

Computational Fluid Dynamics
Prof. Sreenivas Jayanti
Department of Computer Science and Engineering
Indian Institute of Technology, Madras

Lecture – 26
Discretization of time domain

In a last lecture we have seen the Poisson equation and how to discretize that we have equation sixteen as a Poisson equation subject to Dirichlet boundary conditions.

(Refer Slide Time: 00:18)

Example: 2-D Poisson Equation


(16) $\partial^2 u / \partial x^2 + \partial^2 u / \partial y^2 = f \quad 0 \leq x \leq L \text{ and } 0 \leq y \leq W$
with Dirichlet boundary conditions: $u(x,y) = g(x,y)$ on boundary

• Write $\partial^2 u / \partial x^2|_j \approx [(u_{i,j} - 2u_j + u_{i+1,j}) / (\Delta x^2) + O(\Delta x^2)]$
and $\partial^2 u / \partial y^2|_j \approx [(u_{j-1} - 2u_j + u_{j+1}) / (\Delta y^2) + O(\Delta y^2)]$
and substitute in (16) to get

(17)
$$[(u_{i,j} - 2u_j + u_{i+1,j}) / (\Delta x^2) + [(u_{j-1} - 2u_j + u_{j+1}) / (\Delta y^2)] = f_j + O(\Delta x^2, \Delta y^2)$$

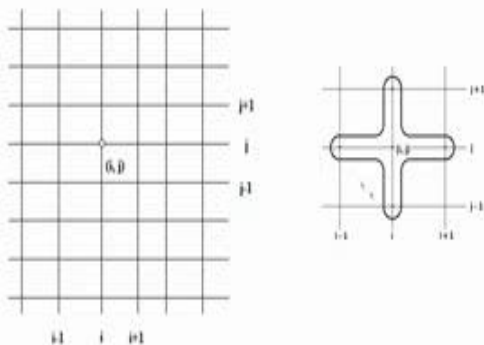

• With Dirichlet boundary conditions, equation (17) would be valid for $2 \leq i \leq N_i \quad 2 \leq j \leq N_j$

• Results in $(N_i - 1) \times (N_j - 1)$ algebraic equations to be solved for $u(i,j)$



(Refer Slide Time: 00:24)

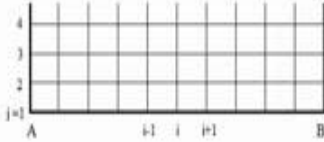
2-d grid

And in which case on a 2 dimensional grid for the point i comma j here we derived a computational molecule consisting of the immediate right and the left neighbors and immediate bottom and top neighbors.

(Refer Slide Time: 00:38)

Boundary conditions



Boundary conditions over AB:

- Dirichlet boundary conditions:
 $u(x_i, y_j) = g(x_i, y_j)$ on AB
- Normal gradient specified:
 $du/dy|_{j=1} = c_i$ for all i at $j=1$
- Convective boundary condition:
 $q''_{j=1} = -k \partial u / \partial y|_{j=1} = h^*(u_{air} - u_{i,1})$; h and u_{air} given

And in case of a boundary we considered three different boundary conditions the Dirichlet boundary condition, on which the value as the variable is specified and normal boundary condition which is the gradient normal gradient is specified. We also considered the convective boundary condition for example, the heat flux given by a convective heat transfer quotient specified and a bulk value of the variable specified and in each case we.


(Refer Slide Time: 01:08)

Poisson Equation: Other Boundary Conditions

- Normal gradient specified, e.g. $du/dy = c_1$ for all i at $j = N_j$
- Values of $u(i, N_j)$ not known and have to be determined
- For these boundary points,

$$du/dy \approx (u_{i,N_{j-1}} - u_{i,N_j}) / \Delta y = c_1 \quad \text{"first order accurate"}$$
 or
$$u_{i,N_j} - u_{i,N_{j-1}} = c_1 \Delta y$$
- Equations for the interior points remain the same
- For second order accuracy, one can write

$$du/dy \approx (a u_{i,N_{j-2}} + b u_{i,N_{j-1}} + c u_{i,N_j}) / \Delta y = c_1$$
- Convective boundary condition: $q''_w = h^*(u_{inf} - u_w)$; h and u_{inf} given
- This can be implemented by noting that $q''_w = -k du/dy$
- Thus, $h^*(u_{inf} - u_{i,N_j}) = -k^*(a u_{i,N_{j-2}} + b u_{i,N_{j-1}} + c u_{i,N_j}) / \Delta y$ which gives the necessary algebraic equation for the boundary point.
- $(N_i - 1) \times (N_j)$ algebraic equations to be solved for $u(i,j)$



