Foundation of Scientific Computing

Prof. T .K. Sengupta

Department of Aerospace Engineering

Indian Institute of Technology, Kanpur

Lecture No. # 32

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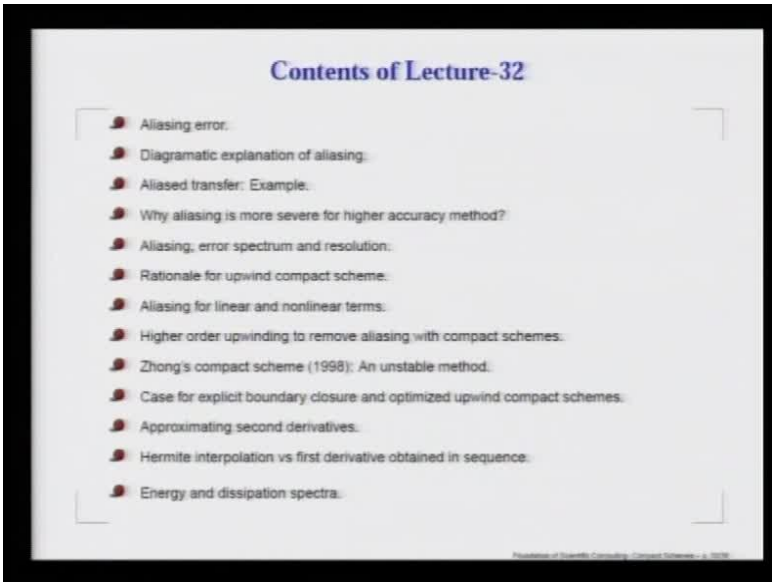

Lecture 32 will begin with a detailed discussion on aliasing error and trying to explain this aliasing error. We will explain it in a diagrammatic fashion, and show, how different components are spuriously wrapped around and put inside. And this alias transfer would lead to major source of error, which we will show through an example. And, what we also note very curiously enough is that, this aliasing problem becomes more and more severe for higher accuracy methods, which do not attenuate the high wave numbers in contrast to low accuracy methods, which so-called naturally removes this high wave numbers, but then, it is at the cost of the accuracy of the solution.

So, it is necessary for one to basically work out a strategy, where we will adopt higher accuracy method, and at the same time, remove the sources of the aliasing. So, this is what we talked about, aliasing - how does it affect the error spectrum and resolution; and then, we have made a case for necessity for adopting upwind compact schemes. These upwind compact schemes have that role of removing aliasing, and that is what we will be

talking about. And having defined aliasing for linear and non-linear terms, we will introduce higher order upwinding to remove aliasing, and then we will show that the Zhong's compact scheme, which is again a higher order up-wind scheme; it is a fifth order upwind scheme, but unfortunately, because of boundary closure problem, once again it turns out to be an unstable method.

This points out the inadequacy of various implicit boundary closure methods that we have been talking about so far, and we make a very strong case for adopting explicit boundary closure, and thereby, using those to optimize, and this is the actual methodology that we have adopted so far, and we will highlight that. Talking about that, we also come next to discussing, how do we approximate second derivatives, and we look at it as a competition between, let us say, direct Hermite interpolation method of directly evaluating the second derivative or evaluating the derivative in sequence by using first derivative algorithms.

We particularly highlight what is required in many simulations, that not only we express the energy content of the system correctly, we must also describe how this dissipation is, while energy may be part in the lower wave number. We know that dissipation keeps increasing with wave number, so, there is a case for uniform resolution of spectrum to balance in an equilibrium flow between the energy and dissipation.

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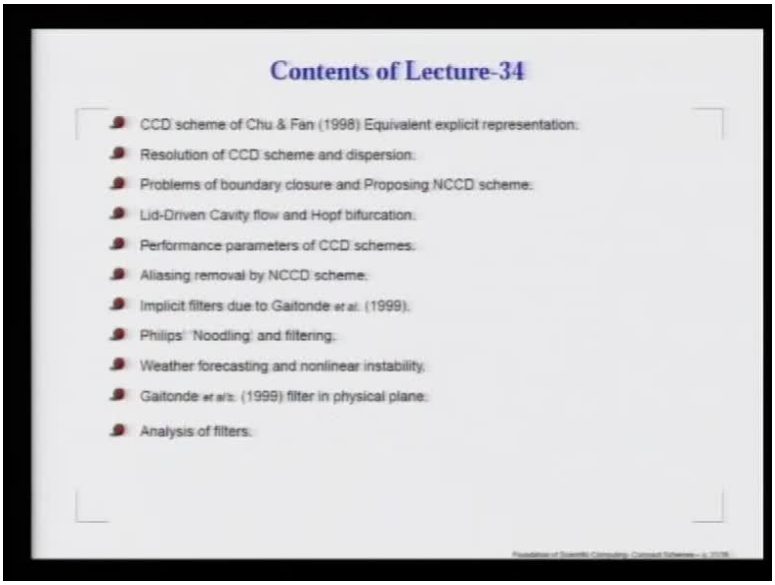

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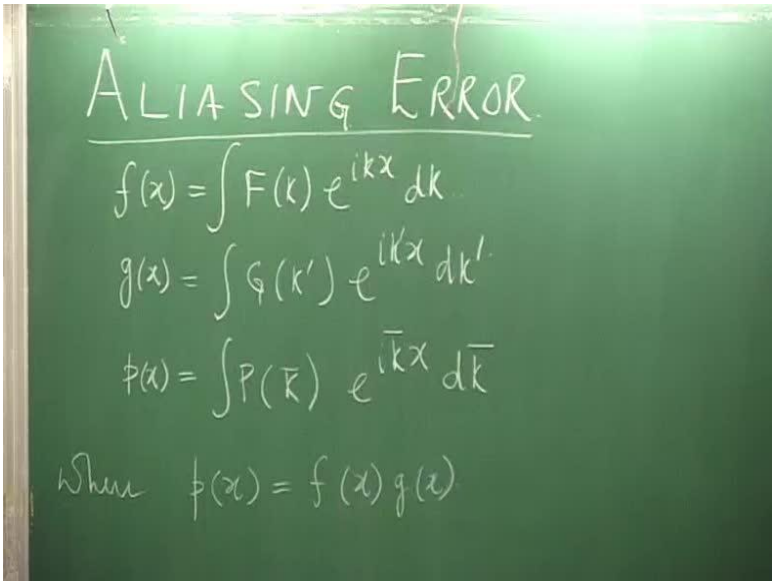

This is a major issue, and this is a major source of error which initially, people did not suspect to be of importance; the reason was that, people are using some kind of low-order method; and as we will see that this kind of error becomes important for large wave numbers; and you have seen in this low order method in evaluating derivatives, we have seen what happens is that, high wave numbers are filtered because of the nature of discretization; that we have seen.

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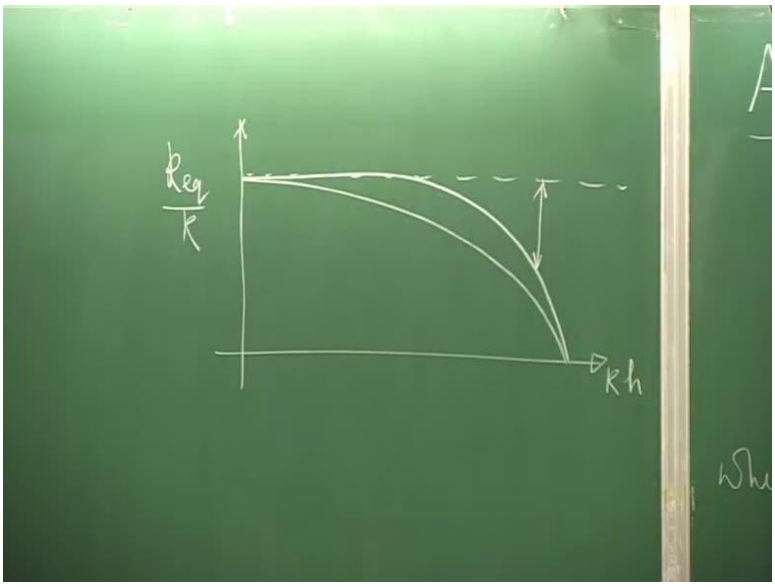

What I mean by filter is the following. That suppose I am trying to evaluate a derivative, and that let us say, we are plotting ((No Audio)) effectiveness parameter, then what we see is that, for the smaller wave number, they remain faithful; it is only towards the

larger wave number, they come down. So, this is what we state, that, this is the amount of attenuation or filtering that that particular wave number suffers, right? If I have a rather low-order method, then I will see much more severe attenuation or filtering, right?

So, what happens is, the, this aliasing error happens whenever you are trying to compute a product of 2 unknown functions. Now, this product operation has been somewhat misunderstood by many; and in many courses and books, you would find they talk about aliasing as a problem to occur due to non-linearity.

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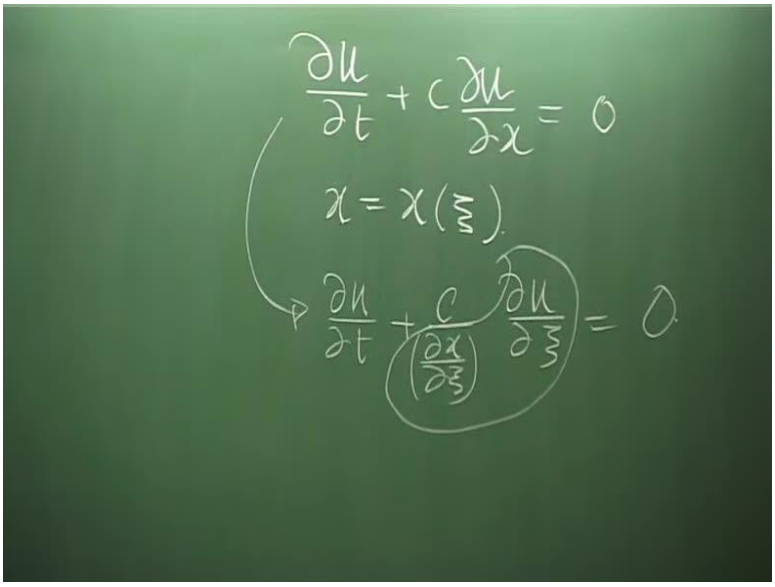

However, as we saw in the last class, that if we are trying to solve a linear equation as simple as 1-d wave equation, and if we do not solve it in the physical plane, instead we got to a transform plane where the transformation metric equation is given like this, then this equation transforms to the following. So, you can see that we have, even on a, for a linear equation, we have to evaluate a product, right? del u del xi as well as del x del xi; they are both functions of xi, so, this is ((No Audio))

We have seen here on this slide. Now, try to understand what causes aliasing. So, we represent these nodes on the right hand side, f of x, g of x, in terms of its Fourier Laplace Transform. So, let us say, f is defined in k plane and g is defined in k prime plane, so, what we could do is, we could draw a portrait here; on this side, let me plot k; on this side, let me plot k prime.

