Direct Algorithms for Sparse Schur Complements and Inverses

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Outline

Examine some less common sparse direct algorithms:

- Partial linear solution.
- Schur complements.
- Sampling the inverse operator.

Apply them as "frontends" for low-rank skeletonization:

- Cross approximation.
- Range estimation.
- Ritz projection.

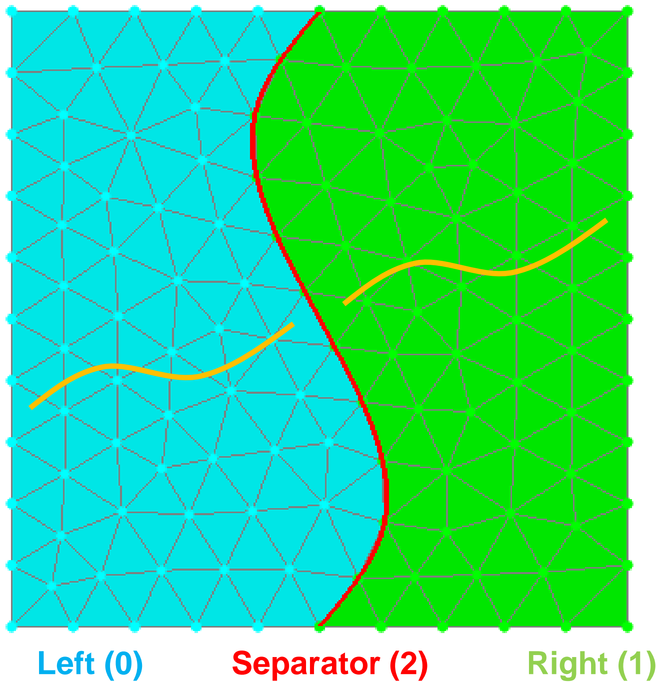
Motivations: fast direct solvers for FE-BI's and FE-DDM's.

Refresher: Factor $A=LL^T$

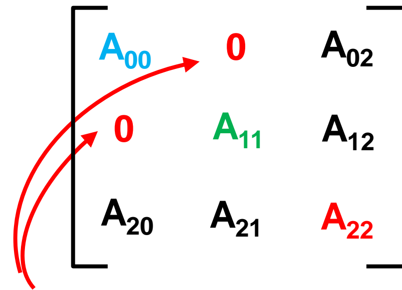
Reorder: Left(0), Right(1), Separator(2). $A_{01} = A_{10}$ **= all zero!**

Right looking. Factor A_{00}/A_{11}**, schur downdate** A_{22}**, factor.**

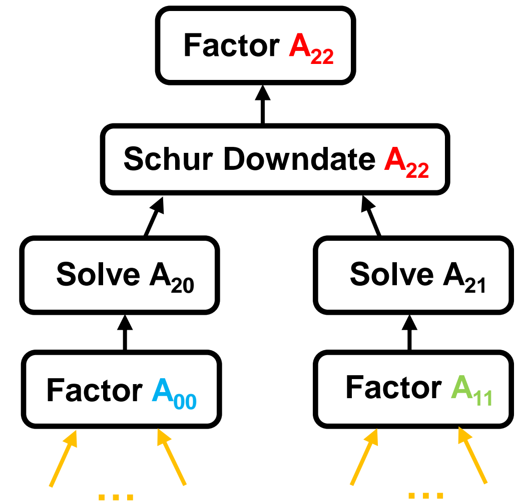
FEM mesh:



Reordered matrix:



Algorithm steps:

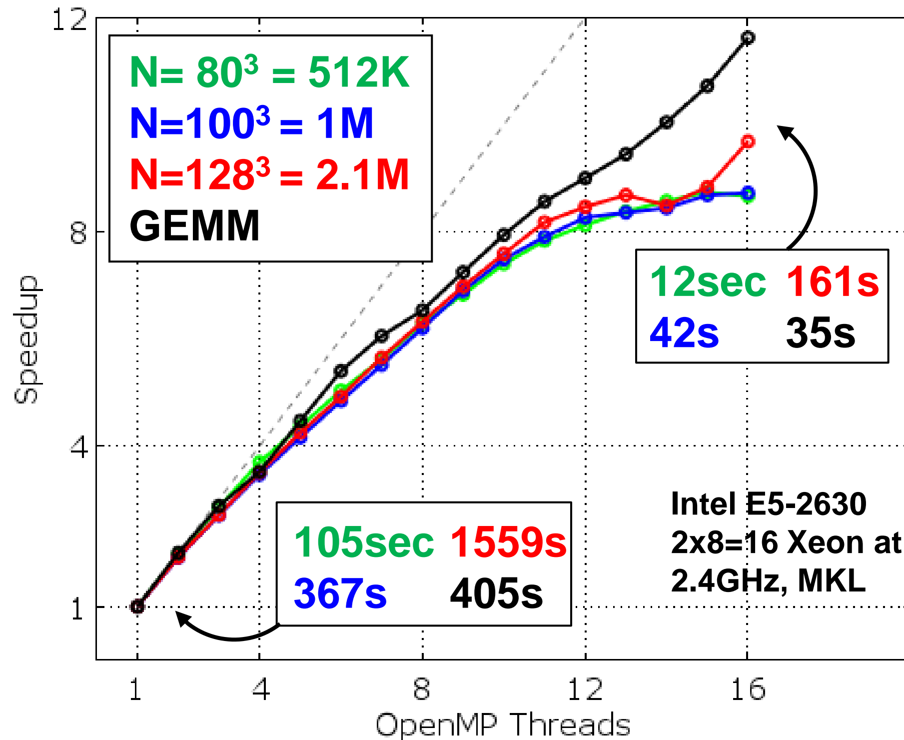


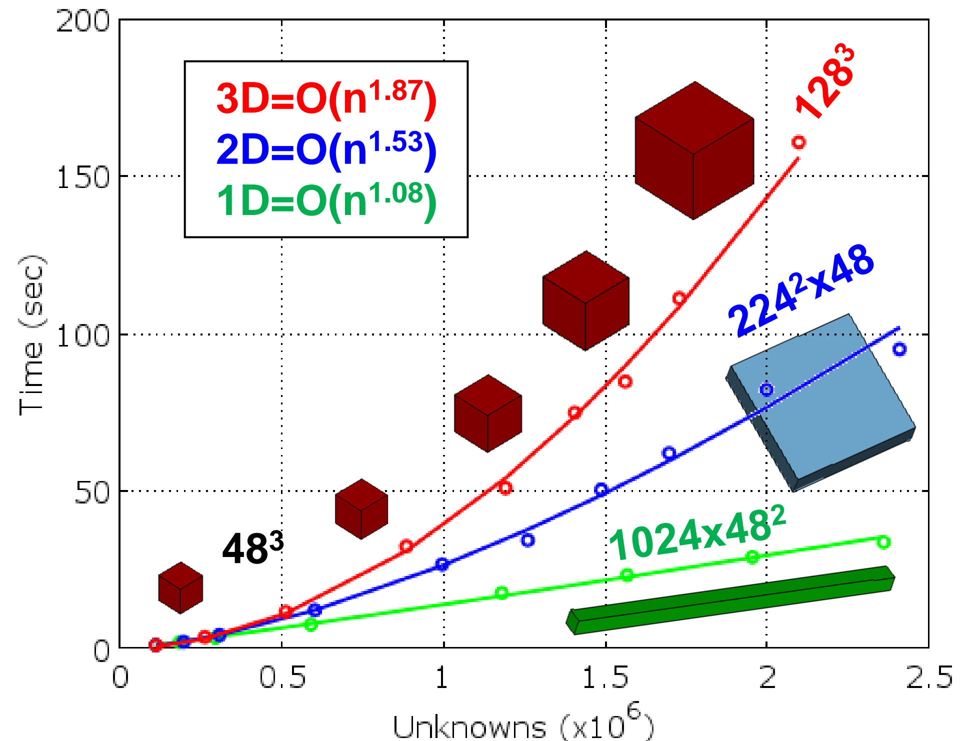
Note A_{00} **and** A_{11} **also sparse, apply idea recursively.**

Leads to a tree of operations, eliminating from bottom up.

Selected profiling data.

Example problem under study: I x J x K brick (N = IJK)



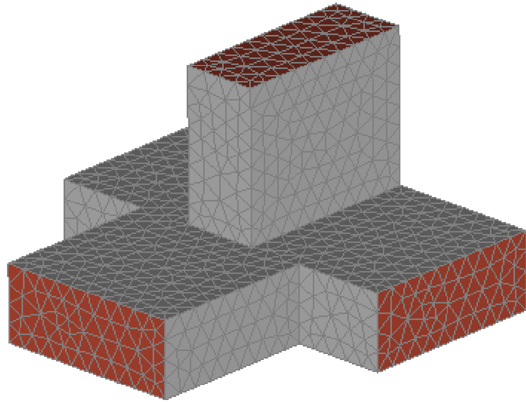


Discrete graph laplacian (7-point): well understood spectrum.

Structured grid: easy to reorder using nested dissection.

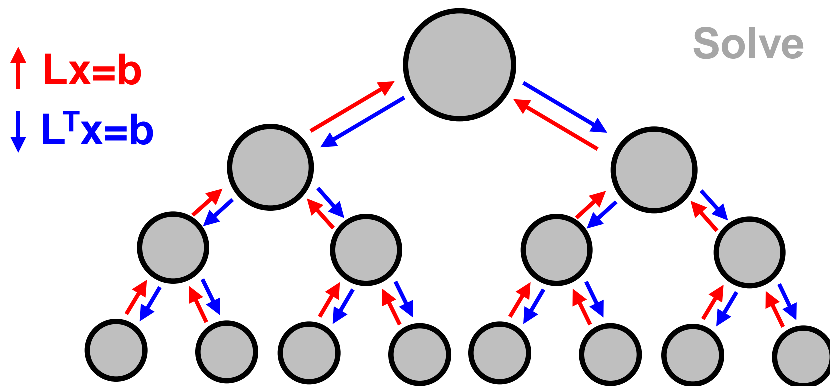
Partial solution $x=R_i^TA^{-1}R_jb$

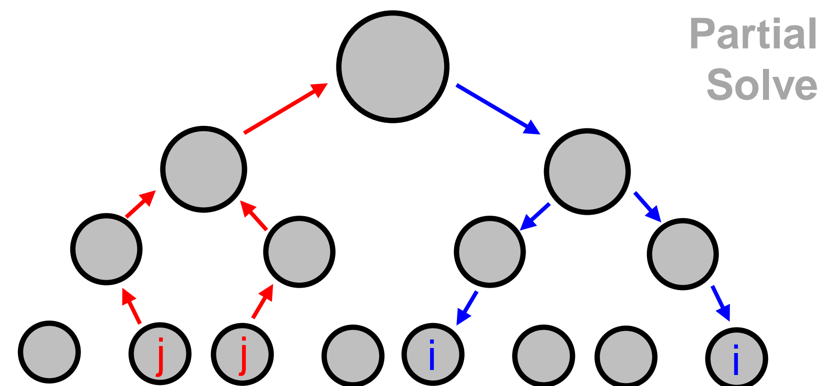
In plain english: only b(j) nonzero, only x(i) is needed.



$$= \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & +1 & +1 \\ 0 & 0 & +1 & -1 \\ +1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \end{bmatrix}$$

Many engineering QoI's use only *boundary-valued* b and x.





