Lecture 15:
More Iterative Ideas

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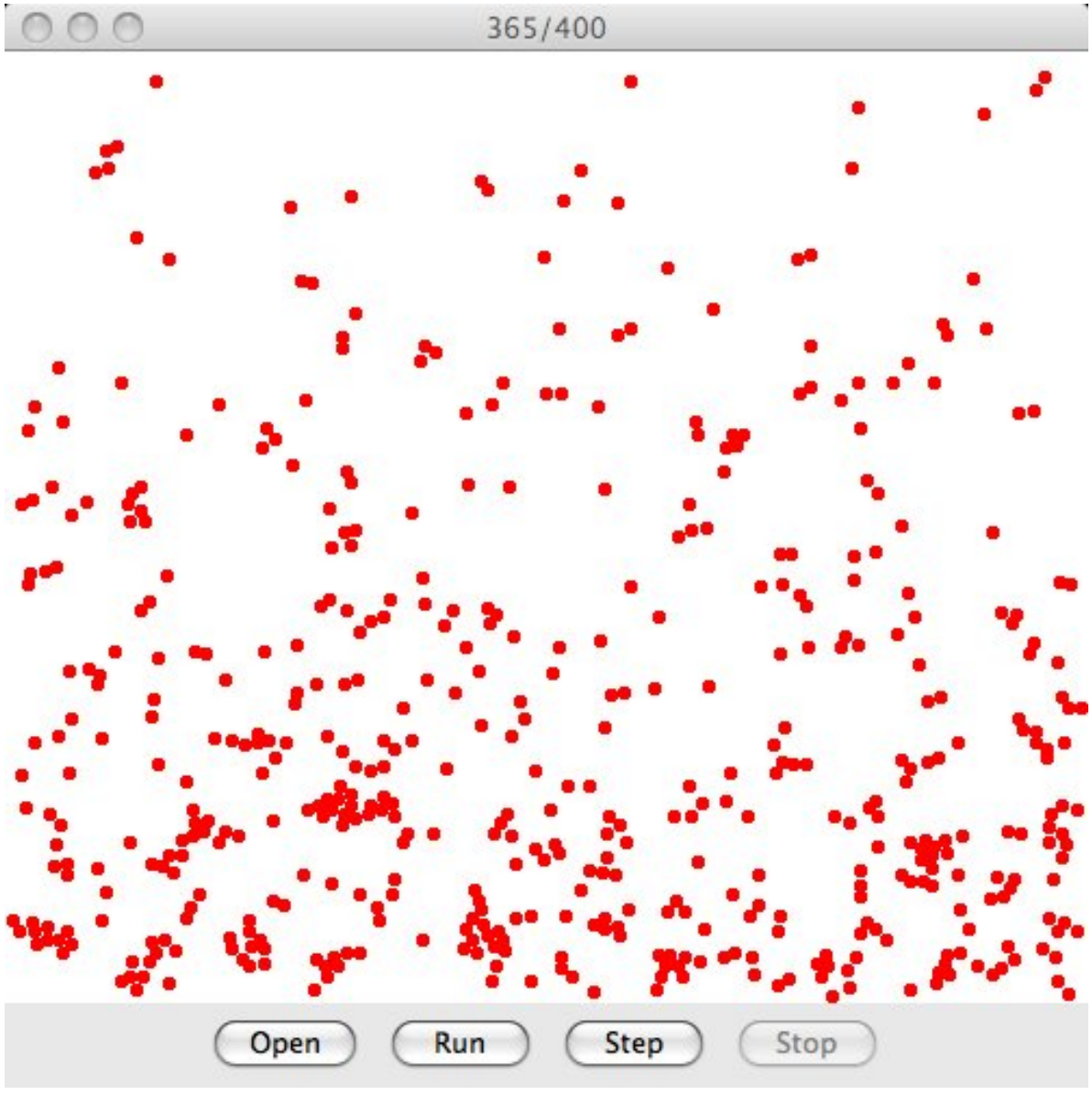
15 Mar 2010

Logistics

- HW 2 due!
- Some notes on HW 2.
- Where we are / where we're going
- More iterative ideas.
- Intro to HW 3.