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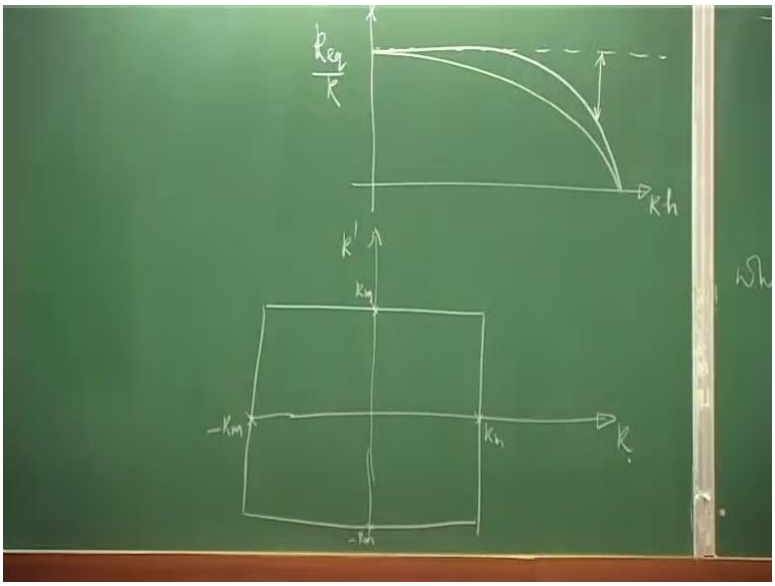

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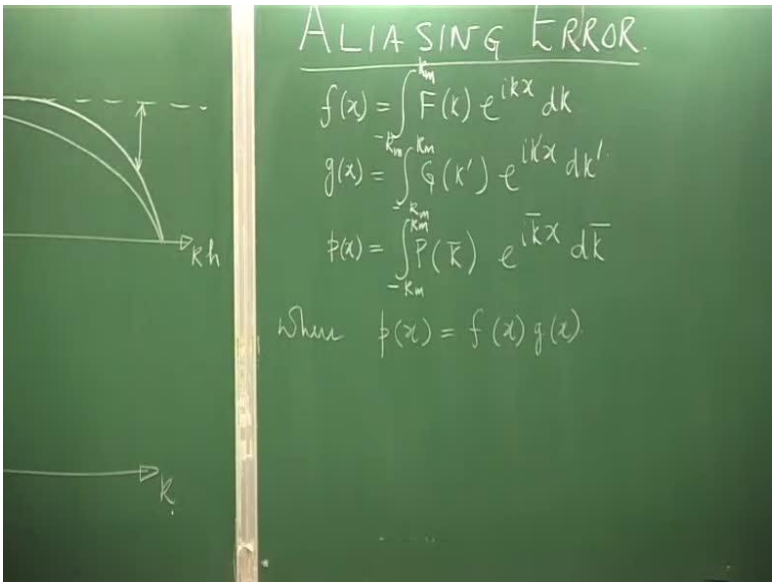

And you know the range of f is going to be, minus k m to plus k m, so, if I am using a same grid, so the range is fixed by the Nyquist criteria, so that will be k m, should be equal to pi by 8; we can do that. And needless to say, that the product also, would be also represented in the same range. Because, we are using the same grid, so, it is very unlikely that you could evaluate p at any other resolution than what you are doing with the primitives, f and g.

Now, if I look at it, then then in this plane, I should be actually focusing upon a box. So, this is your plus k m, and this is your minus k m; and this is also your plus k m, and similarly this will be your minus k m, okay? So, we are in evaluating the product; we are essentially working in this box; that is clearly understood.

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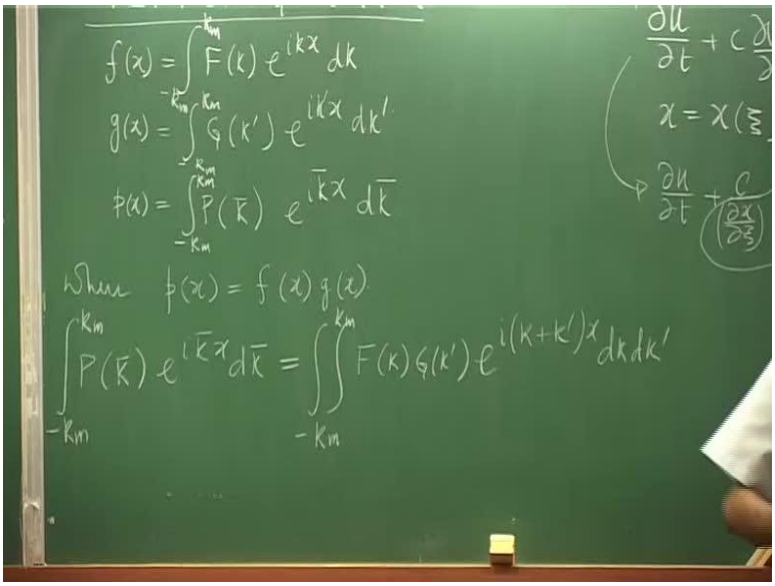

So, what happens is then, I will write from here, that p of k bar e to the power i k bar x d k bar should be equal to double integral f of k, g of k prime. And look at the phase part now; it is going to be i k plus a prime x d k d k prime. So, this integral is evaluated in the this box, right? Because k is varying from minus k m to plus k m, k prime is varying from minus k m to plus k m; however, you also notice that individually, each of these are varying from minus k m to plus k m, so it would appear as if, this phase can vary from minus 2 k m to plus 2 k m. At the same time, on the left hand side, we are saying that, that is not possible; because, using the same grid, I cannot evaluate the phase with a higher precision than what the grid allows, right?

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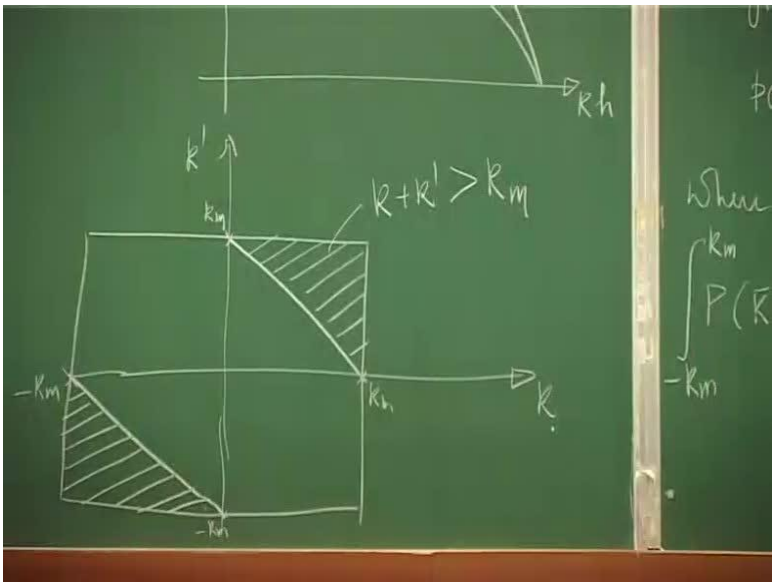

So, something has to give in; when k plus k prime increases above k m, or decreases below minus k m. So, what are those lines where k plus k prime is equal to k m? It would be a line like this, right? And similarly, k plus k prime equal to minus k m would be a line like this; and what about this area? This area would correspond to... This area would correspond to k plus k prime greater than..., right?

All of you see that you are comfortable with the observation. So, same way, this part also represents an apparent phase which goes beyond the other limit; so, this is the region where this space indicates - you would be there. However, this tells you that it is not allowed. So, what happens to this 2 part? This 2 part, this 2 part in a computation, cannot remain there; they have to remain within the ((No Audio)); they actually fold back.

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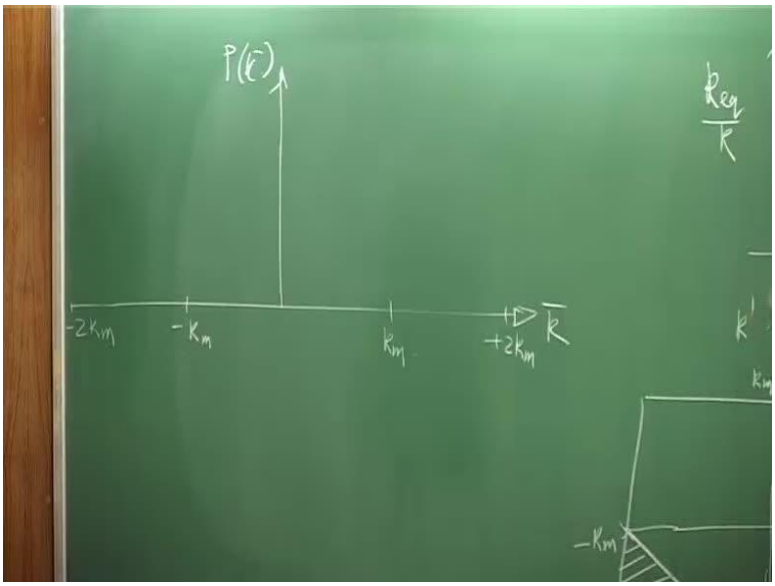

