

Introduction to CFD
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Lecture - 22
Numerical Solution of Unsteady Heat Condition (Parabolic PDE)

In the next few lectures, we are going to look at parabolic partial differential equations. One of the example problems where you could have a parabolic partial differential equation is unsteady heat conduction equation.

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Numerical solution of unsteady heat conduction (Parabolic PDE) using various schemes, implementing initial and boundary conditions

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

$u = u(x, t)$ The function 'u' has both time and space dependence

- Unsteady heat conduction equation
- Boundary layer equations
- Parabolized Navier Stokes equations

$$u(x, t + \Delta t) = u(x, t) + \Delta t \frac{\partial u}{\partial t} \Big|_{x,t} + \frac{(\Delta t)^2}{2!} \frac{\partial^2 u}{\partial t^2} \Big|_{x,t} + \dots$$

$\Delta t \rightarrow$ time step
Small number
 $t \rightarrow n$
 $t + \Delta t \rightarrow n + 1$
 Forward difference approximation of order Δt
 1st order time accuracy

$$\frac{\partial u}{\partial t} \Big|_{x,t} = \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} + \frac{(\Delta t)}{2!} \frac{\partial^2 u}{\partial t^2} \Big|_{x,t} + \dots$$

Apart from that, you could have parabolic partial differential equations in boundary layer equations, where you have a thin viscous layer formed on a surface when you have a relatively high Reynolds number of flow over such a surface. However, the viscous effects do not percolate beyond that thin layer. In such a case, you will have a boundary layer formation on the surface of a body, and the governing partial differential equations are of the parabolic kind.

You could also have parabolised Navier Stokes equations where certain terms are modified in the original, Navier Stokes equations in order to give the equations, a parabolic nature. So, there are several possibilities of occurrences of parabolic partial differential equations. However, we are going to look at only one case where you have an unsteady term on the left hand side of the equation that means a time derivative term of the dependent variable.

So, here we are calling the dependent variable as u , this u could be temperature. It could be a velocity component for different types of problems that we look at of the parabolic kind. And we have to remember that this dependent variable is having a time dependence in addition to the space dependence that we have already looked at in elliptic partial differential equations. So, on the left hand side, you have a partial derivative of the dependent variable in time.

And on the right hand side, you have a spatial derivative a second order spatial derivative of the dependent variable, multiplied by a term, α which can be called as a diffusion coefficient. So, depending on the type of physical problem that we are solving this diffusion coefficient can have different implications. So, the most important thing that we need to notice that; the dependent variable u is now having both a space, as well as time dependence.

Earlier in the elliptic equation category, we have seen that the dependent variable is dependent on one or more than one spatial coordinate. So, the independent variables were the spatial coordinates, they had no connection with time. Now, since we have a partial derivative in time, you would like to see how to represent that partial derivative in an approximate form, and we continue with the Taylor series approach, like we did before.

So, we now expand the function u in time by keeping the spatial coordinate unaltered. And therefore, you end up generating different orders of derivative of the dependent variable, u in time multiplied by terms which are dependent on the time step, Δt . So, Δt here is a time step. And of course, we assume that it is a small number, as usual. Now, if you are to retain only 2 terms here.

Then you could approximate the first derivative of u in time, as this. And then you would be left with a Δt raised to the power of 1 in the truncation error as the leading error term. And therefore, this gives you a first order time accuracy. Of course, in a manner similar to how we have used Taylor series in spatial sense, we could generate more, higher order accurate formula for the time derivative.

But here, let us consider this first order accurate time derivative, we would call it as a forward difference approximation of the order, Δt , because we are going forward in time to a different time step, you will see later that we often call the time steps with a superscript. And

in this case, a time step corresponding to $t + \Delta t$ would be called as $n + 1$, because the time step corresponding to t would be called as n .

So, if you look at the nomenclature that way. We could just show the nomenclature to familiarize ourselves that how the space and time would get indicated simultaneously.

