

Foundation of Scientific Computing

Prof. T. K. Sengupta

Department of Aerospace Engineering

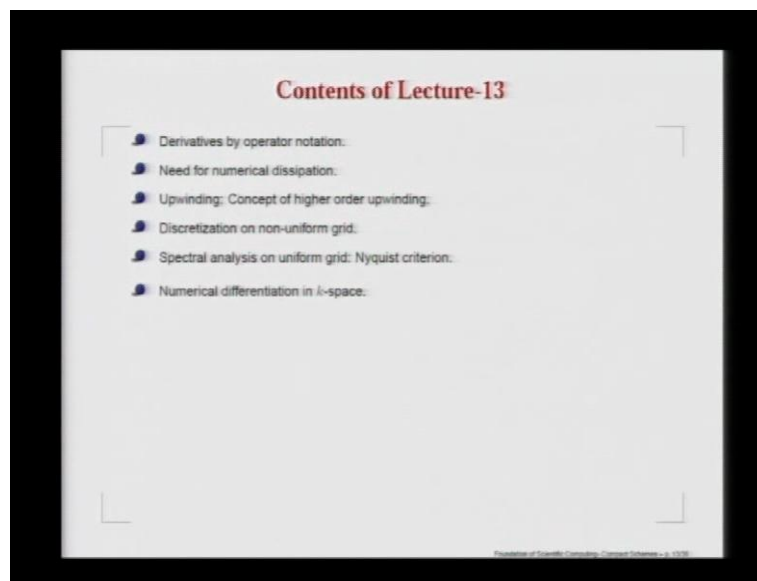
Indian Institute of Technology, Kanpur

Module No. # 01

Lecture No. # 13

In today's lecture number 13, we will again review the derivatives obtained via operator notation. Then we will discuss about why we need upwinding.

(Refer Slide Time: 00:17)



Why do we need numerical dissipation, when we are solving differential equations, which are non-dissipative in nature? While talking about upwinding, we specifically bring the concept of higher order upwinding because in many physical systems, we have dissipative effects, which are represented by second order derivative term. So, to avoid interfering with the physical nature of the problem, we need to bring in higher order upwinding. It means we will be adding numerical dissipation, which are proportional to

fourth or other higher or derivative terms. This is the essence of upwinding and we will see that this is central to many existing methodologies.

So far, we have been talking about discretization on uniform grid, uniform grid of points. Today, I will just introduce you to the topic of discretization on non-uniform grid. We will focus our attention only upon first and second derivatives. Once we set this stage for the discretization, we must be able to analyze the effect of such discretization.

One of the methods that will be central to this course is the spectral analysis. It means, instead of studying the problem in the physical plane, we will be studying the problem in the wave number, frequency plane or k ω plane. So that is the essence of spectral analysis and the moment. We fix our spatial discretization, temporary discretization and the grid spacing. We will see that we do not have unlimited resolution. In this context, we bring in the concept of Nyquist criteria that relates the grid spacing with the maximum number of wave number and that can be resolved by the use of this grid. Having defined the Nyquist criteria, we basically try to show various effects of discretization in the k space or the wave number space and with that we will conclude today's lecture.

(Refer Slide Time: 03:14)

Expressions for Higher Derivatives (Cont.)

As $\delta = 2 \sinh\left(\frac{hD}{2}\right)$ and $\delta_1 = 2 \sinh(hD)$

Therefore, $D = \frac{2}{h} \sinh^{-1}\left(\frac{\delta}{2}\right)$ or $D = \frac{1}{h} \sinh^{-1}(\delta_1)$

$$D = \frac{2}{h} \left[\frac{\delta}{2} - \frac{1}{6} \left(\frac{\delta}{2}\right)^3 + \frac{3}{40} \left(\frac{\delta}{2}\right)^5 - \frac{15}{336} \left(\frac{\delta}{2}\right)^7 + \dots \right] \quad (32)$$

$$D = \frac{1}{h} \left[\frac{\delta_1}{2} - \frac{1}{6} \left(\frac{\delta_1}{2}\right)^3 + \frac{3}{40} \left(\frac{\delta_1}{2}\right)^5 - \frac{15}{336} \left(\frac{\delta_1}{2}\right)^7 + \dots \right] \quad (33)$$

We shall begin. If you note here, it is basically an expression for the first derivative in terms of central difference operators based on half point delta or the integral points delta. You can decide to stop at any point, get expressions of any order and that is one way of doing it.

(Refer Slide Time: 03:43)

6th Order Accurate Symmetric Stencil for First Derivative

Consider an expression for the representation of first derivative that retains only odd derivative terms,

$$\frac{\partial f}{\partial x}\bigg|_i = a (f_{i+3} - f_{i-3}) + b (f_{i+2} - f_{i-2}) + c (f_{i+1} + f_{i-1}) \quad (34)$$

Equating coefficients of derivatives on both sides,

$$f'_i : 1 = 2h (3a + 2b + c)$$

$$f'''_i : 0 = \frac{h^3}{3} (27a + 8b + c)$$

$$f^{(5)}_i : 0 = \frac{h^5}{60} (243a + 32b + c)$$

Solving the above three equations, one gets:

$$a = \frac{1}{60h}, \quad b = -\frac{3}{20h}, \quad c = \frac{3}{4h}$$

Hence,

$$\frac{df}{dx} = \frac{f_{i+3} - 9f_{i+2} + 45f_{i+1} - 45f_{i-1} + 9f_{i-2} - f_{i-3}}{60h} \quad (35)$$

There is another simpler way of doing it and that is what I demonstrated to you in the last class. Suppose, we are interested in finding out a sixth order representation of the first derivative, then we can club the terms in this particular manner. So, this particular clubbing of terms ensures that all the even derivative terms disappear leaving behind only the odd derivative terms. Then in this equation, if you equate the coefficients, it helps you to generate relations for this unknown constants - a, b and c. We are done with collecting coefficients of first, third and fifth derivative. Upon solving those 3 equations, you get an expression of this kind and that it is a central representation. So, you have basically 7 points.

