Foundation of Scientific Computing

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Module No. # 01

Lecture No. # 17

Lecture 17 covers the following topics. We begin by the exact solutions of heat equation and how it is solved numerically. In the context, we try to tell you the importance of applying the boundary conditions because unlike theoretical solution methods, numerical methods need definitive boundary conditions.

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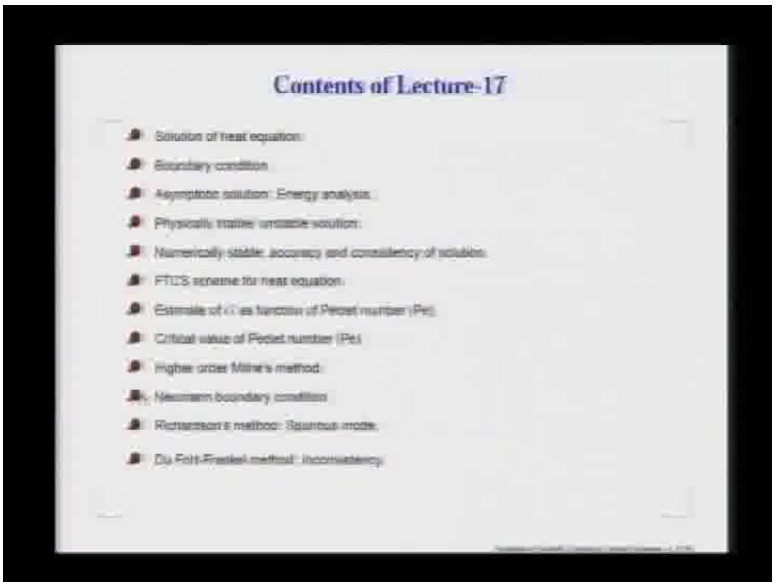

In the context of analyzing numerical methods, we need to talk about, how the solution behaves over large time; this brings us to the topic of asymptotic solution; this we do via an energy analysis and we distinguish what is a physically stable and what is an unstable solution. We need to distinguish between to these two cases. This is what is going to be a constant theme in this course. We need to see that, discretizing physically unstable

solution is a challenge because we need to capture the physical instability, while not allowing any numerical instability of the method.

So, that is why we are going to talk about numerical stability accuracy and the consistency of the method. In the context of the heat equation, we will begin in the same historic manner in which the subject has developed by introducing - forward in time centered in space scheme or the FTCS scheme. For this FTCS scheme, using our spectral analysis, we will obtain an estimate for the numerical amplification factor, which is going to be a function of spacial and time steps given in terms of a number which we will call as the Peclet number. We will figure out what a critical value of Peclet number is for a particular numerical method. For the FTCS method, we will identify a specific range of Peclet numbers, over which solutions will have different types of qualitative behavior.

Having discussed about FTCS method, we will show that, at times, if we are little more restrictive in terms of spacial and tempered discretization, we can get higher accuracy and one such method is due to Milne; we will talk about it. This will be followed by our discussion of handling boundary conditions which are not given in terms of the function value, but in terms of its derivative. So, these are called the Neumann boundary condition. So, we will talk about the Neumann boundary condition and how they are use using ghost boundary concepts.

Since we have realized that, accuracy is one of our requirements, we will also follow an attempt - a failed attempt by Richardson, which was developed to achieve higher accuracy, but what we found people found out that this gives rise to spurious modes because this is a 3 time level method. This spurious method actually makes the method also unstable and we would not the suggesting that any one use Richardson method.

This will be followed by another variation of a higher order approach which was suggested by Du Fort and Frankel. We will notice that, if we are not careful in choosing delta x and delta t, we may actually end up having inconsistency problem; that means, although we are solving a parabolic partial differential equation, numerically it would behave like hyperbolic differential equation.

Direct specifically on purpose for a finite domain x non-dimensionalise so that it lies between 0 and 1. You start off with some initial condition that t equal to 0; that is given in the second line. Then you study the evolution of the solution with space and time.

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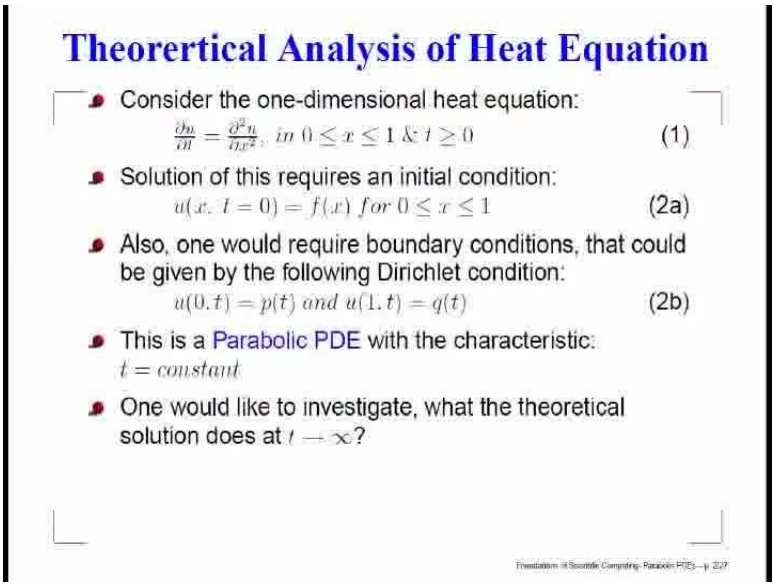

However, because you have a finite domain, there is a possibility that you could apply some input through those boundaries, which we will call as boundary conditions; they are fixed excess at 0 and 1. However, those conditions could be time dependent. So, there is a possibility that you could do that.

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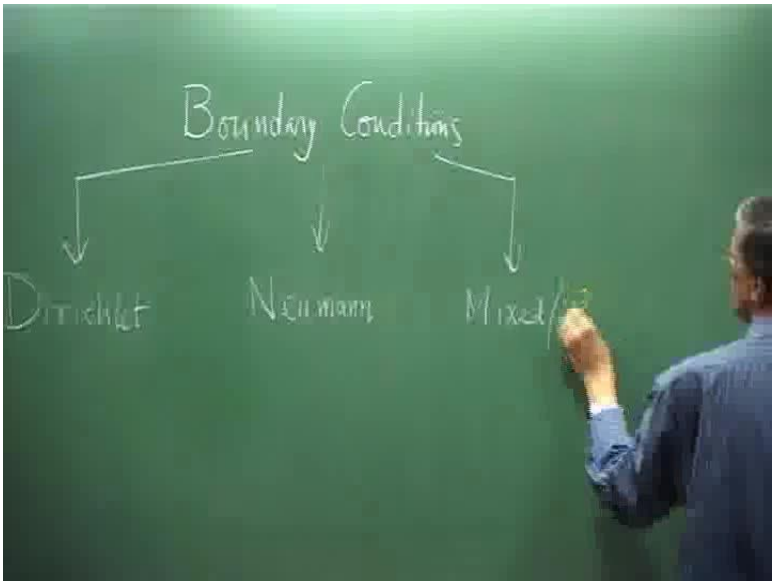

I probably did not amplify boundary conditions that we usually talk about; they are classified into three categories: one is called the Dirichlet condition, then we have Neumann condition, and third is the Mixed or Robin's boundary condition.

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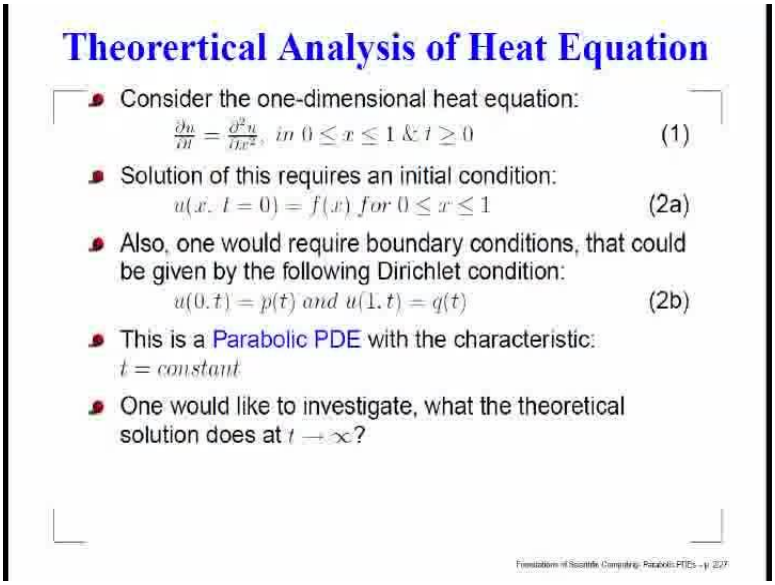

If you give a function, value of the function itself at the boundaries is what you call as Dirichlet condition. So, what you are seeing here is an example of Dirichlet condition. You are prescribing the solution u at the two ends. This we studied that, it is a parabolic

PDE with t equal to constant as the characteristic - single characteristic; it is not plural you just have only one.