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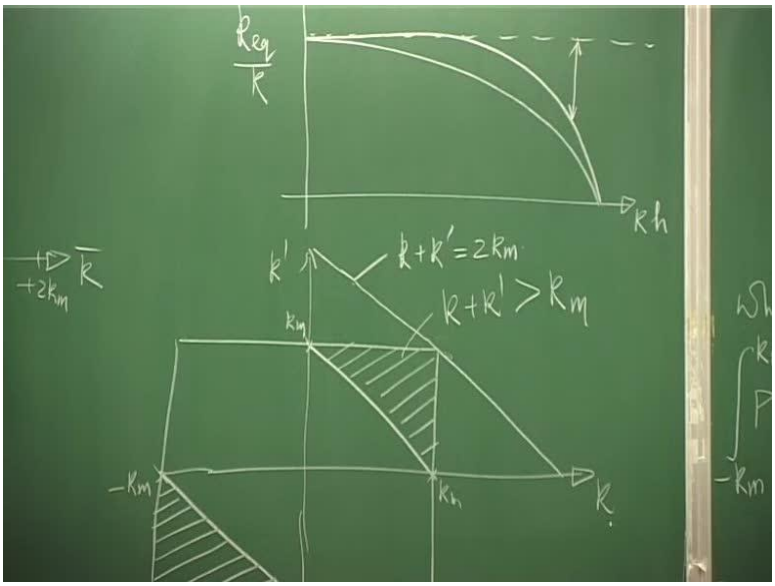

How do they fold back? That is what we explained in the last class. Also, suppose I plot here k bar, and here and let us say any function, that I am plotting, say p of k bar here; and this is going from minus k m to plus k m. Now, the right hand side tells you that this actually can go all the way up to minus 2 k m, and on this side it can go to plus 2 k m. So, that is what we had seen, that is that; so, if this line represents k plus k prime equal to k m, I can draw a similar line parallel to this, and that will go like this; and what is this line? This line is..., right?

So in evaluating the right hand side, what I noticed is that, my phase can also go in this region, but, out of this whole region, this part is not there, right? This does not exist. So, here e of k prime is 0; and here f of k is 0. So, this part, this triangle and this triangle are not coming into play. What is coming into play is what I have shown you here, by the shaded region, right? That is indeed always happening. Now, where would those contributions go? That is the question that we are debating now. So, this region, the shaded region is here, plus k m 2 plus 2 k m, right?

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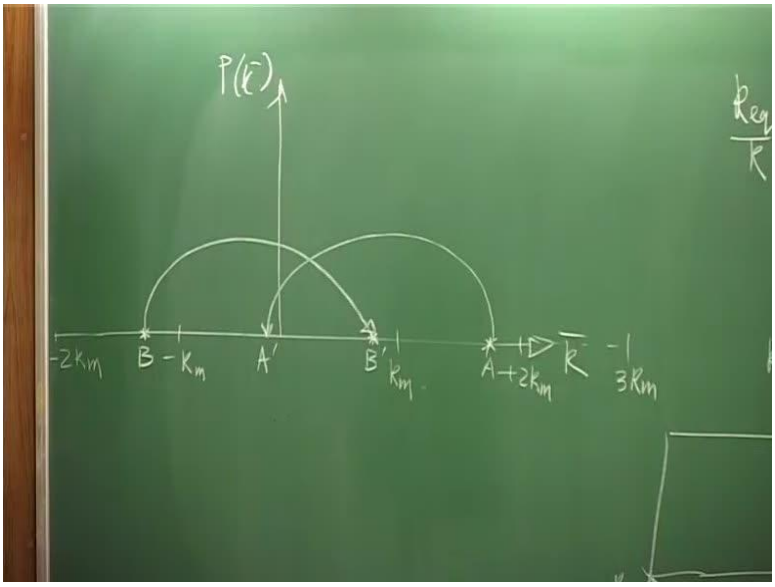

Now, suppose I have a point here, if I call this a point A, where would it go? I have made an observation, a couple of lectures ago, that even though when we are working in a finite domain, in a finite k space, the back of our mind we are talking about a periodic extension in both directions, right? So, what happens is, whatever I am doing from minus k m to plus k m, that event is replicated on either side; so here, if I go up to this 3 k m, the status in this is same as the status in this; that means what? A point 'A' here would be somewhere here, so that this distance is equal to that distance.

All of you follow it clearly. What is the aliasing roll here? So, I have some phase which puts my point beyond the range that has to be folded back within the acceptable range; so, this A will be mapped to a prime. The same way, suppose I had a point here, where will it go? This is towards the end of the the left event, so, I have a similar thing from minus 3 k m to the plus 3 k m, and the point B is to the right of that range.

So, that point should be within this range, almost to the close to the right of this; so, if that is B, it should be mapped here, to B prime; so, this is what will happen. That b will be mapped to B prime; A will go to A prime; so, what is happening is, you are seeing that all these points in the admissible range are also getting spurious, erroneous contribution coming from outside; and they are mapping inside. So, this is what is the dictionary meaning of aliasing, that this B prime or A prime - this should not be there; but they are spuriously taking the roll of those points; that is what is called aliasing, right?

So, you know the source; because, we have this region that is getting mapped inside; this region is getting mapped inside, and we are getting the problem. Now, what happens is, in many computations, as you can see that this kind of a phenomenon of bringing events from outside to inside would be more prevalent near the end of the ranges. How?

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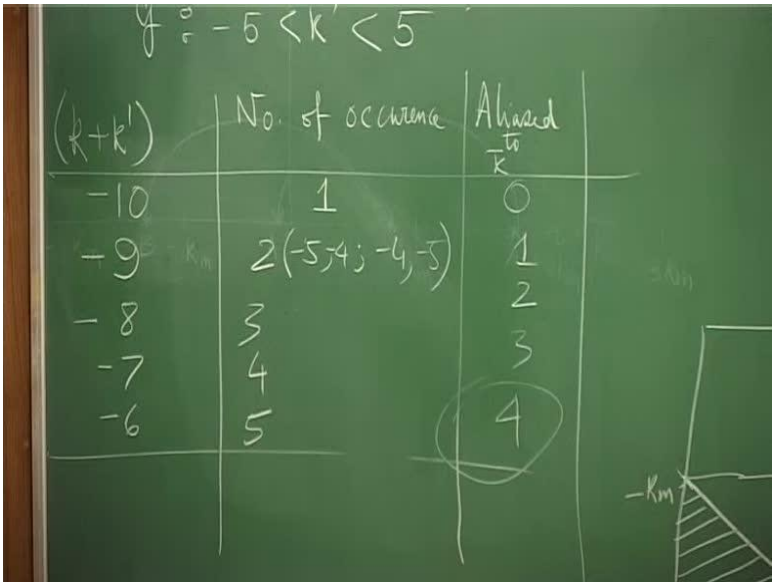

Well actually, I can actually give you a simple example; it is there. I can take a look at the book. Let us do the follow up, let us do a little bit of small accounting. Let us say f, I will talk about that, this the k varies, say discrete values, and talk about Fourier series now. Say, it varies between plus and minus 5; and g similarly, also let us say, varies between plus minus 5; then, what happens is, you can see what I have here is a kind of a table; I will just tell you what will happen. If I look at what k plus k prime can take values; and on this next column, I would find out how many times those kinds of events

occur. So, this is something like number of occurrence of such an event, and those values which were wrongly there, we need to find out where they are going to.

And let me just simply give you this idea; so, what happens is, say both k and k prime goes from minus 5 to plus 5, so the least value it can take would be minus 10; when both are minus 5 that can happen? How many such occurrences are possible? Only once; k is equal to minus 5; and but this is not admissible; because we are saying, that working on the same grid k plus k prime has to be kept within plus, minus 5, that modulus; what about 9? It could be 2, right? k is 5, minus 5, and k prime is minus 4 or either way. So, this will be 2, so, you can say that this will be 5, 4 and minus 4, sorry, minus 5. This, what about this? Then we can have 8, then we can have 7, then we can have 6, 5 is admissible; so, these are the places where things would go aliasing, right?

What about 3, right? Minus 5 minus 3 minus 4 minus 4 minus 3 minus 5, three possibilities, right? So, you can work it out. And this will be 4, and this will be 5 now. Yes, so, I am saying it is like, let us say, Fourier series, you know, go away from Fourier transform, let us say it is a periodic function. So, I have a 5 harmonic for k and 5 harmonic for k prime, so they will be all integer, right? So, it is just for sake of simplicity, otherwise it is going to be dense; so, what we are doing here in-between, you will have to think of (( )). But these are discrete occurrences; even in that table. Now, Now you got to tell me, which is going where?

Minus 10 would go where? 0, right? Good. All of you see that, why it goes to 0. Because, this minus 10 is right in the middle of the left hand extension that would go from minus 15 to minus 5, and minus 10 is middle of that range, and that is in the middle of also minus 5 to plus 5, right? If anybody has any problem, please stop me. So, this actually goes to 0. Where does this go? 1, right?

So, you can see that this will go to (()) and something like this. So, what you are noticing is that, aliasing can occur to every part of the wave number range; but where is it more predominant? See, these are happening many more times; while this is happening only once, this is happening 5 times. So, that is why, based on this observation, people have made a kind of a rule of thumb, that aliasing problem is more severe at higher wave number. Isn't that so?

Because, this is a higher wave number, isn't it? If I am looking at minus 5 to plus 5, so 4 is, of course, higher than compared to 0 and 1. So, what happens is, aliasing is a problem that you actually face mostly at high wave numbers; they are there in the low wave numbers too, but not so significantly more than this. Then what happens is, why did not people notice earlier in computations? That was what we are discussing discussing there.

But how is it that the people only who were doing spectral calculation, they were bothered for decades that, "Oh! Aliasing is a problem in spectral calculations; we have to take care." But while the other people who are using finite difference, finite volume and other discrete methods, they say "Oh! Aliasing is something we do not need to worry about; it does not happen; we never see."

Why it does not happen? It is because of this nature. You see, if I take a low order method, then those high wave numbers where aliasing is predominant, there those quantities are anyway getting attenuated due to filtering. So, it was a kind of a benefit of ignorance, people did not know; but they were being implicitly taken care of by the poor property of the numerical method.

Now, suppose you start coming up with better methods like what we are now discussing, compact scheme, we do not have this. We would probably have something like this; now, what happens is, you can see even this higher wave numbers, they are very much present in your computations and you start seeing those effects of (()). So, what happens is, as we mature, we became better in our ability, we start seeing aliasing which we thought were not there in the first place.