(Refer Slide Time: 05:04)

4th Order Accurate Symmetric Stencil for First Derivative

$$\frac{\partial f}{\partial x}|_i = b(f_{i+2} - f_{i-2}) + c(f_{i+1} + f_{i-1})$$

Equating coefficients of derivatives on both sides.

$$f'_i : 1 = 2h(2b + c)$$

$$f'''_i : 0 = \frac{h^3}{3}(8b + c)$$

Solving the above two equations, one gets:

$$b = -\frac{1}{12h}; \text{ and } c = \frac{8}{12h}$$

Hence,

$$\frac{df}{dx} = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} \quad (36)$$

Although the middle point, i th point would be missing here and that is the way we have constructed it. Same way, if you decide to figure out what the fourth order symmetric stencil would be for first derivative, then you just keep this as first term. Again go through that same process and equate the coefficients of first and third derivative. Solve for it and you get this.

(Refer Slide Time: 05:26)

Symmetric Stencil For 6th Derivative Term

Consider a stencil given by,

$$f''_i = a(f_{i+3} + f_{i-3}) + b(f_{i+2} + f_{i-2}) + c(f_{i+1} + f_{i-1}) + d f_i \quad (37)$$

Correspondingly, only the even derivatives survive, whose coefficients are given by, $f''_i : 2a + 2b + 2c + d = 0$

$$f''_i : 9a + 4b + c = 0$$

$$f^{(iv)}_i : 81a + 16b + c = 0$$

$$f^{(vi)}_i : 729a + 64b + c = \frac{360}{h^6}$$

Solving for a , b , c and d and substituting them in (37), one gets,

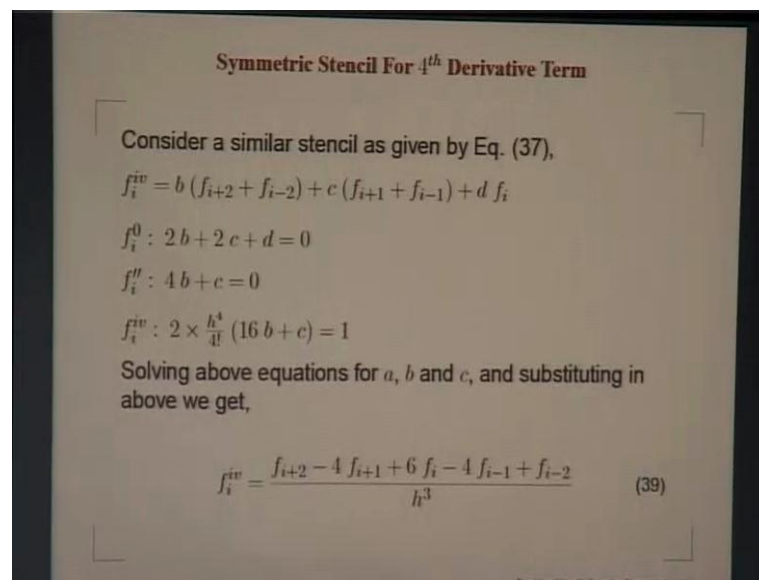
$$f''_i = \frac{f_{i+3} - 6f_{i+2} + 15f_{i+1} - 20f_i + 15f_{i-1} - 6f_{i-2} + f_{i-3}}{h^6} \quad (38)$$

I think, this is where, we were making some point that at times, we need to obtain expressions for even ordered derivatives. Even order derivatives, for example, we have

written down the expression for a sixth derivative as we are interested in even derivative. The clubbing of individual term appears with an intervening plus sign between the pairs. You also have d times f_i and go through that same exercise represented by Taylor series and compare coefficients. For example, a function on the right hand side will have coefficients of this kind and on the left hand side there is none.

The second derivative on the left hand side is none. In fourth also you have nothing. Sixth, you have 1 and then equating the sixth derivative coefficient would give you this. So, once again you have 4 equations for 4 unknowns: a , b and c and d and that will give you the stencil.

(Refer Slide Time: 06:55)



Symmetric Stencil For 4th Derivative Term

Consider a similar stencil as given by Eq. (37),

$$f_i^{iv} = b (f_{i+2} + f_{i-2}) + c (f_{i+1} + f_{i-1}) + d f_i$$

$$f_i^0 : 2b + 2c + d = 0$$

$$f_i'' : 4b + c = 0$$

$$f_i^{iv} : 2 \times \frac{h^4}{4!} (16b + c) = 1$$

Solving above equations for a , b and c , and substituting in above we get,

$$f_i^{iv} = \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^3} \quad (39)$$

Now, the question is why we are doing this and that is where we actually stopped. I mentioned to you that in many physical applications of scientific computing, you would have equations of this kind.

(Refer Slide Time: 07:15)

How

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

Exact \downarrow Dispersion

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1} - u_{i-1}}{2\Delta x} = 0$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i - u_{i-1}}{\Delta x} = 0$$

$$\frac{D\vec{V}}{Dt} = \nabla^2 \vec{V} + \vec{f}$$

$$\frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla) \vec{V} = \nabla^2 \vec{V} + \vec{f}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1} - u_{i-1}}{2\Delta x} = \alpha \frac{\partial^2 u}{\partial x^2}$$

So, substantial derivative would be given by the diffusion term plus additional terms, **if we are not talking about**. So, what happens is, you would be able to write it in a local acceleration form and of course the conductive acceleration form of this kind. So, that is what you noticed. You need to really obtain expressions for first derivative in discretizing. This equation would come from here. Now, what happens is- if you remember when we were solving this simple model equation, depending upon your discretization strategy. For this (Refer Slide Time: 08:32), assume that this is exact and you do not make any error in discretization. Let us make that assumption and then you start noticing that depending on whatever stencil that you would choose for this first derivative, you would have methods, which would be neutrally stable. I mean the solution will behave properly as you expect it to be. In the context, we have some discussion on lectures couple of days ago, where we talked about that. If I do it by first order, a kind of a forward difference or backward difference. Actually, I had dissipation that solution would attenuate and that is something, which we do not like. We also said that if we do some kind of a second order central differencing scheme for this. We notice that this gives rise to dispersion and we discussed it. We made that observation.