You want to study this problem. Before you study it computationally, you would like to investigate what is the attribute of this solution in a theoretical frame work. For example, if we go to very large time, what happens to this solution? Does this solution exist? Does it remain unique? Is it bounded? - All these mathematical questions crap up in our mind.

So, to study that aspect, what we did? We defined a functional which I called as u square by 2. If u is the temperature, u square by 2 does not mean anything, but if u is some kind of a velocity, then this has a connotation of energy. That is why I said energy, but please do understand with in quotes - this is an energy; in that sense, if u is the temperature, then by no means I will called that as physical energy, but still the main property of this function is that, it is not negative.

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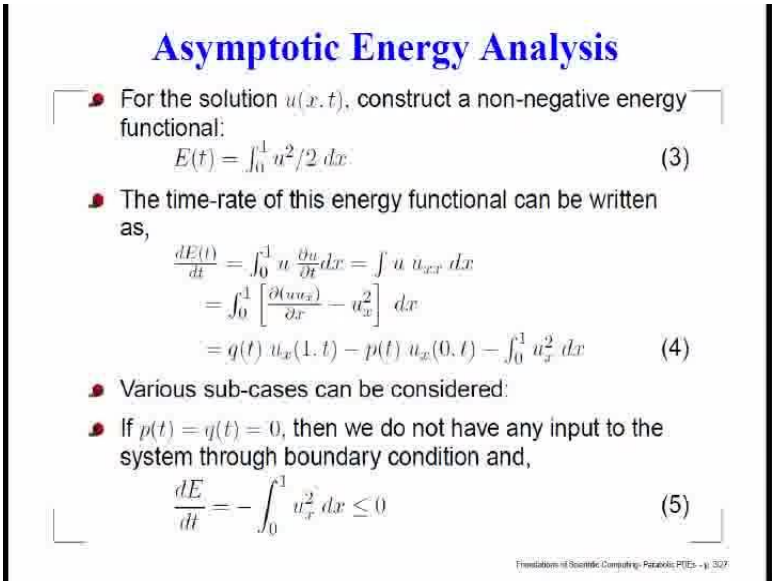

If I have a quantity which is non-negative, I want to find out how this quantity changes with time. So, what we did was just simply differentiated it with respect to time. Then we will get u del u and del t. Since del u and del t is equal to u x x, from the governing equation, I can write this and then do this bit of manipulation. You get a perfect differential in the first part minus u x square. So, I can integrate this part; that will be u u

x at 1 minus u u x at 0. So, those are those two parts of the solution and the last one is simply minus u x square d x.

Now, we could consider various sub-cases. for example, if we do not give in any kind of boundary input, that means this Dirichlet condition we talked about at 0, then you can see, first two parts disappear, leaving behind this time rate minus of u x square. Once again, because of the negative sign and this being a square, you appreciate that this dE by dt is negative - non positive; it could be 0 also. So, it actually means that, we start off with a quantity which itself is positive, but which is decaying with time. So, what happens then? That is an attribute of what I called as a physically stable system. In a physically stable system, what happens that as time progresses, nothing goes unbounded.

So, here is an example where we started with the finite energy E and then that kept on decreasing time. This is quite understandable because if I take this example as a heat in a rod, then what we are doing at t equal to 0? We are providing some kind of a temperature distribution and then we are seeing what is happening with it as time progresses.

What do we expect to happen?

It will slowly conduct and convict heat away and temperature would come down - that is what we expect. So, that is an attribute of a physically stable system; this E would keep on decaying.

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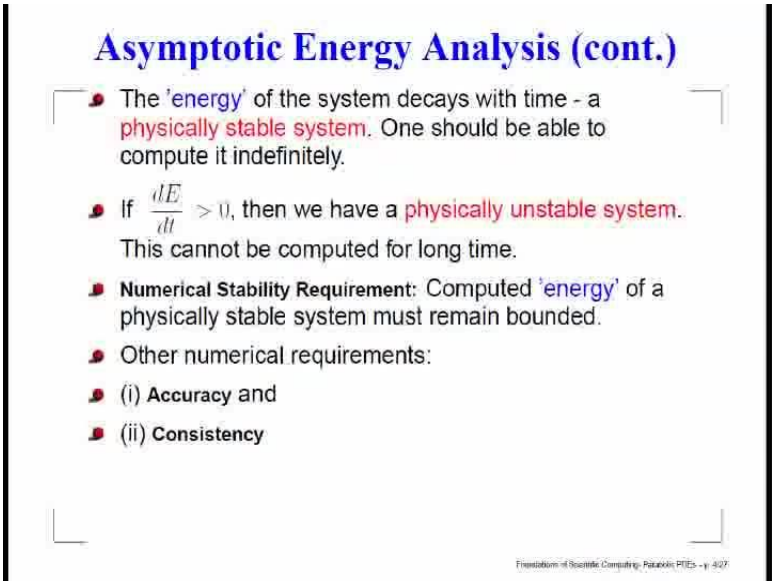

Then, if I am doing my computation quite all right, then one of the big principles that we must satisfy is that, we should be able to compute it for indefinite period of time. We will have this quantity E blowing up on our face.

However, in some physical unstable system, you can see that this quantity dE by dt can be positive; how can it be positive? That clue is given in the previous slide. You can see here that, if I produce some kind of a heat addition through these two terms, I can make this quantity either 0 or plus. So, it is very simple. If I take once again, an example of a rod, if I keep on adding heat from both the sides, then the temperature will grow. If the temperature grows, then this dE by dt can keep on increasing. So, that is what we meant by a physically unstable system.

However, there is a kind of an inherent danger here. If unstable system really goes unbounded, computationally we would not be able to follow unbounded numbers because all computing is done with finite precession, finite ability to represent numbers. So, that is why I added the sentence that, this cannot be computed for very large times. This is the sort of a description of the physical stability and instability of the system.

Now, we have to compare this physical property with what you are doing numerically.

So, if I have a physically stable system, my numerical system should also be stable. It should not block; we are not following the physics of the problem. So, that is what I said that the computed energy of a physically stable system must remain bounded; if it does go unbounded, then we are much sure that there is something wrong with the numerical method.

We also would like to see, if the solution is decaying at a particular rate. So, there is a given temperature distribution. I should be able to also calculate it quite accurately. It is not necessary that I will say I have started with this initial solution. Finally, I know temperature will be 0 everywhere. So, let me rush through and get to that solution. Then what will happen? The solution at the intermediate stages will not be accurate. So, time accuracy is the attribute of a good numerical solution.

The last one that I mentioned here is called consistency. We will see what we mean by consistency. The solution has some physical property. I would like to represent it numerically; in a sense that, it does not value those physical principles.

Suppose, as I explained here, the dE by dt is negative, then what does it mean? The energy will slowly come down. It does not say that energy should keep oscillating up and down. But if my numerical solutions shows that kind of an attribute, then I am perhaps not solving the correct set of equation by correct method; may be the equation is correct, but the method is faulty because I am not consistent to what I see physically. So, that issue we will be talking about; may be today itself. I will give a concrete example.

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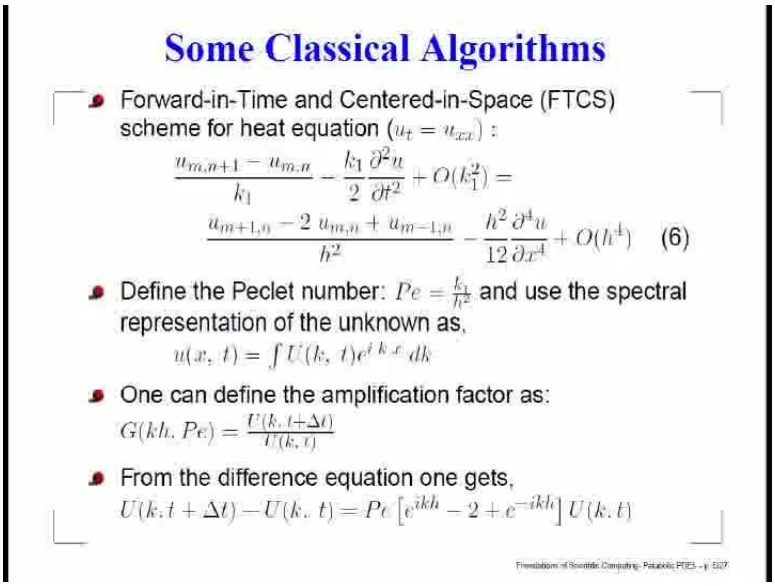

Let us now go through this. This is something which we are familiar. We are solving this equation u t equal to u x x; then, the time derivative here; we are doing it by Euler time integration; that is what we meant by forward in time. So, we are at jth time level; we are trying to find out the solution at j plus 1th level; that is where, this forward in time phrase comes in.

The second derivative u x x has been derived here, also by a central scheme. So, that is why we have this acronym called FTCS standing for Forward-in-Time Centered-in-Space. If you compare this with the 1D wave equation that we have been looking at for so long, this method was unstable, but here what happens? Let us try to see.