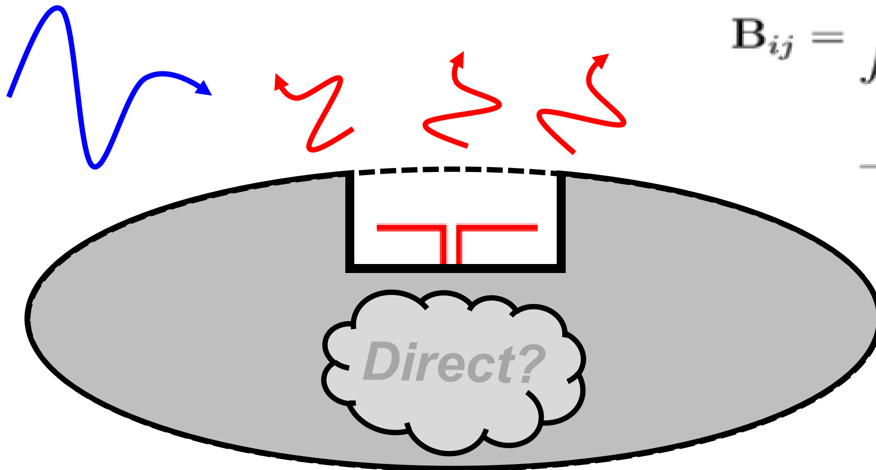
$O(n^{4/3})$ time, like $x=A^{-1}b$. Only $O(n^{2/3})$ space per RHS, not $O(n)$.

Schur complement $S=B^TA^{-1}B$

Concept: form "saddle system" of A and B, then "quit" early.

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{L} & 0 \\ (\mathbf{L}^{-1}\mathbf{B})^T & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{B}^T\left(\mathbf{L}\mathbf{L}^T\right)^{-1}\mathbf{B} \end{bmatrix} \begin{bmatrix} \mathbf{L}^T & \mathbf{L}^{-1}\mathbf{B} \\ 0 & \mathbf{I} \end{bmatrix}$$

Arise from FE-BI hybrids, eg scattering from apertures.



$$\mathbf{A}_{ij} = \int_V \left(\nabla \times \vec{w}_i \cdot \mu_r^{-1} \nabla \times \vec{w}_j - k^2 \vec{w}_i \cdot \epsilon_r \vec{w}_j\right) dv$$

$$\mathbf{B}_{ij} = \int_S \nabla \bullet (\hat{n} \times \vec{w}_i) \cdot \int_{S'} \nabla' \bullet (\hat{n}' \times \vec{w}_j) \cdot g(\vec{r}, \vec{r}')\, dS' dS$$

$$- k^2 \int_S (\hat{n} \times \vec{w}_i) \bullet \int_{S'} (\hat{n}' \times \vec{w}_j) \cdot g(\vec{r}, \vec{r}')\, dS' dS$$

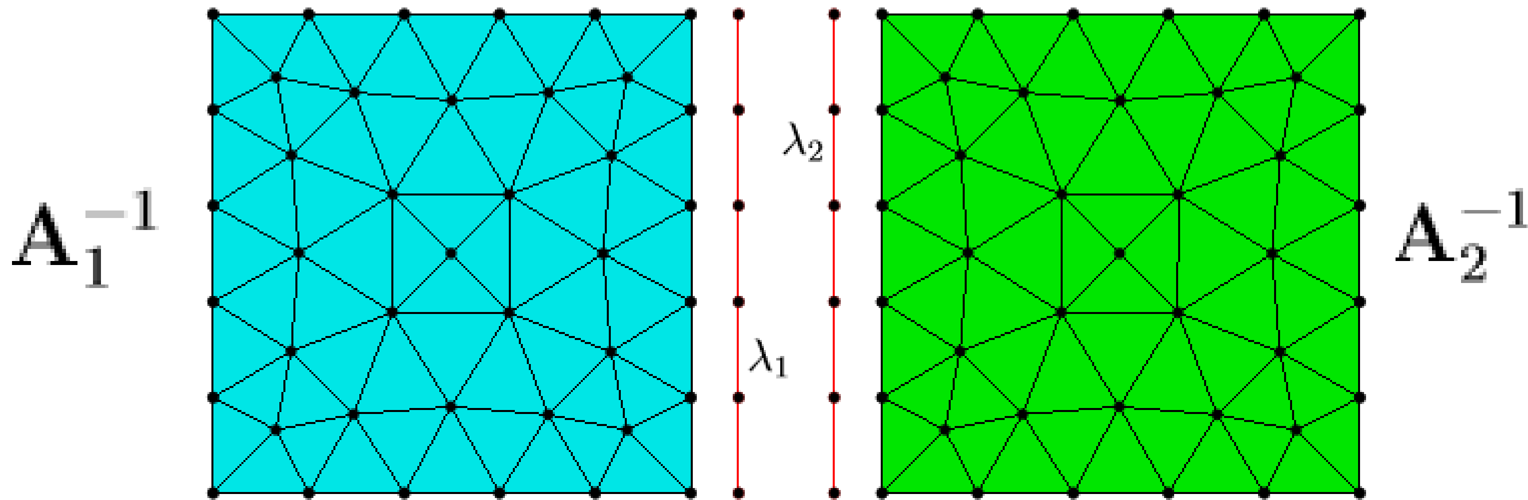
$$\begin{bmatrix} \mathbf{A}_{ee} & \mathbf{A}_{em} \\ \mathbf{A}_{me} & \mathbf{A}_{mm} + 2\mathbf{B}_{mm} \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{m} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{h}_{inc} \end{bmatrix}$$

$$\left[\mathbf{A}_{mm} - \mathbf{A}_{em}^T \mathbf{A}_{ee}^{-1} \mathbf{A}_{em} + 2\mathbf{B}_{mm} \right] \left[\mathbf{m} \right] = \left[\mathbf{h}_{inc} \right]$$

