

Foundation of Scientific Computing

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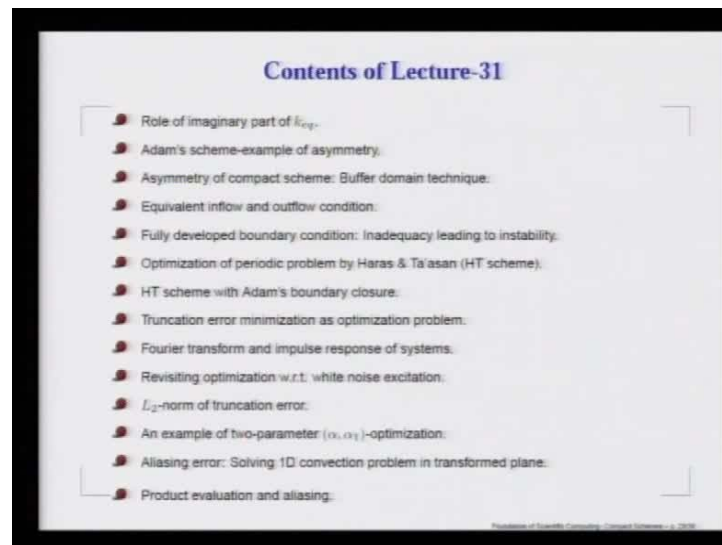
Department of Aerospace Engineering

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Module No. # 01

Lecture No. # 31

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Lecture 31 begins with a review of the imaginary part of the K equivalent that we can obtain the spectral analysis tool we have developed and as an example we saw the Adams scheme which shows the asymmetry in terms of instability near the inflows.

And this can be at times cured by introducing called as a Buffer domain technique which is used near the outflow and the compact scheme. Interestingly, enough actually mimics this Buffer domain technique because it has tremendously high dissipation near the outflow boundary. So, if we are talking about a propagation problem the waves will propagate through the domain.

And when it comes near the outflow boundary it will be attenuated and that will save lots of problem of wave reflection from the boundary which seems to be a major problem of computing.

So, this is what we would be talking about. We also would highlight that, very often used outflow boundary condition as a fully developed boundary condition is not always adequate. Because, it can lead to some kind of wave reflection and if we have developed a method which is stable for a wave that is propagating from left to right then this reflected wave will be unstable with respect to that algorithm.

So, this is a major issue that we will have to be working on and then. We will again switch back to the optimization method of Haras and Ta'asan in developing a scheme for a periodic problem.

And once we adopt this optimum scheme of Haras and Ta'asan and add Adams boundary closure to it, we notice again that the instability problem is retained.

So, this actually tells us that we need to do somewhat better and we talk about truncation error minimization as optimization problem by taking care of boundary closure properly.

And we note that, we use the Fourier transform technique and this relates to its property with respect to the impulse response and we will revisit this optimization problem with respect to white noise excitation; only because any other estimates will be a less conservative estimate. So white noise excitation gives us the outer bound.

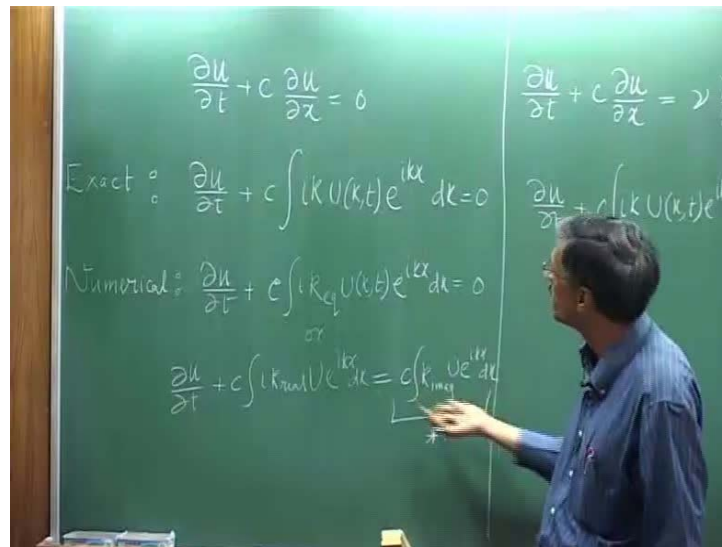
Having defined the mean square error through this norm, we can actually develop an example that is what we will be doing; introducing the optimization problem as a two parameter problem, which will be actually using the grid search technique in identifying the optimum values of these 2 parameters.

This will basically conclude our discussion on developing optimum scheme for compact scheme methodologies and having done that, we also would highlight another source of error which is not covered in the above, that is namely the Aliasing error.

This happens whenever we include product evaluation either in the transform plane as a linear equation or non-linear equation. So, this is something that we will be talking about and we will introduce Aliasing as such.

I think, we were discussing yesterday about what is the role of imaginary part of K equivalent that we have here in this equation 22.

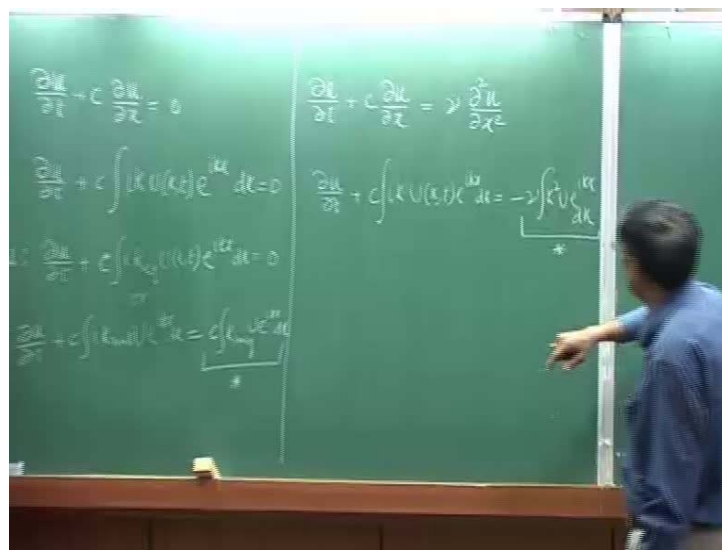
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You can see that while calculating the spatial derivative in a exact form is you multiply $i K$ right and numerically, that this $i K$ is represented by $i K$ equivalent.

If I have this $i K$ equivalent split into the real and imaginary part, the imaginary part goes in the right hand side.

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You look at the corresponding dissipative equation. So this is the source of dissipation here and when I write in the spurious spectral form then, I will get $\frac{\partial u}{\partial t} + c$, this is equal to minus μ ; into this will give me K square.

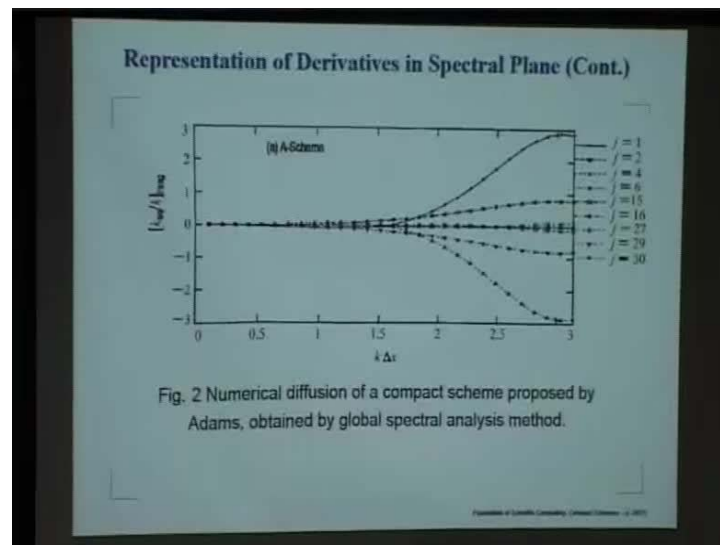
So, what happens is you can see this term appears here with a negative sign. So that is what we have to look for when you obtain K equivalent by K and plot it versus K . you look at the imaginary part,

Wherever you have negative sign that would give you a dissipative effect. If K imaginary is negative that is the dissipative effect.

