

# **Foundation of Scientific Computing**

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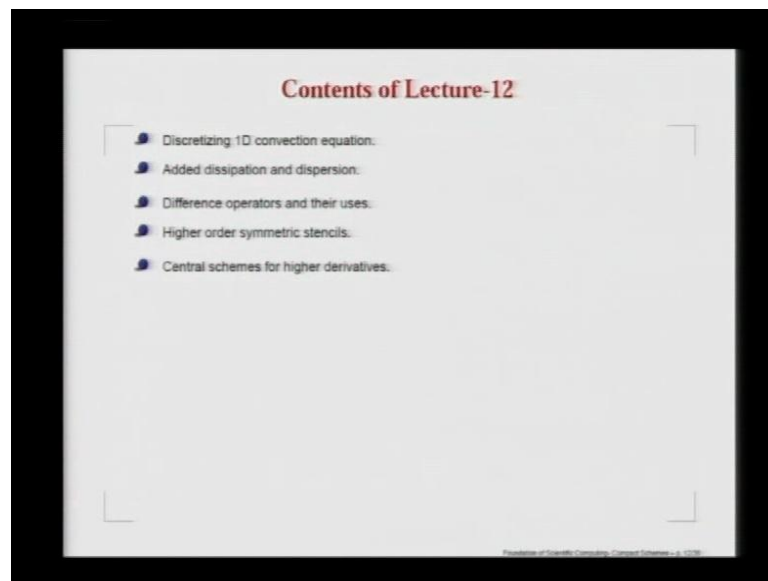
**Indian Institution of Technology, Kanpur**

**Module No. # 01**

**Lecture No. # 12**

We will continue our discussion on discretization on lecture 12. What we are essentially going to do is to display the various concepts by taking up an example of 1D convection equation. This is the most elementary equation that one can talk about.

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However, we would note that discretizing this simple system 1D convection equation which is an example of a non-dissipative, non-dispersive system of solution that will see various discretization methods, actually adds dissipation and dispersion. We will be talking about this in some detail; this will be followed by our discussion of discretization using operators.

This will essentially simplify our expansion methods of differential equations and integral equations. We will develop generic methods of differencing. Specifically, our application for this course will talk about symmetric or the central schemes - that we talked about in yesterday class - but, we will focus our attention on higher order representation, because we are interested in scientific computing. So, we require accuracy and the accuracy would be somewhat related to higher order for explicit schemes and such schemes when they are performed in a central manner do not always function well. That requires, that we use asymmetric stencil and this is what we talked about as upwinding in the last lecture.

In today's lecture, I will show that the upwinding is nothing but a blend of a central scheme using higher order stencil along with a higher order even derivatives, these two together consist of upwinding. After a class, someone came up and asked me that if we use the central difference scheme for discretizing the first derivative in this equation.

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$$\begin{aligned} \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} &= 0 \quad ; \quad c > 0 \\ \left[ \frac{\partial u}{\partial t} \right]_j + c \frac{u_{j+1} - u_j}{\Delta x} &= 0 \\ \left[ \frac{\partial u}{\partial t} \right]_j + \frac{c}{\Delta x} \left[ \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 u}{\partial x^3} - \right] &= 0 \\ \left[ \frac{\partial u}{\partial t} \right]_j + c \left[ \frac{\partial u}{\partial x} \right]_j + \frac{c \Delta x}{2} \left[ \frac{\partial^2 u}{\partial x^2} \right]_j + \frac{c \Delta x^2}{6} \left[ \frac{\partial^3 u}{\partial x^3} \right]_j \dots &= 0 \end{aligned}$$

Why do I say the solution is going to be dispersive? That is the question. To clarify that doubt, what we do is we look at the following two steps: first, we have the continuum equation; from there we come to the discrete equation.

Let me write this part; let us say it is discretized at a node  $j$  without any questions asked about its accuracy. So, the time discretization is accurate and this is what we write. We

do this space discretization using forward difference. So, let us also look at the case with  $C$  positive. If I do a forward differential, I will be doing this at  $\Delta x$  that is what we will be solving.

Now, this is one step; you come from differential equation to difference equation. Now understand, what you are doing? What you can do is, write down the Taylor series of this term and observe, what is the equation that we are in a sense solving? So if I do that, then  $u_j$ ,  $u_j$  will cancel and then I will have  $\Delta x$ ,  $\frac{d}{dx} u \Delta x$  and so on so forth. So this is what we are doing (Refer Slide Time: 05:05).

The first step is from differential equation to difference equation and try to understand what we are doing. We again go to an equivalent differential equation that we are handling numerically - that is what it means. If numerical operation amounts to taking this step 2, that is equivalent to corresponding differential equation of this form. If I do it then of course, this I will get as  $C \frac{d}{dx} u$  and this additional term that will be  $C \Delta x$  by 2 and so on so forth. So, that is equal to 0.

In a sense, what we are doing is that is what I would write by looking at the terms which belong to the parent equation. So this of course is evaluated at  $j$ ; everything is evaluated at the  $j$ th node. So, by discretization we are in a sense solving this equation and every other term being pushed to (Refer Slide Time: 6:49); let me write like this triple  $x$  and so on and so forth, we will have many more terms.