Sampling the inverse Z(i,j), $Z=A^{-1}$

Closely related to Schur complement, $Z(i,j) = R_i^T \cdot A^{-1} \cdot R_j$

Arise in FETI/DDM, iterate/exchange fields at boundaries.



$$\begin{bmatrix} \mathbf{I} & \mathbf{I} - 2\alpha \underline{\mathbf{R}_2^T \mathbf{A}_2^{-1} \mathbf{R}_2} \\ I - 2\alpha \underline{\mathbf{R}_1^T \mathbf{A}_1^{-1} \mathbf{R}_1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 2\alpha R_1^T \mathbf{A}_1^{-1} \mathbf{f}_1 \\ 2\alpha R_2^T \mathbf{A}_2^{-1} \mathbf{f}_2 \end{bmatrix}$$

Direct?

Scatter, solve, gather. Scatter, solve, gather.

Tabulating Z(i,j) opens up reuse/preconditioning options.

Cross Approximating Z(i,j) [1/2]

Alternately sample row/column with largest error modulus.

$\log_{10}(Z-UV^T)$

0
-1
-2
-3
-4
-5

Estimated Error
Actual Error
SVD(Z)

Log10(A-UV')

0 10 20 30 40

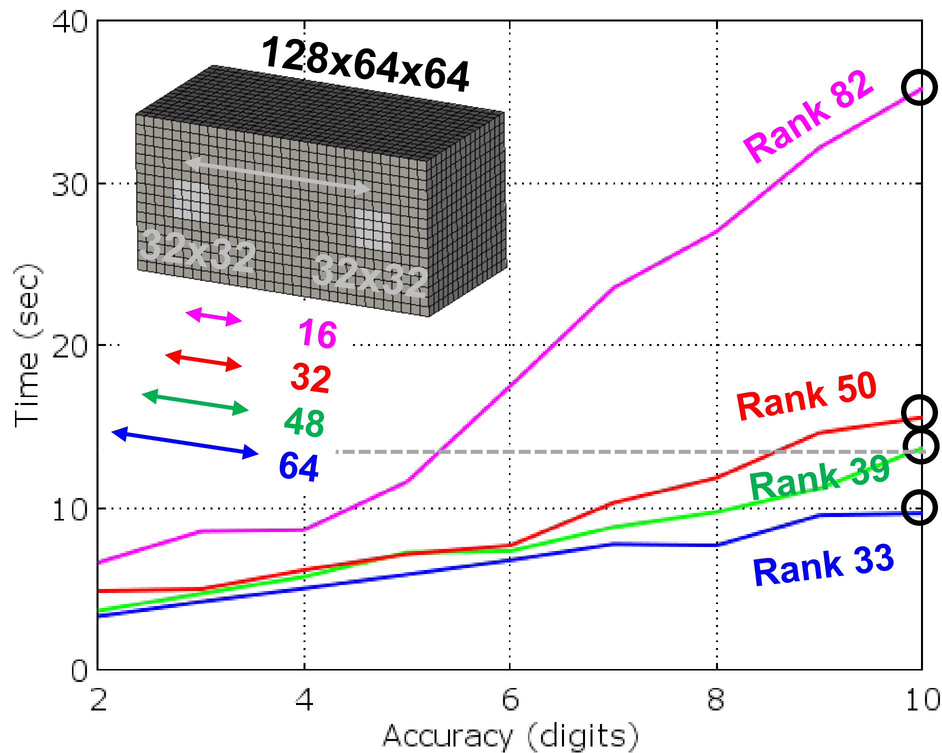
Iteration

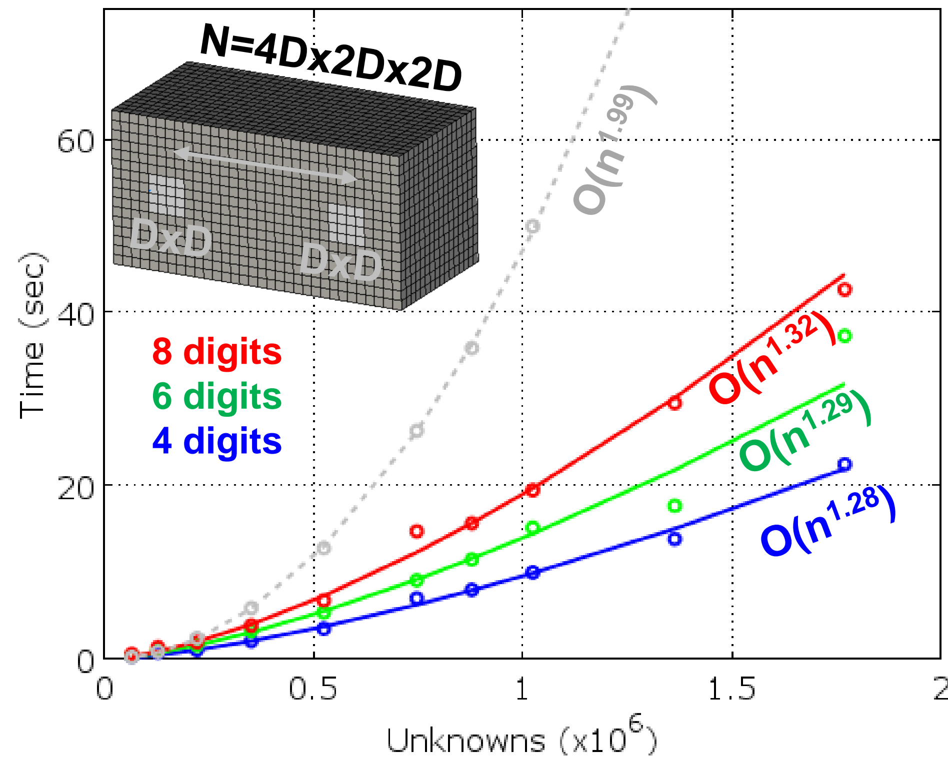
Key idea: partialsolve() can efficiently extract rows/columns:

```
c = Z([i],j) = solver.partialsolve([i],j,x=1.0,'Left')
r = Z(i,[j]) = solver.partialsolve(i,[j],x=1.0,'Right')
```

Cross Approximating Z(i,j) [2/2]

Beats solver.inverse() at large N, especially at low rank/tol.