If K imaginary is positive then what we said yesterday, you would have a anti diffusive effect. So that is what we talk about. Let us say this scheme here,

In this scheme what you see here that for 0.1, 0.2 and 0.4 you see the imaginary part of K equivalent. All these three points you are seeing here are positive.

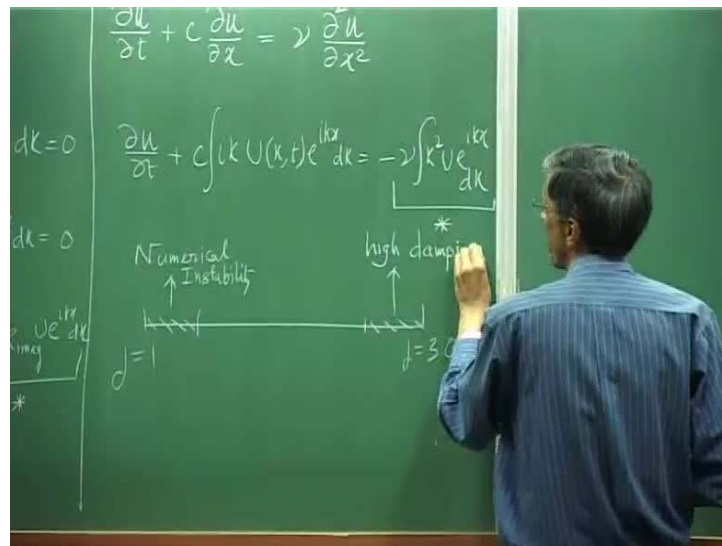
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So, in a numerical exercise these 3 points; well actually would show all the way up to the sixth point. If you see, the sixth point is marginally unstable that is slightly positive on curve. So all these first 6 points you would see numerical instability.

In the same way, if you look on the other side of the domain j equal to 30, you have a massive dissipation. You can see this value and this is j equal to 29 and you can see j equal to 27. So what happens is, near the inflow if, I am solving this problem in a domain like this. Let us call this j equal to 1 and this is at j equal to 30.

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So, what we are seeing up to the first 6 points are getting numerical instability and on the other side of the domain you (()) get to see very high damping.

Right so this is what, I thought I will explain to you clearly; because, I think after the class we had a discussion and I thought everybody would benefit.

So, you can see the role of the imaginary part, that is very interesting and this kind of portrait was obtained only when we could basically do a full domain analysis.

If I do a local analysis, I would not be able to do it. In fact all the way up to two thousand three, many people have come out with local analysis and none of them could actually get a portrait of this kind. And this was shown in two thousand three for the first time with that matrix stability analysis that we talked about in last couple of lectures. We could study the full domain in one go.

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

$$\text{Exact: } \frac{\partial u}{\partial t} + c \int (k U(k, t)) e^{ikx} dk = 0$$

$$\text{Numerical: } \frac{\partial u}{\partial t} + c \int (k_{\text{eq}} U(k, t)) e^{ikx} dk = 0$$

$$\frac{\partial u}{\partial t} + c \int (k_{\text{num}} U(k, t)) e^{ikx} dk = c \int (k_{\text{num}} - k) U(k, t) e^{ikx} dk$$

And the reason that we have chosen this model equation is pretty much obvious. Because, we are trying to take a model equation which is really non dissipative or non-dispersive. So, if you are trying to test out your scheme numerical method, nothing can be better than this. It provides a very critical test on your ability to look at the dissipation and dispersion of numerical scheme.

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Representation of Derivatives in Spectral Plane (Cont.)

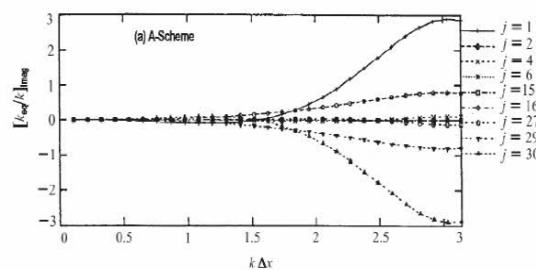
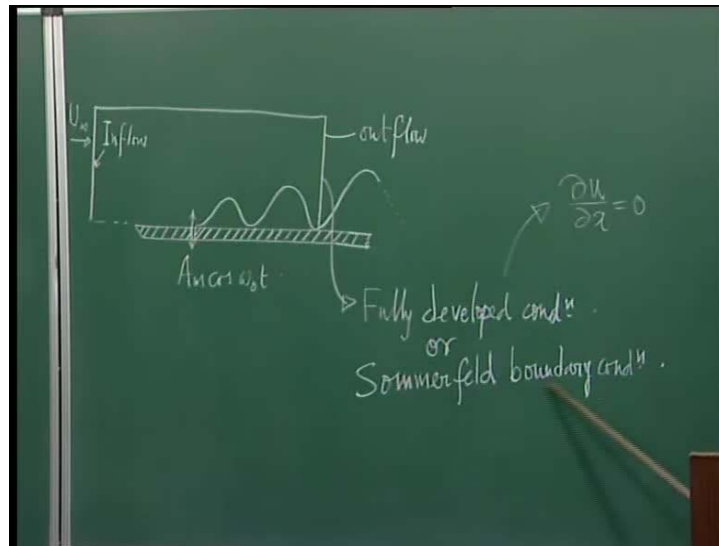


Fig. 2 Numerical diffusion of a compact scheme proposed by Adams, obtained by global spectral analysis method.

So I suppose, this is what we did talk about. Here, we had talked about the dissipative property of the Adams scheme and what we notice that, it becomes more dissipative as you move towards the outer part of the domain.

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And interestingly enough, this could be of very beneficially used in practical computing and let us see how it is done through an example what we are seeing here, called as receptivity of a flow over a flat plane.

What essentially one does here is excite the flow at fixed amplitude on a fixed frequency and the flow is computed in the domain guided by this inflow as well as the outflow here. And what happens during the evolution of the flow is nothing but the growth of periodic disturbances that actually grow in space.

Now if you excite the flow here, these are essentially physically unstable waves that means the amplitude keeps growing as you go down stream.

And, if you are talking about computing such a flow; of course, one cannot take a infinite domain because, eventually this instability will lead this lamina flow into a turbulent state and even there we would not be able to know what precisely the condition would be at the end of the domain. What we have called here is the outflow.

What we notice that this practicality of computing leads to truncating the domain to a finite size. Forces have to consider the inflow and outflow.

Inflow, the conditions are unambiguous but at the outflow we do not know a priori what the solution would be.

And this is rather an interesting aspect of computing as compared to the theoretical aspect of solving a problem. Because, in the theoretical problem we always consider the flow in an infinite domain and we expect the disturbances to decay far away from it and in contrast, in computing we are always forced to take a finite domain and as I mentioned outflow is a major issue.