When we decide to solve this equation and we adopt this algorithm that is equivalent to solving this equivalent differential equation. Now, what you are noticing that ideally you would like the right hand side to be equal to 0 but, the discretization forces you to solve an altered equation where the forcing comes from this sort of terms.

Now, looking at that expression immediately will set the alarm bell ringing, what is this term? This is second derivative term but, it is a negative sign and  $C$  is positive, so this is going to give you some kind of an anti diffusion. So, it will not attenuate the solution, what it would do? If you adopt this method to solve this equation you are going to get into trouble.

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

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \frac{u_j - u_{j-1}}{\Delta x} = 0$$

$$\left[ \frac{\partial u}{\partial t} \right]_j + \frac{c}{\Delta x} \left[ 4x \frac{\partial u}{\partial x} + \frac{4x^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{4x^3}{3!} \frac{\partial^3 u}{\partial x^3} + \dots \right] = 0$$

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \left[ \frac{\partial u}{\partial x} \right]_j + \frac{c \Delta x}{2} \left[ \frac{\partial^2 u}{\partial x^2} \right]_j + \frac{c \Delta x^2}{3!} \left[ \frac{\partial^3 u}{\partial x^3} \right]_j + \dots = 0$$

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \left[ \frac{\partial u}{\partial x} \right]_j = - \frac{c \Delta x}{2} \left[ \frac{\partial^2 u}{\partial x^2} \right]_j - \frac{c \Delta x^2}{3!} \left[ \frac{\partial^3 u}{\partial x^3} \right]_j - \dots$$

Now, why did it happen? Well, it is very easy for you to comprehend this scenario by looking at an analytical solution. Let us say, if I have a solution which is at  $t$  equal to 0 like this (Refer Slide Time: 08:33) at a later time or this solution should have just simply bodily shifted itself at a speed  $C$ , that is what that equation means.

Now that means what? The information is propagating from left to right. If the information propagates from left to right, what we have tried to do here? We are trying to find out the information at the  $j$ th node but, how do we develop that information? By looking at what the function is doing at the point to the right (Refer Slide Time: 09:18).

We have violated physics here; the information should have gone from left to right but, your numerical method adopted tell you that it is going in the opposite direction and that is the reason for this (Refer Slide Time: 09:31). This is of course wrong. We should never do it; you got to follow the physics of the problem. You cannot just mindlessly plugin some mathematical expression without thinking what is the consequence going to be.

What you can do? Well, prescription is this, that instead you follow the physics, you know the information should go from, if I am looking at the  $j$  th node. I should get the information from  $j$  minus 1; not the other way round.

What happens is, I should do this (Refer Slide Time: 10:23) and this without even analyzing, I could just simply write it like this but, if you are not convinced you follow the train of thought that we have written down here. So what would we get? If this will be plus (Refer Slide Time: 10:41) this will be minus, this will be plus, this will be minus and so on so forth. What you are going to get is this will be like this, this will be minus and this will be plus and so on so forth. What happens is and then you will get a plus sign here.

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**Taylor series representation (cont.)**

Both these representations of first derivative by the bracketed quantity are first order accurate. The accuracy is determined by the order of a polynomial that is represented exactly by it. Symbolically we will represent the forward difference by,

$$\frac{\partial u}{\partial x}|_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{h}$$

and the backward difference by,

$$\frac{\partial u}{\partial x}|_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{h} \quad (4)$$

Alternately, central difference approximation is given by,

$$\frac{\partial u}{\partial x}|_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} \quad (5)$$

What happens in this case if I do a backward differencing that is, this second formula if we adopt that, that does not valid to physical principle as such in terms of information propagation, because it is going in the right direction, it is going from left to right.

However, taking that particular stencil for the first derivative amongst to having this kind of terms on them and you do understand that they hold lot of terms there; the one which will dominate the dynamics would be the leading terms, because everything is proportional to this grid spacing. So, if the grid spacing itself is small you could see that the higher derivatives would tray loss in terms of their importance.

The leading term would be of course, the leading truncation error term and that is what we also call as a truncation error itself. So, the truncation error all as refers to the leading omitted term not necessarily the whole set because that is too unwinding.

Now, what you notice that as far as information propagation is concerned directionality is maintained but, we have this problem of attenuating the solution, because we adding a dissipation here. So, that is something we should be worried about. So may be in this case, we will go properly in the right direction but, we would see that has time progresses the amplitude will keep coming down. We are again not commenting upon if there is some effect of dispersion in the process; that we will be doing shortly. We will show which method gives what kind of dispersion.

However, you understand that taking a first order accurate method by the followed difference violates physics of the problem and should never be attempted. Taking the backward difference form, it does not violate the directionality of the information propagation but, it surely attenuates the signal and that is something, we should be worried about.

We should not add on numerical dissipation, so this works like a numerical dissipation, physically there is no dissipation in this problem, but solving it by backward difference formula is equivalent to adding a numerical dissipation why because, it is proportional to  $\Delta x$ . In the theoretical limit of  $\Delta x$  going to 0 it should have gone away, it should not have bother you at all, all the right hand side term should disappear.

