Exercises : Chapter 5-3, PDE problems, Part 3

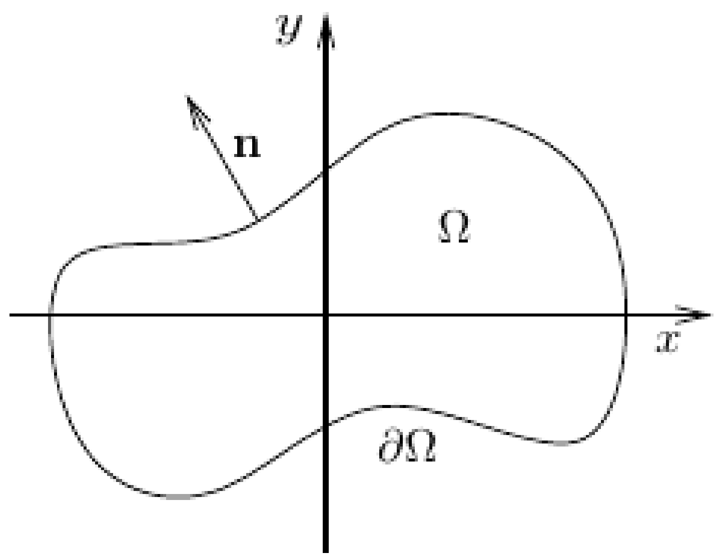
Saravana P T, Date : 24/11/2017, 7th semester , Computational physics

Due : 24/11/2017 before 9 PM

1 What is PDE

A partial differential equation (PDE) is an equation for some quantity u (dependent variable) which depends on the independent variables ($x_1, x_2, ..., x_n$), and involves derivatives of u with respect to at least some of the independent variables.

$$F(x_1, ..., x_n, \partial_{x_1} u, ..., \partial_{x_n} u, \partial^2_{x_1} u, \partial^2_{x_1 x_2} u, ..., \partial^n_{x_1 ... x_n} u) = 0. \tag{1}$$



In applications x_i are often space variables (e.g. x, y, z) and a solution may be required in some region Ω of space. In this case there will be some conditions to be satisfied on the boundary $\partial\Omega$; these are called boundary conditions (BC's).

Also in applications, one of the independent variables can be time (t say), then there will be some initial conditions (IC's) to be satisfied (i.e., u is given at t = 0 everywhere in Ω).

Again in applications, systems of PDEs can arise involving the dependent variables $u_1, u_2, u_3, ..., u_m$,$m \geq 1$ with some (at least) of the equations involving more than one u_i.

The order of the PDE is the order of the highest (partial) differential coefficient in the equation. As with ordinary differential equations (ODE's) it is important to be able to distinguish between linear and nonlinear equations.

A linear equation is one in which the equation and any boundary or initial conditions do not include any product of the dependent variables or their derivatives; an equation that is not linear is a nonlinear equation.
First order PDE of linear form

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \tag{2}$$

Second order PDE of linear form

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = \psi(x, y) \tag{3}$$

A nonlinear equation is semilinear if the coefficients of the highest derivative are functions of the independent variables only.

$$(x+3)\frac{\partial u}{\partial x} + xy^2\frac{\partial u}{\partial y} = u^3 \tag{4}$$

Second order PDE of linear form

$$x\frac{\partial^2 u}{\partial x^2} + (xy + y^2)\frac{\partial^2 u}{\partial y^2} + u\frac{\partial u}{\partial x} + u^2\frac{\partial u}{\partial y} = u^4 \tag{5}$$

A nonlinear PDE of order m is quasilinear if it is linear in the derivatives of order m with coefficients depending only on x, y, . . . and derivatives of order $< m$.

$$[1 + (\frac{\partial^2 u}{\partial y^2})^2]\frac{\partial^2 u}{\partial x^2} - 2\frac{\partial u}{\partial x}\frac{\partial u}{\partial y}\frac{\partial^2 u}{\partial x \partial y} + [1 + (\frac{\partial^2 u}{\partial x^2})^2]\frac{\partial^2 u}{\partial y^2} = 0 \tag{6}$$

Waves propagation, etc.

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u \tag{7}$$

Heat conduction and distribution, etc

$$\frac{\partial u}{\partial t} = k\nabla^2 u \tag{8}$$

1.1 PDE's describe the behavior of many phenomena

- Waves on a string, sound waves, waves on stretch membranes, electromagnetic waves, etc.
- Fluid flow (air or liquid)
- Air around wings, helicopter blade, atmosphere
- Water in pipes or porous media,

- Material transport and diffusion in air or water
- Weather: large system of coupled PDE's for momentum, pressure, moisture, heat.
- Vibration
- Mechanics of solids: stress-strain in material, machine part, structure
- Heat flow and distribution
- Electric fields and potentials
- Diffusion of chemicals in air or water
- Electromagnetism and quantum mechanics

1.2 Objective of this Unit

This part of the chapter will cover the following learning objectives,

1) To distinguish between the 3 classes of 2nd order, linear PDE's. Know the physical problems each class represents and the physical/mathematical characteristics of each.

2) To describe the differences between finite-difference and finite-element methods for solving PDE's.

3)To solve Elliptical (Laplace/Poisson) PDE's using finite differences.

4) To solve Parabolic (Heat/Diffusion) PDE's using finite differences.

$$A\frac{\partial^2 U}{\partial x^2} + B\frac{\partial^2 U}{\partial x \partial y} + C\frac{\partial^2 U}{\partial z^2} + D = 0 \tag{9}$$

$$U(x,y), B(x,y), C(x,y), D(x,y,u,,) \tag{10}$$

The PDE is nonlinear if A, B or C include u, $\frac{\partial U}{\partial x}$, $\frac{\partial U}{\partial y}$, $\frac{\partial U}{\partial z}$, or if D is nonlinear in u and/or its first derivatives.
Classification of PDE follows under the following geometrical conditions:

- $B^2 - 4AC < 0 \rightarrow$ Elliptic (e.g. Laplace Eq.)
- $B^2 - 4AC = 0 \rightarrow$ Parabolic (e.g. Heat Eq.)
- $B^2 - 4AC > 0 \rightarrow$ Hyperbolic (e.g. Wave Eq.)

Each category describes different phenomena. Mathematical properties correspond to those phenomena.

2 Elliptic Equations $(B^2 - 4AC < 0)$ [steady-state in time]

Elliptic equations are typically associated with steady-state behavior. The archetypal elliptic equation is Laplaces equation.

$$\nabla^2 u = 0 \tag{11}$$

and describes, steady, irrational flows, electrostatic potential in the absence of charge, equilibrium temperature distribution in a medium.
Because of their physical origin, elliptic equations typically arise as boundary value problems (BVPs). Solving a BVP for the general elliptic equation

$$L[u] = \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x_i} + cu = F \tag{12}$$

recall: all the eigenvalues of the matrix $A = (aij), i, j = 1n$, are non-zero and have the same sign is to find a solution u in some open region Ω of space, with conditions imposed on $\partial\Omega$ (the boundary of Ω) or at infinity. E.g. inviscid flow past a sphere is determined by boundary conditions on the sphere (u. n = 0) and at infinity (u = Const). There are three types of boundary conditions for well-posed BVPs,

- typically characterize steady-state systems (no time derivative)
- temperature
- torsion
- pressure
- membrane displacement
- electrical potential

Closed domain with boundary conditions expressed in terms of,

$$u(x, y), \frac{\partial u}{\partial \eta} \tag{13}$$

that means $\rightarrow$

$$\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \tag{14}$$

Typical example include :

$\rightarrow$ Laplace Equation.

