CME342/AA220
Parallel Methods in Numerical Analysis

Matrix Computation: Iterative Methods I

Outline:

- Jacobi, Gauss-Seidel, SOR.
- Domain partition (vs matrix partition) computations, & Multicoloring technique.
- CG, GMRES, BiCG.
- Parallel Sparse Matrix Algebra.
- Preconditioning.

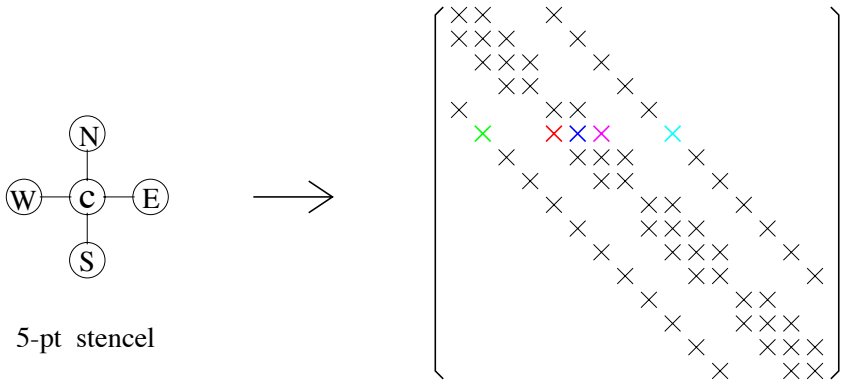
Source of materials: *Numerical Linear Alg*, *Introduction to Parallel Computing* by Kumar et al., Demmel's CS267 course.

Announcements

- Homework 2: Due Monday 5/12 @ 5 pm. Submit electronically through Stanford Box.
- Final project: it is time to think about it!
- If you plan to work on a project, submit a brief ($<$ 1 page) proposal with homework 2. If not, we will assign one to you.
- We strongly encourage you to propose a project of your own. Please feel free to discuss the project with us.
- Please take a few minutes to complete the mid-quarter evaluation by Friday 5/9.

Sparse Matrices + Direct Methods

The discretization matrix of the heat equation solved by an implicit method on a 2D mesh:

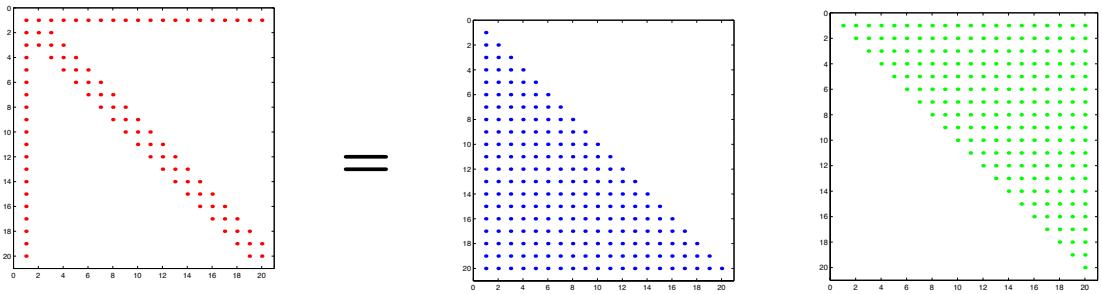


Direct Methods:

- Complexity $= O(n^3) \Rightarrow$ serious computing power challenges when $n \rightarrow \infty$.
- Storage $= O(n^2) \Rightarrow$ Not feasible for large problems.

Sparse Matrices + Direct Methods (cont.)

- Even start with a sparse matrix, the L, U factors can be dense $\rightarrow$ Fill-in occurs during LU factorization:



Observation: Most of the elements are zero $\rightarrow$ no need to store them nor perform any calculation.

Iterative Methods

- Only operate on nonzero elements.
- Typically, max number of nonzeros per row is bounded. Thus,
  - ▷ Work $\propto$ # of unknowns per iteration step.
  - ▷ Storage $= O(n)$.
- No fill-in occurs in iterative methods.
- However, convergence may not be guaranteed.
- Classical relaxation methods: Jacobi, Gauss-Seidel, SOR. (Today)
- Krylov subspace methods: Conjugate gradient, BiCG, GMRES, ...
- Krylov subspace methods + Preconditioning $\Rightarrow$ Fast solution methods.