Now, having noticed that both this method has something bad about themselves. Now, what you could do is, look at the third alternative that we are investigating there. Here, what we would do? We do this (Refer Slide Time: 14:11) and we have already noted that this is higher order equate term, in the sense that you can write down the Taylor series expansion. What would you get is the odd derivatives would disappear isn't it. So,  $u_j$ ,  $u_j$  will go away the first two derivatives, sorry, that will remain. So, I will get this  $C$  by  $2\Delta x$ ,  $u_j$  goes away, so I will get two times this (Refer Slide Time: 14:48) and the second derivative goes away and I will get what? I will put that equal to 0.

Of course, what you are noticing here that is equivalent to solving this equation (Refer Slide Time: 15:28) this  $2\Delta x$ ;  $2\Delta x$  will go away and this is what we are doing and this is again evaluated the  $j$ th node and this term goes to the right hand side. What I am going to get is  $C\Delta x^2$  by 6 and this is my leading omitted terms. So that truncation error is not proportional to the second derivative but, it is proportional third derivative. This is what I noted in the last class, that this brings in dispersion.

Now, the question arose, I think he is missing, whoever asked that question, he is missing today. Why do we say it is dispersion? That is the question; why do we call it dispersion? I am not asking to remember some kind of a mantra that all odd derivatives are dispersion, even derivatives are dissipation; but, we should be able to rationalize, why do we call it dispersion, yes Ravishek, No?

How should we say that it is a dispersion or dissipation? Anyone? I mean we spent about 4 lectures talking about waves touches all about that to make you familiarize, what are these basic physical processes. Shakthi, why do we call it dispersion and how do we name it as yes, it is in the dispersion? No, I will give you a clue, what you do is you try out a so called trial solution. Time amplitude and let us say, e to the power i of kx minus omega t plug this in (( )) that is what we are doing, we are looking at a (( )) plug it in and then you would develop an equation between omega and k, isn't it, that is what we have done for so many days over the last couple of weeks.

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

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \frac{u_{j+1} - u_{j-1}}{2\Delta x} = 0$$

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \left[ \frac{2\Delta x \frac{\partial u}{\partial x}}{2\Delta x} + 2 \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} + \dots \right] = 0$$

$$\left[ \frac{\partial u}{\partial t} \right]_j + c \left[ \frac{\partial u}{\partial x} \right]_j = - \frac{c \Delta x^2}{6} \left[ \frac{\partial^3 u}{\partial x^3} \right]_j \rightarrow \text{Dispersion}$$

Why do I would get then? So del u del t term give me i omega U naught. I am omitting the phase part and this part will give me i k C U naught and what do I get on the right hand side, the leading term will give us C delta x square by 6 and If I take the third derivative then I will get this (Refer Slide Time: 18:50).

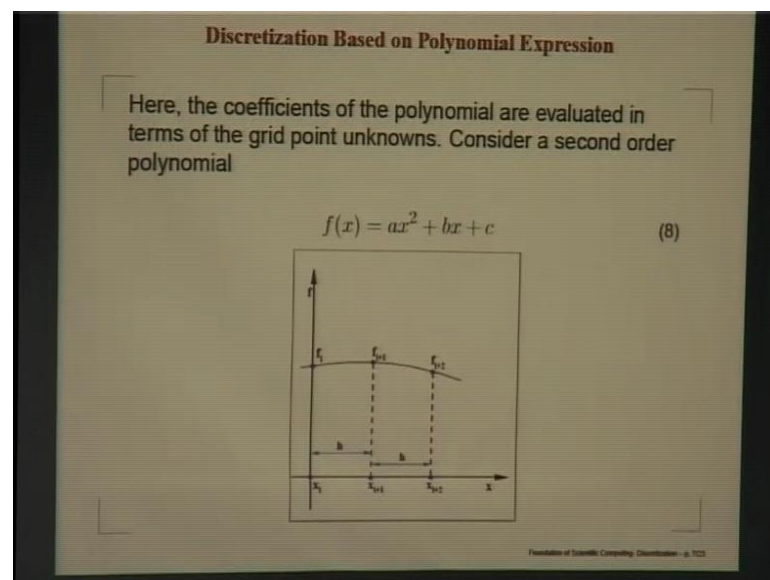


Of course, you can knock off, there will be an  $U$  naught 2, so you can remove this and  $i$  can go away. So, we will get minus  $i$  plus  $i$   $k$   $C$  and on this side. We will get  $k$  cube  $C$   $\Delta x$  square, so  $i$  square will take care of that.

What we get here is then  $\omega$  equal to  $i$   $k$   $C$  minus  $k$  well, this  $i$  will not be there all the  $i$  will go away. So,  $\omega$  equal to  $k$   $C$  minus  $k$  cube  $C$   $\Delta x$  square 6. You have  $\omega$  as a function of  $k$  and how do you find out it is a dispersive or non-dispersive? We calculate the group velocity. If the group velocity happens to be the same for all  $k$  then, we know it is non-dispersive. If group velocity is going to be depended on  $k$  that means, different  $k$  component will transmit its energy at a different speed. So, if I had a compact disturbance at  $t$  equal to zero, it will disperse itself.

You can work it out and you can judge for yourself as why we call that as a dispersive is that clear; if that is clear, you can understand that. We now have our disposal tools to understand what we do numerically and we can observe there potential in solving some given equations.

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Well, I think we started talking about other ways of looking at discretization. The alternative was here; if we try to do a polynomial fit locally and use the function values at discrete nodes then, we can fix this coefficients  $a$ ,  $b$ ,  $c$  in that polynomial representation.