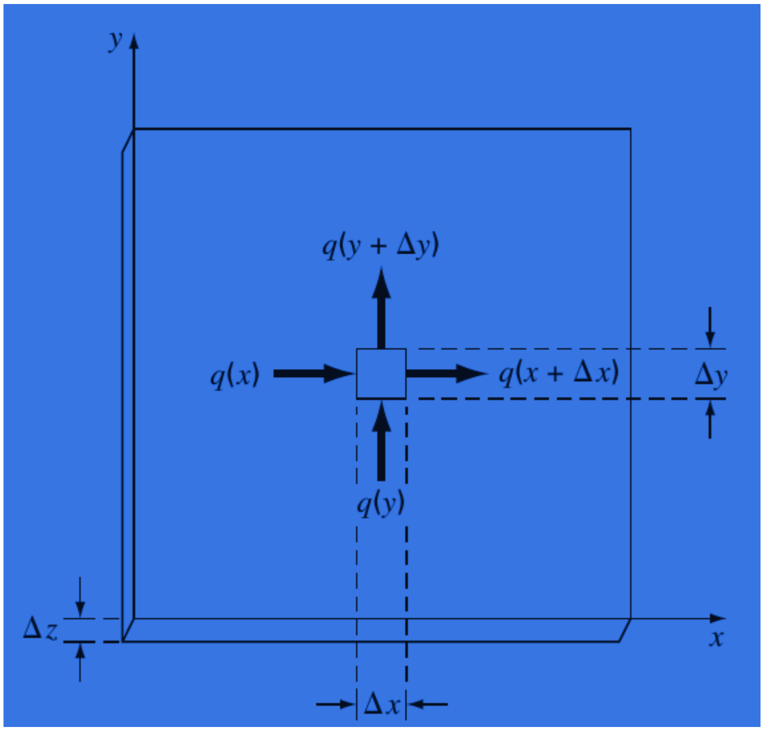
$$\nabla^2 T = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{15}$$

→ Poisson Equation.

$$\nabla^2 T = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -D(x, y, u, \partial u \partial x, \frac{\partial u}{\partial y}) \tag{16}$$

$A = 1, B = 0, C = 1 \rightarrow ==> B^2 - 4AC = 4 < 0$

3 How to obtain



The figure (mentioned above) shows an element on the face of a thin rectangular plate of thickness Δz. The plate is insulated everywhere but at its edges, where the temperature can be set at a prescribed level. The insulation and the thinness of the plate mean that heat transfer is limited to the x and y dimensions. At steady state, the flow of heat into the element over a unit time period Δt must equal the flow out, as in

$$q(x)\Delta y \Delta z \Delta t + q(y)\Delta x \Delta z \Delta t = q(x + \Delta x)\Delta y \Delta z \Delta t + q(y + \Delta y)\Delta x \Delta z \Delta t \tag{17}$$

where q(x) and q(y) = the heat fluxes at x and y, respectively $[\frac{cal}{cm^2 * s}]$. Dividing by Δz and Δt and collecting terms yields

$$[q(x) - q(x + \Delta x)]\Delta y + [q(y) - q(y + \Delta y)]\Delta x = 0 \tag{18}$$

Multiplying the first term by $\frac{\Delta x}{\Delta x}$ and the second by $\frac{\Delta y}{\Delta y}$ gives

$$[\frac{q(x)-q(x+\Delta x)}{\Delta x}]\Delta x\Delta y+[\frac{q(y)-q(y+\Delta y)}{\Delta y}]\Delta y\Delta x=0 \tag{19}$$

Dividing by $\Delta x\Delta y$ and taking the limit results in

$$-\frac{\partial q}{\partial x}-\frac{\partial q}{\partial y}=0 \tag{20}$$

Equation mentioned above is a partial differential equation that is an expression of the conservation of energy for the plate. However, unless heat fluxes are specified at the plates edges, it cannot be solved. Because temperature boundary conditions are given, this equation must be reformulated in terms of temperature. The link between flux and temperature is provided by Fouriers law of heat conduction, which can be represented as

$$q_i=-k\frac{\partial T}{\partial i} \tag{21}$$

where q_i heat flux in the direction of the i dimension $[\frac{cal}{(cm^2*s)}]$, k = coefficient of thermal diffusivity, $(\frac{cm^2}{s})$, ρ density of the material $(\frac{g}{cm^3})$,C = heat capacity of the material $[\frac{cal}{(g*C^\circ)}]$, and T = temperature (C°), which is defined as

$$T=\frac{H}{\rho CV} \tag{22}$$

where H = heat(cal) and V=volume(cm^3). Sometimes the term in front of the differential in Eq mentiond above, is treated as a single term,

$$k^{'}=k\rho C \tag{23}$$

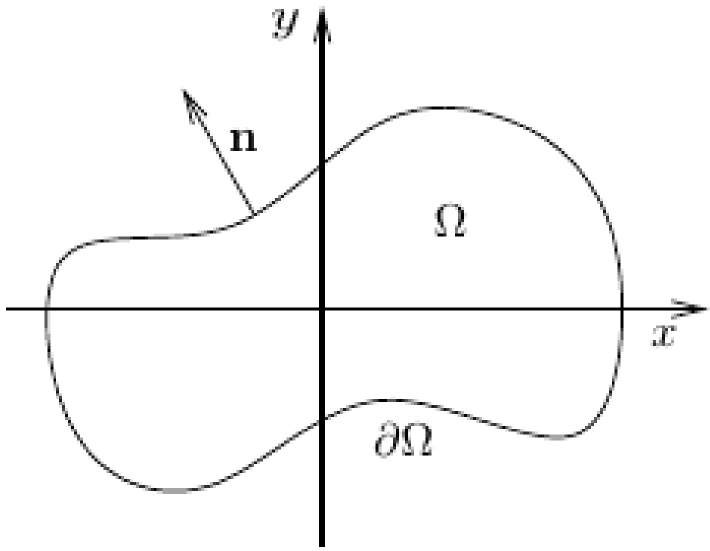
where $k^{'}$ is referred to as the coefficient of thermal conductivity $[\frac{cal}{s*cm*C^\circ)}]$.
In either case, both k and $k^{'}$ are parameters that reflect how well the material conducts heat. Fouriers law is sometimes referred to as a constitutive equation. It is given this label because it provides a mechanism that defines the systems internal interactions. Inspection of equation of flux indicates that Fourier's law specifies that heat flux perpendicular to the i axis is proportional to the gradient or slope of temperature in the i direction. The negative sign ensures that a positive flux in the direction of i results from a negative slope from high to low temperature. Substituting those equation of heat flux and Laplace results in

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0 \tag{24}$$

which is the Laplace equation. Note that for the case where there are sources or sinks of heat within the two-dimensional domain, the equation can be represented as where f(x, y) is a function describing the sources or sinks of heat. Equation is referred to as the Poisson equation.

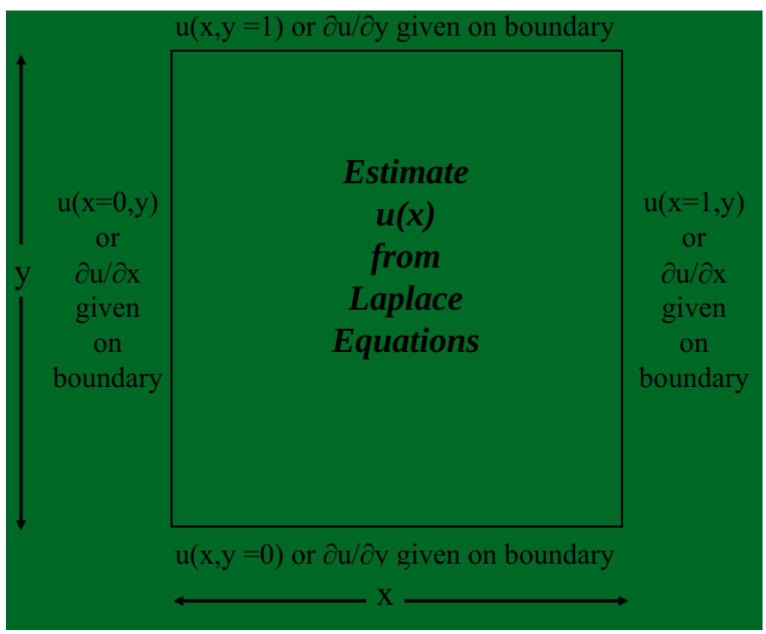
$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=f(x,y) \tag{25}$$