Now because this disturbance is growing downstream; if we abruptly end the domain here and try to forcibly give some condition at the outflow that can lead to either a spurious reflection of this wave or an attenuation of this wave.

If we could attenuate this wave that would be perfectly fine, then we could disregard a part of the flow where it has rapidly attenuated and retain the rest of the flow and that is precisely what one would like to do in an ideal situation.

Now, if you look at various packages available what one does usually is called as a fully developed condition and in this fully developed condition what we do is, we take the physical variable and we enforce its streamwise derivative equal to 0.

Unfortunately this does not tackle a problem, where we are talking about this kind of wavy nature that is where we need to adopt what is called as Sommerfeld boundary condition.

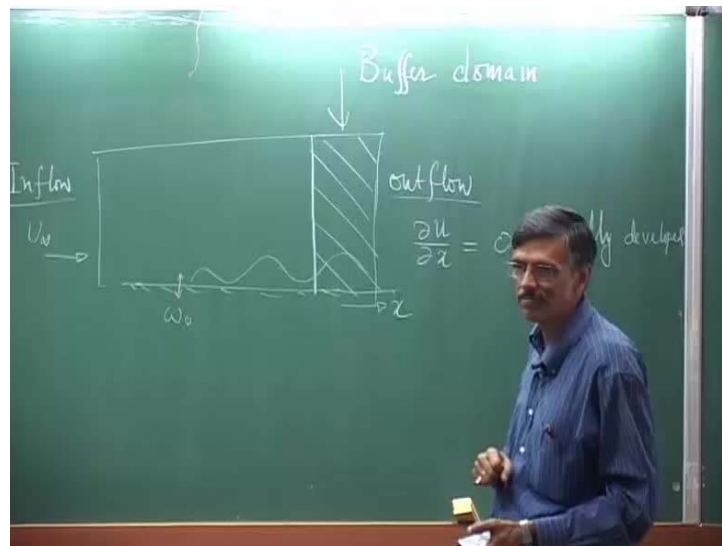
If the wave is reflected back, then you can see what will happen now; if you look at your previous portrait here, what we told that these are dissipative points, right j equal to 30 and 29 but this is dissipative with respect to a signal that is propagating in the downstream direction.

Now suppose I get a reflected wave, what will happen is, it will have numerical instability.

So, you can understand that in actual real life competition; it is so much important for you to appreciate the role of the numerical methods **vis-à-vis** what you are actually computing. Suppose, you are solving laminar flow or say fully developed double inflow, it is not so difficult.

When you try to study certain physical flow, certain physical effects like how disturbances grow and give you a unstable scenario. Physically, these are physical instabilities and are not numerical instabilities that we talked about. We are talking about capturing physical instabilities; those are crucial tests.

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And if you do that and if you are not very sure what you are going to do with this, you are going to get into serious problem. Actually you will not be able to do anything.

Now, **what do you do what** people do and people have found out that, you can create a layer of the flow field, introduce a Buffer domain.

So, what we are actually doing in the Buffer domain is, whatever disturbances are coming here will not allow it to grow, if we have the numerical over stability like this. serious damping that will happen in this path instead of, this wave actually growing numerically will attenuated.

And if we do so much that, when we come to the end of the domain; the wave has artificially been damped out. So, there is no question of its reflection back inside again in the domain.

So, this is the role that Buffer domain plays in actual competition; wherever you have information propagating via waves, you may be better off artificially constructing the Buffer domain like what we have shown in the black board.

This portrait tells you very clearly that, this particular method or methods which actually display this kind of property near the outflow, behaves like a Buffer layer for you.

Because in the outflow path of this domain, any disturbances those are coming will be trivially attenuated and you will not have this problem and this is what we just said in the second. (())

The amount of dissipation added for this outflow points are quite large and this will work like a Buffer layer; used in many flow transition problem. So, I explain to you what this flow transition problem is.

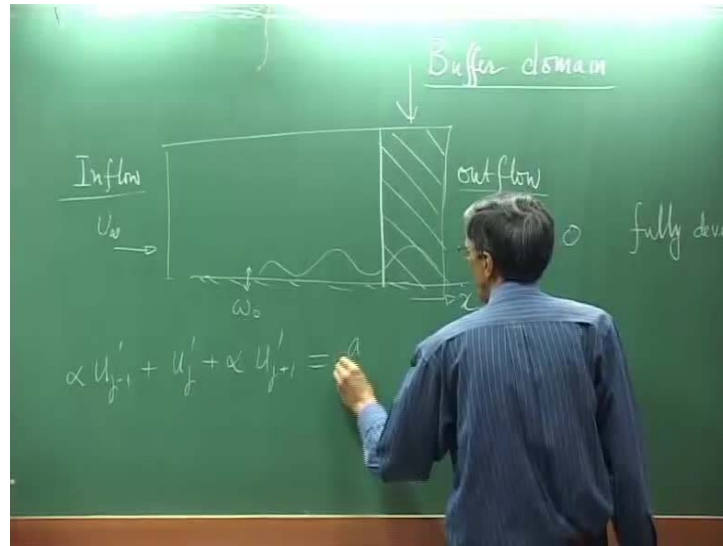
And you can appreciate the utility of such layer that basically, will decay perturbations to 0 at the outflow. So, any spurious reflection from the outflow boundary is a major benefit that we can derive from property of this method.

Now I think we can go back to where we were yesterday and were looking at various schemes and worth looking at how to improve the accuracy of the scheme. I briefly mentioned about these 2 scientist worked on developing new schemes.

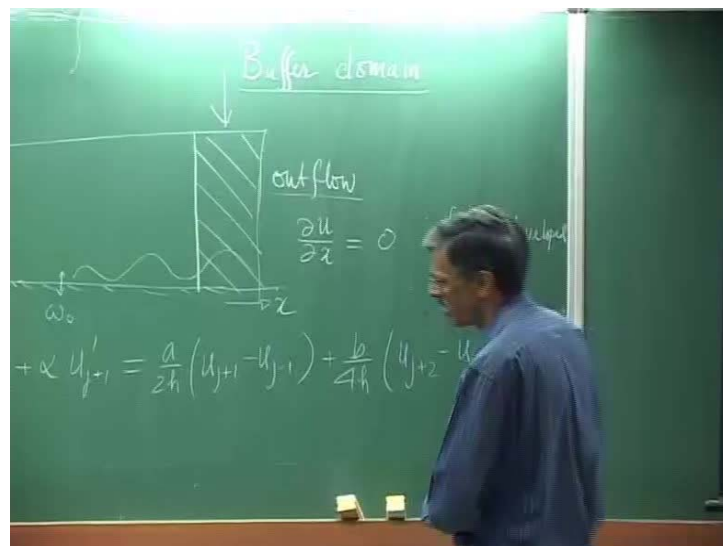
Which had this following property had very high spectral accuracy. You can do it very easily so, the computational speed is quite fast.

However you must notice that they also solved the same problem, the 1 d wave problem, 1 d convection problem.

