

Advanced Computational Techniques
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Lecture no. 18
Linear Parabolic (PDE)

Now so far what we have done is the variable u or y we are taken as a function of x . So, we have dealt with the ordinary differential equation.

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The image shows handwritten notes on a whiteboard. At the top, it says "Transport Equation: $u(x) \rightarrow ODE$ ". Below this, the equation $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2}$ is written, with red annotations: "unsteady" under $\frac{\partial u}{\partial t}$, "convection term" under $u \frac{\partial u}{\partial x}$, and "diffusion" under $\mu \frac{\partial^2 u}{\partial x^2}$. The domain is given as $t \geq 0, 0 < x < l$. The initial condition is $u(x, 0) = f(x), 0 < x < l$. The boundary conditions are $u(0, t) = U_0$ and $u(l, t) = U_L$ for $t > 0$. A graph shows a rectangular domain in the $x-t$ plane with x on the vertical axis and t on the horizontal axis. The top boundary is at $x=l$ and the left boundary is at $t=0$. Below the graph, it says "Burgers equation, nonlinear" and "Linear equation: $\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2}$ - (I)". It notes that if $c(x, t)$ is a known function, then (I) is linear. If $c=0$, the equation becomes $\frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial x^2}$, which is labeled as "diffusion".

In many process particularly in mathematical modeling of any transport phenomena say fluid transport, heat transfer or any reaction diffusion equations what I come across a equation like this

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2}$$

So, in this case u is a function of x, t

$$u = u(x, t)$$

so it is not a single variable it is a function of x and t , x can be space coordinate and t can be so say $t \geq 0$ is the time then say $a < x < l$ say or $0 < x < l$ and the show that means, this set of equations you should have a we need to prescribe one initial condition as $u(x, 0) = f(x)$ that is a $t = 0$ whatever the condition is prescribed at say a value is given for $0 < x < l$ and 2 boundary condition because we have a second derivative with respect to x .

So we should have 2 boundary conditions. So, these boundary conditions are say $u(0, t) = u_0$ say some value is given and $u(1, t)$ is some value is given to be u_1 this can be a function of x also this is for $t > 0$. So, that means, you have a competition or domain is something like this. So, what we have is say if we call this the one for x , x is varying from here 0. So, this is the t axis and this is x axis, so x is varying from 0 to 1, and this is $t = 0$ this is the line.

So, that means, what we have given is the conditions that the SME infinite domain and at the rate marked line these conditions are prescribed. So, we need to solve this. Now, this equation is also referred as the Burgers equation, Burgers equation it is very popular or very important in testing any numerical scheme for any kind of advection diffusion equations or the viscous transport equations, fluid flow or Navier stokes equation in a simple form this Burgers equation is adopted.

So, this is the unsteady term unsteady term this is the convective transferred convection term and this is the diffusion term this is what is referred as the diffusion term. So, there are processes which are by which these u is transported by the mechanism one is the diffusion and fix laws for example, another is the advection or convection.

Now, this is a non-linear equation. Now, it can happen show happen that instead of a non-linear equation, we can the linear situation show if it is a linear equation. So, since the advection term is known, so, one of the linear equation is

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = m\mu \frac{\partial^2 u}{\partial x^2} \quad -(2)$$

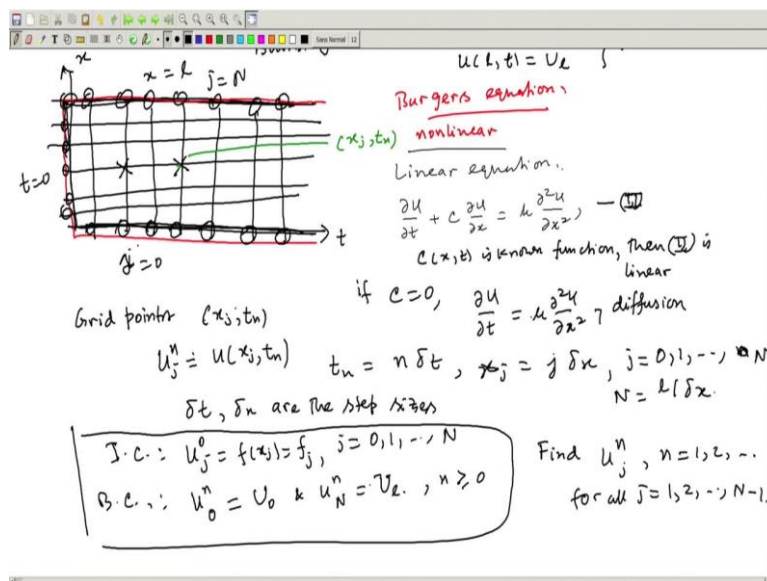
In this case, this is a linear equation and where $c(x, t)$ might be a known function.

