Lecture 16:
Iterative Methods and Sparse Linear Algebra

David Bindel

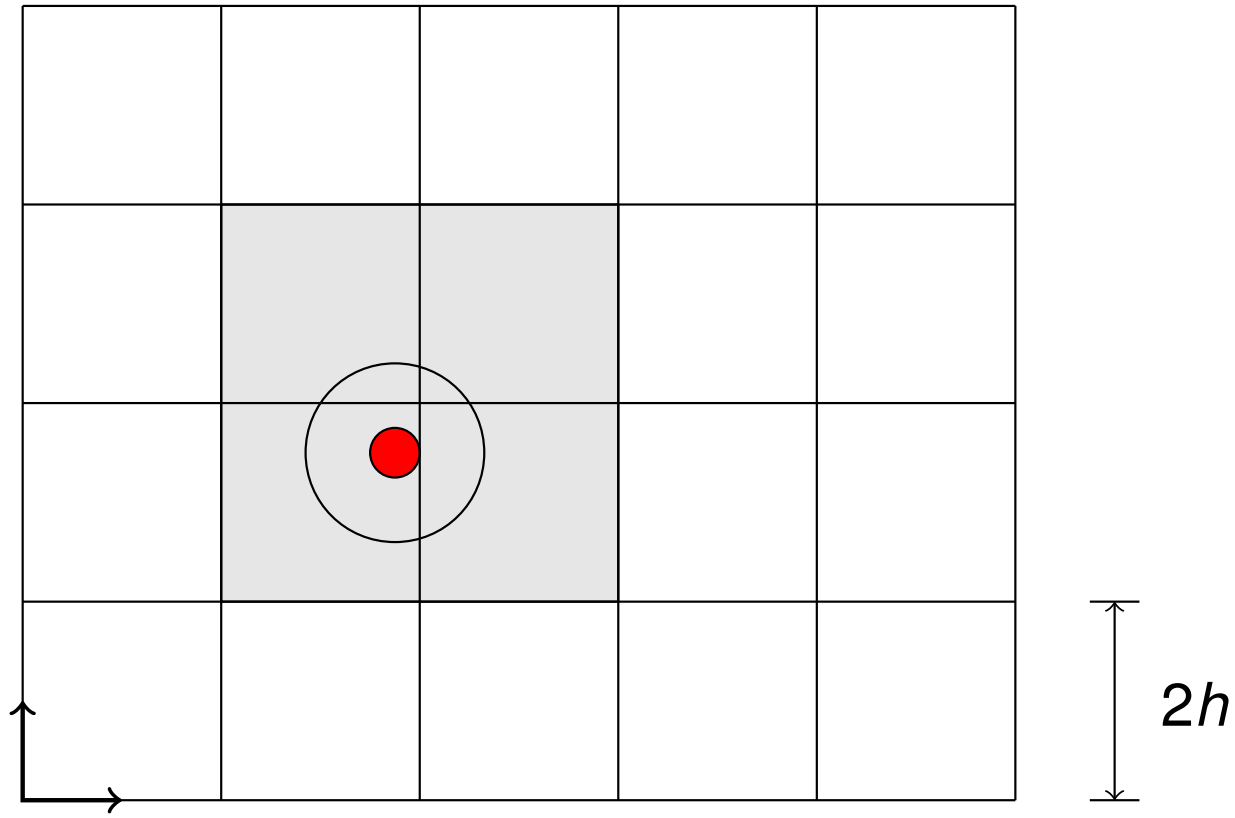
25 Oct 2011

Logistics

- Send me a project title and group (today, please!)
- Project 2 due next Monday, Oct 31

<aside topic="proj2">

Bins of particles




```
// x bin and interaction range (y similar)
int ix   = (int) ( x     /(2*h) );
int ixlo = (int) ( (x-h)/(2*h) );
int ixhi = (int) ( (x+h)/(2*h) );
```

Spatial binning and hashing

- Simplest version
  - One linked list per bin
  - Can include the link in a particle `struct`
  - Fine for this project!
- More sophisticated version
  - Hash table keyed by bin index
  - Scales even if occupied volume $\ll$ computational domain

Partitioning strategies

Can make each processor responsible for

- A region of space
- A set of particles
- A set of interactions

Different tradeoffs between load balance and communication.

To use symmetry, or not to use symmetry?

