An Efficient Solver for Sparse Linear Systems based on Rank-Structured Cholesky Factorization

David Bindel and Jeffrey Chadwick

Department of Computer Science
Cornell University

22 July 2013

```
u = K \ f
```

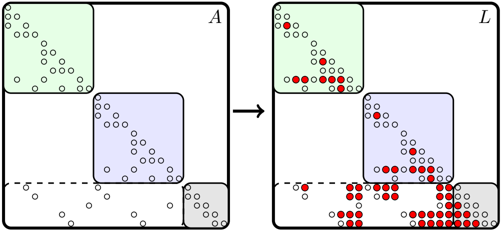
Great for circuit simulations, 1D or 2D finite elements, etc.

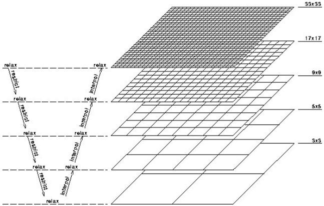
Standard advice to students: Just try backslash for these problems.
Standard response: What about for the 3D case?

"Try PCG with a good preconditioner. Maybe start with the ones in PETSc. You've taken Matrix Computations, right? Blah blah yadda blah..."

(Not an actual student)

Direct or iterative?





CW: Gaussian elimination scales poorly. Iterate instead!

- **Pro:** Less memory, potentially better complexity
- **Con:** Less robust, potentially worse memory patterns

Commercial finite element codes still use (out-of-core) Cholesky.
Longer compute times, but fewer tech support hours.

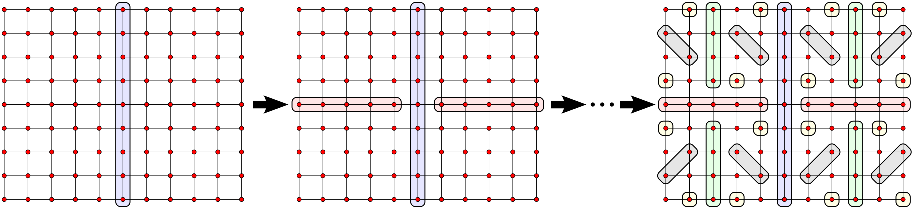
Desiderata

I want a code for sparse Cholesky ($\mathbf{A} = \mathbf{L}\mathbf{L}^T$) that

- Handles modest problems on a desktop (or laptop?)
  - Inside a loop, without trying my patience
  - $\implies$ Does not need gobs of memory
  - $\implies$ Makes effective use of level 3 BLAS
- Requires little parameter fiddling / hand-holding
- Works with general elliptic problems (esp. elasticity)

Idea is in the air – see talks by Darve and Li (bracketing me!), also work by Xia, Gu, Martinsson, Ying, ...

From ND to “superfast” ND



ND gets performance using just *graph* structure:

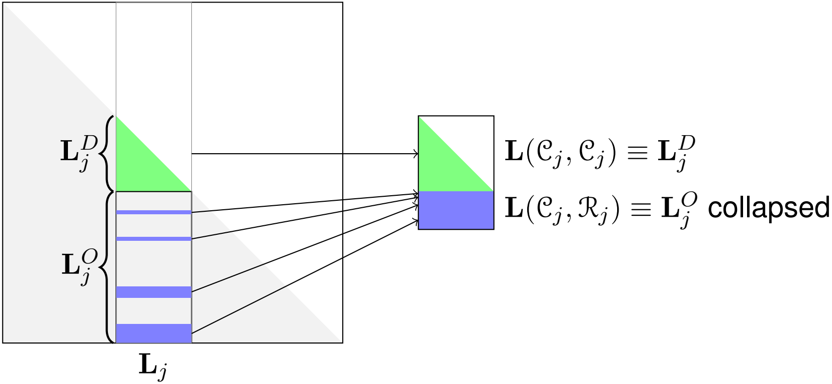
2D: $O(N^{3/2})$ time, $O(N \log N)$ space.
3D: $O(N^2)$ time, $O(N^{4/3})$ space.

Superfast ND reduces space/time complexity via *low-rank* structure.