We are able to make use of the boundary conditions to develop an algebraic equation for the boundary points. This is using a first order accurate scheme a second order accurate scheme in the case of a convective boundary condition we had a slightly different form of discretized equation for the boundary points. So, in this way we have seen that making use of finite different approximations we can convert a partial differential equation into a set of algebraic equations.

In today's lecture we are going to look at the discretization of the time domain.

(Refer Slide Time: 01:51)

Discretization of Time Domain


- Consider the unsteady heat conduction problem: $\partial T / \partial t = \partial^2 T / \partial x^2$ (18)
- Denote $T(x,t) = T(i \Delta x, n \Delta t) = T_i^n$
- We seek discretization of eqn. (18) of the form

$$(19) \quad \partial T / \partial t \Big|_i^n = \partial^2 T / \partial x^2 \Big|_i^n$$

- Evaluate LHS of (19) using forward differencing as

$$(20) \quad \partial T / \partial t \Big|_i^n = (T_i^{n+1} - T_i^n) / \Delta t + O(\Delta t)$$

- But several options for RHS even if we choose, say, central differencing for $\partial^2 T / \partial x^2$



So, far we have looked at the spatial derivatives, but governing equations also have time derivatives, and we would like to see what additional complexities if any arise in the case of discretization of time derivatives. So, let us consider the unsteady heat conduction problem given by equation 18 here that is $\frac{dT}{dt}$ where; capital T is a temperature equal to alpha which is the diffusivity which is taken as 1 in this particular case. Times $\frac{dT}{dx^2}$. So, it is a one dimensional unsteady heat conduction problem with the thermal diffusivity equal to 1. So, if we have this then a of course, the problem is fully specified only when we do the initial conditions and the boundary conditions we will come to that, but now we have T the temperature as a function of both x and t. So, we denote T of x and T as a in the two-dimensional space of x and T we discretize using the index i in the space domain.

So, that x_i is i times Δx and in the time domain T_n is given as $n \Delta T$ and. So, T of x_i T_n is nothing, but $T_{i,n}$ and it is usual to put the space index as a subscript i here and the time index n as a superscript $T_{i,n}$. So, this is the usual convention that is done. So, this implies the value of T at the spatial grid location of i and the time step location of n corresponding to this. So, we would like to discretize this equation here and so; that means, that we would like to discretize at point i, n , just as we are doing it earlier for i, j here we have i, n where n superscript indicates the time index. So, on both sides we are evaluating the derivatives at i, n and i, n like this.

So, if we look at the left hand side then we can write a simple forward difference like this, $\frac{T_{i,n+1} - T_{i,n}}{\Delta T}$ and. So, the first derivative $\frac{dT}{dt}$ at i, n is given as temperature at $i, n+1$ minus temperature at i, n divided the ΔT because it is a variation with respect to time here. So, the index n changes from $n+1$ to n, this is a forward difference approximation for of first ordered forward difference approximation for $\frac{dT}{dt}$ at i, n here. It is order accurate as we have seen earlier.

Now, what about the space index the space spatial derivative on the right hand side, and here even if you choose for example, this is a second derivative and we can use central differencing. So, we can use central differencing for this, but even then we have certain choices to make, the choice is depend on when we talk about $\frac{dT}{dx^2}$ by $\frac{dT}{dx^2}$ using central differencing we get $\frac{T_{i+1,n} - 2T_{i,n} + T_{i-1,n}}{\Delta x^2}$

divide by delta x square. So, that is an approximation here, but what about the index n the time index n. So, that gives us possibilities. So, that is what we have seen here.

