

# CS 5220

## Sparse linear algebra

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Solve

$$Ax = b,$$

where  $A$  is sparse (or data sparse).

- Reminder of stationary iterations
- Krylov idea and performance via
  - Parallelism in algorithm
  - Better convergence (preconditioning)
  - Better memory access (reordering)
- Sparse Gaussian elimination

From splitting  $A = M - K$ , compute:

$$x^{(k+1)} = x^{(k)} + M^{-1}(b - Ax^{(k)}).$$

“Linear” rate of convergence, dependent on  $\rho(M^{-1}K)$ .

What if we only know how to multiply by  $A$ ? About all you can do is keep multiplying!

$$K_k(A, b) = \text{span} \{b, Ab, A^2b, \dots, A^{k-1}b\}.$$

Gives surprisingly useful information!

## Example: Conjugate Gradients

If  $A$  is symmetric and positive definite,  $Ax = b$  solves a minimization:

$$\phi(x) = \frac{1}{2}x^T Ax - x^T b$$
$$\nabla\phi(x) = Ax - b.$$

Idea: Minimize  $\phi(x)$  over  $K_k(A, b)$ . Basis for the *method of conjugate gradients*

Idea: Minimize  $\|Ax - b\|^2$  over  $K_k(A, b)$ . Yields *Generalized Minimum RESidual* (GMRES)

- KSPs are *not* stationary (no constant fixed-point iteration)
- Convergence is surprisingly subtle!
- CG convergence upper bound via *condition number*
  - Large condition number iff  $\phi(x)$  is narrow
  - True for Poisson and company



- *Preconditioned* problem  $M^{-1}Ax = M^{-1}b$
- Whence  $M$ ?
  - From a stationary method?
  - From a simpler/coarser discretization?
  - From approximate factorization?

```
r = b-A*x;
p = 0; beta = 0;
z = Msolve(r);
rho = dot(r, z);
for i=1:nsteps
    p = z + beta*p;
    q = A*p;
    alpha = rho/dot(p, q);
    x += alpha*p;
    r -= alpha*q;
    if norm(r) < tol, break; end
    z = Msolve(r);
    rho_prev = rho;
    rho = dot(r, z);
    beta = rho/rho_prev;
```

- Solve with  $M$
- Product with  $A$
- Dot products and axpys

- Rearrange if  $M = LL^T$  is available
- Or build around “powers kernel”
  - Old “s-step” approach of Chronopoulos and Gear
  - CA-Krylov of Hoemmen, Carson, Demmel
  - Hard to keep stable

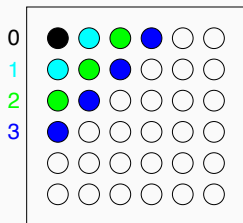
Two real application levers:

- Better preconditioning
- Faster matvecs

Key: fast solve with  $M$ , product with  $A$

- Some preconditioners parallelize better!
- Balance speed with performance.
  - Speed for set up of  $M$ ?
  - Speed to apply  $M$  after setup?
- Cheaper to do two multiplies/solves at once...
  - Can't exploit in obvious way – lose stability
  - Variants allow multiple products (CA-Krylov)
- Lots of fiddling possible with  $M$ ; matvec with  $A$ ?

## Thinking on (basic) CG convergence



Consider 5-point stencil on an  $n \times n$  mesh.

- Information moves one grid cell per matvec.
- Cost per matvec is  $O(n^2)$ .
- At least  $O(n^3)$  work to get information across mesh!

- Time to converge  $\geq$  time to move info across
- For a 2D mesh:  $O(n)$  matvecs,  $O(n^3) = O(N^{3/2})$  cost
- For a 3D mesh:  $O(n)$  matvecs,  $O(n^4) = O(N^{4/3})$  cost
- “Long” meshes yield slow convergence



3D beats 2D because everything is closer!

- Advice: sparse direct for 2D, CG for 3D.
- Better advice: use a preconditioner!

Define the *condition number* for  $\kappa(L)$  s.p.d:

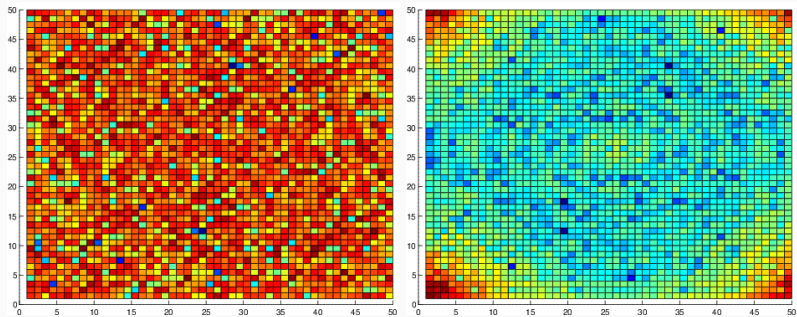
$$\kappa(L) = \frac{\lambda_{\max}(L)}{\lambda_{\min}(L)}$$

Describes how elongated the level surfaces of  $\phi$  are.

