colors [graph of $B^T B$]

Next Issue: Guessing the pattern of B

- Recall that we are dealing with $B := B_\epsilon$ ['pruned' B]
- Assume A diagonally dominant
- Write $A = D - E$, with $D = \mathcal{D}(A)$. Then :

$$A = D(I - F) \quad \text{with} \quad F \equiv D^{-1}E \quad \rightarrow$$

$$A^{-1} \approx \underbrace{(I + F + F^2 + \cdots + F^k)D^{-1}}_{B^{(k)}}$$

- When A is D.D. $\|F^k\|$ decreases rapidly.
- Can approximate pattern of B by that of $B^{(k)}$ for some k.
- Interpretation in terms of paths of length k in graph of A.

Q: How to select k?

A: Inspect $A^{-1}e_j$ for some j

- Values of solution outside pattern of $(A^k e_j)$ should be small.
- If during calculations we get larger than expected errors – then redo with larger k, more colors, etc..
- Can we salvage what was done? Question still open.

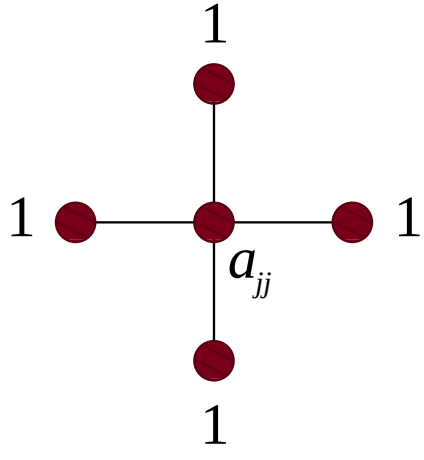
Preliminary experiments

Problem Setup

- **DMFT**: Calculate the imaginary time Green's function
- **DMFT Parameters**: Set of physical parameters is provided
- **DMFT loop**: At most 10 outer iterations, each consisting of 62 inner iterations

- **Each inner iteration**: Find $\mathcal{D}(B)$
- **Each inner iteration**: Find $\mathcal{D}(B)$
- **Matrix**: Based on a five-point stencil

with $a_{jj} = \mu + i\omega - V - s(j)$



Probing Setup

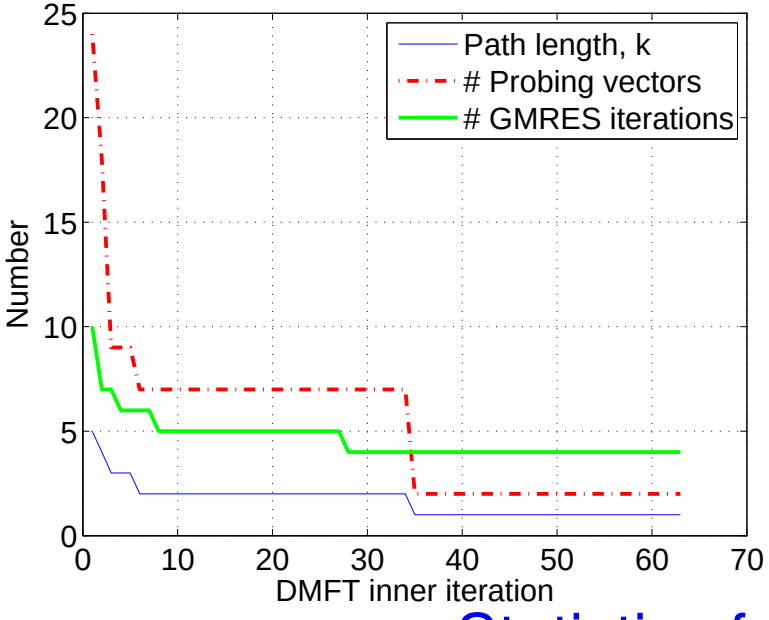
- **Probing tolerance**: $\epsilon = 10^{-10}$
- **GMRES tolerance**: $\delta = 10^{-12}$

