Matrix representation of physical systems- Associated errors

Somnath Roy

Department of Mechanical Engineering

Matrix representation of physical systems

System of linear equations with multiple variables can be expressed as matrix equation

Physical systems with multiple degree of freedom can give matrix equations

Rate equations in a continuum can be converted to matrix equations by Taylor series like approximations

Continuum ideally have infinite degree of freedom, but can be approximated with a large finite number of discrete variables.

Discretization – journey from analytical to numerical

Differential equation -> Difference equations (addition-subtraction operations)

One-dimensional steady heat conduction

$$k\frac{d^2T}{dx^2}=0$$

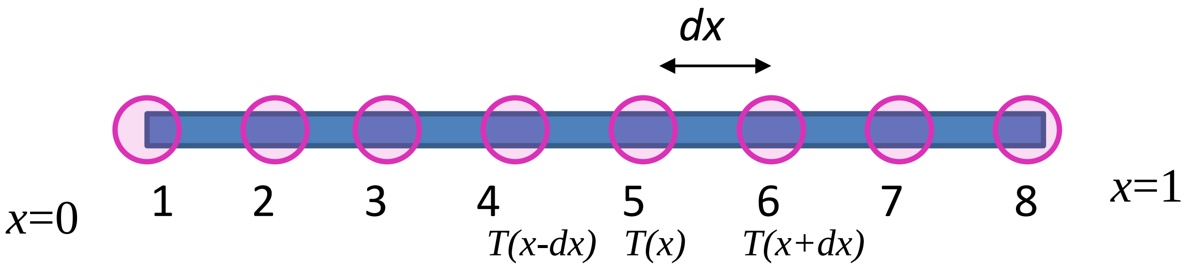
Steady heat flow, constant conductivity

$x=0$ $x=1$

Boundary conditions

$$\begin{cases} T(x=0)=0 \\ T(x=1)=1 \end{cases}$$

Discretization – Finite difference method



uniform mesh

Taylor series expansion

$$T(x+dx) = T(x) + \frac{d\ T}{dx} * dx + \frac{d^2T}{dx^2} * \frac{(dx)^2}{2!} + \frac{d^3T}{dx^3} * \frac{(dx)^3}{3!} + \frac{d^4T}{dx^4} * \frac{(dx)^4}{4!} + \ldots\ldots. \qquad \text{(A)}$$

$$T(x-dx) = T(x) - \frac{d\ T}{dx} * dx + \frac{d^2T}{dx^2} * \frac{(dx)^2}{2!} - \frac{d^3T}{dx^3} * \frac{(dx)^3}{3!} + \frac{d^4T}{dx^4} * \frac{(dx)^4}{4!} + \ldots\ldots. \qquad \text{(B)}$$

Adding (A) and (B)

$$T(x+dx) = T(x) + \frac{dT}{dx} * dx + \frac{d^2T}{dx^2} * \frac{(dx)^2}{2!} + \frac{d^3T}{dx^3} * \frac{(dx)^3}{3!} + \frac{d^4T}{dx^4} * \frac{(dx)^4}{4!} + \ldots\ldots. \qquad \text{(A)}$$

$$T(x-dx) = T(x) - \frac{dT}{dx} * dx + \frac{d^2T}{dx^2} * \frac{(dx)^2}{2!} - \frac{d^3T}{dx^3} * \frac{(dx)^3}{3!} + \frac{d^4T}{dx^4} * \frac{(dx)^4}{4!} + \ldots\ldots. \qquad \text{(B)}$$

$$T(x+dx) + T(x-dx) = 2*T(x) + 0 + 2*\frac{d^2T}{dx^2} * \frac{(dx)^2}{2!} + 0 + 2*\frac{d^4T}{dx^4} * \frac{(dx)^4}{4!}$$

$$\frac{d^2T}{dx^2} = \underbrace{\frac{T(x+dx) - 2*T(x) + T(x-dx)}{(dx)^2}}_{\text{approximation}} + \underbrace{2*\frac{d^4T}{dx^4} * \frac{(dx)^2}{4!} + \ldots\ldots \;(\text{higher orders of dx})}_{\text{error (of order 2)}}$$

Discretization error

$2 * \frac{d^4T}{dx^4} * \frac{(dx)^2}{4!}$ is the largest term in the error.