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Numerical solution of unsteady heat conduction (Parabolic PDE) using various schemes, implementing initial and boundary conditions

$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$ $u = u(x, t)$ The function 'u' has both time and space dependence

- Unsteady heat conduction equation
- Boundary layer equations
- Parabolized Navier Stokes equations

$u(x, t + \Delta t) = u(x, t) + \Delta t \left. \frac{\partial u}{\partial t} \right|_{x,t} + \frac{(\Delta t)^2}{2!} \left. \frac{\partial^2 u}{\partial t^2} \right|_{x,t} + \dots$

$\left. \frac{\partial u}{\partial t} \right|_{x,t} = \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} - \frac{\Delta t}{2!} \left. \frac{\partial^2 u}{\partial t^2} \right|_{x,t} \dots$ Forward difference approximation of order Δt

Handwritten notes:
 $n+1$ n ← Superscript - Time step.
 $n-1$ u_i ← Suffix subscript Spatial grid location
 $i+1, i-1$

So, you would indicate u add the spatial grid point i at the n th time step in this form. So, the suffix continues to be representing the spatial grid location, the subscript indicates that, and the superscript would represent the time step. So like, you could have different spatial grid locations like $i + 1$, $i - 1$, et cetera. You could also have different time steps indicated as $n + 1$, $n - 1$, and so on.

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Forward time central space (FTCS)

$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$ *CD2*

$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$

$n+1$
 n
 $n-1$

u_w u_e

Boundary conditions at W and E boundaries of the domain

Initial condition ($n=0$)

- The solution at each time step in a Parabolic PDE has physical significance. It is a transient solution which is evolving from its initial to final state subject to satisfaction of boundary conditions.
- The solution at each time step in a Parabolic PDE is not to be confused with solution at an iteration in Elliptic PDE. Solutions generated at intermediate iteration levels do not have any physical significance. Only the converged solution has physical significance.

So, the way we derive the formula for the time derivative in u . We use the same formula here to discretize the time derivative, and evolve the finite difference equation. And a spatial second order derivative is written down here in the form of a central difference, second order accurate, central difference. So, you can now notice that this is a familiar expression for us because this we have already used in elliptic equations.

While this expression in a time derivative sense is comparatively new to us; but we have already familiarized ourselves with the approach. It is the same old Taylor series approach. So, the only additional issue over here is that you are using the superscripts, indicating the different time steps. So, if you watch carefully, the time steps that you have for the 5 different terms that you have generated here are containing the n th time step for 4 out of the 5 terms.

And only 1 term contains the $n + 1$ th time step. Now, that would mean that the terms could be arranged in such a manner that the $n + 1$ th time step value, could be represented on the left hand side of the equation, and all the n th time step values could be written on the right hand side. So, all these terms, correspond to n th time step value. And the specific name given to this kind of discretization of the parabolic partial differential equation is called as forward time central space or abbreviated as FTCS.

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Forward time central space (FTCS)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$$

$$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

Explicit & Implicit

explicit

Boundary conditions at W and E boundaries of the domain

Initial condition ($n=0$)

$n=1$

$t=0$

- The solution at each time step in a Parabolic PDE has physical significance. It is a transient solution which is evolving from its initial to final state subject to satisfaction of boundary conditions.
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So, from our earlier discussions on explicit and implicit schemes who can identify this as an explicit scheme because from this one equation, you can solve for the value of u at the i th grid point. I have spatial grid point. And the $n + 1$ th time step, independent of all other spatial

grid point values. So, since a single equation, helps you to update the value of u at the grid point i at the new time step $n + 1$. This is called as an exclusive scheme.

Now, since we are talking about the time dimension as well in this problem, you have to understand that there is a time $t = 0$, from where all the calculations would start. And that would be called as the initial condition. And we can call that as the $n = 0$, time step. And then from that point onwards, you would generate the next time step value using an equation of this kind for the grid point i .