Now, what happens is the moment I withdraw this assumption that we can have temporal discretization exact. Let us say, it is represented like this u_{i+1} at i th point minus u_i at the i th point and like this (Refer Slide Time: 10:18). This is what is Euler method. So,

we did talk about that when we are solving initial value problem and you recall that exercise. If I write this like this, we said that it will not attenuate the solution, but it will disperse a combination of this kind of temporal discretization. With the special discretization, it makes this method unusable.

If you try to solve it, you would see that this solution will blow up in time. This is not a very useful combination of method and we will discuss it very shortly. So, what happened is that the amplitude will keep growing with time. If, I want to moderate that growth in time, what I could do is- I could attenuate that growing solution and try to get a balance. Numerically, I am getting this solution to amplify. Now, if I add numerical dissipation, I will attenuate with a judicious choice of the 2. I could nullify the effect of one by the other. So that whatever I am looking for, I am going to get that and it is one way. Of course, this is unstable. Suppose, if I do this again, let us say I am doing Euler time discretization. If I do it like this, how should I do? The solution is going from left to right, if c is positive and that is what it is. What I should be doing here? I should be discretizing it, such that the information will propagate from left to right. So that would be in $U_i - U_{i-1}$ by Δx and this we agreed.

If I did that and I will leave it as an exercise for you to show me, that this one would actually amount to doing this; some coefficient α . So, what we are essentially saying is that look at this (Refer Slide Time: 13:08). First order apprehending is equivalent to doing a second order stencil plus adding a numerical dissipation term. So, this is not there and this is what I will call it as numerical dissipation. In fact, most of computing activities relate to suitably designing numerical dissipation to do a job. That is what we would see, as we go along.

Now, this is perfectly okay and we know that this solution by itself was unstable. So, the moment I added this numerical dissipation term and bringing into play the possibility that the amplification on this side will be balanced by attenuation on this side. So, this may work. I have to be very careful in choosing this constant alpha. We should be able to do that and it is possible. There are many other ways of doing it. So that is panacea for taking an unstable method like this and making it work. This is quite often done and that is not a very difficult task to perform.

(Refer Slide Time: 14:55)

The image shows a green chalkboard with handwritten mathematical derivations. At the top right, the equation
$$** \frac{\partial u}{\partial t} + \left(c \frac{\partial u}{\partial x} \right)_{\text{st}} = \nu \frac{\partial^2 u}{\partial x^2}$$
 is written. Below it, the same equation is shown with a subscript 'nd' under the convection term:
$$\frac{\partial u}{\partial t} + \left(c \frac{\partial u}{\partial x} \right)_{\text{nd}} = \nu \frac{\partial^2 u}{\partial x^2} + \alpha \frac{\partial^3 u}{\partial x^3}$$
. Arrows point from the terms in this equation to labels: 'Physical' points to the diffusion term $\nu \frac{\partial^2 u}{\partial x^2}$, and 'Numerical' points to the third-order term $\alpha \frac{\partial^3 u}{\partial x^3}$. On the left side of the board, the vector form of the equation is written:
$$\frac{D\vec{V}}{Dt} = \nabla^2 \vec{V} + \vec{f}$$
 and
$$(\vec{V} \cdot \nabla) \vec{V} = \nabla^2 \vec{V} + \vec{f}$$
. Below these, a finite difference approximation is shown:
$$u'' + c \frac{u_{i+1} - u_{i-1}}{2\Delta x} = \left(\alpha \frac{\partial^2 u}{\partial x^2} \right)$$
. An arrow points from the $\alpha \frac{\partial^2 u}{\partial x^2}$ term to the label 'Numerical Dissipation'. At the bottom right, the equation
$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + \beta \frac{\partial^3 u}{\partial x^3}$$
 is written, with an arrow pointing from the $\beta \frac{\partial^3 u}{\partial x^3}$ term to the label 'Higher order upwinding'.

However, suppose, instead of this equation, (Refer Slide Time: 14:47) I have been asked to solve an equation of this kind. Let us say, this is some nu times. So, this is what is called as the convection equation. So, this is called the convection diffusion equation. So, this is the diffusion operator appearing here. Now, what happens is- if you have asked to solve this equation, you again adopt the same kind of a thing to Euler time integration here. Let us say, I decided to do first order apprehending. Then, what happens is if I do the first order apprehending, it would be equivalent to this. That will be a second order quantity. On the right hand side, I have this term; this is physical term and to that I am going to add this term.

So, this is physical and this is numerical. So, this is exactly like what we are looking at here. If I decide to do some kind of approximating this convection term of first order, then that would be equivalent to adding some second derivative term like here α times this. What happens? You are in a dilemma because to numerically stabilize it. What you are doing? You have a physical term and to that you are adding a numerical term. This numerical dissipation added, actually interfere with the physical dissipation and this is dangerous. So, what one can do? Instead of going through this route, we will not do this exercise, suppose I do it like this. So, I have the physical dissipation term and the numerical dissipation. Instead of adding with second derivative, I will add it with even higher order derivative. So, what will happen? This is still a dissipative term, but it is not going to interfere with the physical dissipation. This is what we call as higher order upwinding.

Please keep in mind that there are practically no computing methods, which do not use higher order upwinding or the concept of upwinding is pervading. You cannot avoid this. If we do not do upwinding, we end up getting numerical instability. So, upwinding is a order of the day. You have to do it, but the question is how do you do it? You would do it in a lower order fashion like this or in a higher order fashion. Lower order means, where the numerical dissipation is proportional to the second derivative higher order and it is higher than second, it could be fourth derivative, it could be sixth derivative. Those are few and you may have heard people talk about spectral method, which is supposed to be the most accurate numerical method of computing.

