Overview of Numerical Solution Methods for PDE's

Finite Difference Method:

Functions are represented by their values at certain grid points and derivatives are approximated through differences in these values.

Method of Lines (MOL):

All dimensions are discretized except one (time).

Finite Element Method (FEM):

FEM encompasses all the methods for connecting many simple element equations over many small subdomains, named finite elements, to approximate a more complex equation over a larger domain. (CFD – Computational Fluid Dynamics)

Gradient Discretization Method (GDM):

It is based on the separate approximation of a function and of its gradient.

Finite Volume Method:

"Finite volume" refers to the small volume surrounding each nodal point on a mesh (grid structure). In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem.

Spectral Method:

The idea is to write down the solution of the differential equation as a sum of certain "basis functions" (for example, as a Fourier series, which is a sum of sinusoids) and then to choose the coefficients in the sum that best satisfy the differential equation.

Meshfree Methods:

Simulation of some otherwise difficult types of problems, at the cost of extra computing time and programming effort.

Domain Decomposition Methods:

Solve a boundary value problem by splitting it into smaller boundary value problems on subdomains and iterating to coordinate the solution between adjacent subdomains. Overlapping methods, non-ovelapping methods, etc.

Multigrid (MG) Methods:

The main idea of multigrid is to accelerate the convergence of a basic iterative method by *global* correction from time to time, accomplished by solving a coarse problem.

ELLIPTIC PDE's

Laplace Equation: $$\nabla^2 U = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0$$

Poisson Equation: $$\nabla^2 U = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = g(x,y)$$

Helmholtz Equation: $$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + f(x,y)\,U = g(x,y)$$

where

$0 \le x \le a$ and

$0 \le y \le b$

Boundary conditions: Given U => **Drichlet type**

Given derivative of U => **Neumann type**

Mixed

Pierre-Simon (Marquis de) Laplace

French Mathematician

1749 - 1827

Siméon Denis Poisson

French Mathematician

1781 - 1840

Hermann Ludwig Ferdinand von Helmholtz

German Physicist

1821 - 1894

Johann Peter Gustav Lejeune Dirichlet

German Mathematician

1805 - 1859

John von Neumann

Hungarian (American) Mathematician

1903 - 1957

Physical problems that has elliptic type (mostly steady-state) PDE’s,

- Temperature field
- Pressure field
- Electrostatic potential
- Stress distribution
- Velocity potential
- Torsion
- Membrane displacement
- Others

The existence of the solution of an elliptic PDE and its uniqueness depend heavily on the boundary conditions. This is true for analytical as well as numerical solutions.

Two conditions must exist for a well-posed problem:

- One unambiguous condition at every point of the boundary must be specified;
- The boundary should be closed. If part or all of the boundary is at infinity, the function should stay finite.

Helmholtz Equation: $$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + f(x,y)\,U = g(x,y)$$

Notes:

- This has only two dimensions. There may be a third dimension, z
- This is in Cartesian coordinates. Other coordinate systems exists such as cylindrical (radial direction), spherical (angular directions), curvy-linear, others
- There may be mixed boundary conditions (u as well as derivative(s) of u)

Example: Consider $U_{xx} + U_{yy} = 0 \qquad 0 \le x \le a \;,\; 0 \le y \le b$

Boundary Conditions: $U(0,y) = \text{Given} \quad U(a,y) = \text{Given}$, $U(x,0) = \text{Given} \quad U(x,b) = \text{Given}$ } Drichlet type

