Numerical Solutions of Finite–Volume Equations

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Equation to Be Solved

- $A_N\phi_N + A_S\phi_S + A_E\phi_E + A_P\phi_P + A_W\phi_W = Q_P$
- $A_N\phi_{iJ+1} + A_S\phi_{ij-1} + A_E\phi_{i+1j} + A_P\phi_{ij} + A_W\phi_{i-1j}$
- Have a set of simultaneous linear equation to be solved algebraically
- A_K coefficients different for u, v, p, but all equations seen here link central (P) node to 4 nearest neighbors
- Sparse matrix system, look at iterative methods for solution

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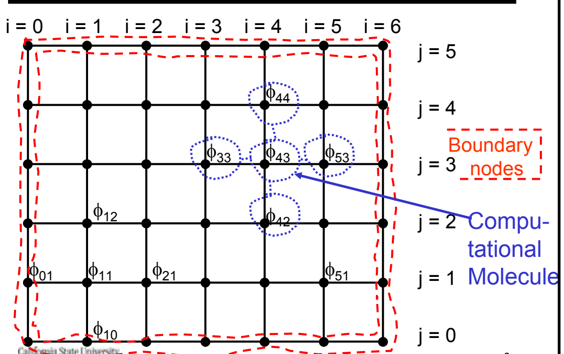
A Small Grid (N = 6, M = 5)



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Grid i,j Notation

- For system typically use this notation in combination with compass points
- Notation A_{ij}^{point} is general coefficient
  - ij refers to a particular node
  - Point = N(orth), S(outh), E(ast), W(est) refers to neighboring nodes by direction
- General equation shown below

$$A_{ij}^S\phi_{ij-1} + A_{ij}^W\phi_{i-1j} + A_{ij}^P\phi_{ij} + A_{ij}^E\phi_{i+1j} + A_{ij}^N\phi_{ij+1} = b_{ij}$$

$$A_{ij}^P = -A_{ij}^S - A_{ij}^W - A_{ij}^E - A_{ij}^N \qquad A_{ij}^S = A_{ij-1}^N \qquad A_{ij}^W = A_{i-1j}^E$$

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Solving the Equations

- Typically have large number of equations forming sparse matrix
  - For $\Delta x = \Delta y = .01$ have 99^2 equations so matrix has $96\text{x}10^6$ potential coefficients
  - Only 48609 (0.051%) are nonzero
- Want data structure and algorithm for handling sparse matrices
- Gauss elimination uses storage for banded matrices
- Iterative methods used for solutions

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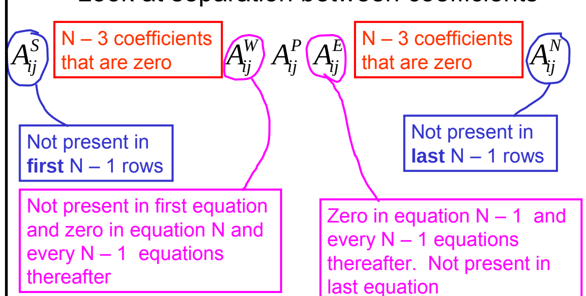
General Equation in a Matrix

- Look at separation between coefficients



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Sparse Matrix Structure

- 20 equations can have 400 coefficients
- Here each equation has no more than five coefficients (100 possible)
- Boundaries give another 2(N + M - 2) zero coefficients (18 in this example)
- Thus, we have 82 nonzero coefficients and 400 – 82 = 318 zeros in matrix
  - Nearly 80% of coefficients are zero
  - Fraction increases for larger grids

How Sparse is the Matrix?

- The M by N grid has (M – 1)(N – 1) nodes with equations giving $(M-1)^2(N-1)^2$ possible coefficients
- Without boundaries we have only 5 (M – 1)(N – 1) nonzero coefficients
- Boundaries give 2(N + M – 2) = 2(M – 1) + 2(N – 1) additional zero coefficients

$$\begin{bmatrix}Nonzero\\Fraction\end{bmatrix} = \frac{5(N-1)(M-1) - 2(N-1) - 2(M-1)}{(N-1)^2(M-1)^2} = \frac{5}{(N-1)(M-1)} - \frac{2}{(N-1)(M-1)^2} - \frac{2}{(N-1)^2(M-1)}$$

What Makes Sparseness?

- Each node is connected only to a small number of nearest neighbors
  - Problem here has four neighbors
  - Higher order schemes and 3D finite-volume equation can have more neighbors
- Can have complex coefficients so long as number of neighbors is limited
- Convection-diffusion coefficients with uneven grid spacing are an example of complex coefficients in a sparse matrix

Iterative Solutions

- Simplest examples are Jacobi, Gauss-Seidel, and Successive Over Relaxation
- Move from iteration n to iteration n+1
- Iteration 0 is initial guess (often all zero)
- Straightforward approach: solve equation for ϕ_{ij} and use this as basis for iteration

$$\phi_{ij} = \frac{b_{ij} - A_{ij}^S \phi_{ij-1} - A_{ij}^W \phi_{i-1j} - A_{ij}^E \phi_{i+1j} - A_{ij}^N \phi_{ij+1}}{A_{ij}^P}$$

$$\phi_{ij} = b_{ij}' - A_{ij}^{S'} \phi_{ij-1} - A_{ij}^{W'} \phi_{i-1j} - A_{ij}^{E'} \phi_{i+1j} - A_{ij}^{N'} \phi_{ij+1}$$

Iterative Solutions II

- Use superscript (n) for iteration number
- Jacobi iteration uses all old values

$$\phi_{ij}^{(n+1)} = b_{ij}' - A_{ij}^{S'} \phi_{ij-1}^{(n)} - A_{ij}^{W'} \phi_{i-1j}^{(n)} - A_{ij}^{E'} \phi_{i+1j}^{(n)} - A_{ij}^{N'} \phi_{ij+1}^{(n)}$$