Even in spectral calculations, people do add such terms and of course they gave a very fanciful name. They call it as hyper viscosity term. So, if this (Refer Slide Time: 19:48) is your viscosity type of term. Since we are doing it with a higher order derivative, you call it a hyper viscosity term. It is something that you must get use to the idea that there are no computing methods, which will perhaps work without some bit of upwinding. So that is what we want to do. What is the way? You do upwinding and you have seen that. When I do first order upwinding here, it is equivalent to discretizing the convection term by the second order plus a second derivative term. So, that is your first order upwinding and I can extend this logic.

(Refer Slide Time: 20:52)

4th Order Accurate Symmetric Stencil for First Derivative

$$\frac{\partial f}{\partial x}|_i = b(f_{i+2} - f_{i-2}) + c(f_{i+1} + f_{i-1})$$

Equating coefficients of derivatives on both sides.

$$f'_i : 1 = 2h(2b + c)$$

$$f''_i : 0 = \frac{h^3}{3}(8b + c)$$

Solving the above two equations, one gets:

$$b = -\frac{1}{12h}; \text{ and } c = \frac{8}{12h}$$

Hence,

$$\frac{df}{dx} = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} \quad (36)$$

Suppose, I do not write it by second order central difference scheme but I want to do with this a fourth order term. Here, we have a fourth order, sorry fourth order accurate representation of the convection term. Again you will notice that keeping it as an Euler time discretization with fourth order central differencing of the kind given by that equation 36 will still make the method unstable.

So, you would have to add some kind of a dissipation. I would make the point that in most of the computing. You do not like to add second derivative term because the physical dissipations appear with the laplacian operator and that is a second derivative. So, we do not like to give a second derivative term. Instead, we would like to have a fourth derivative term. If I have a fourth order representation of the convection term, on the right hand side, I had an equivalent fourth derivative term and that method will be called as third order upwinding.

This is a nomenclature and you understand the logic. If I talk about nth order upwinding, I am talking about n plus 1th order central differencing plus a derivative, which is n plus 1th derivative and that is what we have been doing. See, we have first derived this sixth order accurate and fourth order accurate expressions for the first derivative.

(Refer Slide Time: 22:52)

Symmetric Stencil For 6th Derivative Term

Consider a stencil given by,

$$f_i^{vi} = a (f_{i+3} + f_{i-3}) + b (f_{i+2} + f_{i-2}) + c (f_{i+1} + f_{i-1}) + d f_i \quad (37)$$

Correspondingly, only the even derivatives survive, whose coefficients are given by, $f_i^0 : 2a + 2b + 2c + d = 0$

$$f_i'' : 9a + 4b + c = 0$$

$$f_i^{iv} : 81a + 16b + c = 0$$

$$f_i^{vi} : 729a + 64b + c = \frac{360}{h^6}$$

Solving for a, b, c and d and substituting them in (37), one gets,

$$f_i^{vi} = \frac{f_{i+3} - 6f_{i+2} + 15f_{i+1} - 20f_i + 15f_{i-1} - 6f_{i-2} + f_{i-3}}{h^6} \quad (38)$$

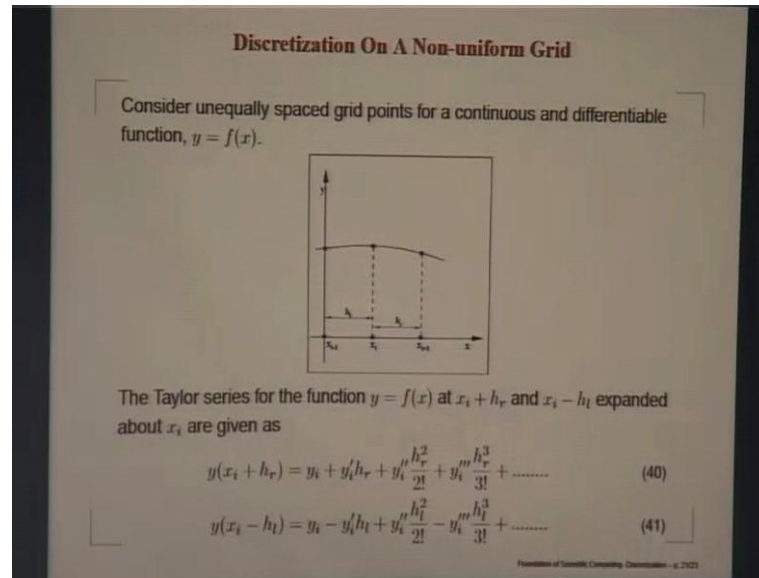
Now, if I want to add a fifth order upwinding, what I would be doing? I will take that sixth order central difference scheme for the diffusion term, sorry convection term to that and I will add the sixth derivative term. If I want to do third order upwinding, then I will do with cd4 or central differencing scheme of fourth order for the convection term. I will add a fourth derivative term as a numerical solution. So that is the whole idea suggested to us and we follow this. Any question? Please tell me, if you have a question, do not feel shy. I mean if you have any confusion, let us discuss it. Well, if you do not have, then we will carry on.

This is a very standard frame, for example, quite a few of you may have even used some of that commercial software like the fluent. It is the one that is quite often used. In fluent software, what you find is that it has options for you. Either you can do it by first order upwinding or if you do not suggest anything, without your knowledge it will do first order upwinding. Then you understand what it does? The added numerical dissipation actually interferes with the physical dissipation and the results are in suspect for most of the time. However, if you go back and look at the fluent code, you will notice that they will also give you an option to do with third order upwinding case. So that is equivalent to what I just now explained to you.

So, this is just for you to get familiar with how these things are done. So, here, we have shown you how a sixth derivative term is obtained. So, that we can construct a fifth order

upwind scheme or we can obtain a fourth derivative term that would fit to this, if we blend that fourth order central differencing scheme, then we can generate the third order upwinding scheme.