Results

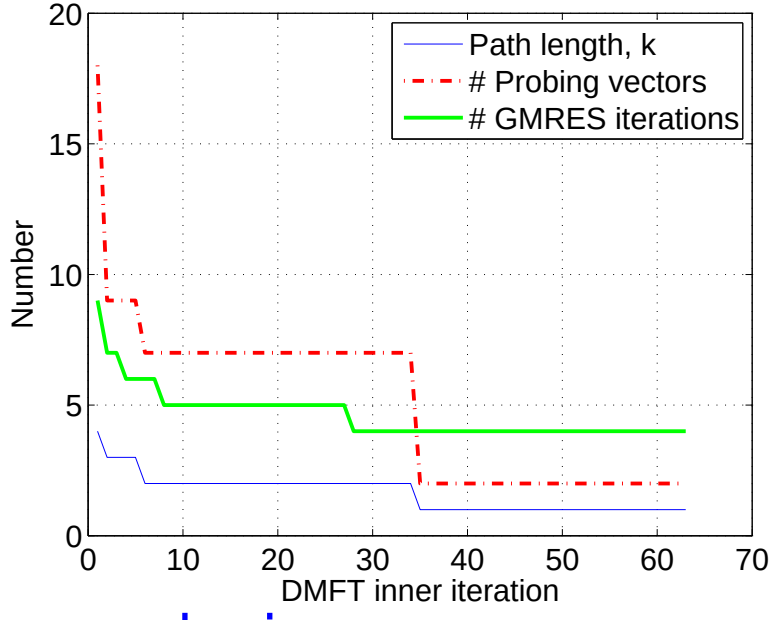
CPU times (sec) for one inner iteration of DMFT

$n \rightarrow$	21^2	41^2	61^2	81^2
LAPACK	0.5	26	282	> 1000
Lanczos	0.2	9.9	115	838
Probing	0.02	0.19	0.79	2.0

$n = 21 \times 21$



$n = 81 \times 81$



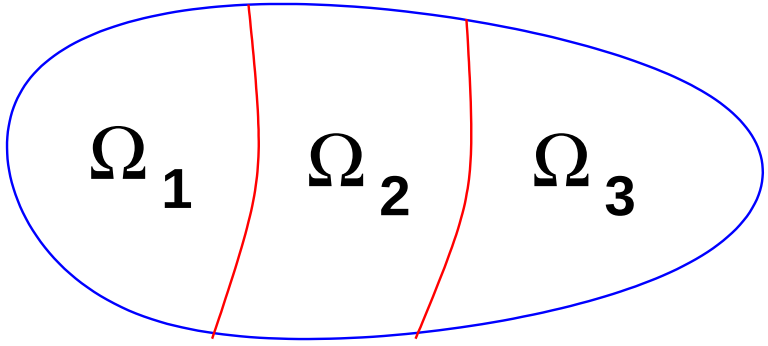
Statistics for two mesh sizes

Challenge: The indefinite case

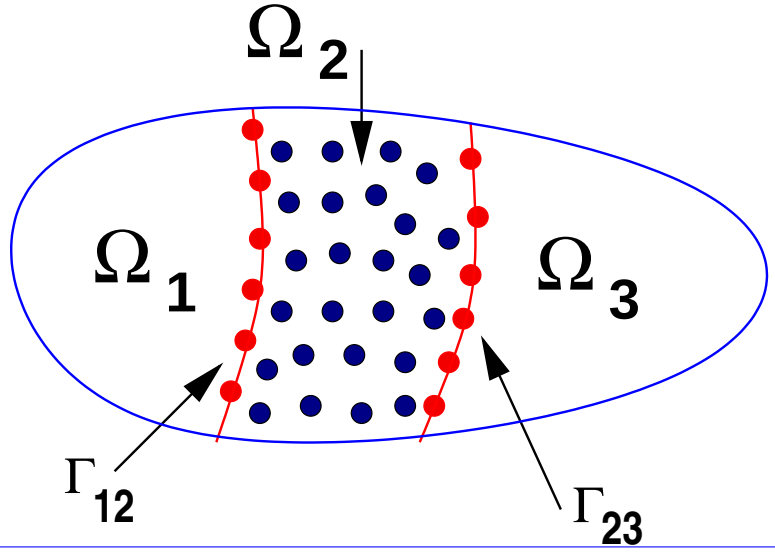
- The DMFT code deals with a separate case which uses a "real axis" sampling..
- Matrix A is no longer diagonally dominant – Far from it.
- This is a much more challenging case.
- Plan for now: solve $Ax_j = e_j$ FOR ALL j's - with the ARMS solver using ddPQ ordering.