- Gauss–Seidel uses most-recent values

$$\phi_{ij}^{(n+1)} = b_{ij}' - A_{ij}^{S'} \phi_{ij-1}^{(n+1)} - A_{ij}^{W'} \phi_{i-1j}^{(n+1)} - A_{ij}^{E'} \phi_{i+1j}^{(n)} - A_{ij}^{N'} \phi_{ij+1}^{(n)}$$

- Relaxation basis: Gauss–Seidel provides a correction that can be adjusted

$$\phi_{ij}^{(n+1)} = \phi_{ij}^{(n)} + \omega\left[\phi_{ij}^{(n+1,GS)} - \phi_{ij}^{(n)}\right]$$

Relaxation Factor

Example Problem

- Look at simple system of equations
  - Could solve exactly to find x = 1, y = 2
  - Use to illustrate iteration

Original system: $6x + y = 8$, $2x + 5y = 12$

Iteration Form: $x = \frac{8-y}{6}$, $y = \frac{12-2x}{5}$

- Jacobi – general form and first steps

$$x^{(n+1)} = \frac{8 - y^{(n)}}{6} \qquad x^{(0)} = 0 \qquad x^{(1)} = \frac{8 - y^{(0)}}{6} = \frac{8}{6}$$

$$y^{(n+1)} = \frac{12 - 2x^{(n)}}{5} \qquad y^{(0)} = 0 \qquad y^{(1)} = \frac{12 - 2x^{(0)}}{5} = \frac{12}{5}$$

Jacobi Example Continued

$$x^{(2)} = \frac{8 - y^{(1)}}{6} = \frac{8 - 12/5}{6} = \frac{28}{30}$$
$$y^{(2)} = \frac{12 - 2x^{(1)}}{5} = \frac{12 - 2(8/6)}{5} = \frac{56}{30}$$

$$x^{(3)} = \frac{8 - y^{(2)}}{6} = \frac{8 - 56/30}{6} = \frac{184}{180}$$
$$y^{(3)} = \frac{12 - 2x^{(2)}}{5} = \frac{12 - 2(28/30)}{5} = \frac{304}{150}$$

- What is next iteration?
- How do we know we're finished?

Concluding Iterations

- In general, do not know correct answers
- Two common measures
  - Residual: $r_i = \Sigma_j a_{ij} x_j - b_i$
  - Difference in one iteration $|x_i^{(n+1)} - x_i^{(n)}|$
- Can use relative or absolute measure
- Need vector norm such as maximum absolute value or root mean square
- Look at summary of iterations for Jacobi

Jacobi Iteration History

n	x_n	y_n	x residual	y residual	x change	y change
0	0	0	8	12		
1	1.33333	2.4	-2.4	-2.66667	1.333333	2.4
2	0.93333	1.86667	0.533333	0.8	-0.4	-0.53333
3	1.02222	2.02667	-0.16	-0.17778	0.088889	0.16
4	0.99556	1.99111	0.035556	0.053333	-0.02667	-0.03556
5	1.00148	2.00178	-0.01067	-0.01185	0.005926	0.010667
6	0.9997	1.99941	0.00237	0.003556	-0.00178	-0.00237
7	1.0001	2.00012	-0.00071	-0.00079	0.000395	0.000711
8	0.99998	1.99996	0.000158	0.000237	-0.00012	-0.00016
9	1.00001	2.00001	-4.7E-05	-5.3E-05	2.63E-05	4.74E-05

Gauss-Seidel Iteration

- Apply Gauss-Seidel Iteration to same set of equations

Original system
$$6x + y = 8 \qquad 2x + 5y = 12$$

Iteration Form
$$x = \frac{8 - y}{6} \qquad y = \frac{12 - 2x}{5}$$

- Gauss-Seidel – general iteration form and first step (uses most recent values)

$$x^{(n+1)} = \frac{8 - y^{(n)}}{6} \qquad y^{(n+1)} = \frac{12 - 2x^{(n+1)}}{5}$$
$$x^{(0)} = 0 \qquad y^{(0)} = 0$$
$$x^{(1)} = \frac{8 - y^{(0)}}{6} = \frac{8}{6} \qquad y^{(1)} = \frac{12 - 2x^{(1)}}{5} = \frac{12}{5} - \frac{2}{5}\frac{8}{6} = \frac{56}{30}$$

Gauss-Seidel Iteration II

$$x^{(2)} = \frac{8 - y^{(1)}}{6} = \frac{8 - 56/30}{6} = \frac{184}{180}$$
$$y^{(2)} = \frac{12 - 2x^{(2)}}{5} = \frac{12 - 2(184/180)}{5} = \frac{1792}{900}$$

$$x^{(3)} = \frac{8 - y^{(2)}}{6} = \frac{8 - 1792/900}{6} = \frac{5408}{5400} = 1.00148\ldots$$
$$y^{(3)} = \frac{12 - 2x^{(3)}}{5} = \frac{12 - 2(5408/5400)}{5} = 1.9941\ldots$$

- Faster convergence in Gauss-Seidel

Relaxation Methods

- Relaxation factor, ω, greater than or less than 1 is over- or underrelaxation
  - Underrelaxation procures stability in problems that will not converge
  - Overrelaxation procures speed in well-behaved problems

$$\phi_{ij}^{(n+1)} = \phi_{ij}^{(n)} + \omega\left[\phi_{ij}^{(n+1,GS)} - \phi_{ij}^{(n)}\right] = (1-\omega)\phi_{ij}^{(n)} + \omega\phi_{ij}^{(n+1,GS)} = (1-\omega)\phi_{ij}^{(n)} - \omega\Big[-b_{ij}^{'} + A_{ij}^{S'}\phi_{ij-1}^{(n+1)} + A_{ij}^{W'}\phi_{i-1j}^{(n+1)} + A_{ij}^{E'}\phi_{i+1j}^{(n)} + A_{ij}^{N'}\phi_{ij+1}^{(n)}\Big]$$

