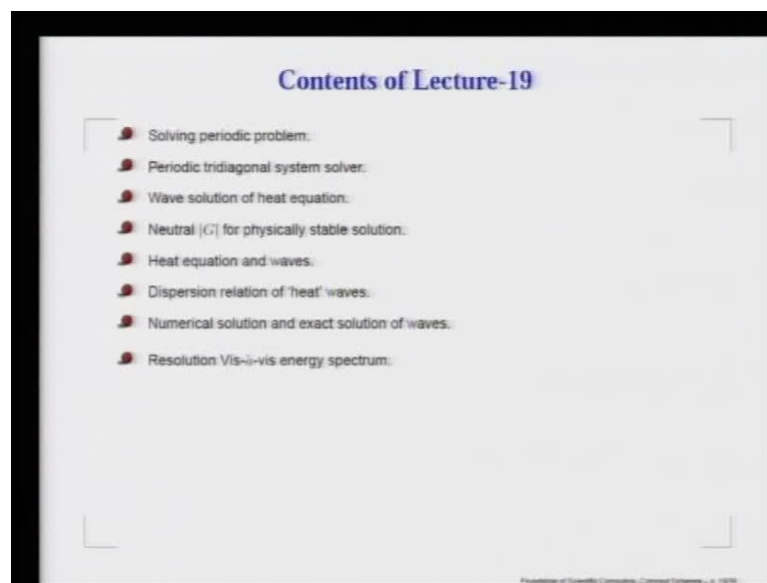


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**Module No. # 01**

**Lecture No. # 19**

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On lecture 19 today, we are going to once again explore - how do we solve the periodic problem? And in this context, we develop in detail, steps how this periodic tridiagonal system solver is obtained. And it shows that the number of operations does increase, but we still end up having an analytic solution and this is certainly a plus point for any numerical method that involves, invokes tridiagonal matrices.

We have talked about waves in this course and we have noticed that even parabolic equation can give rise to waves, and in this context we want to study the heat equation and show how wavy solutions are possible. This comes about through the application of time harmonic periodic boundary condition and for such a solution, once again, we need to establish that the modulus of the numerical amplification factor has to be neutral, so that we can obtain physically stable solution.

Continuing our discussion on heat equation and waves, we obtain analytically its dispersion relation, and then we set up quite standard numerical solution techniques for this wave solution and compare it with the exact version of it. And that will tell us what are our requirements of obtaining wavy solutions, and in this context, we do talk about the spectrum of the solution and how to resolve this energy spectrum? That would be what we will be discussing finally on this lecture.

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So, we can begin today. In the last class, we were discussing about the distinction between periodic and non-periodic problems and what we noticed for this simple equation. If we have periodic problem, then we still end up getting the same linear algebraic equation from unknown vector  $x$ , evaluated by solving this linear algebraic equation.

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$$u_t = u_{xx} \text{ periodic in } x$$

$$[A]\{x\} = \{b\}$$

$$A = \begin{bmatrix} b_1 & c_1 & & & \\ u_2 & b_2 & 0 & & \\ & & \ddots & & \\ a_n & b_n & & & \\ c_n & & & & \end{bmatrix} = \begin{bmatrix} q_1 & 0 & & & \\ p_2 & q_2 & & & \\ & & \ddots & & \\ r_1 & r_2 & & & \\ q_{n-2} & b_n & q_n & & \end{bmatrix}$$

$$\{x\} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}$$

$$\{b\} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$A = L + U$$

I suppose, by now all of you are pretty much conversant, and you can see it very clearly that the whole activity of computing revolves around having either a differential equation or integral equations or any other forms of discrete equations, that you can develop by say, Monte Carlo technique or Lattice Boltzmann. Whatever you do, at the end of the day all you have to do is solve linear algebraic equation; so, linear algebraic equation actually occupies a huge space in this study.

Here also, you notice that this equation looks the same, but A matrix had a specific structure that we talked about. So, we note it down like this, and what we notice that due to periodicity, we had an entry at the last column and the first row. Now, the other lines do behave as before because we do not have any problem there, and we can go on all the way getting  $b_n$  here and we get  $a_n$  here and again we get  $c_n$  as the first entry on the last row.

So, this is the structure of this A matrix. If it was not periodic, what we suggested that we will do a l u d composition. We will show it as a product of a lower and an upper triangular matrix. Here also, let us be ambitious and try to do the same thing and what we would do? We will write it like this. So, the lower triangular matrix, I will write it like this, let us say  $q_1$ , let me first write then we will discuss. Why we write the way we are writing? And here on we have zeroes, and I will leave something blank in the last row,

but let me first write down the matrix and then you will understand, why we are doing, what we are doing?

So, we will have again an upper triangular matrix with diagonal entry as 1 and the super diagonal terms, we would write it like  $u_1$  and there would be  $u_2$  and all the way up to  $u_{n-1}$ . Now, you see, to account for this entry a 1 here, you cannot afford to have all these things 0, the otherwise you will not be able to match that a 1, is not it? To match that a 1, I must have a non-zero entry here. So, to do that what I would do, I will introduce a stack of unknowns, let me call them as  $w_1, w_2$  all the way up to  $w_{n-2}$ .

Now you can see, that if I multiply this row with the last column, I can account for a 1, so that should actually help me in getting some of these last columns of this upper triangular matrix. The same way, the  $c_n$  over here would force us to look at the structure of this lower triangular matrix and what we do here, of course, we need to have a stack of unknowns and that would be something like  $n-2$ . So, then if I can do all this, so these are zeroes and that is how we look at it.

So, you see, the very fact that due to periodicity we have these two odd entries at this extreme points in the matrix, forces us to have a nonzero last row in the lower triangular matrix, and nonzero last columns in the upper triangular matrix.