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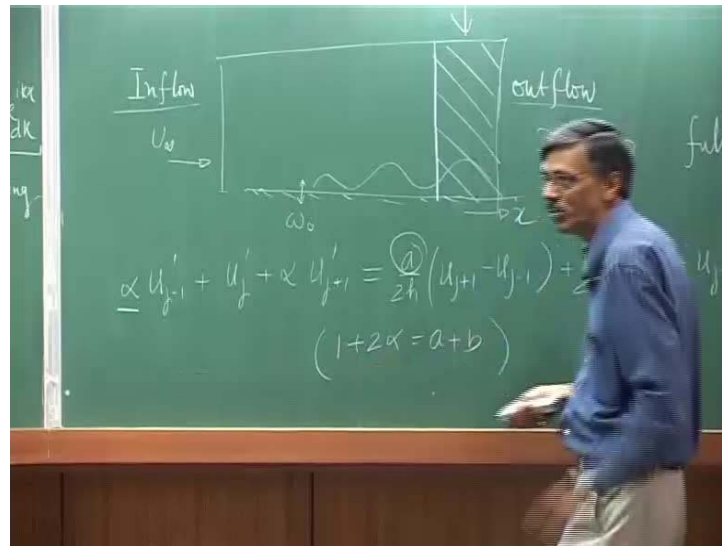


And then what they did is, they started off from that equation that we wrote. This is the stencil with which we actually start working and then because they were looking at a periodic problem, periodic one d problem; all you need to do is tweak this to get you the accurate solution.

So this is applicable at all points periodic problem. So, we do not have to worry about near boundary closure and all this issues have been side stepped by considering the periodic problem .

Now, what you do actually is try to minimize the error that is created by this compact scheme with respect to a spectral method over the full range. Then you can see that, departure is going to be a function of this 3 parameters alpha, a and b.

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And we have already noted that what we need to do is, we need to ensure this consistency condition to be satisfied exactly. So, this is what we wanted.

So, essentially this objective function that you are setting up as the departure of the compact scheme from the spectral method have to satisfy this equation and from that objective function, you can derive 2 more equations to solve this 3 unknowns.

And they did that and they found that, this values of alpha, a and b are this given by equation this relation 34.

And you can see that, this is what we are anticipating. You do not have those fancy numbers, you know rational quotient like i by j kind of thing; what you get is truly real number and (()) nice spectral property of the scheme. You can ensure by looking at that, this is valid that $1 + 2\alpha$ would be equal to $a + b$.

And we noted that, this has a much better property than the sixth order scheme. Now what has happened in this optimization issue is, we have only satisfied the equality of u' .

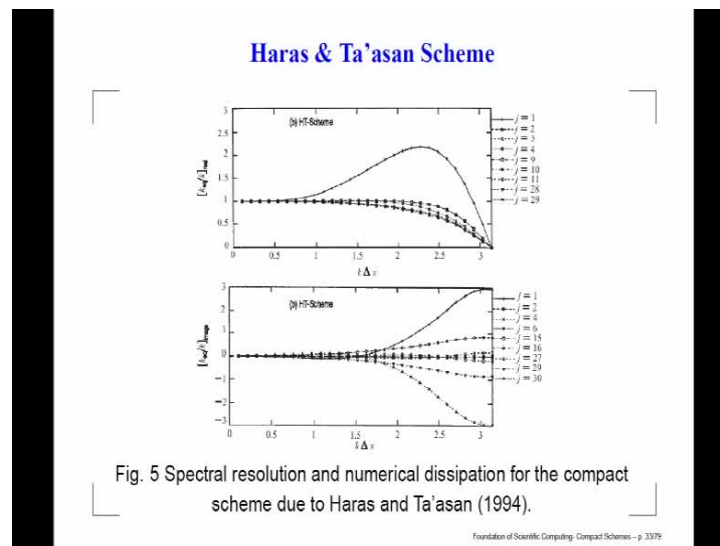
So, what is the order of the scheme. Order of the scheme is second order scheme. So, even within the compact scheme, earlier we showed that compact schemes are much superior to the explicit scheme.

Now, within the family of the compact scheme we are noticing that, if you do a careful optimization, you are going to get a much better resolution of this second order scheme, as compare to the sixth order scheme proposed by Adams.

So, this was quite interesting and if we do one thing that we try to investigate how this scheme will function. suppose if I want to solve a non-periodic problem.

So, if I want to do the non-periodic problem what I could do; I could borrow those boundary closures that has been given by Adams scheme. We have already noted their fourth order accurate schemes, as far as that order accuracy is concerned. It is not going to go any inferior because your basic interior stencil is second order; but you are giving fourth order boundary closure for j equal to 1 and 2 at $n-1$ and n .

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And then what happens is, you get this picture now. This may look slightly better than the Adams scheme but, it is still you can notice for j equal to 1, j equal to 2 and although you have to j equal to 6. You are going (()) numerical instability because the imaginary part is positive for this first 6 point.

So what happens is Haras and Ta'asan scheme was a eye opener in a sense that, it does open up possibilities of developing schemes with very high resolution. why do we say high resolution; now you see Adams scheme, we had K equivalent by K , the real $\frac{\Delta t}{\Delta x}$ was close to 1 up to 1.5 and after that it started falling off.

But you notice here, for the interior stencils, the middle of the domain if you leave out the boundary points, then it remains flat all the way of up to about 2.2 2.3.

So, maximum you can go up to $\frac{\pi}{5}$ and this scheme actually helps you go all the way up to that theoretical limit.

So, this was a good thing. But still, we notice that despite its excellent spectral resolution, imaginary part actually shows the large instability for those inflow part of the domain. We do get intermediate wave numbers, where you have large instabilities and milder instabilities.

At extreme wave number for j equal to 2 and for j equal to 5, this instability property actually starts coming down.

But that lead us to making a confession that, you are still not ready to use it for practical application because, the numerical instabilities are there.

However this analysis tells us the efficiency of optimization process and we could perhaps exploit it and that is what we can do.

What we would do is let us say that, we are trying to find out the first derivative by a via optimization process. So, what we could do is we could obtain the exact representation of the first derivative as l of $K h$.

And the corresponding discrete representation is $l h$ of $K h$; then we can find out this l^2 norm that, we have being talking about.

So basically what we are doing we are finding out the mean square departure of the error and this is obtained at let us say at the j th node so this is a local property.

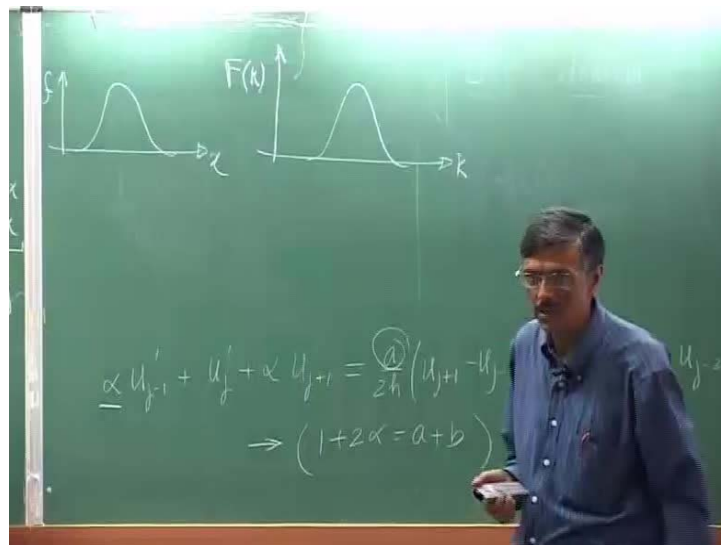
So what we could do is, we could sum such departure across all the nodes in a domain and we can construct a global objective function which is sum of all these and this is what it would like.

Now what happened in Haras and Ta'asans exercise is they were solving this problem with periodic boundary conditions. So, they took some initial conditions and those initial conditions were kind of restrictive in a sense they were band limited.