(Refer Slide Time: 05:52)

Explicit and Implicit Schemes

- Put $\frac{\partial^2 T}{\partial x^2} \Big|_n = (T_{i+1,n} - 2T_{i,n} + T_{i-1,n}) / \Delta x^2 + O(\Delta x^2)$ (21)
and substitute (20) and (21) in (19) to get
- Explicit equation for $T_{i,n+1}$:

$$(T_{i,n+1} - T_{i,n}) / \Delta t = (T_{i+1,n} - 2T_{i,n} + T_{i-1,n}) / \Delta x^2$$
or $T_{i,n+1} = T_{i,n} + \Delta t / \Delta x^2 (T_{i+1,n} - 2T_{i,n} + T_{i-1,n}) + O(\Delta t, \Delta x^4)$ (22)
- Put $\frac{\partial^2 T}{\partial x^2} \Big|_n = (T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}) / \Delta x^2 + O(\Delta x^2)$ (23)
and substitute (20) and (21) in (19) to get
- Implicit equation for $T_{i,n+1}$:

$$(T_{i,n+1} - T_{i,n}) / \Delta t = (T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}) / \Delta x^2$$
 or

$$(1 + 2 \Delta t / \Delta x^2) T_{i,n+1} = T_{i,n} + \Delta t / \Delta x^2 (T_{i-1,n+1} + T_{i+1,n+1}) + O(\Delta t, \Delta x^4)$$
 (24)

For example we can write double square T by double x square at i comma n s T i plus 1 n 2 T i n 2 T i n T i minus 1 n divide by delta x square plus terms of the order delta x square this is the second order central difference approximation, but double square T by double x square at i comma n.

Now, what this means is that even though we are looking at time evolving solution, time dependent problem, we are choosing to evaluate the right hand side at the time step n not a n plus 1 not at somewhere else. So, this is 1 particular choice that we are made here. So, this is consistent with our earlier choice of not disturbing the n while changing only i because it is a space index. So, if you now substitute this approximation and this approximation into equation 19 here, we get an expression for T i n plus 1 like this. So, this is T i n plus 1 minus T i n times delta t.

So, here i just put comma n and not used n as a superscript it is a same thing it is much easy to write like this type like this. So, we have this equal to T i plus 1 n minus 2 T i n plus T i minus 1 n divide by delta x square. And you can rearrange the terms here and take this 1 to the right hand side and then you can explicit as T i n plus 1 equal to T i n plus delta T by delta x square this delta T goes here, delta x square times T i plus 1 n minus 2 T i n plus T i minus 1 n.

Now, what is the accuracy of this order of accuracy of this scheme this is first order in time because we made use of a first order accurate approximation here. And it is second order in space. So, if you have all space indices x, y, z like that then we tend to have the same order of accuracy in all the x, y, z coordinates, but if we have time as an independent variable then, it is possible for us in some times it is desirable for us, to make use of a forward differencing, as a as a discretization. Simply because that you get a started for example, if you want evaluate a equation 22 this problem is a time dependent problem it requires in initial solution so; that means, that n equal to 0 we can say or n equal to 1 is the initial guess or initial condition, and the initial condition is given for over this entire space domain. So, as part of this specification of this bound this problem we have given the values of T_{i+1} at every point now making use of these of values of T known values of T_{i+1} at $i, i+1$ and $i-1$ and all that i can get T_{i+n+1} so; that means, that i can sweep through all this values which correspond to n equal to 1 are given here. So, if i want to know this value here then i make use of these values which are known and then get a value for this and then i move here i make use of these values and then get this value like this. So, i go through all these values.

So, that at time steps of 1 equal to 2, everything is known and then i move to the next time level this is part of the boundary conditions. So, this may be given to us. So, i do not need to evaluate these boundary points, but i need to evaluate the interior points and the way that i am doing with equation 22 is that all this is known and even this point and this point is known from the boundary condition. So, in order to do these i can make use of known values of T_{i+n} in order to get this and then once i get this i move on to this and then i solve this and then solve this. So, i evaluate this 1 first this 1 first and then half from in the x direction from i equal to 1 or i equal to 2, to the end point depending on what type of boundary condition is given, and then after sweeping through all the spatial nodes at that particular time step i move on to the next time step.