Relaxation Code (f is ϕ)

```
do iter = 1, maxIter
  maxResid = 0
  do i = 1, N – 1
    do j = 1, M – 1
      old = f(i,j)
      f(i,j) = (omega – 1) * f(i,j)
        + omega * ( AN(i,j) * f(i,j+1)
        + AE(i,j) * f(i+1,j) + AS(i,j)
        * f(i,j-1) + AW(i,j) * f(i-1,j)
        - b(i,j) )
      resid = abs( ( f(i,j) – old ) /
          f(i,j) )
      if ( resid > maxResid ) then
        maxResid = resid;
      end if
```

One set of iterations (omitted on next page)

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Relaxation Code II

```
do iter = 1, maxIter
  maxResid = 0;
  do i = 1, N - 1
    do j = 1, M - 1
       !compute new f(i,j) and maxResid
    end do
  end do
  if ( maxResid <= errTol ) exit
end do
if ( maxResid > errTol ) then
  print *, "Not converged"
else
  call doOutput( f, N, M )
end if
```

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Converging Iterations

- Have three different "solutions"
  - Correct solution to differential equation
  - Exact solution to finite-difference equations
  - Current and previous iteration values
- Iterations should approach correct solution to finite-difference equations
- Since neither correct solution is known, we use norm of error estimates
  - Residual in finite-difference equations
  - Change in iteration value

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Converging Iterations II

- At each grid node we can compute a relative change or a residual
  - Both are zero at convergence

$$\begin{bmatrix}\text{Relative} \\ \text{Change}\end{bmatrix}_{ij} = \frac{\phi_{ij}^{(n+1)} - \phi_{ij}^{(n)}}{\phi_{ij}^{(n+1)}}$$

$$[\text{Residual}]_{ij} = \phi_{ij}^{(n+1)} + A_{ij}^{S'}\phi_{ij-1}^{(n+1)} + A_{ij}^{W'}\phi_{i-1j}^{(n+1)} + A_{ij}^{E'}\phi_{i+1j}^{(n)} + A_{ij}^{N'}\phi_{ij+1}^{(n)} - b_{ij}'$$

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Converging Iterations III

- Need some overall measure of convergence error
- Consider error (relative change or residual) at each point as one component of a vector
- Use vector norm for overall error
  - Maximum absolute value (zero norm)
  - Root mean squared error (two norm)

$$\varepsilon_{overall} = \sqrt{\frac{\sum_{all\ nodes} \varepsilon_{node}^2}{N_{nodes}}}$$

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Simple Numerical Example

- Look at simple, two-dimensional case with diffusion only (velocities are zero)
- Dirichlet (fixed ϕ) boundary conditions
- Use finite-volume equation from original work on diffusion with a source term
- Set source term to zero and use constant grid sizes and Γ
- Solve finite-volume equation for this case (**v** = **0**, Δx, Δy fixed, constant Γ)

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v = 0, Δx, Δy, Γ constant

$$\left[\Gamma_e^{(\phi)}\frac{\phi_E-\phi_P}{x_E-x_P}\right]\Delta y+\left[\Gamma_n^{(\phi)}\frac{\phi_N-\phi_P}{y_N-y_P}\right]\Delta x+$$
$$\left[\Gamma_w^{(\phi)}\frac{\phi_W-\phi_P}{x_P-x_W}\right]\Delta y+\left[\Gamma_s^{(\phi)}\frac{\phi_S-\phi_P}{y_P-y_S}\right]\Delta x=0$$

- Divide by ΓΔy/Δx

$$\phi_E-\phi_P+(\phi_N-\phi_P)\left(\frac{\Delta x}{\Delta y}\right)^2+\phi_W-\phi_P+(\phi_S-\phi_P)\left(\frac{\Delta x}{\Delta y}\right)^2=0$$

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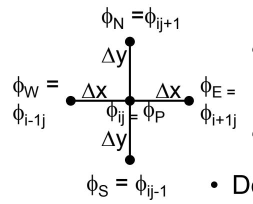
v = 0, Δx, Δy, Γ constant II



$$\phi_E-\phi_P+(\phi_N-\phi_P)\left(\frac{\Delta x}{\Delta y}\right)^2+$$
$$\phi_W-\phi_P+(\phi_S-\phi_P)\left(\frac{\Delta x}{\Delta y}\right)^2=0$$

- Define β = Δx/Δy and rearrange terms

$$\phi_E+\phi_W+\beta^2(\phi_N+\phi_S)-2(1+\beta^2)\phi_P=0$$
$$\phi_{i+1j}+\phi_{i-1j}+\beta^2(\phi_{ij+1}+\phi_{ij-1})-2(1+\beta^2)\phi_{ij}=0$$

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Finite-difference Equation

- Finite-volume form typical of two-dimensional Laplace equation
- If β = Δx/Δy = 1, ϕ_{ij} is the average of its four nearest neighbors

$$\phi_{ij-1}+\phi_{i-1j}-4\phi_{ij}+\phi_{i+1j}+\phi_{ij+1}=0$$

- Consider Dirichlet boundary conditions
  – ϕ_{ij} known at all boundary nodes
  – Need to find (N – 1)(M – 1) unknown values of ϕ_{ij} on grid