But in parallel the gap narrows, BLAS3 vs BLAS1 effects.

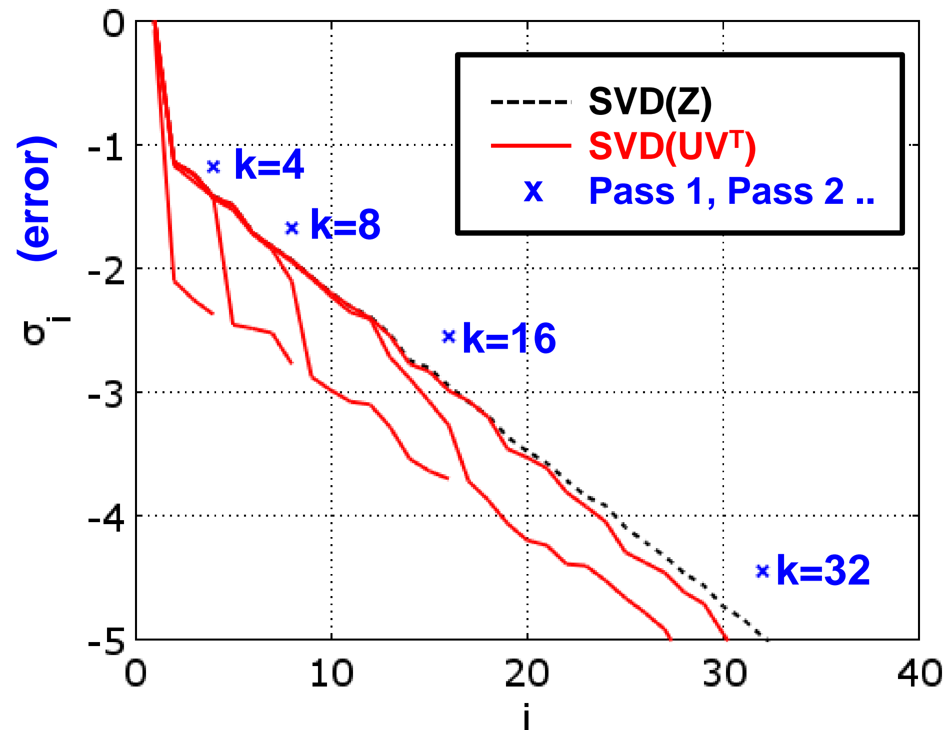
Range estimation of Z(i,j) [1/2]

Apply action of Z to random vectors X, form image Y=ZX.

If Z has rapidly decaying σ's, Y probably spans range(Z).

```
// Find Q = span(Z)
X = rand(Z.cols,k)
Y = Z.apply(X)
[Q,R,π] = QR(Y,0)

// Build k-SVD from Q
W = Z'.apply(Q)
[U,Σ,V] = svd(W,0)
Z≈(QU)·Σ·(V)
```