- Simplest version is prone to race conditions!
- Can not use symmetry (and do twice the work)
- Or update bins in two groups (even/odd columns?)
- Or save contributions separately, sum later

Logistical odds and ends

- Parallel performance starts with serial performance
  - Use flags — let the compiler help you!
  - Can refactor memory layouts for better locality
- You will need more particles to see good speedups
  - Overheads: open/close parallel sections, barriers.
  - Try -s 1e-2 (or maybe even smaller)
- Careful notes and a version control system *really* help
  - I like Git's lightweight branches here!

```
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```

Reminder: World of Linear Algebra

- Dense methods
  - Direct representation of matrices with simple data structures (no need for indexing data structure)
  - Mostly $O(n^3)$ factorization algorithms
- Sparse direct methods
  - Direct representation, keep only the nonzeros
  - Factorization costs depend on problem structure (1D cheap; 2D reasonable; 3D gets expensive; not easy to give a general rule, and NP hard to order for optimal sparsity)
  - Robust, but hard to scale to large 3D problems
- Iterative methods
  - Only *need* $y = Ax$ (maybe $y = A^T x$)
  - Produce successively better (?) approximations
  - Good convergence depends on *preconditioning*
  - Best preconditioners are often hard to parallelize

Linear Algebra Software: MATLAB

```
% Dense (LAPACK)
[L,U] = lu(A);
x = U\(L\b);

% Sparse direct (UMFPACK + COLAMD)
[L,U,P,Q] = lu(A);
x = Q*(U\(L\(P*b)));

