Numerical Methods for Partial Differential Equations (PDE) (3)

Finite Difference Methods

PDE - Elliptic Equations

Poisson Equation

$$-\Delta u = f \quad \text{in } \Omega \subseteq \mathrm{R}^2$$

$$\Delta u = \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

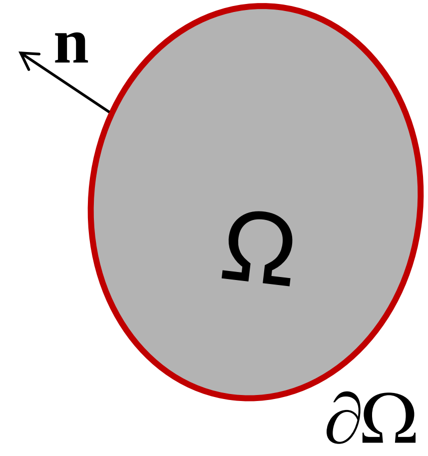
If $f = 0$ -> Laplace's Eq.

Solutions to Laplace's equation are called *harmonic functions*.

Dirichlet BC $\quad u\big|_{\partial\Omega} = g$

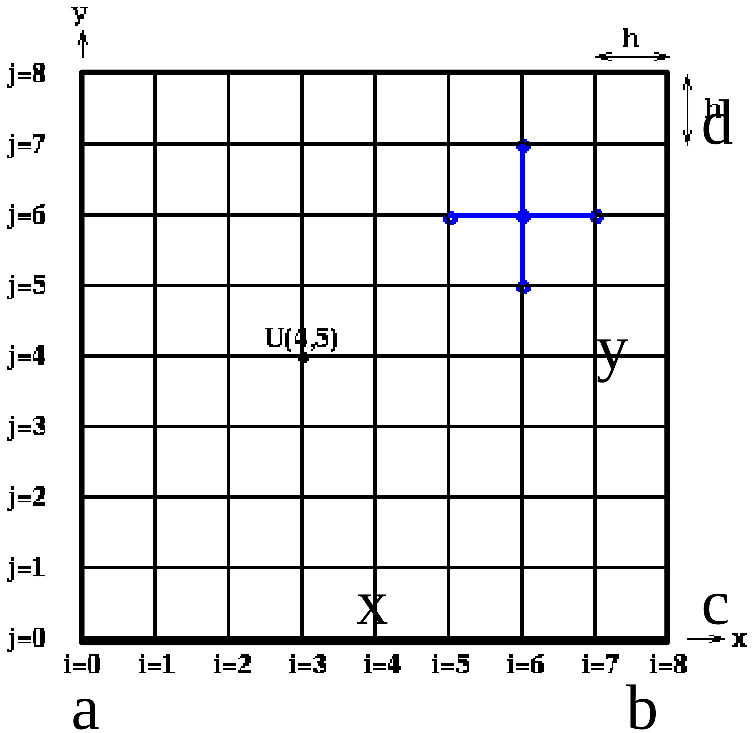
Neumann BC $\quad \left.\frac{du}{d\vec{n}}\right|_{\partial\Omega} = g$

Robin BC $\quad au + b\left.\frac{du}{d\vec{n}}\right|_{\partial\Omega} = g$



Poisson Problem
domain discretization

$$\begin{cases} -\Delta u(x,y) = f(x,y) \\ u(a,y) = g_1(y) \\ u(b,y) = g_2(y) \\ u(x,c) = g_3(x) \\ u(x,d) = g_4(x) \end{cases}$$



Let $\Omega=[a,b]x[c,d]$

be the grid of points in the plane xy:

$$x_i = a + ih \qquad h = (b-a)/N$$
$$y_j = c + jk \qquad k = (d-c)/M$$

Poisson Problem
differential operators discretization

$$-\frac{\partial^2 u}{\partial x^2}-\frac{\partial^2 u}{\partial y^2}=f$$

Replace the x-and y- derivatives with centered finite differences

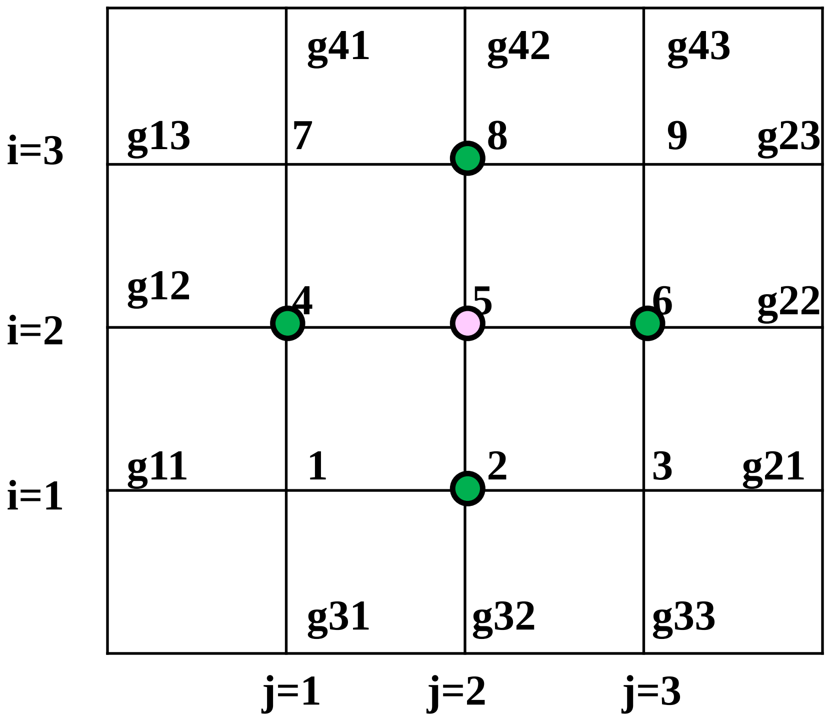
$$-\left[\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}\right]-\left[\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{h^2}\right]=f(x_i,y_j)$$

Determine the values of the solution u(x, y) in the internal nodes of the grid with step h = k:

$$\boldsymbol{-u_{i-1,j}-u_{i+1,j}+4u_{i,j}-u_{i,j-1}-u_{i,j+1}=h^2 f_{ij}}$$

Poisson Problem
set the linear system

For N=M=4 we get a grid 4x4:



Order the $(N\text{-}1)^2$ unknowns,

u_{ij} i,j=1,..,N-1

row by row

Natural Row-wise ordering:

$$(u_{1,1}, u_{1,2}, u_{1,3}, \ldots, u_{1,N-1}, u_{2,1}, \ldots, u_{N-1,N-1})$$

Associate an equation for each point of the mesh:

$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$

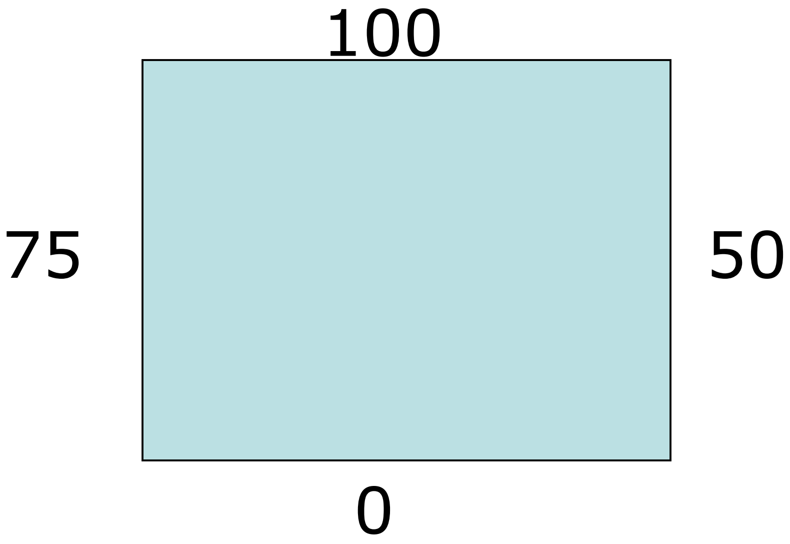
Poisson Problem
solving the linear system

$$\begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ u_{3,1} \\ u_{3,2} \\ u_{3,3} \end{bmatrix} = \begin{bmatrix} h^2 f_{1,1} + g_{11} + g_{31} \\ h^2 f_{1,2} + g_{32} \\ h^2 f_{1,3} + g_{21} + g_{33} \\ h^2 f_{2,1} + g_{12} \\ h^2 f_{2,2} \\ h^2 f_{2,3} + g_{22} \\ h^2 f_{3,1} + g_{13} + g_{41} \\ h^2 f_{3,2} + g_{42} \\ h^2 f_{3,3} + g_{43} + g_{23} \end{bmatrix}$$

Symmetric diagonally dominant in the weak sense. It is also positive definite (M-matrix)

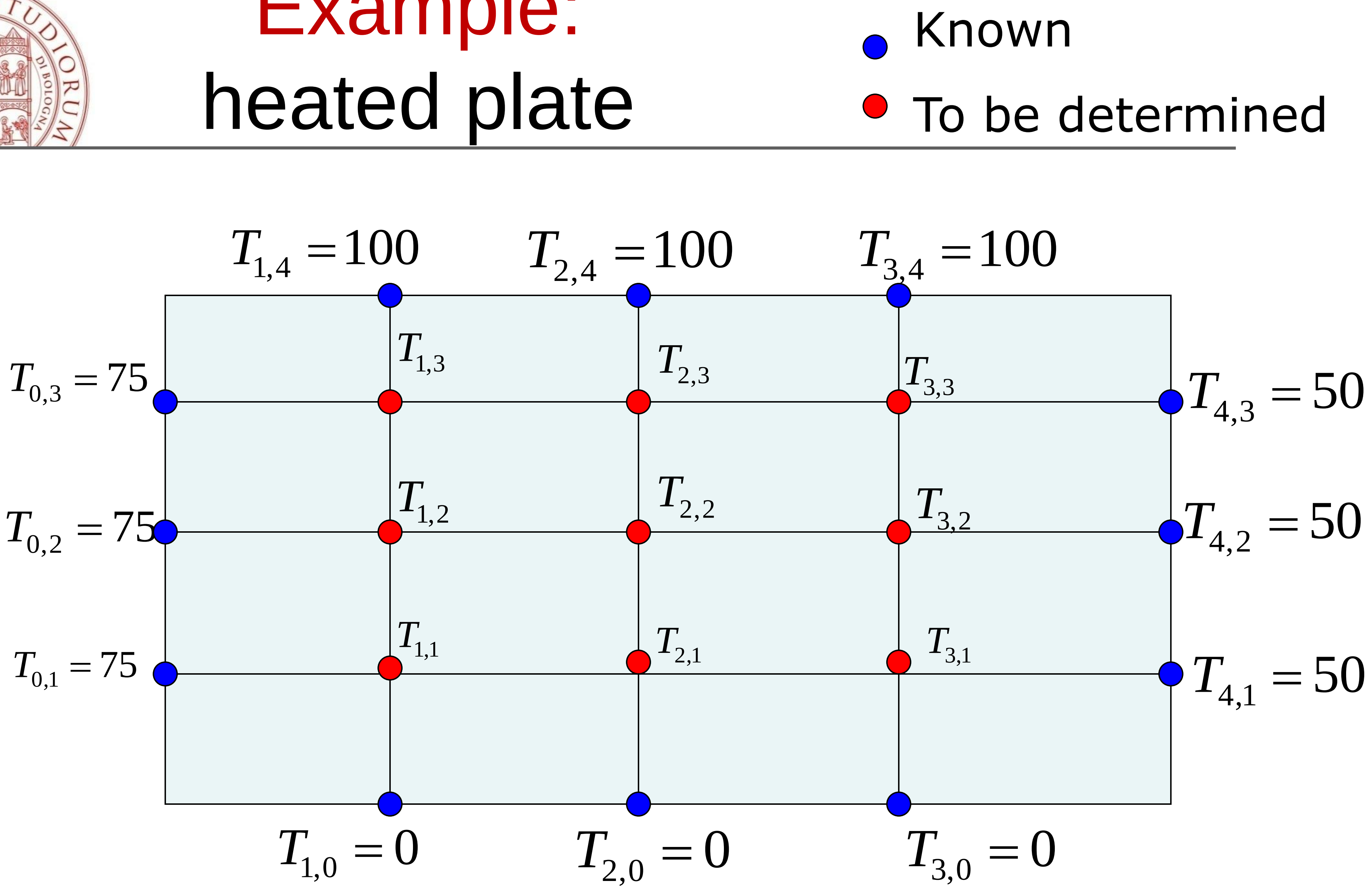
Example: heated plate

It is required to determine the steady state temperature at all points of a heated sheet of metal. The edges of the sheet are kept at a constant temperature: 100, 50, 0, and 75 degrees.