Now, I have written down the leading truncation error term in time discretization; that is proportional to the second derivative and it is also proportional to the time step. So, this is basically a first order, accurate in time; this is the part, which we had quite a bit of discussion. In terms of h, I will say it is a second order; in terms of the order of the polynomial, I will say it is a third order.

Let us try to now analyze this. So, numerically what we do? We drop out all these truncation error terms; we write this term is equal to this term; then I would have quantity called k 1 by h square; that is like your delta t by delta x square and this has a name called the Peclet number. So, we call this as a Peclet number which defines the ratio of the time step by the space step squared.

Now, let us follow our spectral representation of the unknown. So, what would I do is - I express the x variation in terms of the corresponding wave number to avoid confusion; that is why I wrote here k 1; so, you understand k 1 refers to delta t; k is the wave number.

Now, as before, we can also define an amplification factor which will be this Fourier Laplace amplitude evaluated at the advance time divided by the same value at the prior time step. Now, if I take this representation and plug it in there, then from here, I will get u of k t plus delta t j plus 1 will give me t plus delta t; u i j here will give me U k t and this k 1 has gone up stairs and divided by h square gives you the Peclet number. What I have here - u i plus 1, I could write it as e to the power i k h times U of k t; that we have done in the last few classes; you know how to handle that. 2 u i j is nothing but simply 2 into U k t and u minus 1 j will be e to the power minus i k h U k t.

So, having obtained this difference equation in the k t space, I could divide both side U of k t. If I do that, then what do I get?

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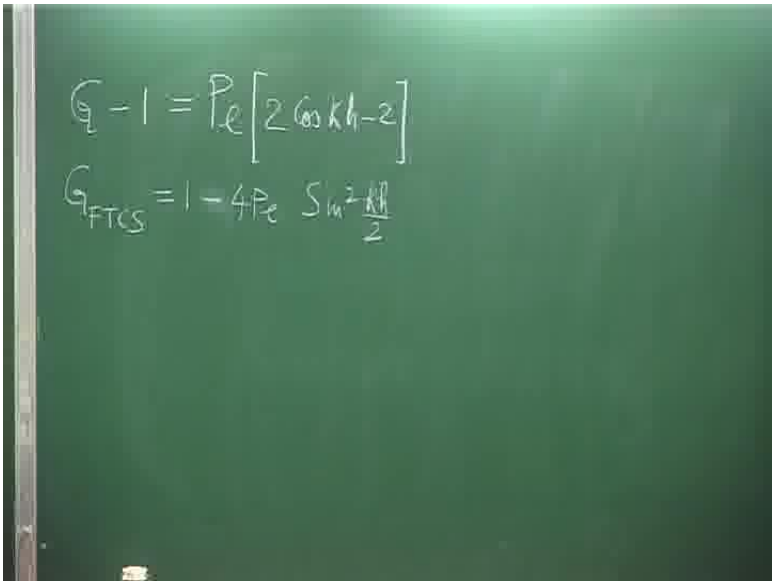

This one here, this divided by U k t will give me G; then I will have minus 1. In the right hand side, I will have the Peclet number. What about this? (Refer Slide Time: 17:48) e to the power i k h plus e to the power minus i k h will give me 2 cos k h minus 2; that is what we have.

So, what I am getting here then G of this algorithm which I called as FTCS would be equal to 1 plus, what about this? I could take 2 out; I could also write 1 minus cos minus 2 sin square; so, I could write here with a minus sign; I will write it here as 4 P e Sin square k h by 2.

So, that is precisely written as equation 7.

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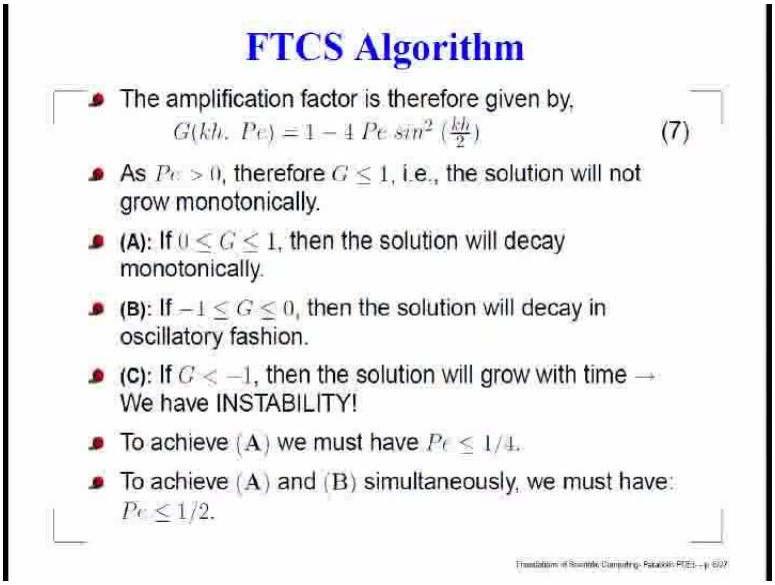

Now, what do we want numerically? Numerically, we do not want G to be greater than 1. If G is greater than 1, then it is numerically unstable method; so, we cannot afford to have that. That part - G value exceeding 1 is out of question because you can see, it is 1 minus 4 times this. So, this is a positive quantity 1 minus 4. So, the whole quantity has to less than 1. So, Peclet number is positive; it is a time step by space state square; so, it is positive; so, the solution will not grow monotonically. What does it mean? If G is greater than 1, then every time it keeps on growing retaining the same time. So, that is what I mean by monotonic growth. So, if I have Peclet number, as Peclet number is positive, this is assured if G is less than plus 1.

However, if I have the value of G lying between 0 and 1, then what will happen? Then the solution will not grow and it will slowly come down retaining the same sign because G has a plus sign. So, you should see the solution decaying monotonically.

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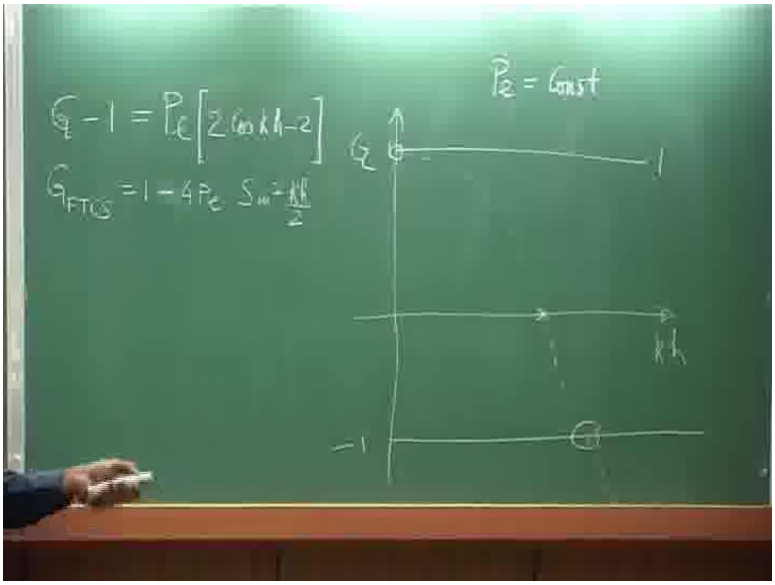

However, if I try to plot G versus k h, we have seen the upper bound is plus 1. So, that is always satisfied. Now, if g is between 0 and 1, I could have some solution like this (Refer Slide Time: 20:33).

So, what are we doing? We are fixing some value of Peclet number and then we are plotting G versus k h; this can happen. For small values of k h, what happens? When k h goes to 0, this part goes to 0 and you get 1. That is why we start from 1, as k h keeps increasing, slowly comes down and you can see there would be a limiting value of k h for which 1 minus 4 is going to be 0. So, you can locate what is the k h for which the G is 0.

So, if I have my G bracketed in between this (Refer Slide Time: 21:20 to 21:50), then the solution will monotonically decay, but then, we are seeing that, for higher values of k h, it takes a negative value. So, it is this condition that we have talked about here that I could have a situation where g is less than 0, but bounded on the bottom side by minus 1. So, this is my minus 1. So, I could just simply come up like this. So, in this range, what happens? Solutions still decay because G is less than 1 modulus; but what happens? Every time you do that, you multiply by G. So, you switch sign; so, that is what I said, that you will have a solution that will decay, but in an oscillatory fashion.

Now, this figure shows the possibility that I could go below minus 1 also. If I do that, what happens? That means numerical instability. Please do not confuse it with physical instability. We are talking about physically stable system and we are looking at the property of the numerical method. So, these are the possibilities determined by the value of G.