% Sparse iterative (PCG + incomplete Cholesky)
tol = 1e-6;
maxit = 500;
R = cholinc(A,'0');
x = pcg(A,b,tol,maxit,R',R);
```

Linear Algebra Software: the Wider World

- Dense: LAPACK, ScaLAPACK, PLAPACK
- Sparse direct: UMFPACK, TAUCS, SuperLU, MUMPS, Pardiso, SPOOLES, ...
- Sparse iterative: too many!
- Sparse mega-libraries
  - PETSc (Argonne, object-oriented C)
  - Trilinos (Sandia, C++)
- Good references:
  - *Templates for the Solution of Linear Systems* (on Netlib)
  - Survey on “Parallel Linear Algebra Software” (Eijkhout, Langou, Dongarra – look on Netlib)
  - ACTS collection at NERSC

Software Strategies: Dense Case

Assuming you want to *use* (vs develop) dense LA code:

- Learn enough to identify right algorithm
  (e.g. is it symmetric? definite? banded? etc)
- Learn high-level organizational ideas
- Make sure you have a good BLAS
- Call LAPACK/ScaLAPACK!
- For n large: wait a while

Software Strategies: Sparse Direct Case

Assuming you want to use (vs develop) sparse LA code

- Identify right algorithm (mainly Cholesky vs LU)
- Get a good solver (often from list)
  - You *don't* want to roll your own!
- *Order your unknowns* for sparsity
  - Again, good to use someone else's software!
- For n large, 3D: get lots of memory and wait

Software Strategies: Sparse Iterative Case

Assuming you want to use (vs develop) sparse LA software...

- Identify a good algorithm (GMRES? CG?)
- Pick a good preconditioner
  - Often helps to know the application
  - ... *and* to know how the solvers work!
- Play with parameters, preconditioner variants, etc...
- Swear until you get acceptable convergence?
- Repeat for the next variation on the problem

Frameworks (e.g. PETSc or Trilinos) speed experimentation.

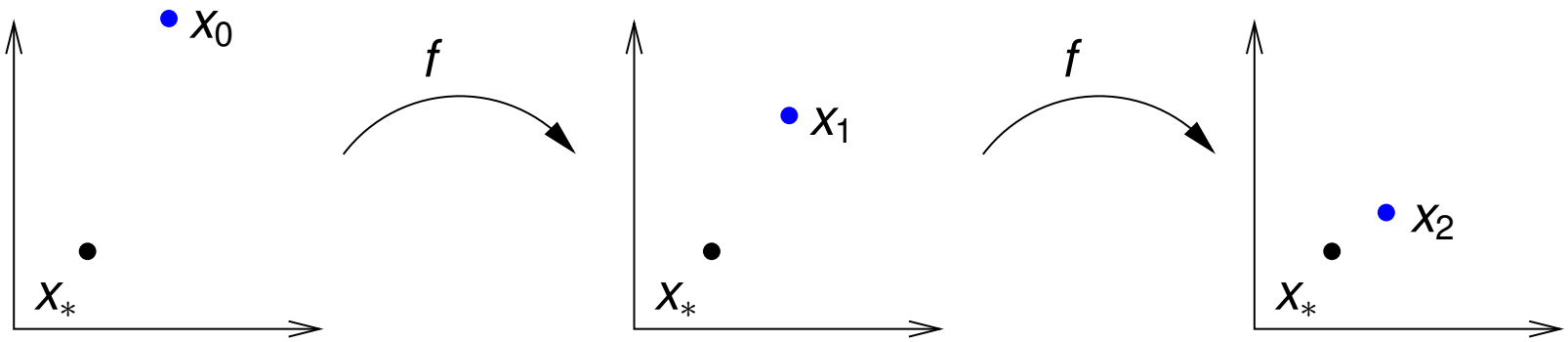
Software Strategies: Stacking Solvers

(Typical) example from a bone modeling package:

- Outer load stepping loop
- Newton method corrector for each load step
- Preconditioned CG for linear system
- Multigrid preconditioner
- Sparse direct solver for coarse-grid solve (UMFPACK)
- LAPACK/BLAS under that

First three are high level — I used a scripting language (Lua).

Iterative Idea



- f is a *contraction* if $\|f(x) - f(y)\| < \|x - y\|$.
- f has a unique *fixed point* $x_* = f(x_*)$.
- For $x_{k+1} = f(x_k)$, $x_k \to x_*$.
- If $\|f(x) - f(y)\| < \alpha\|x - y\|$, $\alpha < 1$, for all x, y, then

$$\|x_k - x_*\| < \alpha^k \|x - x_*\|$$

- Looks good *if* α not too near 1...

Stationary Iterations

Write $Ax = b$ as $A = M - K$; get fixed point of

$$Mx_{k+1} = Kx_k + b$$

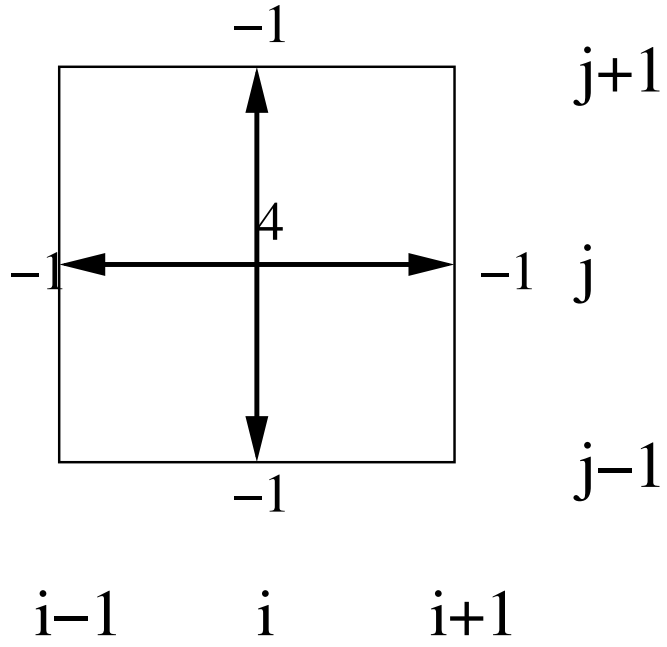
or

$$x_{k+1} = (M^{-1}K)x_k + M^{-1}b.$$

- Convergence if $\rho(M^{-1}K) < 1$
- Best case for convergence: $M = A$
- Cheapest case: $M = I$
- Realistic: choose something between

Jacobi	$M = \text{diag}(A)$
Gauss-Seidel	$M = \text{tril}(A)$

Reminder: Discretized 2D Poisson Problem



$$(Lu)_{i,j} = h^{-2}\left(4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1}\right)$$

Jacobi on 2D Poisson

Assuming homogeneous Dirichlet boundary conditions

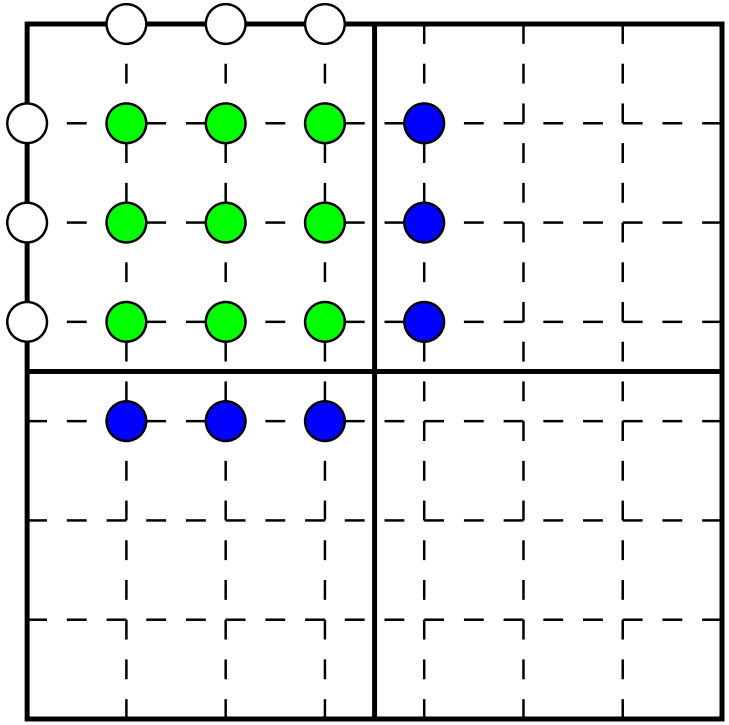
```
for step = 1:nsteps