Set: $h = a / M \qquad k = b / N$

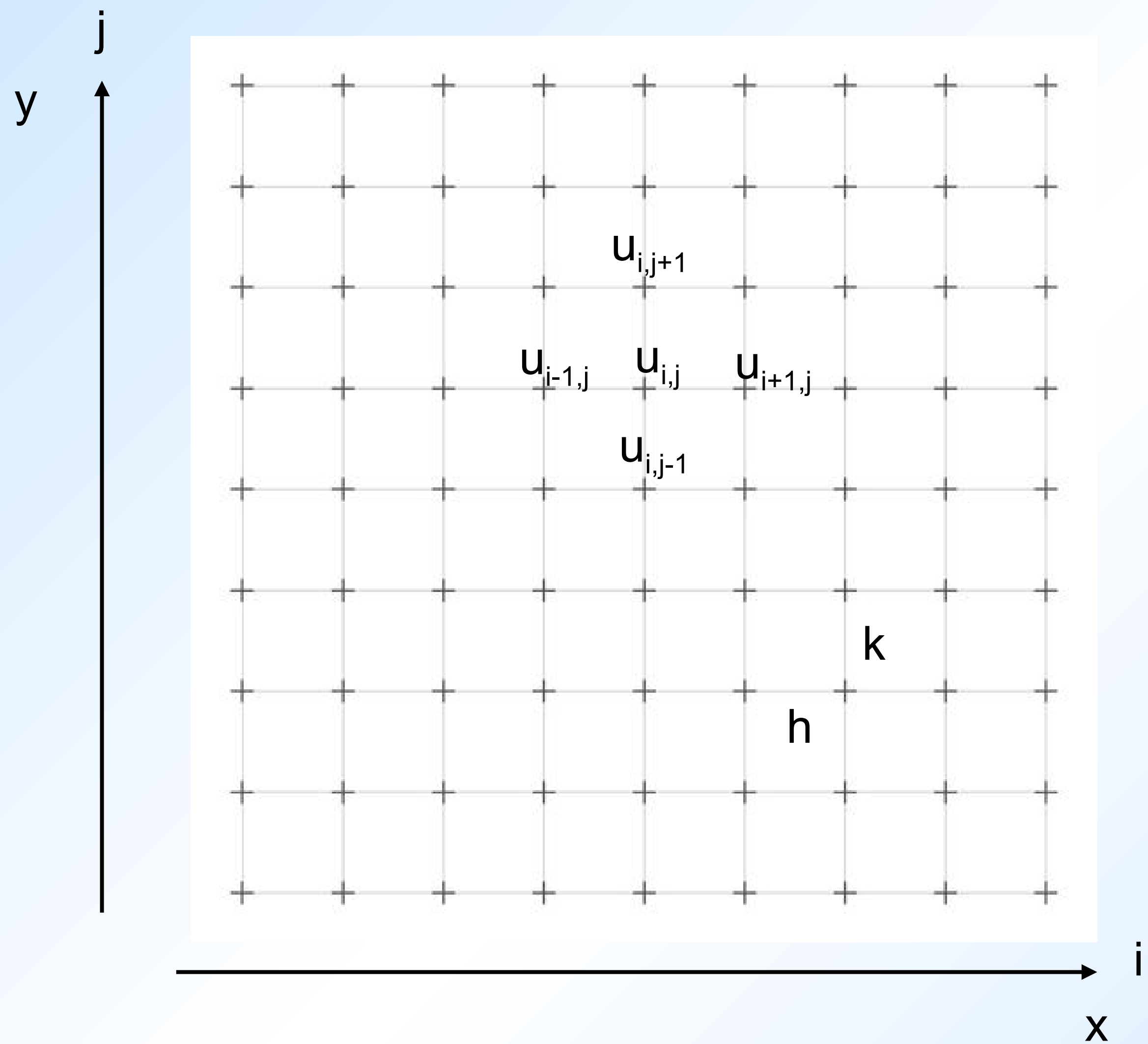
Using central differences:

$$\frac{u_{i-1,j} - 2\,u_{i,j} + u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2\,u_{i,j} + u_{i,j+1}}{k^2} = 0$$