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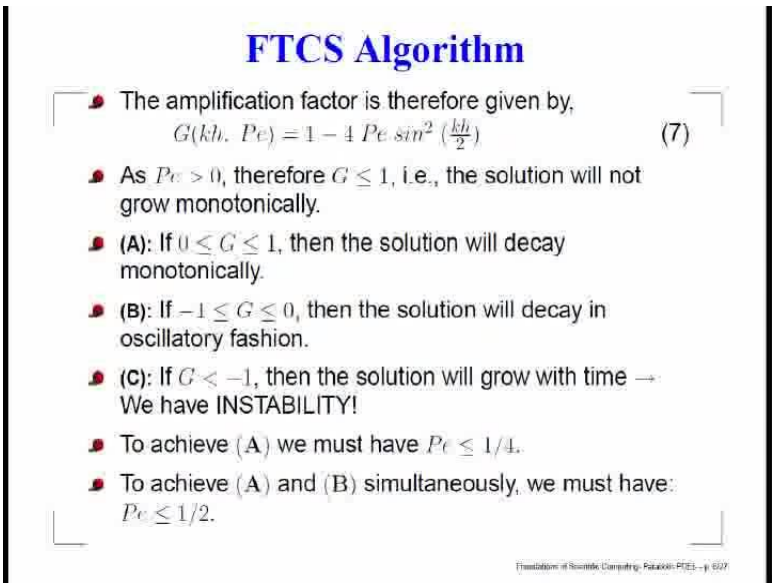

So, C is the case is what we do not like to happen, where solution actually blows up.

Now, as you can see, this sin square k h by 2 at the most can be 1. So, if I want to achieve this condition, G should lie between 0 and 1. This is assured only up to where it becomes equal to 0. As I showed you, it would happen if you keep your Peclet number less than one-fourth; if you do that you are assured. So, this is sort of a limit prescribed to you to keep your calculations stable. So, to solve, use this method and solve this equation. You should endeavor to keep this Peclet number less than one-fourth; then you will have a solution to decay monotonically.

Now, if I also want to allow this possibility that not only there I want to go from here to here (Refer Slide Time: 23:48). So, I start from here; so, I would like my solution to be bounded between minus 1 and plus 1. So, that means achieving a and b simultaneously; how can that happen?

I have to see what is the additional range of Peclet number I can allow so that I can go and reach up to here (Refer Slide Time: 24:12). You can very clearly see that, that will happen if I put this equal to minus 1. Then, you will see, the Peclet number should be equal to half. So, what happens is you have the following recipe in front of you now.

We are saying that, if we keep the Peclet number less than one-fourth, then we will have a decaying solution which will retain its sign at every time step. But if I keep my solution - the Peclet number, between one-fourth and one-half, then solution will still decay, but it will flip sign every time step. So, you can now understand what it does.

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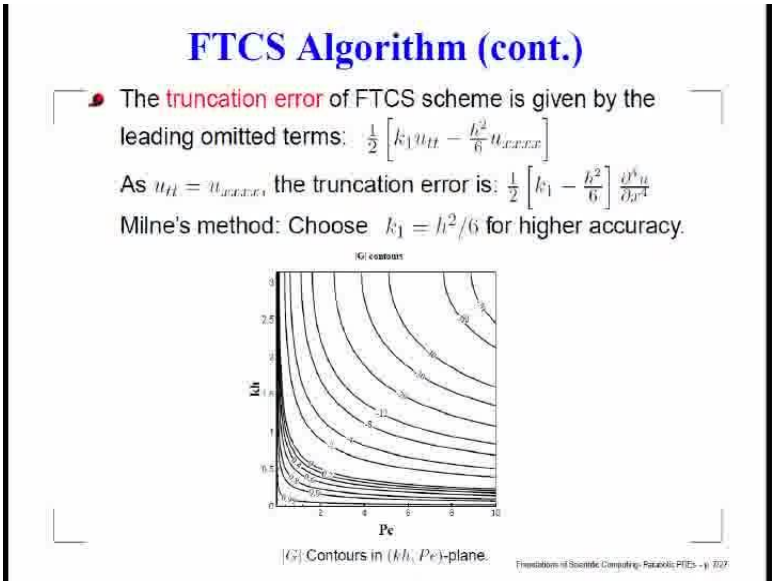

Now, before I go to anything else, let me also point out one interesting aspect that if you look at the leading truncation error term, from the time derivative, we had this term k 1 by 2 into u t t; if you look at the space discretization, that was h square by 12 into fourth derivative.

However, what happens? u t is equal to u x x. So, I can find out u t t will be this fourth derivative of u with respect to x. So, these two quantities are essentially same; so, I can just take it out. Then, what I see inside? a quantity which is k 1 minus h square by 6. What does it mean? If I choose my time step k 1 in such a way that k 1 is equal to h square by 6, then this leading truncation error term will be 0. So, that would give you the additional degree of freedom, where the error is further minimized.

This method was suggested by Milne. So, this is called the Milne's Method.

Now, think of the consequence of such a requirement. What we found out? So, what is this? This means that the Peclet number should be less than one-sixth. So, if you can keep your Peclet number less than one-sixth, then you will not only get a solution which will monotonically decay, but it will also give you more accurate solution.

So, this is what we do and what you could do is you realize that, G - that expression, that we have written there (Refer Slide Time: 26:56) are functions of two parameters: one is the Peclet number and the other one is the wave number k h non-dimensional. So, what we could do is - we could represent the health of this method by plotting G contours in Peclet number k h plane. What do you notice here? Though there is a line here, that is your G equal to 0 line, anything above this line on this side are all unstable; so, they are all less than minus 1. So, you are forbidden to go there. You can stay in this region, but you also realize that, depending on the choice of your Peclet number means depending on your choice of time step, you can only resolve those k h which lies below that G equal to 0 line.

So, actually we should be drawing a G equal to minus 1 line; basically that is your stability limit.

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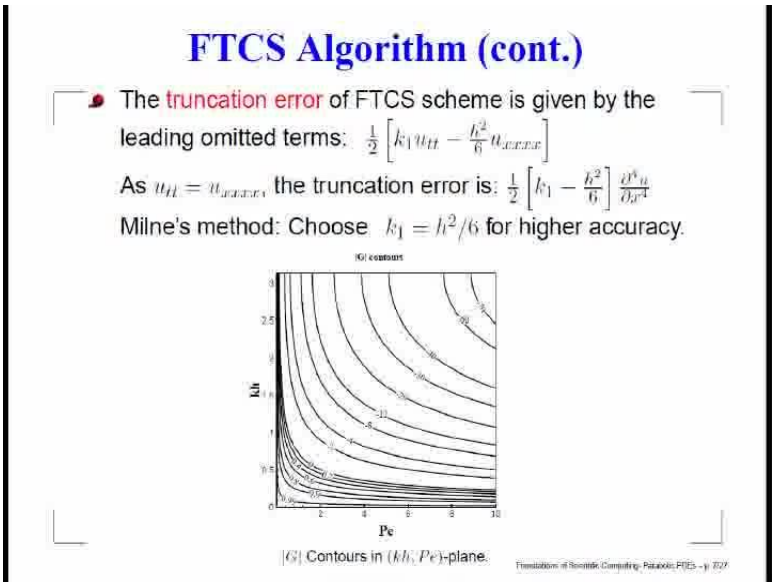

So, basically, we are saying that, if I want to represent all k h values faithfully without incurring any instability or error then, my Peclet number should be very small because you have seen this last line that we draw here is point 0.99.

What does it mean? It means that every time step you are computing, your solution is decreasing by 1 percent. So, if I use this method in matter of 100 steps, you can see that I am actually incurring so much of error. So, what you ideally want? Recall back what we say. Ideally we always want G should be equal to 1.

So, you can see that this method - this forward-in-time centered-in-space scheme is a quite a restrictive method. If I now go back to the stencil, how do we do it operationally?

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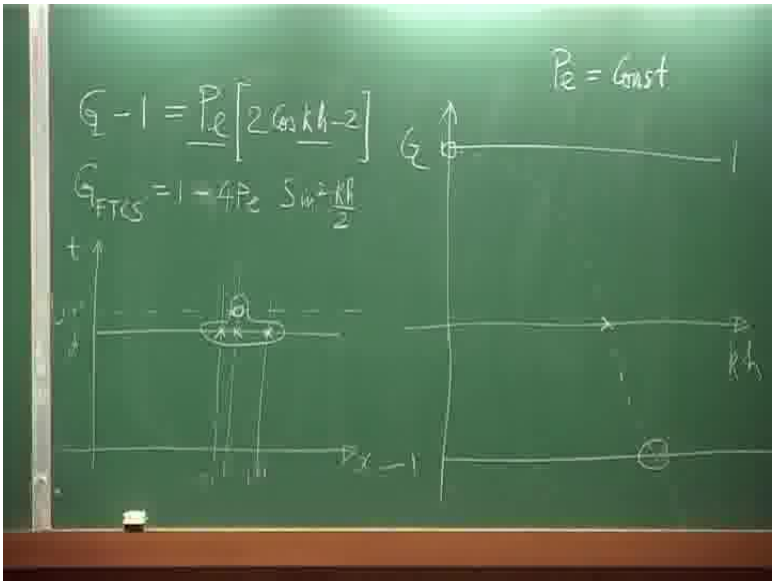

Operationally it is like this that, I will try to get the solution in the x t plane.

Now, if I write this index as j and the next line is j plus 1, and let us calls this as i and this is i minus 1 and this is i plus1 (Refer Slide Time: 29:40 to 29:58). So, what does this discrete equation difference equation tell us? It tells us that u i at j plus 1, that means this point solution depends on u i j, the point just below. So, I will mark it there and these three points are also one level below.