  for i = 2:n-1
    for j = 2:n-1
      u_next(i,j) = ...
        ( u(i,j+1) + u(i,j-1) + ...
          u(i-1,j) + u(i+1,j) )/4 - ...
        h^2*f(i,j)/4;
    end
  end
  u = u_next;

end
```

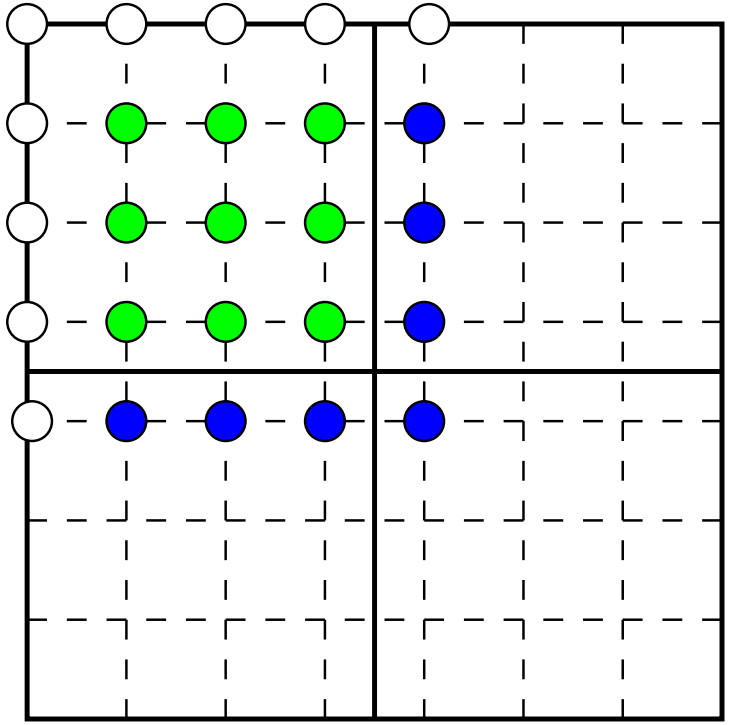
Basically do some averaging at each step.

Parallel version (5 point stencil)



Boundary values:	white
Data on P0:	green
Ghost cell data:	blue

Parallel version (9 point stencil)