Strategy

- Start with CHOLMOD (a good supernodal left-looking Cholesky)
  - Supernodal data structures are compact
  - Algorithm + data layout $\Longrightarrow$ most work in level 3 BLAS
  - Widely used already (so re-use the API!)
- Incorporate compact representations for low-rank blocks
  - Outer product for off-diagonal blocks
  - HSS-style representations for diagonal blocks
- Optimize, test, swear, fix, repeat

Supernodal storage structure



Supernode factorization

$\mathfrak{U}_j^D \longleftarrow \mathbf{A}(\mathcal{C}_j, \mathcal{C}_j)$
$\mathfrak{U}_j^O \longleftarrow \mathbf{A}(\mathcal{R}_j, \mathcal{C}_j)$

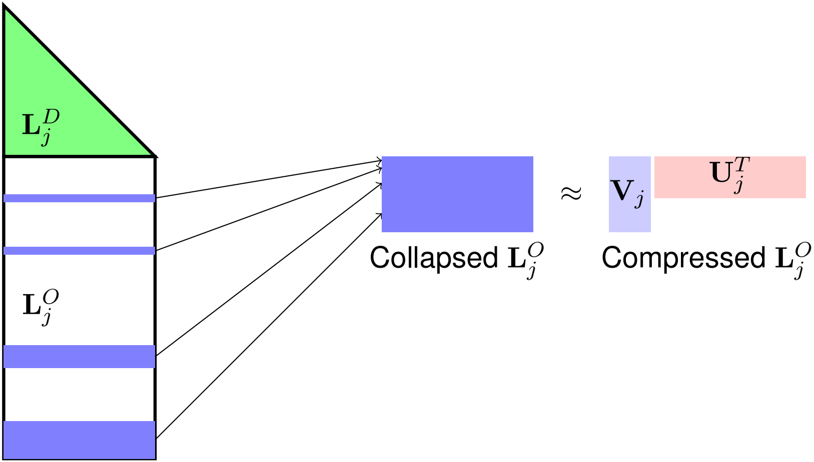
for each $k \in \mathbb{D}_j$ **do**
    Build dense updates from $\mathbf{L}_k^O$
    Scatter updates to $\mathfrak{U}_j^D$ and $\mathfrak{U}_j^O$

$\mathbf{L}_j^D \longleftarrow \mathrm{cholesky}(\mathfrak{U}_j^D)$
$\mathbf{L}_j^O \longleftarrow \mathfrak{U}_j^O (\mathbf{L}_j^D)^{-T}$

- Initialize storage
- Pull Schur contributions
- Finish forming $\mathbf{L}_j^D$

What changes in the rank-structured Cholesky?

Off-diagonal block compression



Collapsed off-diagonal block is a (nearly low-rank) dense matrix

Off-diagonal block compression

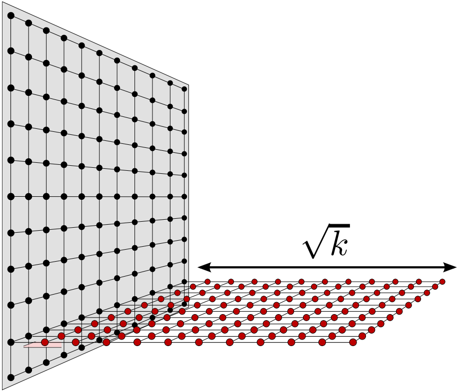
$\mathbf{G} \longleftarrow \text{rand}(|\mathcal{C}_j|, r+p)$
$\mathbf{C} \longleftarrow (\mathbf{L}_j^O)^T \mathbf{G}$
for $i = 1, \ldots, s$ **do**
  $\mathbf{C} \longleftarrow (\mathbf{L}_j^O)\mathbf{C}$
  $\mathbf{C} \longleftarrow (\mathbf{L}_j^O)^T \mathbf{C}$
$\mathbf{U}_j = \text{orth}(\mathbf{C})$
$\mathbf{V}_j = \mathbf{L}_j^O \mathbf{U}_j$

Compress *without* explicit $\mathbf{L}_j^O$:

- Probe $(\mathbf{L}_j^O)^T$ with random $\mathbf{G}$
- Extract orth. row basis $\mathbf{U}_j$
- $\mathbf{L}_j^O = \mathbf{V}_j \mathbf{U}_j^T \implies \mathbf{V}_j = \mathbf{L}_j^O \mathbf{U}_j$