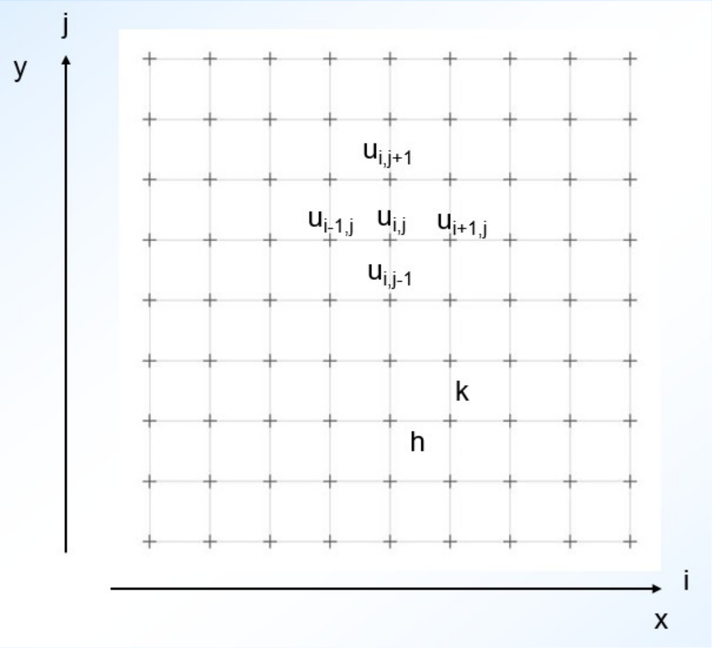
$$2\left(h^2 + k^2\right) u_{i,j} = k^2 \left(u_{i-1,j} + u_{i+1,j}\right) + h^2 \left(u_{i,j-1} + u_{i,j+1}\right)$$

where $1 \le i \le M - 1$ and $1 \le j \le N - 1$

The given BC's determine $u_{0,j}$, $u_{M,j}$, $u_{i,0}$, and $u_{i,N}$



Grid structure or mesh in Cartesian coordinates



$$\frac{u_{i-1,j} - 2\,u_{i,j} + u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2\,u_{i,j} + u_{i,j+1}}{k^2} = 0$$

If $h = k$:

$$u_{i,j} = \frac{1}{4}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\right)$$

This means that the value of u at an interior node is equal to the average of u at four adjacent nodes. This is the well-known mean-value theorem for harmonic functions that satisfy the Laplace equation.

If h = k: $$u_{i,j} = \frac{1}{4}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\right)$$

We have (M-1) (N-1) number of unknown $u_{i,j}$ values at the interior nodes when boundary conditions are given in terms of u's (not derivatives).

It can be shown that the solution of the finite difference equation converges to the exact solution as h and k -> 0.

The proof of existence of a solution and its convergence is essentially based on the Maximum Modulus Principle.

It follows from the finite difference equation that the value of |u| at any interior grid point does not exceed the value at any of the four adjoining nodal points.

If $h = k$: $$u_{i,j} = \frac{1}{4}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\right)$$

The successive application of this argument at all interior grid points leads to the conclusion that $|u|$ at the interior grid points cannot be greater than the maximum value on the boundary.

This is analogous to the Maximum Modulus Principle.

The solution obtained from this representation, like the exact solution, has no maxima or minima at interior nodes of the solution domain. If extreme values exist, they must lie on the boundary.

The **maximum modulus principle** or maximum modulus theorem for complex analytic functions states that the maximum value of modulus of a function defined on a bounded domain may occur only on the boundary of the domain. If the modulus of the function has a maximum value inside the domain, then the function is constant.

Thus, the maximum modulus principle states the nature of the local maximum of an analytic function within a domain. The maximum value could only be attained on the boundary unless the function is constant.

See OdtuClass for an e-book on complex numbers and complex functions.