Sir, Yes ((student talks)) Yes. ((student talks)) No, we have written everything at  $j$  th node you see, that is what it is. ((student talks )) But look at it, it is symmetry.

The symmetry of this with respect to this cancels all those information that is what actually happened. So eventually what happened is this; we look at this. What happened as a consequence for the forward difference case was an anti diffusion that lead to numerical instability but here, there is no such thing happening.

What is happening here again, you write that we have not being truthful because, that is the price we pay for discretization; differential equation all has given you a point property and whenever we discretize, we are getting in information from the surrounding point. So, in the hope that  $\Delta x$  going to 0, all this surrounding points will collapse into the pointing question but, at the same time we need to understand what happens to our numerical procedure. The numerical procedure should not lead to some kind of self sustained instabilities that is what happened with forward difference but - in this case it does not - but, instead what happens? Instead of amplification of numerical solution, you are generating Fourier dispersion that is what you see, if this part was not there then,  $d\omega/dk$  is equal to  $C$  that is a non-dispersive solution that is what you wanted.

Now, because of this  $k \cdot q$  term is there, you will see the group velocity is becoming a function of  $k$  and that is the price you are paying. So, I am not for any movement suggesting that if I ask you to solve this equation adopt this, all that we are doing we not able to analyze and say what algorithm gives us what? So, this also is a faulty what because this is going to lead to Fourier dispersion the physical solution does not have this.

Now, coming back to this suppose, we decide to fit a parabola, we can do any order polynomial that we want. If we want to treat a cubic then of course, you will have to fit it with respect to 4 points but, let us keep ambition modest and try to fit a parabola here with respect to  $f_i$ ,  $f_i + 1$  and  $f_i + 2$  and if we do that and can shift the origin to  $x_i$ .

So, if this point has spaced at a distance  $h$ , so  $x_i + 1$  is at  $h$  and this is at  $2h$ . Basically, I will successively plug in  $f$  of  $x_i$  would correspond to this  $x$  equal to 0;  $f$  of  $x_i + 1$  will correspond to  $x$  equal to  $h$  and  $f$  of  $x_i + 2$  would correspond to  $x$  equal to  $2h$ . So we did that and got these three equations, we did solve them and we got these three values.

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**Discretization Based on Polynomial Expression (Cont.)**

In the previous figure the origin is fixed at  $x_i$ , so

$$f(x_i) = f_i = c \quad (9a)$$
$$f(x_{i+1}) = f_{i+1} = ah^2 + bh + c \quad (9b)$$
$$f(x_{i+2}) = f_{i+2} = 4ah^2 + 2bh + c \quad (9c)$$

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**Discretization Based on Polynomial Expression (Cont.)**

Solving above equations for  $a$ ,  $b$  and  $c$ , one gets

$$c = f_i$$
$$b = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$$
$$a = \frac{f_{i+2} - 2f_{i+1} + f_i}{2h^2}$$
$$\left. \frac{df}{dx} \right|_i = b \quad (12)$$
$$\left. \frac{d^2f}{dx^2} \right|_i = 2a \quad (13)$$

The procedure followed here is same as in one-sided difference formulae obtained using Taylor series. Since the expressions satisfy exactly a second order polynomial, we will call it second order accurate.

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Once you have that polynomial expansion you could calculate the derivative. What you have here is a bit of a advantage because, you going to get both the derivatives - the first and the second derivatives at the node  $i$ . If I look at this, we are basically following the same kind of strategy. We are trying to get the information at the  $i$ th node in terms of the information obtain from  $i$  plus 1 and  $i$  plus 2.

Now you see, this kind of artifice of trying to generate information from one side alone is sometimes unavoidable why? Because, if I am trying to solve the problem in a given domain then, I do not know what is outside the domain.

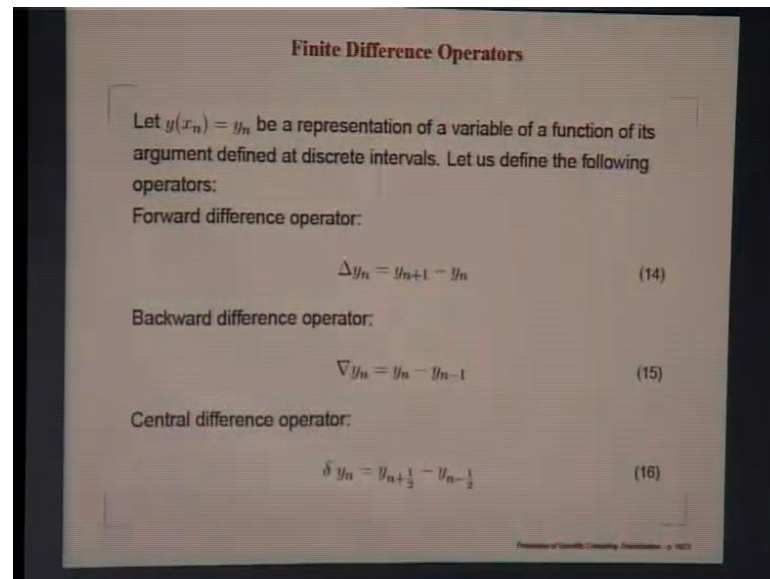
If I am looking at a point on the domain, I have got all the information from inside only. So, I cannot do that this kind of thing central difference; if  $j$  happens to be the boundary node, if it happens to be the left boundary node then, I do not have this and if  $j$  happens to be the right boundary node, I do not have this. Your hand will be forced to adopt one side and this is a major issue; it is not a trivial issue.