What one could perhaps do is make that restrictions also disappear so, what you do is you take u of K as equal to 1. what does u of K equal to 1 mean,

I think this is something also I wanted to discuss with you because, I noticed that not all of you are familiar with the property of Fourier transform so, if I just briefly state that if I have a function here

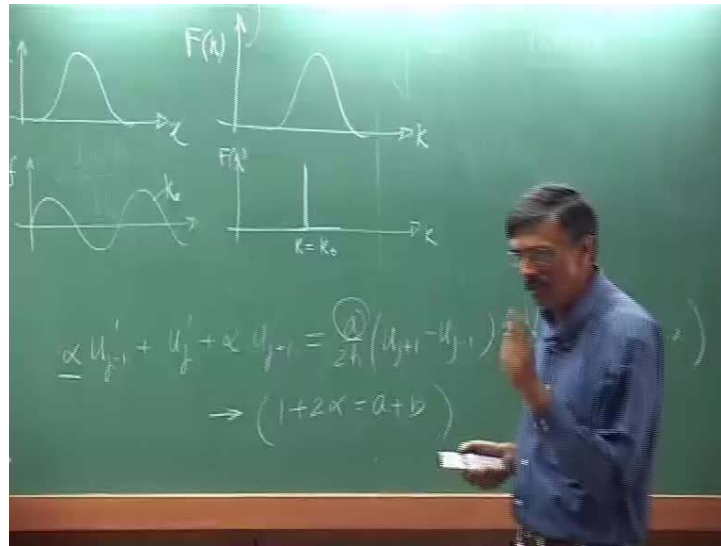
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Like this, then of course I can plot it is Fourier transform. I would perhaps see if it is a Gaussian then, it will also be a kind of a Gaussian.

This is a very nice well behaved function; the Gaussian functions are from a member of permission functions. They have this unique property that, the original and its transform has identical appearance.

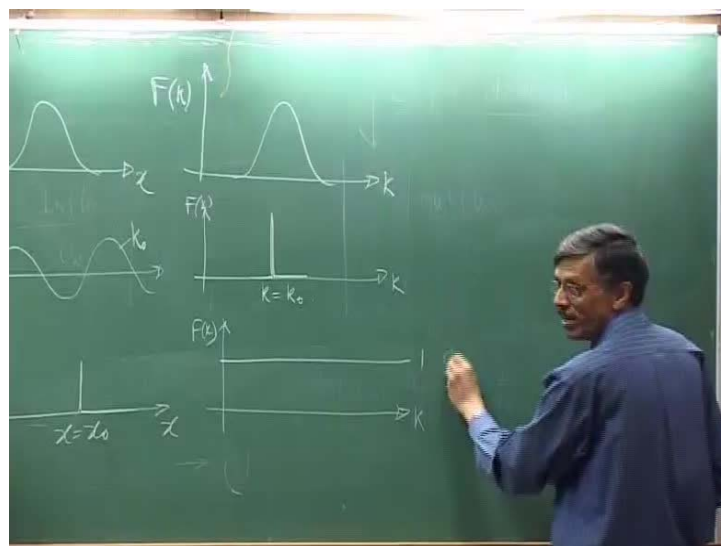
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However, if I take a function like this a periodic function what do I get. So, what would be its transform, here its transform would be given by a wave number and what it would be a delta function so, if this corresponds to K naught then the spike in spectral plane is also at K naught.

That, if in the physical plane the function is all pervading. It goes from minus infinity to plus infinity in the K plane. It is very localized and it is present only in 1 point.

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Now, if I look at the other extreme; that, in the physical space i have a delta function. So, if I have a delta function let us say at x , equal to x naught. what will I get here,

You will get what is called as a **(())** white noise. you will get this F of K is equal to 1 everywhere that means what all the wave numbers are equally excited.

Now you will understand that, in all those high school experiments when you started doing all those vibration of a pendulum, you always gave a impulsive excitation.

You took the pendulum in one point and let it go so that, was like this an impulse that is imparted into the system. The moment you impart an impulse, it excites all the wave numbers and frequency in the system.

So that, you are not doing any discrimination. So, what happen, your input to the system is equally spread over all wave numbers and all frequencies and what the system does. System actually picks up the natural frequency and displaces it. That is what you see the pendulum eventually settles down to its natural frequency.

So, you have already done it. So what you are seeing that if, you have a very localized disturbance that is going to be a very very tough condition case for you to consider. Because now you can see all case are excited.

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Optimization Problem With Evaluation of First Derivatives (Cont.)

- In Eq. (36) the left hand side functions are the parameters over which the problem is to be minimized. The corresponding objective function used in Haras & Ta'asan (1994) is given by

$$\bar{G} = \int_{-k_m}^{k_m} |L_h(kh) - L(kh)|^2 [U(k)]^2 dk \quad (37)$$
- Here $U(k)$ was taken corresponding to the initial condition of the wave equation that was solved.
- Haras & Ta'asan (1994) considered a wave equation with particular type of band-limited spectrum for $U(k)$ corresponding to initial data.
- Using Eqs. (21) and (35) we can write,

$$g_j = \int_{-k_m}^{k_m} \left| \sum_{l=1}^N C_{jl} R_{lj} + i \left(\sum_{j=1}^N C_{jl} I_{lj} - kh \right) \right|^2 dk \quad (38)$$

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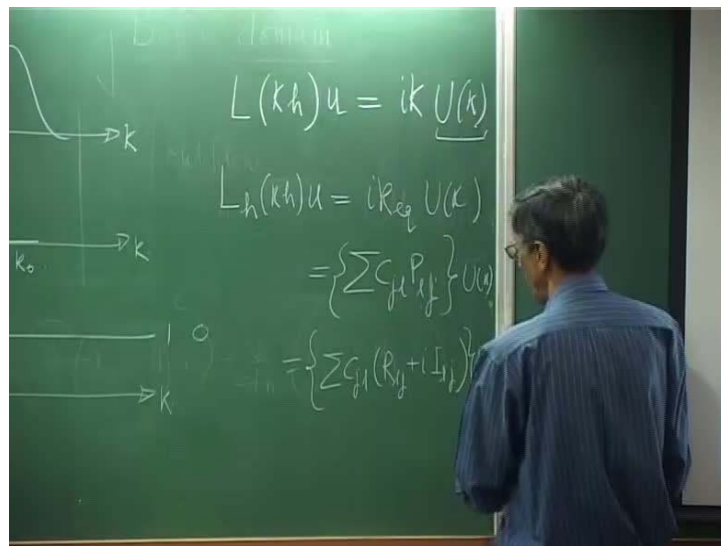
And so, when we are also going to do this optimization business exercise, what we are going to do is instead of U of K square, we just simply put it equal to 1.

So, what we are doing; we are not discriminating like Harass and Ta'asan. They may have done something like this, a band limited thing. So, what happens, that optimization becomes somewhat like a problem dependent exercise. It is restrictive.

So, we wanted to restrict that and we did that and that is what you see in equation 36. We have put U of K equal to 1 so that, we can talk about the toughest possible problem that you can have.

Now, so this is what I have been talking about. So, this is what is explained now. what you notice here L of K .

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If I am obtaining the first derivative, what is L of K going to be its operating on u . So, this actually give me in K space as $i K U$ right.

That is our theoretical estimate of the derivative. So, for each K all I need to do is take the transform multiply by $i k$.

And that is what we are going to substitute in equation 37 here. L of K I will just simply write it as i of K .

Now what about this discrete operation. If you recall yesterday, we wrote it as $i k$ equivalent U and this we wrote it as your $i k$ equivalent and [then/there] you multiply and this itself $P l j$. We wrote it as the real part and the imaginary part. So, that is this part time.