Domain Decomposition approach

Domain decomposition with $p = 3$ subdomains



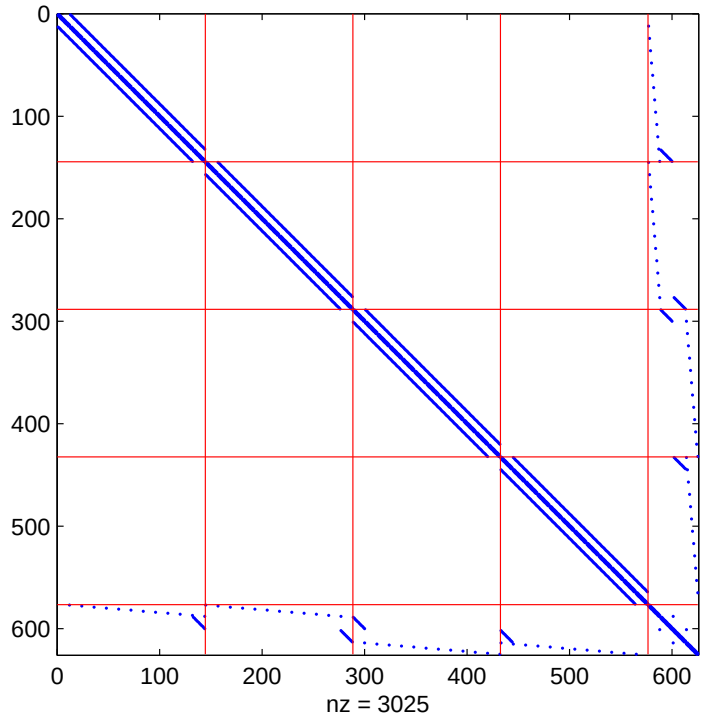
Zoom into Subdomain 2



Under usual ordering [interior points then interface points]:

$$A = \begin{pmatrix} B_1 & & & F_1 \\ & B_2 & & F_2 \\ & & \ddots & \vdots \\ & & B_p & F_p \\ F_1^T & F_2^T & \cdots & F_p^T \quad C \end{pmatrix} \equiv \begin{pmatrix} B & F \\ F^T & C \end{pmatrix},$$

Example of matrix A based on a DDM ordering with $p = 4$ subdomains. ($n = 25^2$)



Inverse of A [Assuming both B and S nonsingular]

$$A^{-1} = \begin{pmatrix} B^{-1} + B^{-1}FS^{-1}F^TB^{-1} & -B^{-1}FS^{-1} \\ -S^{-1}F^TB^{-1} & S^{-1} \end{pmatrix}$$

$$S = C - F^TB^{-1}F,$$

$$\mathcal{D}(A^{-1}) = \begin{pmatrix} \mathcal{D}(B^{-1}) + \mathcal{D}(B^{-1}FS^{-1}F^TB^{-1}) & \\ & \mathcal{D}(S^{-1}) \end{pmatrix}$$

- Note: each diagonal block decouples from others:

Inverse of A in i-th block (domain)

$$(A^{-1})_{ii} = \mathcal{D}(B_i^{-1}) + \mathcal{D}(H_i S^{-1} H_i^T)$$
$$H_i = B_i^{-1} F_i$$

- Note: only nonzero columns of F_i are those related to interface vertices.

- Approach similar to Divide and Conquer but not recursive..

Experiments

- Simple model problem for the DMFT application: Shifted 2-D Laplacien

$$-\Delta - \tau(1+i), \quad \tau \in \mathbb{R}, \quad i^2 = -1,$$

- Time vs. $\sqrt{n}$ (mesh-size in each direction)
- PROBE: number of probing vectors in parentheses

$\tau = 10.$

$\sqrt{n}$	INV	PROBE	D&C	DD
25	.7	.1 (52)	.1	.1
50	12	.6 (53)	1.5	.6
75	66	1.7 (53)	5.5	2.1
100	n/a	3.7 (54)	16	5.9
150	n/a	11 (54)	64	23
200	n/a	30 (54)	238	64

$\tau = 1$

$\sqrt{n}$	INV	PROBE	D&C	DD
25	.7	.3 (165)	.1	.1
50	11	1.7 (170)	1.3	.6
75	64	4.9 (171)	5.3	2.1
100	n/a	9.9 (169)	14	5.8
150	n/a	73 (171)	64	23
200	n/a	n/a	173	62

$\tau = 0.1$.