In fact, satisfying boundary conditions happens to be  $(( ))$  for all the computing people. I mean, this is not a problem which has been equivocally answered by anyone. We do actually look at specific problem and we do sort of series of investigations, we try to understand how this happens. I will also tell you there are some approaches, which tries to in work physics and get boundary condition information, but it is not necessarily easy.

One thing you notice that we wrote down the first and second derivate at  $i$ , but since you have the polynomial expansion, you could have use the same thing for  $i$  plus 1, then that would be equivalent to your central difference kind of formula.

You are generating information at  $i$  plus 1 in terms of  $i$  and  $i$  plus 2 or you could have used that expression to get that information at  $i$  plus 2, so that would be like your backward difference. What we are written here is like your forward difference, we could have it by using the same thing as the central difference as well as backward difference, so there you have it.

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This looks like all bit off adhoc thing, I will have to juggle and struggle with all this polynomial plugging points. So, mathematicians have tried to formalize it by using operator notation. Suppose, I have a sequence of points for the independent variable  $x$  located at  $n$ ; I will call the dependent variable  $y$  as  $y_n$  then, we can define some of these operators like the forward difference operator would be something like  $y_{n+1}$  minus  $y_n$ . The backward difference operator, we could write it as  $y_n$  minus  $y_{n-1}$ .

The central difference operator, you notice that it is half a point to the right, half a point to the left where we could also do it integral points but then, what happens? The accuracy depends on  $\Delta x$ . If I instead of taking  $\Delta x$  if I take  $\Delta x$  by 2 that you should improve. So, that is the motivation by taking this half node points to the right and left in defining this.

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**Finite difference operators (Cont.)**

In terms of integral nodal values, define a new operator

$$\delta_1 y_n = [y_{n+1} - y_{n-1}] \quad (17)$$

Averaging operator:

$$\mu y_n = \frac{1}{2} [y_{n+\frac{1}{2}} + y_{n-\frac{1}{2}}] \quad (18)$$

Shift operator:

$$E y_n = y_{n+1}, \quad E^{-1} y_n = y_{n-1} \quad (19)$$

Differential operator:

$$D y = \frac{dy}{dx} \quad (20)$$

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As I told you, we could also adopt integral node values then, you realize that I may have to divided by factor 2, because that is the distance between the extreme nodes to delta x. Now, we can also bring in what we call as averaging operation? Averaging operator is mu that means, you are taking the function values with the left and right and average it - with equal rate it.

Now given a point  $y_n$ , I could write  $y_{n+1}$  as if some shift operator is working on it that is, the definition and the same way if I do a inverse operation  $E^{-1}$ , then I go to the point on the left and this is something you all know; you have done it n number of times differentially operated D.

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**Finite Difference Operators (Cont.)**

Using the expressions in the previous slide, relations among different operators are obtained.

$$\Delta y_n = y_{n+1} - y_n = E y_n - y_n = (E - 1)y_n \quad (21)$$

Hence the following identities are obtained,

$$\Delta = E - 1 \text{ and } \nabla = 1 - E^{-1}. \quad (22)$$

Similarly,

$$\mu = \frac{E^{\frac{1}{2}} + E^{-\frac{1}{2}}}{2} \text{ and } \mu^2 = \frac{E + E^{-1} + 2}{4} \quad (23)$$

$$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}} \text{ and } \delta^2 = E + E^{-1} - 2 \quad (24)$$

Therefore,

$$\mu = \left(1 + \frac{\delta^2}{4}\right)^{\frac{1}{2}} \quad (25)$$

Now, we can actually play around with all this operators and definitions and see if we could get something meaningful out of it. For example, the forward difference operator here is defined as  $y_{n+1} - y_n$ ,  $y_{n+1}$ ; I could write in terms of the shift operator  $e$  of  $y_n$  basically, then this forward difference operator operating on  $y_n$  is equal to nothing but  $e - 1$  operating on  $y_n$ . So  $\Delta$  is  $e - 1$ , so this is simple.

Same way, I could write down the backward difference operator. So, this corresponds to actually  $y_n - y_{n-1}$ , so that we have written as  $e^{-1} y_n$  and that is what gives us this. Now,  $\mu$  was the average where you have taken the point shifted half to the right and half to the left. So, shifting half would be equivalent to  $e$  to the power half and shifting half a point to the left would be  $e$  to the power minus half. So, that is your  $\mu$  operator related to the shift operator. So, you can square it and this is what you are going to get.

Now, I think there is the mistake here. This is  $\Delta^2$ ; this  $\Delta^2$  is  $y_{n+1} - y_n$  minus  $y_n - y_{n-1}$ . So this is  $\Delta^2$ , so after squaring we should get that. So, if  $\Delta^2$  is this and  $\mu^2$  is this, you can relate  $\mu$  and  $\Delta$ . The essential idea that we are trying to derive the benefit from is to obtain - some kind of - one kind of operation and try to generate information based on them for the other operators.