So this is how we write in equation 37 - the expression for the theoretical estimate of the derivative and this is the corresponding numerical estimate of the derivative and you substitute that and workout the details. So, this is how it would look like.

$C j l$ into $R l j$ and the imaginary part will be i times $C j l I l j$ minus $k h$ and this is the complex number. So, you take its multiplied by conjugate and you get a squared quantity at that is what this is going to be your local optimization function g of j .

Well there is a bit of algebra involved, you can go through it and what you find that everything depends on what now few numerical method that fixes the C matrix and once you have the C matrix this is what your optimization function is going to look like.

So, it involves if you are looking at the j th node it involves some constant part that of course, comes from this part L of $K h$ part that gives raise to this first 2 terms and the rest of the term comes from this numerical approximation of the derivative and it comes out in the following 3 groups the way we have written down.

Once corresponds to the node itself $C j j$ square and then we have this type of product term which involves interaction of the neighbors of the j th node. Because, you see we are restricting it to L naught equal to j so it is summed over L , equal to 1 to n (()) j is equal to j is a written now they are separately ok.

(()) In addition, we have this kind of term where $C j l$ is divided by L minus j . Now, if you are focusing at the j th point you notice that, if $C j l$'s are non-zero they are going to be affected by all the neighbors.

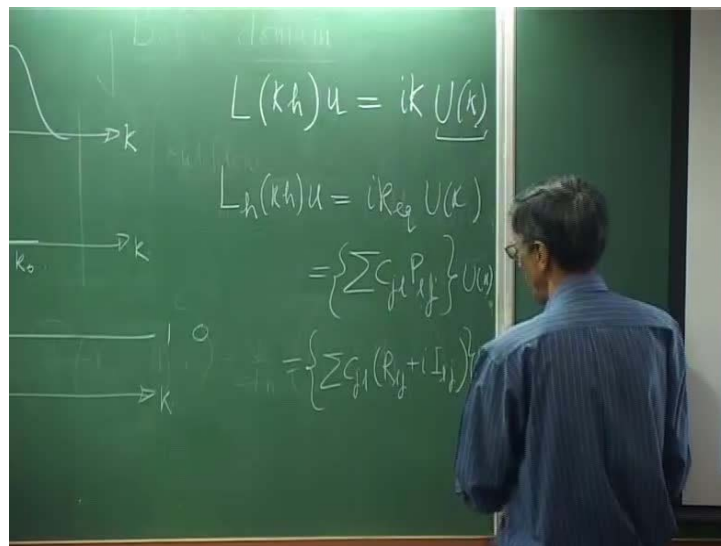
So, this is what we get now. You can actually use this representation or this formula for any particular method you choose, provided you know the corresponding C matrix. So, that is the clue.

Now, we have also noted that in general for a general discrete scheme, C is essentially equal to a inverse b . However, if you look at explicit scheme a matrix is the identity matrix. So, C is equal to b .

And you also notice that the thing is $(())$ error. So, this g_j is some kind of an error so, g_j actually scales with n . More you have larger the number of points, the error will be more.

So, it is somewhat little counter intuitive because, we are given to believe that we refine the grid more and more, error will come down. But, you are noticing that n comes here as a scaling parameter. So, actually g_j is directly proportional to n . So n increases the error also would increase.

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That is that and you also notice $(())$ that this is a squared term. So, this you cannot minimize and you cannot choose any particular $C_{j,j}$ for which your g_j can be reduced except the condition that you choose the $C_{j,j}$ itself as 0.

So, if $C_{j,j}$'s are 0; if I construct the C matrix and if I maneuver to get $C_{j,j}$ equal to 0 then that would be a good thing to happen because that will minimize g_j .

This one is also a quadratic set of term and this will also not going to help you much because $(())$ that we have neighboring points on either side and they come in a anti symmetric form. So this is also a squared set of terms so this will not be able to get you

any way by which you can minimize g_j . So only thing that will allow you to minimize g_j is this term - this second term that would be what you can actually do.

That is the nature of the term that you are seeing and you can also very clearly see the way this neighbors of j th point contribute.

The next point would be $j + 1$ so $1 - j$ would be so, that quantity would be 1 depending on $1 - j$ is plus 1 or minus 1; you are going to get a minus 1 sign. So, the next point on either side of the j th node actually reduce.

And the very next point again you are going to see that is this will become positive. so we will have to prove a little closer and see what we get.

The first and foremost is you can see that if this quantity is going to be minimized, it would be in our interest to keep the scheme as compact as possible. Because,

more number of C_j l's are involved; they can give you a constructive as well as destructive interference. So we do not want it. In a better way, it should be that the immediate neighboring points produce the maximum effect because it is divided by $1 - j$.

So, if I look at the second point it will be half $1 - j$ equal to one; it is going to give you the most contribution. $1 - j$ equal to 2 will reduce the contribution of C_j and so on so forth.

So that is what we note here, that this should keep our scheme as compact as possible. Because then we would be able to minimize that. If you now look at those set of terms, look at the contribution coming from 1 equal to $j + 1$ and $j - 1$ that is this contribution given here four times $C_{11} - 1 - C_{11} + 1$.

So, just to minimize g_j we must have this point to the right should be positive and the point to the right should be much greater than point to the left or the point to the left must be negative.

So what happens is $(())$ to $(())$ compact scheme $(())$ explicit scheme C itself is b matrix so the b matrix are chosen by us. .

We can see what happens and you notice that inspecting the b matrix we can talk about least error schemes and we have already noted that we want to do something, The diagonal term should be equal to zero and that is what you get in all central scheme.

If I look at the jth node I always put that coefficient equal to 0 so that is something that will tell you why central schemes are preferred. Central schemes inherently give you $C_{j,j}$ equal to 0.

If you now look at second order central difference scheme $C_{j,j}$ is 0 and these are what you get $C_{j,j+1}$ is plus half and $C_{j,j-1}$ is minus half and you can work out that expression and this is what you are going to get for the second order central scheme.

Now, if you look at the corresponding fourth order central difference scheme you notice that $C_{j,j}$ is once again 0 and then next neighbors are two thirds and the subsequent neighbors give a contribution of which is 1 by 12.

And you now look at the expression given in 42 and 43 and you can very clearly note that a fourth order scheme is a better scheme than this as $(())$ estimate. Because there we are subtracting 3.5 and here we are subtracting 4.76. So of course fourth order scheme is better from this analysis point of view also.

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Optimized Compact Scheme for First Derivative

Let us consider the following stencils used in Lele (1992) for evaluation of first derivatives:

$$j = 1 : u'_1 + \alpha u'_2 = (au_1 + bu_2 + cu_3 + du_4)/h \quad (44)$$

$$j = 2 : u'_1 + 4u'_2 + u'_3 = 3(u_3 - u_1)/h \quad (45)$$

$$3 \leq j \leq N-2 : \alpha_1 u'_{j-1} + u'_j + \alpha_1 u'_{j+1} = \frac{b_1}{4h}(u_{j+2} - u_{j-2}) + \frac{a_1}{2h}(u_{j+1} - u_{j-1}) \quad (46)$$

α and α_1 are the free parameters used in optimizing the above stencil.

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If we now come to optimizing compact scheme for first derivative, we can actually follow the route which Lele had taken already earlier and what he did was of course, try to obtain a fourth order internal stencil. So, that is the stencil given here in 46 for internal points starting from j equal to 3 with j equal to n minus 2.