4 Boundary Conditions for Elliptic PDE's:



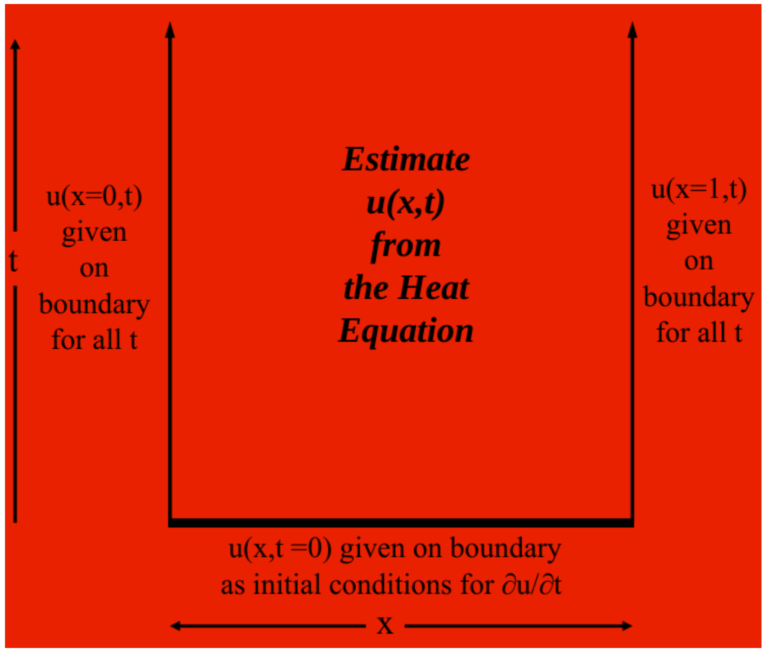
4.1 Dirichlet:

"u" provided along all of edge. "u" takes prescribed values on the boundary Ω (first BVP).



4.2 Neumann:

$\frac{\partial u}{\partial \eta}$ provided along all of the edge (derivative in normal direction)

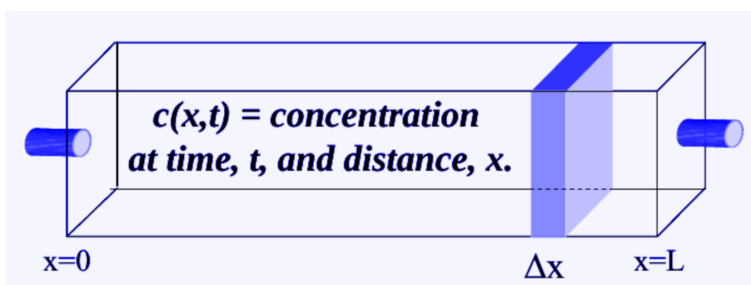


the normal derivative, $\frac{\partial u}{\partial \eta} = nu$ is prescribed on the boundary $\partial\Omega$ (second BVP). In this case we have compatibility conditions (i.e. global constraints): E.g., suppose u satisfies $\nabla^2 u = Fon\Omega$ and $n\nabla u = \partial_n u = f$ on $\partial\Omega$. Then,
Based on divergence theorem

$$\int_\Omega \nabla^2 u dV = \int_\Omega \nabla.\nabla u dV = \int_{\partial\Omega} \nabla u.nds = \int_{\partial\Omega} \frac{\partial u}{\partial n} dS \tag{26}$$

for the problem to be well defined.

$$= \int_\Omega F dV = \int_{\partial\Omega} f dS \tag{27}$$



4.3 Mixed (Robin):

u provided for some of the edge and $\frac{\partial u}{\partial \eta}$ for the remainder of the edge.
A combination of u and its normal derivative such as $\frac{\partial u}{\partial \eta} + \alpha u$, is prescribed on the boundary $\partial\Omega$ (third BVP).

Sometimes we may have a mixed problem, in which u is given on part of $\partial\Omega$ and $\frac{\partial u}{\partial n}$ given on the rest of $\partial\Omega$. If Ω encloses a finite region, we have an interior problem; if, however, $\Omega$is unbounded, we have an exterior problem, and we must impose conditions "at infinity". Note that initial conditions are irrelevant for these BVPs and the Cauchy problem for elliptic equations is not always well-posed (even if Cauchy-Kowaleski theorem states that the solution exist and is unique).As a general rule, it is hard to deal with elliptic equations since the solution is global, affected by all parts of the domain. (Hyperbolic equations, posed as initial value or Cauchy problem, are more localised.) From now, we shall deal mainly with the Helmholtz equation $\nabla^2 u + Pu = F$, where P and F are functions of x, and particularly with the special one if P = 0, Poisson's equation, or Laplaces equation, if F = 0 too. This is not too severe restriction; recall that any linear elliptic equation can be put into the canonical form

$$\sum_{k=1}^{n} \frac{\partial^2 u}{\partial x_k^2} + ... = 0 \tag{28}$$

Elliptic PDE's are analogous to Boundary Value ODE's, this is how they will be implemented.
u(x,y =1) or $\frac{\partial u}{\partial y}$ given on boundary

u(x=0,y) or $\frac{\partial u}{\partial x}$ given on boundary

u(x=1,y) or $\frac{\partial u}{\partial x}$ given on boundary

u(x,y=0) or $\frac{\partial u}{\partial y}$ given on boundary

4.4 Parabolic PDE's

Unlike elliptic equations, which describes a steady state, parabolic (and hyperbolic) evolution equations describe processes that are evolving in time. For such an equation the initial state of the system is part of the auxiliary data for a well-posed problem. The archetypal parabolic evolution equation is the heat conduction or diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{29}$$

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \tag{30}$$

Problems which are well-posed for the heat equation will be well-posed for more general
Parabolic Equations ($B^2 - 4AC = 0$) [first derivative in time]
variation in both space (x,y) and time, t,
typically provided are: (i) initial values: u(x,y,t = 0) (ii) boundary conditions:
$u(x = x_o, y = y_o, t)$ for all t
$u(x = x_f, y = y_f, t)$ for all t

all changes are propagated forward in time, i.e., nothing goes backward in time; changes are propagated across space at decreasing amplitude.
Typical example: Heat Conduction or Diffusion (the Advection-Diffusion Equation)
1D:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + D(x, u, \frac{\partial u}{\partial x}) \tag{31}$$

A = k, B = 0, C = 0 →B$^2 - 4AC = 0$
2D:

$$\frac{\partial u}{\partial t} = k[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}] + D(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) \tag{32}$$

$$= k\nabla^2 u + D \tag{33}$$

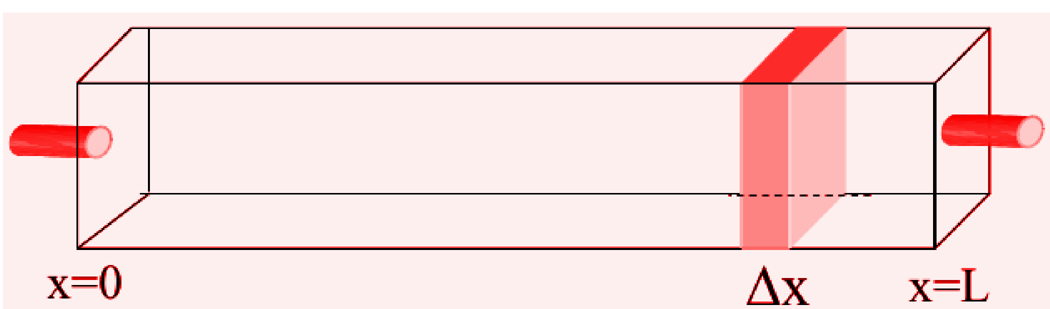
u(x=0,t) given on boundary for all t
u(x=1,t) given on boundary for all t
u(x=0,t) given on boundary as initial conditions for $\frac{\partial u}{\partial t}$
An elongated reactor with a single entry and exit point and a uniform cross-section of area A. A mass balance is developed for a finite segment Δx along the tank's longitudinal axis in order to derive a differential equation for concentration ($V = A\Delta x$).