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**Finite Difference Operators (Cont.)**

An expression of the differential operators in terms of the forward difference operator:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots \quad (26)$$

Therefore,

$$Ef(x) = \left(1 + \frac{h}{1!}D + \frac{h^2}{2!}D^2 + \frac{h^3}{3!}D^3 + \dots\right)f(x) = e^{hD}f(x) \quad (27)$$

Which implies

$$D = \frac{1}{h} \ln[E] = \frac{\ln(1+\Delta)}{h} = \frac{\ln(1-\nabla)}{h} \quad (28)$$

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For example, if I write a Taylor series of a function about effects for its neighbor  $x$  plus  $h$ , then of course, you write this in terms of the Taylor series and you note this  $f'$  of  $x$ , where this all should have been with in parenthesis, they actually refer to  $D$  of  $f$ . So, this will be  $D$  square; this will be  $D$  cube, so it effectively occurs like this. So, what you notice that quantity with in this bracket is nothing but  $e$  to the power  $hD$ .

So what happens is, we can write  $e$  equal to  $e$  to the power  $hD$  or take log and defined  $D$  as  $1$  over  $h \ln$  of  $e$ . Recall in the previous slide, we had related  $e$  with delta. So,  $e$  is  $1$  plus delta, if I do that then I get  $D$  is equal to  $\ln$  of  $1$  plus delta by  $h$ . In the same way, I could have also written in terms of the backward operator that would be  $\ln$  of  $1$  minus delta by  $h$ .

So basically, what we are trying to do is to obtain say expression for  $D$ . We are obtaining the expression for  $D$  in terms of either the forward difference operator or the backward difference operator and since, you can write out expression for  $\ln$  of  $1$  plus delta, you can actually get this.



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**Finite Difference Operators (Cont.)**

These are exact relations between  $D$  and  $\Delta$  or between  $D$  and  $\nabla$ .  
Expanding the logarithmic term in a series and retaining terms up to specific order, one obtains derivatives expanded up to that order.

$$D = \frac{1}{h} \left[ \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \dots \right] \quad (29)$$
$$D = \frac{1}{h} \left[ \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \dots \right] \quad (30)$$

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So, this is a much more neater way of obtaining the derivatives either in terms of forward or backward operator, provided you know what this delta is and if you know what delta is, you can get this and you can actually derive formula of higher and higher accuracy by including more and more terms. Say for example, if I just keep the first term then, I would have got the forward difference operator that you have to written.

If I retain the first two terms which is going to be a higher accurate formula, because the omitted term would come from delta cube, so that would give you some second order accurate formula. You can actually take one sided formula and obtain higher accuracy representation by taking either this 29 or 30, so that depends on where you are looking at.

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**Expressions for Higher Derivatives**

$$\frac{d^k y}{dx^k} = D^k y$$

$$= \frac{1}{h^k} \left( \Delta^k - \frac{k}{2} \Delta^{k+1} + \frac{k(3k+5)}{24} \Delta^{k+2} - \frac{k(k+2)(k+3)}{48} \Delta^{k+3} + \dots \right) y \quad (31)$$

As  $\delta_1 = E - E^{-1}$ ,  $\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}$  and  $E = e^{hD}$

$$\delta = e^{\frac{hD}{2}} - e^{-\frac{hD}{2}} = 2 \left[ \frac{e^{\frac{hD}{2}} - e^{-\frac{hD}{2}}}{2} \right]$$

$$\delta_1 = e^{hD} - e^{-hD} = 2 \left[ \frac{e^{hD} - e^{-hD}}{2} \right]$$

Having formally obtained the expression for D in terms of those forward or backward operator; you could get any derivatives. If I say for example, I am looking for the k th derivative, so that is D to the power k operating on y and since, I have D as a function of - let us say - delta I could take that whole series and raise it to the power k and simplify. This is what we are going to get.

Now, once again I suppose there would be a factor of 2 coming here because, these are based on integral nodes. So this delta 1, we defined as  $y_{n+1} - y_n$  by 2, so that 2 is missing; there is a mistake here, I will correct it whereas, central difference operator based on half node is delta that is given here. Since, we have already established e is equal to e to the power h of D, so I could plug this here and write delta in terms of this.

So, e to the power hD by 2 minus e to the power minus hD by 2, I can write it like this. So, the quantity in the square bracket resembles that sign hyperbolic function, so that is what we get. In terms of integral nodes, we could write this and I suppose, there is a factor of 2 missing then, this 2 will not be there.

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**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  $D = \frac{1}{h} \sinh^{-1}(\delta_1)$

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

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

What happens is, then we could write the central difference operator as 2 times sign hyperbolic  $hD$  by 2 or delta 1 in terms of - please ignore this 2 part the sin hyperbolic  $h$  of  $D$ . So, what I could do is then from here, I could write  $D$  as 2 by  $h$  sin hyperbolic inverse this quantity. You look up any mathematics hand book, you will find out they will happily give you all kinds of series expansion for the sign of hyperbolic inverse function and that is what your 32 is; 32 is nothing but this expression.

So, what you got here is this. So, this is an alternative form where you are getting the first derivative in terms of only central differencing, because this deltas are the central difference operators; these are not one sided or you could write it in terms of those integral node values. Then, you would have delta 1 and then, you can write this. So, these are formal ways of simplifying your task and getting as high and accurate formula that you want.