For j equal to 2 and j equal to n minus 1 we can use that same fourth order scheme we talked about. This is a central scheme so this points towards the correct direction.

Whereas, at j equal to 1 we do not know what to do. So we write the scheme like this. For j equal to 1 we say the derivative at first point is related to derivative of the second point with respect to this coefficient α and on the right hand side in the function value we take four points because our experience in eighties have shown that we could do a up winding scheme for this j equal to one point and that should be.

So, basically if I look at this, I could try to get this a , b , c and d here in terms of α and the same way I could get a_1 and b_1 in terms of α_1 then what happens is my optimization function $G_1(\alpha, \alpha_1)$ exercise would be function of α and α_1 .

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Optimized Compact Scheme for First Derivative (Cont.)

• A third order accuracy requirement for Eq. (44) and the fourth order accuracy requirement for Eq. (46), allows one to relate the rest of the parameters in terms of α and α_1 . This gives:

$$a = -\frac{(11 + 2\alpha)}{6}; b = \frac{6 - \alpha}{2}; c = \frac{2\alpha - 3}{2}; d = \frac{2 - \alpha}{6}$$

and

$$a_1 = 2\left(\frac{\alpha_1}{3} + 2\right); b_1 = \frac{4\alpha_1 - 1}{3} \quad (47)$$

Thus, the global optimization requires minimizing the following objective function,

$$G_1(\alpha, \alpha_1) = \sum_{j=1}^N g_j(\alpha, \alpha_1)$$

where g_j is as given in Eq. (40).

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$G_1(\alpha, \alpha_1)$ this is what was attempted there so we could do that as I said that with the help of the stencil given at the first point and equating the Taylor series coefficients we can work out this expression for a , b , c and d in terms of α like this

This gives us a third order accuracy; whereas, the internal stencil we can work for fourth order accuracy and we can get a 1 and b 1 in terms of α .

So what happens is the global optimization requires basically looking into α space and which we can do it because now we can estimate g_j at α and α .

And one thing you notice though, if I go back here and look at this equation written only for one point whereas, this equation we have written it for many many points.

Now you look back to what you did in your exam or an elliptic equation. We have seen that one of the attribute that we must try to do is to keep the corresponding linear algebraic equation diagonally dominant.

So, what that would do? That gives you some limit on the value of α . what should be that α then? it should be less than half.

If it is less than half because you see diagonal term has a coefficient 1 so the half diagonal terms have give you a contribution of 2α . So, $1 - 2\alpha$ should be means $1 - 2\alpha$ should be positive. So α has to be less than half.

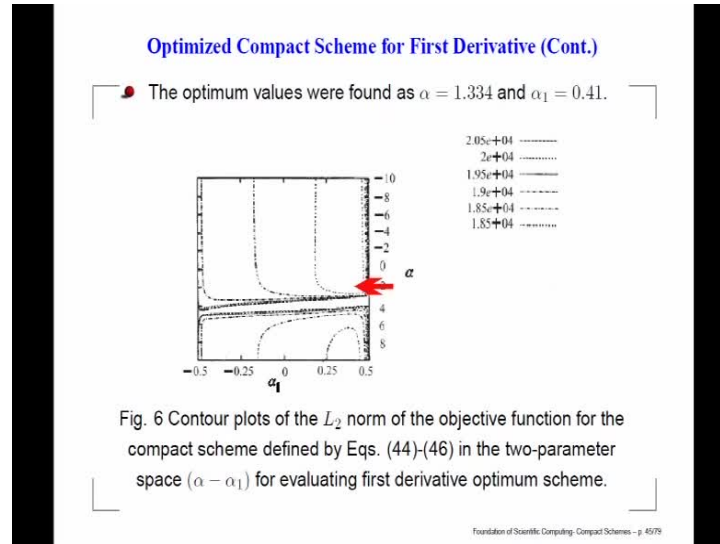
Whereas this point is only applied at one point and we do not perhaps need to be that hussy about the diagonal dominance and with. (()) It says that α should be equal to less than 1 but if we violate marginally it should not cause tremendous problem.

So, that is what we make the point here that α should be less than equal to half. So that we get the corresponding a matrix has dominant and we should be able to use Thomas algorithm without any problem.

The same logic requires that α should be less than 1 but we can still obtain the c matrix with this condition mildly violated and this is what we are going to show.

What we are going to do is, we are going to obtain this value of g that we have shown in the bottom of this slide and plot this g in α plane.

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So, that is basically we are showing you this error that optimization function g global optimization in α α_1 plane.

what you notice is along this groove the function actually goes up. So, instead of having a maximum along this line you get this going to be very large.

Whereas a optimum value somewhere here in the middle and this is also the region where your diagonal dominance actually break downs. So, that is estimated here also that if you calculate you see the corresponding error is also going to be very large.

Now so having obtained this value of α and α_1 we have $((C))$ for the whole domain with non-periodic boundary condition.

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Optimized Compact Scheme for First Derivative (Cont.)

- The real and imaginary part of $\frac{k_{eq}}{k}$ are displayed as a function of kh for the optimal parameters mentioned in the previous slide.

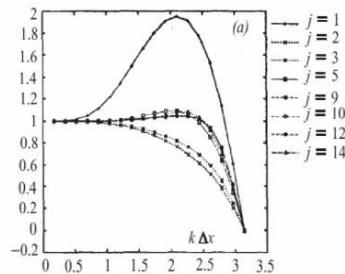


Fig. 7(a) Spectral resolution corresponding to the optimum scheme of Fig. 6 for the first derivative.

How does it function so you can plot it; the real part k_{eq} equivalent by k real part in the kh or $k\Delta x$ explain and you can see various points behave like this. So this is your j equal to one point and these are the other points.

You see a slight over shoot here and some bit of degradation here for close to the boundary points here. So, those we have shown only half the domain and we did not show the latter half of the domain. So, that is what we are seeing that this is the real part so we do see that there is some benefit.

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Optimized Compact Scheme for First Derivative (Cont.)

- The imaginary part of (k_{eq}/k) , however, displays instability for $j = 2, 3$ and 5 for high wave numbers. This is due to the fact that the objective function $G_1(\alpha, \alpha_1)$ did not have any constraint on the imaginary part.

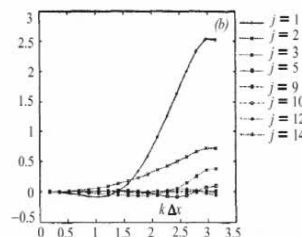


Fig. 7(b) Added numerical dissipation corresponding to the optimum scheme of Fig. 6 for the first derivative.

However if you plot the imaginary part this is what it is and this is not variant encouraging at all. Because, you can see the j equal to 1 have very severe instability for any $k h$ about 1 point 5.

And if j equal to 1 is not also considered important then you look at j equal to 2,3,5 etcetera. They are also selectively scale and selectively unstable but j equal to 2 perhaps all wave numbers are unstable.

For j equal to 3 you will see that high wave numbers are unstable and j equal to 5 you see a very interesting thing; there is a intermediate range over which it is unstable then that is followed by another intermediate range where it is stable again at very high wave number close to the Nyquist limit again. **this is the quite.**

So, of course we should not be surprised because we did not put any constraint on the g to avoid numerical instability and we are paying the price here right.

So, if we do not have any constraint on the g we end up developing super optimum scheme which will have numerical instability.