$$\frac{\Delta c}{\Delta t} = Qc(x) - Q[c(x) + \frac{\partial c(x)}{\partial x}\Delta x] - DA\frac{\partial c(x)}{\partial x} + DA[\frac{\partial c(x)}{\partial x} + \frac{\partial}{\partial x}\frac{\partial c(x)}{\partial x}\Delta x] - kVc(x)$$

(34)

As, Δt and $\Delta x \to 0$

$$\frac{\Delta c}{\Delta t} \to= \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - \frac{Q}{A}\frac{\partial c}{\partial x} - kc \tag{35}$$



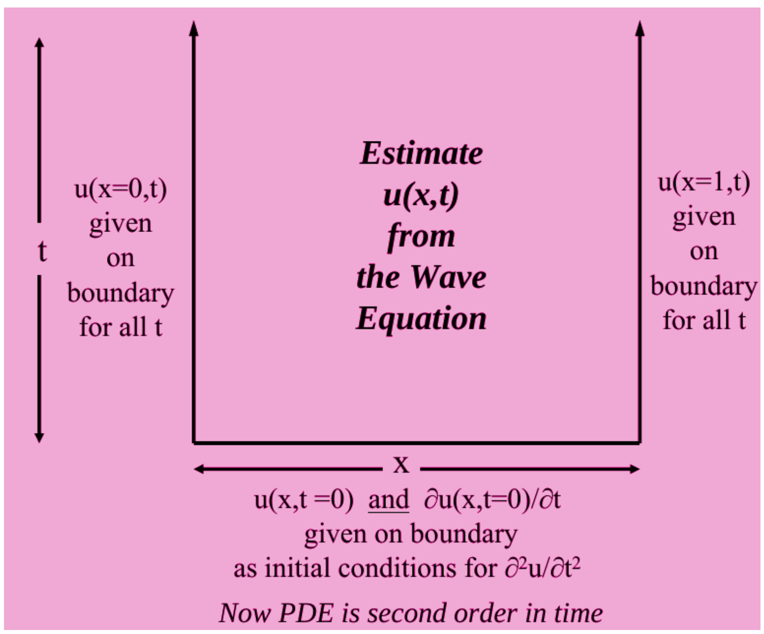
As Δt and $\Delta x \to 0$, $\frac{\Delta c}{\Delta t} \to= \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - \frac{Q}{A}\frac{\partial c}{\partial X} - kc$

5 Hyperbolic Equations ($B^2 - 4AC > 0$)[2nd derivative in time]

variation in both space (x, y) and time, t, requires: initial values: u(x,y,t=0), $\frac{\partial u}{\partial t}(x, y, t = 0)$ "initial velocity"
boundary conditions: $u(x = x_o, y = y_o, t)$ for all t
$u(x = x_f, y = y_f, t)$ for all t
all changes are propagated forward in time, i.e., nothing goes backward in time.
Hyperbolic Equations ($B^2 4AC > 0$)
Typical example: Wave Equation 1D :

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} + D(x, y, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t} \tag{36}$$

$A = 1, B = 0, C = -1/c^2 \Rightarrow B^2 - 4AC = 4/c^2 > 0$
Models: vibrating string, water waves, voltage change in a wire



6 Numerical Methods for Solving PDE's

Numerical methods for solving different types of PDE's reflect the different character of the problems. Laplace - solve all at once for steady state conditions. Parabolic (heat) and Hyperbolic (wave) equations. Integrate initial conditions forward through time.

6.1 Methods

Finite Difference (FD) Approaches: Based on approximating solution at a finite of points, usually arranged in a regular grid. Finite Element (FE) Method : Based on approximating solution on an assemblage of simply shaped (triangular, quadrilateral) finite pieces or "elements" which together make up (perhaps complexly shaped) domain. In this course, we concentrate on FD applied to elliptic and parabolic equation.

6.2 Finite Difference for Solving Elliptic PDE's

Solving Elliptic PDE's: (i) Solve all at once (ii) Liebmann Method. Based on Boundary Conditions (BCs) and finite difference approximation to formulate system of equations. Use Gauss-Seidel to solve the system

→ Laplace Equation.

$$\nabla^2 T = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{37}$$

→ Poisson Equation.

$$\nabla^2 T = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -D(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) \tag{38}$$

$A = 1, B = 0, C = 1 \rightarrow ==> B^2 - 4AC = 4 < 0$

6.3 Finite Difference Methods for Solving Elliptic PDE's

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1. Discretize domain into grid of evenly spaced points 2. For nodes where u is unknown:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2} + O(\Delta x^2) \tag{39}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{(\Delta y)^2} + O(\Delta y^2) \tag{40}$$

$\frac{w}{\Delta x} = \Delta y = h$, substitute into main equation

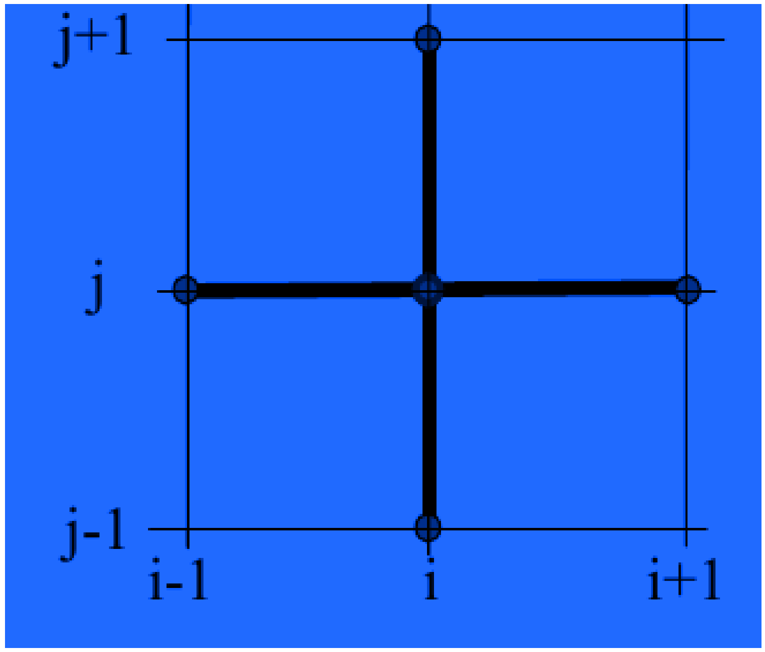
$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} + O(h^2) \tag{41}$$

Using Boundary Conditions, write, n*m equations for $u(x_{i=1:m}\ ,y_{j=1:n})$ or n*m unknowns.

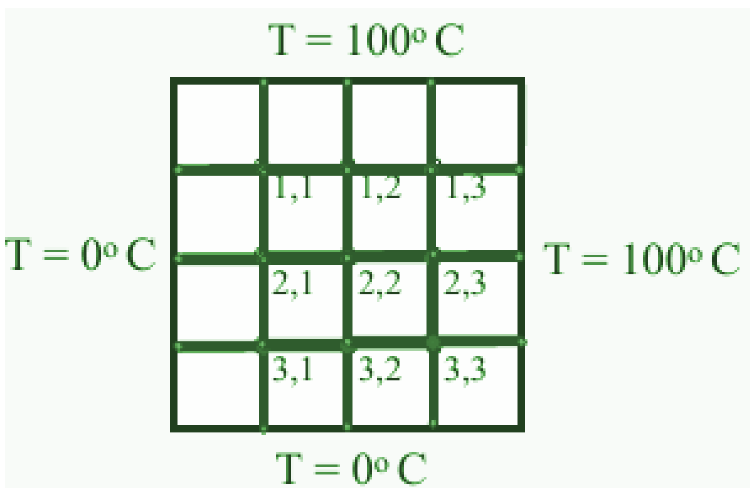
Solve this banded system with an efficient scheme. Using Gauss-Seidel iteratively yields the Liebmann Method .