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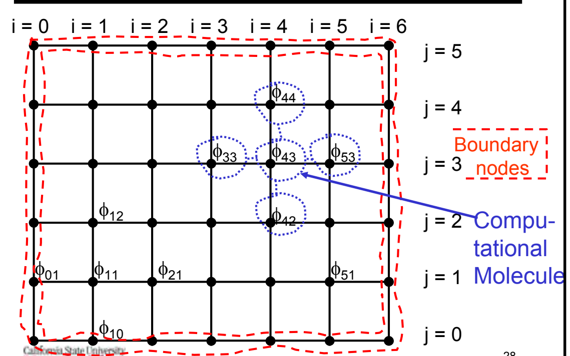
A Small Grid (N = 6, M = 5)



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Grid Equations (β = 1)

$$\begin{array}{lllllllllll}
-4\phi_{11} & +\phi_{21} & & & & +\phi_{12} & & & & & =-\phi_{10}-\phi_{01}\\
\phi_{11} & -4\phi_{21} & +\phi_{31} & & & & +\phi_{22} & & & & =-\phi_{20}\\
& \phi_{21} & -4\phi_{31} & +\phi_{41} & & & & +\phi_{23} & & & =-\phi_{30}\\
& & \phi_{31} & -4\phi_{41} & +\phi_{51} & & & & +\phi_{24} & & =-\phi_{40}\\
& & & \phi_{41} & -4\phi_{51} & & & & & +\phi_{25} & =-\phi_{40}-\phi_{61}\\
\phi_{11} & & & & & -4\phi_{12} & +\phi_{22} & & & +\phi_{31} & =-\phi_{02}\\
& \phi_{21} & & & & +\phi_{12} & -4\phi_{22} & +\phi_{23} & & +\phi_{32} & =0\\
& & \phi_{31} & & & & +\phi_{22} & -4\phi_{23} & +\phi_{24} & +\phi_{33} & =0
\end{array}$$

- N = 6 and M = 5 gives (6 – 1)(5 – 1) = 20 equations – only eight shown
- Diagonal structure incorrect here

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Execution Times and Errors

- Examine square region with zero boundary conditions at x = 0, x = x_{max}, and y = 0; two cases for y = y_{max}
  – Case 1: constant value of ϕ_N(x) = 1
  – Case 2: ϕ_N(x) = sin(πx)
- First case has discontinuity for y = y_{max} at x = 0 and x = x_{max}
- Use overrelaxation (SOR) with variable relaxation factors

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Execution Times and Errors II

- Iterate until maximum iteration difference in ϕ_{ij} is about machine error
  - Case 1: constant value of $\phi_N(x) = 1$
  - Case 2: $\phi_N(x) = \sin(\pi x)$
- First case has discontinuity for $y = y_{max}$ at $x = 0$ and $x = x_{max}$
- Compare solutions to exact solution of differential equation and exact solution of finite difference equations

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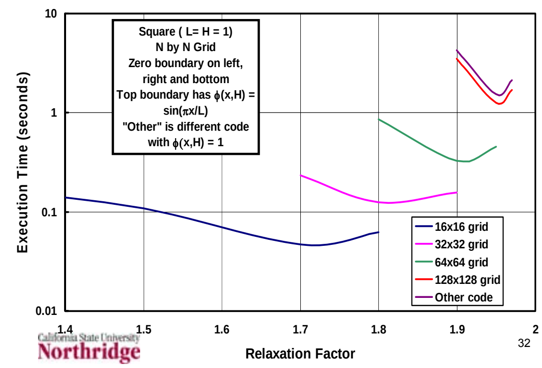
Effect of Relaxation Factor on Execution Time



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Effect of Iterations on Errors

- Compare three error measures using the maximum value on the grid
  - True iteration error: difference between the current value and the value found by an exact solution of the ***difference*** equations
  - Difference in ϕ_{ij} between two iterations
  - Residual = $\phi_{i+1j} + \phi_{i-1j} + \phi_{ij+1} + \phi_{ij-1} - 4\phi_{ij}$
  - Exact error is difference between iteration value and exact solution of ***differential*** equation

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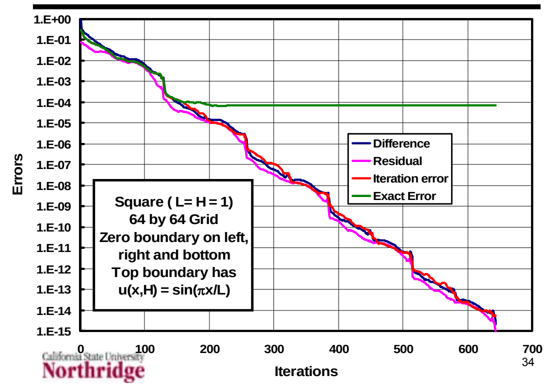
Effects of Iterations on Laplace Equation Errors



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Will Iterations Converge?

- How do we ensure that an iterative process converges?
- Look at general example of solving a system of simultaneous equations by iteration
- Write equation in matrix form $\mathbf{A}\phi = \mathbf{b}$
- Develop general iteration algorithm in matrix form
- Look at criterion for error to decrease

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Matrix Equation Form

- Advanced solution techniques treat matrix for finite-difference equations
- Leads to dimensional confusion
  - Start with 2D grid (x and y indices)
  - Treat as matrix equation where unknowns ϕ_{ij} form a column vector (one-dimensional)
  - The coefficients in the matrix form a two-dimensional display
  - Examine small grid example
  - Take $A_E = A_W = A_N = A_S = 1$, $A_P = -4$

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General Matrix Structure

- Confusion about two two-dimensional representations
- Grid has two space dimensions with (N – 1)(M – 1) unknown nodes
- ϕ_{ij} forms a one dimensional column matrix of unknowns (at right)
- Coefficient matrix has five diagonals
- Right-hand side has boundary values

$$A^S_{ij}\phi_{ij-1} + A^W_{ij}\phi_{i-1j} + A^P_{ij}\phi_{ij} + A^E_{ij}\phi_{i+1j} + A^N_{ij}\phi_{ij+1} = b_{ij}$$

$$\begin{bmatrix} \phi_{11} \\ \phi_{12} \\ \phi_{13} \\ \phi_{14} \\ \phi_{15} \\ \phi_{21} \\ \phi_{22} \\ \phi_{23} \\ \vdots \\ \phi_{45} \end{bmatrix}$$