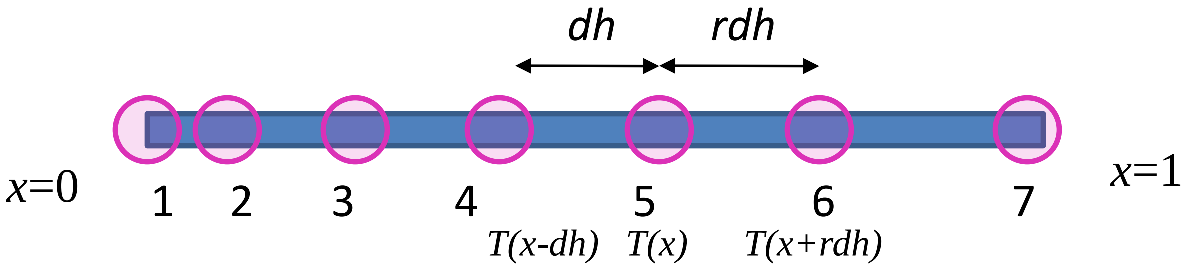
The rod has a length L=1

dx=1/N <1

So, $(dx)^2$ <<1

As we will increase number of grid points, error will be smaller

Non-Uniform mesh



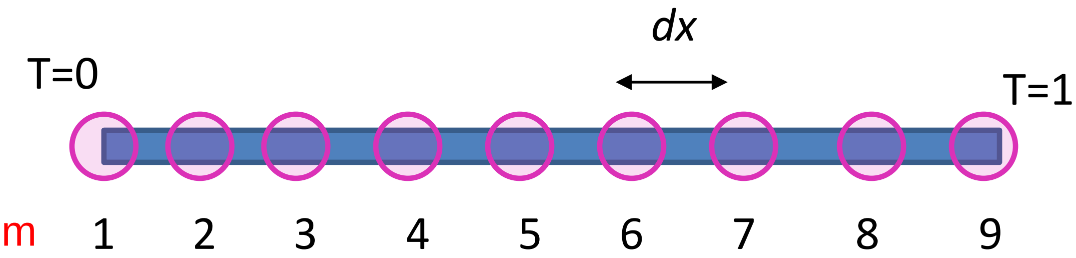
$$T(x+rdh)=T(x)+r\frac{dT}{dx}*dh+r^2\frac{d^2T}{dx^2}*\frac{(dh)^2}{2!}+r^3\frac{d^3T}{dx^3}*\frac{(dh)^3}{3!}+r^4\frac{d^4T}{dx^4}*\frac{(dh)^4}{4!}+\ldots\ldots \qquad (A)$$

$$T(x-dh)=T(x)-\frac{dT}{dx}*dh+\frac{d^2T}{dx^2}*\frac{(dh)^2}{2!}-\frac{d^3T}{dx^3}*\frac{(dh)^3}{3!}+\frac{d^4T}{dx^4}*\frac{(dh)^4}{4!}+\ldots\ldots \qquad (B)$$

$A+rB::$

$$\frac{d^2T}{dx^2}=\frac{T(x+rdh)-(1+r)*T(x)+rT(x-dh)}{\left(r/2\right)(1+r)(dh)^2}+O(dh)$$

Finite difference method- equation system



Uniform mesh

$$k\frac{d^2T}{dx^2} = 0$$

$$\Rightarrow \frac{d^2T}{dx^2} = \frac{T(x+dx) - 2*T(x) + T(x-dx)}{(dx)^2} = 0$$

with error of order (dx^2)

T=0

$$T_1 - 2T_2 + T_3 = 0$$

$$T_2 - 2T_3 + T_4 = 0$$

.