And similarly, you will repeat these calculations for all the grid points that you have in the domain. So, that you then have the value of i , available at all spatial grid points at the next time step, which would then be called as $n = 1$, and so on. So, as these calculations progress with time, you would reach a general time step n . And then what you have generated before that time step n would be called as the $n - 1$ at time step.

So, everything would be calculated and updated till the n th time step. And then from then onwards you are looking at the $n + 1$ th time step which is the next upcoming time step where you are not able to figure out what the values will be like. So, you would make use of the discretized governing equation then to know that what the values would turn out to be at the next time step $n + 1$.

So, this is essentially an evolution problem where you are actually proceeding with the solution over all the physical grid points and marching the solution in time. So, this is often called as time marching.

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Forward time central space (FTCS)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$$

$$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

time marching

Boundary conditions at W and E boundaries of the domain

Initial condition (n=0)

- The solution at each time step in a Parabolic PDE has physical significance. It is a transient solution which is evolving from its initial to final state subject to satisfaction of boundary conditions.
- The solution at each time step in a Parabolic PDE is not to be confused with solution at an iteration in Elliptic PDE. Solutions generated at intermediate iteration levels do not have any physical significance. Only the converged solution has physical significance.

Now, there are certain very important aspects about the solution that you generate at each of these time steps that you cross. So, it is very important to understand that all these different time steps solutions that you are generating when solving the parabolic partial differential equation in its discrete form, have physical significance. It is a time dependent solution that you are generating, which is often called as a transient solution.

That means the solution changes with time, and is evolving with time, evolving from where it is evolving from an initial condition that you had set at $n = 0$ to a final state, which could come up at a large value of n . And again, there would be a certain check that you would have to carry out in order to ensure that you have reached a final equilibrium state. And all this while, you have been satisfying the boundary conditions.

As you do the time marching, or the repetitive recursive calculations. So, there is an initial state from where you begin. And right from the initial state, you keep satisfying some boundary conditions and evolve the solution in both space and time till you reach a final state which is supposedly an equilibrium state. So, each time step that you cross in the process, and you generate these intermediate solutions which form a part of this transient solution has physical significance.

That means, if you were to study the problem experimentally. Then if you could measure the evolution of these properties by a suitable experimental technique, then you would be able to gather some data, which could be directly comparable with what you are generating

numerically through this exercise. At least they are expected to be of the same order, which means these are measurable quantities, by and large, and they have physical significance.

Now, how does it compare with the iterative steps that we crossed in solving elliptic equations, where we said that we are iterating the solution. And we are trying to start from a guess solution or an initial solution and reach an equilibrium solution finally about intermediate steps, only generate some intermediate values which do not have physical significance.

So, if we revisit these issues regarding what we faced in elliptic equations, we see that when we iterate in the elliptic partial differential equations, the solutions that we generate in the intermediate iteration levels, they do not have any physical significance. They are just iterated values. They are just lying on the path, which we are following to reach an equilibrium state finally, but they as such, do not have any physical significance.

So what has physical significance, it is only the converged solution that will reach at the end at large, iteration levels, usually, that we see physical significance. So, only the equilibrium solution has physical significance. While in parabolic partial differential equations when we solve all intermediate time step calculations have physical significance. This is a very important difference that you need to keep in mind when dealing with solutions, involving elliptic and parabolic partial differential equations.

So, as far as the parabolic equation solution is concerned, we said that we need an initial condition, so, at $n = 0$. You have a certain distribution of values of u . So, if this is the i th grid point. So you have a u_i^0 , which you are prescribing through initial condition. And likewise, you would have suitable values of u at other grid locations.

But all at the time level 0. So that would form the initial condition. And what you pose, at the ends of the domain, because this is a one dimensional domain spanning only along x . So, you have two boundary conditions imposed at the two ends of the domain. One is say at $x = 0$, and another is say at $x = L$, if L is the length of the domain. And what you impose at the West boundary, if we call this as the west boundary and this as the east boundary.