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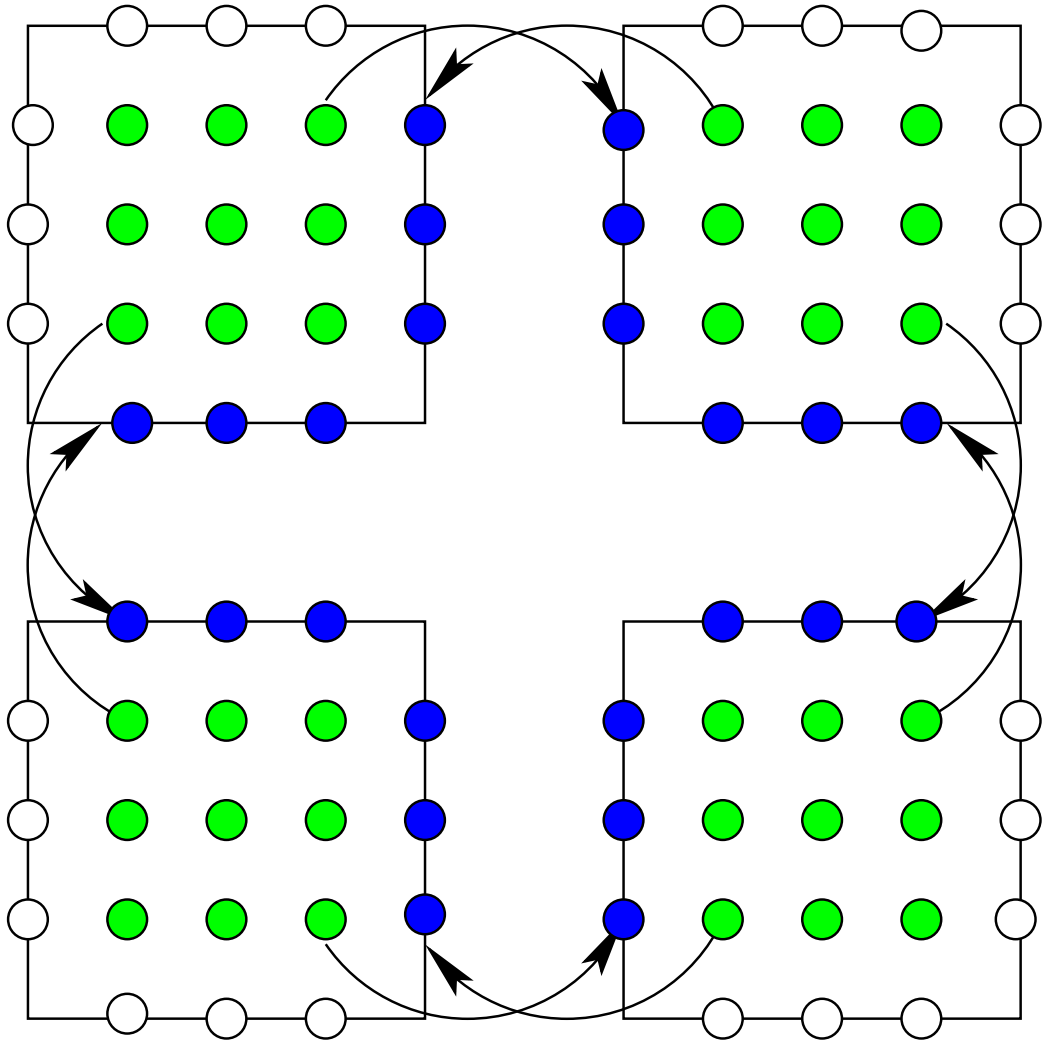
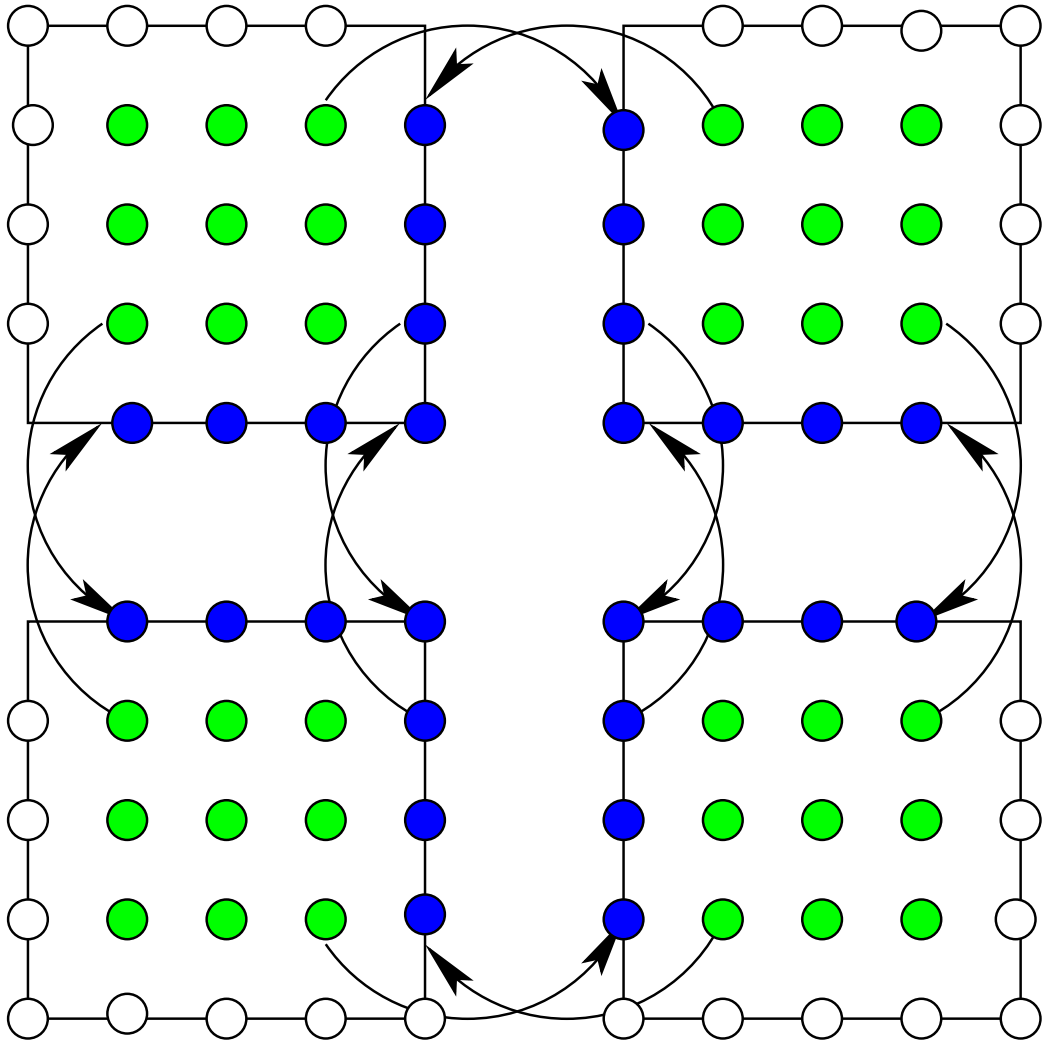
Parallel version (5 point stencil)



Communicate ghost cells before each step.

Parallel version (9 point stencil)



Communicate in two phases (EW, NS) to get corners.

Gauss-Seidel on 2D Poisson

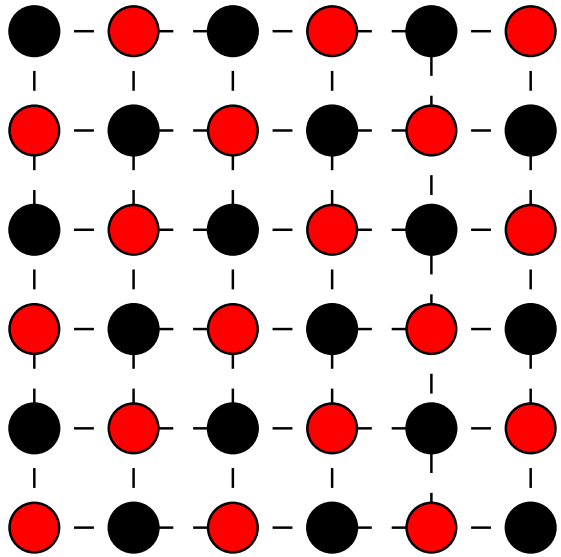
```
for step = 1:nsteps