- For Poisson,  $\kappa(L) = O(h^{-2})$
- Steps to halve error:  $O(\sqrt{\kappa}) = O(h^{-1})$ .

Similar back-of-the-envelope estimates for some other PDEs. But these are not always that useful... can be pessimistic if there are only a few extreme eigenvalues.

## Frequency-domain approach

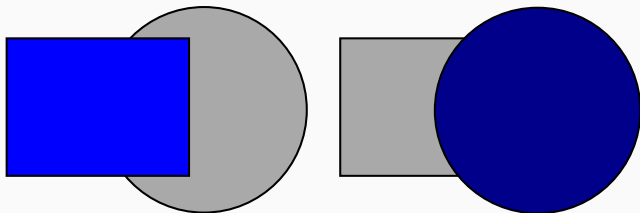


Error  $e_k$  after  $k$  steps of CG gets smoother!

- CG already handles high-frequency error
- Want something to deal with lower frequency!
- Jacobi useless
  - Doesn't even change Krylov subspace!

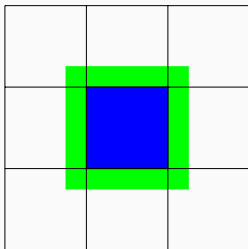
Better idea: block Jacobi?

- Q: How should things split up?
- A: Minimize blocks across domain.
- Compatible with minimizing communication!



Generalizes block Gauss-Seidel

## Restrictive Additive Schwartz (RAS)



- Get ghost cell data (green)
- Solve *everything* local (including neighbor data)
- Update local values for next step (local)
- Default strategy in PETSc



- RAS moves info one processor per step
- For scalability, still need to get around this!
- Basic idea: use multiple grids
  - Fine grid gives lots of work, kills high-freq error
  - Coarse grid cheaply gets info across mesh, kills low freq

Can also tune matrix multiply

- Represented implicitly (regular grids)
  - Example: Optimizing stencil operations (Datta)
- Or explicitly (e.g. compressed sparse column)
  - Sparse matrix blocking and reordering
  - Packages: Sparsity (Im), OSKI (Vuduc)
  - Available as PETSc extension

Or further rearrange algorithm (Hoemmen, Demmel).

```
for (int i = 0; i < n; ++i) {  
    y[i] = 0;  
    for (int jj = ptr[i]; jj < ptr[i+1]; ++jj)  
        y[i] += A[jj]*x[col[jj]];  
}
```

Where is the problem for memory access?

Memory access patterns:

- Elements of  $y$  accessed sequentially
- Elements of  $A$  accessed sequentially
- Access to  $x$  are all over!

Can help by switching to block CSR. Switching to single precision, short indices can help memory traffic, too!

- Each processor gets a piece
- Many partitioning strategies
- Idea: re-order so one of these strategies is “good”

SpMV performance goals:

- Balance load?
- Balance storage?
- Minimize communication?
- Good cache re-use?

Reordering also comes up for GE!

Permute unknowns for better SpMV or

- Stability of Gauss elimination,
- Fill reduction in Gaussian elimination,
- Improved performance of preconditioners...

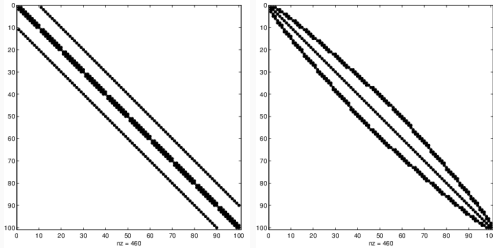
Want to partition sparse graphs so that

- Subgraphs are same size (load balance)
- Cut size is minimal (minimize communication)

Matrices that are “almost” diagonal are good?



# Reordering for bandedness



## Reverse Cuthill-McKee

- Select “peripheral” vertex  $v$
- Order according to breadth first search from  $v$
- Reverse ordering

- RCM ordering is great for SpMV
- But isn't narrow banding good for solvers, too?
  - LU takes  $O(nb^2)$  where  $b$  is bandwidth.
  - Great if there's an ordering where  $b$  is small!

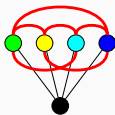
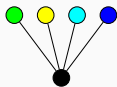
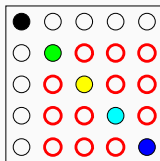
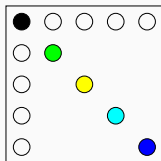
- *Profile* solvers generalize band solvers
- Skyline storage for lower triangle: for each row  $i$ ,
  - Start and end of storage for nonzeros in row.
  - *Contiguous* nonzero list up to main diagonal.
- In each column, first nonzero defines a profile.
- All fill-in confined to profile.
- RCM is again a good ordering.

