Lecture 18: More Fun With Sparse Matrices

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Life lessons from SPH?

- Where an error occurs may not be where you observe it!
- Check against a slow, naive, obvious calculation.
- `assert` is your friend.
- Use version control (`git`, `cvs`, `svn`, ...).

Reminder: Conjugate Gradients

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

$$\mathcal{K}_k(A, b) = \text{span}\left\{b, Ab, A^2b, \ldots, A^{k-1}b\right\}.$$

Gives surprisingly useful information!

If A is symmetric and positive definite, $x = A^{-1}b$ minimizes

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

Idea: Minimize $\phi(x)$ over $\mathcal{K}_k(A, b)$.
Basis for the *method of conjugate gradients*

Convergence of CG

- KSPs are *not* stationary (no constant fixed-point iteration)
- Convergence is surprisingly subtle!
- CG convergence upper bound via *condition number*
  - Large condition number iff form $\phi(x)$ has long narrow bowl
  - Usually happens for Poisson and related problems
- *Preconditioned* problem $M^{-1}Ax = M^{-1}b$ converges faster?
- Whence M?
  - From a stationary method?
  - From a simpler/coarser discretization?
  - From approximate factorization?

PCG

```
Compute $r^{(0)} = b - Ax$
for $i = 1, 2, \dots$
    solve $Mz^{(i-1)} = r^{(i-1)}$
    $\rho_{i-1} = (r^{(i-1)})^T z^{(i-1)}$
    if $i == 1$
      $p^{(1)} = z^{(0)}$
    else
      $\beta_{i-1} = \rho_{i-1}/\rho_{i-2}$
      $p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$
    endif
    $q^{(i)} = Ap^{(i)}$
    $\alpha_i = \rho_{i-1}/(p^{(i)})^T q^{(i)}$
    $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$
end
```

Parallel work:

- Solve with M
- Product with A
- Dot products
- Axpys

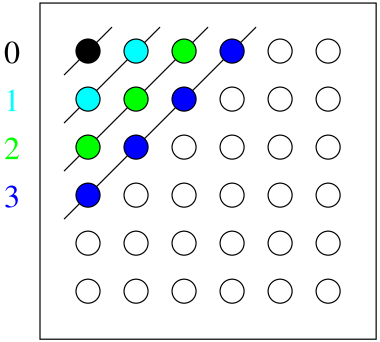
Overlap comm/comp.

PCG bottlenecks

Key: fast solve with M, product with A

- Some preconditioners parallelize better! (Jacobi vs Gauss-Seidel)
- 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 — Hoemmen's thesis
- Lots of fiddling possible with M; what about matvec with A?

Thinking on (basic) CG convergence



Consider 2D Poisson with 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!

CG convergence: a counting approach

- Time to converge $\geq$ time to propagate info across mesh
- 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!

CG convergence: an eigenvalue approach

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

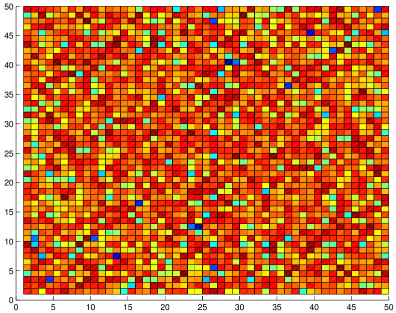
$$\kappa(L) = \frac{\lambda_{\max}(L)}{\lambda_{\min}(L)}$$

Describes how elongated the level surfaces of ϕ are.

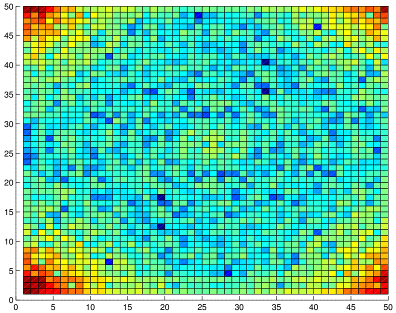
- For Poisson, $\kappa(L) = O(h^{-2})$
- CG steps to reduce error by $1/2$ = $O(\sqrt{\kappa}) = O(h^{-1})$.

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.