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{42}$$

If, $\Delta x = \Delta y$ then, Laplace Molecule,



$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$



The Laplace molecule: $T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}4T_{i,j} = 0$.
The temperature distribution can be estimated by discretizing the Laplace equation at 9 points and solving the system of linear equations.

$$
\begin{array}{c}
\begin{array}{ccccccccc} T_{11} & T_{12} & T_{13} & T_{21} & T_{22} & T_{23} & T_{31} & T_{32} & T_{33} \end{array} \\
\begin{bmatrix}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{bmatrix}
\end{array}
\begin{Bmatrix} T_{11} \\ T_{12} \\ T_{13} \\ T_{21} \\ T_{22} \\ T_{23} \\ T_{31} \\ T_{32} \\ T_{33} \end{Bmatrix}
=
\begin{Bmatrix} -100 \\ -100 \\ -200 \\ 0 \\ 0 \\ -100 \\ 0 \\ 0 \\ -100 \end{Bmatrix}
$$

Primary (solve for first):

u(x,y) = T(x,y) = temperature distribution

Secondary (solve for second):

Heat flux :

$$q_x = -k' \frac{\partial T}{\partial x} q_x = -k' \frac{\partial T}{\partial x} \tag{43}$$

Obtain by employing,

$$\frac{\partial T}{\partial x} \approx \frac{T_{i+1,j} T_{i-1,j}}{2\Delta x} \tag{44}$$

$$\frac{\partial T}{\partial y} \approx \frac{T_{i+1,j} T_{i-1,j}}{2\Delta y} \tag{45}$$

then obtain resultant flux and direction:
$q_n = \sqrt{q_x^2 + q_y^2}$

$\theta = tan^{-1}(\frac{q_y}{q_x})$, where $q_x > 0$

$\theta = tan^{-1}(\frac{q_y}{q_x}) + \pi$, where $q_x < 0$ (θ in radians)

$q_x = -k' \frac{\partial T}{\partial x} \approx -k' \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x}$;
$q_y = -k' \frac{\partial T}{\partial y} \approx -k' \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y}$

$q_x \approx \frac{-0.49(50-0)}{(210cm)} = -1.225 \frac{cal}{(cm^2 s)}$; $q_y \approx \frac{-0.49(50-14.3)}{(210cm)} = -0.875 \frac{cal}{(cm^2 s)}$

$q_n = \sqrt{q_x^2 + q_y^2} = \sqrt{1.225^2 + 0.875^2} = 1.851 \frac{cal}{(cm^2 s)}$

$\theta = tan^{-1} \frac{q_y}{q_x} = tan^{-1}(\frac{-0.875}{-1.225}) = 35.5° + 180° = 215.5°$

Neumann Boundary Conditions (derivatives at edges): Employ phantom points outside of domain. Use FD to obtain information at phantom point,

$T_{1,j} + T_{-1,j} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0[*]$

If given $\frac{\partial T}{\partial x}$ then use $\frac{\partial T}{\partial x} = \frac{T_{1,j} - T_{i-1,j}}{2\Delta x}$

$T_{1,j} = T_{1,j} - 2\Delta x \frac{\partial T}{\partial x}$

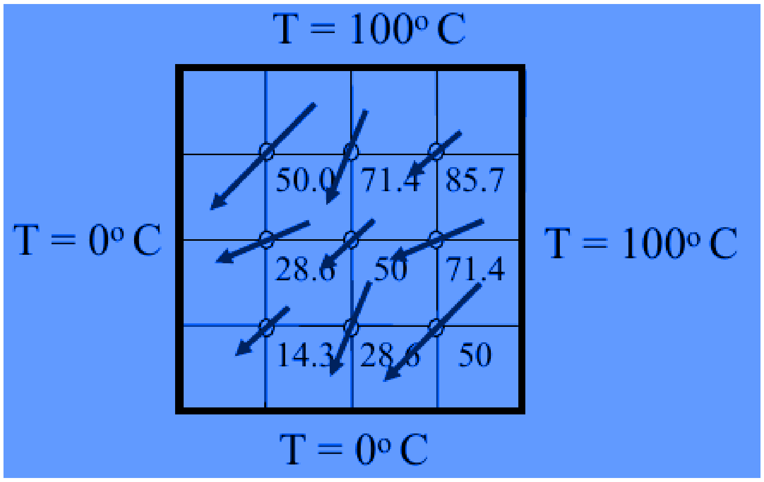
Substituting [*]: $2T_{1,j} - 2\Delta \frac{\partial T}{\partial x} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0$

Irregular boundaries: use unevenly spaced molecules close to edge, use finer mesh.

The Laplace molecule: $T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$

Derivative (Neumann) BC at (4,1):

$\frac{\partial T}{\partial y} = \frac{T_{3,1} - T_{5,1}}{2\Delta y}$



$T_{5,1} = T_{3,1} - 2\Delta y \frac{\partial T}{\partial y}$

$T_{4,2} + T_{4,0} + T_{3,1} + T_{5,1} - 4T_{4,1} = 0$

$T_{4,2} - T_{4,0} + 2T_{3,1} - 2\Delta y \frac{\partial T}{\partial y} - 4T_{4,1} = 0$, where, $\frac{\partial T}{\partial y} = 0$

7 Solution of Parabolic PDE's by FD Method:

Use B.C.'s and finite difference approximations to formulate the model, integrate I.C's forward through time,
for parabolic systems will investigate: (i) explicit schemes,(ii) stability criteria
implicit schemes: (i) Simple Implicit,(ii) Crank-Nicolson (CN), (iii) Alternating Direction (A.D.I), (iv) 2D-space
To find T(x,t):1D

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \tag{46}$$

To find T(x,t):2D

$$\frac{\partial T}{\partial t} = k(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial x^2}) \tag{47}$$

Given the initial temperature distribution as well as boundary temperatures with $K = \frac{K^{'}}{C_\rho}$ = Coefficient of thermal diffusivity.
where, $k^{'}$ = coefficient of thermal conductivity, C = heat capacity, ρ=density

Discretize the domain into a grid of evenly spaces points (nodes). Express the derivatives in terms of Finite Difference. Approximations of $O(h^2)$ and $O(\Delta t)$ [or order $O(\Delta t^2)$].

$\frac{\partial^2 T}{\partial x^2}, \frac{\partial^2 T}{\partial y^2}, \frac{\partial T}{\partial t} \rightarrow$ Finite Difference.

Choose $h = \Delta x = \Delta y$, and Δt and use the I.C's and B.C.'s to solve the problem by systematically moving ahead in time.

8 Time derivative:

Explicit Schemes: Express all future (t + Δt) values, T(x, t + Δt), in terms of current (t) and previous (t-Δt) information, which is known.

Implicit Schemes: Express all future (t + Δt) values, T(x, t + Δt), in terms of other future (t + Δt), current (t), and sometimes previous (t-Δt) information.

Use subscript(s) to indicate spatial points. Use superscript to indicate time level: $T_i^{m+1} = T(x_i, t_{m+1})$. Express a future state, T_i^{m+1}, only in terms of the present state, T_i^m.