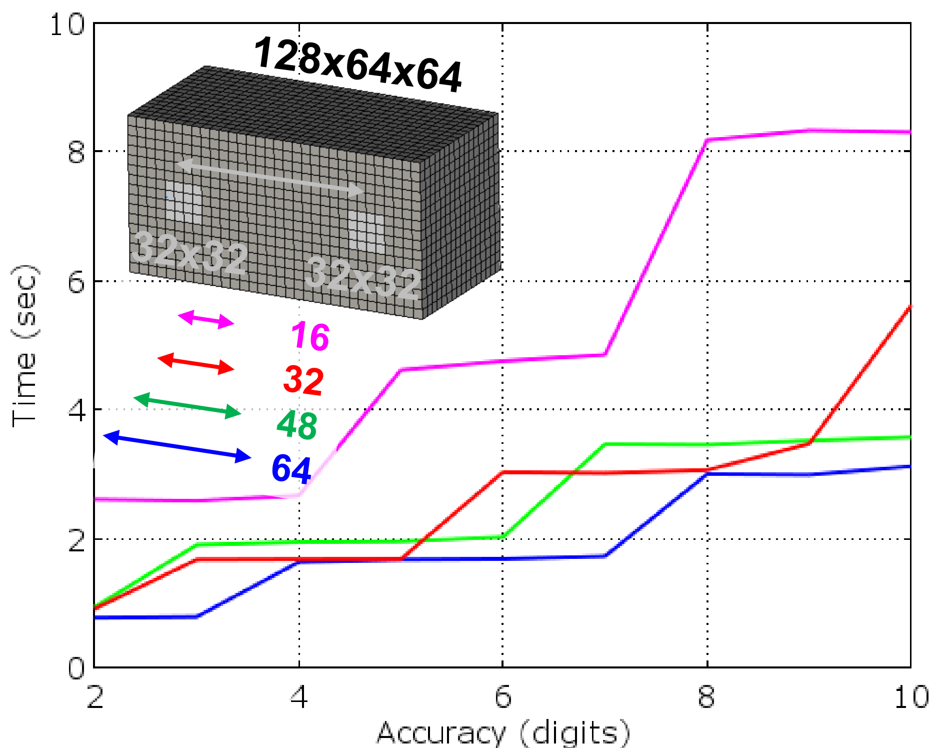


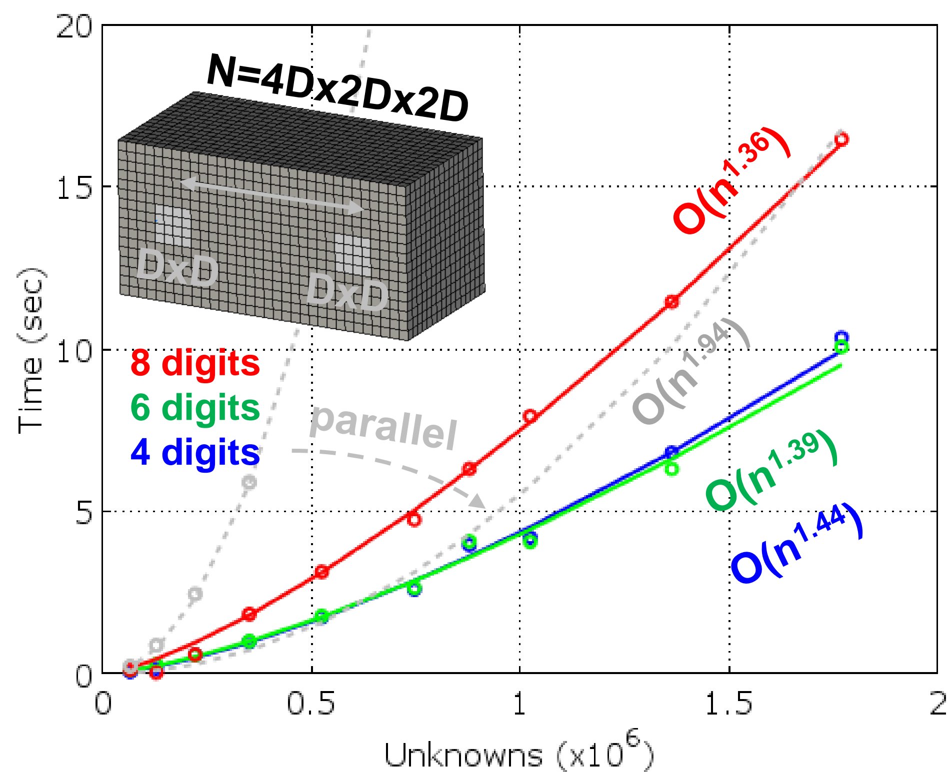
Key idea: partialsolve() can efficiently apply Y=Z(i,j)·X:

```
Y = Z([i],[j])*X = solver.partialsolve([i],[j],X,'Left')
```

Range estimation of Z(i,j) [2/2]

All the same problem instances as before (sizes,shapes).





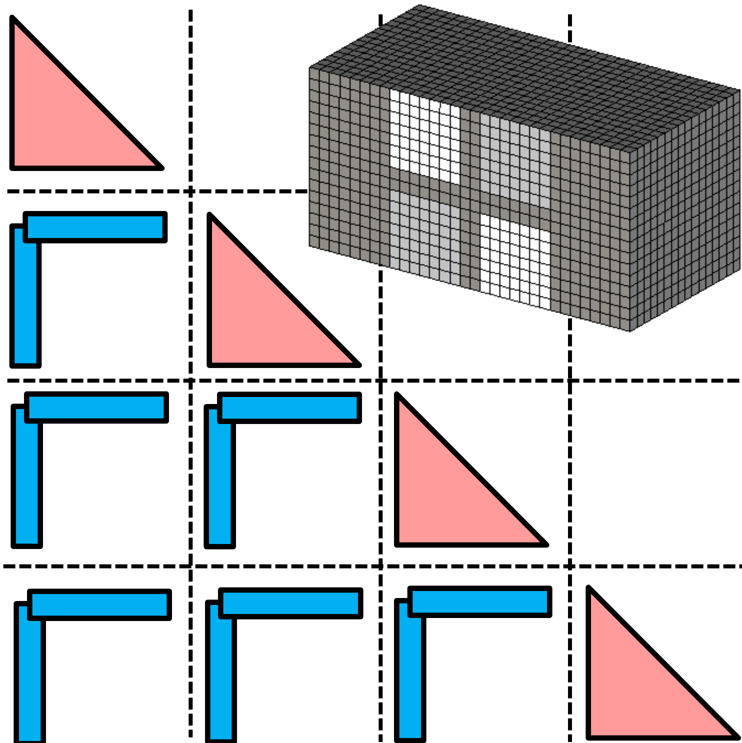
Availability of all forcing data up front leads to speedup.

Can be faster than parallel solver.inverse(), even at modest N.

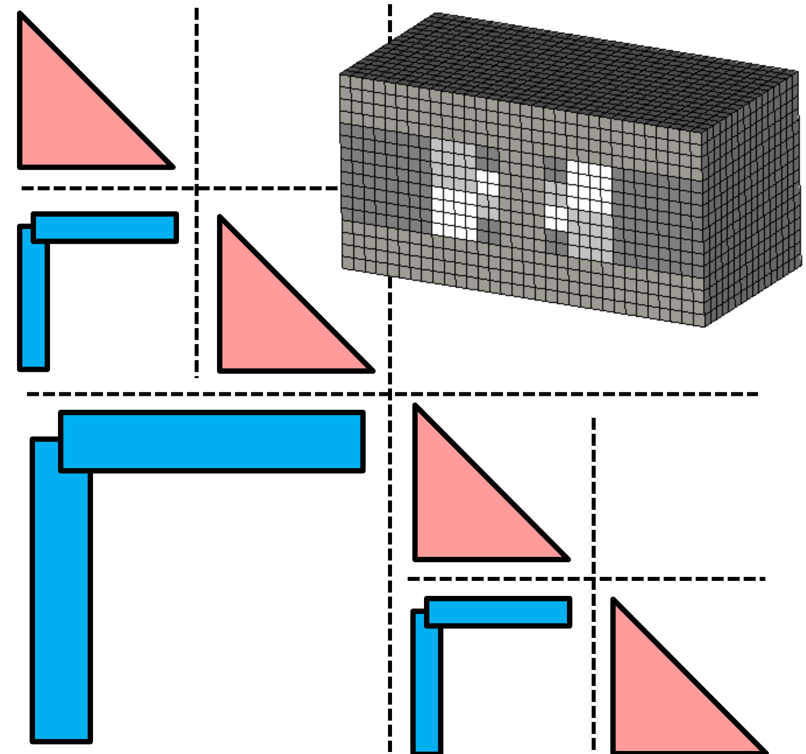
Ritz Projection of Z(i,j) [1/3]