More HW 2 notes



See solution code!

Life lessons from HW 2?

- 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`, ...).

Where we've been

So far: some basic technology and algorithmic ideas

- Architectural ideas (serial and parallel)
- Parallel programming models
- OpenMP and MPI programming
- Overview of parallel simulation ideas
- Overview of dense and sparse linear algebra

Where we're going

Still up (technology side):

- UPC programming
- CUDA programming
- Performance analysis tools
- Scripting, code generation, mixed-language coding
- Library use and PETSc/Trilinos

Where we're going

Still up (algorithmic side):

- Sparse direct methods
- FFT and spectral methods
- Multigrid and domain decomposition
- Hierarchical methods for N-body
- Graph partitioning
- Parallel sort

... and some applications as time permits.

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

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

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 $i = 1, 2, \ldots$
  solve $Mz^{(i-1)} = r^{(i-1)}$
  $\rho_{i-1} = (r^{(i-1)})^T z^{(i-1)}$
  if $i == 1$
    $p^{(1)} = z^{(0)}$
  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

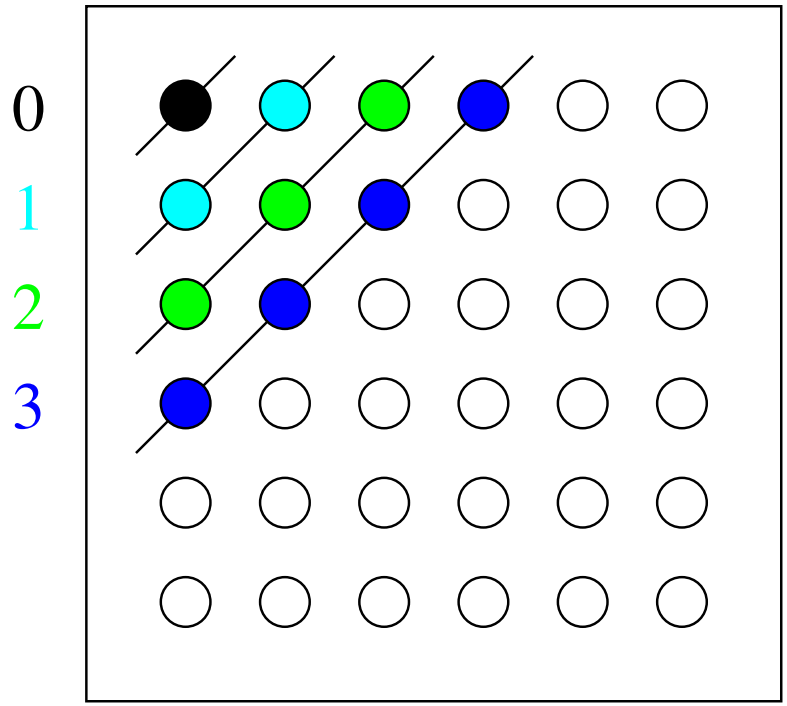
Overlap comm/comp.

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:

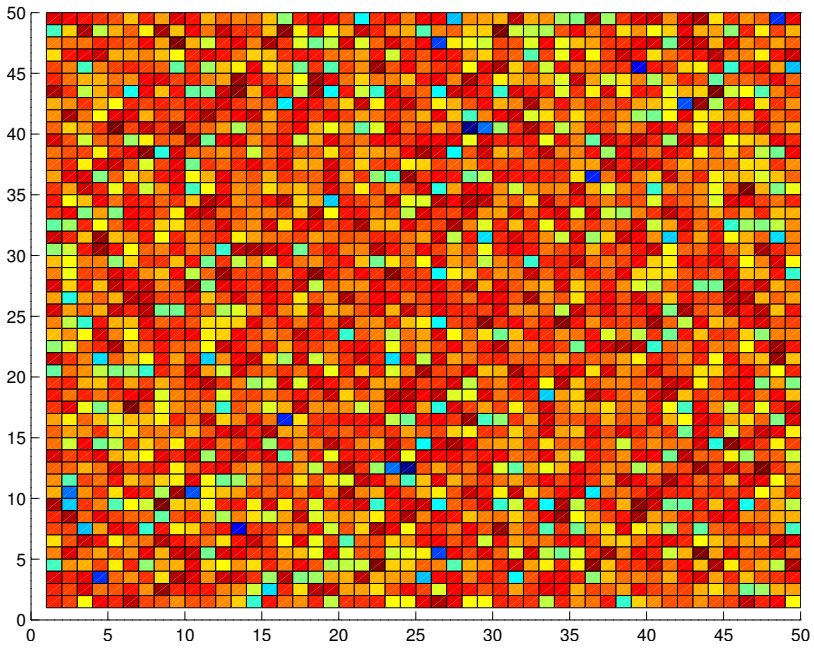
$$\kappa(L) = \frac{\lambda_{\max}(L)}{\lambda_{\min}(L)}$$

Describes how elongated the level surfaces of ϕ are.

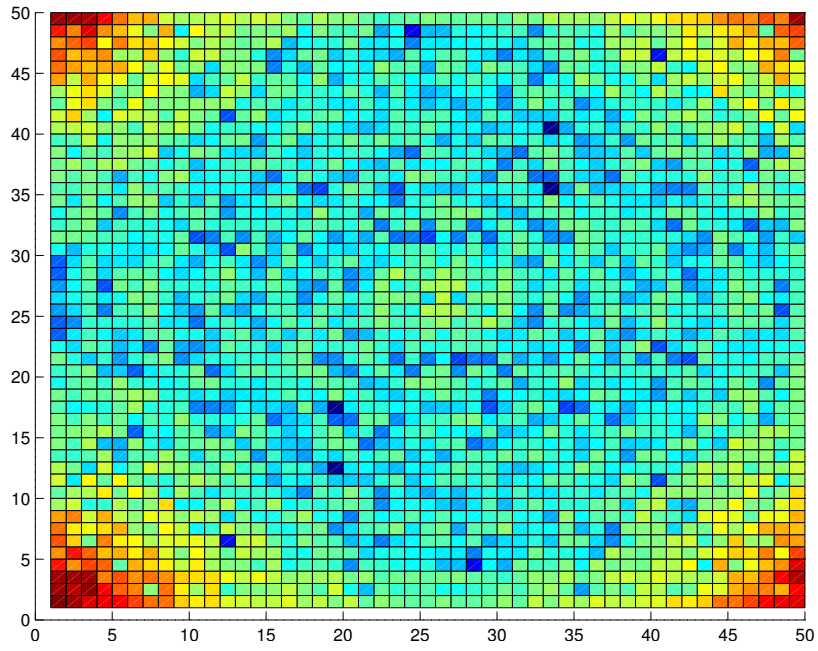
- For Poisson, $\kappa(L) = O(h^{-2})$
- CG steps to reduce error by $1/2$ = $O(\sqrt{\kappa}) = O(h^{-1})$.