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Handwritten mathematical derivations on a green chalkboard:

Left side (Matrix structure):

$$\begin{bmatrix} 1 & u_1 & 0 & \dots & 0 \\ 0 & 1 & u_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_{n-2} \\ 0 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Right side (Derivations):

$$\begin{aligned} b_1 &= q_1 & w_1 &= a_1/b_1 \\ c_1 &= q_1 u_1 & u_1 &= c_1/b_1 \\ a_2 &= p_2 & p_2 &= a_2 \\ b_2 &= p_2 u_1 + q_2 & q_2 &= b_2 - a_2 q_1/b_1 \\ c_2 &= q_2 u_2 & u_2 &= c_2/q_2 \end{aligned}$$

For  $j = 2$  to  $n-1$ :

$$\begin{aligned} p_j &= a_j \\ q_j &= b_j - q_{j-1} c_{j-1}/b_{j-1} \\ u_j &= c_j/q_j \end{aligned}$$

So, we have this and it is now easy for us to do those multiplication of this  $l$  and  $u$  matrix and equate to a matrix entry and we will get this. As I told you, if I were to look for a 1 then what should I do? I should multiply this with the last column here, and that would give me  $q_1 w_1$  so that is easily seen.

How about  $b_1$ ?  $b_1$ , I should be multiplying this with the first column here and that would be simply equal to  $q_1$ . And similarly, we could write  $c_1$ , would be nothing but the first row with the second column, so that should give us  $q_1$  into  $u_1$ .

So, this basically helps you in what you are looking for? You are looking for those unknowns, so  $q_1$  is this; then you get  $w_1$  as nothing but  $a_1$  by  $b_1$  and  $u_1$  would be nothing but  $c_1$  by  $b_1$ .

So, that is the way systematically we will begin with this elements  $q_1 w_1 u_1$ . Let us look at the **second row of a 2**, second row of a 2, what should we get?  $a_2$  should be equal to simply  $p_2$ , so I am just multiplying this with the first column that would yield  $a_2$  equals to  $p_2$ .

What about the second one? We will multiply the again the second row with the second column, so that would give me  $p_2 u_1$  plus  $q_2$ . And you look at  $c_2$ , that would be a multiplication of the second row of  $l$  with the third column of  $u$  matrix and that should give you nothing but equal to  $q_2 u_2$ .

So, again you have an handle to the problem and that tells you your  $p_2$  is nothing but  $a_2$ , and then we estimate  $q_2$  from the second equation, that would be  $b_2$  minus  $a_2 u_1$  is here, so  $c_1$  by  $b_1$ .

So, that is what we should get as  $q_2$  and finally you would like to get  $u_2$  is equal to  $c_2$  by  $q_2$ . So  $q_2$  is here, so you can substitute and you have, you have done.

So, this is the usual way of doing it, so you can generalize it to any  $i$ th row. If I do that, what I am going to see or say, let us call it a  $j$ th row; so, I would see that for  $j$  equal to 2 onwards itself, I am going to get the same sequence.

So, we have already done that part. If I know what  $j$  equal to 2 is, I can do that and this I will do it up to  $x$  bar in the last line. So, I would do this recursion, whatever I derive here

for  $j$  equal 2 to  $n$  minus 1, and that would give us this relation that we have written  $p_j$  equal to  $a_j$  and from here we write  $q_j$  equal to  $b_j$  minus  $a_j c_j$  minus 1 by  $b_j$  minus 1.

And the same way, we could write  $u_j$  is equal to  $c_j$  by  $q_j$ , so you have done this part quite o.k. Now, only thing that we need to do is we have to do it for the last line, we have the starting value here and then you can fill this up.

Now, what we can see is that if I multiply these rows with this last column, that will give me what? That will give me the entries here for which the first one is a 1, rest of them are 0.

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The image shows a green chalkboard with handwritten mathematical derivations. On the left side, the following equations are written:

$$q_1 = b_1$$

$$w_1 = a_1/b_1$$

$$u_1 = c_1/b_1$$

$$p_2 = a_2$$

$$q_2 = b_2 - a_2 q_1/b_1$$

$$u_2 = c_2/q_2$$

$$q_j = c_{j-1}/b_{j-1}$$

On the right side, the following equations are written:

$$p_j w_{j-1} + w_j q_j = 0 \text{ for } j=2 \text{ to } n-2$$

Last row of  $A$  :

$$c_n = x_1$$

$$x_j + x_{j-1} u_{j-1} = 0 \text{ for } j=2 \text{ to } n-2$$

$$x_{n-2} u_{n-2} + p_n = a_n$$

$$\sum_{j=1}^{n-2} x_j w_j + p_n u_{n-1} + q_n = b_n$$

So, if I leave out that first one a 1 then what do I get? I get a relation that will give me  $p_j$  into  $w_j$  minus 1 plus  $w_j q_j$  equal to 0, I am just talking about all these nonzero entries.

That is what you will be doing, you will be just taking each of this rows one at a time and multiply with the last column, that will give you that kind of a relationship.

And well, you can do it for basically  $j$  equal to 2 to  $n$  minus 2 and what you notice, that here the starting value, because we have  $w_1$ ,  $w_1$  is obtained here; so, if I have the  $w_1$ , I could keep on recursively obtaining the other quantities, all this  $w_j$ 's.

So, essentially what we are trying to do is, we are trying to figure out what these nonzero entries in the last columns are? That is helped by that equation. So, so, this is from the last column of  $a$ . Similarly, I could look at last row of  $a$ .

If I start looking at the last row of  $a$ , then what do I get? What is  $c_n$ ?  $c_n$  would be this, multiplied by the first column, so that gives you simply equal to  $r_1$ , that is easy. Now, I can keep doing it with different columns one by one and those 1s are going to be 0.

So, that is exactly like what we have here. So, if I look at it that way, then I will see that  $r_j$  plus  $r_j$  minus 1  $w_j$  minus 1, sorry this will be  $u_j$  minus 1, that should be equal to 0 and this is true for  $j$  equal 2 to  $n$  minus 2.

And the last, second last entry that we notice there, that will give us  $r_{n-2} u_n$  minus 2 plus  $p_n$  is equal to  $a_n$ .

So, what we have done, we have just multiplied this one with the second last element that gave us this relationship; so, this is what we have done.

And what about this one? This is the most cumbersome, this multiplied by this will give you nothing but summing over  $r_j w_j$  and  $j$  would go from 1 to  $n$  minus 2 and  $p_{n-1} u_n$  minus 1 plus  $q_n$  is equal to  $b_n$ .

So, now I think we have done our job, you can see that all the entries of  $l$  and  $u$  matrices have been obtained. Having done that, you can follow the same procedure of solving these equations that we have done for the non-periodic case also.