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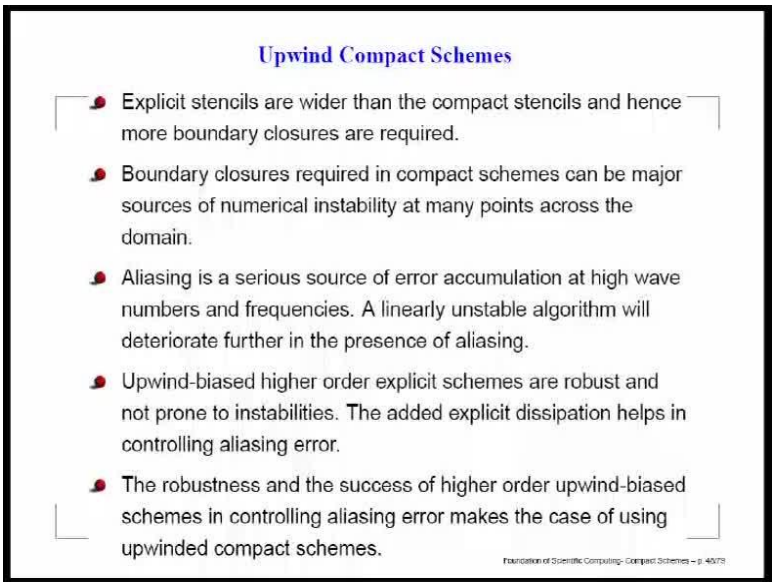

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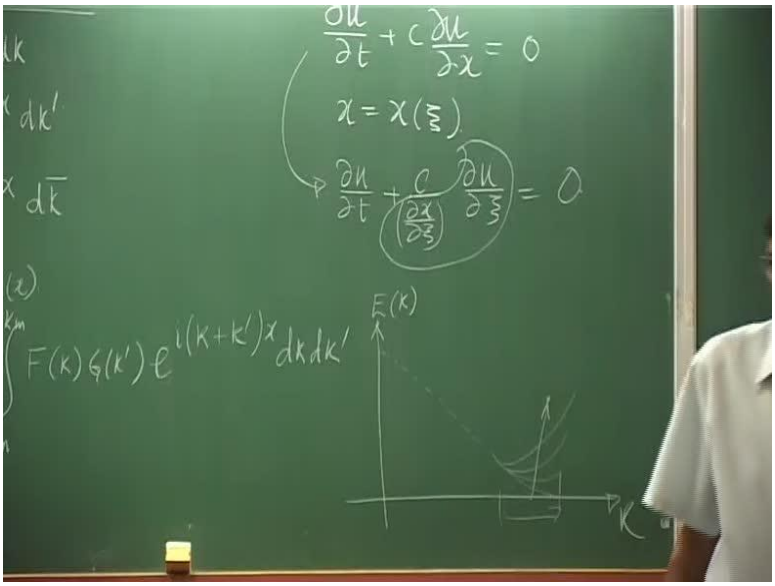

So, that is what we made in this observation, in the last class; that aliasing is a serious source of error accumulation at high wave number and frequency. Now, you understand why I kept that. A linearly unstable algorithm will deteriorate further in the presence of aliasing. So, what happens? These things, the energy or the events, seem to unnaturally pile up at the higher wave numbers; so, if I am looking at, let us say, some physical events, and I am plotting, let us say, the energy of the system, right? And I am trying to compute those, then what happens is, in most of the cases, as you know, physical systems are band limited; it it it comes down like this.

These are the all kinds of certainties, different system, it shows different variation; but eventually, they are kind of band-limited; they come and stop somewhere. If you are trying to compute some subsystem, and if aliasing is present, what would you hope to expect? You would hope to expect, that as your computing, because of this, it is not a good thing to happen; but, if aliasing is present, those alias component will start piling up in the higher wave number range.

And as you are computing, let us say, time dependent problem, you will see that with time, spuriously, energy will pile up at high wave number; and of course, you realize by now, that most of the problems are related to high wave number, high frequency phenomena, that is, what we are saying also here; that suppose I already have a linearly unstable algorithm, then in addition, if I have aliasing, that will be accentuated; that will happen more readily. So, this is something that you do; and as I also told you, that aliasing is a typical problem of whenever you get a product term, most of the act, sort of diagnosis of aliasing came from fluid mechanics. And there, actually, we have problems of this kind; the terms of this kind, say conductive acceleration terms etcetera, etcetera.

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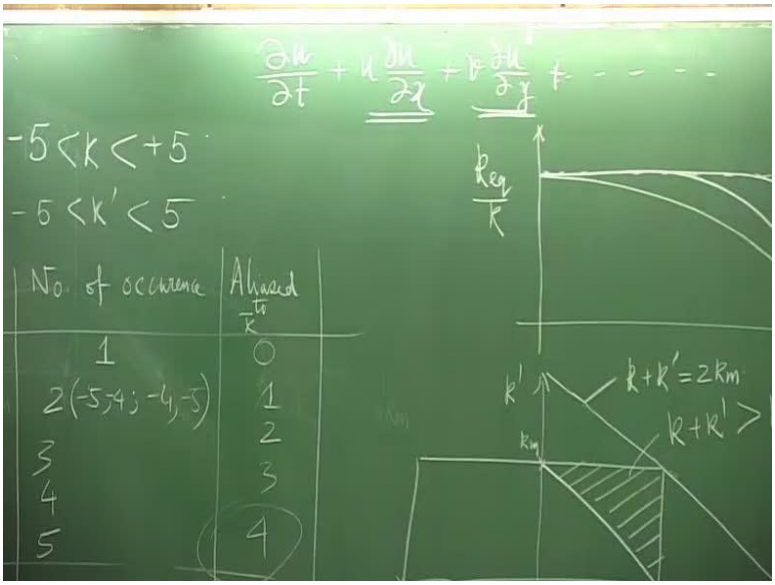

So, you can see, these are the natural product terms occurring in the governing equation, and they are essentially kind of non-linear. So, there has been a, sort of a, sort of a mistake in belief that aliasing error is a non-linear instability problem; that that is the misperception in most of the literature and books you would find. However, from this

simple example we showed, that even for a linear system, you can have a product term, and such a product term can give rise to… You have also seen another example which we had done before, so, that was that Laplacian in the transform plane.

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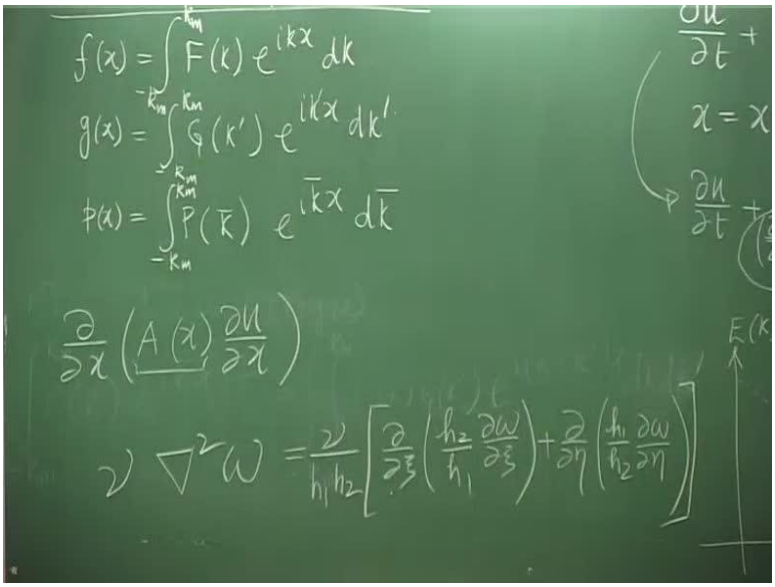

If you recall, that we wrote terms of this kind while talking about A d e or some, sorry, a d i method, we had this kind of a term. So, this will be a kind of a known function of x; it is not an unknown. But still, you can see, there is a double product here, so, this can also give rise to aliasing. In fact, if you look at fluid dynamical equations, you always have to do this. If suppose, I have to get this as the dissipation term, and now, if I am looking at in the transform plane, it would be something like this; unfortunately, we will not be able to do it, but it would look like this.

So, that is how it would look like; and you can see, even though this is a linear operator, it involves a triple product here, h 2 is a function of xi n eta h 1. These are all grid transformation quantities, so they are not constants; they themselves are functions of xi and eta. So, here, you can see the triple product, here is the triple product; and when you try to differentiate them, those triple products, actually, the problem becomes even more acute. You all would agree with me, that in numerical operation, if you do some kind of integration, you actually smooth out. Whereas, when you differentiate, you accentuate. If I have some error quantity, and I am differentiating, that gets magnified; I am integrating it kind of as an effect of smoothing on, okay.

So, we have a term, and further more differentiating, and it, can be a serious source of aliasing. So, please do not be swayed by any of such statement, where people say aliasing is a non-linear, discretizing problem. Aliasing is equally bad for linear problems, right? So, let us keep that in mind. Now, we have noted that when it comes to explicit methods, we can use this higher order upwinding schemes, like, we have talked about third order up-wind schemes, right. We did work out those stencils when we were talking about discretization quite some time ago, before your first mid sem; and there we found that, if we take higher order upwind schemes, explicit schemes, they are quite robust; and they have this tendency to suppress numerical instabilities. Because, upwinding involves an implicit dissipation term, right. Suppose, I do first order upwinding, what is the equivalent dissipation term? We have is a second derivative term.