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



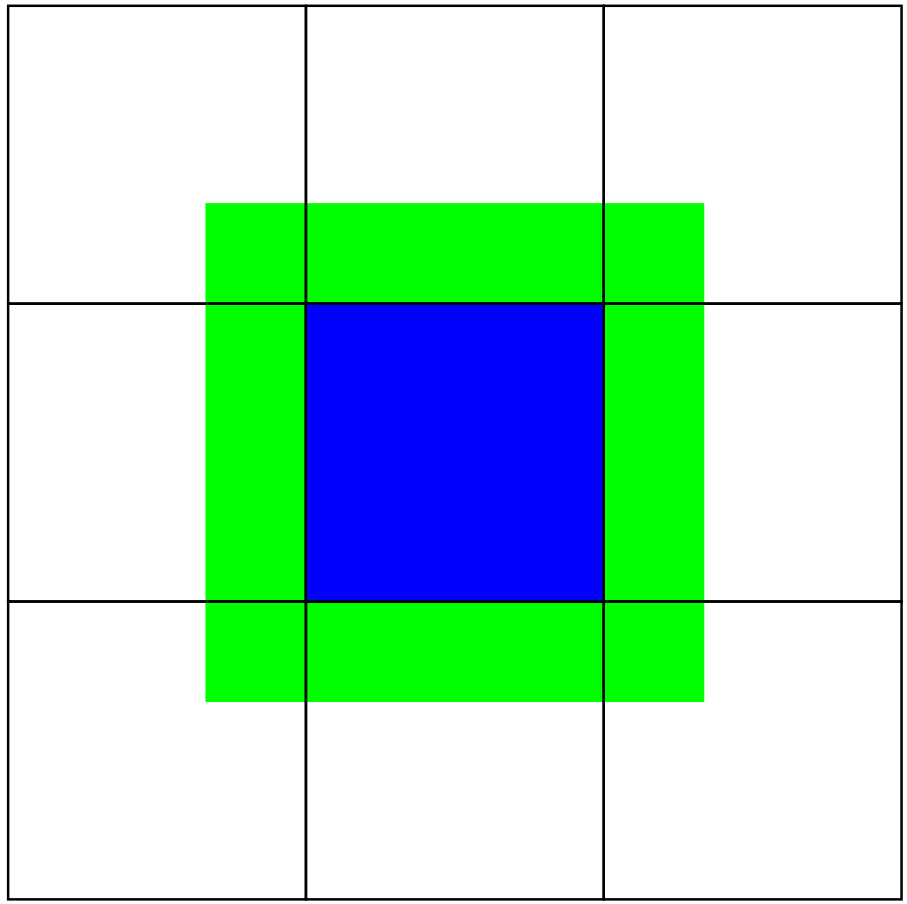
FFT of e_{10}

Error e_k after k steps of CG gets smoother!

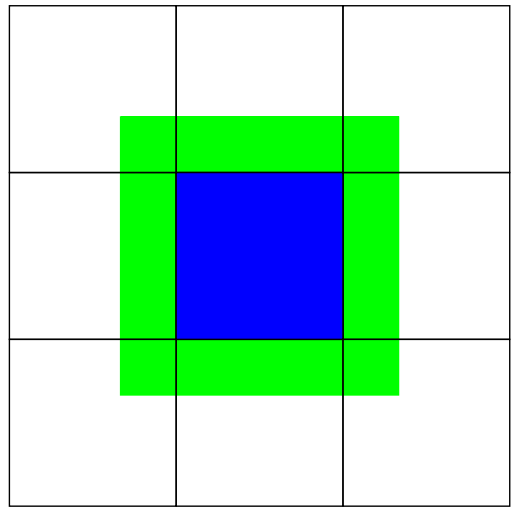
Choosing preconditioners for 2D Poisson

- 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 $i == 1$
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  $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$
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 $i = 0, 1, 2, \ldots$
  $w_i = L^{-T} s$
  $p_i = w_i + \beta_{i-1} p_{i-1}$
  $q_i = A p_i$
  $\gamma = p_i^T q_i$
  $x_i = x_{i-1} + \alpha_{i-1} p_{i-1}$
  $\alpha_i = \rho_i / \gamma_i$
  $r_{i+1} = r_i - \alpha q_i$
  $s = L^{-1} r_{i+1}$
  $\rho_{i+1} = s^T s$
  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

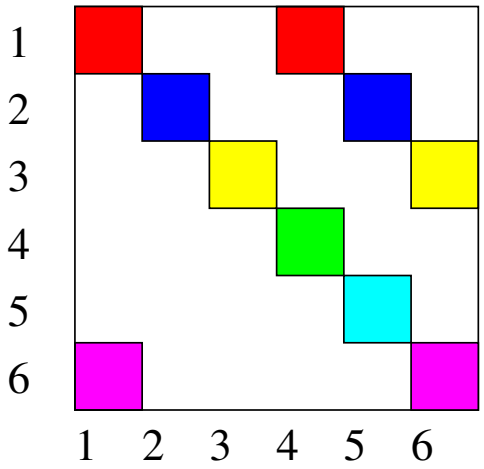
- Preconditioner solve (hooray!)
- Matrix multiply
  - Represented implicitly (regular grids)
  - Or explicitly (e.g. compressed sparse column)