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$$\begin{aligned} [A]\{x\} &= \{b\} \\ [L][U]\{x\} &= \{b\} \\ A &= [L][U] \end{aligned}$$

Under  $[U]\{x\}$  is a bracket labeled  $\{V\}$ .

From  $[L]\{V\} = \{b\}$ , an arrow points to "Solve for  $\{V\}$ ".

From  $[U]\{x\} = \{V\}$ , an arrow points to "Solve for  $\{x\}$ ".

You recall that what we did was basically we wrote, if I can now erase this part, so we will be simply writing the same thing that we have done before -  $L$  times  $U$  multiplying with  $X$  is equal to  $b$  vector. And then, what we could do is if I could define this as some  $v$  vector, then this equation actually implies  $L$  times  $V$  is equal to  $b$ . So, you can first solve for  $V$  vector, and once you have that then you solve  $U X$  equal to  $b$ , then you basically solve this in the sequence and you are done.

So, basically even you understand that it is somewhat more work, I did not do any accounting business, but if you have counted the number of operations, you would have noticed that the non-periodic matrix, tridiagonal matrix, operation requires roughly about  $5n$  operations.

If  $n$  is the matrix rank, then you do not do  $n^3$  like what you would be doing for direct inversion, you get it by  $5n$  operation and this is a great saving. You can imagine when  $n$  is of the order of few thousands, you can think of the amount of saving that you can get by making use of the sparsity of the matrix information.

So, I suppose, we are now there to make use of this. Please be comfortable with these, so that if need arises, you should be able to write out your small subroutines or procedures to solve equations arising out of this.



Now, in keeping with the sentiment of this course, if you have noticed that we have spent lots and lots of time talking about waves and I have been often accused that I have a fascination for waves. Well, the reason is, we understood it by now that waves are there everywhere, so we can just simply hope it is not there and it disappears.

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$$u_t = u_{xx} \quad 0 \leq x \leq 1$$

$$i.c.: u(x,0) = u_0(x)$$

$$b.c.s.: u(0,t) = f(t) \quad u(1,t) = g(t)$$

$$E(t) = \frac{1}{2} \int_0^1 u^2(x,t) dx$$

$$\frac{dE}{dt} = \int_0^1 u u_t dx = \int_0^1 u u_{xx} dx$$

$$= \int_0^1 \left( \frac{\partial}{\partial x} (u u_x) - u_x^2 \right) dx$$

For example, next thing that I am trying to tell you is even for a parabolic PDE we can create waves, so let us do that. So, the type of thing that we like to do, suppose we did this exercise before, but none the less let me just jog your memory and tell you what we try doing there; so, we are trying to solve a problem in a boundary domain and we have some kind of initial **conditions**, condition, which I will write it as  $u(x,0)$ , I will write it as  $u_0(x)$  and the boundary conditions could be like,  $u(0,t)$  and  $u(1,t)$ .

Let me call that as  $f(t)$  and  $u(1,t)$ , let me call this is  $g(t)$ . If you recall, in the previous part we defined an energy functional, which I called as  $e(t)$  and which we defined as  $\frac{1}{2}$  square of the **mineral** solution integrated over the whole domain, so 0 to 1.

And then, when we looked at  $\frac{dE}{dt}$ , we found out that this was  $\int_0^1 u u_t dx$ ; using  $u_t$  is equal to  $u_{xx}$ , so we reached up to there and then we also wrote it down as a partial of  $u u_x$  minus  $u_x^2$  dx.

Now, with the help of these two boundary conditions, this part, first part could be exactly integrated and the values substituted there, then I get this  $\frac{dE}{dt}$  is equal to  $g(t)f(t) - \int_0^1 u_x^2 dx$ .

So, that is at the upper bound, what the boundary condition required times  $u_x$  of 1 and  $t$   $u_x$ , means **of course**, the partial of  $u$  there minus the condition at the lower limit. And I think, we did reach up to here and then **we made**, took the fork in the road by saying that suppose  $f$  and  $g$  are 0 and we just trigger the problem by an initial condition alone. And then we made that observation that energy functional is a decay function of time, and we have a damp system, and that was what we were calling it as a kind of a physically stable system, and we wanted to compute it. And we said that to be proper and accurate, we must preserve that property and to do that we also said that our method should have a numerical amplification factor that should be perfectly neutral.

I think some of you would find it difficult, trying to reconcile the fact that I have a system which is physically stable, that means its amplification factor is less than 1, and I am suggesting that you pick up a method for which the numerical amplification factor should be completely neutral. Is there a conflict of interest? Are we following the same route that we should be? Think of it the way we have defined that numerical amplification factor.

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The chalkboard contains the following handwritten equations:

- Boundary conditions:  $0 \leq x \leq 1$ ,  $u(0,t) = f(t)$ ,  $u(1,t) = g(t)$
- Initial condition:  $u(x,0) = u_0(x)$
- Energy functional:  $\frac{dE}{dt} = g(t)u_x(1,t) - f(t)u_x(0,t) - \int_0^1 u_x^2 dx$
- Numerical amplification factor:  $G_2(k, h, P_e) = \frac{U(k, t + \Delta t)}{U(k, t)}$
- Limit as  $\Delta t \rightarrow 0$ :  $\lim_{\Delta t \rightarrow 0} G_2(k, h, P_e) = 1$
- Other equations:  $\int_0^1 u u_{xx} dx$ ,  $\sum_{j=1}^n u_j + k_1 u_{j-1} + q_1 = b_n$

If you recall, we defined a numerical amplification factor, which I wrote for various heat equation, was something like this -  $U$  of  $K$   $t$  plus  $\Delta t$  divided by  $U$  of  $K$  and  $t$ .

So, of course, for a finite time calculations this will be not equal to 1, but what is your ideal? Although you are doing numerical computing, you basically want to get the

solution for all space coordinate at all times. So, you really want to compute it in the limit  $\Delta t \rightarrow 0$ ; that is your ideal goal.

So, what happens when  $\Delta t$  goes to 0? You have no other option than having it as equal to 1. So, what are we doing then? Well, we are doing the simple thing that let the physics decide for itself what the problem has to do. My numeric should not interfere with the physical process; I should stay neutral and like a referee in a game.