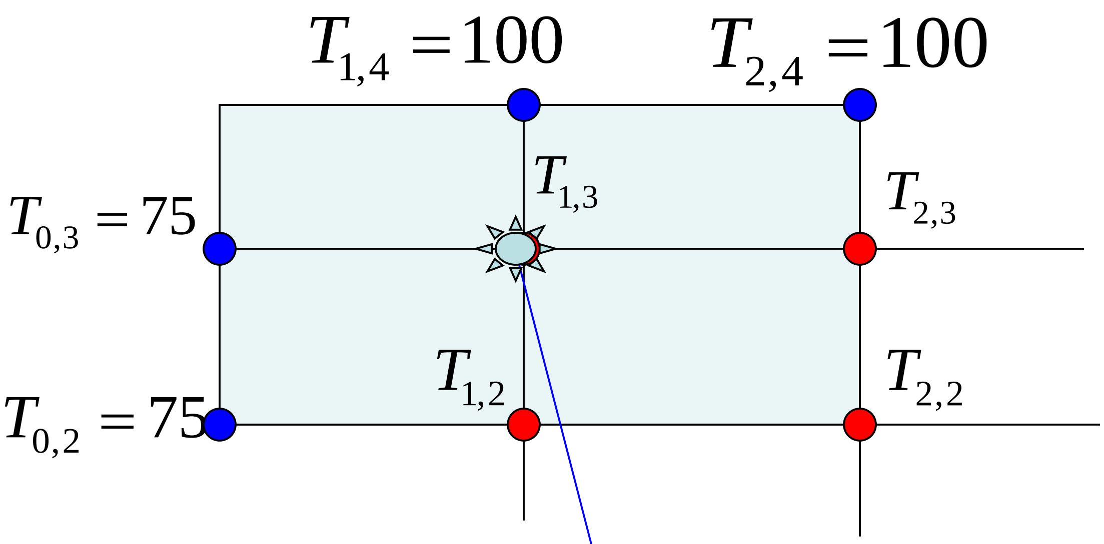
The sheet is divided to 5X5 grids.

Example: heated plate



First Equation

- Known (blue)
- To be determined (red)