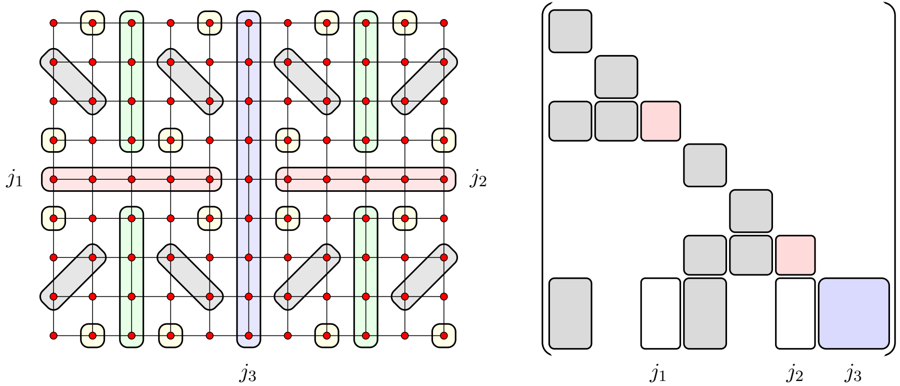
Where do we get the estimated rank bound r?

Interaction rank



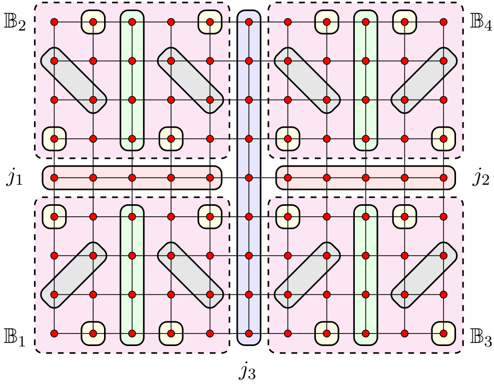
Could dynamically estimate the rank of L_j^O.
Practice: empirical rank bound $\approx \alpha\sqrt{k}\log(k)$.

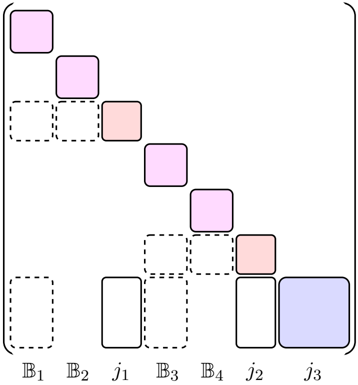
Optimization: Selective off-diagonal compression



Compress off-diagonal blocks of sufficiently large supernodes (j_1, j_2).

Optimization: Interior blocks





Don't store *any* of $\mathbf{L}_j^O$ for "interior" blocks
(Represent as $\mathbf{L}_j^O = \mathbf{A}_j^O(\mathbf{L}_j^D)^{-1}$ when needed)

Diagonal block compression

$$\mathbf{L}_j^D = \left(\begin{array}{cc:cc} \mathbf{L}_{j,1}^D & \mathbf{0} & \multicolumn{2}{c}{\multirow{2}{*}{$\mathbf{0}$}} \\ \hdashline \mathbf{L}_{j,2}^D & \mathbf{L}_{j,3}^D & & \\ \hdashline \multicolumn{2}{c:}{\multirow{2}{*}{$\mathbf{L}_{j,4}^D$}} & \mathbf{L}_{j,5}^D & \mathbf{0} \\ \cdashline{3-4} & & \mathbf{L}_{j,6}^D & \mathbf{L}_{j,7}^D \end{array}\right)$$

Basic observation: off-diagonal blocks are *low-rank*.
(H-matrix, semiseparable structure, quasiseparable structure, ...)