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**6<sup>th</sup> Order Accurate Symmetric Stencil for First Derivative**

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

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

Equating coefficients of derivatives on both sides.

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

$$f''_n : 0 = \frac{h^2}{3} (27a + 8b + c)$$

$$f'''_n : 0 = \frac{h^3}{60} (243a + 32b + c)$$

Solving the above three equations, one gets:

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

Hence,

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

Well, in those are very nice; I could have gone back and done, what we are trying to do here. If I want to obtain formally higher order, let us say sixth order accurate stencil for first derivative. You realize that most of the time, your governing equations usually have the first derivatives and second derivatives. You look at any branch of physics at the most you will get byquadratic - fourth derivative. So, we will try to get some of those expressions explicitly and we have also realized by now that we can derive higher accuracy by taking higher order formula and that is what we are trying to do.

So, our basic aim is to obtain a first derivative which will be of sixth order accuracy. At the same time, we would like to do it like central differencing because, we have seen if we try to do one side and we have to be careful because, we may like to add numerical dissipation that in the process we have seen that it could instead add anti diffusion.

So, one of the safest way in computing is always try to begin with symmetric operator - symmetric stencil, so that you do not add either dissipation or anti diffusion, both the cases are bad. If you add dissipation, it is going dump out the signal. If you of course, add anti diffusion, you do not have to worry, the code will block on your face; you will know that you are wrong.

The problem is the other way, the problem is when you have a working code but the solutions are wrong unfortunately, that is the story of all commercial software. They are

all wrong, most of them know and because they **un physically** attenuate the solution. So, to avoid that pitfall, it is always better that you go to a symmetric stencil and if I want to write a asymmetric stencil, what have we seen so far? That the first round of accurate formula for that first derivative involved two points; second order accurate formula required three points  $j + 1$  and  $j - 1$ , if I am trying to find out at  $j$ .

If I extend the logic, so sixth order accurate formula would require seven points. If, I am looking at  $i$  th node; excluding that  $i$  th node, I need to take three points to left, three additional points to the right and if I club them in this clever manner, then what do I notice? All the even derivatives will disappear, because of this minus sign you see,  $f_{i+3} - f_{i-3} + 2f_{i+2} - 2f_{i-2}$ .

So, we are trying to develop an expression, where we do not want even derivatives to be there because, they can do both the things that we have talked about. So, we would club them like this since the coefficients ask 1. So, all those even derivatives go away and expand this right hand side and on the left hand side, we have only first derivative.

If, I look at the first derivative, I do not know why I mixed it up with  $i$  and  $n$ . So, this could be  $i$ , so  $f'_i$ , left hand side could sufficient is 1 and on the right hand side, what do I get from here, I will get  $3h$  into the first derivative of derivative 2; one coming from here, one coming from there, so that is what I have  $6h$  here. So, this combination will give you everything the factor of 2, so I have taken the 2 out and the lead term has  $h$  there so that is what we are getting. So this will give me  $3a$ ; this will give me  $2b$  and this will give me  $C$ , so that is what we are getting.

The higher derivatives of course, there will be 0; there is nothing on this side, so the third derivative is 0 whereas the right hand side gives me this. So, what is this? This is 3 cube, this is 2 cube, this is 1 cube. This one is 3 to the power 5, 2 to the power 5, 1 to the power 5. So, you can see a very neat order there and we are trying to fix this three unknown coefficients  $a$ ,  $b$  and  $c$ . So I just stop here, because we have adequate number of equations for this three unknowns and we solve them and this is what you get.

So, this is we have sixth order accurate formula, which will involve  $i + 3$  to  $i - 3$ .

You also notice one interesting feature of this formula. Looking at the formula, you can tell that this is a non-dissipative formula why? There is no term involving  $f_i$ .

If there was a term involving  $f_i$  then you are sure there is some dissipation involved in. See, that is what we have done; we have not included in  $f_i$  term to keep the even derivatives away, so that is what we are seeing here. So, this is what you get. So, If, I am saying it is a sixth order accurate. So, what is the leading truncation error term that would be proportional to that will be proportional to the seventh derivative term. We have stopped here at  $f_5$ . So, the next term will be  $f_7$ .

So, as far as the polynomial expansion of  $\phi_4$  is concerned its satisfies exactly a sixth order polynomial, because we are fixing  $a$  and  $b$  and  $c$  by equating right and left hand side. Anything that is unbalance is at the seventh derivative, so that is why we would call this as a sixth order accurate method.

(( ))

Yes

(( ))

What I did on the right hand side? I just simply wrote at a Taylor series. So, we writing the Taylor series about the node  $i$  th node because, left hand side the first derivative as at the  $i$  th node right So, once you do that you are basically equating the coefficients on either side and once you have three equations - three unknowns - if solve them and this is what you get. So, this is a sixth order accurate stencil for first derivative.

Now, what happens suppose, I would have try to do that with a fourth order accurate stencil then of course, this is super flows.

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**4<sup>th</sup> Order Accurate Symmetric Stencil for First Derivative**

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

Equating coefficients of derivatives on both sides.