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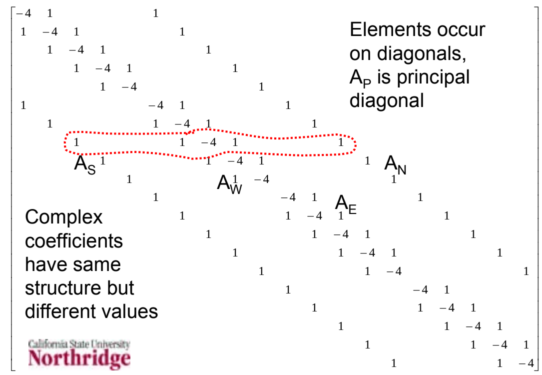
Previous Solution Matrix



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General Solution Matrix, A

- Like the one on the previous chart
  - Has more rows for more grid points
  - Coefficients may not be the same
  - Will be generally sparse
  - Has regular structure for simple grids
  - Unstructured grids do not give simple structure, but keep a sparse matrix
  - We want to solve **A**ϕ = **b** where ϕ is a vector of all the unknowns on the grid

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General Iteration Approaches

- We want to solve **A**ϕ = **b** by iteration
- As the solution to the finite-difference equations, ϕ has truncation error even with perfect iteration solution
- Define iteration error as $\varepsilon^{(n)} = \phi - \phi^{(n)}$
- Define residual, $\mathbf{r}^{(n)} = \mathbf{b} - \mathbf{A}\phi^{(n)}$
- Combine equations: $\mathbf{r}^{(n)} = \mathbf{b} - \mathbf{A}\phi^{(n)} = \mathbf{A}\phi - \mathbf{A}\phi^{(n)} = \mathbf{A}(\phi - \phi^{(n)}) = \mathbf{A}\varepsilon^{(n)}$
- $\mathbf{r}^{(n)} = \mathbf{A}\varepsilon^{(n)}$ relates computable $\mathbf{r}^{(n)}$ to $\varepsilon^{(n)}$ that we want to control but can't compute

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General Iteration Approaches II

- One iteration step takes the old values, $\phi^{(n)}$, to the new values, $\phi^{(n+1)}$
- General iteration: $\mathbf{M}\phi^{(n+1)} = \mathbf{N}\phi^{(n)} + \mathbf{b}$
- Methods select **M** and **N** to accelerate convergence of iterations
- At convergence, $\phi^{(n+1)} = \phi^{(n)} = \phi$, so that $\mathbf{M}\phi^{(n+1)} = \mathbf{N}\phi^{(n)} + \mathbf{b}$ is $(\mathbf{M} - \mathbf{N})\phi = \mathbf{b}$
- We are solving **A**ϕ = **b**, so we must have **M** – **N** = **A**

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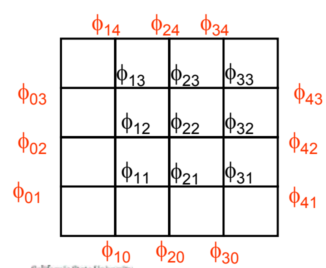
Example of M and N Matrices

- Heat conduction with constant properties and no source term with $N_x = N_y = 4$



- System of equations with nine unknowns
- Boundary values known
- Solve **A**ϕ = **b**

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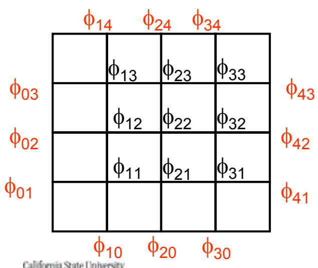
Example of **M** and **N** Matrices II

- Iterate Gauss Seidel from lower left to upper right using newest values



$$\phi_{ij-1}^{(n+1)} + \phi_{i-1j}^{(n+1)} + \phi_{ij}^{(n+1)} + \phi_{i+1j}^{(n)} + \phi_{ij+1}^{(n)} = 0$$

When solving for ϕ_{22} we will have current iteration values for ϕ_{12} and ϕ_{21}

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Aϕ = b and M$\phi^{(n+1)}$ = N$\phi^{(n)}$ + b

$$\begin{bmatrix} -4 & 1 & & 1 & & & & & \\ 1 & -4 & 1 & & 1 & & & & \\ & 1 & -4 & & & 1 & & & \\ 1 & & & -4 & 1 & & 1 & & \\ & 1 & & 1 & -4 & 1 & & 1 & \\ & & 1 & & 1 & -4 & & & 1 \\ & & & 1 & & & -4 & 1 & \\ & & & & 1 & & 1 & -4 & 1 \\ & & & & & 1 & & 1 & -4 \end{bmatrix} \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \\ \phi_{12} \\ \phi_{22} \\ \phi_{32} \\ \phi_{13} \\ \phi_{23} \\ \phi_{33} \end{bmatrix} = \begin{bmatrix} -\phi_{10}-\phi_{01} \\ -\phi_{20} \\ -\phi_{30}-\phi_{41} \\ -\phi_{02} \\ 0 \\ -\phi_{42} \\ -\phi_{03}-\phi_{14} \\ -\phi_{24} \\ -\phi_{43}-\phi_{34} \end{bmatrix}$$

GS **M** matrix

GS **–N** matrix

$$\phi_{ij-1}^{(n+1)} + \phi_{i-1j}^{(n+1)} - 4\phi_{ij}^{(n+1)} = -\phi_{i+1j}^{(n)} - \phi_{ij+1}^{(n)} + b_{ij} \qquad b_{ij} = 0$$