So, in that sense evaluation of this is very, very simple and we can say that the value of T_{i+n+1} is given in an explicit form involving the solution variables at the previous times step. So, this is known as an explicit formulation of this particular problem. So, the unsteady heat conduction equation can be solved in a fairly simple way like this, but we can also choose to evaluate the right hand side $\text{dou square } T \text{ by } \text{dou } x \text{ square}$ at $i+n$ in terms of the values at $n+1$. This is also an approximation for $\text{dou square } T \text{ by } \text{dou } x$

square a central difference of approximation, but here all the values are being evaluate at n plus one.

Now, if you do this if you were to do this then and substitute this approximation and this approximation into the equation 19 then, we will get an equation like this $T_{i,n+1} - T_{i,n}$ divide by ΔT equal to $T_{i+1,n+1} - 2T_{i,n+1} + T_{i-1,n+1}$ and $T_{i,n+1} - T_{i,n}$ divide by Δx square, and by rearranging all these things we can get $1 + 2\Delta T$ by Δx square times $T_{i,n+1}$ equal to $T_{i,n} + \Delta T$ by Δx square $T_{i+1,n+1} + T_{i-1,n+1}$ and the order of approximation is still second order accurate in space and first order accurate in time.

So, there is no difference in the accuracy between this formulation given by equation 21 and this formulation given by equation 23, they both from an accuracy point of view they are the same, but from an evaluation point of view they are very different in the case of $T_{i,n}$ in the case of equation 22 here, $T_{i,n+1}$ is given explicitly in terms of all known values corresponding to previous times step, in the case of 24 equation 24. If i need to note if i want to evaluate this i need to know this this is known and i need to know this $T_{i,n+1}$ and $n+1$ this is not known because i am still at step i here $T_{i-1,n+1}$.

So, if we go back to discrete here. So, if i want to evaluate for example, this 1 here then, this will involve the value of $T_{i,n}$ here this is known from the initial condition, but it will also involve the left neighbor at the same time step and the right right neighbor at the same time step. So, if i am coming from this side i may know the left neighbor at this stage when i am here, i do not know the right neighbor. So, that mean i cannot explicitly evaluate this i will have to wait and till this is evaluated.

Now, if i want to evaluate this i need to know this value and this value. So, i need to wait until this is evaluated like that. So, if i come to this then i need to know this value and this value and. So, it becomes a coupled equation, i cannot explicitly evaluate only 1 value i have to evaluate all these values simultaneously, at n equal to 2 i need to evaluate all the i value simultaneously by solving a set of algebraic equations which i given like this. So, this is a tri diagonal equation from we will come back to that at a later stage, but this. So, the evaluation of $T_{i,n+1}$ in this particular case is given implicitly. So, $T_{i,n+1}$ is given implicitly in the form of other variables, where as in the case of equation

22 it is given explicitly. So, there is a difference in the way that how we evaluate double square T by double x square makes a difference between an explicit solution or an implicit solution and this is not all we can also evaluate in a different way.

(Refer Slide Time: 15:17)

Other Schemes

- Put $T_{i,n} = (T_{i,n+1} + T_{i,n-1})/2$ to get
- the DuFort-Frankel scheme:

$$(25) \quad (T_{i,n+1} - T_{i,n}) / (\Delta t) = (T_{i,n} - T_{i,n-1} + T_{i,n+1} + T_{i,n}) / \Delta x^2 + O(\Delta t^2, \Delta x^2)$$
 - Explicit, second order accurate and unconditionally stable
- Evaluate RHS at $(n+1/2)$ as $(RHS_n + RHS_{n+1})/2$ and put in (19) to get
- the Crank-Nicolson scheme:

$$(26) \quad -r T_{i,n+1} + (2+2r) T_{i,n} + r T_{i,n-1} = r T_{i,n+1} + (2-2r) T_{i,n} + r T_{i,n-1}$$
 where $r = \Delta t / \Delta x^2$
 - Implicit, second order accurate and unconditionally stable

For example we can put $T_{i,n}$ equal to $(T_{i,n-1} + T_{i,n+1})/2$. So, you take the average of the 2 and then we get different expression here. So, now, if you look at this using a Taylor series approximation we can show that this is second order accurate in time, and also second order accurate in space. So, and we are looking at $T_{i,n+1}$ here and this is given in terms of $T_{i,n-1}$. So, this is an old value. So, this is we can say is known $T_{i,n-1}$ this is the previous time step value. So, known $T_{i,n+1}$. So, this is what we are actually trying to evaluate. So, we can bring this here. So, this is not a new term $T_{i,n-1}$ this is old value $T_{i,n-1}$ this is a old value. So, the resulting expression here 25 is an explicit way of calculating $T_{i,n+1}$ just like in the case of equation 22 here except that this is second order accurate in time.