1D heat Equation: $\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$

Centered FDD:

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-1}^m - 2T_i^m + T_{i+1}^m}{(\Delta x)^2} + O(\Delta x)^2 \tag{48}$$

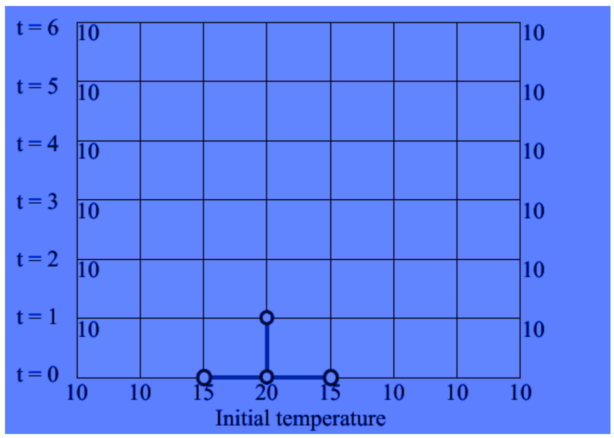
Forward FDD:

$$\frac{\partial T}{\partial t} = \frac{T_i^{m+1} - T_i^m}{\Delta t} + O(\Delta t) \tag{49}$$

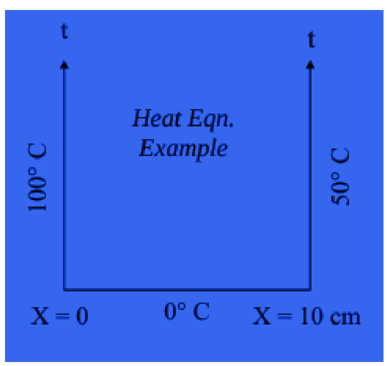
Solving for T_i^{m+1} results in:

$$T_i^{m+1} = T_i^m + \lambda(T_{i-1}^m - 2T_i^m + T_{i+1}^m)\lambda = k\Delta t/(\Delta x)^2 \tag{50}$$

$$T_i^{m+1} = (1 - 2\lambda)T_i^m + \lambda(T_{i-1}^m + T_{i+1}^m) \tag{51}$$



9 Example solution



1D heat Equation:

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \tag{52}$$

$k = 0.82\frac{cal}{s*cmC^{\circ}}$, 10-cm long rod, $\Delta t = 2$ secs, $\Delta x = 2.5$ cm

$$I.C.'s : T(0 < x < 10, t = 0) = 0^{\circ} \tag{53}$$

$$B.C.'s : T(x = 0, \forall t) = 100^{\circ} \tag{54}$$

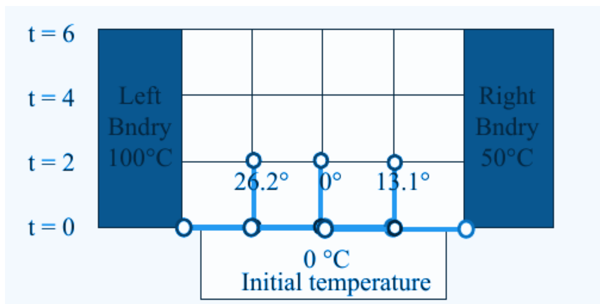
$$T(x = 10, \forall t) = 50^\circ \tag{55}$$

with

$\lambda = k\frac{\Delta t}{(\Delta x)^2} = 0.262(56)$

$$T_i^{m+1} = T_i^m + \lambda(T_{i-1}^m - 2T_i^m + T_{i+1}^m) \tag{57}$$

Starting at t = 0 secs. (m = 0), find results at t = 2 secs. (m = 1):

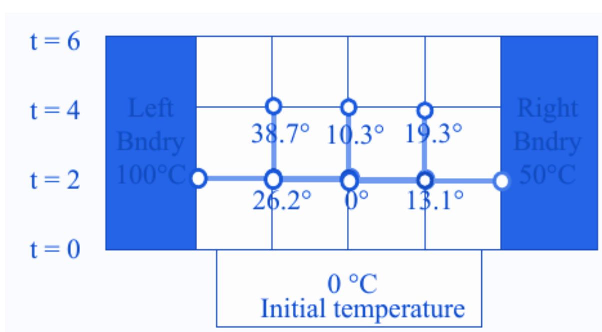


$T_1^1 = T_1^0 + (T_0^0 + T_1^0 + T_2^0) = 0 + 0.262[1002(0) + 0] = 26.2^\circ$

$T_2^1 = T_2^0 + (T_1^0 + T_2^0 + T_3^0) = 0 + 0.262[02(0) + 0] = 0^\circ$

$T_3^1 = T_3^0 + (T_2^0 + T_3^0 + T_4^0) = 0 + 0.262[02(0) + 50] = 13.1^\circ$

From t = 2 secs. (m = 1), find results at t = 4 secs. (m = 2):



$T_1^2 = T_1^1 + (T_0^1 + T_1^1 + T_2^1) = 26.2 + 0.262[1002(26.2) + 0] = 38.7^\circ$

$T_2^2 = T_2^1 + (T_1^1 + T_2^1 + T_3^1) = 0 + 0.262[26.22(0) + 13.1] = 10.3^\circ$

$T_3^2 = T_3^1 + (T_2^1 + T_3^1 + T_4^1) = 13.1 + 0.262[02(13.1) + 50] = 19.3^\circ$

Parabolic PDE's: The Explicit Method is Conditionally Stable.

For the 1-D spatial problem, the following is the stability condition:

$$\lambda = \frac{k\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \tag{58}$$

or

$$\Delta t = \frac{(\Delta x)^2}{2k} \tag{59}$$

$\lambda \leq \frac{1}{2} \rightarrow$ can still yield oscillation (1D)
$\lambda \leq \frac{1}{4} \rightarrow$ ensures no oscillation (1D)
$\lambda \leq \frac{1}{6} \rightarrow$ tends to optimize truncation error
We will also see that the Implicit Methods are unconditionally stable.

10 Summary:

Solution of Parabolic PDE's by Explicit Schemes.
Advantages: (i) very easy calculations, (ii) simply step ahead
Disadvantage:
(i) low accuracy, $O(\Delta t)$ accurate with respect to time
(ii) subject to instability; must use "small" Δt's. and require many steps.

11 Parabolic PDE's: Implicit Schemes

Implicit Schemes for Parabolic PDEs, Express T_i^{m+1} terms of T_j^{m+1}, T_i^m and possibly also T_j^m (in which j = i-1 and i+1). Represents spatial and time domain. For each new time, write m (of interior nodes) equations and simultaneously solve for m unknown values (banded system).

Simple Implicit Method. Substituting:
Centered FDD:

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-1}^m - 2T_i^m + T_{i+1}^m}{(\Delta x)^2} + O(\Delta x)^2 \tag{60}$$

Forward FDD:

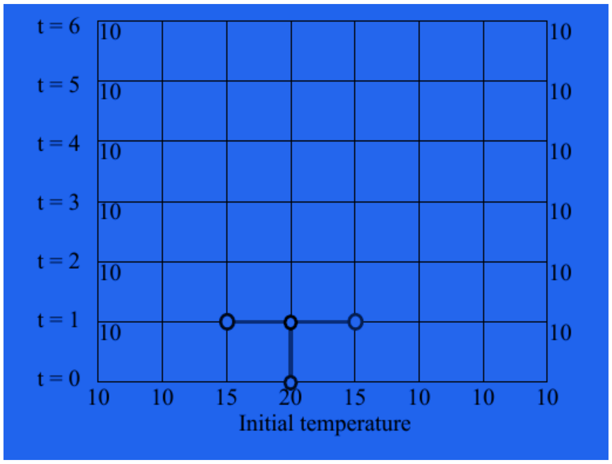
$$\frac{\partial T}{\partial t} = \frac{T_i^{m+1} - T_i^m}{\Delta t} + O(\Delta t) \tag{61}$$

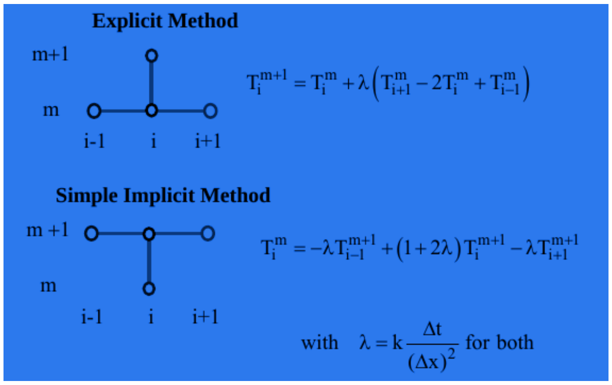
$$-\lambda T_{i-1}^{m+1} + (1+2\lambda)T_i^{m+1} - \lambda(T_{i+1}^{m+1} = T_i^m) \tag{62}$$

with

$$\lambda = \frac{k\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \tag{63}$$

Requires I.C's for case where m = 0: i.e., T_i^0 is given for all i. Requires B.C's to write expressions at 1st and last interior nodes (i=0 and n+1) for all m.