What about approximating *more* than just one block?

(B)lock (L)ow (R)ank



(H)eirarchical Matrix

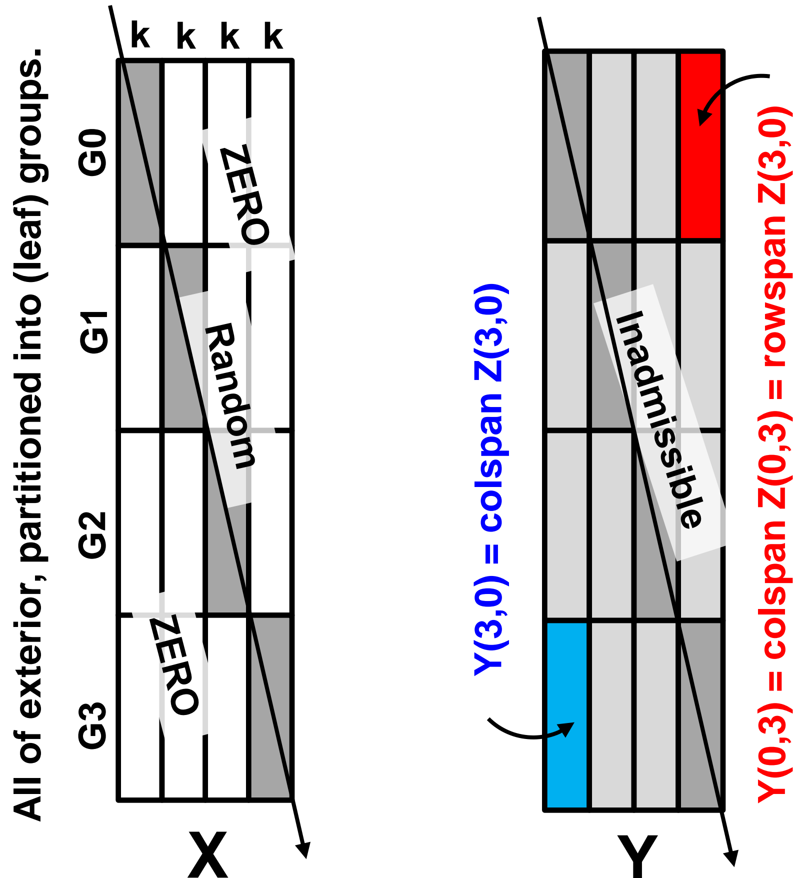


Optimization(BLR)/amortization(H) opportunities do exist.

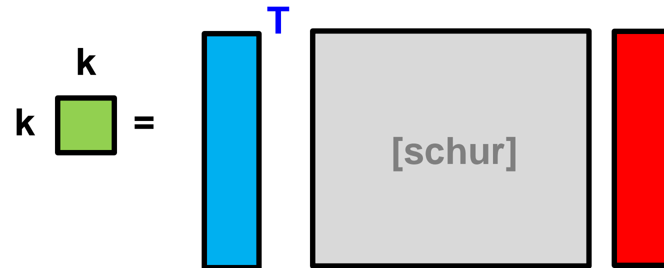
Ritz Projection of Z(i,j) [2/3]

First pass: find row/column spans using "fat" partialsolve()

```
Y = partialsolve([all],[all],X)
```