Jacobi Method

- Want to solve $Ax = b$ iteratively (k is the iteration index).
- Start with an approximate solution x^k. Then, in general, the residual vector $r^k \neq 0$:

$$r^k \equiv b - Ax^k \neq 0.$$

- Considering the ith component, improve $x_i^k \rightarrow x_i^{k+1}$ by forcing $r_i^k = 0$, i.e.

$$b_i - (a_{ii}x_i^{k+1} + \sum_{i \neq j} a_{ij}x_j^k) = 0.$$

  After rearranging terms,

$$x_i^{k+1} = \frac{b_i - \sum_{i \neq j} a_{ij}x_j^k}{a_{ii}}.$$

  Repeat for all $i = 1, \ldots, n$.

- Note: Jacobi method requires nonzero diagonal entries.

Jacobi Method (cont.)

- Algorithm:

  `for i = 1:n,`

  $x_i^{k+1} = (b_i - \sum_{i \neq j} a_{ij} x_j^k)/a_{ii}$;

  `end;`

- Matrix form: Write $A = D - L - U$, where

  D = diagonal of A

  L = strict lower triangular part of $(-A)$

  U = strict upper triangular part of $(-A)$

  Jacobi iteration:

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

- Thus, Jacobi iteration essentially consists of (sparse) matrix-vector multiplications.

- Convergence: Jacobi converges for diagonal dominant matrices:

$$|a_{ii}| > \sum_{j \neq i}^{n} |a_{ij}|.$$

Parallel Jacobi Method

- Parallelization of Jacobi method is straightforward:

  for $i = localstart : localend$,
  $x_i^{k+1} = (b_i - \sum_{i \neq j} a_{ij} x_j^k)/a_{ii}$;
  end;

- Key observations:

  ▷ x_i^{k+1} is updated using previous $\{x_j^k\}$ only.

  ▷ Update is independent of ordering.

  $\Rightarrow$ Can be done in parallel!

- Consider the matrix form:

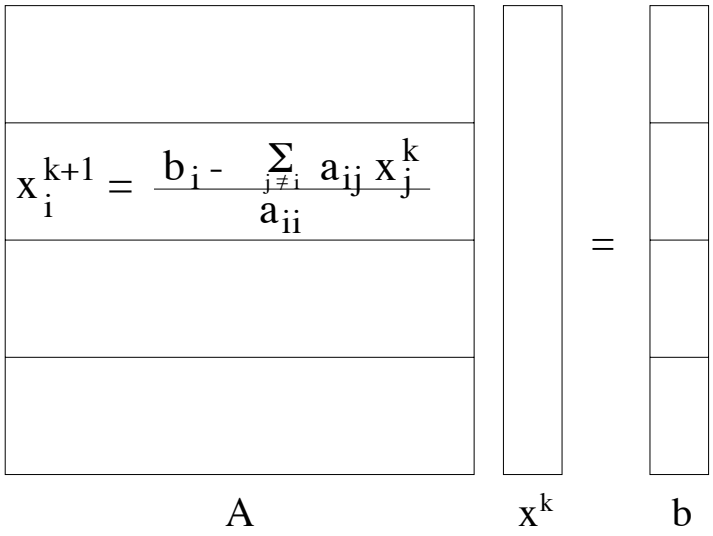
$$x^{k+1} = x^k + D^{-1}(b - Ax^k).$$

  Need to perform parallel (sparse) matrix-vector product. (Will discuss later.)

Parallel Jacobi Method (cont.)

Suppose A is a *general sparse matrix*...

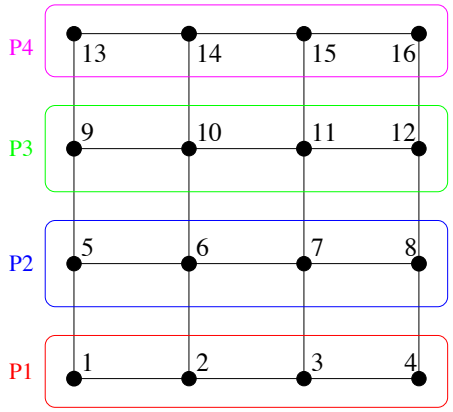
- Distribute A and b by row partitions, and an entire x^k among processors (since each row i can have nonzero a_{ij} in any columns):



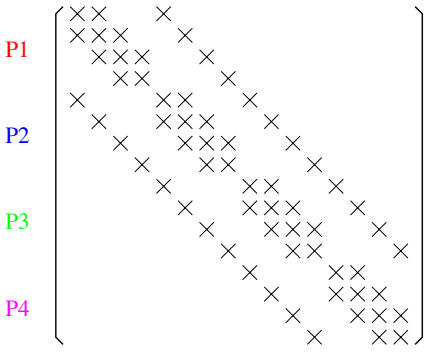
- Each processor updates its local x_i^{k+1} *without* any communication.
- At the end, each processor broadcasts its x_i^{k+1}'s to one another (MPI Allgather operation).