In a way you can see that it is involving time steps of time values of $n+1$ and $n-1$ here. So, that makes it in a way second order accurate thing which, we can demonstrate through Taylor series expansion and we need to do that demonstration in order to get that proper accuracy. So, this is an explicit second order accurate scheme which is different from either 22 or 25, 23 and we can also evaluate the right hand side not at n or not at $n+1$ that at intermediate values. So, it is all equation of we are

saying that you have a space derivative and do we evaluate based on previous time step or the future time step or we evaluate based on some intermediate time step value.

So, this is an intermediate time step value. So, we can say that the r h s is given as r h s at n plus r h s n plus 1 divide by 2. So, this plus this divide by 2. So, we are effectively evaluating these temperatures which are continuously changing with time we are evaluating at n intermediate value. So, if you do that then, you have an expression which can be finally, brought into this particular form here where you are using the symbol r equal to delta T by delta x square and the form after if i simple algebraic manipulation comes out as minus r T i minus 1 n plus 1 plus 2 plus 2 r times T i i n plus 1 minus r T i plus 1 n plus 1 equal to r T i minus 1 n 2 minus 2 r T i n r T i plus 1 n.

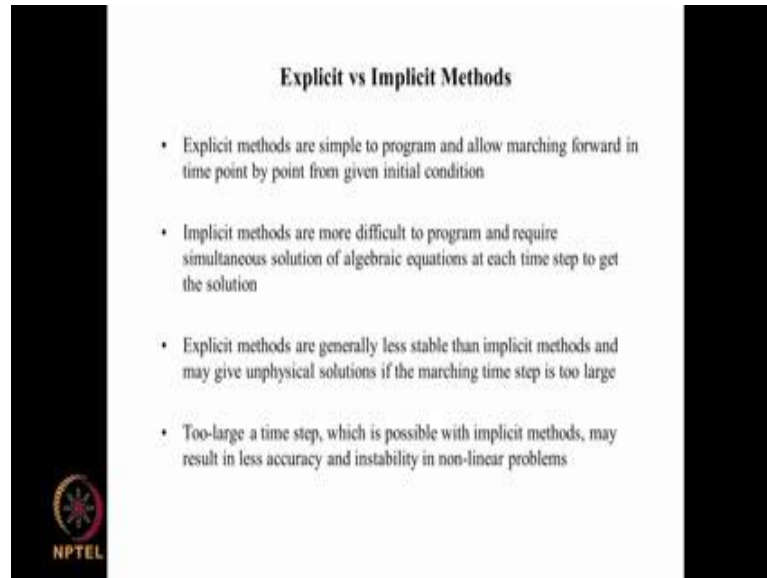
Now, what is a significant about this structure is that all the values that belong to the previous time step values are put on the right hand side. So, the right hand side is known from the previous time step or from the initial condition and the left hand side contains all the values are at n plus 1, which are not at known. So, even if you take the average of these 2 like this there is some component of this which is not known and we cannot solve this explicitly again at a given time step we have to solve for we have to write the equations corresponding to all the space values, and then that gives us a matrix a T equal to b type of matrix and then we can solve that matrix to get a solution here now. So, in that sense this is an implicit and we can show that this is a second order accurate scheme.

So, for the same equation that we have unsteady heat equation we can have very different ways of calculating the temperature variation with both space and time 1 method 1 type of approach is the explicit method, where the calculation of the current value at a particular grid point is expressed in terms of known values at all previous times step or the values which are already computed for example, if you are at T i n plus 1 it may involve T i minus 1 n n plus 1 that is already known. So, once you have an explicit form you can go from grid point to grid point and sweep; sweep through all the grid point at a particular time step and then come back then you can evaluate we can evaluate it in a very simple form.

The other case involving the evaluation of the right hand side term either at n plus 1 or at mid way point or in some other intermediate point weighted average point like that all those things will result in an implicit form and implicit forms requires matrix solution in

order to get $T_{i,n} + 1$. Whereas, an explicit form does not require matrix type of solution, so there is a difference in the way that the 2 solutions evolve and that is summarized over here.