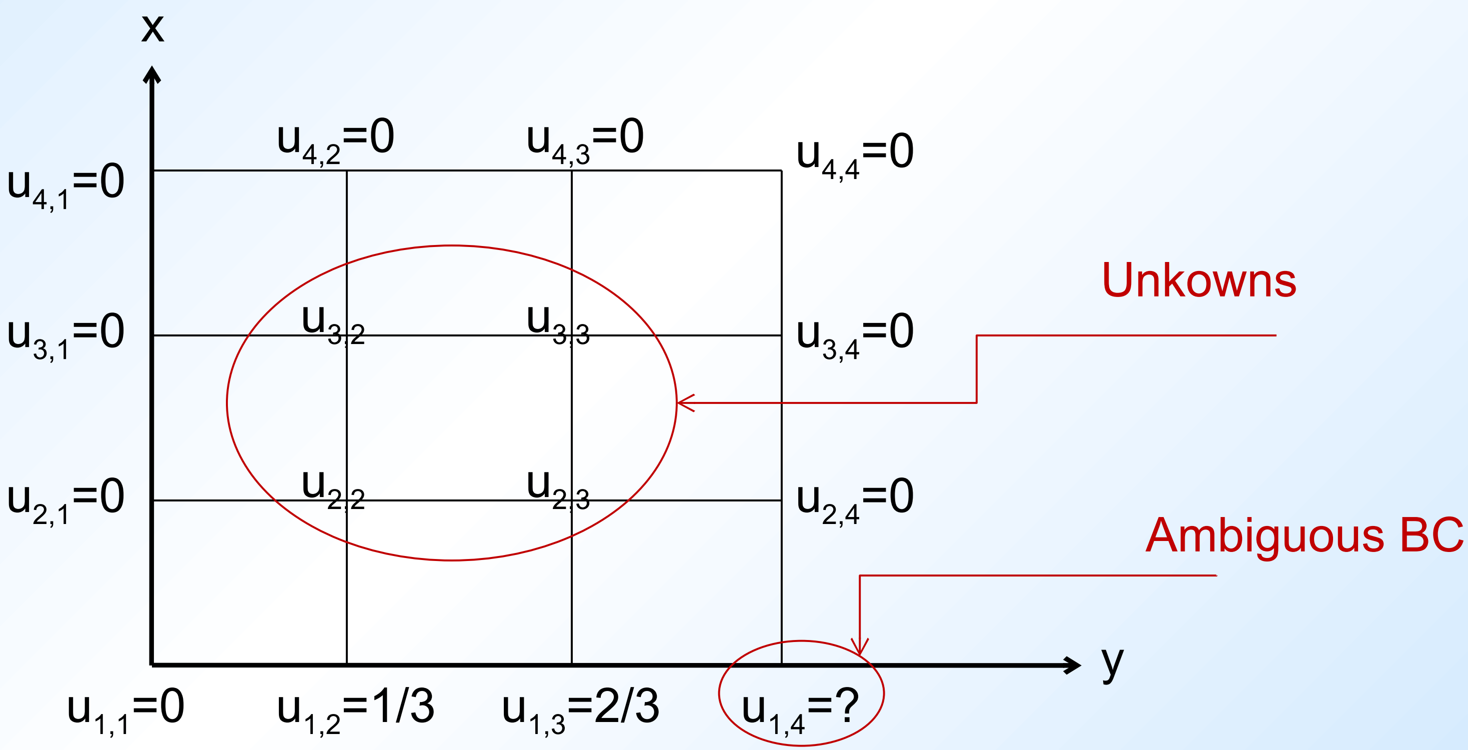
See OdtuClass for an e-book on PDE's.

Example: $U_{xx} + U_{yy} = 0 \quad 0 \leq x \leq 1 \;,\; 0 \leq y \leq 1$

Boundary Conditions:

$U(0,y) = y \quad U(1,y) = 0 \quad \text{on} \quad 0 \leq y \leq 1$

$U(x,0) = 0 \quad U(x,1) = 0 \quad \text{on} \quad 0 \leq x \leq 1$



Finite difference equations in ***natural order***:

$$\begin{pmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{pmatrix} \begin{pmatrix} u_{2,2} \\ u_{2,3} \\ u_{3,2} \\ u_{3,3} \end{pmatrix} = \begin{pmatrix} -1/3 \\ -2/3 \\ 0 \\ 0 \end{pmatrix}$$

Natural order: Left to right , Bottom to top

Then, the coefficient matrix becomes diagonal (penta-diagonal in this case)

Solution: $u_{2,2} = 11/72$ $u_{2,3} = 16/72$ $u_{3,2} = 4/72$ $u_{3,3} = 5/72$

Example: Given Helmholtz equation $\nabla^2 U + f(x,y)\, U = g(x,y)$

f and g are continuous functions defined in the solution domain.