Parallel Jacobi Method (cont.)

Suppose A is a *planar graph*...
e.g., discretization of a PDE on a 2D mesh.



Graph of A (in this case, also = mesh)



Matrix A

- Partition the planar graph associated with A by blocks $\Rightarrow$ Distribute A, b *and* x^k by block of rows.
- Each processor updates its local $\{x_i^{k+1}\}$ *with* comm. to its *neighboring* procs only.
- Thus, the amount of comm. depends only on the number of boundary nodes. No global communication (Allgather) is needed.

Gauss-Seidel Method

- Start with x^k. Update x_i^{k+1} using the most recent values of x_j, $j \neq i$:

$$x_i^{k+1} = \frac{b_i - \sum_{j<i} a_{ij} x_j^{k+1} - \sum_{j>i} a_{ij} x_j^k}{a_{ii}}.$$

- Note: Gauss-Seidel method also requires nonzero diagonal entries.

- Matrix form:

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

- Convergence:
  - ▷ Gauss-Seidel converges for diagonal dominant matrices and symmetric positive definite matrices.
  - ▷ If both Jacobi and GS convergence, GS typically converges twice as fast as Jacobi.

SOR Methods

- Weighted average of x^k and x^k_{GS}:

$$\begin{aligned} x^{k+1} &= (1-\omega)\, x^k + \omega\, x^k_{GS} \\ x^{k+1}_i &= (1-\omega)\, x^k_i + \omega\, \frac{b_i - \sum_{j<i} a_{ij} x^{k+1}_j - \sum_{j>i} a_{ij} x^k_j}{a_{ii}} \end{aligned}$$

- Pre-selected relaxation parameter ω chosen to accelerate convergence:

$$\omega \begin{cases} < 1 & \text{under-relaxation} \\ = 1 & \text{GS} \\ > 1 & \text{over-relaxation} \end{cases}$$

- With optimal value of ω (usually > 1), the convergence rate of SOR can be an order of magnitude faster than GS and Jacobi.

Parallel GS (or SOR)

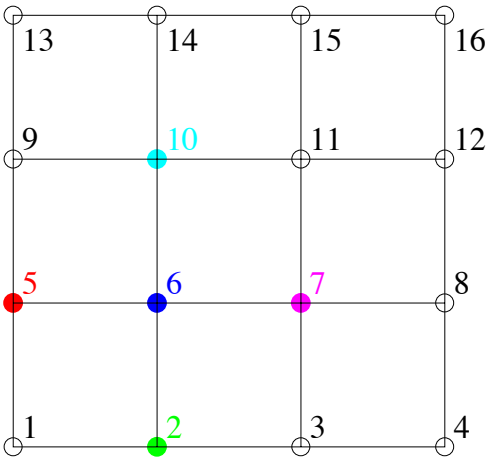
- Parallelization turns out to be nontrivial.
- Consider the component equation:

$$x_i^{k+1} = \frac{b_i - \sum_{j<i} a_{ij} x_j^{k+1} - \sum_{j>i} a_{ij} x_j^k}{a_{ii}}.$$

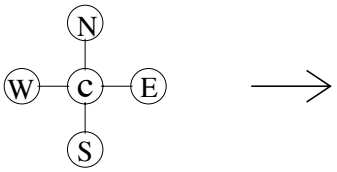
  - ▷ Require the updated values x_j^{k+1}, $j < i$, which are not available if the processor does not own them.
  - ▷ Every processor will have to wait for the updated values from other processors $\rightarrow$ sequential bottleneck.

- Key observation:
  If $a_{ij} = 0$ for $j < i$, then no communication nor waiting is needed $\rightarrow$ same scenario as Jacobi method.
- Use multi-coloring technique to order the unknowns such that $a_{ij} = 0$, $j < i$.