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M Matrix for SOR

$$\begin{bmatrix} -4 & & & & & & & & \\ \omega & -4 & & & & & & & \\ & \omega & -4 & & & & & & \\ \omega & & & -4 & & & & & \\ & \omega & & \omega & -4 & & & & \\ & & \omega & & \omega & -4 & & & \\ & & & \omega & & & -4 & & \\ & & & & \omega & & \omega & -4 & \\ & & & & & \omega & & \omega & -4 \end{bmatrix} \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \\ \phi_{12} \\ \phi_{22} \\ \phi_{32} \\ \phi_{13} \\ \phi_{23} \\ \phi_{33} \end{bmatrix}^{(n+1)} =$$

$$\omega\phi_{ij-1}^{(n+1)} + \omega\phi_{i-1j}^{(n+1)} - 4\phi_{ij}^{(n+1)} = -\omega\phi_{i+1j}^{(n)} - \omega\phi_{ij+1}^{(n)} + (4\omega - 4)\phi_{ij}^{(n)} = 0$$

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N Matrix for SOR

$$\begin{bmatrix} d & -\omega & & -\omega & & & & & \\ & d & -\omega & & -\omega & & & & \\ & & d & & & -\omega & & & \\ & & & d & -\omega & & -\omega & & \\ & & & & d & -\omega & & -\omega & \\ & & & & & d & & & -\omega \\ & & & & & & d & -\omega & \\ & & & & & & & d & -\omega \\ & & & & & & & & d \end{bmatrix} \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \\ \phi_{12} \\ \phi_{22} \\ \phi_{32} \\ \phi_{13} \\ \phi_{23} \\ \phi_{33} \end{bmatrix}^{(n)} - \omega \begin{bmatrix} \phi_{10}+\phi_{01} \\ \phi_{20} \\ \phi_{30}+\phi_{41} \\ \phi_{02} \\ 0 \\ \phi_{42} \\ \phi_{03}+\phi_{14} \\ \phi_{24} \\ \phi_{43}+\phi_{34} \end{bmatrix}$$

$$d = 4\omega - 4$$

$$\omega\phi_{ij-1}^{(n+1)} + \omega\phi_{i-1j}^{(n+1)} - 4\phi_{ij}^{(n+1)} = -\omega\phi_{i+1j}^{(n)} - \omega\phi_{ij+1}^{(n)} + (4\omega - 4)\phi_{ij}^{(n)} = 0$$

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Next Steps

- Look at general iteration equation: **M**$\phi^{(n+1)}$ = **N**$\phi^{(n)}$ + **b**
- Get equation for evolution of error vector, $\varepsilon^{(n)}$, representing error in each unknown ϕ at step n
- How does error at new step, $\varepsilon^{(n+1)}$ depend on error at old step, $\varepsilon^{(n)}$
- How can we guarantee that error does not grow at each step?

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Convergence

- Start with **M**$\phi^{(n+1)}$ = **N**$\phi^{(n)}$ + **b**
- Subtract **M**$\phi^{(n)}$ from each side
- Result is **M**($\phi^{(n+1)}$ – $\phi^{(n)}$) = **b** – (**M** – **N**)$\phi^{(n)}$
- But we said that **M** – **N** = **A**, so result is
- **M($\phi^{(n+1)}$ – $\phi^{(n)}$) = b – (M – N)$\phi^{(n)}$ = b – A$\phi^{(n)}$**
- We defined **b – A$\phi^{(n)}$** = **r**$^{(n)}$ = **A**$\varepsilon^{(n)}$, so
- **M($\phi^{(n+1)}$ – $\phi^{(n)}$) = b – A$\phi^{(n)}$ = r$^{(n)}$ = A$\varepsilon^{(n)}$**

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Convergence II

- From last chart: $\mathbf{M}(\phi^{(n+1)} - \phi^{(n)}) = \mathbf{r}^{(n)} = \mathbf{A}\varepsilon^{(n)}$
- Define update = $\delta^{(n)} = \phi^{(n+1)} - \phi^{(n)}$
- $\mathbf{M}(\phi^{(n+1)} - \phi^{(n)}) = \mathbf{M}\delta^{(n)} = \mathbf{r}^{(n)} = \mathbf{A}\varepsilon^{(n)}$
- Have two computable measures of error, $\varepsilon^{(n)}$; these are $\delta^{(n)}$ and $\mathbf{r}^{(n)}$
- What makes error decrease?

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Does the Error Decrease?

- Iteration equation: $\mathbf{M}\phi^{(n+1)} = \mathbf{N}\phi^{(n)} + \mathbf{b}$
- At convergence, $\phi^{(n+1)} = \phi^{(n)} = \phi$, so that $\mathbf{M}\phi = \mathbf{N}\phi + \mathbf{b}$
- Subtract $\mathbf{M}\phi = \mathbf{N}\phi + \mathbf{b}$ from $\mathbf{M}\phi^{(n+1)} = \mathbf{N}\phi^{(n)} + \mathbf{b}$ giving $\mathbf{M}(\phi^{(n+1)} - \phi) = \mathbf{N}(\phi^{(n)} - \phi)$, which gives $\mathbf{M}\varepsilon^{(n+1)} = \mathbf{N}\varepsilon^{(n)}$
- New error given by $\varepsilon^{(n+1)} = \mathbf{M}^{-1}\mathbf{N}\varepsilon^{(n)}$
- Does the error go to zero as we take more iterations?