.

$$T_6 - 2T_7 + T_8 = 0$$

$$T_7 - 2T_8 + T_9 = 0$$

T=1

So, a set of linear equations are obtained for temperature at points 2,3,....8

Matrix representation

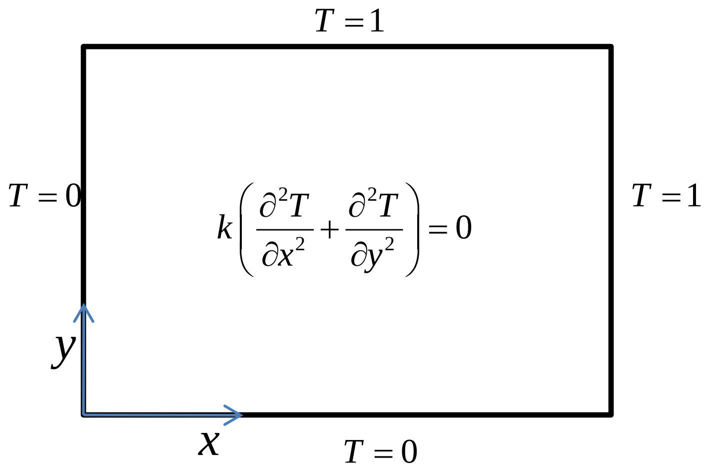
$$
\begin{bmatrix}
-2 & 1 & 0 & 0 & . & . & \\
1 & -2 & 1 & . & & & \\
0 & 1 & -2 & 1 & & & \\
0 & 0 & 1 & -2 & 1 & & \\
. & . & & 1 & -2 & 1 & \\
 & & & & 1 & -2 & 1 \\
 & & & & & 1 & -2
\end{bmatrix}
\begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}
$$

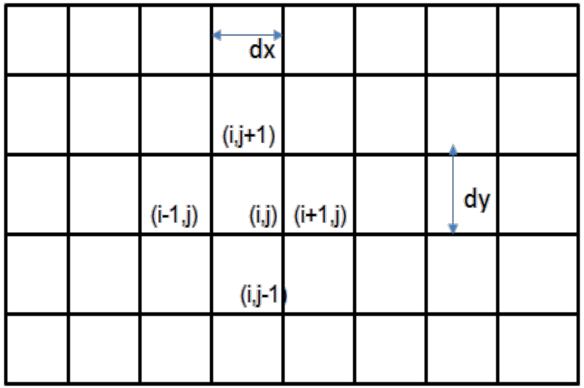
Banded sparse matrix—Tridiaginal matrix

It is important to have boundary conditions

If both boundary has T=0, trivial solution T=0 at all points are obtained

Two dimensional problem





$$\frac{T_{i-1,j}-2T_{i,j}+T_{i+1,j}}{(dx)^2}+\frac{T_{i,j-1}-2T_{i,j}+T_{i,j+1}}{(dy)^2}=0$$

with error of order $O\left(dx^2, dy^2\right)$

Can be expressed as a matrix equation after sequential numbering of (i,j) points

Finite difference method

- Method based on Taylor series expression of difference terms
- Unknown variable is solved at fixed number of pre-defined discrete points or nodes
- Error is bounded by the truncated term of difference approximation
- This error is a function of spacing between consecutive nodes or grid-spacing

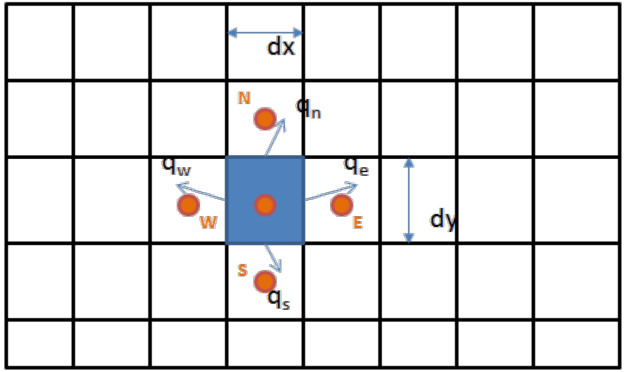
Finite difference method

- Banded diagonal matrix is obtained
- For Laplace/Poisson equation gives tridagonal matrix in 1D
- Pentadiagonal in 2D and septadiagonal in 3D!
- For uniform mesh, matrix is symmetric

$$\begin{bmatrix} -2 & 1 & 0 & 0 & . & . & \\ 1 & -2 & 1 & . & & & \\ 0 & 1 & -2 & 1 & & & \\ 0 & 0 & 1 & -2 & 1 & & \\ . & . & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \\ & & & & & 1 & -2 \end{bmatrix} \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}$$