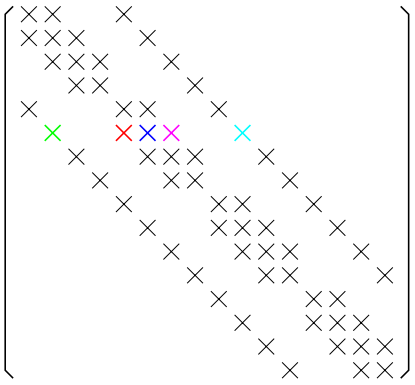
2D Mesh: Natural Ordering



- 5-pt stencil discretization of the Laplacian operator results in a matrix of the form:

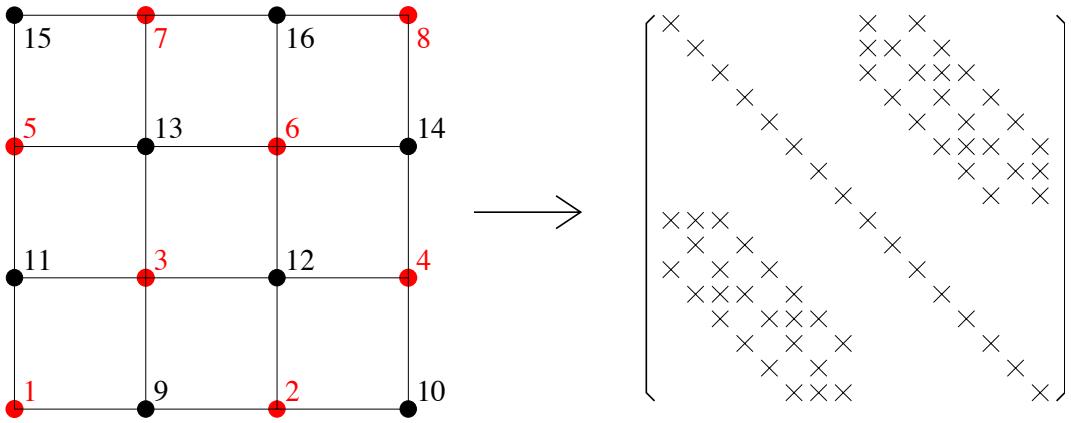


5-pt stencel



- For each node C, there are, in general, 4 neighbors (E, S, W, N). Using natural ordering, the update at C requires the updated values at S and $W \rightarrow$ sequential bottleneck.

2D Mesh: Red-Black Ordering



- In RB ordering, the update of red nodes (e.g. 3) depends only on black nodes; thus can be done independently in parallel. Afterwards, broadcast the values to their neighbors, and then update black nodes in parallel.
- Parallelization can be realized from the 2×2 block structure in the RB ordered matrix where the diagonal blocks are diagonal matrices.

Parallel Implementation

- Distribute the red nodes equally among p procs; same for the black nodes.
- Algorithm:

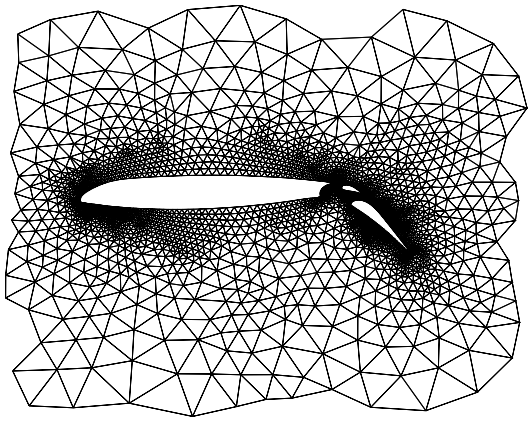
`for each color=`$\{$`red, black`$\}$

`All procs update its local` x_i^{k+1} `simultaneously:`

$$x_i^{k+1} = \frac{b_i - \sum_{j<i} a_{ij} x_j^{k+1} - \sum_{j>i} a_{ij} x_j^k}{a_{ii}};$$

`end;`

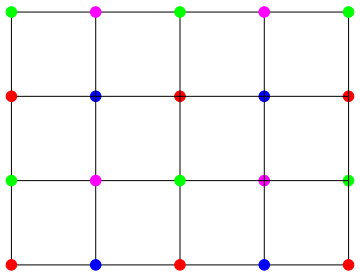
General Mesh: Multicoloring



- For general matrix graph, use multicoloring.
- Nodes for each color can be updated simultaneously, i.e. in parallel.
- The fewer the # of colors, the more parallel the algorithm is.
  - ▷ RB Gauss-Seidel has 2 colors $\rightarrow$ parallel.
  - ▷ Gauss-Seidel has n colors $\rightarrow$ sequential.
- Convergence: The fewer the # of colors, the slower the convergence is.
- Hence tradeoff between parallelism & efficiency.