So, this is one of the equation so, then let us call this to equation (2), then (2) is linear and also some cases if $c = 0$ so, then we have a pure diffusion equation so

$$\frac{\partial u}{\partial t} = m\mu \frac{\partial^2 u}{\partial x^2}$$

that is a equation governed only by the diffusion processes like heat transfer process where there is no advection term are involved.

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So, we will talk about solving these kinds of equations numerically so now, if you want to solve this numerically so first of all we have to define the grids so we define the grid points as (x_i, t_j) . And we define this as $u(x_i, t_j) = u_j$ say better we write instead of, because i we may use for some other purpose show let us write this as x and (x_j, t_n) and so, that is the grid points are defined as (x_j, t_n) and we define $u_j^n = u(x_j, t_n)$

So that means, we are choosing the grid points like this way if we draw some vertical line it is spacing say δt . So, that means $t_n = n \delta t$ and the horizontal line we define like this. So, maybe this was not straight, x_j we are defining as $x_j = j \delta x$ so δt and δx are the steps size and grid points step size is along x direction and t direction. So, first let us see that what are the conditions we have been given.

So, initial condition which can be written as $u_j^0 = f(x_j) = f_j$ for all these $j = 0, 1, 2, \dots, N$, so let us call j , different values because n already we have used so $N = \frac{1}{\delta x}$ and so $j = 0, 1, \dots, N$ and what the conditions are prescribed at the 2 end as boundary conditions can be written as

$$u_{0j}^n = u_0 \text{ and } u_N^n = u_1 \text{ for } n \geq 0.$$

So, these are the conditions are prescribed so you need to find, find u_j^n for $n \geq 0$ or strictly > 0 or the other $n = 1, 2, \dots$ for all $j = 1, 2, \dots, N-1$ because $N = n - 1$ so, this is equal to $j = 0$ line and this is $j = n$ line, so along this line all the solutions are prescribed so if I say that grid points manner so all these circled if I define this as where the solutions are prescribed so along this all the circles are .

So, you need to find out at the across point so if I call this as (x_j, t_n) grid points so I need to find out the solution at these grid points.

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I. $\frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial x^2}$, Discretize FTCS
 Forward time marching procedure
 $\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}$ T.E.: $O(\delta t, \delta x^2)$
 $r = \mu \delta t / (\delta x)^2$
 $u_j^{n+1} = r u_{j+1}^n + (1 - 2r) u_j^n + r u_{j-1}^n, j = 1, 2, \dots, N-1$
 Explicit scheme T.E. $O(\delta t, (\delta x)^2)$.
 Conditionally stable, stable if $r \leq 1/2$

II. Implicit Scheme:
 $\frac{\partial u}{\partial t} \Big|_j^{n+1} = \mu \frac{\partial^2 u}{\partial x^2} \Big|_j^{n+1}$, BTCS

So, first let us talk about the simple situation that means, u satisfy the equation

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

if u satisfy this equation, so, then if we discretize this equation so what I do is forward time and central space. Now, one thing is that we adopt a forward time marching procedure so, that means, what I do is say this $t = 0$ is known, we want to find out first at $t = t_1$ then $t = t_2$ like this way if I want to go.

So, we get a FTCS so we can write as

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}$$

So obviously, already can see that, because we have used a forward time first order in t and second order in x , so this truncation error obviously, is $O(\delta t, \delta x^2)$. So, in that case we can write very simply u_j^{n+1} by introducing a parameter say $r = \mu \frac{\delta t}{(\delta x)^2}$

So, if I introduce this so what I again get is u_j^n or other if I take in inside. So, this can be written as

$$u_j^{n+1} = r u_{j+1}^n + (1 - 2r) u_j^n + r u_{j-1}^n, j = 1, 2, \dots, N-1$$

so r is unknown parameter. So this is an explicit formula explicit scheme with truncation error order δt first order in δt and second order in δx $O(\delta t, \delta x^2)$ because we have used FTCS. So, this is one way.