So, what you impose on the west boundary let it be u_W . What you impose at the east boundary let it be u_E . So, these are the boundary conditions which you are imposing at the ends of the domain. And these boundary conditions would remain unchanged. All along the calculations, as you proceed from 1 time step to the other. Right. Till the end is reached, the final state is reached, these boundary conditions remain invariant.

Usually this is the case when we are talking about Dirichlet boundary conditions. However, if we are imposing gradient based boundary conditions then the values at the boundary would get updated based on updates of u in the internal part of the domain, close to that boundary. So, we have seen a small example of solving Laplace equation, using a mixed Dirichlet Von Neumann boundary condition and then we saw that as the iterations proceed.

The values at the Von Neumann boundary were changing with each iteration because they were getting influenced by updating of values in the inner domain, close to that boundary. So, likewise similar thing can happen here. Now, if you are following a particular grid points a grid point i with the FTCS scheme. We can see that we have all these grid points involved in the stencil. So, this is $i - 1$ at n , this is i at n , this is $i + 1$ at n . And this is i at $n + 1$.

So, if you notice the 5 different terms that we have in the discretized equation, all the values belong to these grid points in some way or the other. So, how information propagates in space and time can be indicated through the arrows that we have put on this figure. So, if you watch carefully, the value at the grid point i at $n + 1$ th time step is essentially dependent on all these values that are coming from the n th time step.

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Forward time central space (FTCS)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$$

$$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad (n+1)?$$

n=0

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- The solution at each time step in a Parabolic PDE is not to be confused with solution at an iteration in Elliptic PDE. Solutions generated at intermediate iteration levels do not have any physical significance. Only the converged solution has physical significance.

all the u_is are known.

Boundary conditions at W and E boundaries of the domain

Initial condition (n=0)

Because those are coming from these terms in the discrete or the equation. So, if you notice, they all belong to either $i - 1$ or i or $i + 1$ at grid points at the previous time level that is the n th time level. And remember that till the n th time level, all the u_i s are known, they have already been calculated. While we do not yet know what the values are at $n + 1$ th time level. So, this is being solved.

And how the points are influencing the solution at $n + 1$ th time level is essentially indicated by those arrows in the figure.

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When solving an Elliptic PDE using an explicit technique we ask the question: 'Will the iterations converge to an equilibrium solution?'
Values of main diagonal and off diagonal elements in all the rows of the coefficient matrix determine whether the iterations would converge or not.

When solving a Parabolic PDE with an explicit technique we ask the question: 'Will the time stepping calculations converge to a steady state solution?'
Stability of the finite difference scheme needs to be investigated using Von Neumann stability analysis.

FTCS

Implicit schemes are inherently stable. This can be shown by using Von Neumann stability analysis.

When we were solving elliptic partial differential equations using an explicit technique, we asked the question, or we could ask a question that will be iterations converge finally to an equilibrium solution. This is something that we discussed in the previous lecture. And we got

to know that this would depend on values of the main diagonal and off diagonal elements in all the rows of the coefficient matrix.

So, if this satisfies certain properties, then the iterations are going to converge. If not, they will not converge. So, the properties of the question metrics would decide on reaching convergence in an iterative manner, when we are solving elliptic partial differential equations. How is it, in the case of parabolic partial differential equation, because here we are talking not about iterations, but rather marching the solution in space and time.

So it is, it is like this that you are actually proceeding in time by solving all the values at the range of grid points that you have disposed over space. So, as this process continues; and you are doing it through an explicit technique. The question that one would ask is that will the time stamping calculations finally converges to a steady state solution. So, again we are asking the question of convergence, to a steady state.