- Minimum bandwidth for 2D model problem? 3D?
- Skyline only gets us so much farther

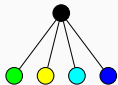
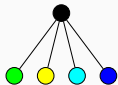
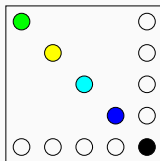
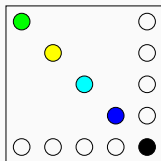
But more general solvers have similar structure

- Ordering (minimize fill)
- Symbolic factorization (where will fill be?)
- Numerical factorization (pivoting?)
- ... and triangular solves

## Troublesome Trees



One step of Gaussian elimination *completely* fills this matrix!



Full Gaussian elimination generates *no* fill in this matrix!

How many fill elements are there for elimination on

$$A = \begin{bmatrix} x & x & 0 & 0 & x & 0 & 0 & x \\ x & x & x & 0 & 0 & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & x & x & 0 & 0 & 0 \\ x & 0 & 0 & x & x & x & 0 & 0 \\ 0 & 0 & 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & 0 & 0 & x & x & x \\ x & 0 & 0 & 0 & 0 & 0 & x & x \end{bmatrix}$$



Consider first steps of GE

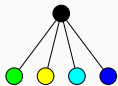
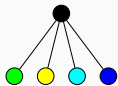
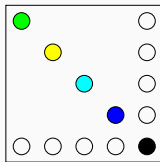
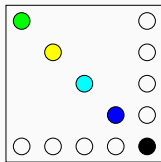
$$A(2:\text{end},1) = A(2:\text{end},1)/A(1,1);$$

$$A(2:\text{end},2:\text{end}) = A(2:\text{end},2:\text{end}) - \dots \\ A(2:\text{end},1)*A(1,2:\text{end});$$

Nonzero in the outer product at  $(i, j)$  if  $A(i,1)$  and  $A(j,1)$  both nonzero — that is, if  $i$  and  $j$  are both connected to 1.

General: Eliminate variable, connect remaining neighbors.

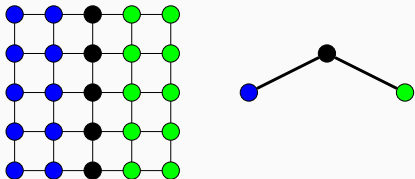
## Terrific Trees Redux



Order leaves to root  $\implies$

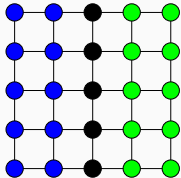
on eliminating  $i$ , parent of  $i$  is only remaining neighbor.

## Nested Dissection



- Idea: Think of *block* tree structures.
- Eliminate block trees from bottom up.
- Can recursively partition at leaves.

# Nested Dissection



- Rough cost estimate: how much just to factor dense Schur complements associated with separators?
- Notice graph partitioning appears again!
  - And again we want small separators!

Model problem: Laplacian with 5 point stencil (for 2D)

- ND gives optimal complexity in exact arithmetic (George 73, Hoffman/Martin/Rose)
- 2D:  $O(N \log N)$  memory,  $O(N^{3/2})$  flops
- 3D:  $O(N^{4/3})$  memory,  $O(N^2)$  flops

- Locally greedy strategy
  - Want to minimize upper bound on fill-in
  - $\text{Fill} \leq (\text{degree in remaining graph})^2$
- At each step
  - Eliminate vertex with smallest degree
  - Update degrees of neighbors
- Problem: Expensive to implement!
  - But better variants via *quotient graphs*
  - Variants often used in practice

- Variables (columns) are nodes in trees
- $j$  a descendant of  $k$  if eliminating  $j$  updates  $k$
- Can eliminate disjoint subtrees in parallel!

Basic idea: exploit “supernodal” (dense) structures in factor

- e.g. arising from elimination of separator Schur complements in ND
- Other alternatives exist (multifrontal solvers)



Pivoting is painful, particularly in distributed memory!

- Cholesky — no need to pivot!
- Threshold pivoting — pivot when things look dangerous
- Static pivoting — try to decide up front

What if things go wrong with threshold/static pivoting?

Common theme: Clean up sloppy solves with good residuals

Can improve solution by *iterative refinement*:

$$PAQ \approx LU$$

$$x_0 \approx QU^{-1}L^{-1}Pb$$

$$r_0 = b - Ax_0$$

$$x_1 \approx x_0 + QU^{-1}L^{-1}Pr_0$$

Looks like approximate Newton on  $F(x) = Ax - b = 0$ .

This is just a stationary iterative method!

Nonstationary methods work, too.

If we're willing to sacrifice some on factorization,

- Single precision factor + double precision refinement?
- Sloppy factorizations (marginal stability) + refinement?
- Modify  $m$  small pivots as they're encountered (low rank updates), fix with  $m$  steps of a Krylov solver?

- Sparse direct for 2D problems
- Gets more expensive for 3D problems
- Approximate direct solves make good preconditioners