I should not be biased, although I know the system is damp, I could devise a method which will make the method more than it should be damped physically and reach the eventual steady state, that is a possibility.

But if I am interested in the time accurate solution, so even when the solution is decaying and going towards its steady state, if I am interested in those transients, then accuracy is of concern. So, I should not adapt a method which will take me faster to the steady state; that temptation is always there and that had motivated most of the people working in competitions, where at one point in time computing time accurately was a kind of a luxury.

People somehow, wanted to get the steady state solution and in the process, if you reach the steady state faster, you felt better that I have done my job quicker than the other guy. The other guy may be actually be doing more accurate calculations, but taking more time and let me tell you, I mean, in my own personal professional life I have been given all kinds of unwanted advice.

People said why are you doing so and so, it is tough, follow so and so, they have done it very quickly, but the point is what you really want? If you are interested in those transient solutions, if you are interested in accurate solutions, you do not want anything other than  $G$  equal to 1.

I think this discussion was necessary because I was talking to Sonam over the weekend, she asked this question and I have very very old students who has been working with me for 3-4 years, quite often they try to raise this question from the side.

So what happens, so they are still not convinced after 3-4 years that there should be something more than what I am saying, but as you can see it for yourself, that what we are looking for is basically the limit.

See, if I do finite time calculations, there is a likelihood that I will have  $g$  less than 1, but please be assured that is not a most desirable solution. The most desirable one would be where I stay neutral. In fact, after this I will get back to the spectral analysis once again to refine these ideas little more.

So, now coming back to this case, we need to have a method now to solve this problem where, let us say, the boundary conditions are non-trivial. So,  $g$  of  $t$  f of  $t$  are non-zero, then what is the possibility? I could make the energy go with as a function of time, I could do that. What are these terms? Where do they come from? What is the meaning of  $u_x$ ? Those of you are from mechanical, should be very very apparent; Abhimanyu where is he?

Tell me, what is  $u_x$ ?  $U_x$  relates to what? The heat flux; so if I start giving heat flux from the end, either at the right extreme or at the left extreme, I can control this dynamics of energy. So, I can really set up myself a case where I could keep the whole thing in a kind of a dynamic balance and which will not show a complete monotonic decay, like what people have done classically.

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## The 1-D Heat Equation

- Consider a long thin bar or rod of constant cross-sectional area and homogenous material insulated laterally.
- The heat conduction in such a body is essentially one-dimensional and is given by the 1-D heat equation,

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (1)$$

where  $u(x, t)$  is the temperature distribution in the body and  $\alpha$  is the thermal diffusivity.

- For heat conduction in a bar of finite length,  $L$  we would like to solve Eqn. (1), say on a finite  $x$ -interval  $[0, L]$ , with initial condition for  $u$  at  $t = 0$ , and boundary conditions at  $x = 0$  and  $x = L$ .

So, here, what we are trying to do is basically revisit the same problem, but look at it in the slightly different way. So, this is what we have already talked about, equation 1 was the heat equation, and you realize, which I have not talked about that this  $\alpha$  is the thermal diffusivity.

And in many a times, you know, you would like to solve problems where you non-dimensionalize the system; so, the  $\alpha$  could be somehow embedded inside the equation itself and you can write it this form, but just for the sake of physical understanding, I broad the concept of thermal diffusivity here.

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### The 1-D Heat Equation (cont.)

- For example, consider the boundary conditions

$$u(0, t) = 0 \quad (2a)$$

$$u(L, t) = 0 \quad (2b)$$

and initial condition

$$u(x, 0) = f(x) \quad (2c)$$

- The above represent one of the classical ways of providing boundary conditions for Eqn. (1).
- The solution of Eqn. (1) with Eqn. (2a), Eqn. (2b) and Eqn. (2c) give **dissipative solutions** which exponentially **decay with time**.

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### Analytical solution: Classical case

- The analytical solution for Eqn. (1) can be found by separation of variables and is given by

$$u(x, t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) e^{(-\lambda_n^2 t)} \quad (3a)$$

where  $\lambda_n^2 = \frac{\alpha n^2 \pi^2}{L^2}$

- The  $B_n$ 's must be coefficients of the Fourier sine series and is given by

$$B_n = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx \quad (3b)$$

- The exponential factor in Eqn. (3a) ensures that the temperature,  $u(x, t) \rightarrow 0$  as  $t \rightarrow \infty$

Parashar: DPM - p. 4/11

Now, if I am solving in that finite domain between 0 and l and well, if I do this, like what we talked before and the initial condition like this, then we have those classical way of providing a solution which gives a dissipative solution that exponentially decays with time, and this you must have done in your first course in PDE where you split the solution by separating the variables and you get it two parts - one is the space dependent part one is the time dependent part.

And you can see indeed, the time dependent part is exponentially decaying. So, that is something you do and of course, from the initial condition you could find out this Fourier series coefficients,  $b_n$ ; this is quite familiar to you. So you should be very comfortable with this step.

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## The Heat Equation and Waves

- We have seen that when boundary conditions in Eqn. (2a) and Eqn. (2b) are used, then the solutions decay with time.
- The **Unsteady Heat equation** is a **parabolic** PDE.
- But what would happen if we had **time-harmonic** boundary conditions?
- It is quite interesting to note that such boundary conditions impose a **time-scale** and we get **Dispersive wave-solutions**.

Paravathi DPE - p. 5/11

Now, we found out a case where solution decays with time. We have also seen, the unsteady heat equation is a parabolic PDE, but what would happen if we had time harmonic boundary condition?

So, what I am talking about that  $f$  and  $t$  and  $g$  of  $t$  are functions of time and that actually introduces a time scale. So, something like this, I have a rod, say heat transfer problem on the end, I have some kind of a heater which is periodically part of the cycle, it is pumping in energy, part of the cycle, it is cooling, so I could do that.

So, I basically have the ability to trick the problem and introduce some kind of a time scale; so, that is what we mean by time harmonic boundary condition and what happens then? Well, the moment you introduce a time scale, you will get a dispersive wave solution and how do you get it is what we are talking about now.