CG convergence: a frequency-domain approach



FFT of e_0



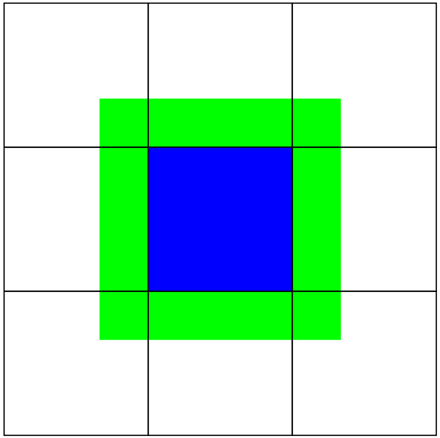
FFT of e_{10}

Error e_k after k steps of CG gets smoother!

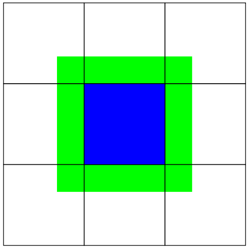
Choosing preconditioners for 2D Poisson

- 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!

Restrictive Additive Schwartz (RAS)



Restrictive Additive Schwartz (RAS)



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

Multilevel Ideas

- RAS propogates information by 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

More on this another time.

CG performance

Two ways to get better performance from CG:

1. Better preconditioner
   - Improves asymptotic complexity?
   - ... but application dependent
2. Tuned implementation
   - Improves constant in big-O
   - ... but application independent?

Benchmark idea (?): no preconditioner, just tune.

Tuning PCG

```
Compute $r^{(0)} = b - Ax$
for $i = 1, 2, \ldots$
    solve $Mz^{(i-1)} = r^{(i-1)}$
    $\rho_{i-1} = (r^{(i-1)})^T z^{(i-1)}$
    if $i == 1$
      $p^{(1)} = z^{(0)}$
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    $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$
end
```

- Most work in A, M
- Vector ops synchronize
- Overlap comm, comp?

Tuning PCG

```
Compute $r^{(0)} = b - Ax$
$p_{-1} = 0; \beta_{-1} = 0; \alpha_{-1} = 0$
$s = L^{-1} r^{(0)}$
$\rho_0 = s^T s$
for $i = 0, 1, 2, \dots$
    $w_i = L^{-T} s$
    $p_i = w_i + \beta_{i-1} p_{i-1}$
    $q_i = A p_i$
    $\gamma = p_i^T q_i$
    $x_i = x_{i-1} + \alpha_{i-1} p_{i-1}$
    $\alpha_i = \rho_i / \gamma_i$
    $r_{i+1} = r_i - \alpha q_i$
    $s = L^{-1} r_{i+1}$
    $\rho_{i+1} = s^T s$
    Check convergence ($\|r_{i+1}\|$)
    $\beta_i = \rho_{i+1} / \rho_i$
end
```

Split $z = M^{-1} r$ into s, w_i
Overlap

- $p_i^T q_i$ with x update
- $s^T s$ with w_i eval
- Computing p_i, q_i, γ
- Pipeline r_{i+1}, s?
- Pipeline p_i, w_i?

Parallel Numerical LA,
Demmel, Heath, van der Vorst

Tuning PCG

Can also tune

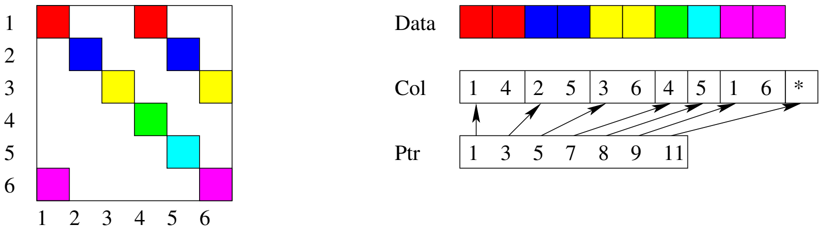
- Preconditioner solve (hooray!)
- Matrix multiply
    - Represented implicitly (regular grids)
    - Or explicitly (e.g. compressed sparse column)

Or further rearrange algorithm (Hoemmen, Demmel).