(Refer Slide Time: 21:06)



Explicit vs Implicit Methods

- Explicit methods are simple to program and allow marching forward in time point by point from given initial condition
- Implicit methods are more difficult to program and require simultaneous solution of algebraic equations at each time step to get the solution
- Explicit methods are generally less stable than implicit methods and may give unphysical solutions if the marching time step is too large
- Too-large a time step, which is possible with implicit methods, may result in less accuracy and instability in non-linear problems

NPTEL

So, when you are looking at time discretization. When we are looking at time dependent problems, we have the possibility of an explicit evaluation of $T_{i,n} + 1$ or an implicit evaluation. Explicit methods are simple to program and allow marching forward in time point by point from given initial condition. Implicit methods are more difficult to program and require simultaneous solution of algebraic equations at each time step to get the solution.

So, because you are looking at matrix solution then it is a slightly more complicated now I would say why we want to have explicit methods or why we want to have implicit methods, at this stage we have not brought into play the concept of stability we can ensure it till we understand that in the case of explicit methods we are depending on old values of the variables in order to estimate how the temperature evolves it is like trying to make a forecast of a next year's budget plans based on this year's or previous year's performance. So, past performance is always not a guaranty of future success.

So, this is a rule of stock market everywhere and so; that means, that we cannot take too large time steps, if we do that then there is a potential trouble that is in store in many cases. So, that is expressed in the form of stability constant. So, most of the explicit

methods suffer from this stability problem implicit methods have a certain constraint in the sense that the special variation of T is evaluated at $n + 1$. So, of balancing both sides are a going to be much easier more accurate and it usually will not lead to stability problems.

So, in that sense there is definitely an advantage in going towards implicit methods because you can use large ΔT without having to worry about stability. Whereas, explicit methods because you are forecasting based on previous performance you are limited to take in small time steps and that creates a; that means, that in order to find out what is the state of the system at a say 10 seconds or 100 seconds with an explicit methods may be we will have to take 0.1 or 0.01 times step within implicit method may be you can take 1 time step or 1 second, and then you can get that quickly, but at each with time step you will have to solve a matrix equation. So, there is a difficulty in terms of solving at each time step, but you can take larger time steps we also have to keep in mind there to whether it is implicit or explicit the accuracy of the time derivative approximation $\frac{du}{dt}$ by $\frac{du}{dt}$ that depends on whether it is first order accurate or second order accurate even though implicit method allows you to have large time steps, the error introduced in having a large time step.

The truncation error may mean that you would have to really you cannot effort to have very large time step from an accuracy point of view we will have to reduce to a small time step. And also when we are solving non-linear equations or coupled equations there again, because when you are looking at a coupled equations is like Navier stokes equations as you are trying to evaluate u v is also changing w is also changing so; that means, that you have to freeze the value of v and w while evaluate u and that kind of thing makes demand on what how large time step you can evaluate even with the implicit methods.

So, there are those kind of a problems, but implicit methods are generally more stable you can have larger time step than explicit methods, but explicit methods are much easier to program and evaluate and we can choose those things depending on our preference what type of solution we want and our ability to do computer program and constants on accuracy all those factors coming to picture. So, we can say at this stage we have looked at making finite difference approximations, but time derivatives and space derivatives of any derivative of any order of accuracy and we have also seen how we can put all these

derivatives together in a for a given equation for example, Poisson equation for unsteady heat conduction equation and convert the governing partial differential equation into an algebraic equation at a grid point. And we also seen how we can introduce the boundary conditions into the set of equations and there by converting the entire mathematical problem involving a partial differential equation and a set of initial and boundary conditions into a set of algebraic equations which can be solved as per the formulation of the problem.

In case of explicit method may be we do not need to solve them simultaneously in case of implicit methods or in case of steady state problems involving Poisson elliptic type of things may be we will have to solve them simultaneously. So, with this think we can claim that we are ready to go in to solution of the actual equations. So, in the next lecture we will take a small tutorial problem, and test our knowledge of finite difference approximations and see whether we can solve a problem which is typical of the kind of problems that we would have when we are dealing with fluid flow equations. So, that is in the next lecture in the form of a tutorial.