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Matrix Eigenvalues: $\mathbf{Ax} = \lambda\mathbf{x}$

- Used to determine convergence
- If a matrix, **A**, multiplies a vector **x** and produces a constant λ times **x**
  - **x** is an eigenvector of **A**
  - λ is the eigenvalue associated with **x**
  - An n by n matrix can have up to n linearly independent eigenvalues
  - If the n eigenvectors are linearly independent we can expand any n component vector in terms of the eigenvectors

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Error Decrease Depends on $\mathbf{M}^{-1}\mathbf{N}$

- Assume that $\mathbf{M}^{-1}\mathbf{N}$ has a complete set of K eigenvalues, $\mathbf{x}_{(k)}$ so we can expand the initial error vector in terms of these eigenvectors $\varepsilon^{(0)} = \Sigma_k a_k\mathbf{x}_{(k)}$
- Iteration process gives following results where λ_k is eigenvalue ($\mathbf{M}^{-1}\mathbf{N}\mathbf{x}_{(k)} = \lambda_k\mathbf{x}_{(k)}$)

$$\boldsymbol{\varepsilon}^{(1)} = \mathbf{M}^{-1}\mathbf{N}\boldsymbol{\varepsilon}^{(0)} = \mathbf{M}^{-1}\mathbf{N}\sum_{k=1}^{K} a_k\mathbf{x}_{(k)} = \sum_{k=1}^{K} a_k\mathbf{M}^{-1}\mathbf{N}\mathbf{x}_{(k)} = \sum_{k=1}^{K} a_k\lambda_k\mathbf{x}_{(k)}$$

$$\boldsymbol{\varepsilon}^{(2)} = \mathbf{M}^{-1}\mathbf{N}\boldsymbol{\varepsilon}^{(1)} = \mathbf{M}^{-1}\mathbf{N}\sum_{k=1}^{K} a_k\lambda_k\mathbf{x}_{(k)} = \sum_{k=1}^{K} a_k\lambda_k\mathbf{M}^{-1}\mathbf{N}\mathbf{x}_{(k)} = \sum_{k=1}^{K} a_k\lambda_k^2\mathbf{x}_{(k)}$$

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General Error Equation

- Reasoning by induction from the last two equations gives $\varepsilon^{(n)}$ as follows

$$\boldsymbol{\varepsilon}^{(n)} = \sum_{k=1}^{K} a_k\lambda_k^n\mathbf{x}_{(k)}$$

- For error to become small as iterations increase, we must have all $|\lambda_k| < 1$
  - Largest $|\lambda_k| = |\lambda_1|$, called spectral radius, will dominate sum for large n
  - $\varepsilon^{(n)} \approx a_1\lambda_1^n\mathbf{x}_{(1)}$
  - Want this to reach desired error, δ

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General Error Equation II

- To control error in $\varepsilon^{(n)} \approx a_1\lambda_1^n\mathbf{x}_{(1)}$ require factor $a_1\lambda_1^n \approx \delta$ or $\lambda_1^n = \delta/a_1$
- Take logs of both sides and solve for n

$$n \approx \frac{\ln\left(\dfrac{\delta}{a_1}\right)}{\ln\lambda_1}$$

- Recall that ln(1 + x) ≈ x for small x
- When λ_1 is close to 1, ln λ_1 will be a small number and n will be large
- Seek iteration matrices with small λ_1

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SOR Spectral Radius

- Use MATLAB to compute the spectral radius, λ_1 = maximum $|\lambda|$ for SOR
  - Find optimum ω (minimum λ_1) by trial and error

N = M = 11		N = M = 21		N = M = 41	
ω	λ_1	ω	λ_1	ω	λ_1
1	0.9206	1	0.9778	1	0.9941
1.56	0.5759	1.74	0.7562	1.85	0.8968
1.57	0.5700	1.75	0.7500	1.86	0.8600
1.58	0.5800	1.76	0.7600	1.87	0.8700

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Diagonal Dominance

- The real requirement is that the largest eigenvalue be less than one in absolute value
- This is guaranteed in the solution matrix is diagonally dominant
- This means that the diagonal coefficient (in absolute value) is greater than or equal to the sum of the absolute values of all other coefficients in the equation

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Diagonal Dominance II

- If the coefficients in the **A** matrix are a_{km}, the rules for diagonal dominance in an N x N matrix are
- $|a_{kk}| >= \Sigma_m |a_{km}|$ for $1 \le k \le N$
- $|a_{kk}| > \Sigma_m |a_{km}|$ for at least one value of k
- General finite-difference equations satisfy the >= condition and boundary conditions satisfy the > condition
- Upwind difference diagonally dominant

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Advanced Methods

- See text for greater discussion
- Methods use different iteration matrices to get faster convergence
  - Alternating Direction Implicit (ADI)
  - Stone's Method
  - Conjugate Gradient
  - Multigrid
- Multigrid generally considered fastest method for CFD calculations

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Multigrid Method

- Solve equations on a set of different grids
- Analysis of error shows that convergence rate depends on grid size
- Getting a solution to a coarse grid then using those results for the fine grid gives solution faster
- Use prolongation and restriction to get results between fine and coarse gride

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Multigrid Method II

- Different patterns used; example below
  - Start with fine grid
  - After partial convergence on find grid use coarser grid and do iterations to get more convergence on that grid
  - Continue to coarsest grid and get convergence there
  - Prolong solution to finer grids and get converged solution on each grid
  - Finally get converged solution on finest grid

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Thomas Algorithm

- Used for simple solution of one-dimensional problems
- Can be extended to improved iteration approach for two- or three-dimensional problems
- Basic problem: $a_W\phi_W + a_P\phi_P + a_E\phi_E = b_K$
- Generalized one-dimensional problem
  - $A_kf_{k-1} + B_kf_k + C_kf_{k+1} = D_k$
  - Look at matrix form