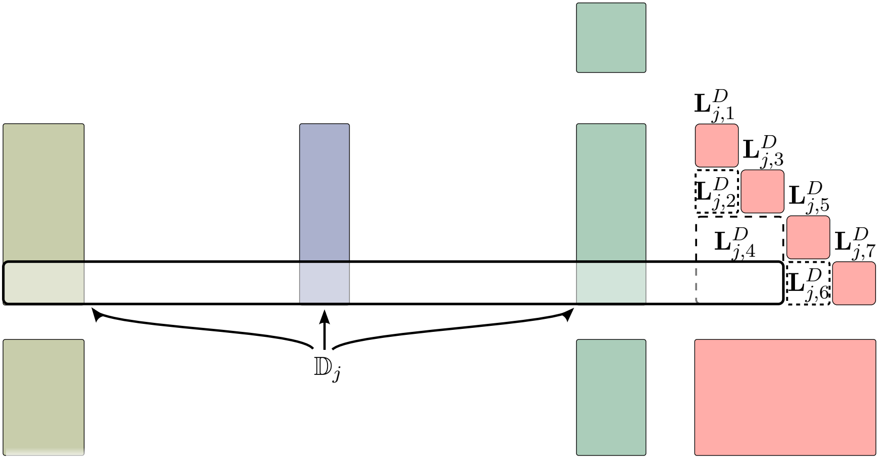
Assumes reasonable ordering of unknowns!

Diagonal block compression

$$
\mathbf{L}_j^D \approx \left(\begin{array}{cc|cc}
\mathbf{L}_{j,1}^D & \mathbf{0} & \multicolumn{2}{c}{\multirow{2}{*}{$\mathbf{0}$}} \\
\mathbf{V}_{j,2}^D(\mathbf{U}_{j,2}^D)^T & \mathbf{L}_{j,3}^D & & \\
\hline
\multicolumn{2}{c|}{\multirow{2}{*}{$\mathbf{V}_{j,4}^D(\mathbf{U}_{j,4}^D)^T$}} & \mathbf{L}_{j,5}^D & \mathbf{0} \\
 & & \mathbf{V}_{j,6}^D(\mathbf{U}_{j,6}^D)^T & \mathbf{L}_{j,7}^D
\end{array}\right).
$$

How do we get *directly* to this without forming $\mathfrak{U}_j^D$ explicitly?

Forming compressed updates



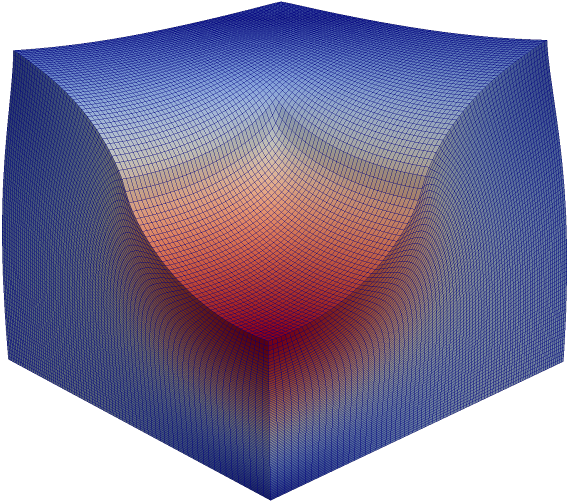
Rank-structured supernode factorization

Basic ingredients:

- Randomized algorithms form $\mathfrak{U}_j^D$
- Rank-structured factorization of $\mathfrak{U}_j^D$
- Randomized algorithm forms $\mathbf{L}_j^O$ (involves solves with $\mathbf{L}_j^D$)

Plus various optimizations.