$\sqrt{n}$	INV	PROBE	D&C	DD
25	.6	n/a	.1	.1
50	11	n/a	1.2	.6
75	62	n/a	5.0	2.0
100	n/a	n/a	14	6.1
150	n/a	n/a	66	24
200	n/a	n/a	189	67

SPARSE MATRIX COMPUTATIONS ON GPUS

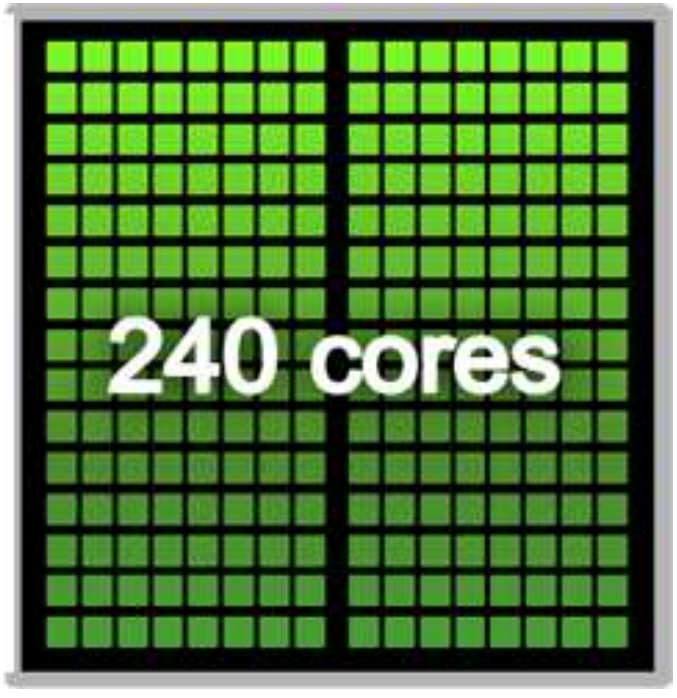
Sparse matrix computations with GPUs **

- GPUs Currently a very popular approach to: inexpensive supercomputing
- Can buy $\sim$ one Teraflop peak power for around $1,350.

Tesla C1060

** Joint work with Ruipeng Li

Tesla:



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

➤ Fermi promises to be more impressive

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 → GPU

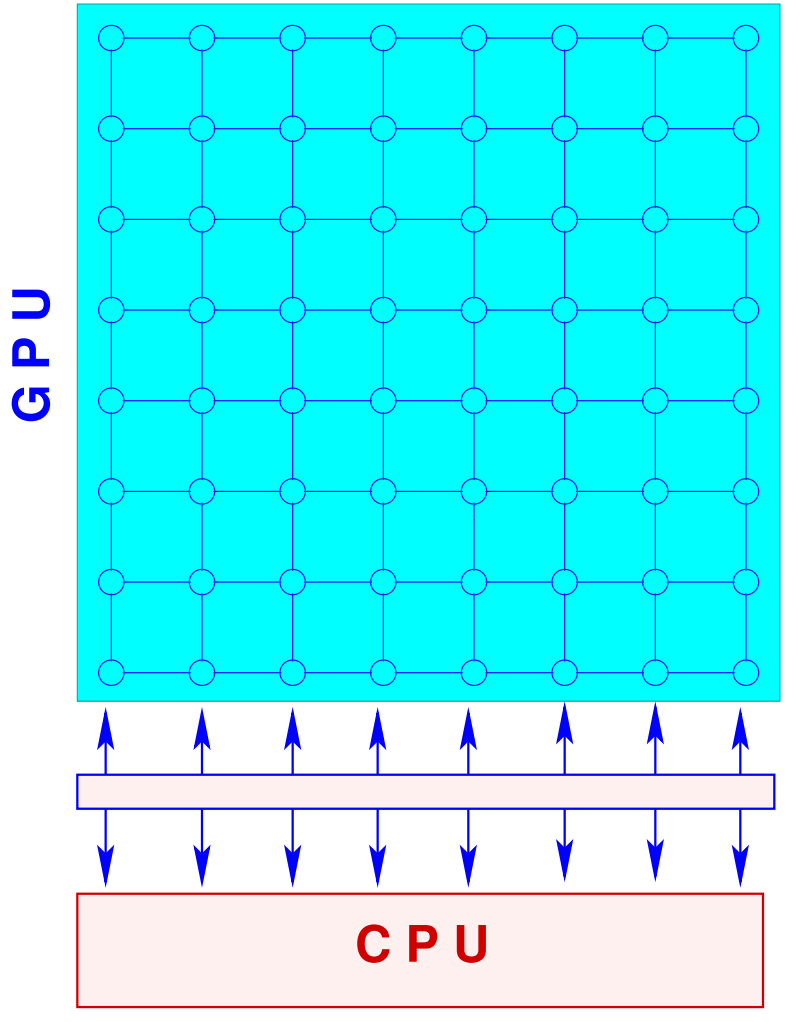
```
cudaMemcpy(...)
```

4. Execute GPU 'kernel':

```
kernel <<<(...)>>>(..)
```

5. Copy data GPU →CPU

```
cudaMemcpy(...)
```



Sparse Matvecs on the Tesla

- Preliminary results are mixed [high programming cost, very good performance for some calculations]
- Performance of matvec [GLOPS] on a Tesla C1060
- Matrices:

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

	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

ILU: Sparse Forward/Backward Sweeps

- Exploit Level-Scheduling.. [Topological sort]
- Poor performance relative to CPU
- Extremely poor when #levs is large
- In the worst case, #levs=n, ≈ 2 Mflops

Matrix	N	CPU	GPU-Lev	
		Mflops	#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

Alternative: Polynomial Preconditioners

- $M^{-1} = s(A)$, where $s(t)$ is a polynomial of low degree
- Solve: $s(A) \cdot Ax = s(A) \cdot b$
- $s(A)$ need not be formed explicitly
- $s(A) \cdot Av$: Preconditioning Operation: a sequence of matrix-by-vector product to exploit high performance Spmv kernel
- Inner product on space $\mathbb{P}_k$ ($\omega \geq 0$ is a weight on (α, β))

$$\langle p, q \rangle_\omega = \int_\alpha^\beta p(\lambda) q(\lambda) \omega(\lambda)\, d\lambda$$

- Seek polynomial s_{k-1} of degree $\leq k-1$ which minimizes

$$\| 1 - \lambda s(\lambda) \|_\omega$$

L-S Polynomial Preconditioning

Tol=1.0e-6; MaxIts=1,000; *:MD reordering applied

Matrix	ITSOL-ILU(3)		GPU-ILU(3)		L-S Polyn		
	iter.	sec.	iter.	sec.	iter.	sec.	Deg
bcsstk36	FAILED		**351***	**10.58***	31	1.34	100
ct20stif	27	9.4	**21***	**2.22***	16	0.70	50
ship_003	27	25.8	27	21.1	10	2.90	100
msc23052	181	18.5	181	6.0	37	1.28	80
bcsstk17	46	1.8	46	2.8	22	0.55	120

ILU(3) & L-S Polynomial Preconditioning

Preconditioner Time

- High level fill-in ILU preconditioner can be very expensive to build
- L-S Polynomial preconditioner set-up time $\approx$ very low
- Example: ILU(3) and L-S Poly with 20-step Lanczos procedure (for estimating interval bounds).

Matrix	N	ILU(3) sec.	LS-Poly sec.
Boeing/ct20stif	23,052	15.63	0.26

Preconditioner Construction Time

Conclusion

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

➤ Recent work on generalizing nonsymmetric permutations to symmetric matrices [Duff-Pralet, 2006].

➤ Complex shifting strategy quite useful even for real matrices

➤ Diag(inv(A)) problem - fairly easy for D.D case. Very challenging in indefinite case: B is dense and 'equimodular'

➤ GPUs for irregular sparse matrix computations: Much remains to be done both in hardware and in algorithms/software

Software:

`http://www.cs.umn.edu/~saad/software`

- ARMS-C [C-code] - available from ITSOL package..
- Parallel version of ARMS available. pARMS3 released
- See also: ILUPACK – developed mainly by Matthias Bollhoefer and his team

`http://www.tu-berlin.de/ilupack/.`