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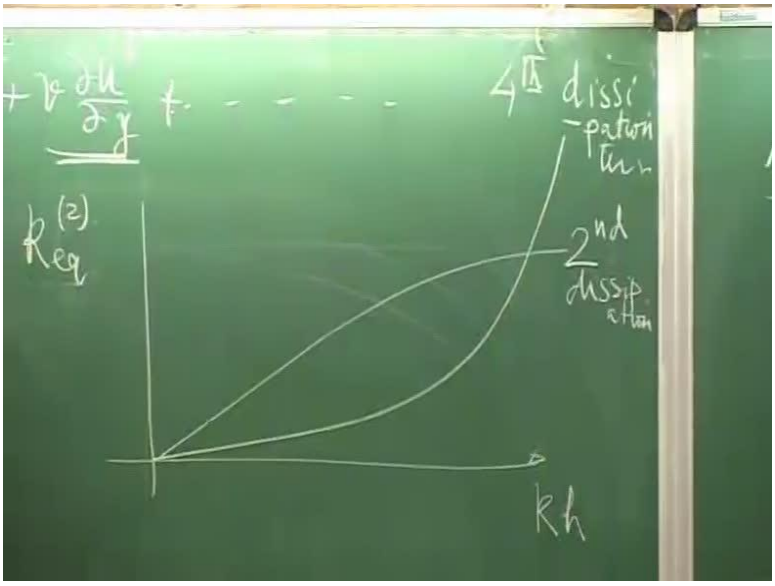

If I am taking a third order upwind scheme, then what will happen? I have equivalently added a fourth derivative term, so all those, even derivative terms actually adds explicitly or implicitly; those dissipations term; and, if you have this dissipation term, what it does is, of course, it attenuates, and what happens? We have done this exercise; if you just recall that if we discretize, let us say the second derivative term versus k h; well, let me just simply just show the dissipation term itself, versus k h; you will notice that this goes like this. So, as k increases, your added dissipation actually increases, right? And this is, let us say, for second dissipation, right? And if I add a fourth derivative term, it would behave like this; so, this is your fourth dissipation term.

So, what is the essential difference between second and fourth dissipation term? In the second dissipation term, you see, even low-cases are getting affected by dissipation; whereas, if you take a higher order dissipation, they remain much more smaller at i k, but, at larger k h, they actually overshoot the second dissipation. So, if I have to add a dissipation, which one would I prefer? I would prefer a fourth dissipation term, why? For two reasons. Because, we said that this dissipation is added to control numerical instabilities, and numerical instabilities always occur at high wave number; that is what we discussed when we were talking about multi-grid method also.

You see, that was one of your question, that, why in restriction you smooth, and in prolongation, you do not? That was essentially the same idea which we are talking about; that, at low wave numbers, they are not such a source of problem, but, at high wave numbers, they are; and there is a second reason, you see, most of the physical processes are physical dissipation.

What is the nature of physical dissipation term? They are always a second derivative term, right? So, if I add second derivative term for numerical stabilization, there is a very good chance that I am going to tamper with the physical dissipation also. So, that is why, low order dissipation are not a very good idea. If you have to do, you would always account for higher order dissipation, because they will not tamper with the physical dissipation; at the same time, they will be able to control numerical instabilities which are more severe at high wave numbers; and I have you can see, at height k h, this amount of dissipation added by higher ordered up-winding is much more, and that gives you additional control. So, this is what we are saying here, that if we have an upwind bias higher order schemes; they are robust, they prevent instabilities and the added dissipation would also help controlling aliasing, isn't it?

See, aliasing, as we said that it is a more of a high wave number phenomenon, so, if I dissipate the solution at high wave number, the tendency for aliasing also comes down. There are other ways of controlling aliasing, so I am not going to go into that, but it is just that, we are talking about here, about upwind schemes; so, I am just telling, what are the plus points of upwind schemes; so, we learnt, what is an aliasing? We are now making an observation that higher order up-winding actually helps controlling aliasing error.

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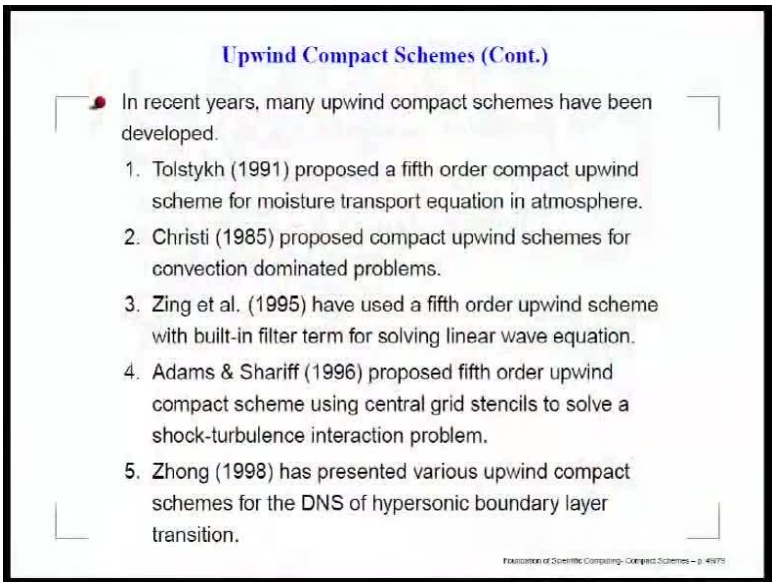

So, if if they are so for explicit scheme, they have to be so for compact schemes which are implicit scheme, that is, what we note down there. Now, many many people have done this work. Tolstykh in Russia has used some fifth order compact schemes for atmospheric science; then, all this other people have done, starting from simple linear wave equation to all the way to Zhong at the UCLA, claim to do direct numerical simulation of re-entry vehicle flow transition.

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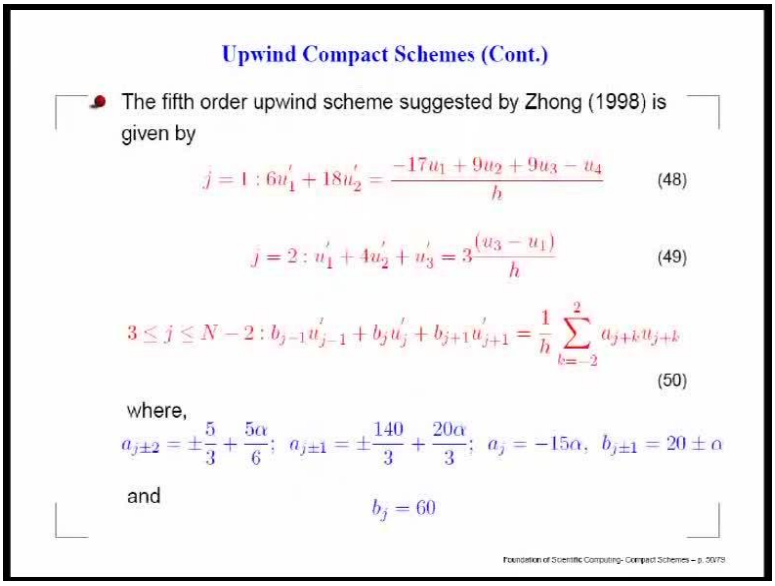

Now, they are there. Let us look at one such scheme. This was what Zhong proposed in '98; it is basically a fifth order upwind scheme. What is it that means by fifth order? Well, that is all embedded in equation-50; and what you would notice? That if it was a central scheme, then b j minus 1 should be equal to b j plus 1; that that is one of the key-ideas of central scheme; that they are to be perfectly symmetric. However, by design, you can see b j plus 1 and j minus 1 are tweaked; they are not same 20, they are, means 1 is added with alpha; another is subtracted by alpha, right? So, that is how we are actually introducing up-winding there. The same thing happens; on the right hand side, also with the function value coefficient, a j plus k, they are given in terms of this. You notice that alpha seems to be kind of a parameter; by the choice of alpha, you can control whatever the up-winding you want to; for example, of course, you put alpha equals to 0 you get the central scheme right.

So, alpha is the parameter by which you are actually switching in the switching in the instability, I mean the up-winding. Now, as you can see, if I put alpha equal to 0, then b j is 60 and b j plus minus 120; so, what is that scheme? That is exactly the central scheme that was used in by Adams, right? Adams had a sixth order scheme that was exactly like this; that 1 3 1 here, here, it was 1 here, it was 3, and here it was 1, it is a same thing; if you divided by 20, you will get the same value.

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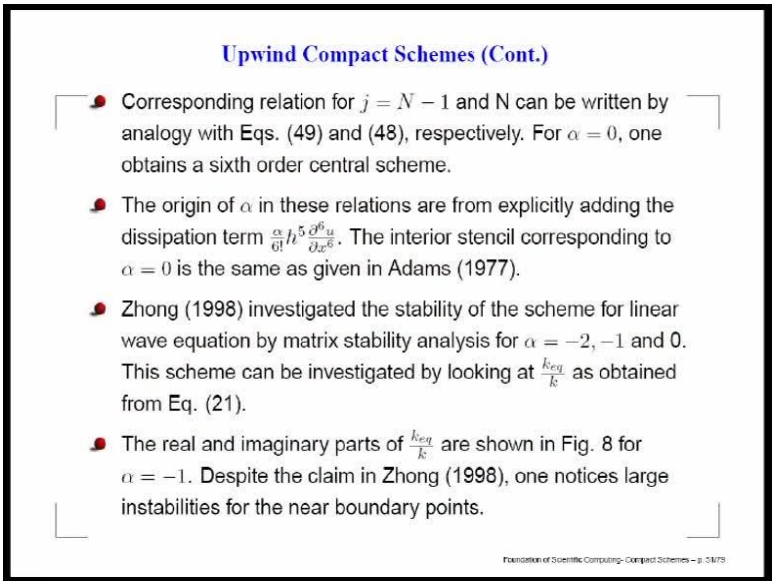

So, of course, the stencil is written like this; it is penta-diagonal on the right hand side and tri-diagonal on the left hand side. So, you would require two more auxiliary relation boundary closures at j equal to 1, j equal to 2; they seem to be what others have done before, and it was proposed; and Zhong continued working on it for quite some time, so, of course, we now know what we could do. Now, the choice of alpha is given by the second bullet; you can see that it is given by adding a term which is alpha by 6 factorial h to the power of 5, the sixth derivative.

So, this is really higher order up-winding, right? Sixth order term has been added now; Zhong actually investigated various possible cases taking values of alpha as minus 2 minus 1 and 0. 0 takes you back to Adams' schemes. Now, what we could do is, we have learnt how to do a global analysis, so we could subject this scheme, that we have 48 to 50 and calculate k equivalent by k and find out what is being done in this scheme.