Boundary conditions: $U(x,y) = q(x,y)$ on the perimeter R of the solution domain

Define: $x_i = i\,h$, $y_i = j\,h$ $i\,,j > 0$, The same spacing on x and y

$$u_{i,j} = u(x_i\,, y_j) \quad , \quad f_{i,j} = f(x_i\,, y_j) \quad , \quad g_{i,j} = g(x_i\,, y_j)$$

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

The corresponding difference equation is:

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

Take: $h = 1/10$

There is one equation for every interior point. In matrix notation, A U = B where the matrices are:

$$
A = \begin{pmatrix}
4-h^2 f_{22} & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4-h^2 f_{32} & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 4-h^2 f_{42} & 0 & 0 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 4-h^2 f_{23} & -1 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -1 & 4-h^2 f_{33} & -1 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -1 & 4-h^2 f_{43} & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 & 0 & 4-h^2 f_{24} & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 4-h^2 f_{34} & -1 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4-h^2 f_{44}
\end{pmatrix}
$$

$$U = \begin{pmatrix} u_{2,2} \\ u_{3,2} \\ u_{4,2} \\ u_{2,3} \\ u_{3,3} \\ u_{4,3} \\ u_{2,4} \\ u_{3,4} \\ u_{4,4} \end{pmatrix} \qquad B = \begin{pmatrix} -h\,g_{2,2} + u_{1,2} + u_{2,1} \\ -h\,g_{3,2} + u_{3,1} \\ -h\,g_{4,2} + u_{5,2} + u_{4,1} \\ -h\,g_{2,3} + u_{1,3} \\ -h\,g_{3,3} \\ -h\,g_{4,3} + u_{5,3} \\ -h\,g_{2,4} + u_{1,4} + u_{2,5} \\ -h\,g_{3,4} + u_{3,5} \\ -h\,g_{4,4} + u_{5,4} + u_{4,5} \end{pmatrix}$$

This is natural ordering.

Note that A is symmetrical and diagonal . The main diagonal elements are dominant when $f \leq 0$.

ITERATIVE METHODS
- Point Iterative Methods
- Block Iterative Methods

PROPERTIES OF A GOOD ITERATIVE METHOD

1. Simple algorithm;
2. Requires small storage memory on the computer by making use of the sparseness of the coefficient matrix;
3. Rapid convergence to true solution;
4. Independent of initial guess, so self correcting (even the round-off error).

Gauss-Seidel Iteration Method:

In numerical linear algebra, the **Gauss–Seidel method**, also known as the **Liebmann method** or the **method of successive displacement**, is an iterative method, similar to Jacobi's method, used to solve a system of linear equations. It is named after the German mathematicians Carl Friedrich Gauss and Philipp Ludwig von Seidel.

The name successive displacement is because the second unknown is determined from the first unknown in the current iteration, the third unknown is determined from the first and second unknowns.

Though it can be applied to any matrix with non-zero elements on the diagonals, convergence is only guaranteed if the matrix is either strictly diagonally dominant, or symmetric and positive definite.

Johann Carl Friedrich Gauss

German Mathematician

1777 - 1855

Philipp Ludwig von Seidel

German Mathematician

1821 - 1896

Let us assume a set of linear equations in the matrix form is as follows:

$$A\,X = B$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \ldots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \ldots & a_{2n} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & a_{n3} & \ldots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \ldots \\ \ldots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \ldots \\ \ldots \\ b_n \end{pmatrix}$$

$$\begin{aligned} a_{11}\,x_1 + a_{12}\,x_2 + \ldots + a_{1n}\,x_n &= b_1 \\ a_{21}\,x_1 + a_{22}\,x_2 + \ldots + a_{2n}\,x_n &= b_2 \\ \ldots + \ldots + \ldots + \ldots &= \ldots \\ a_{n1}\,x_1 + a_{n2}\,x_2 + \ldots + a_{nn}\,x_n &= b_n \end{aligned}$$

If the diagonal elements are non-zero, each equation is rewritten for the corresponding unknown, that is, the first equation is rewritten with x_1 on the left hand side, the second equation is rewritten with x_2 on the left hand side and so on as follows.

$$\left.\begin{aligned} x_1 &= \frac{b_1 - a_{12}\,x_2 - \ldots - a_{1n}\,x_n}{a_{11}} \\ x_2 &= \frac{b_2 - a_{21}\,x_1 - \ldots - a_{2n}\,x_n}{a_{22}} \\ \ldots &= \ldots \\ x_n &= \frac{b_n - a_{n1}\,x_1 - \ldots - a_{n\,n-1}\,x_{n-1}}{a_{nn}} \end{aligned}\right\} \quad a_{ii} \neq 0$$

These equations can be rewritten in a summation form for any row i:

$$x_i = \frac{b_i - \sum_{\substack{j=1 \\ j \neq n}}^{n} a_{ij}\, x_j}{a_{ii}}$$

To find x_i's, assume an initial guess for the x_i's (all the x_i's) and then use the rewritten equations to calculate the new estimates.