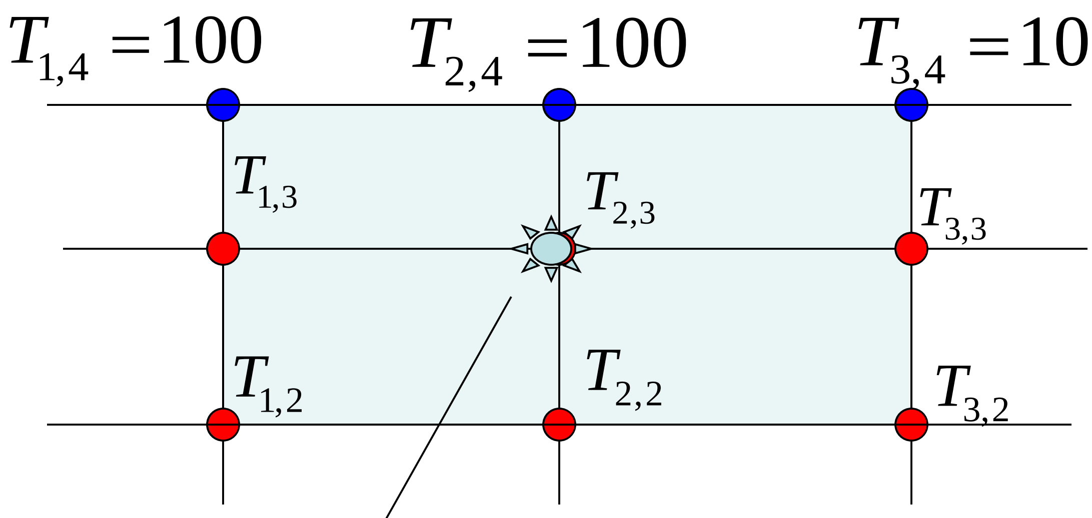


$$T_{0,3} + T_{1,4} + T_{1,2} + T_{2,3} - 4T_{1,3} = 0$$

$$75 + 100 + T_{1,2} + T_{2,3} - 4T_{1,3} = 0$$

Another Equation

- Known
- To be determined



$$T_{1,3} + T_{2,4} + T_{3,3} + T_{2,2} - 4T_{2,3} = 0$$

$$T_{1,3} + 100 + T_{3,3} + T_{2,2} - 4T_{2,3} = 0$$

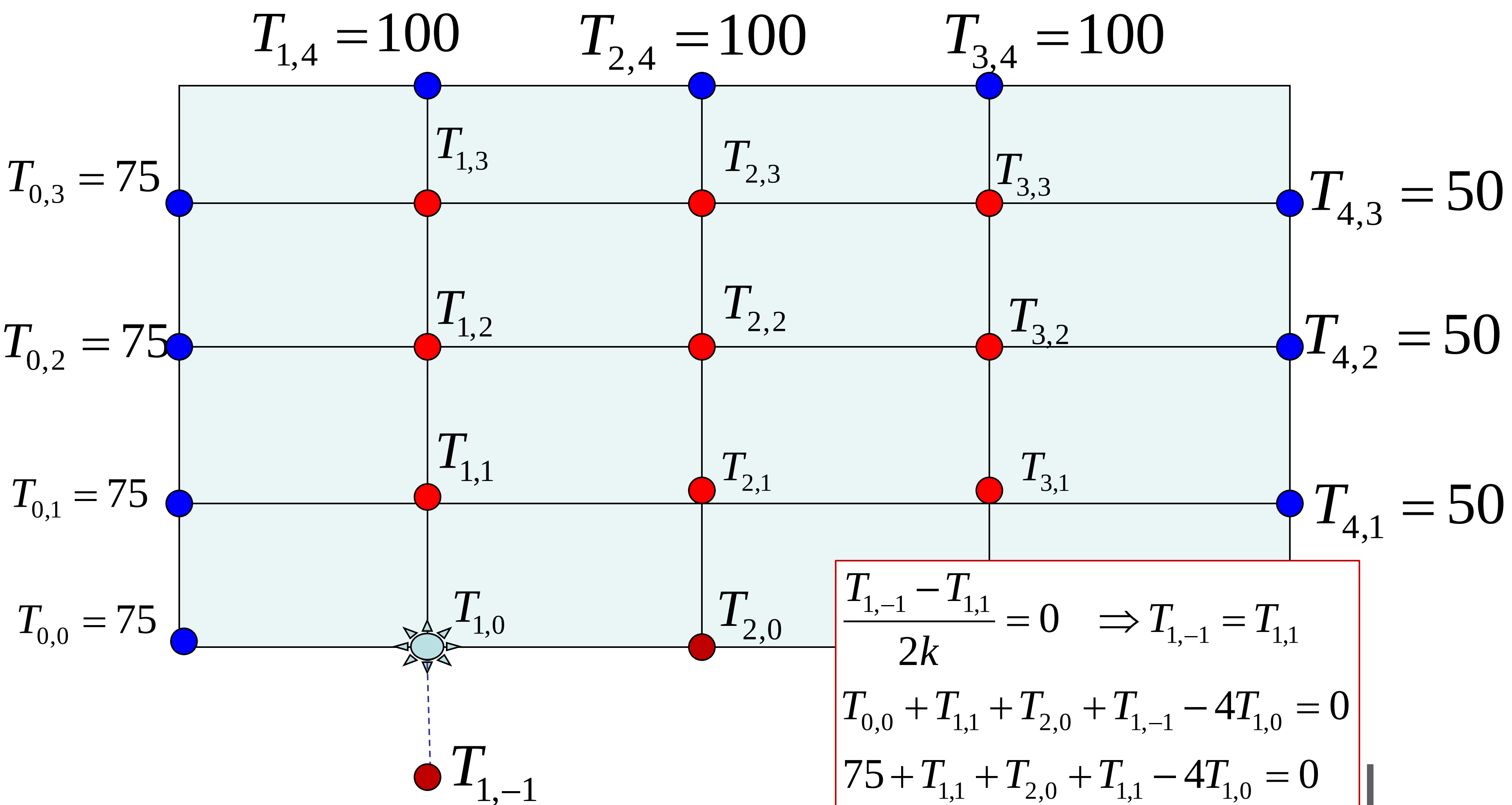
Solve the linear system

$$\begin{pmatrix} 4 & -1 & 0 & -1 & & & & & \\ -1 & 4 & -1 & 0 & -1 & & & & \\ 0 & -1 & 4 & 0 & 0 & -1 & & & \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & & \\ & -1 & 0 & -1 & 4 & -1 & 0 & -1 & \\ & & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ & & & -1 & 0 & 0 & 4 & -1 & 0 \\ & & & & -1 & 0 & -1 & 4 & -1 \\ & & & & & -1 & 0 & -1 & 4 \end{pmatrix} \begin{pmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \\ T_{1,2} \\ T_{2,2} \\ T_{3,2} \\ T_{1,3} \\ T_{2,3} \\ T_{3,3} \end{pmatrix} = \begin{pmatrix} 75 \\ 0 \\ 50 \\ 75 \\ 0 \\ 50 \\ 175 \\ 100 \\ 150 \end{pmatrix}$$

Example: Heated Plate with an Insulated Edge

- Known
- To be determined

Neumann boundary condition: the lower edge is insulated, derivative is 0



$$\frac{T_{1,-1} - T_{1,1}}{2k} = 0 \quad \Rightarrow T_{1,-1} = T_{1,1}$$

$$T_{0,0} + T_{1,1} + T_{2,0} + T_{1,-1} - 4T_{1,0} = 0$$

$$75 + T_{1,1} + T_{2,0} + T_{1,1} - 4T_{1,0} = 0$$

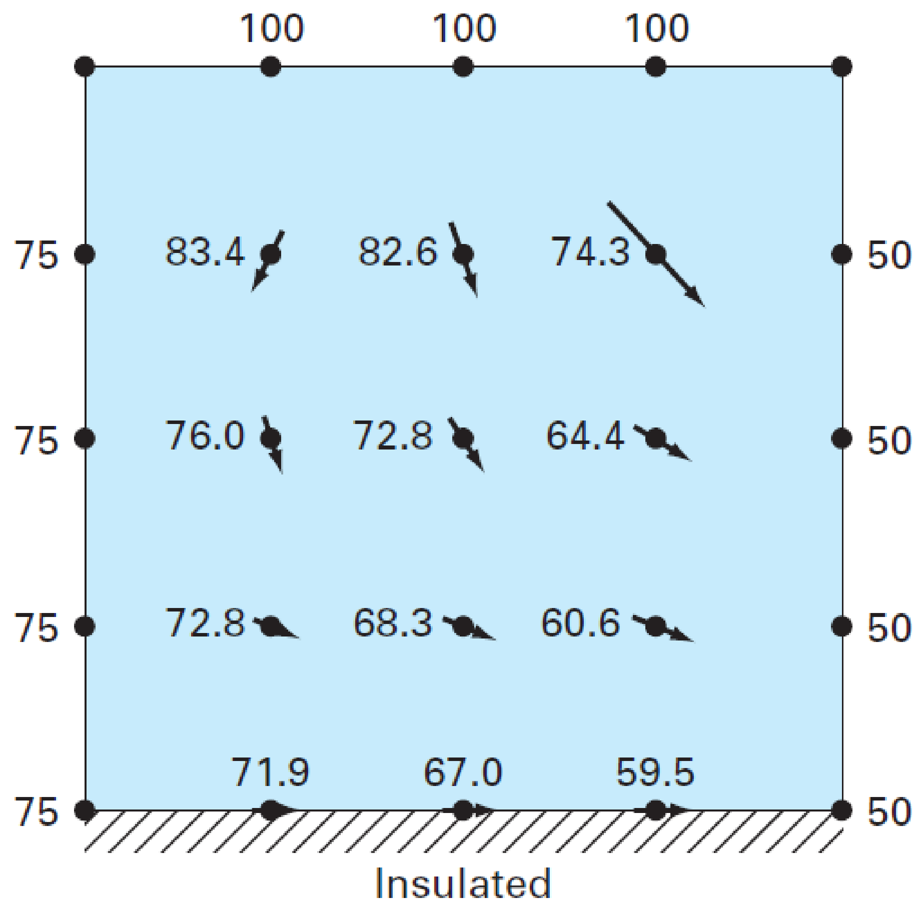
$$75 + 2T_{1,1} + T_{2,0} - 4T_{1,0} = 0$$