At the Left boundary:

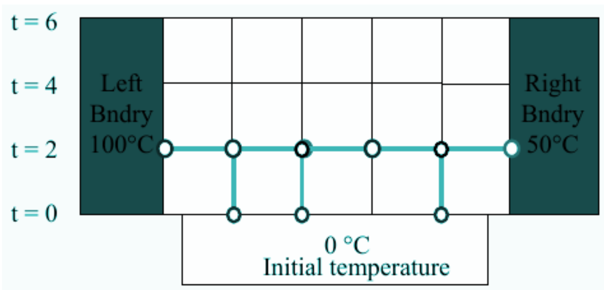
$$(1+2\lambda)T_1^{m+1} - \lambda T_2^{m+1} = T_1^m + \lambda T_0^{m+1} \tag{64}$$

Away from boundary:

$$-\lambda T_{i-1}^{m+1} + (1+2\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = T_i^m \tag{65}$$

At the Right boundary:

$$(1+2\lambda)T_i^{m+1} - \lambda T_{i-1}^{m+1} = T_i^m + \lambda T_{i+1}^{m+1} \tag{66}$$



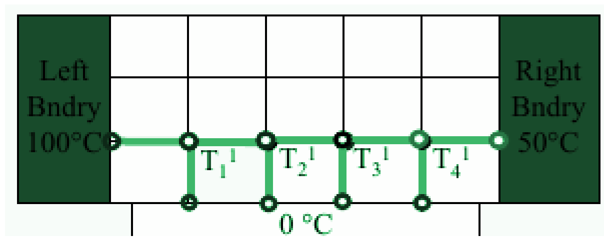
At the Left boundary:

$$(1+2\lambda)T_1^1 - \lambda T_2^1 = T_1^0 + \lambda T_0^1 \tag{67}$$

$$1.8T_1^1 - 0.4T_2^1 = 0 + 0.8 * 100 = 40 \tag{68}$$

Away from boundary:

$$-\lambda T_{i-1}^1 + (1+2\lambda)T_i^1 - \lambda T_{i+1}^1 = T_i^0 \tag{69}$$



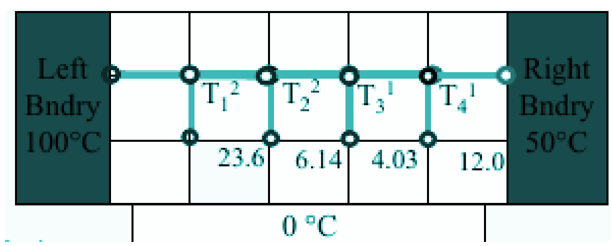
$$-0.4T_1^1 + 1.8T_2^1 - 0.4T_3^1 = 0 \tag{70}$$

$$-0.4T_2^1 + 1.8T_3^1 - 0.4T_4^1 = 0 \tag{71}$$

At the Right boundary:

$$(1+2\lambda)T_i^3 - \lambda T_{i-1}^2 = T_3^0 + \lambda T_4^1 \tag{72}$$

$$1.8T_i^{m+1} - 0.4T_{i-1}^{m+1} = 0 + 0.4 * 50 = 20 \tag{73}$$



At the Left boundary:

$$(1+2\lambda)T_1^2 - \lambda T_2^2 = T_1^1 + \lambda T_0^2 \tag{74}$$

$$1.8T_1^2 - 0.4T_2^2 = 23.6 + 0.4 * 100 = 78.5 \tag{75}$$

Away from boundary:

$$-\lambda T_{i-1}^2 + (1+2\lambda)T_i^2 - \lambda T_{i+1}^2 = T_i^1 \tag{76}$$

$$-0.4T_1^2 + 1.8T_2^2 - 0.4T_3^2 = 6.14 \tag{77}$$

$$-0.4T_2^2 + 1.8T_3^2 - 0.4T_4^2 = 4.03 \tag{78}$$

At the Right boundary:

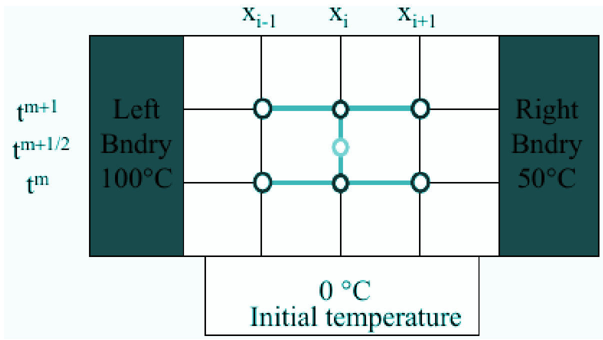
$$(1+2\lambda)T_3^2 - \lambda T_4^2 = T_3^1 + \lambda T_4^2 \tag{79}$$

$$1.8T_3^2 - 0.4T_4^2 = 12.0 + 0.4 * 50 = 32 \tag{80}$$

12 Parabolic PDE's: Crank-Nicolson Method

Implicit Schemes for Parabolic PDE's.

Crank-Nicolson (CN) Method (Implicit Method),Provides 2nd-order accuracy in both space and time. Average the 2nd-derivative in space for t^{m+1} and t^m.



$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}[\frac{T_{i-1}^m - T_i^m + T_{i+1}^m}{(\Delta x)^2} + \frac{T_{i-1}^{m+1} - T_i^{m+1} + T_{i+1}^{m+1}}{(\Delta x)^2}] + O(\Delta x)^2 \tag{81}$$

$$\frac{\partial T}{\partial t} = \frac{T_i^{m+1} - T_i^m}{\Delta t} + O(\Delta t^2) \tag{82}$$

Then Equation of the Crank-Nicholson:

$$-\lambda T_{i-1}^{m+1} + 2(1+\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = \lambda T_{i-1}^m + 2(1-\lambda)T_i^m - \lambda T_{i+1}^m \tag{83}$$

13 Stability of the Crank-Nicolson Implicit Method

$$-\lambda T_{i-1}^{m+1} + 2(1+\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = \lambda T_{i-1}^m + 2(1-\lambda)T_i^m - \lambda T_{i+1}^m \tag{84}$$

Worst case solution: $T_i^m = r^m(-1)^i$

$$-\lambda r^{m+1}(-1)^{i-1} + 2(1+\lambda)r^{m+1}(-1)^i - \lambda r^{m+1}(-1)^{i+1} = -\lambda r^m(-1)^{i-1} + 2(1-\lambda)r^m(-1)^i + \lambda r^m(-1)^{i+1} \tag{85}$$

$$r[\lambda(1)1 + 2(1+\lambda) - \lambda(1) + 1] = \lambda(1)1 + 2(1\lambda) + \lambda(1) + 1 \tag{86}$$

$$r = [12\lambda]/[1+2\lambda] \tag{87}$$

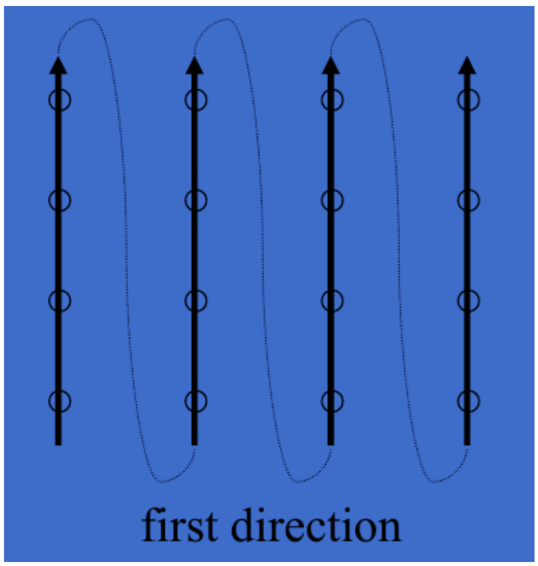
14 Summary: Solution of Parabolic PDE's by Implicit Schemes

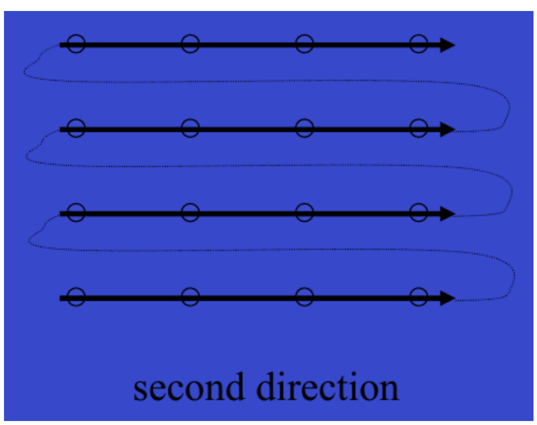
Advantages: Unconditionally stable, Δt choice governed by overall accuracy. [Error for CN is $O(\Delta t^2)$]. May be able to take larger $\Delta t \rightarrow$ fewer steps.