(Refer Slide Time: 25:16)



So far we have been talking about all expressions that have grid points spaced equidistantly. However, in most of the calculations that you would notice like the assignment you are doing. If you have a boundary layer very close to the wall, then you need to have very fine spacing near the wall. It would not be very smart to continue with that kind of discretization for the whole domain and that would amount to taking astronomically high number of points. So, what one ends up doing is basically take points, which are non-uniformly distributed. Wherever, you have flow gradients, you have finer spacing. As you go away to regions of interest, where the gradients are not so large, you can keep on increasing.

So, if we do this, how do we obtain derivatives? I have just given a very simple example. Let us say, we have a function of x , y is distributed over non-uniform point. I have this space saying about this central point x_i , which I call as h_l to the left and h_r to the right. Now, what happens? I could obtain this value from this value by Taylor series. So, x_i plus h_r should be written as y obtained at x_i plus y' into h_r and so on. So, you

have couple of expressions for the function to the right and to the left here. So, one can basically use this Taylor series information and obtained derivatives.

(Refer Slide Time: 27:19)

Discretization on a non-uniform grid (Cont.)

Writing the above Taylor series expansion in terms of $\frac{h_r}{h_l} = \beta$, one gets

$$y(x_i + h_r) = y_{i+1} = y_i + y'_i(\beta h_l) + y''_i \frac{\beta^2 h_l^2}{2!} + y'''_i \frac{\beta^3 h_l^3}{3!} + \dots \quad (42)$$

$$y(x_i - h_l) = y_{i-1} = y_i - y'_i h_l + y''_i \frac{h_l^2}{2!} - y'''_i \frac{h_l^3}{3!} + \dots \quad (43)$$

Composing Eqs. (42) and (43), we get

$$y_{i+1} - \beta^2 y_{i-1} = y_i - \beta^2 y_i + y'_i(\beta h_l) + y'_i(\beta^2 h_l) + O(h_l^3)$$

$$y_{i+1} - \beta^2 y_{i-1} = y_i(1 - \beta^2) + y'_i \beta h_l(1 + \beta) + O(h_l^3)$$

Upon simplification one gets

$$y'_i = \frac{y_{i+1} - y_i(1 - \beta^2) - \beta^2 y_{i-1}}{\beta(1 + \beta)h_l} + O(h_l^2) \quad (44)$$

For example, if I decide to write the ratio of this grid spacing h_r by h_l as some quantity called beta, then the right hand neighbour can be written in terms of this. So that is quite understood. So, what we have done? Instead of writing h_r , I have written beta into h_l . It is as simple as that and then this left neighbour has been written in terms of h_l . We have tried to write everything in terms of h_l and this grid parameter, the ratio beta. So, if I look at these two expressions and perform this combination, left hand side is nothing but $y_{i+1} - \beta^2 y_{i-1}$. If I multiply by beta square and subtract from there, then of course you can see the second derivative term will go away. I will have the function itself minus beta into beta square into y_i , then the first derivative will remain. So, first derivative remains like this and the next high order term will be proportional to h_l cube. So, what I could do? I could simplify it and from this I could obtain the first derivative in terms of this.

Since, I have divided both sides by h_l . So, the leading truncation error term is proportional to h_l square. So, by the classical sense, we will be talking about it as a kind of a second order accurate, as well as in terms of a polynomial series and that also is a second order accurate representation. So, this is an expression for the first derivative. We

can similarly manipulate those two equations by multiplying the second equation with beta cube. We can add it to the first equation and then we will get an expression of this kind.

(Refer Slide Time: 29:41)

Discretization on a non-uniform grid (Cont.)

Addition of $\beta^3 \times \text{Eq. (43)}$ to Eq. (42) gives

$$y_{i+1} + \beta^3 y_{i-1} = y_i(1 + \beta^3) + y'_i \beta(1 - \beta^2) + y''_i \frac{h_i^2}{2} \beta^2(1 + \beta) + O(h_i^4) \quad (45)$$

Substituting y'_i from Eq. (44) in Eq. (45) and simplifying one gets

$$y_{i+1} + \beta^3 y_{i-1} = y_i(1 + \beta^3) + \frac{y_{i+1} - y_i(1 - \beta^2) - \beta^2 y_{i-1}}{\beta(1 + \beta)h_i} \beta h_i \times (1 - \beta^2) + y''_i \frac{h_i^2}{2} \beta^2(1 + \beta) + O(h_i^4) \quad (46)$$

Further simplification provides the second derivative expression as

$$y''_i = \frac{2\beta y_{i+1} - 2\beta(1 + \beta)y_i + 2\beta^2 y_{i-1}}{\beta^2(1 + \beta)h_i^2} + O(h_i^2) \quad (47)$$

By performing this, what we have done? We have obtained an expression, which involves everything including y prime at x i. You know already, we have expressions for this quantity. We can use that and when we use that this is what we get. Basically, this is what we are getting. This is an expression, again a second order accurate expression. So, this is something that I think we spent more time. That is adequate for discretization and we will come back to it, when we go to different thing.

(Refer Slide Time: 31:14)

Spectral Analysis of Computing

- Consider the one-dimensional convection equation:

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \quad (1)$$
- This has analytic solution that is non-dissipative and non-dispersive.
- The general solution is written in numerical framework, in the spectral plane by:

$$u(x_m, t^n) = u_m^n = \int U(k, t) e^{ikx_m} dk \quad (2)$$
- With the initial condition given by,

$$u_m^0 = \int U_0(k) e^{ikx_m} dk \quad (3)$$
- Numerically, we can at the most resolve any quantity up to the Nyquist Limit (k_{max}):

$$u(x) = \frac{1}{2\pi} \int_{-k_{max}}^{k_{max}} U(k) e^{ikx} dk$$

where, for a grid of uniform size (h): $k_{max} = \frac{\pi}{h} \quad (4)$

Foundations of Scientific Computing, Springer, 2012

Now, let us start off with a lecture or maybe we will spill over to the next one. We will talk about analyzing computing methods and a few groups including us essentially developed this. This actually refers to expressing the quantities like k in ω plane, wave number, circular frequency plane. That was one of the reason, I spent disproportionate amount of time in familiarizing you with the waves.