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

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

Solving the above two equations, one gets:

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

Hence,

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

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As I explain to you, the fourth order would involve five points; two to the left, two to the right, so we should have began with d and c and once we do that, this is what we get. So, even this is unnecessary and then, we equate this to fix this two constants b and c by equating the coefficients of f prime and f triple prime and solve them to get this. So, this is your fourth order accurate expansion for the first derivative. Again this is a non dissipative formulas and symmetric stencil.

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**Symmetric Stencil For 6<sup>th</sup> 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,  $f'' : 2a + 2b + 2c + d = 0$

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

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

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

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

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

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Now this is something I would first derive it and then, I will explain why we are doing this. Let us say, we are trying to find out an expression for the sixth derivative term. So far we have been looking at the first derivative, so let us try to derive an expression for sixth derivative by using symmetric stencil. Now sixth derivative means, it is an even derivative. So, if I want to write a symmetric stencil, what should I do? I would again club them and not only should the point should be there this should be also in equal proportion.

So, if I have  $f_{i+3}$  and  $f_{i-3}$  look at their coefficients; coefficients are same. So, I cannot write  $2f_{i+3} + 3f_{i-3}$  that is not the symmetry. So, symmetry requires this coefficients to be same and that coefficient has been brought out here as a, b, c etcetera. The point that I made that if I am looking for even derivatives, I should have to add the point itself, so D into  $f_i$  (Refer Slide Time: 48:33).

You also noticed that we are interested in looking at the even derivatives that is why the intervening sign are now all plus. First derivative, we did it like, coupled them over with minus sign in between. Now, we are putting all of them with the plus sign. So, when we add this up, what will happen? The odd derivatives will disappear and all we would be left with the even derivative terms including the function. So, if I look at that the function value  $f_i$  has of course, D coming from there. From here I will get  $2c$ ; from here I will get  $2b$  and from here I will get  $2a$  that is your first equation, so this is the  $f$  of 0 (Refer Slide Time: 49:24).

Now, the second derivative term of course, will come from each one of them except the D term and this is what we get. So, we have a four unknowns; we stop at  $f_7$  and we can solve for this a, b, c, d. I plug it in there. So that is what I observed that, if I am looking at an expression for the even derivative by symmetric stencil, you will notice that the coefficients have to be same. So, this is plus 15, this is plus 15. This is minus 6, that is also minus 6 and this plus 1 the last 1 is plus 1 and the D is of course, standing out by itself that is minus 20. So, this is what we do this is what we do. Now, you should ask why all this gymnastics that we are doing but, before I do that I will just simply conclude this part that if I am trying to find out an expression, let us say for now not the sixth derivative but the fourth derivative.



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**Symmetric Stencil For 4<sup>th</sup> 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,

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

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We will go through that same exercise again and look for three equations for three unknowns, solve them and this is what we get. ((students talks)). We are just calculating the derivative itself. Now, it depends on how you use it in your difference equation. If you use it, keep it on the right hand side and keep it with a plus sign that will be a diffusion term. If you do it with a minus sign, that will be anti-diffusive. So, we are getting the expressions and giving the degree of freedom to choose the way you want to use it in actual equation. Now, why we do what we have done? I mean why did we do all this? Well, whatever we have here on the board, we can make use of it and see what we are doing.

Now, let see if we would have done this for that equation then well, we have got term like this and what we find that this is anti-diffusive and if instead I had written it like this then, I would have got an similar equation like what we have here. So, you see some times taking one side stencil and let say here, what we have here is a first order accurate expression is equivalent to solving the given equation by having some next higher order even derivative. So, this was a first order accurate method.

So, that is equivalent to solving this equation - actual given equation - plus a next higher order derivative. So it has first order method; so you have a second derivative appearing there; this is a simple equation. In your actual application, what you would be doing is a

complex equation may be with the second derivative, first derivative terms coming they would be with the non-linearity so, on so, forth.

So, if this has the simple constant coefficient linear equation and we are seeing this; that solving this method by a odd order accurate method is equivalent to solving the actual equation and spiking it with the next higher order dissipative term. So, then we have seen that if we develop a method, let say will show it in the next class perhaps. What we find is that, solving it by a central method leads to some kind of numerical instability. So, what we can do is, if we know the method is numerically unstable, we can try to stabilize it numerically and how do I stabilize it? So, the amplitude is growing because of numerical instability, so I would add some dissipation how do I add dissipation? We have seen this first order up winding is equivalent to adding a second derivative term.

In many physical problems, you will find that the governing equation already have second derivative term, then is it safe to add second derivative term for numerical stabilization? Answer is no, because you are going to alter the physics of the problem, because physically itself, there is second derivative term.

So, what you may like to do is numerically stabilize those cases adding higher derivative terms. So, I would not add second derivative term but, I would add fourth derivative or sixth derivative and that is what you have been trying to do. We are trying to find out expressions for fourth derivative here or in the previous case; we are trying to find out the sixth derivative here (Refer Slide Time: 56:24).

So what I would do is, I may decide to take a symmetric stencil for the first derivative but application of the symmetric stencil on the first derivative gives me a method, which is unstable - numerically unstable. So, what is stable? What is unstable? We will discuss it in the very next class, then how do I rectify? The rectification can come through by selective explicit addition of even derivative term and when you do that this is what we call it as up winding. Basically, we are creating a proper **bias** to the solution and that is what we will talking about in the next class.