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## Analytical solution: Dispersive Waves

- Consider the 1D heat equation again

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \quad (4)$$

to be solved in a domain that extends from  $x = 0$  to  $x = \infty$

- The solution can be found by the method of separation of variables

$$\phi(x, t) = G(x)H(t) \quad (4a)$$

- Use the above in Eqn. (4) we get

$$\frac{H'}{H} = \frac{\alpha G''}{G} = p(a \text{ constant}) \quad (4b)$$

Ramanujan DPG - p. 6/11

So, let us say we are trying to solve a problem and we have, just for the ease, extended the right hand all the way up to infinity, so that we can get rid of looking at one of the boundary condition.

And once again we resort to the same thing that we do before - separate it into a space and time dependent function, substitute it over here and then you get this. So, after this part, there is nothing very spectacular or new; only is, how we define this constant in the previous case? We put it as minus lambda n square. That is that is how we got that time decaying solution.



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## Analytical solution: Dispersive Waves

- As we are looking for dispersive wave solutions set  $p = -i\omega$ , where  $\omega$  is the circular frequency of the exciter placed at  $x = 0$

- Hence we obtain from Eqn. (4b)

$$\frac{H'}{H} = -i\omega \quad (4c)$$

$$\frac{\alpha G''}{G} = -i\omega \quad (4d)$$

- From Eqn. (4c) we have

$$H(t) = C e^{-i\omega t} \quad (4e)$$

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However, what happens if we take this constant as equal to minus i omega, the pure imaginary quantity? So, basically, that is something like what we have defined as the circular frequency.

If I do that, then my time dependent solution looks like this - H prime by H is equal to minus i omega. So, immediately I get a solution which tells you that time dependent part is harmonic; so, I have got a harmonic solution in time.

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## Analytical solution: Dispersive Waves

- From Eqn. (4d) we get

$$\alpha G'' + i\omega G = 0 \quad (4f)$$

Characteristic equation is given by  $\alpha\lambda^2 + i\omega = 0$ . The roots are

$$\lambda_{1,2} = \pm i \left[ \sqrt{\frac{\omega}{2\alpha}} + i \sqrt{\frac{\omega}{2\alpha}} \right]$$

Let

$$\lambda_{1,2} = \pm i [k_r + i k_i]$$

where

$$k_r = k_i = \sqrt{\frac{\omega}{2\alpha}} \quad (4g)$$

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You then substitute that constant also here and this is the space dependent part. Look at the characteristic equation that will give you alpha lambda square plus i omega, and you solve it, you get two parts - a real part and an imaginary part; the magnitude of both of it are the same.

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### Analytical solution: Dispersive Waves

- Solving Eqn. (4f) we have

$$G(x) = A_1 e^{i(k_r + ik_i)x} + A_2 e^{-i(k_r + ik_i)x} \quad (4h)$$

- From Eqn. (4a) we get

$$\phi(x, t) = B_1 e^{-k_i x} e^{i(k_r x - \omega t)} + B_2 e^{k_i x} e^{-i(k_r x + \omega t)} \quad (4i)$$

- As we have a domain which is unbounded on the right,  $B_2$  must be zero so that the solution does not blow up.
- Therefore we have

$$\phi(x, t) = B_1 e^{-k_i x} e^{i(k_r x - \omega t)} \quad (5)$$

- Eqn. (5) represents a **dispersive wave propagating to the right**.

RaoBali: 2019a-p. 9/11

But you do see this now, that the space dependent part would have a harmonic variation in space also, and if you substitute all of it together; so, this is your space dependent part and you construct your total solution.

And what you see is this,  $k x$  minus  $\omega t$  part, that reminds us of our dispersive waves; remember, that is what we spent lot and lot of time discussing water waves. We have seen in all those cases as an example, that we do see a phase speed, etcetera, etcetera; and the group velocity, we get the same thing here, we get the same thing here.

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## Analytical solution: Dispersive Waves

From Eqn. (4d) we get

$$\alpha G'' + i\omega G = 0 \quad (4f)$$

Characteristic equation is given by  $\alpha\lambda^2 + i\omega = 0$ . The roots are

$$\lambda_{1,2} = \pm i \left[ \sqrt{\frac{\omega}{2\alpha}} + i \sqrt{\frac{\omega}{2\alpha}} \right]$$

Let

$$\lambda_{1,2} = \pm i [k_r + ik_i]$$

where

$$k_r = k_i = \sqrt{\frac{\omega}{2\alpha}} \quad (4g)$$

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Now, of course, we have taken a problem which is unbounded in x direction, so then you must have  $b_2$  equal to 0; otherwise, of course, this part e to the power  $k_i x$  will blow. We can afford to keep that solution, you notice that  $k_i$  is given by this  $\omega$  by  $\alpha$ .

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## Analytical solution: Dispersive Waves

Solving Eqn. (4f) we have

$$G(x) = A_1 e^{i(k_r + ik_i)x} + A_2 e^{-i(k_r + ik_i)x} \quad (4h)$$

From Eqn. (4a) we get

$$\phi(x, t) = B_1 e^{-k_i x} e^{i(k_r x - \omega t)} + B_2 e^{k_i x} e^{-i(k_r x + \omega t)} \quad (4i)$$

As we have a domain which is unbounded on the right,  $B_2$  must be zero so that the solution does not blow up.

Therefore we have

$$\phi(x, t) = B_1 e^{-k_i x} e^{i(k_r x - \omega t)} \quad (5)$$

Eqn. (5) represents a **dispersive wave propagating to the right**.

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So, it depends on what frequency you are doing and what is the thermal diffusivity that determines the magnitude of  $k_r$  and  $k_i$ , and that of course, precludes the second part of the solution; that means, you have to choose  $b_2$  equal to 0.

So, if I take a solution from  $x$  equals to 0 to infinity, then the surviving part of the solution would be this.

Now, of course, this is a dispersive wave and that is propagating to the right; and  $x$  minus  $c t$ , **that is**, that is the way we have figured out that if it was  $x$  plus  $c t$ , it would have gone the upstream direction; so, it is going in the downstream direction.