But in this case, we are essentially talking about the fact that, because this additional issue of marching the solution in time is concerned, what will be the additional worries, would there be any additional worries. So, here, we would do some kind of a stability analysis of the discrete form of the governing equation. So, the stability of the finite difference scheme that we are using.

Let us say the FTCS scheme that we already came across that needs to be investigated and investigated using a certain method, which is called as the Von Neumann stability analysis. So, we have to use the stability analysis tool, in order to investigate that whether the finite difference scheme has these properties which will ensure reaching of a steady state solution stably.

So, whether it does have the desired stability inherent to it that as the calculations proceed in time. No values would start becoming very erratic or errors will build up in such a manner that the calculations become fraught with error and then finally become unstable and crash. So, this is something that we have to learn how to do. So, we learn about the Von Neumann stability analysis.

Now, one thing that we emphasize that you must have noted is that here we emphasized about the behaviour of explicit techniques because explicit techniques are vulnerable to the stability issues.

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When solving an Elliptic PDE using an explicit technique we ask the question: 'Will the iterations converge to an equilibrium solution?'
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When solving a Parabolic PDE with an explicit technique we ask the question: 'Will the time stepping calculations converge to a steady state solution?'
 Stability of the finite difference scheme needs to be investigated using Von Neumann stability analysis.

Implicit schemes are inherently stable. This can be shown by using Von Neumann stability analysis.

Implicit schemes in general are inherently stable, by and large, and in fact, this can also be displayed through the Von Neumann stability analysis that implicit schemes are not troubled with the stability issue, but explicit schemes are. And therefore, whenever we are handling explicit schemes, we need to be very careful. Especially, when we are marching the solution in time to do a stability analysis and ensure that the scheme will actually work.

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Von Neumann Stability analysis

- The solution of the FD form of a PDE is expanded in a Fourier series.
- A Fourier component contains an **amplitude term** which represents the **temporal level (time level)** of a **grid point** multiplied with an **exponential term with complex argument** (like the one used for **modified wavenumber analysis**) which represents the **spatial location of grid point**.
- Through Fourier representation, **time and space components of the function are represented in a decoupled manner**.
- For a **linear PDE**, various solutions may be linearly combined. Hence taking **one component** of the Fourier series is sufficient in carrying out the Von Neumann stability analysis.
- Linearity of the governing PDE** is a requirement for application of Von Neumann stability analysis

L= domain length
 N= number of grid intervals

$$x_i = \frac{L}{N} i$$

$$u_i^n = U^n e^{jkx_i} = U^n e^{jk\Delta x i}$$

$$u_{i+1}^{n+1} = U^{n+1} e^{jkx_{i+1}} = U^{n+1} e^{jk\Delta x (i+1)}$$

u is assumed to be periodic over length L

So, we will begin the discussion on Von Neumann stability analysis. So, in this method, what we do is, we look at the finite difference form of the partial differential equation and we try to

expand it in a Fourier series. And here when we use the Fourier series, the Fourier components contain 2 terms, essentially.

So, there is an amplitude term, which is representing the temporal level or time level or the time step of a grid point and that is multiplied with an exponential term with complex argument, like the one we use for modified wave number analysis, which represents the spatial location of the grid point. So, we remember that when we were looking at modified wave number analysis, we just looked at the spatial distribution of a function.

And therefore, we had an exponential term, which had a complex argument, which would just take care of the spatial location of the grid point, and through the complex argument, we could look at both the real, as well as the imaginary part of the function, which will be represented through the cosine and sine terms, respectively. Now here, when we have a problem, or both space and time are involved.

We would have to incorporate both the dimensions in some way into the Fourier component. So, what we do is we have 1 term, which takes care of the temporal level or the time level and another term, which looks at this spatial location of the grid point. So, that way, both the dimensions, both the coordinates, the space and time for coordinates get represented. And again, the way we do it also ensures that space and time components are represented in a decoupled manner.

So, we will discuss more about these aspects of the Von Neumann stability analysis in the next lecture. Thank you.