Finite volume method

PDEs are expressed as flux differenced between two surfaces

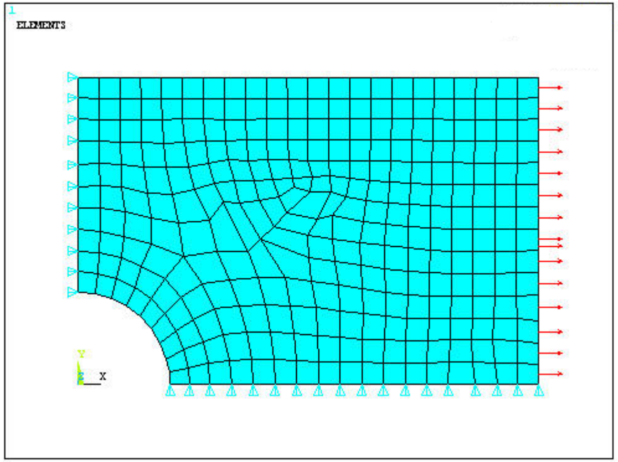


Heat generation: $Q.dx.dy.1 = (q_n + q_s)*dx.1 + (q_w + q_e)*dy.1$

Or, $Q=0= (q_n + q_s)/dy + (q_w + q_e)/dx$

$$0 = ((T_N - T_P)/dy + (T_S - T_P)/dy)/dy + ((T_E - T_P)/dx + (T_W - T_P)/dx)/dx$$

Finite element method



- Entire domain is discretized into a number of smaller elements
- A trial/test solution is assumed within each element
- Error is estimated from the trial solution
- Total error inside each element is integrated and the integral is minimized to get a trial solution with least error, i.e., maximum accuracy

Advantage: Mathematically sound, element shape can vary, complex geometries can be easily handled

Disadvantage: Difficult mathematics, discretization along flow direction is difficult

Errors associated

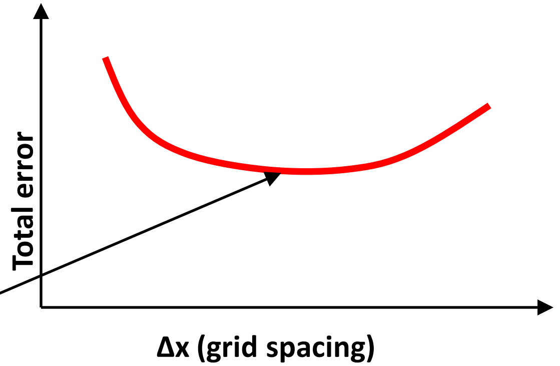
- Discretization error (due to difference approximation, vanishes as grid-spacing decreases or no. of discrete point (*N*) increases)

- Round-off error (precision of the computer to round of after few decimal places)

increases with increase in no of calculation steps or with higher no of discrete points (*N*)

22/7=3.142857

Optimal solution

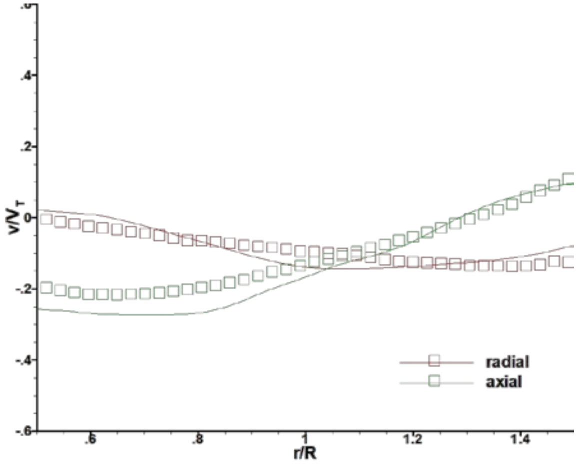


$\Delta x = L/N$

Grid independent solution
preferred grid size

Validation and verification

Validation: Comparison with available experimental/ analytical results



Verification: verifying the accuracy of the code error is 2^{nd} (or higher) order function of grid-spacing