Tuning sparse matvec

- Sparse matrix blocking and reordering (Im, Vuduc, Yelick)
  - Packages: Sparsity (Im), OSKI (Vuduc)
  - Available as PETSc extension
- Optimizing stencil operations (Datta)

Reminder: Compressed sparse row storage



```
for i = 1:n
  y[i] = 0;
  for jj = ptr[i] to ptr[i+1]-1
    y[i] += A[jj]*x[col[j]];
  end
end
```

Problem: `y[i] += A[jj]*x[`**col[j]**`];`

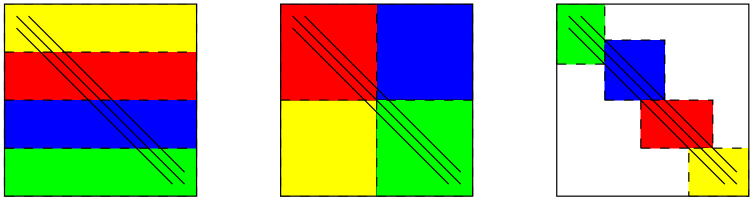
Memory traffic in CSR multiply

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!

Parallelizing matvec



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

Reordering for matvec

SpMV performance goals:

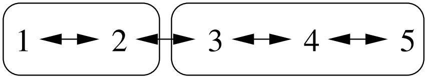
- Balance load?
- Balance storage?
- Minimize communication?
- Good cache re-use?

Also reorder for

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

Reminder: Sparsity and partitioning

$$A = \left[\begin{array}{cc:ccc} * & * & & & \\ * & * & * & & \\ \hdashline & * & * & * & \\ & & * & * & * \\ & & & * & * \end{array}\right]$$

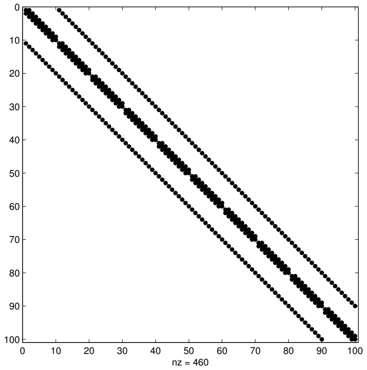


Want to partition sparse graphs so that

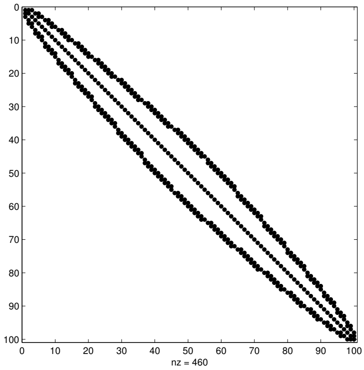
- Subgraphs are same size (load balance)
- Cut size is minimal (minimize communication)

Matrices that are “almost” diagonal are good?

Reordering for bandedness



Natural order



RCM reordering

Reverse Cuthill-McKee

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

From iterative to direct

- 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!

Skylines and profiles

- *Profile* solvers generalize band solvers
- Use skyline storage; if storing 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.

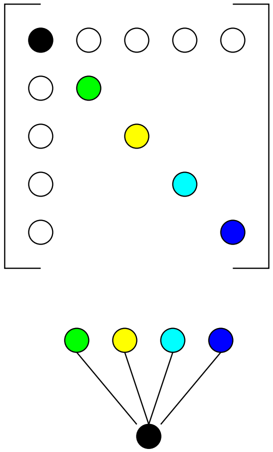
Beyond bandedness

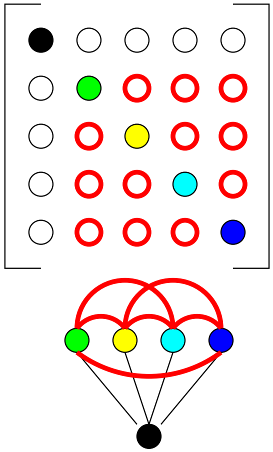
- Bandedness only takes us so far
  - Minimum bandwidth for 2D model problem? 3D?
  - Skyline only gets us so much farther
- But more general solvers have similar structure
  - Ordering (minimize fill)
  - Symbolic factorization (where will fill be?)
  - Numerical factorization (pivoting?)
  - ... and triangular solves