So, this is the reason and let us see how we go about doing this. As I have been telling you, this is our favorite equation because this has special property. The property is that the solution is non-dissipative and the solution is non-dispersive. We are talking about the analytical or the exact solution behavior. Now, what we like to do is- represent a solution in a discrete plane. So, the points are at discrete x locations, which are indicated by u of x n . Let us say, we are defining the solutions discrete times, which are indicated by t superscript n . This will be written like this u subscript m superscript n . So, the subscript refers to space and superscript refers to time. What I would be doing? I would be writing that quantity in the k plane and this is your fourier transform.

So, what is it? The fourier laplace amplitude and that will be a function of k , the time dependence and I am putting it in here. So, this is like t to $d t$ n and x variation. We write in terms of k integral. Now in same way, we can define the initial condition and that would be given in solving equation 1. So, initial condition is defined as n equal to 0 and that would be defined by the spectrum at t equal to 0. Whatever initial condition I give, I

can do a fourier transform. The quantity, I will write it as ν naught of k and that is distributed in the k plane and that is what we get.

Now, the next thing that we want to do is try to understand, what we want to do. If you look at equation 3, I have been silent on the limit of integration. Ideally, the peaking one would like to basically extend the limit from minus infinity to plus infinity. You take all possible wave numbers. After that I do not know what the initial condition is. So, in writing 3, we did not put any lower limit or an upper limit, but the moment we decide to work on a finite grid, what happens is something that I would like you to pay attention to.

(Refer Slide Time: 34:23)



Think of the following that we have. Let us say, for ease of understanding, we will talk about uniform spacing. I will write down and let us say this is my initial condition, which I will write it as a function of x . It could be something like this (Refer Slide Time: 34:34). So, what I would be doing? Dividing this domain into equispace points, so Δx and let me just define it as h . Now, if I work on such a grid, what is the smallest wavelength wave I can describe on that grid? What should be the smallest wavelength wave I can describe? 2π by Δx . So, what we are saying? I want to adequately describe a wave. let us say, this is the wave.

(Refer Slide Time: 35:52)



Let us say, this is the wave. How do I define a wave? Let us say, the amplitude and I define a phase and it could also have a phase shift. So, how many quantities? There are 3. So, I need to obtain a , obtain k , obtain ϕ . If I want to fix these 3 quantities, I should be able to substitute it at 3 distinct independent points. I have 3 equations, 3 unknowns and I solve it. I know everything about it. So, what happens is you can very clearly see that with this kind of a grid, I really can describe the smallest wave that is equal to $2h$. These are those 3 points that I could think off because, if I try to do it like this, I do not have a complete description of the wave and the wave is not completely described.

Basically, to describe a complete wave, I would require the full wavelength to be spread over $2h$. So that is your λ_{\min} and λ_{\min} is $2h$. So, what I will get? The corresponding k would be the maximum. k_{\max} would be the number of waves in length to π . So, I will write 2π by λ_{\min} and this is the definition of wave number. What I get is π by h . So, having picked up a grid; a discretization, which is characterized by spacing h . I immediately can say the maximum wave number and I can resolve this. This is what is called as the Nyquist limit. I think most of you are familiar with it. You must have heard of it in your electrical engineering course. If you sample a data at interval of Δt , you immediately say what the maximum frequency is. You can

resolve and that frequency you call as a Nyquist frequency. So, it is the same thing and you can understand.

The logic is exactly same. So, what happens? The very fact that we are constrained to work on a grid of size h . It tells us, despite I have fervent wish that we should like to take it from minus infinity to plus infinity and we could go from minus k max to plus k max. So, this is the first lesson that you understand in performing discrete computing. Your ability to resolve a function is limited by the choice of the grid that you have made. So, that is your Nyquist limit. Now, after this, you should not have any confusion.

(Refer Slide Time: 39:08)

Spectral Analysis of Computing (cont.)

- One can represent first derivative evaluated by any discrete method:

$$\frac{\partial u}{\partial x} = \frac{1}{h} [C] \{u\} \quad (5)$$
- In the spectral plane this can be written as,

$$\frac{\partial u}{\partial x} \bigg|_{x_j} = \frac{1}{2\pi} \int_{-\pi}^{\pi} i k_{eq} U(k) e^{i k x_j} dk \quad (6)$$
- For spectral method: $k_{eq} = k$
- For discrete computing methods:

$$[i k_{eq}]_j = \frac{1}{h} \sum_{l=1}^N C_{jl} e^{i k (x_l - x_j)} \quad (7)$$
- For second order central differencing:

$$k_{eq}^{(2)} = \left[\frac{\sin(kh)}{h} \right] \quad (8)$$
- For fourth order central differencing:

$$k_{eq}^{(4)} = \left[\frac{\sin(kh)}{h} \right] \left[\frac{4 - \cos(kh)}{3} \right]$$

What happens? If I am trying to evaluate a derivative, what do I do? We have written quite a few including today's class. If I want to do it by second order central scheme, a fourth order or a sixth order. What I end up doing? I get the derivative in terms of a matrix operation, C matrix operating on the u r a and that is how we pick up the points. If I do it, I can symbolically write it in a linear algebraic form in this fashion. We do not want to go into the ((.)) of x method versus y method. Let us keep it as general as possible. We talked about the C matrix; you choose your c matrix and do the analysis and that is your part of the deal.

(Refer Slide Time: 40:23)

$$\Delta x \equiv h$$

$$u = \int a e^{ikx} dk$$

$$\frac{\partial u}{\partial x} = \int ika e^{ikx} dk$$

Now, what happens? If I represent a function like what we have written there, if I write it like this (Refer Slide Time: 40:23), well, I would prefer to write it in complex notation and this makes life much easier. So, we understand that we take the real part of that expression and that is where writing in the complex form is necessary. You can explain phase shift. If I excite a system at a wave number k , the response need not necessarily be following with the input. The output could be phase shifted and that is what we wrote. Remember, kx plus ϕ and that ϕ comes from here.