So, basically what you are getting is a computational molecule of this shape. so this is how you get to solve the problem.

What is the attribute of this method? At each and every point, I can explicitly work the value here because we already have the information at the time step. So, that is why this method is called the explicit method.

This is a sort of a rule of term, as we will also prove and show that all explicit methods have this kind of a restriction like what we have talked about. As we saw in that figure, to be close to G equal to 1, we really need to keep Peclet number very very small. We are talking about say 10 to the power minus 3, 10 to the power minus 4.

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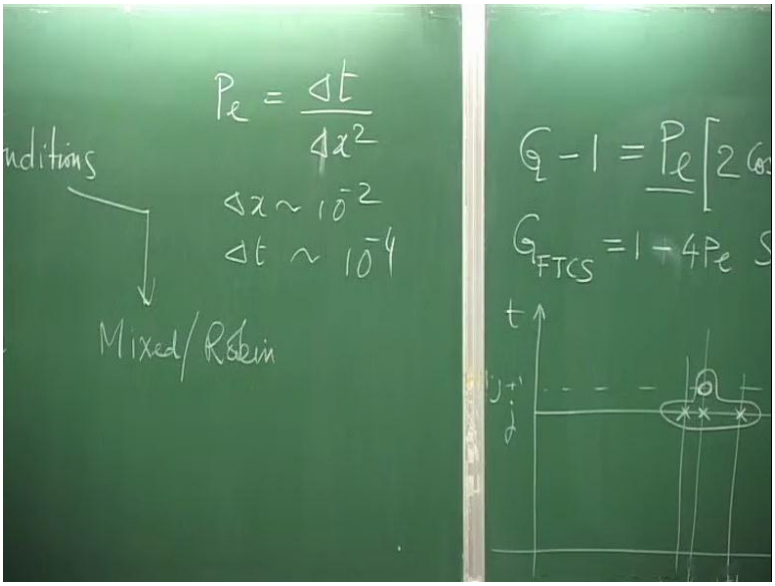

What is Peclet number? Peclet number is basically your delta t by delta x square. So, what happens is - suppose I take delta x as 0.01, what is delta t? This is of the order of 10 to the power minus 4. So, you can see that how much of a refined time step you will have to adopt to be able to compute. Not only that, I mean we have to keep the Peclet number, for accuracy reason if we adopt Milne's method, that itself should be one-sixth. So, your time will be further reduced.

So, this sort of restrictions keep piling up one over the other and make this method little difficult to use.

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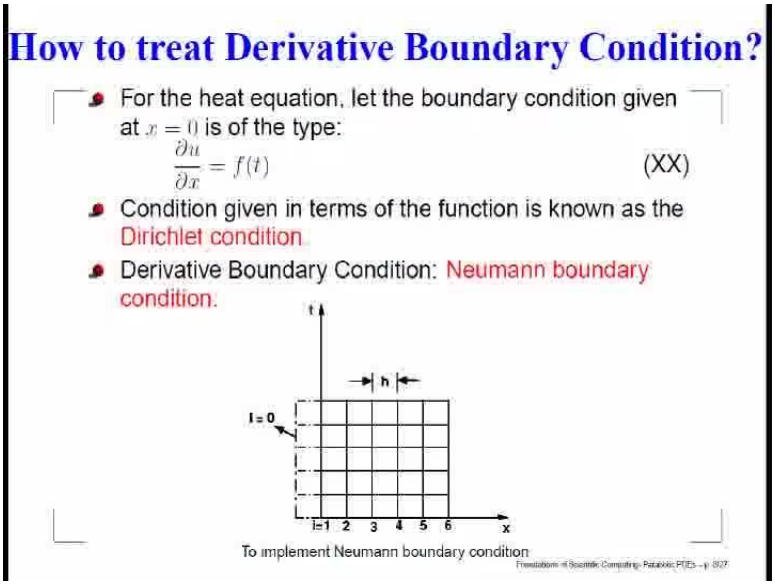

Before we go any further, let us try to see what happens if we do not have Dirichlet condition, but instead, we have the Neumann condition; that is something like a derivative condition.

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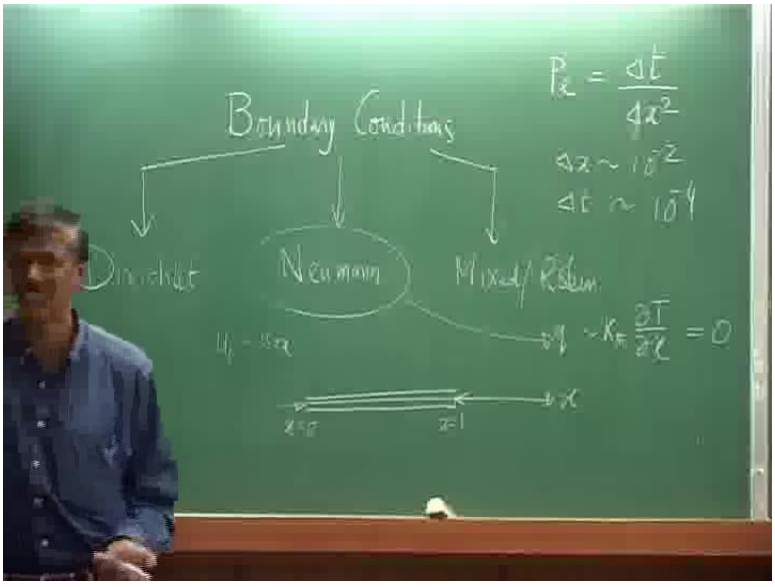

If you recall, the problem that we are talking about, if this is my x plane, then I was talking about a rod here. So, this is x equal to 1 and this is x equal to 0, and then we have some kind of boundary conditions given at this end and at that end. (Refer Slide Time:

32:35). That is the problem that we are solving. So, when I say I am solving u t equal to u x x, this could be one of the representations.

Many a times, what you could do? If it is an engineering problem, you can put it at a constant temperature bath; you can fix the temperature. If I fix the temperature, then I will get the Dirichlet type of condition. I am fixing the function itself. However, many a times, what you do? You have all done thermodynamics; most of you have hopefully done. You know that you also have this kind of conditions where you say, I will keep it insulated; I would not allow any heat transfer to occur from one of them.

If I do that, what will happen? I will basically say something like this q is some… I should be careful to say, this is the heat transfer rate (Refer Slide Time: 33:41). Suppose I put this equal to 0, then I am basically giving a condition on the derivative and that is what we are calling as Neumann condition.

So, this is quite common. For a heat transfer problem, having a Neumann condition is a very routine state of affair. So, that is what we are saying.

For example, a heat equation we have on the left boundary. We put del u by del t is equal to some f of t. Then, how do I solve the problem? What is the problem? The problem is the following: let us look at the computational molecule and how we go about solving it.

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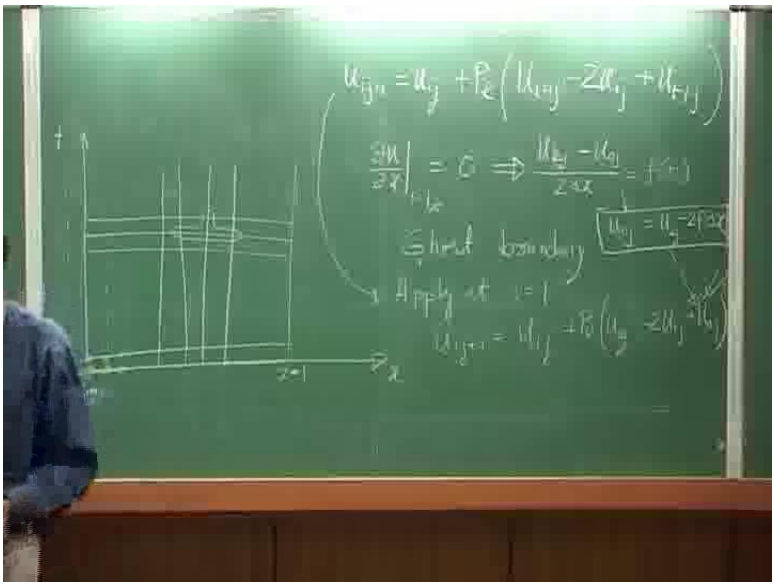

So, basically what we are doing? I will talk about solution in the x t plane and this is one of the boundaries; that is equal to x equal to 1 and this is condition x equal to 0. Then, we have seen that, if we look at few lines - time lines and the corresponding space discretization by lines of this kind, then we have seen that, we have a computational molecule which is something like this.

Now, that equation we had written was this - u i j plus 1 is equal to u i j and what do we have there? plus Peclet number into u i plus 1, j minus 2 u i j plus u i minus 1. So, this is our strategy.

Suppose, I give you the solution at t equal to 0, then what do you do? You go to the next line and what you see is…If a Dirichlet condition is given to us, then this is already known to us. Then I will start using this equation (Refer Slide Time: 36:12 to 36:23) from the second point onwards. So, you can see, applying a Dirichlet type of boundary condition is much easier because we can then straight ahead start from here. This solution would depend on this value, this value and the next value. Then I will come to the next point and so on and so far I could do.