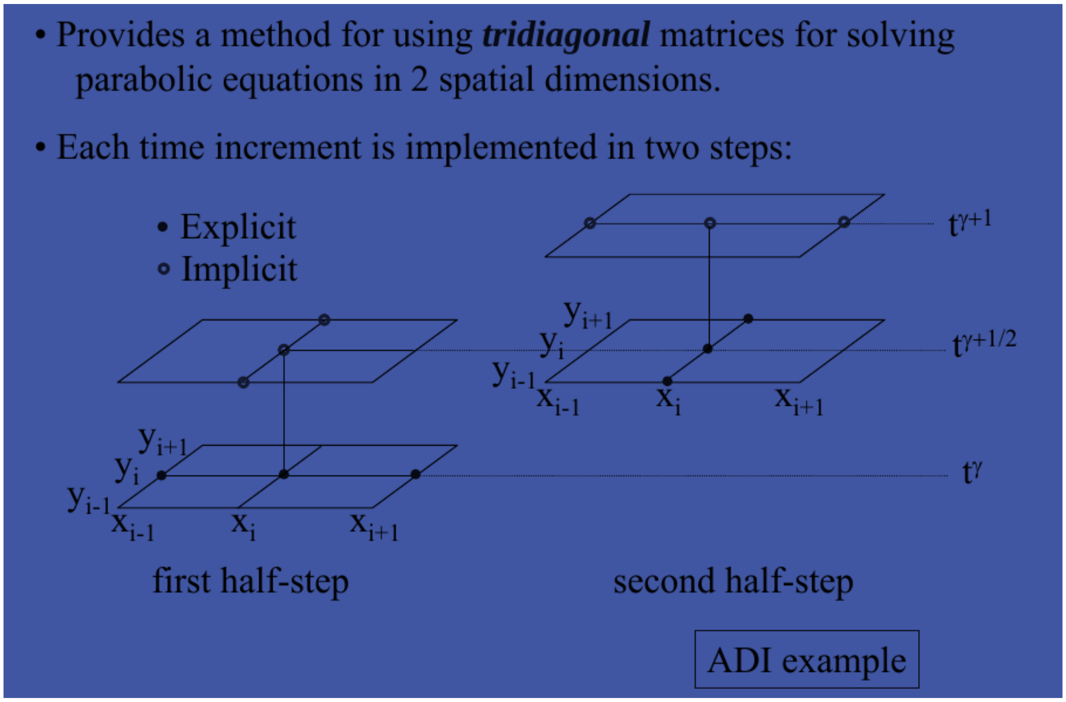
Disadvantages: More difficult calculations, especially for 2D and 3D spatially, For 1D spatially, effort same as explicit because system is tridiagonal.

15 Parabolic PDE's:Alternating-Direction Implicit (ADI) Method

Provides a method for using tridiagonal matrices for solving parabolic equations in 2 spatial dimensions.

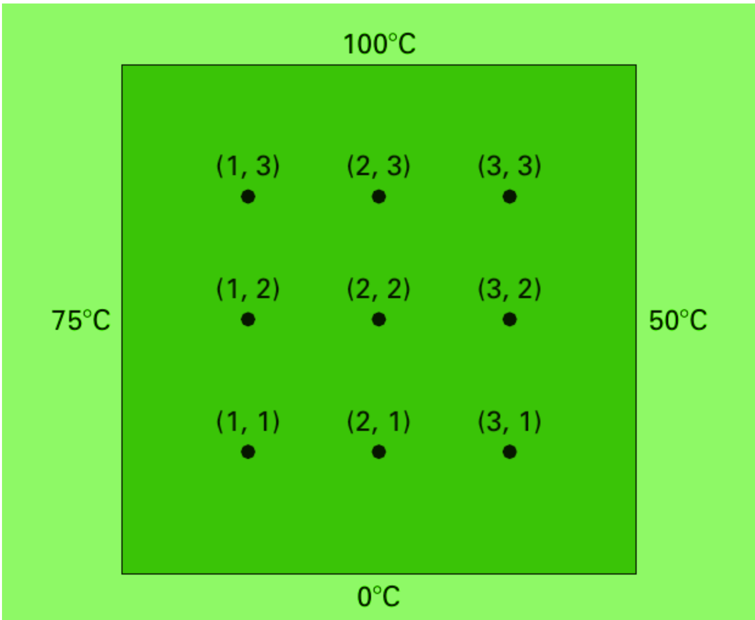






16 Problems to solve

1.Use Liebmanns method (Gauss-Seidel) to solve for the temperature of the heated plate as shown in the given below figure. Employ overrelaxation with a value of 1.5 for the weighting factor and iterate to $\varepsilon_s = 1\%$.



2. Repeat the same problem, but with the lower edge insulated.

3. Use the explicit method to solve for the temperature distribution of a long, thin rod with a length of 10 cm and the following values:

$k' = 0.49\frac{cal}{s*cm*C^{\circ}}$, $\Delta x = 2cm$, and $\Delta t = 0.1s$. At t = 0, the temperature of the rod is zero and the boundary conditions are fixed for all times at $T(0) = 100^{\circ}$ and $T(10) = 50^{\circ}$. Note that the rod is aluminum with C = 0.2174 $\frac{cal}{(g*C^{\circ})}$ and $\rho = 2.7\frac{g}{cm^3}$. Therefore, $k = \frac{0.49}{(2.7*0.2174)} = 0.835\frac{cm^2}{s}$ and $\lambda = 0.835(0.1)2^2 = 0.020875$.

4.Use the simple implicit finite-difference approximation to solve problem 3.

5.Use the Crank-Nicolson method to solve the same problem as in 3 and 4.

17 Examination Point of View/Model Questions for the Exam(as discussed earlier)

1.The unsteady one dimensional heat conduction in solids is given by the following PDE, using:

a) Implicit Finite Difference method
Thickness $= L = 10cm$, $\Delta x = 1cm$

b) Explicit Finite Difference method

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{88}$$

T=T(x,t); x is the space coordination m and t is the time in seconds

The initial condition; $T(x, 0) = 100C^{\circ}$
The boundary Conditions:

Left hand BC: $T(0, t) = 25C^{\circ}$

Right hand BC: $T(L, t) = 0C^{\circ}$

α is the thermal conductivity, for example for copper $\alpha = \frac{k}{\rho C_p} = 14x10^{-6}\frac{m^2}{s}$
2). Approximate the solution to the following Parabolic PDE of heat conduction along a thin rod of length 10 cm using explicit method. Use h=2 and k=0.1. At t=0, the temperature of the rod is zero and the boundary conditions are fixed at all times.

$$\frac{\partial u(x,t)}{\partial t} - 0.835.\frac{\partial^2 u(x,t)}{\partial x^2} = 0, \tag{89}$$

$0 < x < 10.0, 0 < t$

$u(0,t) = 100C^\circ and u(10,t) = 50C^\circ$

(i) Use the implicit method to solve the problem

(ii) Use Crank-Nicolson method to solve the problem

3. The 1D heat conduction equation can be presented in the form:

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} \tag{90}$$

(i) Discretise this equation using the explicit finite difference approach

(ii) Discretise this equation using the implicit finite difference approach