Reminder: Matrices to graphs

- $A_{ij} \neq 0$ means there is an edge between i and j
- Ignore self-loops and weights for the moment
- Symmetric matrices correspond to undirected graphs

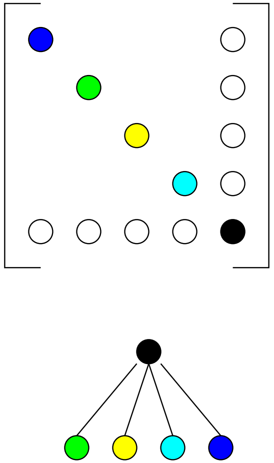
Troublesome Trees

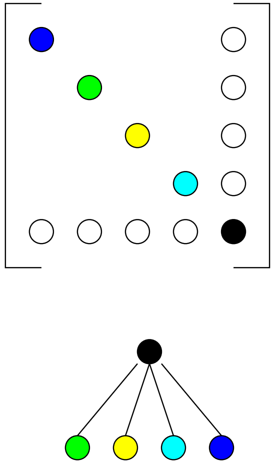




One step of Gaussian elimination *completely* fills this matrix!

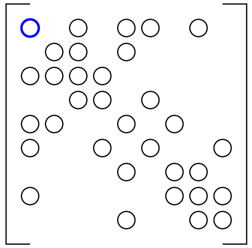
Terrific Trees

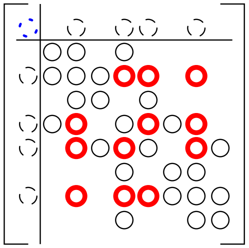


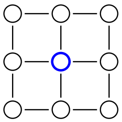


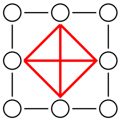
Full Gaussian elimination generates *no* fill in this matrix!

Graphic Elimination









Eliminate a variable, connect all neighbors.

Graphic Elimination

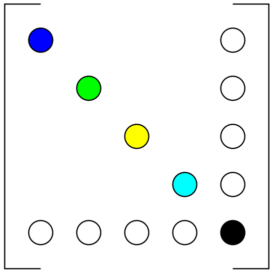
Consider first steps of GE

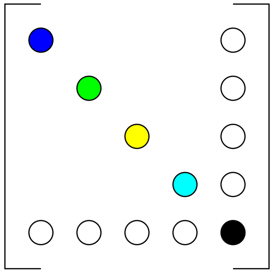
```
A(2:end,1)       = A(2:end,1)/A(1,1);
A(2:end,2:end) = A(2:end,2:end)-...
                   A(2:end,1)*A(1,2:end);
```

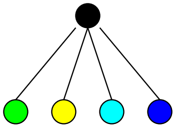
Nonzero in the outer product at (i, j) if `A(i,1)` and `A(j,1)` both nonzero — that is, if *i* and *j* are both connected to 1.

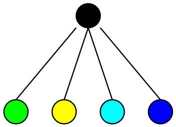
General: Eliminate variable, connect remaining neighbors.

Terrific Trees Redux



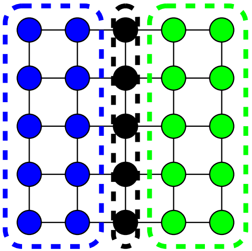


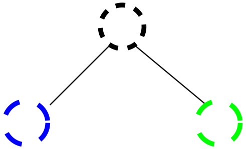




Order leaves to root $\Longrightarrow$
on eliminating *i*, parent of *i* is only remaining neighbor.

Nested Dissection





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

Nested Dissection

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

Minimum Degree

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

Elimination Tree

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

Cache locality

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

Pivoting is a tremendous pain, 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

Direct to iterative

Can improve solution by *iterative refinement*:

$$
\begin{aligned}
PAQ &\approx LU \\
x_0 &\approx QU^{-1}L^{-1}Pb \\
r_0 &= b - Ax_0 \\
x_1 &\approx x_0 + QU^{-1}L^{-1}Pr_0
\end{aligned}
$$

Looks like approximate Newton on $F(x) = Ax - b = 0$.
This is just a stationary iterative method!
Nonstationary methods work, too.

Variations on a theme

If we're willing to sacrifice some on factorization,

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