  for i = 2:n-1
    for j = 2:n-1
      u(i,j) = ...
        ( u(i,j+1) + u(i,j-1) + ...
          u(i-1,j) + u(i+1,j) )/4 - ...
        h^2*f(i,j)/4;
    end
  end

end
```

Bottom values depend on top; how to parallelize?

Red-Black Gauss-Seidel



Red depends only on black, and vice-versa.
Generalization: multi-color orderings

Red black Gauss-Seidel step

```
for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 0
      u(i,j) = ...
    end
  end
end

for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 1,
    u(i,j) = ...
  end
end
```

Parallel red-black Gauss-Seidel sketch

At each step

- Send black ghost cells
- Update red cells
- Send red ghost cells
- Update black ghost cells

More Sophistication

- Successive over-relaxation (SOR): extrapolate Gauss-Seidel direction
- Block Jacobi: let M be a block diagonal matrix from A
  - Other block variants similar
- Alternating Direction Implicit (ADI): alternately solve on vertical lines and horizontal lines
- Multigrid

These are mostly just the opening act for...

Krylov Subspace Methods

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!

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 $\mathcal{K}_k(A, b)$.
Basis for the *method of conjugate gradients*

Example: GMRES

Idea: Minimize $\|Ax - b\|^2$ over $\mathcal{K}_k(A, b)$.
Yields *Generalized Minimum RESidual* (GMRES) method.

Convergence of Krylov Subspace Methods

- 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?