Another way now, we will show that where if we take a explicit scheme so then the scheme can be conditionally stable. So, that means it is stable, we will prove that stable if $r \leq 1/2$, if we choose the grid point in such a way that it is $r \leq 1/2$ then the scheme is stable. Now, if $r \leq 1/2$ creates the restriction for δt , so, δt has to be very small okay.

So, that means we have to go for a larger number of steps to solve this. So, instead show that is stable, conditionally stable if $r \leq 1/2$. So, instead of that what we do is an implicit scheme should that means what we do is we satisfy this equation at the unknown time level

$$\frac{\partial u}{\partial t} \Big|_j^n = \mu \frac{\partial^2 u}{\partial x^2} \Big|_j^{n+1}$$

satisfy instead of satisfying the previous one we are satisfying as n, j . Here we are satisfying at $n + 1$ and j and apply BTCS that means, backward in time and central in space.

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$$u_j^{n+1} = r u_{j+1}^n + (1-2r)u_j^n + r u_{j-1}^n, \quad j=1, 2, \dots, N-1$$
 Explicit scheme T.E. $O(\delta t, \delta x^2)$,
 Conditionally stable, stable if $r \leq 1/2$

II: Implicit Scheme:

$$\frac{\partial u}{\partial t} \Big|_j^{n+1} = \mu \frac{\partial^2 u}{\partial x^2} \Big|_j^{n+1}, \quad \text{BTCS}$$

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + O(\delta t, (\delta x)^2)$$
 Stable for any choice of $\delta t, \delta x$.

$$r u_{j-1}^{n+1} - (1-2r)u_j^{n+1} + r u_{j+1}^{n+1} = -u_j^n, \quad j=1, 2, \dots, N-1$$

$$u_0^{n+1} = u_0^n, \quad u_N^{n+1} = u_N^n$$

$$AX = b, \quad X = [u_1^{n+1}, u_2^{n+1}, \dots, u_{N-1}^{n+1}]$$
 which is a tri-diagonal system.
 Implicit scheme are unconditionally stable.

So in that case we get

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + O(\delta t, (\delta x)^2)$$

here truncation error wise is no improvement, but only improvement is the stability wise shows that this will become stable. So, again this is $\delta t, \delta x^2$. So, this is stable for any choice. So, this is an implicit scheme which is stable for any choice of r .

So, that means, that implies δt and δx so immaterial of whatever the choice of $\delta t, \delta x$ we can have a stability for this scheme. So, this can be now, obviously, this does not look like as simple as that because u^{n+1} is appearing in both sides.

So, that means it will lead to a system of equation linear system in a couple function so which can be written as

$$r u_{j-1}^{n+1} - (1 - 2r) u_j^{n+1} + r u_{j+1}^{n+1} = -u_j^n, j=1, 2, \dots, N-1$$

So, for $j=1, 2, \dots, N-1$.

So, which leads to a tri-diagonal system $AX = d$, X is the variable here it is $X^T = [u_1^{n+1}, u_2^{n+1}, \dots, u_{N-1}^{n+1}]$ and this is A and you what to know at the 2 end points $u_0^{n+1} = u_0, u_j^{n+1} = u_1$ which forms a tri-diagonal system. So, this forms $AX = d$ which is tri-diagonal system.

So, this tri-diagonal system can be inverted using Thomas algorithm as we discussed before and we get the solution X . Now so, unconditionally implicit scheme or unconditionally stable. So, that means, for any choice of $\delta t, \delta x$ you have a stability of the numerical scheme.

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$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + O(\delta t, (\delta x)^2)$$

$$\bar{j} = 1, 2, \dots, N-1$$

Stable for any choice of $\delta t, \delta x$.
 $\Rightarrow \delta t, \delta x$.

$$r u_{j-1}^{n+1} - (1-2r) u_j^{n+1} + r u_{j+1}^{n+1} = -u_j^n, \quad \bar{j} = 1, 2, \dots, N-1$$

$$u_0^n = U_0, u_N^n = U_N$$

$$AX = d, \quad X^T = [u_1^{n+1} \quad u_2^{n+1} \quad \dots \quad u_{N-1}^{n+1}]$$

\rightarrow which is a tri-diagonal system.