Example: Heated Plate with an Insulated Edge

$$
\begin{bmatrix}
4 & -1 & & -2 & & & & & & & & \\
-1 & 4 & -1 & & -2 & & & & & & & \\
& -1 & 4 & & & -2 & & & & & & \\
-1 & & & 4 & -1 & & -1 & & & & & \\
& -1 & & -1 & 4 & -1 & & -1 & & & & \\
& & -1 & & -1 & 4 & & & -1 & & & \\
& & & -1 & & & 4 & -1 & & -1 & & \\
& & & & -1 & & -1 & 4 & -1 & & -1 & \\
& & & & & -1 & & -1 & 4 & & & -1 \\
& & & & & & -1 & & & 4 & -1 & \\
& & & & & & & -1 & & -1 & 4 & -1 \\
& & & & & & & & -1 & & -1 & 4
\end{bmatrix}
\begin{Bmatrix} T_{10} \\ T_{20} \\ T_{30} \\ T_{11} \\ T_{21} \\ T_{31} \\ T_{12} \\ T_{22} \\ T_{32} \\ T_{13} \\ T_{23} \\ T_{33} \end{Bmatrix}
=
\begin{Bmatrix} 75 \\ 0 \\ 50 \\ 75 \\ 0 \\ 50 \\ 75 \\ 0 \\ 50 \\ 175 \\ 100 \\ 150 \end{Bmatrix}
$$

- Note that because of the derivative boundary condition, the matrix is increased to 12 × 12 in contrast to the 9 × 9 system to account for the three unknown temperatures along the plate’s lower edge.

Temperature and flux distribution for a heated plate subject to fixed boundary conditions except for an insulated lower edge.



$$A = \begin{bmatrix} B & -I & & & & \\ -I & B & -I & & & \\ & & \dots & \dots & & \\ & & & -I & B & -I \\ & & & & -I & B \end{bmatrix}, \quad B = \begin{bmatrix} 4 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & & \dots & \dots & & \\ & & & -1 & 4 & -1 \\ & & & & -1 & 4 \end{bmatrix}$$

$$A \in R^{(n-1)^2 x (n-1)^2}$$

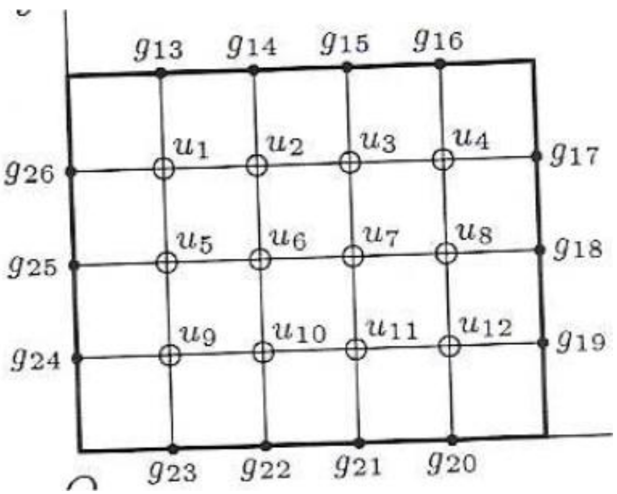
$$cond_2(A) = |\lambda_{\max}| / |\lambda_{\min}| = O(h^{-2})$$

The matrix A is very sparse, block tridiagonal (for the above numbering) and SPD.

Caution: convergence of iterative solvers deteriorates as the mesh is refined

The matrix structure depends on the ordering of the points in the grid

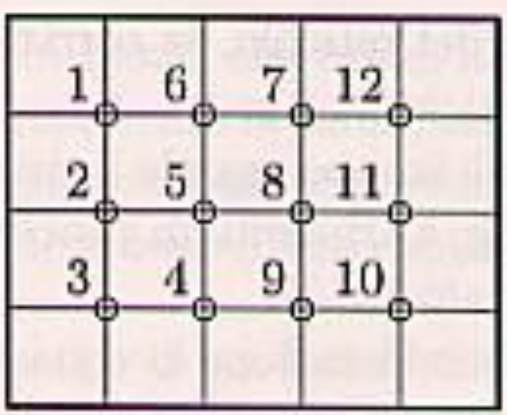
(1) **Natural row-wise ordering**



$$A = \left(\begin{array}{cccc|cccc|cccc}
4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
\hline
-1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 \\
\hline
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4
\end{array}\right)$$

Block Tridiagonal

(2) **Zig-Zag ordering**



$$A = \left(\begin{array}{ccc|ccc|ccc|ccc}
4 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & -1 & 4 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 4 & -1 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 4
\end{array}\right)$$

Ordering the unknowns and equations

Given a spatial grid m x m.
The linear system has a matrix of dimension $m^2 \times m^2$ that is very sparse as each equation involves at most 5 unknowns, and then each row has at most 5 coefficients different from zero and the matrix has nonzero elements only on 5 diagonals.
The diagonals have an offset of more distant m^d-1 (d = number of spatial dimensions) from the main diagonal, very bad for direct methods as Gaussian elimination. We use iterative methods.

Theorem. **If a matrix $A \in \mathbf{R}^{nxn}$ strictly diagonal dominant, is such that**

$$a_{ij} \le 0 \quad i \ne j \quad \text{and} \quad a_{ii} > 0 \quad i = 1, 2, \ldots, n$$

then A is an M-matrix.

Poisson Problem
solving the linear system

Iterative Gauss-Seidel method

At iteration k:

$$x^{(k+1)} = D^{-1}(b - Lx^{(k+1)} - Ux^{(k)})$$

$$-u_{i,j-1} - u_{i-1,j} + 4u_{i,j} - u_{i+1,j} - u_{i,j+1} = h^2 f_{ij}$$

! We don't need to form the matrix, the computation is row by row

Poisson Problem
solving the linear system

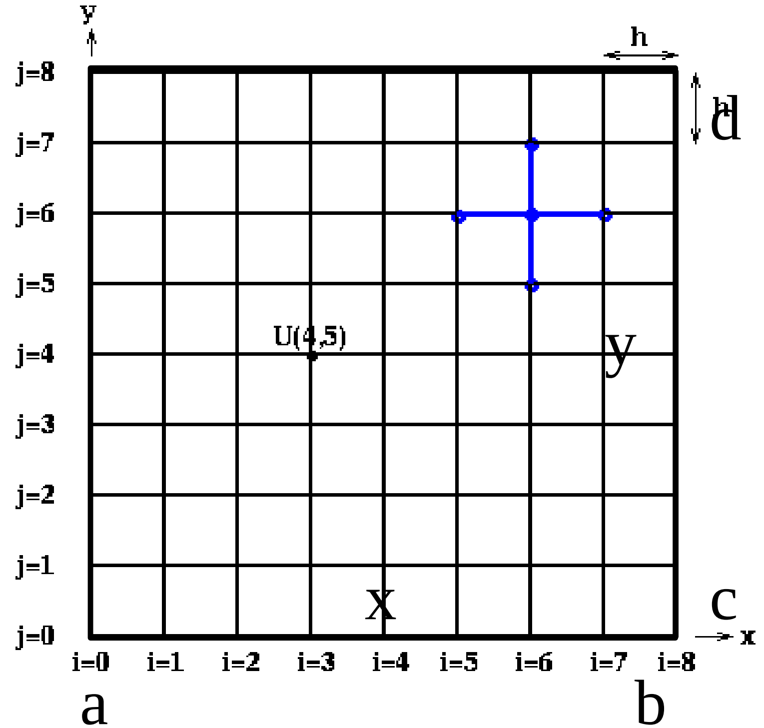
$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$

$$
\begin{array}{l}
\text{Gauss – Seidel algorithm for the linear system} \\
\;\; for \quad k = 1, 2, \ldots \\
\qquad for \quad i = 2, .., N+1 \\
\qquad\qquad for \quad j = 2, .., N+1 \\
\qquad\qquad\qquad u^{(k+1)}{}_{i,j} = \dfrac{1}{4}\left(u^{(k+1)}{}_{i-1,j} + u^{(k)}{}_{i+1,j} + u^{(k+1)}{}_{i,j-1} + u^{(k)}{}_{i,j+1} + h^2 f_{ij}\right) \\
\qquad\qquad end \\
\qquad end \\
end
\end{array}
$$

Poisson Problem + reaction term

$$\begin{cases} -\Delta u(x,y) + cu(x,y) = f(x,y) \\ u(a,y) = g_1(y) \\ u(b,y) = g_2(y) \\ u(x,c) = g_3(x) \\ u(x,d) = g_4(x) \end{cases}$$

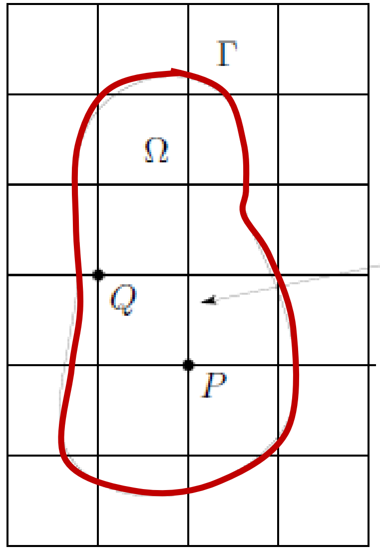
$c \geq 0$



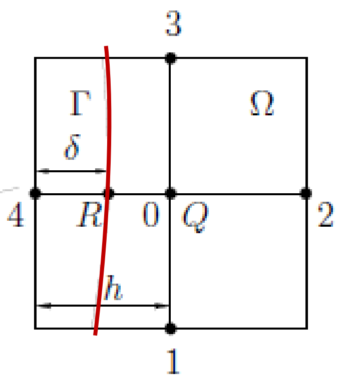
$$\frac{-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1}}{h^2} + c\,u_{ij} = f_{ij}$$

$$-u_{i-1,j} - u_{i+1,j} + (4 + h^2 c_{i,j})u_{i,j} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$

Treatment of Irregular Boundaries



curvilinear boundary



stencil of Q

$$u = g_0 \quad su\ \Gamma$$

$$-\frac{u_1 + u_2 - 4u_0 + u_3 + u_4}{h^2} = f_0$$

Linear Interpolation

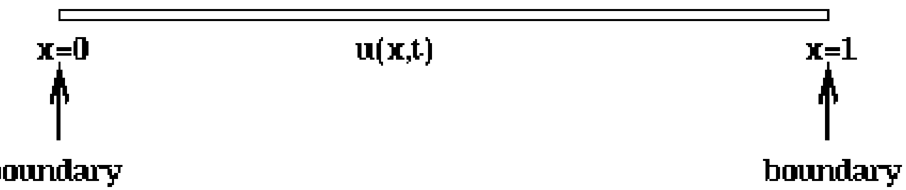
$$u(R) = \frac{u_4(h-\delta) + u_0\delta}{h} = g_0(R) \quad \Rightarrow u_4 = -u_0\frac{\delta}{h-\delta} + g_0(R)\frac{\mathrm{h}}{\mathrm{h}\text{-}\delta}$$

substitution yields

$$-u_1 - u_2 + (4 + \frac{\delta}{h-\delta})u_0 - u_3 = h^2 f_0 + g_0(R)\frac{h}{h-\delta}$$

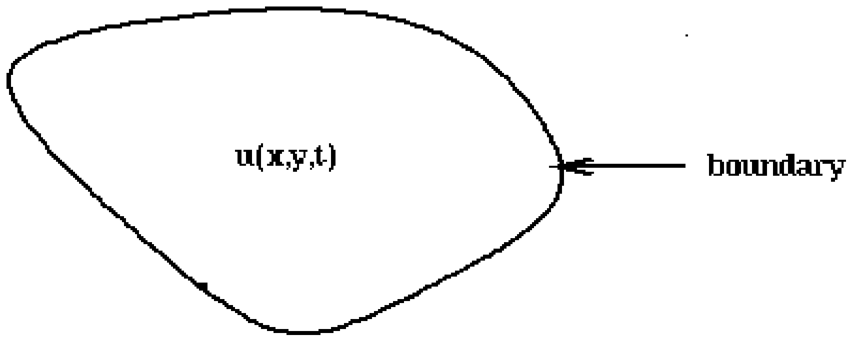
PDE - Heat equations multidimensional problems

1 – Dimensional Heat Equation



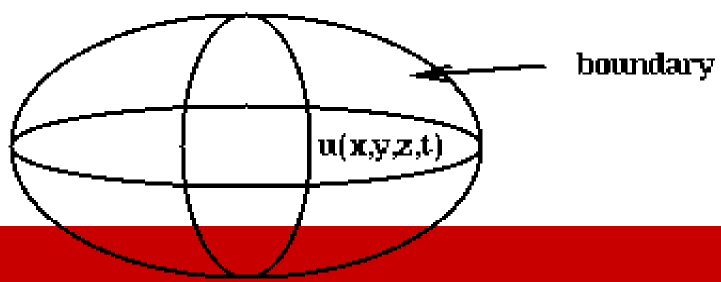
$$\frac{d\,u(x,t)}{dt} = C\left(\frac{d^{\wedge}2\,u(x,t)}{d\,x^{\wedge}2}\right)$$