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### Analytical solution: Dispersive Waves

- The initial condition is given by

$$\phi(x, 0) = B_1 e^{(k_r + i k_i)x} \quad (5a)$$

and the boundary condition is

$$\phi(0, t) = B_1 e^{-i\omega t} \quad (5b)$$

- Recall Eqn. (4g) which gives the **dispersion relation**,

$$\omega = 2 \alpha k_r^2 \quad (6)$$

- The **group velocity** can be calculated as

$$V_g = \frac{d\omega}{dk_r} = 4 \alpha k_r \quad (7)$$

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So, initial conditions can be used here and the boundary conditions. So, basically, what we have done? We have basically doing the inverse trick, we have generated a solution which looks like a dispersive wave and then we are going backwards.

And from this general solution, we are looking at what is the corresponding initial condition and admissible boundary condition? So, this initial and boundary conditions are very compatible with a general solution.

And what about the dispersion relation? Dispersion relation, that you noticed was given here in the last line, if I just simply square it or dispersion relation comes from where? The real part of  $k$ . So, I would write that equal to  $k_r$  square equal to  $\omega$  by  $2 \alpha$  and that is what we have done. So,  $\omega$  is nothing but  $2 \alpha k_r$  square, you can calculate it, group velocity  $d\omega/dk_r$  and this is it.

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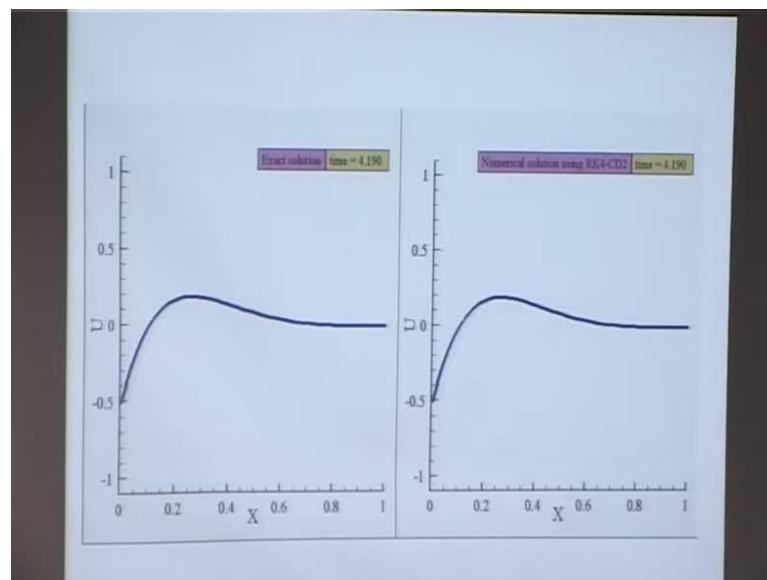
## Numerical Solution: Dispersive Waves

- For the numerical solution, the spatial discretization is done using **CD2** and time integration is performed by **RK4** method.
- Here is an animation showing the analytical and numerical solution

Parabolic PDEs - p. 15/11

So, basically, you can really see what the solution is going to be. So, just for interest, **just to pay**, very simple method that second order central difference scheme in space and fourth order Runge-Kutta scheme for time integration, and we solved it.

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So, now you have both the case, you have an analytical solution and you also have a numerical solution, and this is the way both the solutions go in time. So, you see as the time counter keeps going you can very clearly see that there is hardly any difference between the exact solution on the left and the numerical solution on the right.

So, I hope now you are convinced that we have a case where we actually can get even a wavy solution for a parabolic case.

Now, the question is for the mechanical engineers to go in the lab and try to measure such heat transfer, weight, etcetera, time varying. I am told it is not so easy, so we will leave it to them to set such experiments up and then we will see what we can do if that could be experimentally verified to.

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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** ( $k_{max}$ ):  

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

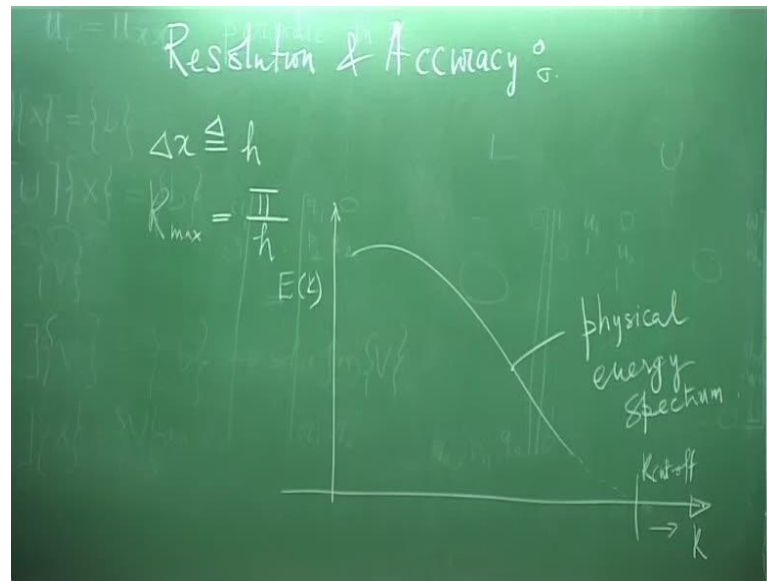
where, for a grid of uniform size ( $h$ ):  $k_{max} = \frac{\pi}{h} \quad (4)$

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Now, let me now go back and see what we were doing before and come back to it. This is what we are talking about. Now, you see why you were so fascinated by waves because irrespective of classification of the PDE, we can generate waves.

And let me try to summarize what we have done because this is **very** very central to what we do in the following; so, let me give you an overview of what we have done here, so it is a kind of a recapitulation of what we have done before.

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But let us try to understand what we mean by it. See, the point is we talked about resolution. What exactly we mean by resolution and accuracy?

Now, I told you that if I solve the problem where I choose, let us say, a discretized, uniformly discretized space as  $h$ , then we immediately talk about  $k_{\max}$ .

So,  $k_{\max}$  is this, that we discussed because that is the maximum wave number that we can express having three points in  $2h$ , that will define one wave that fixes this  $k_{\max}$ . So, what actually happens in real life? Let us say, I am looking at some simple problem, a flow of water in a pipe that we are all familiar with.

So, if I try to find out, how the energy is a function of wave number in that flow inside a pipe? So, what you find, the spectrum looks like this, what it does mean that it has a non-zero value up to something, so this is your physical energy spectrum.