Always use the most recent estimates to calculate the next estimates, x_i.

At the end of each iteration, calculate the absolute relative approximate error for each x_i as

$$\left|\varepsilon_a\right|_i = \left|\frac{x_i^{new} - x_i^{old}}{x_i^{new}}\right| (100)$$

where new x_i is the recently obtained value of x_i , and old x_i is the previous value of x_i. When the absolute relative approximate error for each x_i is less than the pre-specified tolerance, the iterations are stopped.

Example

The upward velocity of a rocket is given at three different times in the following table:

Time, t (s)	Velocity, V (m/s)
5	106.8
8	177.2
12	279.2

The velocity data is approximated by a polynomial as:

$$V(t) = a_1 t^2 + a_2 t + a_3$$

Find the values of a_1 a_2 a_3 using the Gauss-Seidel method.

Assume the initial guesses: $a_1 = 1$ $a_2 = 2$ $a_3 = 5$

$$25\,a_1 + 5\,a_2 + a_3 = 106.8$$
$$64\,a_1 + 8\,a_2 + a_3 = 177.2$$
$$144\,a_1 + 12\,a_2 + a_3 = 279.2$$

$$a_1 = \frac{106.8 - 5\,a_2 - a_3}{25}$$
$$a_2 = \frac{177.2 - 64\,a_1 - a_3}{8}$$
$$a_3 = \frac{279.2 - 144\,a_1 - 12\,a_2}{1}$$

Assume the initial guesses: $a_1 = 1$ $a_2 = 2$ $a_3 = 5$

$$a_1 = \frac{106.8 - 5\,a_2 - a_3}{25} = \frac{106.8 - (5)\,(2) - 5}{25} = 3.672$$

$$a_2 = \frac{177.2 - 64\,a_1 - a_3}{8} = \frac{177.2 - (64)\,(3.672) - 5}{8} = -\,7.815$$

$$a_3 = 279.2 - 144\,a_1 - 12\,a_2 = 279.2 - (144)\,(3.672) - (12)\,(-7.851) = -\,155.36$$

Iteration	a_1	a_2	a_3
1	3.672	-7.851	-155.36
2	12.056	-54.882	-798.34
3	47.182	-255.51	-3448.9
4	193.33	-1093.4	-60072

The solution estimates are not converging.

The true solution is: $a_1 = 0.29048$ $a_2 = 19.690$ $a_3 = 1.0857$

The pitfall of most iterative methods is that they may or may not converge.

However, the solution to a certain classes of systems of simultaneous equations does always converge using the Gauss-Seidel method. This class of system of equations is where the coefficient matrix is diagonally dominant, that is

$$|a_{ii}| \geq \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{ij}|$$

$$25\,a_1 + 5\,a_2 + a_3 = 106.8 \qquad 25 < 5 + 1 \quad \text{NO}$$

$$64\,a_1 + 8\,a_2 + a_3 = 177.2 \qquad 8 < 64 + 1 \quad \text{NO}$$

$$144\,a_1 + 12\,a_2 + a_3 = 279.2 \qquad 1 > 144 + 1 \quad \text{NO}$$

The criteria are not satisified for any of the rows (equations). Therefore. it is always divergent no matter what the initial guesses are.

If the criterion is satisfied for most of the rows, there is possibly convergence. But, there is no guarantee.

If the critirion is not satified for most of the rows, there is possibly no convergence. But, there is no guarantee.