2 – Dimensional Heat Equation



$$\frac{d\,u(x,y,t)}{dt} = C\left(\frac{d^{\wedge}2\,u(x,y,t)}{d\,x^{\wedge}2} + \frac{d^{\wedge}2\,u(x,y,t)}{d\,y^{\wedge}2}\right)$$

3 – Dimensional Heat Equation



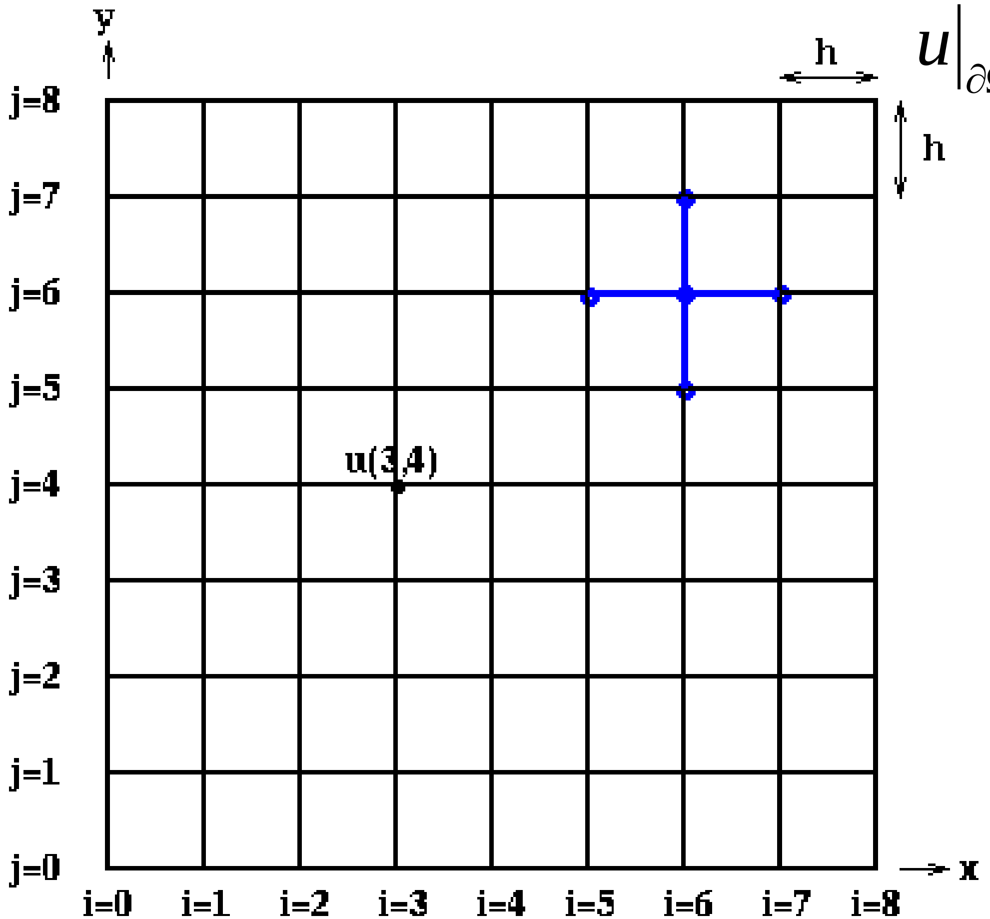
$$\frac{d\,u(x,y,z,t)}{dt} = C\left(\frac{d^{\wedge}2\,u(x,y,z,t)}{d\,x^{\wedge}2} + \frac{d^{\wedge}2\,u(x,y,z,t)}{d\,y^{\wedge}2} + \frac{d^{\wedge}2\,u(x,y,z,t)}{d\,z^{\wedge}2}\right)$$

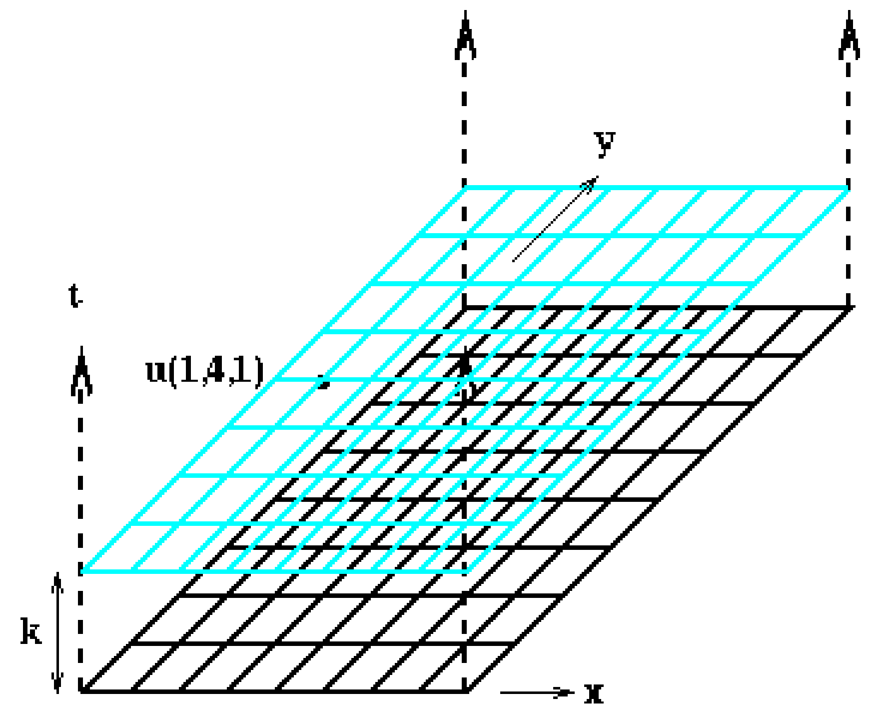
PDE - 2D Heat equations

$$u_t = c\Delta u = c(u_{xx} + u_{yy}) \quad \text{in } \Omega \subseteq \mathrm{R}^2$$

$$u(x,y,0) = u_0(x,y)$$

$$u\big|_{\partial\Omega} = \bar{u}(x,y)$$





Method of lines (MOL)

- Consider a **semidiscretization in space** of the PDE that provides a large system of ODEs with each component of the system that corresponds to the solution in a certain grid point as a function of time.