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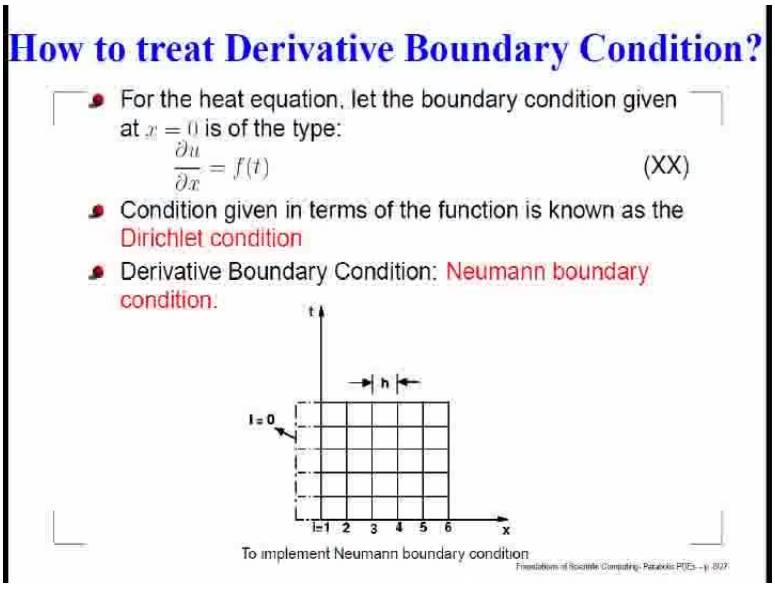

However, we are seeing here that, here the boundary condition given on the left hand is given in terms of a derivative. So, this solution itself is not known to us. So, what do we do? We have been given del u del x at i equal to 1 equal to 0 and what we do since we

are doing Centre-in-space, I could also write like this. So, I will write u. So, I am trying to evaluate the condition.

If I try to do a central difference, I need a point to the right and also point to the left; point to the left does not exist physically. So, what we do is - we add a fictitious line which I have shown here by this dotted line.

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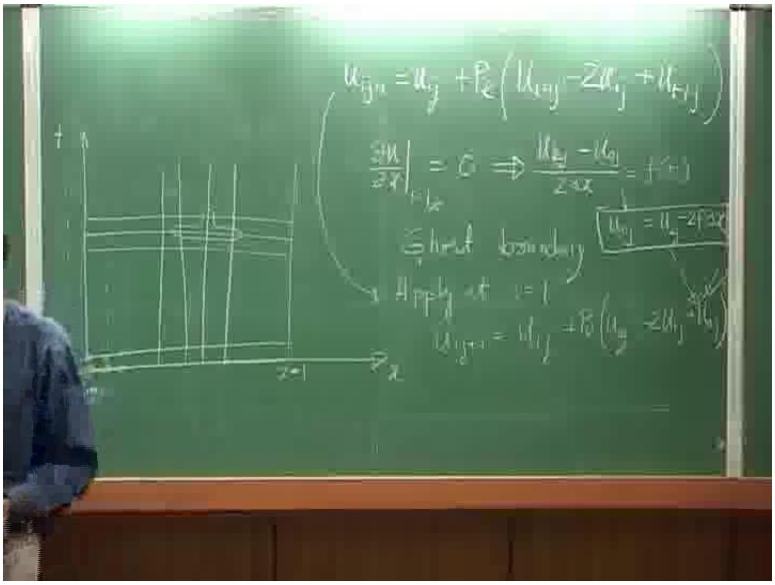

So, this dotted line that you are seeing here is what is called as the ghost boundary. So, we add an extra line here. So, this was i equal to 1. So, I am basically introducing a line i equal to 0; so, this is my ghost boundary.

Now, what I should be doing? The difference equation that we have - where would we apply it from? We start applying it right from i equal to 1. Then what happens? If I apply this, what do I get? u 1 j plus 1 should be equal to u 1 j plus Peclet number and u 2 j minus 2 u 1 j and plus u 0 j. Now, your worry is this does not exist, but you could do this (Refer Slide Time: 38:50). What I could do? I am trying to find it out at i equal to 1. So, I will write it as the point to the right. So, this if it is like this, I will write it as u 2 j minus u 0 j by 2 delta x; that is equal to 0. That is what this condition means.

That means what? This gives us some… what we have taken is not 0. Let us say, we have taken it like f; so, let us keep it f of t. Then, what I get from this equation? then I will be able to write u 0 j is nothing but u 2 j minus 2 f into delta x. So, I have used the

boundary condition to relate the fictitious point with some point inside. So, we can do that. Then what I do is required here; so, I just simply use it here (Refer Slide Time: 40:08). So, what happens now, in this equation you are trying to find out the solution at the next time step; everything is known because this u 0 is nothing but related to u 2 and your boundary condition is also prescribed; if it is known, you can actually use it.

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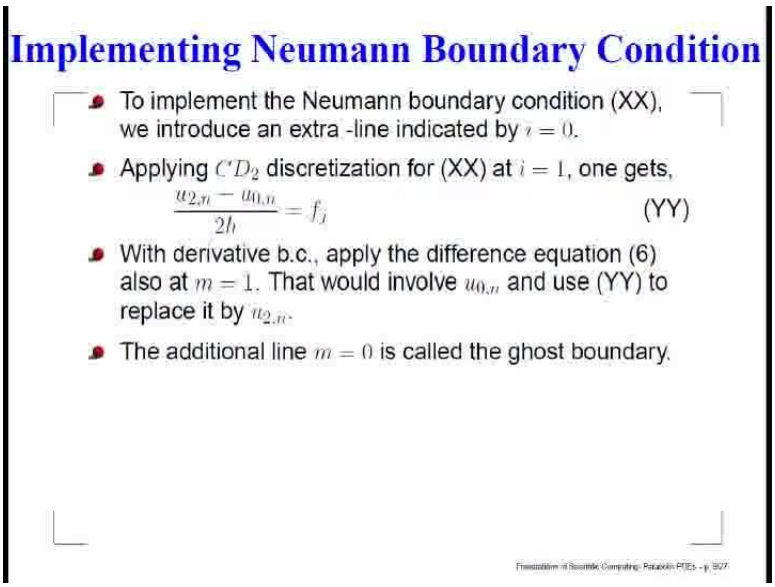

This is what is being demonstrated here in this slide. If I have derivative boundary condition, I call that as the Neumann boundary condition and I used up that boundary condition writing this equation what I have written here as y y.

So, with the derivative boundary condition, you start applying the difference equation from the first point in the physical boundary because that is where you do not even know the solution. You know the derivative condition; so, you need to know the temperature there also. That is what we do and we end up getting what we called as the ghost boundary. So, this is something that we need to know; how to handle derivative boundary conditions.

Now, we made the comment that, FTCS method is restrictive in terms of allow you time steps, in terms of accuracy. So, various people were the vanguard of this development of this subject; one of them was Lewis Fry Richardson from Cambridge and he was so very optimistic about the future of this subject that he wrote a book in I think 1904 or 1903

saying, how weather will be predictable very soon. So, he wrote a book then and there; he was actually looking at this problem and he said – look, we have a problem for the FTCS method in terms of accuracy. So, if we increase the order of the method, there is a chance that will have a better accuracy.

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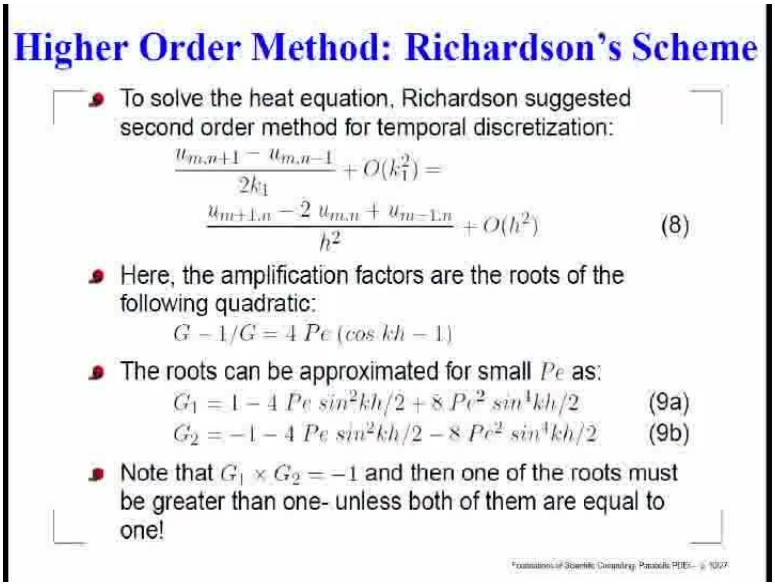

That lead him to suggest that – look, we are doing second order accurate in space if I look at in terms of h square; so, why not make the time discretization also second order accurate? So, what happens? What I would do if I am applying this equation at the j? I will take the solution one level up related to one level below. This has an alternative name also. This is what is also called as the Leapfrog Method.