Now, you want to, let us say, solve this problem. So, how would you choose your  $k_{\max}$ ? Your  $k_{\max}$  must be greater than this value, the cut off value; so, this is your physical cut off value, so your  $k_{\max}$  must be greater than this.

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However, do you think that itself would be adequate? That itself will not be adequate because if I have to solve that problem, that would require solving some differential equations and those differential equations will have all those kinds of derivatives that we have been discretizing, and when we discretize the derivative, what did we do? We found out that the effectiveness of those discretization was written like this,  $k$  equivalent by  $k$  which, let us say this is my  $k$  max, which shows that **cumulate** choice of a method, I actually do not keep this equal to 1, this is what we want it to be 1.

Because we do not want any loss of information,  $k$  equivalent should be equal to  $k$ , **so that whatever the derivative has....** So, recall basically what we are doing is this, if I write the derivative as this, so any discrete method, I am doing this; so, if I am doing this, so this is say, any discrete method.

And we have seen, if we do spectral method, that means, we take the **space-time**, space dependence part in terms of those trigonometric functions, orthogonal functions, then this becomes equal to  $i K U$  of  $K$   $e$  to the power  $i K x$   $d K$ .

So, you see the difference comes in here. Instead of multiplying by  $K$ , we multiply by  $K$  equivalent, and that is why we accumulate error and what do we do? We actually get some curve like this, which shows that we begin with what we want. So, at  $k h$  equal to 0, this value is equal to 1, so there is no problem. But as  $k$  increases, the wave numbers increases, I start seeing the departure from the ideal limit by this.



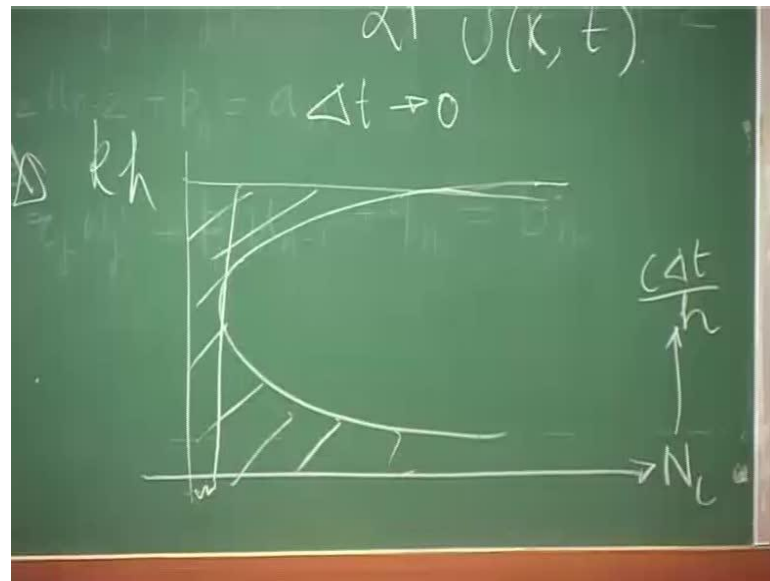
So, basically, let us say if this is 0.95, what does it mean? That every time I evaluate the derivative, I am losing 5 percent of the information and in an actual solution procedure, you would be doing it endlessly almost. If it is a time dependent problem, you will have to be doing it at every time step; so, you can see why it is so much sacrosanct that we do not settle for any of those departures.

So, my  $k_{\max}$  is here, I, I, I, I was very pleased here by saying my  $k_{\max}$  is more than  $k_{\text{cut off}}$ , so I should be o.k., but here we are seeing we are not. What we are seeing that we are actually getting somewhere here? So, what I call as the Nyquist criteria, that may be a Laxmanrekha, but you have opinions within opinions like issues within issues. So, I cannot just simply say I am happy here, I should be content with only this part, I should be content with only this part in terms of representing the governing differential equation; this is the second step.

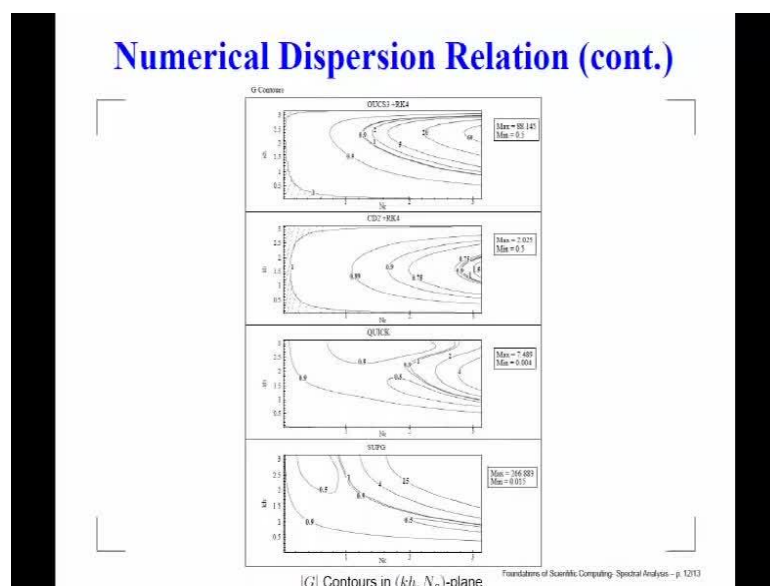
So, the first step is choosing the spacing that fixes the Nyquist limit, then the second step is choosing the discretization method that tells me which is actually really the useable range; rest of it is basically collecting garbage, accumulating error. So, those results are not trustworthy, one should not be taking them seriously, although most of the time people do that.

So, after that what happens? Do you think we are out of woods? Not yet because we have talked about the other properties of computing. What was the next thing that we looked at? G.

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If I, If I now keep looking at, remember what we did? I think we have it here, so you can take a look at that picture and then we can... Can you see it all? Let us keep our attention focused on the second frame because that is related to ACD 2 and RK 4; other methods we have not covered, so you will not understand, so do not at all bother about it.

So, if I have this, what you notice that we have a region which is shown by dashed line, that is where  $g$  equal to 1. Anywhere on this side, it so happens, it is less than 1; so, if I

am trying for accuracy, I should actually choose this abscissa here to a value which should be to the left of this extreme tangent that I can draw.