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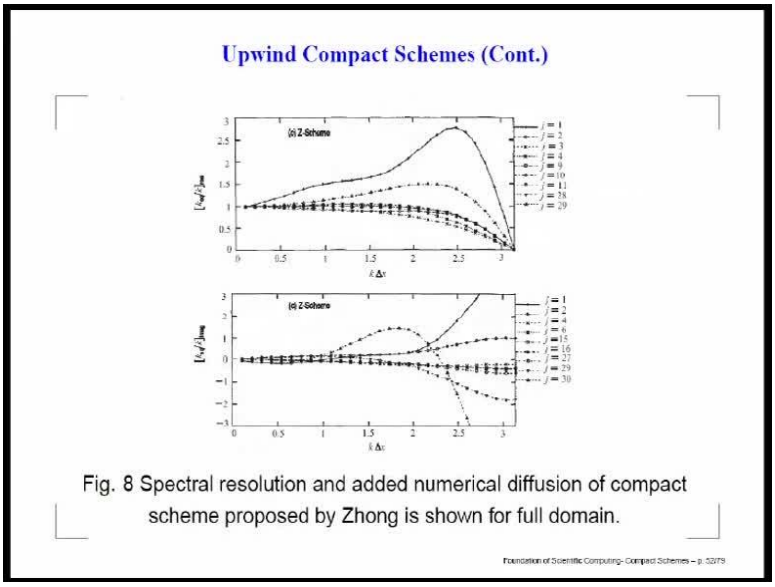

And this is what we find; the top figure tells you about the real part of k equivalent by k, and the bottom one tells you the imaginary part; and you could see that even the real part shows a kind of real variable mixed values of k equivalent by k, for different k h. Although, of course, you can see, it takes you to pretty much high value of almost, above 5 by 2; however, that is not the thing that one should be really worried about. It is the imaginary part that should tell you what is happening here.

What is happening here is, j equal to 1 is truly unstable point that you can see; look at j equal to 2 in the intermediate range; it is unstable, then of course, it becomes stable at later stage. Then, you can see this other points, all these points, it shows your value to be positive; they are all unstable points, so I think our analysis became very unpopular with Zhong, because he did not know; when he saw this, he was quite upset that method is full of holes.

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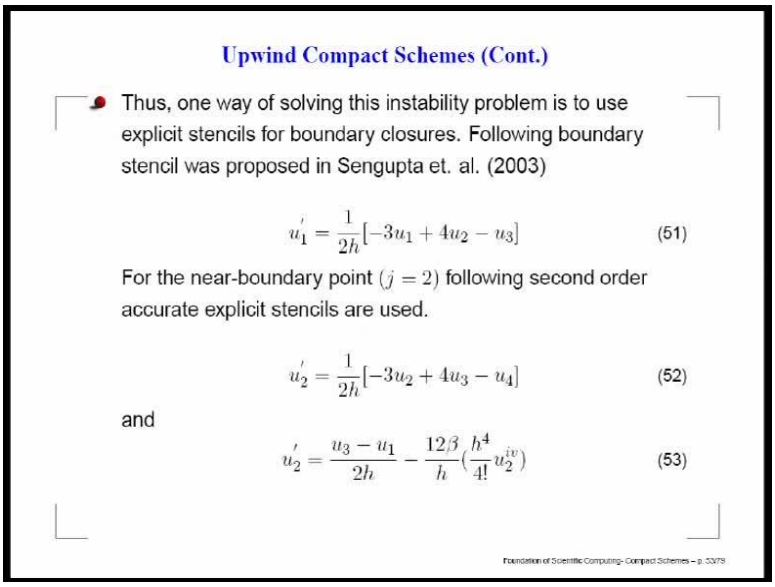

Anyway, we are noticing that even attempt in introducing upwind scheme and trying to get stable method are not always very successful; and they are unsuccessful for the reason that you are trying to have this boundary stencils, one sided right boundary suspensions, in the near boundary stencils as we can see here. In j equal to 1 and j equal to 2, j equal to 2 is still its central scheme, right? j equal to 2 is a central scheme. As you can see, there is no problem, but j equal to 1 is seems to be the culprit, and so bad that the effect is not confined to j equal to 1, but it is confined to many many points inside. And that is happening, because of the implicit nature of the scheme, so, that is where we stepped in and we said - look this probably can be prevented if for the boundary closure.

We revert back to explicit schemes; we do not have implicit schemes because, explicit schemes are truly local in nature. If I add something on the j equal to 1 node, it will only affect the j equal to 1 and not that they were significant; and that is what is done here. Equation-51 is basically a representation of a first derivative; again it is an up-winded

form, but whatever effect that will be there, it will be localized; it will not percolate in the interior of the domain.

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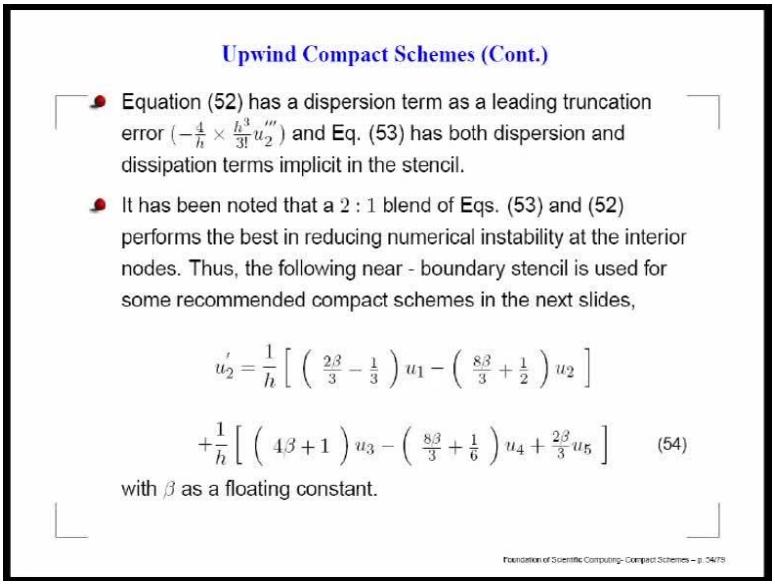

The same way, we have done something the second point; we have used an explicit scheme, and to that, we have tried to add a kind of a stabilized fourth derivative term, so that, we can introduce some kind of an explicit up-winding, even for the 0.2; and this is what happens. It may look unusual, but this is explained here that, we add a dispersion term, and then it also has dissipation, so, what we do is, we to blend two of those terms to get this explicit scheme with beta as a control parameter; we choose beta in such a way that, overall scheme is comes out to be good.

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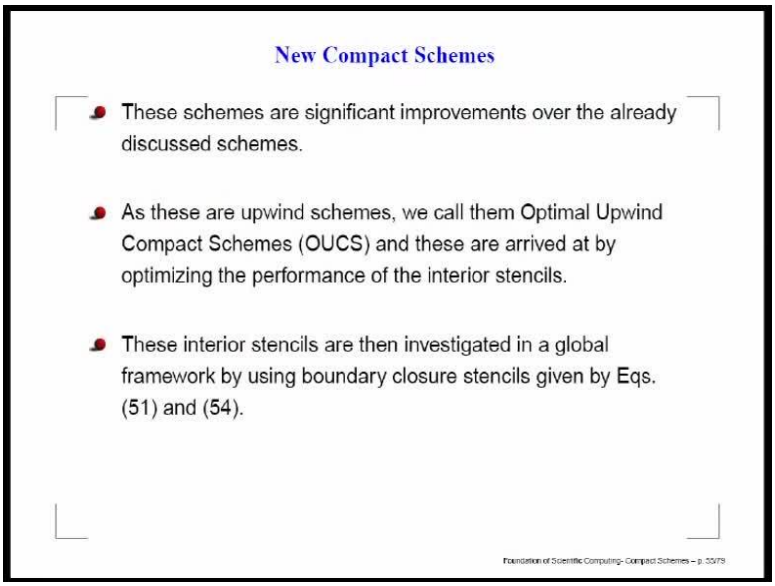

Now, this actually is something we do not make lot of claim. But the point is we diagnose the problem, what is the problem with the existing scheme, and we propose the solution; and this is what we called as some kind of an optimal upwind - compact scheme optimal - in the sense that, we try to figure out those constants that would appear in the scheme, like alpha and beta, that we have manually optimized and we figured it out, and then we have the global analysis tool and we can check what we are getting.

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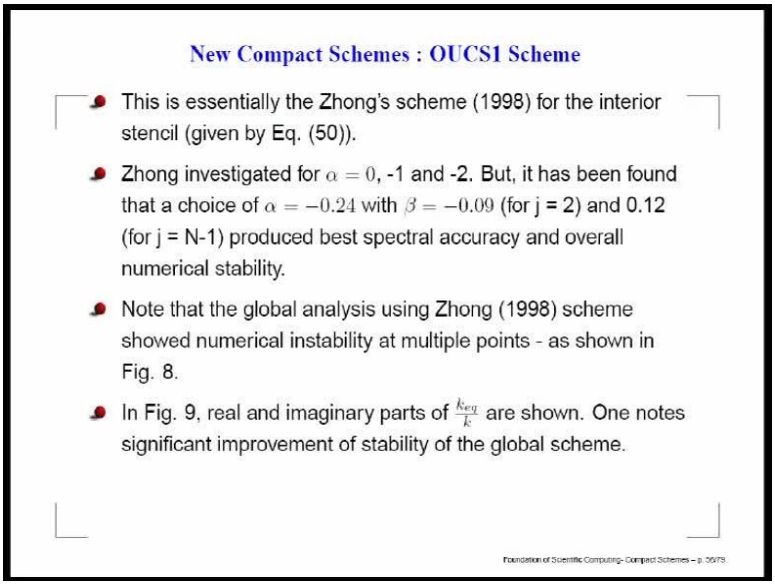

So, there are a series of methods proposed by us, and they are essentially dependent upon what others have already done, for example, this scheme that we are writing here as o u c s 1 scheme, which is nothing, but removing all the problems of Zhong, right? So we took the Zhong's scheme and we did not take such large values of alpha; we figure out in optimization process, that if we take alpha equal to minus 0.24 and that beta, beta is that formula that we have used in this second node parameter for explicit closure, and then with that, we found pretty good method