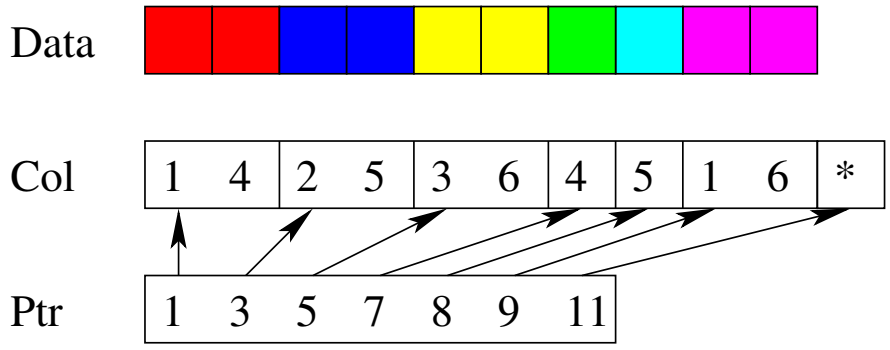
Or further rearrange algorithm (Hoemmen, Demmel).

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]];`

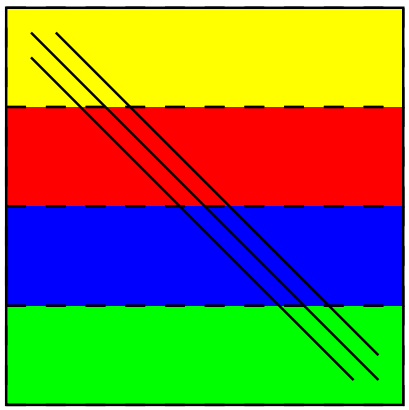
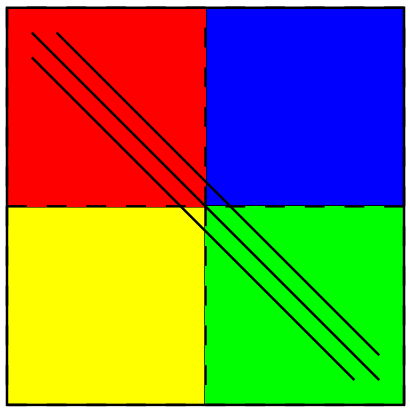
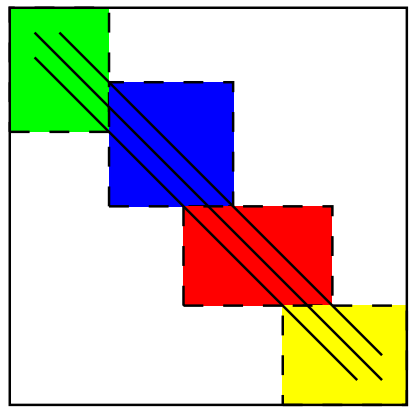
Memory traffic in CSR multiply

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:

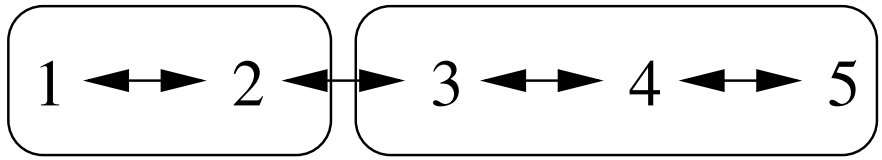
- Balance load?
- Balance storage?
- Minimize communication?
- Good cache re-use?