I will have a real part plus imaginary part and I explained that now. If I write it like this in the spectral form, if I take a derivative with respect to x , what do I get? Well, I will get this (Refer Slide Time: 41:27). So, taking a derivative is rather simple. What will you do? You take the Fourier Laplace Amplitude- a , multiply by the corresponding i, k and perform that integral. There is a very specific name to that integral. Those of you, who are from maths, may have heard it or you may not have heard it. It is called a Bromwich integral. So, we will not talk about it more than that. Do understand that in performing the Bromwich integral, I will take the Fourier Laplace Amplitude. I will multiply by individual i, k and I get this. So, this is my exact representation (Refer Slide Time: 42:17). Isn't it? However, when I am going to do it numerically, then what happens? I do not get that and so what do we get? Let me just demonstrate that to you via an example.

(Refer Slide Time: 42:58)

The image shows a chalkboard with handwritten mathematical derivations. At the top, the central difference formula for the derivative is written: $\frac{\partial u}{\partial x} \Big|_{x_n} = \frac{u_{n+1} - u_{n-1}}{2h}$. Below this, the function u_n is expressed as an integral: $u_n = \int U(k, t_n) e^{ikx_n} dk$. A curved arrow points from this integral to the next line, which shows the derivative being taken under the integral sign: $\frac{\partial u}{\partial x} \Big|_{x_n} = \frac{\partial}{\partial x} \left[\int U(k, t_n) e^{ikx_n} dk \right]$. The final line shows the result of the differentiation: $= \int U(k, t_n) e^{ikx_n} (ik) dk$.

Let us say, we decide to show you the derivative at the m th point, in terms of CD2 formula that we have been talking about. Now, of course, n is implied here. So, you can write n . So, I have no quarrel with that. What happens is we have already written this as U of k, t_n into e to the power $i k x_m dk$. So, what do I get from for this? At x_m and t_n , write this 1 over $2h$. What about this quantity, m plus 1 ? m plus 1 means $i k x_m$ plus h , is not it? So, I would write this as the integral remains, u remains the same for all the methods. Here, I will write this as e to the power $i k x_m$ plus h and this part will give me e to the power $i k x_m$ minus h and this will be performing. So, that is what we get. What happens here? I could see that it is 1 over $2h$. I will do this and I will keep U here. What about this (Refer Slide Time: 44:57)? e to the power $i k x_m$ is same. So, I have e to the power $i k h$ minus e to the power minus $i k h$. So, I have e to the power $i k h$ minus e to the power minus $i k h$. I have e to the power $i k x_m dk$ and this.

(Refer Slide Time: 45:28)

The image shows a green chalkboard with handwritten mathematical expressions. The top expression is:

$$\left[\frac{\partial^2}{\partial x^2} \right]_2 = \int U(k, t) \frac{(2i \sin kh)}{h} e^{ikx} dk$$

Below this, there is an equation for k_{eq} :

$$k_{eq} = \frac{(2i \sin kh)}{h}$$

And finally, an equation for $\frac{k_{eq}}{k}$:

$$\frac{k_{eq}}{k} = \frac{\sin kh}{kh}$$

So, what we are getting? I will write this because we have taken a second order central scheme. What is this (Refer Slide Time: 45:45)? This is $2i \sin kh$. So, we are getting it. So, I can cancel the 2 present in the outside. I could write it like this and U , which is of course, a function of k and t into $i \sin kh$ by h . This is multiplied by e to the power ikx in dk . So, if you now compare this expression with the one that I deleted, it is in your notebook. What you notice? In the exact case, what you did? You took the Fourier Laplace Amplitude and multiplied by ik . Here, in discrete operation, first you should not do by ik , but some kind of an equivalent quantity. This ik equivalent and basically I could knock off this. What I could write here? k equivalent by k would be equal to...

(Refer Slide Time: 49:34)

Spectral Analysis of Computing (cont.)

- One can represent first derivative evaluated by any discrete method:

$$\frac{\partial u}{\partial x} = \frac{1}{h} [C] \{u\} \quad (5)$$
- In the spectral plane this can be written as,

$$\frac{\partial u}{\partial x} \Big|_{x_j} = \frac{1}{2\pi} \int i k_{eq} U(k) e^{ikx_j} dk \quad (6)$$
- For spectral method: $k_{eq} = k$
- For discrete computing methods:

$$[i k_{eq}]_j = \frac{1}{h} \sum_{l=1}^N C_{jl} e^{ik(x_l - x_j)} \quad (7)$$
- For second order central differencing:

$$k_{eq}^{(2)} = \left[\frac{\sin(kh)}{h} \right] \quad (8)$$
- For fourth order central differencing:

$$k_{eq}^{(4)} = \left[\frac{\sin(kh)}{h} \right] \left[\frac{4 - \cos(kh)}{3} \right]$$

Now that is what you are seeing in equation 6. When I am doing some kind of discrete operation, of course, I have to sacrifice. I cannot have $i k$, but I will have $i k$ equivalent. If I were doing spectral method, k equivalent is k . You know spectral method represent the function; in terms of some orthogonal basis like the trigonometric function here. So that itself will give you $i k$ equivalent and it should be equal to k itself. Now, what about this? If you look at this expression, what you have? I am looking at the derivative at the m th node. What is it? I should look at on the right hand side. I should look at the m th row of C matrix multiplying the whole vector U and all of you see that. What does the right hand side represent? This will be nothing but, various rows operating on the U vector. So, if you do that on the left hand side, information is for the m th node. Whereas, on the right hand side, U 's or all the U 's. So, you want to U, M . What I am suggesting to you? If I am looking at j th node, then what I should be doing is basically project all the different points that we have.