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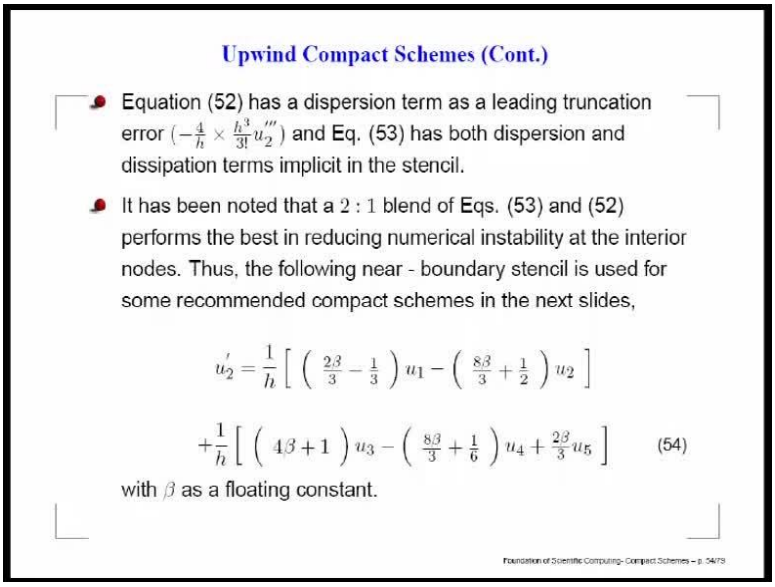

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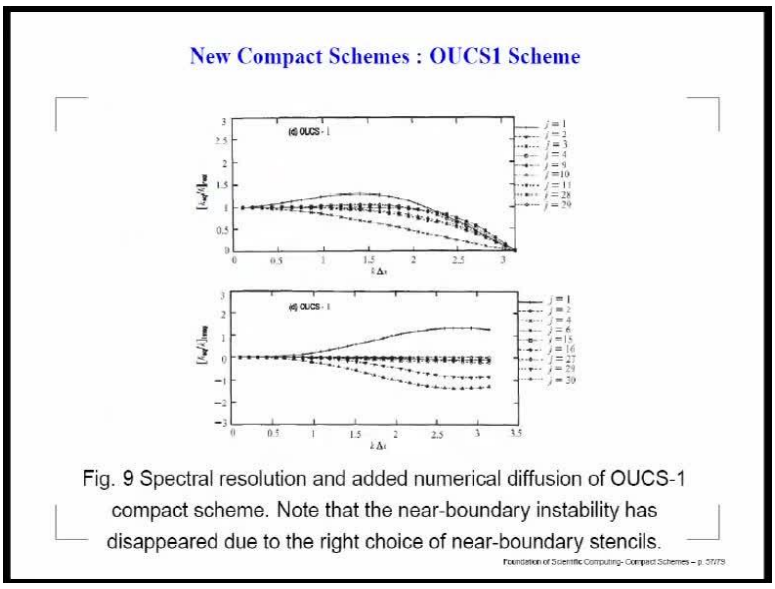

Now, in Zhong's scheme, we have seen numerical instability at multiple points, but, when we plotted our results, this is how it looks. Please note, that we have done one thing. What we have done is the 0.2 we have done something like a c d 2 kind of a stencil, right? And that is what you had seen, that j equal to 2, we have a degraded property here, where as any point inside they they they get better and better; what is important for us though to remember? That The imaginary part that was the source of all kinds of problem before, and what we found in our method that apart from j equal to 1, all the other points are stable or neutrally stable; there is no hint of numerical instability anywhere expect j equal to 1.

And j equal to 1 is of course, not a problem at all. Now, I told you time and again, because this is what we do to calculate all the derivative, but j equal to 1 is a boundary point; that is where you do not discretize the equation, right? So, you do not need that value. This value, it does not go into the calculation; you can see they are at the back points, so this was the first scheme which is a variation of Zhong's scheme.

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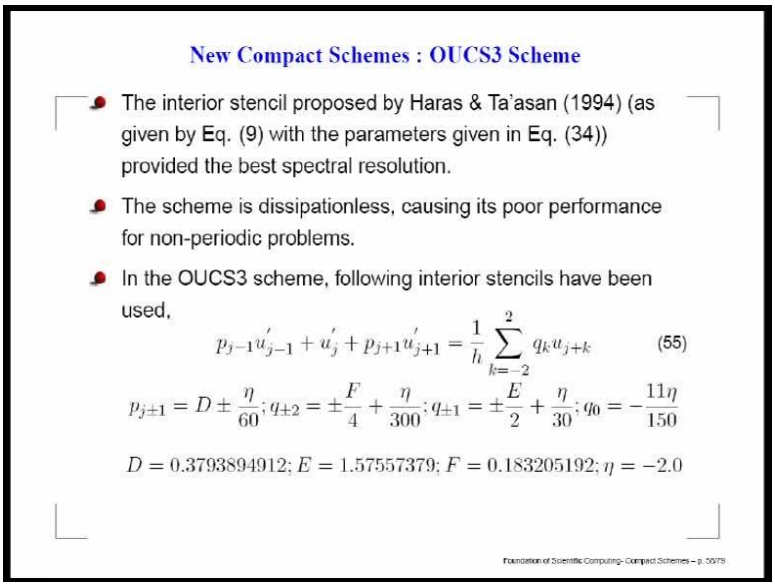

Then, we went and tried to pick that Haras and Ta'asan scheme, because we were quite happy to see that Haras and Ta'asan scheme probably gave a very very good, very very good spectral resolution, so, we said that we will build a scheme. But we will add little bit of up-winding to that scheme and that is what we did. You look at this left hand side, p j minus 1 and p j plus 1, we have added an up-winding term which is given by eta by t.

So, this d, e and f, these are the value that is essentially given by Haras and Ta'asan; so, we did not change those, but we added a little bit of dissipation so that we can get bit of an up-winding.

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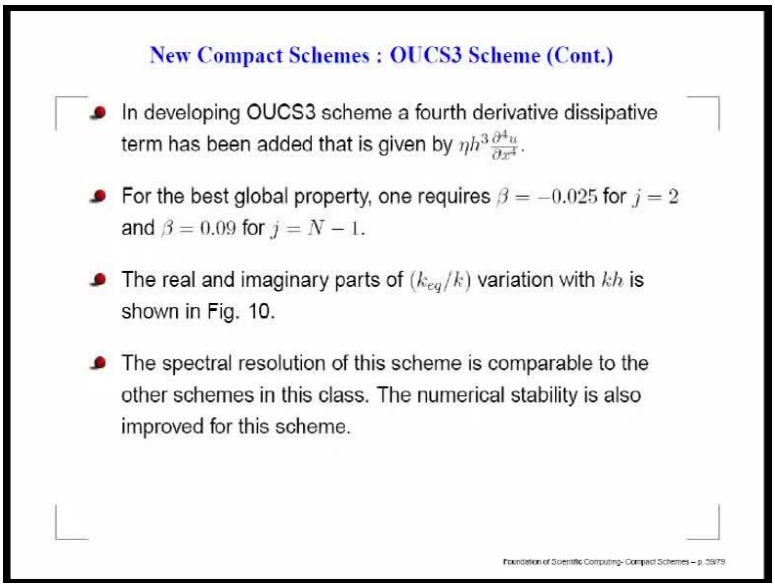

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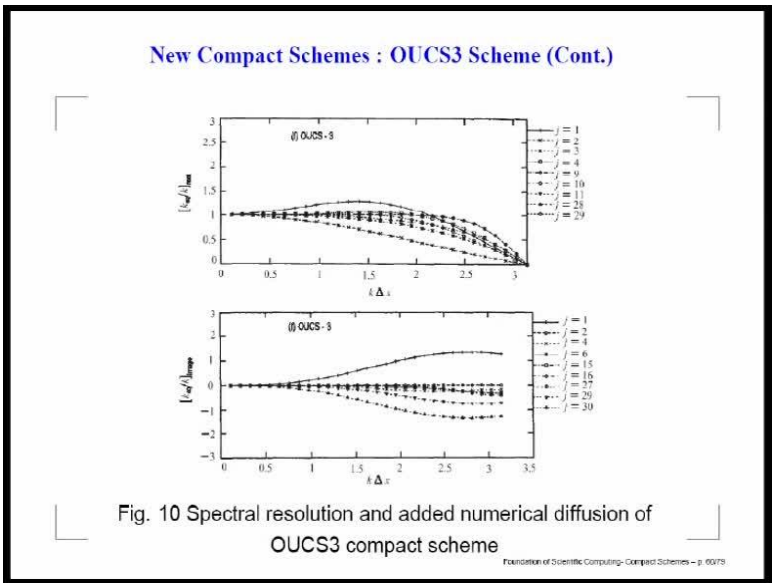

Both on the left hand side and right hand side, and not only that Haras and Ta'asan scheme was kind of for a periodic problem; so, for non-periodic problem, we tried to use our own closure that we have shown for j equal to 1 and j equal to 2. We blended all that together and we figured out that, for this scheme, we need to take beta equal to minus 1,

0 to 5; and for j equal to n minus 1, we take beta equal plus 0.09, and this is what you get. Once again, you have a perfectly stable method, absolutely no problem here, in the imaginary part; and the real part, we retain the good property of the basic Haras and Ta'asan scheme. We may have overshoot at j equal to 1, but that is of no concern.

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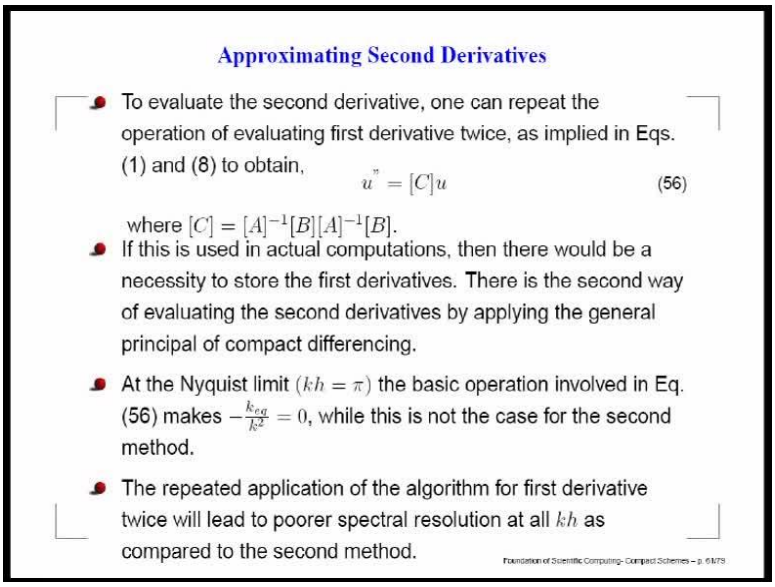

J equal to 2 is the only one which has the lower accuracy, but otherwise, this method seems to perform very well; and let me tell you for the last 7, 8 years, this has been the workhorse in all the things that we been doing here. So, basically, now we have a pretty good well-settled approach to using high accuracy method by compact scheme. As we have shown here, I have just shown you only two schemes. If you are interested, we have developed few more that is something which one can do as and when (( )).