Example

$$12x_1 + 3x_2 - 5x_3 = 1$$
$$x_1 + 5x_2 + 3x_3 = 28$$
$$3x_1 + 7x_2 + 13x_3 = 76$$

$$x_1 = \frac{1 - 3x_2 + 5x_3}{12}$$
$$x_2 = \frac{28 - x_1 - 3x_3}{5}$$
$$x_3 = \frac{76 - 3x_1 - 7x_2}{13}$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

Iteration	x_1	$\lvert\epsilon_a\rvert_1 \%$	x_2	$\lvert\epsilon_a\rvert_2 \%$	x_3	$\lvert\epsilon_a\rvert_3 \%$
1	0.50000	100.00	4.9000	100.00	3.0923	67.662
2	0.14679	240.61	3.7153	31.889	3.8118	18.874
3	0.74275	80.236	3.1644	17.408	3.9708	4.0064
4	0.94675	21.546	3.0281	4.4996	3.9971	0.65772
5	0.99177	4.5391	3.0034	0.82499	4.0001	0.074383
6	0.99919	0.74307	3.0001	0.10856	4.0001	0.00101

Gauss-Seidel Method for Elliptic PDE's:

Given Helmholtz Equation: $\nabla^2 U + f(x,y)\, U = g(x,y)$

Corresponding Finite-difference Equation:

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

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

Gauss-Seidel Iterations, in natural order:

$$u^{n+1}_{i,j} = \frac{1}{4 - h^2\, f_{i,j}} \left(u^{n+1}_{i-1,j} + u^{n}_{i+1,j} + u^{n+1}_{i,j-1} + u^{n}_{i,j+1} - h^2\, g_{i,j}\right)$$

where n denotes iteration step

Gauss-Seidel Method with SOR (Successive Over Relaxation):

Gauss-Seidel Iterations, in natural order:

$$u_{i,j}^{n+1} = \frac{1}{4 - h^2\ f_{i,j}} \left(u_{i-1,j}^{n+1} + u_{i+1,j}^{n} + u_{i,j-1}^{n+1} + u_{i,j+1}^{n} - h^2\ g_{i,j} \right)$$

Gauss-Seidel Iterations with SOR, λ = relaxation factor between 1 and 2:

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{\lambda}{4 - h^2\ f_{i,j}} \left(u_{i-1,j}^{n+1} + u_{i+1,j}^{n} + u_{i,j-1}^{n+1} + u_{i,j+1}^{n} - \left(4 - h^2\ f_{i,j}\right) u_{i,j}^{n} - h^2\ g_{i,j} \right)$$

$$\left(u_{i,j}^{n+1}\right)^{*} = u_{i,j}^{n} + \lambda \left(u_{i,j}^{n+1} - u_{i,j}^{n} \right)$$

↑ GS with SOR estimate

↑ GS estimate

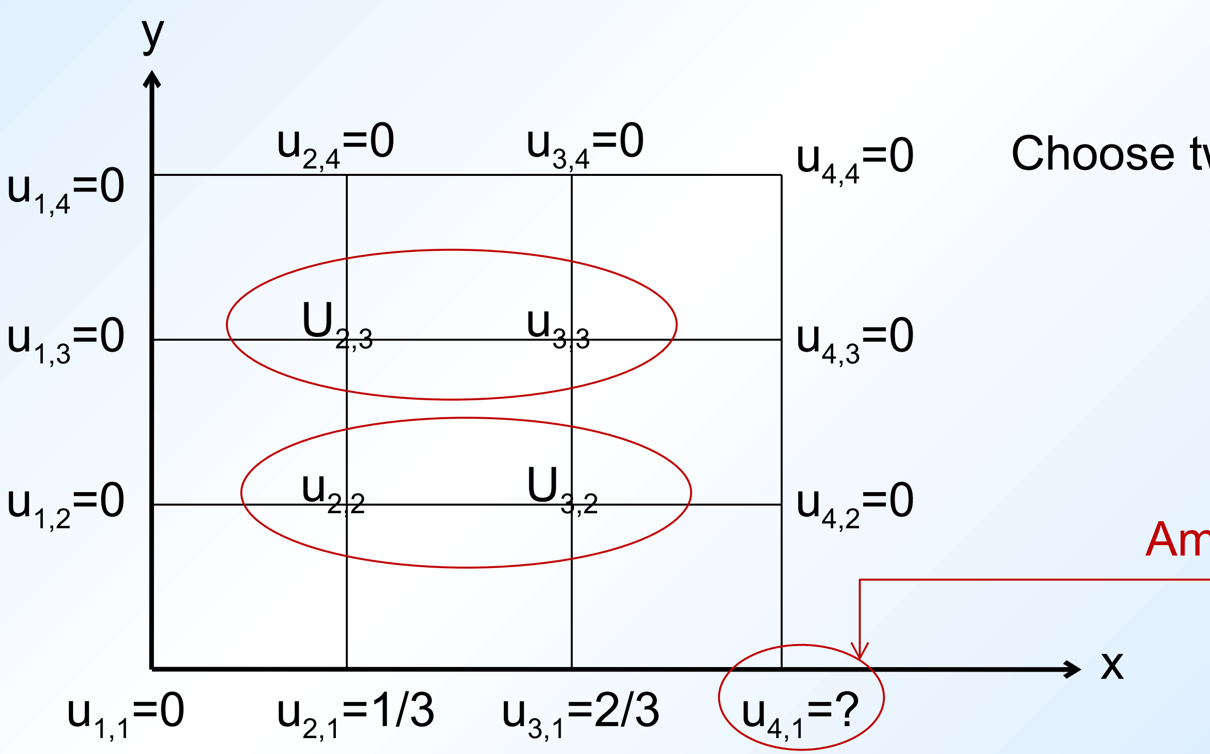
Example (block iterative): $U_{xx} + U_{yy} = 0 \quad 0 \le x \le 1 \;,\; 0 \le y \le 1$