Example: Large deformation of an elastic block



Example: Large deformation of an elastic block

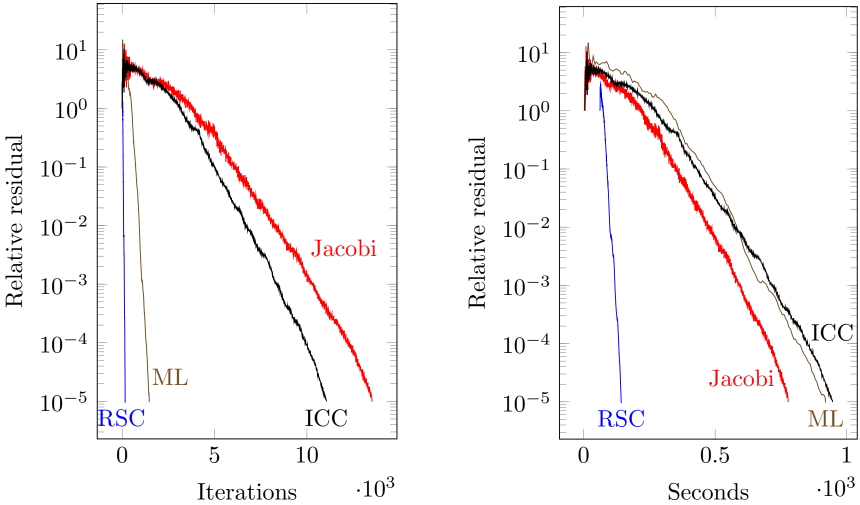
Benchmark based on example from deal.II:

- Nearly-incompressible hyperelastic block under compression
- Mixed FE formulation (pressure and dilation condensed out)
- Tried both $p = 1$ and $p = 2$ finite elements
- Two load steps, Newton on each (14-15 steps)

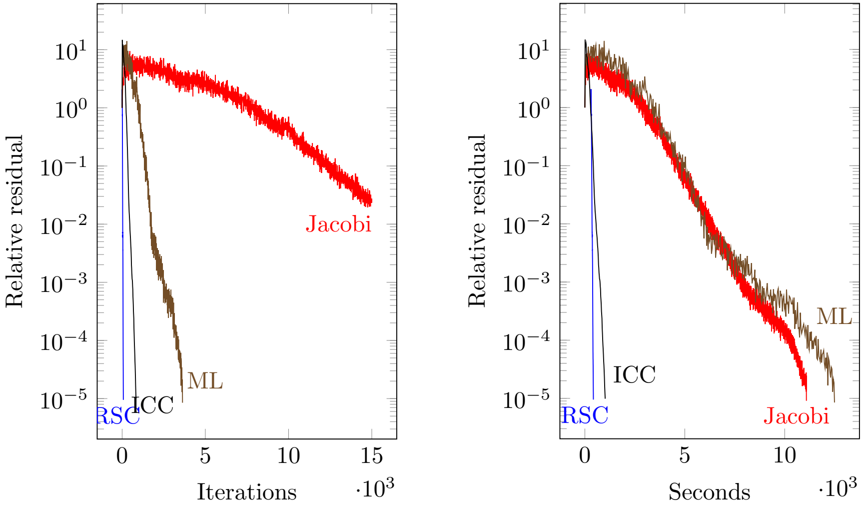
Experimental setup:

- 8-core Xeon X5570 with 48 GB RAM
- LAPACK/BLAS from MKL 11.0
- PCG + preconditioners from Trilinos

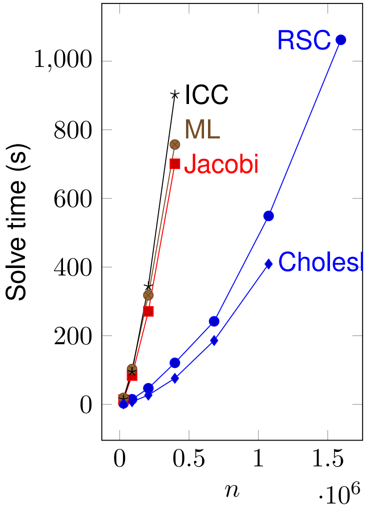
RSC vs standard preconditioners ($p = 1, N = 50$)

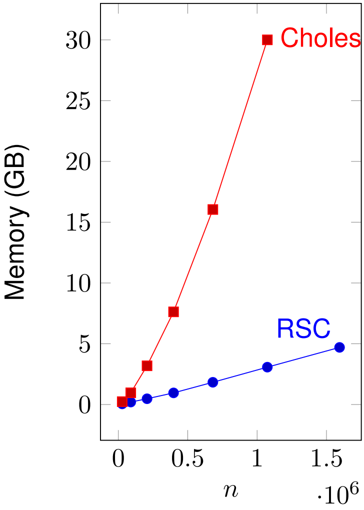


RSC vs standard preconditioners ($p = 2, N = 35$)