Now, let us now talk about calculating the second derivative, because those are also equally important in calculations; and we have already seen that, we can use the first derivate method twice, calculate the second derivative as given in that equation-56. However, you notice that if you are doing a calculation, then you would have to store the first derivative, and from that stored value, you will calculate the second derivative; and what happens is, also that, if we use general principle of compact differencing, general principle of compact differencing, what do we mean?

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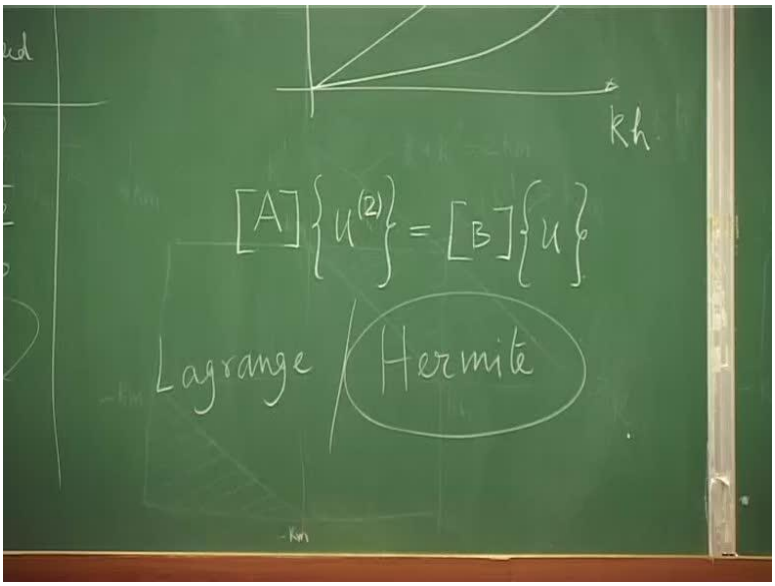

See, the compact differencing scheme is generally, if you are calculating the n th derivative, you can always write this. I do not have time to discuss, but those of you who have done any course on interpolation; you would note that there are two general classes of interpolation; it is the Lagrange interpolation versus the Hermite interpolation, right? In Lagrange interpolation, you interpolate the function values; in Hermite interpolation, you interpolate the derivatives also. So, what happens is, this compact scheme actually belongs to a Hermite interpolation scheme and general interpolation strategies of this kind, so for any n th derivative, you can write in terms of function value.

So you so far what we have done? We have done it for first derivative, so instead of n equal to 1, if you put n equal to 2, you can write out a similar general scheme for second derivative. That is what we are taking about, that we can apply general principle of compact differencing. Now, there is something interesting about this difference between first and second derivative and that is the following.

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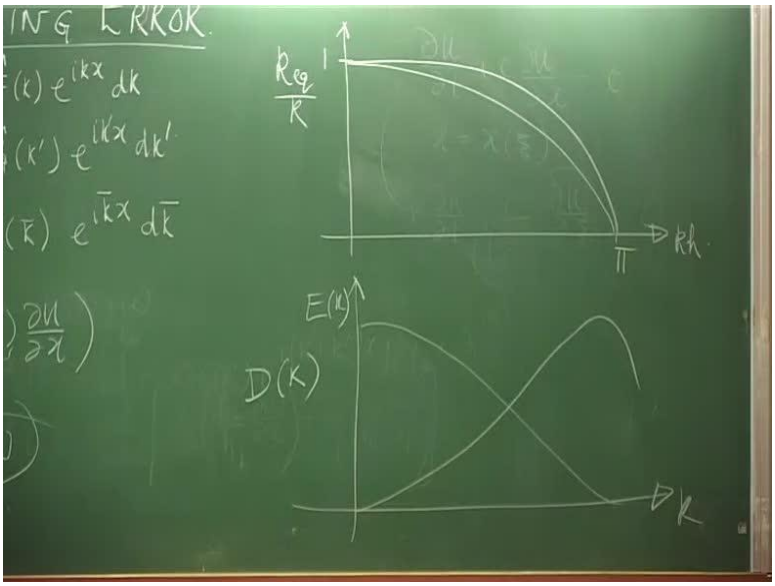

Now, when we evaluated the first derivative, we figured its resolution by k equivalent by k, right? And what we found? That it starts off with a value of 1; and at pi, it ends becoming 0, depending on the method chosen, right? So, now what happens is, if I use the first derivative evaluation method twice, to calculate second derivative, what will happen? So that will be like doing it twice, right?

So, what happens is, basically you would see that it would degrade to something like this, and that means, that at Nyquist limit, your second derivative is totally ineffective 0, right? Now, this is something now related to properties of some physical systems, mostly, let us say fluid dynamical system, that may involve your chemical engineering, metallurgical engineering, everywhere you would see the same thing if I plot energy of the system. Then, as I told you that it could be something like this, it could be a band-limited quantity, right? So you may be happy to choose a method where your Nyquist limit is on this side, where you are saying, "My all energy has been resolved."

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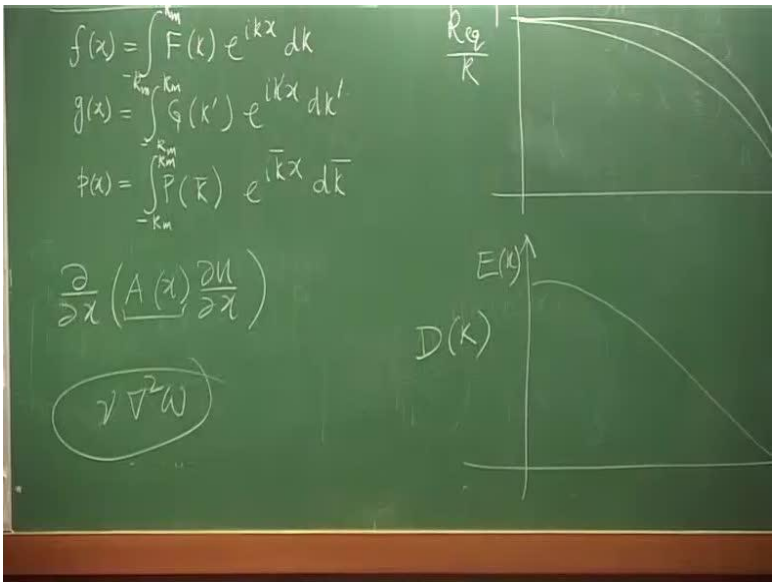

However, when you look at the dissipation term in your governing equation, there are dissipation terms like what we wrote there, nu times… Recall, I wrote this this as a dissipation term, right? If I plot this dissipation term as a function of k, what I find that dissipation terms actually happens like this. So, dissipation term is a sort of a complementary picture of the energy, so at small wave, number dissipations are less effected, but as wave number increases, dissipation keeps increasing so much, so that, at very high wave number, you actually get the peak of dissipation.

Now, if I use the first derivative twice, and if that Nyquist limit happens to be in the vicinity of the d max, you are doing a very poor job, right? You are you are actually doing a very poor job; that is where you need lots of physical, so, these d of k, this is physical dissipation, we are not talking about; so, this is what you want to actually represent, but if you use a method of this kind where at the Nyquist limit, the second derivative turns out to be almost 0, you are not able to do what you want to do.

Your dissipation term is becoming totally ineffective, in fact, now having said and come this far, now you can go back and see in the talk that I gave last summer, at MIT; that is where we did talk about all these issues. What happens is that some of this method, you know, sometimes we are so much obsessed by Nyquist criteria, we say, “Oh! I have resolved everything in the grid.”

But these are the major issues that we have to worry about. One by one, we have seen the various sources of error. Now, this is what today we are talking about; how to represent dissipation term effectively and that would be a pretty bad thing to do if I use a compact scheme; and do it twice, then I know there, the Nyquist limit, the effectiveness of dissipation discretization is virtually 0, and we will not do it very good way so, this is a poor method.

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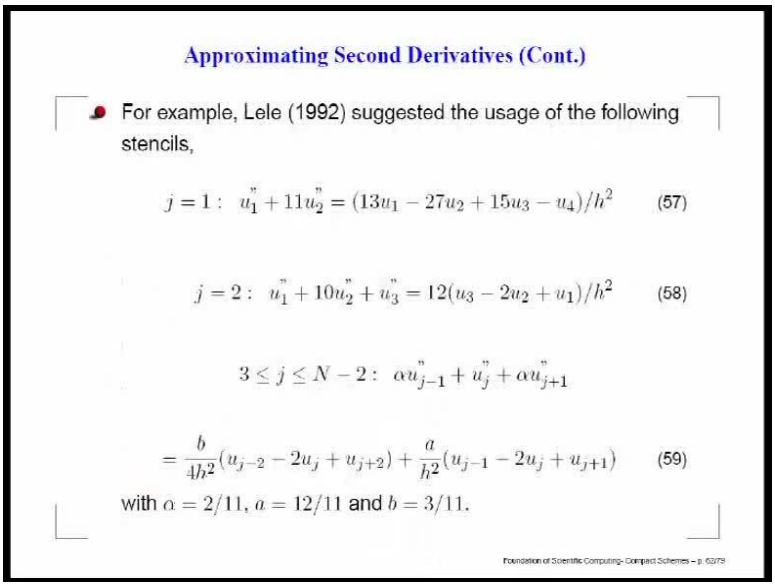

So, what we can do instead, as I told you, we will take general principle of evaluating the second derivative directly from the function itself; and this is what in fact Lele has already done it. So, as you can see, the Lele's method for j equal to 1 uses this stencil j equal to 2, uses this stencil and j equal to 3 uses this; and all that remains is to figure out this alpha a and b, i think in the next meeting, we should be able to wrap this thing up. We are virtually done there; its time I suppose I will also load these notes today, so you can take a look at it, and again when we meet on next class, we should able to wrap this topic up.