Implicit Scheme are unconditionally Stable.
 $n = 0, 1, \dots$

So, one can proceed starting from $n = 0$. First to find out all these first time step, then $n = 1$ and so on up to the desire level of time one can solve this and get the solution by solving the tri-diagonal system. Now, no improvement though it is stability wise improvement, but no improvement in the accuracy.

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II Crank-Nicolson Scheme:

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

$$\int_{t_n}^{t_{n+1}} \frac{\partial u}{\partial t} dt = \mu \int_{t_n}^{t_{n+1}} \frac{\partial^2 u}{\partial x^2} dt \quad \text{at } x = x_j$$

\rightarrow Trapezoidal rule

$$u_j^{n+1} - u_j^n = \mu \cdot \frac{\delta t}{2} \left[\frac{\partial^2 u}{\partial x^2} \Big|_j^{n+1} + \frac{\partial^2 u}{\partial x^2} \Big|_j^n \right]$$

derivatives w.r.t. x we discretize by central difference

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \mu \left[\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2} \right]$$

So, for the accuracy there is the most important and most popular scheme is the Crank Nicolson Scheme. So, this can be expressed in this manner so what I do is

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

so integrate both sides between t_n to t_{n+1} , with respect to t ,

$$\int_{t_n}^{t_{n+1}} \frac{\partial u}{\partial t} | x_j dt = \mu \int_{t_n}^{t_{n+1}} \frac{\partial^2 u}{\partial x^2} | x_j dt$$

So, obviously this side it is at at $x = x_j$. So, what I get here is

$$u_j^{n+1} - u_j^n = \mu \frac{\delta t}{2} \left[\frac{\partial^2 u}{\partial x^2} |_j^{n+1} + \frac{\partial^2 u}{\partial x^2} |_j^n \right]$$

and this side what we do we apply because this cannot be integrated $\frac{\partial u}{\partial t}$ directly can be integrated directly because that is the derivative form so which can be expressed straight away this manner so this one we approximate by trapezoidal rule, so the trapezoidal rule what we do here.

So, n and j , we $n + 1$ and n at the 2 points we take the average so now, what we do now is we apply so, this is a derivative involves so, all these derivatives with respect to x we discretize by central difference scheme.

$$u_j^{n+1} - u_j^n = \frac{\mu}{2} \left[\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2} \right], j=1, 2, \dots$$

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$$u_j^{n+1} - u_j^n = \mu \frac{\delta t}{2} \left[\frac{\partial^2 u}{\partial x^2} |_j^{n+1} + \frac{\partial^2 u}{\partial x^2} |_j^n \right]$$
 derivatives w.r.t. x we discretize by central difference

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \frac{\mu}{2} \left[\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2} \right] \quad n \geq 0$$
 unknowns are u_j^{n+1} appearing implicitly, $j=1, 2, \dots, N-1$, $r = \mu \delta t / (\delta x)^2$

$$-\frac{r}{2} u_{j-1}^{n+1} + (1-r) u_j^{n+1} - \frac{r}{2} u_{j+1}^{n+1} = \frac{r}{2} u_{j+1}^n + (1-r) u_j^n + \frac{r}{2} u_{j-1}^n$$

$$j=1, 2, \dots, N-1$$
 Which leads to a tri-diagonal system $Ax = d$
 Which can be solved by the Thomas Algo.
 to set $X^T = [u_1^{n+1}, u_2^{n+1}, \dots, u_{N-1}^{n+1}] \quad n \geq 0$

So, here the unknowns are u^{n+1} so $j = 1, 2, \dots$, etc, $n \geq 0$ so unknowns are u_j^{n+1} appearing implicitly what is the advantage of this? Advantage is now, this is order $\delta t^2, \delta x^2$ because δt^2 because it is δt^3 but we are dividing by δt .