Also reorder for

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

Reminder: Sparsity and partitioning

$$A = \begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & * & \\ & & * & * & * \\ & & & * & * \end{bmatrix}$$

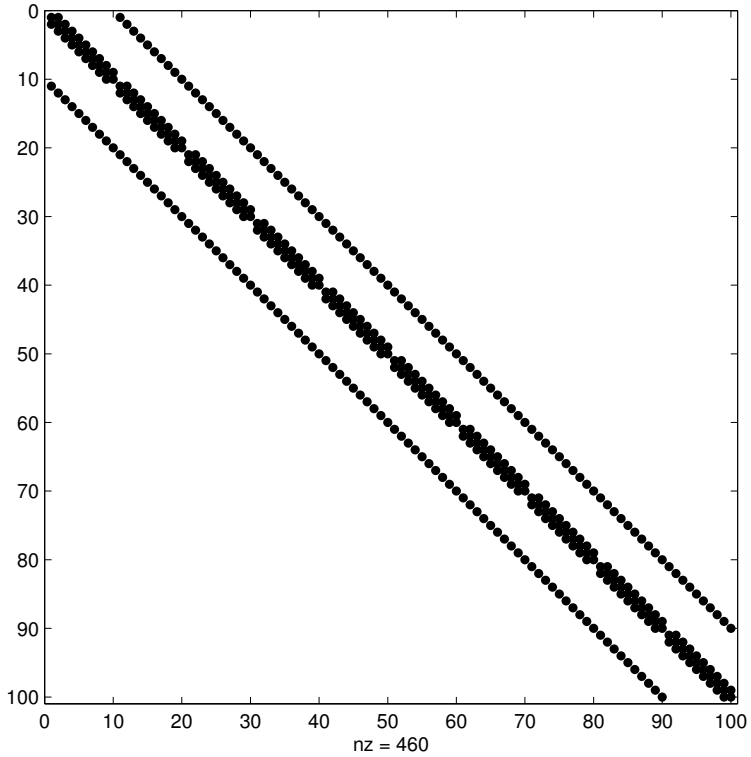


Want to partition sparse graphs so that

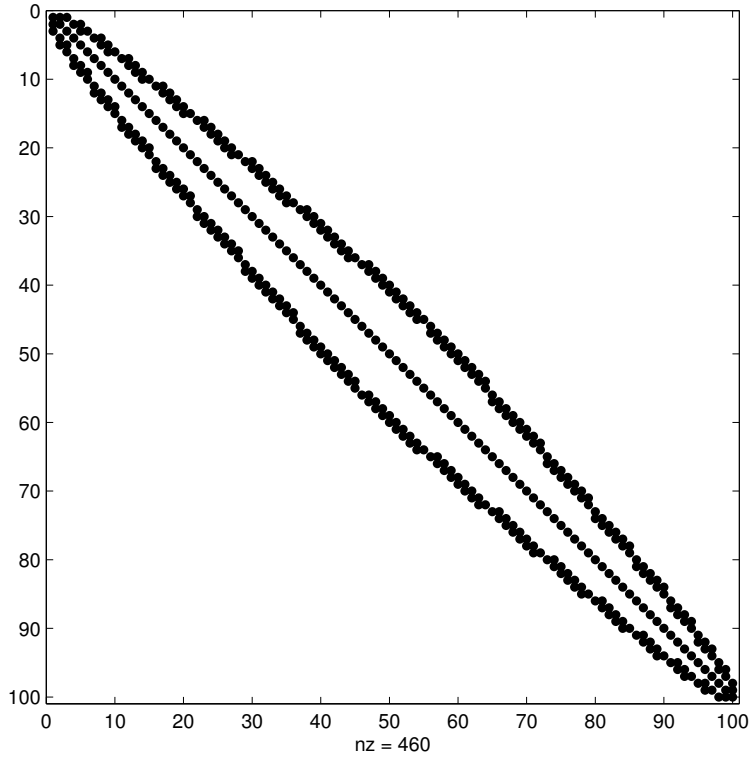
- Subgraphs are same size (load balance)
- Cut size is minimal (minimize communication)

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

HW 3 preview

Given serial implementation of:

- 3D elastic finite element code
- Regular mesh, variable material properties
- PCG solver with an RAS preconditioner

Wanted:

- Parallelized CG solver (MPI or OpenMP)
- Study of scaling with n, p
- Some fun tuning (e.g. matrix layout)