Multicoloring

- Coloring of the 9-pt stencil graph:



- To color a general graph with min. # of color (for max. parallel efficiency) is NP-hard.
- There are heuristics to color most graphs arising from applications using a small # of colors.

- A sequential algorithm:
(color=$\{0, 1, 2, \ldots\}$)

V = set of vertices;
for $i = 1$ to n do
  Choose vertices $v_i \in V$ according to an ordering algorithm;
  Choose the smallest possible color for v_i;
  $V = V \backslash \{v_o\}$;
end

Multicoloring (cont.)

- Examples of ordering algorithm:
  LFO: order vertices in V such that

$$\deg(v_1) \geq \deg(v_2) \geq \cdots \geq \deg(v_n).$$

  IDO: v_i is choosen with max incidence degree, i.e. max # of adjacent colored vertices.

- A parallel coloring algorithm:
  Given a good partitioning & good assignment of partitions to processors (each process has about the same # of vertices; minimal boundary edges)

  1. Color the global boundary vertices.
  2. Color the local vertices independently on each processor by a sequential algorithm.

Jacobi vs RB Gauss-Seidel

- RB GS converges twice as fast as Jacobi, but requires twice as many parallel steps; about the same run time in practice.
- Parallel efficiency alone is not sufficient to determine overall performance.
- We also need fast converging algorithms.

Run Time Complexity: Jacobi

- Assume on a 2D mesh.
- Notations:

  N = # of unknowns

  p = # of processors

  f = time per flop

  α = startup for a message

  β = time per word in a message

  Time = # of steps $\times$ cost per step

- Sequential run time:

  Time(Jacobi) $= O(N) \times O(N) = O(N^2)$.

- Parallel run time:

  $$\begin{aligned}\text{Time(Jacobi)} &= O(N) \times [(N/p)f + \alpha + (\sqrt{N}/p)\beta] \\ &= O(N^2/p)\ f + O(N)\ \alpha + O(N^{3/2}/p)\ \beta\end{aligned}$$

  Note: $O(N/p)$ flops to update local values, α for the start up of message passing, $O(\sqrt{N}/p)$ boundary nodes communicated to neighbors.

Parallel Run Time: Comparison

Notations:

N = # of unknowns

p = # of processors

f = time per flop

α = startup for a message

β = time per word in a message

Time = # of steps $\times$ cost per step

Methods	Parallel run time
Jacobi	$O(N) \times [O(\frac{N}{p})f + \alpha + O(\frac{\sqrt{N}}{p})\beta]$
RB GS	$O(N) \times [O(\frac{N}{p})f + \alpha + O(\frac{\sqrt{N}}{p})\beta]$
RB SOR	$O(\sqrt{N}) \times [O(\frac{N}{p})f + \alpha + O(\frac{\sqrt{N}}{p})\beta]$

Block Methods

- Block Jacobi:

$$x^{k+1} = x^k + \tilde{D}^{-1}(b - Ax^k),$$

  $\tilde{D}$=block diagonal of A.

- E.g. Given $p \times p$ mesh, partition 5-pt stencil matrix A into p block rows where each proc has one line of variables. Then $\tilde{D}_j$=tridiagonal matrix.

- Suppose subvector $x^k_{\vec{j}}$ is the jth portion of vector x^k possessed by proc p_j.

  Parallel Algorithm:

  for each proc p_j,
  $x^{k+1}_{\vec{j}} = x^k_{\vec{j}} + \tilde{D}^{-1}_{\vec{j}}(b - Ax^k)_{\vec{j}}$;
  end;

Block Methods (cont.)

- A variant of block Jacobi method is to substitute the inversion of $\tilde{D}_j$ by one iteration of GS:

```
for each proc p_j,
  for i=localstart to localend,
```

$$x_i^{k+1} = (b_i - \sum_{j<i \ \&\ j=local} a_{ij} x_j^{k+1} - \sum_{j>i \text{ or } j=nonlocal} a_{ij} x_j^k)/a_{ii};$$

```
  end;
end;
```

- Similar to GS except that only use the updated x_i^{k+1} which are local.