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Thomas Algorithm II

- General format for tridiagonal equations

$$\begin{bmatrix} B_0 & C_0 & 0 & 0 & \cdots & 0 & 0 \\ A_1 & B_1 & C_1 & 0 & \cdots & 0 & 0 \\ 0 & A_2 & B_2 & C_2 & \cdots & 0 & 0 \\ 0 & 0 & A_3 & B_3 & & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & B_{N-1} & C_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & A_N & B_N \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{bmatrix} = \begin{bmatrix} D_0 \\ D_1 \\ D_2 \\ \vdots \\ \vdots \\ D_{N-1} \\ D_N \end{bmatrix}$$

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Thomas Algorithm III

- The matrix is called a tridiagonal matrix
  - Has principal diagonal,
  - one diagonal above principal diagonal, and
  - one diagonal below principal diagonal
- Can apply traditional Gauss elimination for solution of simultaneous linear equations to get simple upper triangular form
- Simple equations to obtain this

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Thomas Algorithm IV

- Gauss elimination upper triangular form

$$\begin{bmatrix} 1 & -E_0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -E_1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -E_2 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -E_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{bmatrix} = \begin{bmatrix} F_0 \\ F_1 \\ F_2 \\ \vdots \\ \vdots \\ F_{N-1} \\ F_N \end{bmatrix}$$

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Thomas Algorithm V

- Forward computations
  - Initial: $E_0 = -C_0 / B_0$ $F_0 = D_0 / B_0$
  - For i = 1,… N-1:

$$E_i = \frac{-C_i}{B_i + A_iE_{i-1}} \qquad F_i = \frac{D_i - A_iF_{i-1}}{B_i + A_iE_{i-1}}$$

- Get last x value first $x_N = F_N = \dfrac{D_N - A_NF_{N-1}}{B_N + A_NE_{N-1}}$
- Back substitute: $x_i = F_i + E_ix_{i+1}$

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Thomas Example

$$\begin{bmatrix} 1 & 2 & 0 & 0 \\ 3 & 4 & 5 & 0 \\ 0 & 6 & 7 & 8 \\ 0 & 0 & 9 & 10 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} = \begin{bmatrix} 10 \\ 34 \\ 40 \\ 28 \end{bmatrix} \qquad E_0 = \frac{-C_0}{B_0} = -\frac{2}{1} = -2 \qquad F_0 = \frac{D_0}{B_0} = \frac{10}{1} = 10$$

$$E_1 = \frac{-C_1}{B_1 + A_1E_0} = \frac{-5}{4+3(-2)} = \frac{5}{2}$$

$$F_1 = \frac{D_1 - A_1F_0}{B_1 + A_1E_0} = \frac{34-3(10)}{4+3(-2)} = -2$$

- Continue to find E_2, F_2, E_3, and F_3

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Thomas Example II

- Back substitution (shows F and E results)

$$\phi_3 = F_3 = 1$$
$$\phi_2 = F_2 + E_2\phi_3 = \frac{26}{11} + \left(-\frac{4}{11}\right)1 = \frac{22}{11} = 2$$
$$\phi_1 = F_1 + E_1\phi_2 = -2 + \frac{5}{2}2 = 3$$
$$\phi_0 = F_0 + E_0\phi_1 = 10 + (-2)3 = 4$$

- Original equation set shows results are correct

$$\begin{bmatrix} 1 & 2 & 0 & 0 \\ 3 & 4 & 5 & 0 \\ 0 & 6 & 7 & 8 \\ 0 & 0 & 9 & 10 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} = \begin{bmatrix} 10 \\ 34 \\ 40 \\ 28 \end{bmatrix}$$

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Thomas for Two Dimensions

- Two dimensional equation: $a_N\phi_{ij+1} + a_S\phi_{ij-1} + a_E\phi_{i+1j} + a_P\phi_{ij} + a_W\phi_{i-1j} = b_{ij}$
- Look at one-dimensional approach in x direction: $a_E\phi_{i+1j} + a_P\phi_{ij} + a_W\phi_{i-1j} = b_{ij} - a_N\phi_{ij+1} - a_S\phi_{ij-1}$
- Use Thomas algorithm in x-direction

$$a_W\phi_{i-1j}^{(n+1)} + a_P\phi_{ij}^{(n+1)} + a_E\phi_{i+1j}^{(n+1)} = b_{ij} - a_N\phi_{ij+1}^{(n)} - a_S\phi_{ij-1}^{(n)}$$
$$A\phi_{i-1j}^{(n+1)} + B\phi_{ij}^{(n+1)} + C\phi_{i+1j}^{(n+1)} = D$$

- Next apply algorithm in y direction

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Thomas for Two Dimensions II

- y-direction form

$$a_S\phi_{ij-1}^{(n+1)} + a_P\phi_{ij}^{(n+1)} + a_N\phi_{ij+1}^{(n+1)} = b_{ij} - a_E\phi_{i+1j}^{(n)} - a_W\phi_{i-1j}^{(n)}$$
$$A\phi_{ij-1}^{(n+1)} + B\phi_{ij}^{(n+1)} + C\phi_{ij+1}^{(n+1)} = D$$

- This approach involves more calculations per iteration, but it can reduce error more quickly by getting simultaneous solutions of results along one coordinate direction
- Can be extended to three dimensions

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Unstructured Grids

- Do not have ijk indexing system that regular grids have
- Nodes numbered sequentially with single index
- Must store information on numbers of nearest neighbors for each node
- Equation matrix is still sparse, but not so well structured
  - Do not have all coefficients on 5 or 7 diagonals

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Nonlinear Problems

- CFD equations are nonlinear system of difference equations
- Have terms like $u\phi$ and uu
- Have to solve for u, v, w, T, p, etc.
- Typically linearize problem by writing terms like $u\phi$ as $u^{(n)}\phi^{(n+1)}$ to solve for $\phi^{(n+1)}$
- Once iteration n is complete, update linearized terms
- Usually requires underrelaxation

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