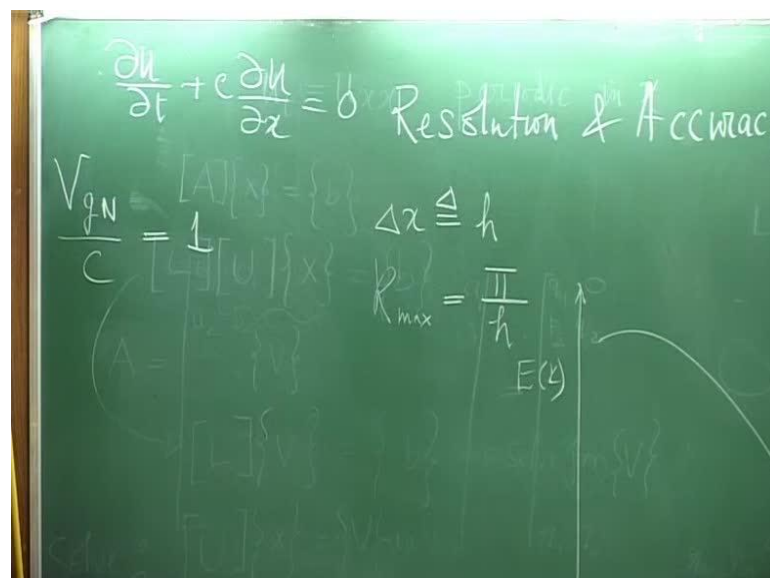
So, what we are seeing? To even have faithful computation, my abscissa, what is this?  $n c$ ; so, on this side we have plotted  $n c$  and  $n c$  is  $c \Delta t$  by  $h$ . So, if I have fixed  $h$ , this tells me how to choose my  $\Delta t$ ; this tells me that if I am too greedy, I may be on this side and then a part of  $k h$  component will be damped out every time I integrate.

So, you see that is what I said, issues within issues. Nobody wants to talk about that Orwellian's peak, we talked about; so, if I talk about this then I have to choose my  $\Delta t$  over here and what would have happened if I would have chosen some value here?

Well, a part of it will be faithfully reproduced, part of it will be done properly here, but in the intermediate segment I would accumulate error.

So, after you have done that..., so this is the story that you would like to get those G contours. So, let us say this is your region where you can confine yourself, so I would say this is my useable  $n c$  range for which whatever  $k_{\max}$  we have chosen; everything is resolved without any numerical attenuation.

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So, now you see this is the third step. Are we done yet? Not so, because after this having done that, we also had shown that how the energy propagates. The energy propagation speed is given by this group velocity and in drawing this figure, we have used the model

equation. So, for every equation you will have a different story, for this equation this is the outcome that you are seeing on them.

So, this ideally should be equal to 1, so that your energy should go at the correct speed as the governing equation suggests. And what you notice in the second frame, that this line, this horizontal line shows about 7 percent dispersion, it is 0.93 instead of 1.

So, whatever  $\Delta t$  I choose, do you realize that I am going to accumulate error quite rapidly if I am here? Now you see, that is where we developed some method over the last 8-9 years, where we actually show that we can go all the way up to one, up to this range.

So, there are methods of doing it, we will be talking about it, but just notice this. So, what you see, that in any small value of chosen value of  $n_c$ , you have dispersion error because the energy will propagate at a lower speed than what you wanted to be.

So, of course, those results are inaccurate to have accuracy. What you should really do is, you should confine yourself as close to the origin as possible. You draw another horizontal line parallel to it, but at a lower level, that **may be**, may be 0.999; so, that is 1 percent dispersion.

So, if you decide to accept 1 percent error, so that is where you should be, but then that further restricts your  $k_h$ . So, you can see now what we had gone through, first we have chosen the grade to ensure that we include the cut off, then we see the discretization process has restricted us to a smaller subset of the  $k_{max}$ , then we are seeing that  $G$  more or less determines what should be the  $\Delta t$  we choose.

But then again, this picture tells you that, look, do not be sure about that  $\Delta t$ , you may have to really further refine your expectations, and how do you do that?

Well, if I want to get my operating point very close here, so I need to basically have this physical thing in the  $k$  space, I multiplied by  $h$ , that is what that scale is  $k_h$ . So what I am trying to do is, instead of plotting it versus  $k$  I if I plot versus  $k_h$ , then I by taking small and small smaller  $h$  value, I can shrink this up, I can telescope it into smaller region.

So, now you see that this is a basically the way that you choose your space and time step.

So, what happens, although I narrated 1 2 3 4, but you would go other way first; you come to the fourth step to see what is the kind of  $h$  you can choose so that you have virtually dispersion free results.

Then, you go to a  $G$  contour and you find out where you get nearly neutral solution or completely neutral solution, **that you choose your...**, and then of course this things, you just check it for the sake of checking that if those ranges are here also.

This is the larger subset that  $G$  and  $v$   $g$   $n$  by  $c$  are more conservative ones; so, if you satisfy those two, these other ones could be o.k. too. So, I suppose this is what I told you about a pipe flow of water in a pipe, for a particular velocity, for a particular flow rate.

The moment I change the flow rate, my spectrum may change; I could get something like this. Those of you are familiar you would know there is something called Reynolds number. If you increase the Reynolds number, your spectrum becomes wider.

So, for every problem, you should be aware of what your physics demands and then you should go through this set of analysis tools that we talked about, that is, when you are convinced that everything is done properly, that is where we start computing.

So, computing is the least interesting part of this whole exercise. It all begins with your ability to grasp the physical nature of the problem and your ability to analyze the problem, numerically what method you would like to choose.

For example, if I look at some of this method, this four methods that we have shown here. This is a method which we have pioneered here, it is called compact schemes which have some extremely good properties, this is the classical finite difference scheme, this is your finite volume scheme that is used in fluent.

The fluent has the most accurate component which run on this algorithm called quick; it has even worst part, but this is the best fluent gives, that this quick scheme. And this is what the finite element, well, as do and you can see this last two - you do not have any region where  $g$  equal to 1; so everything is nice and quiet after a battle, everybody is dead, solution is gone, your signal is gone, everything is attenuated and you are happy with colorful pictures, that is your CFD.

Thank You.