Some of you have played these games; child's play like, they call this Leapfrog or Hopscotch Method. You have heard of people jump from leaving one square alternatively and jumping. It is something like your checker's game. So, that is exactly what is suggested in this method. So, what happens? You could now look at the difference equation and use the same methodology of analysis that we have looked at so far.

So, we define G and what do I get from here? I will get u i j plus 1 divided by u i j that should give me a G.

What about this? I am saying that, if I have a term like this (Refer Slide Time: 43:46) and relate it with this relationship should come via the G because the Fourier amplitude is related by G.

What happens? When I am looking at i j minus 1, I am trying to relate with i j. What happens? Then it will become 1 over G; that is what happened here. If I divide both sides by u i j, this will be u i j minus 1 by u i j. So, that would give me this - 1 over G. So, you can see, this term will give us G; the next term will give us 1 over G; we just take this 2 on the other side and everything remains as before.

Now, what happens? We have now two roots: G 1 and G 2 given by this. You do not need to even solve it to find out what is happening. But you can very clearly see it is a quadratic with the last term; the product term of the root is minus 1. You can see that G square minus 1 into 4 Pe into this. So, G 1 into G 2 is minus 1. So, what does it mean? If one of them is less than 1, it is stable; the other one has to be unstable.

So, without even solving here is a naive approach - just because you apply a higher order method, does not mean that you are going to get what you want: more accuracy, faster calculation, stable calculations.

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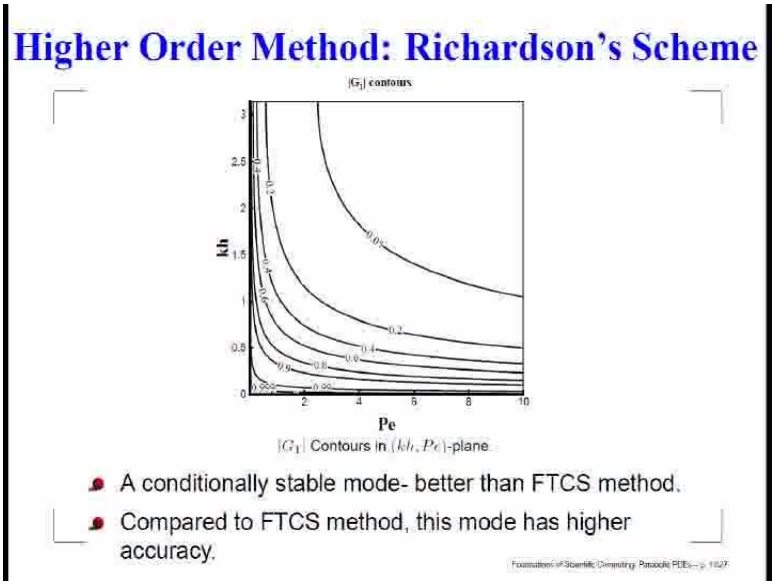

Now, here is an example where you actually end up in trouble. If you do not believe me, you can use up writing a small program and find out, is G 1 and G 2 contours?

So, G 1 expression we have seen given by 9 a, and G 2 is 9 b. So, if I look at G 1, this is what I get.

Now, what happens is this picture is somewhat reminiscent of what we did for FTCS. The only thing is - here all the lines are shifted to the right because it is more accurate method. So, every line actually got shifted there. Now, even this line you are seeing is still plus 0.05. So, 0 lines would be even further on this side; so unstable region for G 1 has been shifted on that side. You can also see that, the last line I have shown here is actually triple 9 - 0.999. So, every time step you are accumulating error of 0.1 percent.

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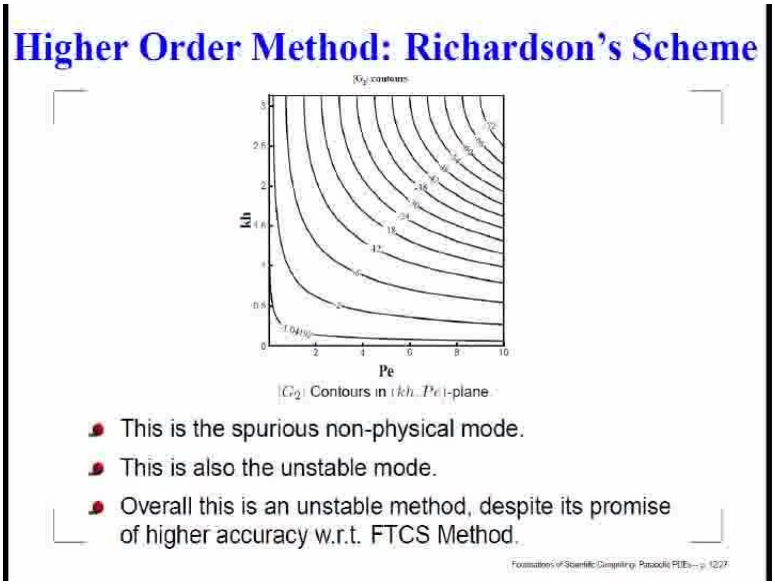

So, you would say, there is an improvement. So, why are we complaining? We are complaining because of this other part - look at this G 2; you can see there, this line is less than minus 1. So, this G 2 mode is unstable mode. So, when you are actually going to compute, it is going to be a combination of G 1 and G 2. One mode is more stable and the other mode is violently unstable. So, net result is - you will not be able to use this.

There is other thing also. You must understand that this happened because we tried to use a method which required information at 3 time levels. That is why we ended up with a quadratic in G.

If you recall, in FTCS we got a single value of G because there was just a linear relation G is equal to 1 minus 4 Pe sin square k h by 2, but here instead we got a quadratic. So,

we get one mode - the G 1 mode, which resembles the actual physical mode; whereas, the G 2 is an attribute of our numerical method. So, we will call this as a numerical mode or non-physical mode and it is spurious. It does not exist; it has come about because of a numerical strategy. So, we conclude that, despite its promise of higher accuracy with respect to FTCS method, this is essentially a unstable method.

So, please do not be taken in by any such claim that, higher order methods are better methods. Always you will have to come back to the drawing board; do your own analysis; find out whether its works fine or not. We learnt our lesson that always you may not get the same thing.

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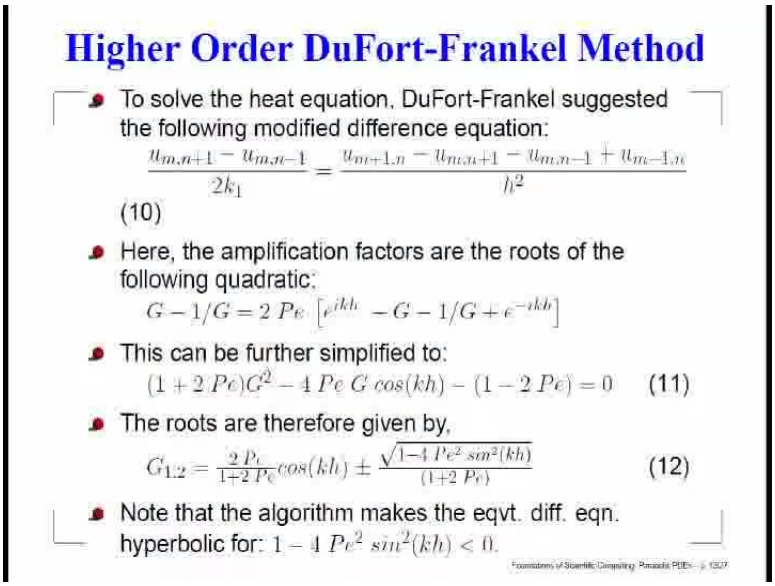

Now, this is a method which was pioneered by these two gentlemen: Du Fort and Frankel. What they did was somewhat very suspicious. You can see the equation 10; what has been changed compared to the other method - that Richardson method. What did we do there?

So, there, it was the Richardson Method. So, Richardson method is written like this (Refer Slide Time: 49:01).

Now, Du Fort and Frankel realized that, that method is unstable. So, they said - let us play a trick. What do we do is instead of this quantity here which is this point (Refer Slide Time: 49:21), what I do is I take as this as average of these two points; that is what

they have done; you see 2 i j has been replaced by u i j plus 1 and u i j minus 1. This looks adhoc. So, we do not let it lie there just like that and we can go ahead and start investigating it. Once again you will agree with me that it is a 3 time level method because you have j minus 1 j and j plus 1. So, you end up with a quadratic in G and that is what you have here.

It looks somewhat little more daunting and complex, but you can get this; you simplify it; you get this quadratic and you get these two roots.

Now, this is something that we should pass and ponder. Our method demand G to be what? A real quantity; we are looking at a solution which is monotonically decaying. We do not want it to oscillate right. So, G should be real, but if you look at this expression here, this quantity under the radical sign depending upon your choice of Peclet number and depending on the k h that you are looking at, that quantity can become negative. When you take a square root, what will happen? You will get a G which will be complex.