Boundary Conditions:

$U(0,y) = 0 \quad U(1,y) = 0 \quad \text{on} \quad 0 \le y \le 1$

$U(x,0) = x \quad U(x,1) = 0 \quad \text{on} \quad 0 \le x \le 1$

Choose two groups, or blocks:



Ambiguous BC

Initial guess: $u_{2,2}^{0} = u_{3,2}^{0} = u_{2,3}^{0} = u_{2,3}^{0} = 0$

Gauss-Seidel iterations with each group:

$$u_{2,2}^{1} = \frac{1}{4}\left(u_{3,2}^{1} + u_{1,2}^{1} + u_{2,1}^{0} + u_{2,3}^{0}\right) = \frac{1}{4}\left(u_{3,2}^{1} + 0 + \frac{1}{3} + 0\right) = \frac{1}{4}u_{3,2}^{1} + \frac{1}{12}$$

$$u_{3,2}^{1} = \frac{1}{4}\left(u_{2,2}^{1} + u_{3,1}^{0} + u_{4,2}^{1} + u_{3,3}^{0}\right) = \frac{1}{4}\left(u_{2,2}^{1} + \frac{2}{3} + 0 + 0\right) = \frac{1}{4}u_{2,2}^{1} + \frac{1}{6}$$

$$\begin{pmatrix} 1 & -\frac{1}{4} \\ -\frac{1}{4} & 1 \end{pmatrix}\begin{pmatrix} u_{2,2}^{1} \\ u_{3,2}^{1} \end{pmatrix} = \begin{pmatrix} \frac{1}{12} \\ \frac{1}{6} \end{pmatrix} \qquad u_{2,2}^{1} = \frac{2}{15} \quad \text{and} \quad u_{3,2}^{1} = \frac{1}{5}$$

$$u_{2,3}^{1} = \frac{1}{4}\left(u_{2,4}^{0} + u_{1,3}^{1} + u_{2,2}^{1} + u_{3,3}^{1}\right) = \frac{1}{4}\left(0 + 0 + \frac{2}{15} + u_{3,3}^{1}\right) = \frac{1}{4}u_{3,3}^{1} + \frac{1}{30}$$

$$u_{3,3}^{1} = \frac{1}{4}\left(u_{4,3}^{1} + u_{3,4}^{0} + u_{2,3}^{1} + u_{3,2}^{1}\right) = \frac{1}{4}\left(0 + 0 + u_{2,3}^{1} + \frac{1}{5}\right) = \frac{1}{4}u_{2,3}^{1} + \frac{1}{20}$$

$$\begin{pmatrix} 1 & -\frac{1}{4} \\ -\frac{1}{4} & 1 \end{pmatrix} \begin{pmatrix} u_{2,3}^{1} \\ u_{3,3}^{1} \end{pmatrix} = \begin{pmatrix} \frac{1}{30} \\ \frac{1}{20} \end{pmatrix} \qquad u_{2,3}^{1} = \frac{11}{225} \quad \text{and} \quad u_{3,3}^{1} = \frac{14}{225}$$