$$R = Y(3,0)^T \cdot Z(3,0) \cdot Y(0,3)$$



$R = \text{solver.schur}(Y_{30}, Y_{03})$

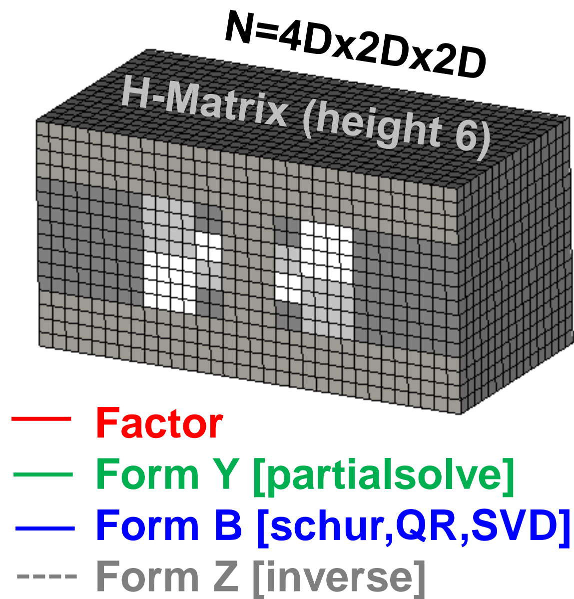
$[U, \Sigma, V] = \text{svd}(R)$

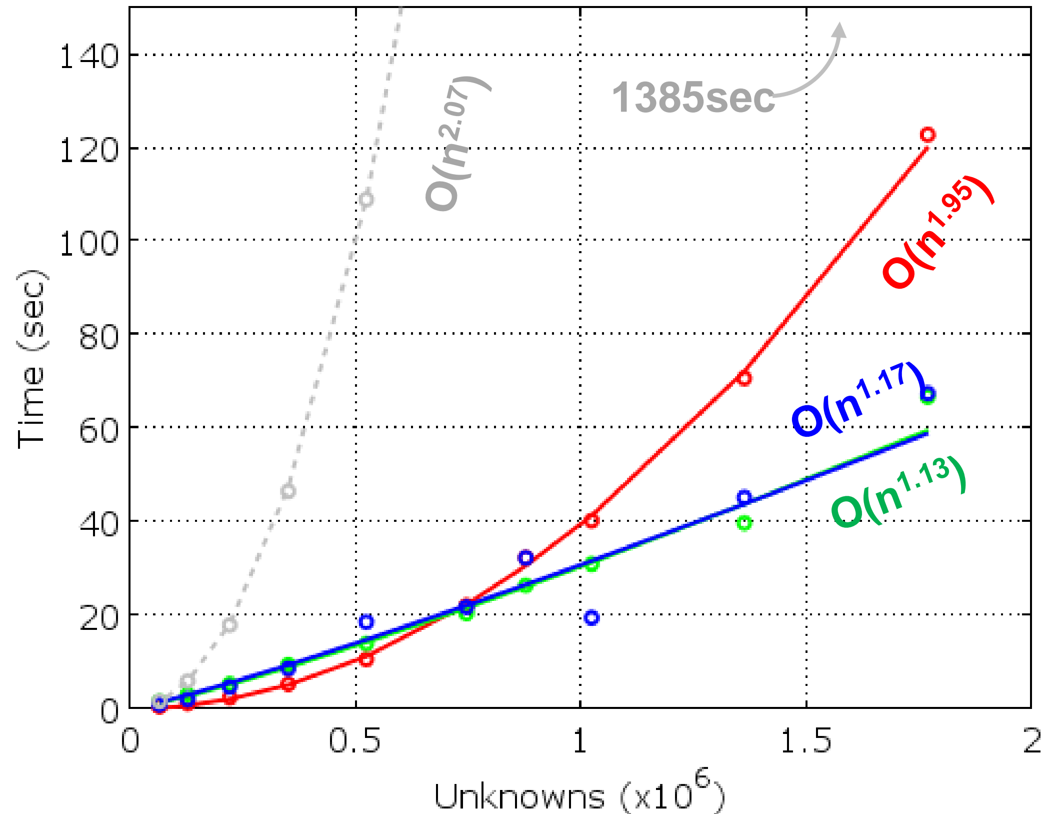
$Z_{30} \approx (Y_{30} \cdot U) \cdot \Sigma \cdot (V \cdot Y_{03})$

Second pass: Ritz projection using solver.schur(), k-SVD

Ritz Projection of Z(i,j) [3/3]

Fill an H-matrix representation of Z restricted to boundary.





Algorithm quickly furnishes all (admissible) blocks.

Can form H-matrix of $S=B^TA^{-1}B$ with a few minor changes.

Wrapping Up

Examined several uncommon sparse direct algorithms:

Partial linear solution: $x=R_i^T A^{-1} R_j b$ (sparse b, sifted x)

Schur complements: $B^T A^{-1} B$, $B^T A^{-1} C$, all sparse

Sampling the inverse operator: $Z(i,j) = R_i A^{-1} R_j$

Used them as "frontends" for low-rank/skeletonization:

Cross approximation: partialsolve() can extract row/column

Range estimation: partialsolve() can apply Z(i,j) quickly

Ritz projection: schur()+partialsolve(), amortization over blocks

Essential tools for FEBI/DDM methods (sparsity+lowrank).

Contact: myracore.com

e pluribus rapidum

MyraMath: sparse factor/solve/schur/inverse/partialsolve.

MyraKL: BLAS/LAPACK API for MyraMath, or use MKL.

MyraMath

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API Tutorials

MyraMath provides an ecosystem of algebraic containers, wrappers for BLAS/L
deal with this large "API surface", some example-driven tutorials are provided be
the most important part of the library, this sequence of tutorials tries to master th

- Step 1: Read the Tutorial for /dense routines
- Step 2: Read the Tutorial for /sparse routines
- Step 3: Read the Tutorial for /multifrontal solvers (part 1)
- Step 4: Read the Tutorial for /multifrontal solvers (part 2)

MyraMath also provides additional algebraic functionality beyond sparse direct s
library but are not essential. Browse them in any order you like:

- Browse the Tutorial for /iterative routines
- Browse the Tutorial for /pdense routines
- Browse the Tutorial for /expression templates.
- Browse the Quick reference for converting Matlab/Octave programs.

Finally, there are a few tutorials that discuss general-purpose/non-algebraic cor

- Browse the Tutorial for /io routines.
- Browse the Tutorial for /jobgraph routines
- Browse the Summary of /test programs.

MyraKL

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Instructions for building on Windows

Overview

MyraKL can be built natively on Windows using the Microsoft Visual C+
Visual Studio are similar. The first step is to generate a .sln (solution)
library (myrakl.dll) and the accompanying test suite is straightforward.
the LAPACK/BLAS tests (within the folders /dense/tests and /dense

Below are links to the sections of this page:

- Running CMake
- Opening MyraKL in Visual Studio
- Building the library and tests
- Running test executables
- Creating new projects of your own

Running CMake

A native Windows installer for CMake can be found at CMake.org. If yo
hold the original source code and the other to hold the products of the
labeled "Where is the source code:", type in the path to MyraKL'
build folder. Alternatively, you use can the browse buttons on the right
"Visual Studio 14 2015 Win64" (for 64 bit systems).

Free software (GPL), or dual license (info@myracore.com)