-Then **solve the system of ODEs** using one of the methods already seen for ODEs.

- Then, apply the **BC**.

This method also allows you to understand the theory for stability for evolutionary PDEs in terms of stability for time dependent ODEs.

We know how to analyze the (absolute) stability of methods for ODEs

MOL: 2D Heat Equation
space discretization

Use the 5-points stencil for the Laplacian about the point (i,j)

$$\nabla_5^2 u_{i,j} = \left[\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \right] + \left[\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2} \right]$$

Semi-discretization about the point (i,j) (space only):

$$(u_{ij})_t = \nabla_5^2 u_{ij}(t) \quad i,j = 1,..,N-1$$

System of (N-1)x(N-1) ODEs for the unknowns $u_{ij}(t)$

$$U'(t) = LU(t) + b(t) \qquad L = L_x + L_y$$

L pentadiagonal matrix, b vector for BC

MOL: time discretization
Explicit Euler Method

$$U^{n+1} = U^n + k\,f(U^n)$$

$$U^{n+1} = U^n + k\frac{1}{h^2}LU^n = (I + \frac{k}{h^2}L)U^n$$

k time step

$$h = h_x = h_y$$

$$u_{ij}^{n+1} = u_{ij}^n + k\left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h_y^2}\right)$$

The method is stable for

$$k\lambda_L \in RA \quad |1 + \lambda_L k(\frac{1}{h_x^2} + \frac{1}{h_y^2})| \le 1 \quad \forall \lambda_L = eig(L)$$

$$-2 \le -4k(\frac{1}{h_x^2} + \frac{1}{h_y^2}) \le 0 \quad \to k(\frac{1}{h_x^2} + \frac{1}{h_y^2}) \le \frac{1}{2}$$

If $h_x=h_y=h$ then $k \le \frac{h^2}{4}$ in general $k \le \frac{\min(h_x^2, h_y^2)}{4 * c}$

The stability for convergence depends on the absolute stability, and on the shape of the stability region for the time-discretization. This is called strong stability.

$$U_{j+1} = A(k)U_j + b_j$$

But note that this is not necessary for Lax–Richtmyer stability :

$$\exists C_T > 0 \quad s.t.$$

$$\left\| A(k)^j \right\| \leq C_T$$

$$\forall k > 0, \textit{ and integers } j \textit{ for which } kj \leq T$$

MOL

Explicit Euler Method

$$U^{n+1} = (I + r\,L)U^{n}$$

Conditioned stability $k \le \frac{1}{8}\frac{(h_x)^2 + (h_y)^2}{c}$

Implicit Euler Method

$$(I - r\,L)U^{n+1} = U^{n}$$

Involve a large linear system,
computationally expensive,
unconditionally stable

Local Truncation error $O(k + h_x^2 + h_y^2)$

MOL: time discretization
Crank-Nicolson Method

$$U^{n+1} = U^n + \frac{k}{2}\frac{1}{h^2}(LU^n + LU^{n+1})$$

$$U^{n+1} = U^n + \frac{k}{2}(f(U^n) + f(U^{n+1}))$$

k time step

$$(I - \frac{k}{2}\frac{1}{h^2}L)U^{n+1} = (I + \frac{k}{2}\frac{1}{h^2}L)U^n$$

$$(I - \frac{r}{2}L)U^{n+1} = (I + \frac{r}{2}L)U^n$$

The method is implicit, we need to solve a system of equations for each time step , the matrix is large and sparse, and it has the same nonzero structure as for the elliptic system

The method is stable.

Stability of the Crank-Nicolson Method

$$(I-\frac{r}{2}L)U^{n+1}=(I+\frac{r}{2}L)U^{n}$$

the eigenvalues of $(I - \frac{r}{2}(L_x+L_y))$ are:

$$\lambda_{p,q}=1-\frac{k}{h^2}[(\cos(p\pi h)-1)+(\cos(q\pi h)-1)] \qquad p,q=1,2,..,N-1, \quad h=1/N$$

$cond(A)=O(\frac{k}{h^2})$ smaller than the $cond(L)=O(\frac{1}{h^2})$

The CN method for ODEs is A-stable (Ra is the negative part of the complex plane). Thus CN is stable for each k>0

Local Truncation Error

$$O(k^2+h_x{}^2+h_y{}^2)$$

ADI Method (Douglas, Rachford, 1956) (Alternating-Direction Implicit)

A disadvantage of the Crank–Nicolson method is that the matrix in the equation is banded with a band width that is generally quite large. Modify the CN method

$$(I - \frac{r}{2}L)U^{n+1} = (I + \frac{r}{2}L)U^{n}$$

$$(I - \frac{r}{2}L_x - \frac{r}{2}L_y)U^{n+1} = (I + \frac{r}{2}L_x + \frac{r}{2}L_y)U^{n} \qquad (*)$$

The idea behind the ADI method is to split (*) into two

$$(1 - \frac{r}{2}L_x)(1 - \frac{r}{2}L_y)U^{j+1} = (1 + \frac{r}{2}L_x)(1 + \frac{r}{2}L_y)U^{j} \qquad (**)$$

Extra term

$$(1 + \frac{r}{2}L_x)(1 + \frac{r}{2}L_y) = (1 + \frac{r}{2}L_x + \frac{r}{2}L_y + \frac{r}{2}\frac{r}{2}L_x L_y)$$

ADI Method (Alternating-Direction Implicit)

$$(1-\frac{r}{2}L_x)(1-\frac{r}{2}L_y)U^{j+1} = (1+\frac{r}{2}L_x)(1+\frac{r}{2}L_y)U^{j} \qquad (**)$$

$$(1+\frac{r}{2}L_x)(1+\frac{r}{2}L_y) = (1+\frac{r}{2}L_x+\frac{r}{2}L_y+\frac{r}{2}\frac{r}{2}L_xL_y)$$

(**) is equivalent to

Extra term

$$(I-\frac{r}{2}L_x)U^{j+1/2} = (I+\frac{r}{2}L_y)U^{j}$$

$$(I-\frac{r}{2}L_y)U^{j+1} = (I+\frac{r}{2}L_x)U^{j+1/2}$$

Solution obtained by two decoupled tridiagonal systems to solve in each step

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