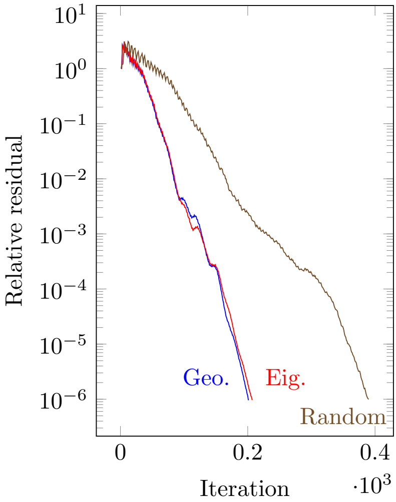


Time and memory comparisons ($p = 1$)





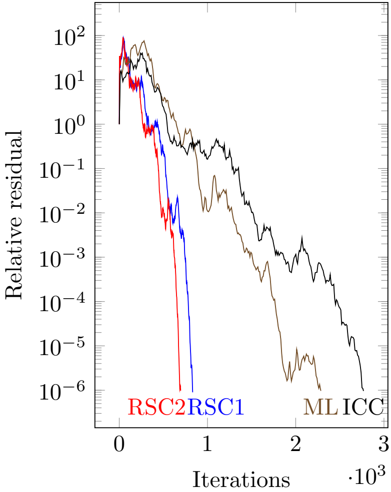
Effect of in-separator ordering

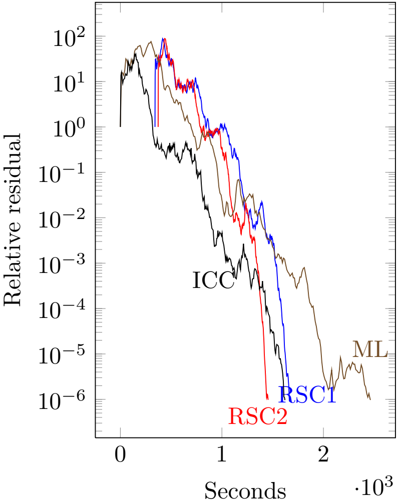


Semi-sep diag relies on variable order – don't want any old order!

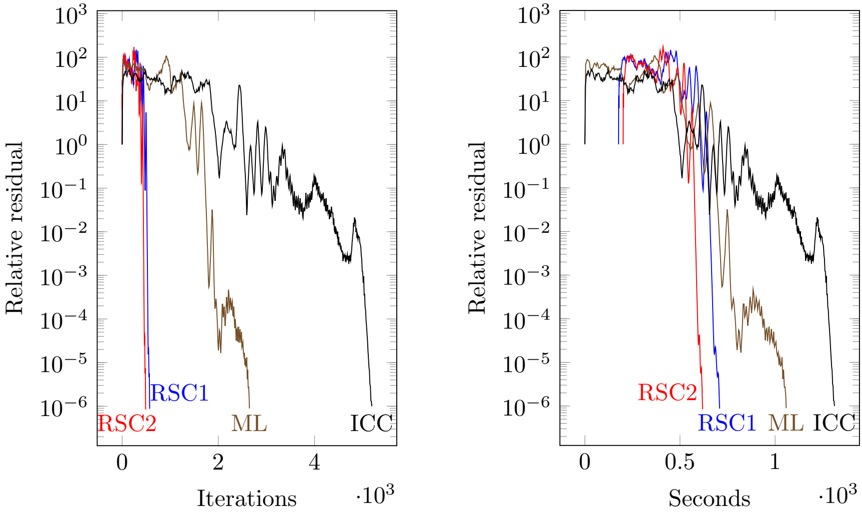
- Apply recursive bisection based on spatial coords
- Use coordinates if known
- Else assign spectrally

Example: Trabecular bone model ($\approx 1M$ dof)

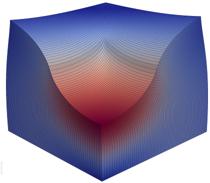




Example: Steel flange ($\approx 1.5M$ dof)



Conclusions



For more:

`www.cs.cornell.edu/~bindel`
`bindel@cs.cornell.edu`

Current status:

- Jeff has graduated! But...
- Code basically ready (still tweaking build system)
- Paper is mostly there (submit+arXiV before September)