So, what happens? You started looking at a solution which should have been monotonically decaying with t equal to constant, but here you are going to get a sort of an oscillatory solution. What you could actually do? You could write down the Taylor series expansion for this equation 10 which will do and we will show that if we are not careful in choosing the spacial steps with the time step, our actual equation can turn out to be hyperbolic.

So, in trying to solve a parabolic equation, somewhat careless approach like what has been suggested here, can lead as to a parameter space, where the solution actually becomes hyperbolic. This is a problem of consistency; this is what I meant by consistency.

If I want to solve the problem which is parabolic in nature, solution should follow that principle faithfully; if it does not, then we have an inconsistent method. Du Fort-Frankel method has to be handled rather carefully. So, you have to ensure, you have to choose your Peclet number in such a way that, the last relation is not violated so that you get truly real values of G 1 and G 2.

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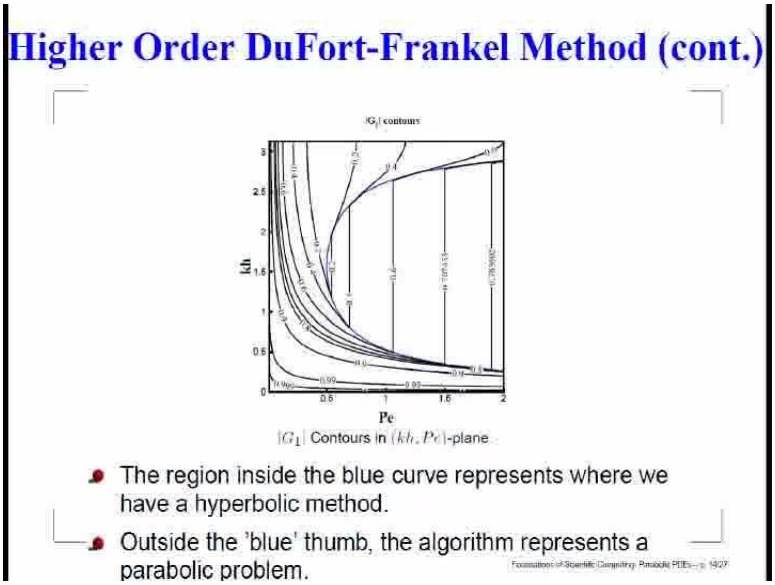

We can actually work it out. We can work it out once again in Peclet number k h plane and this is your G 1 contour and you can see various values here, like what we have seen before. But I have also drawn a line here, which is thumb shaped, which is blue in color; inside that region you have that quantity, negative. So, that is where your G 1 will have a complex value, somewhere in this region - thumb shaped region; outside it is real; so, outside there is no problem.

So, what you need to do is - you can actually choose a value of critical Peclet number. If you keep it below, you are on this side; so, you have no problem of being inconsistent. You will be inconsistent only when you take larger k h. Then some ranges of k h will display hyperbolic wave nature. Whereas, other values of k h will display parabolic nature. So, this is your G 1 contour.

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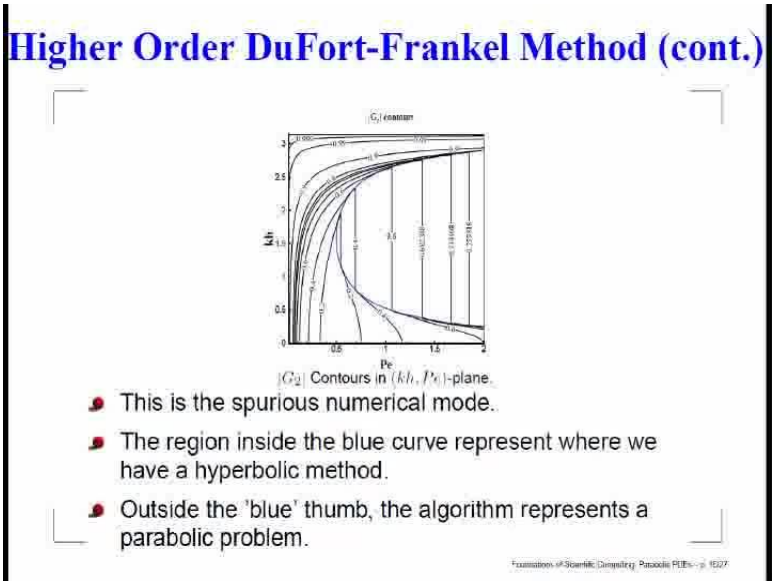

You can also similarly look at the G 2 contour and this is what we get. Needless to tell you that G 2 is the numerical mode; it is not there physically. Why do we call it a numerical mode?

Physically why should we expect that G should be only 1.

(( )) [Noise]

Pardon

Absolutely. So, what he said is the following: In the limit delta t going to 0, you are actually looking at the local time; numerically you may take 3 time step or 4 time step as many as you want, but your definition of continuum derivatives relates it is to derivatives to be calculated at that time. That is why you should always try to avoid this temptation of involving more than two time levels.

So, this is something that we have seen for the Richardson method as well as Du Fort Frankel method that, we do end up having a spurious numerical mode.

Once again, I told you the region inside the blue curve is where we have the hyperbolic equation. Outside this term there, algorithm represents the original parabolic problem. But you also realize that, this mode values; actually you will see it is loaded.

Now, you can take a look and download the material. You can see that most of the small values of k h, for very small values of Peclet number, they are close to 1. So, it does not hard very much. That is why Du Fort Frankel method has been introduced, sometimes if I am not wrong, some sometimes in 30s or 40s and you may actually even do a little of bit search you will find that there are still people who use this method, but you have to be careful because you have to really taken Peclet number very small; otherwise this spurious mode is going to really hurt your solution because if I take larger value, you see this is 0.3 lines, then this is 0.4 lines and so on and so forth.

So, you can actually get into a problem where you may lose physical information. Why do I say that? The fact is - any time I prescribe you some initial condition and you have two modes, what does the solution do? The solution distributes this initial energy into these two modes. If one of the modes keeps on dumping it by factor of 80 percent every time step, that part of the solution is lost. So, your initial condition information is irreversibly lost. I do not know how many of you have taken a course on topic called chaos dynamics - there they swear by initial condition; they say like there are many physical systems including our weather. If I make a very small error in the initial condition, after some time the solution diverges from the actual solution.

So, you understand that these multi-level methods have this perennial problem of invoking spurious numerical modes. They can take away a chunk of initial conditions and the resultant solution, despite the other part being physical, still would be deficient and wrong.

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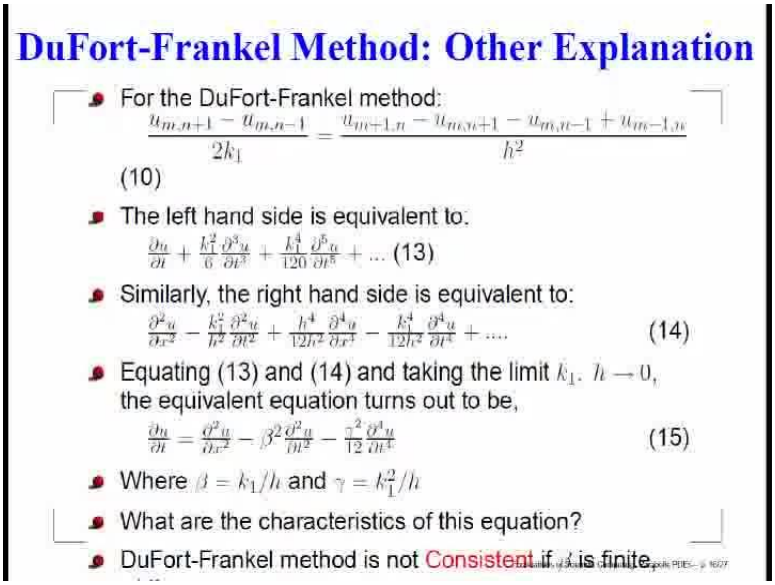

This is something that we should always keep remembering. We can also do a Taylor series and see what happens. The left hand side that we have here, v is nothing but del u by del t plus k 1 square by 6, the third derivative; then k 1 to the power 4 by 120, 5th derivative and so on so forth and the right hand side gives you this.

So, what happens is - when you equate this, you get an equation of this form. What is this beta? Beta is k 1 square by h square. We call it here as beta square. We also have this part - last part of the solution, where if I call k 1 square by h as gamma then this part is this.

Now, what happens? We look at the limit; your k 1 is small, h is small; so, what would you expect? You should get back to your continuum equation. However, in the process, if k 1 by h remains a finite value, it is not 0. Then what happens? This term remains; these beta square terms will not go away, despite the part that individually k 1 is vanishing, h is vanishing, but their ratio is finite.

So, what happens to your wave equation? Any time you have second derivative of time, related to second derivative of x, you end up like what you have seen that d'alembert's wave equation.

So, you need not to believe me. You just plug in the trial solution u is equal to some i k x minus omega t and convince yourself that you are getting a real dispersion relation. That would imply it is a hyperbolic equation.

So, we concluded that DuFort-Frankel method is not consistent if beta is finite, even though k 1 and h may go to 0.

So, I stop here.