So, that is why this becomes a order δt^2 approximate and δx^2 . So that is why it has the advantage of higher order scheme so now if we introduce that $r = \mu \frac{\delta t}{(\delta x)^2}$ so, and bring these unknowns one side so what I get is

$$-\frac{r}{2}u_{j-1}^{n+1} + (r-1)u_j^{n+1} - \frac{r}{2}u_{j+1}^{n+1} = -\frac{r}{2}u_{j-1}^n + (r-1)u_j^n - \frac{r}{2}u_{j+1}^n$$

and that is the all the terms remaining u_j^n and so, that means, here all the terms whatever remaining terms will appear here.

So, this is $n \geq 0$ $j = 1, 2, \dots, N - 1$. So, again this forms a tri-diagonal matrix which leads to a tri-diagonal system $AX = d$. A is a tri-diagonal matrix which can be solved.

So, at every time level N which can be solved by the Thomas algorithm to get X transpose which is $X^T = [u_1^{n+1}, u_2^{n+1}, \dots, u_{N-1}^{n+1}]$ for any $n \geq 0$. Now, we are starting from $n = 0$ which is already the solution known.

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Ex. $u_t = u_{xx}$, $u(x, 0) = \sin \pi x$, $0 < x < 1$
 $u(0, t) = u(1, t) = 0$, $t > 0$
 Crank-Nicolson Scheme
 $-\frac{r}{2}u_{j-1}^{n+1} + 2(r-1)u_j^{n+1} - \frac{r}{2}u_{j+1}^{n+1} = r u_{j-1}^n + 2(1-r)u_j^n + r u_{j+1}^n$
 $r = \delta t / (\delta x)^2$, $r = 1/2$, $\delta x = 1/4$
 $i = 1, 2, 3$, $u_0^{n+1} = 0 = u_4^{n+1}$

$$\begin{bmatrix} 14/6 & -1/6 & 0 \\ -1/6 & 14/6 & -1/6 \\ 0 & -1/6 & 14/6 \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$$

 Stability Scheme
 Consistent if T.E. $\rightarrow 0$ as $\delta t, \delta x \rightarrow 0$.
 Lax equivalence:

So, let us take one example for this case and one simple example will be so, this can be written as so, this can be expressed we say one example is

$$u_t = u_{xx}, u(x, 0) = \sin \pi x, 0 < x < 1 \text{ and}$$

$$u(0, t) = u(1, t) = 0, t > 0$$

So, we can discretize this equation and write as

$$-r u_{j-1}^{n+1} + 2(r-1) u_j^{n+1} - r u_{j+1}^{n+1} = r u_{j-1}^n + 2(r-1) u_j^n - r u_{j+1}^n, r = \mu \frac{\delta t}{(\delta x)^2}$$

since it is unconditionally stable one can choose, so this is the Crank Nicholson scheme.

So, r can be taken to be so, you can choose $r = 1/2$ and $\delta x = 1/4$. So, one can solve this system of equation so $\delta x = 1/4$ means you have the solution to be obtained for $i = 1, 2, 3$, three number of equations and you have $u_0^{n+1} = 0 = u_4^{n+1}$ which is two boundary.

$$\begin{pmatrix} 14/6 & -1/6 & 0 \\ -1/6 & 14/6 & -1/6 \\ 0 & -1/6 & 14/6 \end{pmatrix} \begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}$$

this can be obtained and this provides a with a solution for the Crank Nicolson Scheme for the numerical procedure.

So, this is how the Crank Nicolson Scheme or any implicit scheme or proceeding so that means, you have the solution, so with the knowledge of the solution you are going to t_{n+1} then we are going to t_{n+2} and so on. Now, obviously, since we are starting from a initial condition or from certain stage of time, which we call as the initial condition where it is prescribed and proceeding in time.

So, that means at any stage if we commit any error, so, any mistakes, so, that error will be propagate to the numerical scheme and that will contaminate the successive steps. So, that is why stability of the numerical scheme is very important to know, stability of the numerical scheme.

Now, another thing is that consistency that can be proved that as we define consistency if we define as truncation error T.E. $\rightarrow 0$ as $\delta t/\delta x \rightarrow 0$ as the step size goes to 0, if the truncation error tends to 0 then it is the stable consistent numerical scheme. Now, there is a theorem what is referred as the Lax equivalence theorem states that if numerical scheme is stable and consistent, then it is a converged solution. So this thing we will discuss in the next class. Thank you.