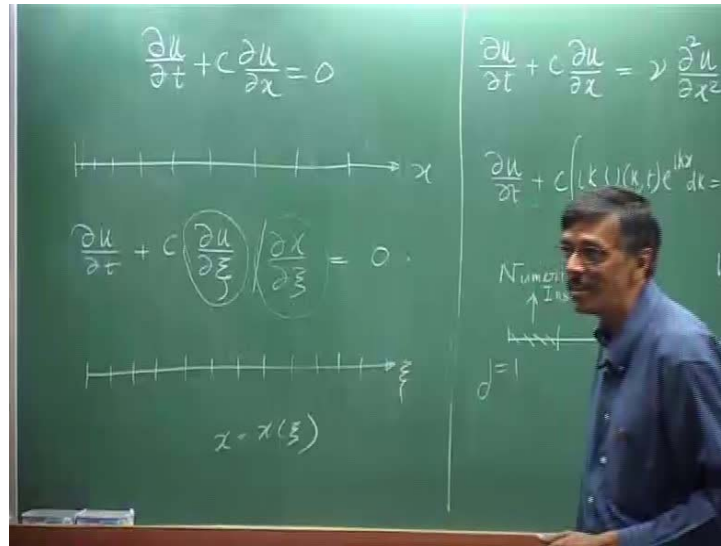
I suppose, we now have come to realize that even in when we are trying to develop compact schemes and if we keep the stencil like what we have done here.

What we have here the basic stencil is given here and they are central. So central schemes appears to be not holding up lot of promise for us so what we could do is we could look for the alternate **(())** should be able to develop for under the umbrella of compact schemes.

So, what we are going to do is basically try to develop some upwind scheme. However, we need to really talk about another source of error which we have kind of avoided talking about so far.

We do not think we can postpone it any longer and that source of error is what is called as Aliasing error.

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So, this is something I need to spend some time now (()) is that as compare to this convection equation. If I try to solve it in a grid which is non-uniform; basically what we are talking about that I have a domain like this.

Now say I know that initially I have (()) structured in such a way that I need to resolve it and I need to have. Let us say (()) grid like this.

We talked about it before also that if we want to use compact scheme in a non-uniform grid what we should be doing. well, we would transform the x plane into a transform plane which I will call as psi. This I should divide it by del x del xi.

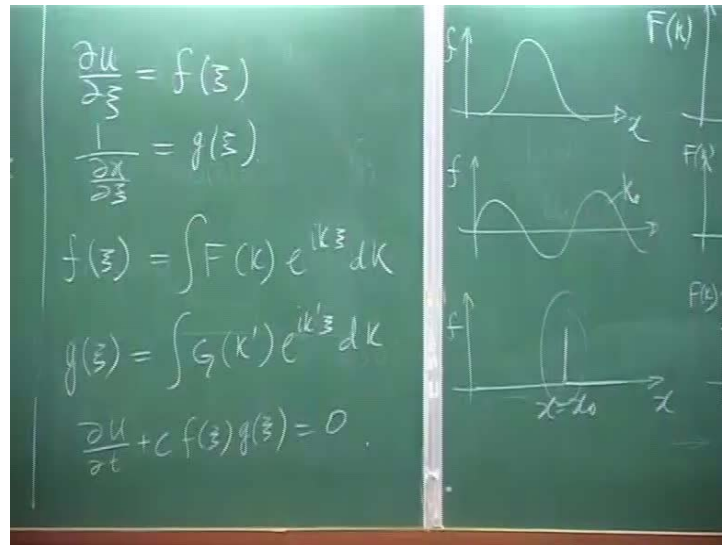
So, basically if that is your x plane in the xi plane I would have uniformly spaced point and now whatever we have developed so far can use them. Because they were all developed for uniform space point. So, if we do this what has happened now.

You see this is a quantity that is a function of xi independent variable in addition, this transformation function that we have tried to get. So x is a function of xi.

If we may actually do it analytically we may do it numerically that we will have to (()) called sort of a linear term. But what has happened now here (())

It has become a product of two functions $(())$ dependent on x . How do we represent it in sets of in the K space?

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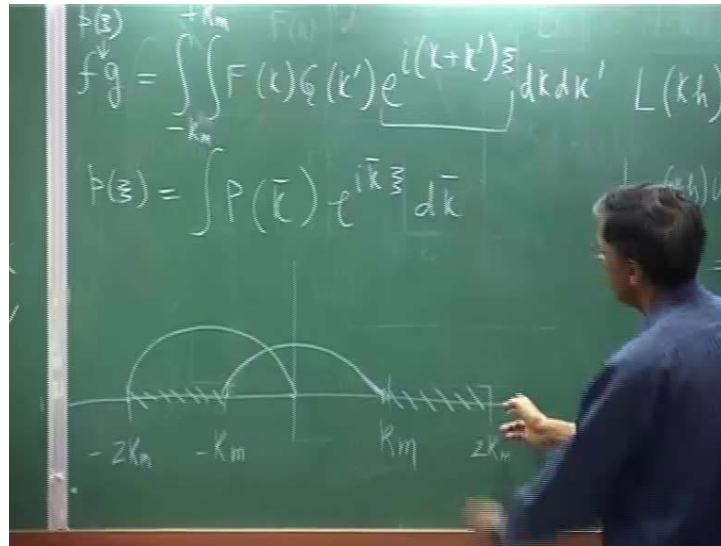


This is what we anticipate. Let me write for simplification of that this is f of x and let me call $1/\partial x/\partial \xi$. Let me write it as g of x .

Now if I am writing this, I could write it as f of K e to the power $i K x$ $d K$ that is $(())$ definition of Fourier transform. Let us write this as call dummy variable; I change it to g K prime and e to the power $i K$ prime x .

Now what we are trying to do there is we are trying solve an equation of this kind. Now what happens, this is where we actually get into a bit of a problem now.

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Now if I am trying to estimate f times g , what we are noticing that this product may call this as p of ξ . I could write that $(())$ product functions p of ξ would be some, let me call that as P of K bar $(())$.

Now what has happened here, K and K prime. What is its range of variability - the Nyquist limit that we need to do here will be minus K max to plus K max

So what happens to this? This shows a variation this phase variation to shown here as minus $2 K$ max to plus $2 K$ max but given a grid can I do that? We cannot.

Because our grid is capable of handling only from minus K max to plus K max. But trying to take the product, we see that $(())$ we are trying to spill out of the region. What happens is I have already told you what happens in computing.

Even though we are working in a limited region we always take it is periodic extension on either side. So, if I am trying to resolve a problem from minus k max to plus k max and in the process I spill out $(())$ to say minus $2 K$ max to plus $2 K$ max.

What happens to this region? They cannot physically stay there. At the same time this problem is repeated. So what does that mean is we are seeing from minus k m to plus k m. The same thing should have happened here minus $3 k$ m to minus k m.

So, these points have a corresponding image inside here because, they are the periodic extension. So what happens is this point would map first point and here that should be the first point. So, what happens to this point. This point would $(())$ so what has happened is the one that is supposed to have gone there numerically will be transposed to this region.

So, same way this part also would map this part. $(())$ so anything that spills out is reassigned in a new region new point and this is something you must have to understand that what is happening now is some component of the product cannot be resolved properly and they have been given a new name this is what we call by Aliasing.

Alias means that you know all those bad people have some $(())$ nick names which we called as x Alias y Alias z.

So, this is also something happening very bad here which should not be kept. But we are pushing them and contaminating the good region where we do not have error. So this phenomenon is called aliasing error.

So, we will talk about it little more on the next class. This is a major issue and it is not very trivial so we will talk about it.