Say x_1 , which I am writing. Basically, look at this; it is integrated for all the nodes, l equal to 1 to M . So, I have those expressed in terms of $i k \times l$. What I am trying to do is I will try to project all those x_k into x_j . Basically, I would take the entries of the C matrix, which I will call it as... This is the j th row for all possible l and this is a kind of a projection operator that would project every point into the j th point. So, for example, if I

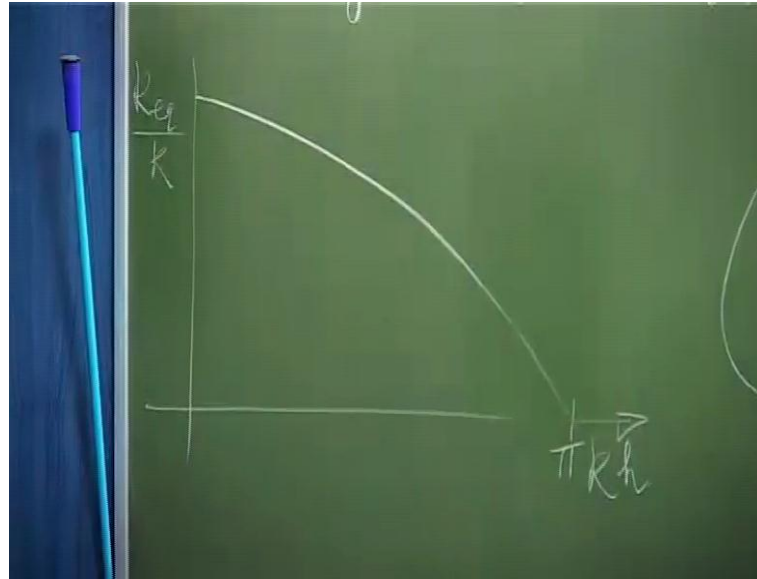
take x_1 , I will multiply by e to the power $i k x_1$ minus x_j into e to the power of $i k x_j$. This is just as simple as sleight of hand. There is not much about it. So, what I find is that, we have been able to really get this information of what this k equivalent is at different point, in terms of the C matrix and this projection operator.

This is a nice way of looking at information in a matrix form. It actually allows you to take a look at the k equivalent at all the points. Why we are talking about all the points? This is something you must realize that this $\frac{\partial u}{\partial x}$ in the equation 5, I have written. It will have different type of formula for different point. For example, say, if you are trying to obtain the derivative in terms of the fourth central representation and that you can do it only from the third point onwards. You realize that you need 5 points. If I try to do it at second point, I go outside the domain. If I try to do it at n minus 1, you can go outside the domain on the right hand side. So, what will happen? The entries of C may not be homogenous for all the lines. It will depend on how you have tackled different points, given the circumstances.

So, what happens is the C matrix that we are writing here has all the information about what you do in the middle or what you do at the boundary. All that information is built in C matrix. With the help of that you can actually obtain this k equivalent for different nodes. This is something you can take advantage of. You can find out, how these things are doing. For the time being, I will look at second order central differencing and I have derived it for you here, what that k equivalent is. It is a $CD2$ method (Refer Slide Time: 52:19). So, I simply added a superscript inside the bracket to indicate it is a second order form and that is $\sin k h$ by h .

Now, we have written down those expressions for the fourth order accurate derivative, for the first derivative and you simplify the way as we have done it. So, what you would be doing? You would be writing the stencil in terms of all those points. That would have n plus 2 to n minus 2 and you could go through all this. You will have some kind of combinations. Those combinations will simplify and give you this. So, the expression I have written in the end. Since it is a fourth order representation, we indicate it by a 4 in the parenthesis. That would be nothing, but $\sin k h$ by h into this factor. So, what does it mean? Actually it means the following.

(Refer Slide Time: 53:31)



On this side, I will plot $k h$ and in this side, I will plot k equivalent by k . Why I am doing it? Because, this is the best way of representing it in a non-dimensional form, K has a dimension 1 over length. k times h would be dimensionless and what is the k max? k max is π by h . So, $k h$ will go from 0 to π . So, this π is your Nyquist limit. This is a universal description of the thing. Now, what about k equivalent by k ? Ideally, I want it to be equal to 1. I do not want any loss of information, but what happens? What is this? This (Refer Slide Time: 54:21) is less than 1. What you are going to find? This goes like this. Well, you do not need to plot anything on the other side. If I had plotted, then the other side would have been like this. You recall, we have done it in your Fourier Transform course and this is what you get.

So, this is your (Refer Slide Time: 54:58) and ideally it should have been equal to 1. So, what is happening in performing discretization? I am losing out this much of information at every k . Ideally, I should have been there, but I am here and my loss of information is more at higher wave number than at lower wave number. So, you see discrete computing brings its baggage of loss of accuracy and this is what you are seeing as the effectiveness of the first derivative. What about k equivalent 4? If I plot it, it will come to 0 at π at the Nyquist limit. So, what you find is that increasing the order of representation, you are actually getting higher accuracy. So, we have done the sixth order representation. You

could go ahead and do it like this. You will see that might be something like this (Refer Slide Time: 56:27). These are all explicit method of representing derivatives. Explicitly, I am obtaining the derivative in terms of the functions. So, that is why these are called explicit methods. For explicit methods, you find out that higher the order, you get higher accuracy and that is what we are seeing here. We can generalize it. I can show it, if I have to obtain this.

(Refer Slide Time: 57:27)

Spectral Analysis of Computing (cont.)

- Using (6) in (1), one obtains,

$$\frac{dU}{U} = - \left[\frac{c \, dt}{h} \right] \sum_{l=1}^N C_{jl} e^{ik(x_l - x_j)}$$
- Define the CFL number as $N_c = \frac{c \, \Delta t}{h}$. If we perform Euler time integration, then the amplification factor $\left[G(k) = \frac{U(k, t + \Delta t)}{U(k, t)} \right]$ is given by,

$$[G_j]_{Euler} = 1 - N_c \sum_{l=1}^N C_{jl} e^{ik(x_l - x_j)}$$

Since we are trying to solve the convection equation, I have just written the derivative in terms of $1 - N_c \sum C_{jl} e^{ik(x_l - x_j)}$. So, I have basically written down the expression for the governing equation in the k plane. Look at these, all are capital U , the Fourier amplitude. So, plugging the Fourier Laplace representation in equation 1, we get this. I will stop here.