Foundation of Scientific Computing

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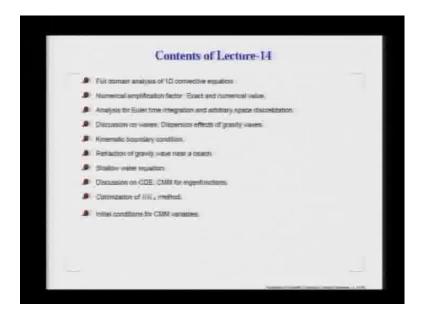
Indian Institute of Technology, Kanpur

Module No. # 01

Lecture No. # 14

Today, we are talking about various topics, because today's lecture is going to be followed by your mid semester. So, we will talk about various topics that would be of specific interest to you; so I will invite questions from you. In this topic, in this lecture, we will begin our discussion actually with a full domain analysis of 1D convective equation.

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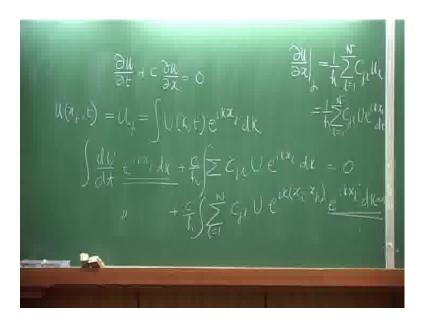
We will talk about numerical amplification factor; its exact and numerical values. As an example, we will use Euler time integration along with arbitrary space discretization. Then, we will actually start our discussion on various topics. I would expect that we will have some discussion on waves. We can talk about dispersion effects of gravity waves.

We would like to emphasize that these waves are essentially created due to kinematic boundary conditions.

We will talk about the various refraction mechanisms that are related to gravity waves near a beach, to explain some of the properties of wave propagation. We have actually spent lot of time in discussing about shallow water equations, so we will be opening up the discussion on that. Then, before that we have talked about solution methods of ordinary differential equation.

In this context, we have specifically talked about CMM or the Compound Matrix Method, which was used for Eigen value and Eigen function evaluations for stability problems. Coming back to time discretization, we will talk about the four stage Runge-Kutta method and its optimization; how this thing comes about. We will also, if necessary, talk about the initial conditions for compound matrix methods.

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Laplace-Fourier transform framework: If I am trying to do it at the jth point that means, actually U at x of j and some t. Then, the argument would be at that point; that is how this is evaluated at jth point; this is what we do. Substitute it in this, the first term would give you dU dt and of course, I have e to the power x j d k plus c.

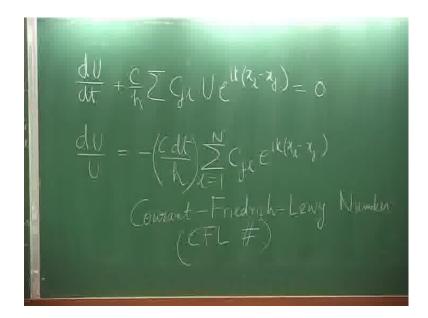
Remember, we have already noted that if we are using explicit method; what we do is we evaluate it as this (Refer Slide Time: 03:51). This is your usual stencil, so I am just

generalizing, writing it in terms of a C matrix. Operating on the U vector would be giving you this derivative.

So, if I plug that in over there, what this would be? Using this representation, this will be 1 over h and summed over C j l. Instead of U l, I will write this expression U of e t, so ik, this is evaluated at l dk. So again, this is what we are going to do.

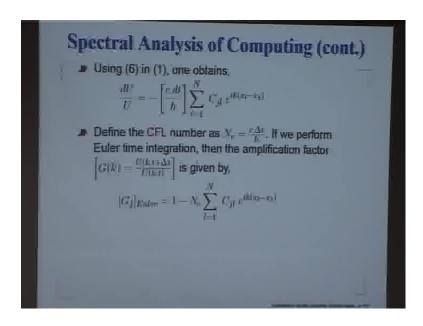
Substitute it over here. You are going to get C by h sum over C jl U e to the power ikxl dk. We are still not ready to directly look at the k space, because here the argument is e to the power ik x j; here it is e to the power ik x l. What I am going to do is I am going to do a little bit of modification. So, this term will remain as it is. Here, we would perform the same operation that we have, but we will project every this xl point to x j. So that means, I will just simply do this, this is what I mean by a projection (Refer Slide Time: 06:09).

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Now, what are you seeing? This equation as it is written everything for flux to the jth node here. What I could do is, of course, I could write this equation for every k. It would be simply C by h summation Cj l u and e to the power ik x l minus x j.

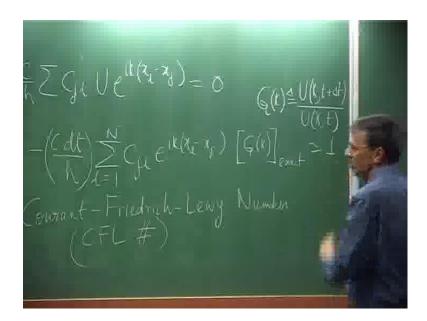
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So, if I have done that I get that equation over there. Now, you can see this is what we get. So, I could just simply transpose it on the right hand side and just simply write it as dU by U, it should be equal to minus Cdt by h and summation of I equal to 1 to N C jl e to the power ik of x I minus x j. You would see most of the time in computing this quantity appears and this is non-dimensional. This is a velocity times dt by h, so it is a non-dimensional quantity. This is what is called as Courant-Friedrich-Lewy number or by its acronym, it is called the CFL number (Refer Slide Time: 07:39).

We can see that CFL number directly comes into play, we are going to use that as the notation and write it as N c. What happens is we need to integrate this equation. What is this u? Look at the argument; this is u as a function of k at that particular time t, we are investigating.

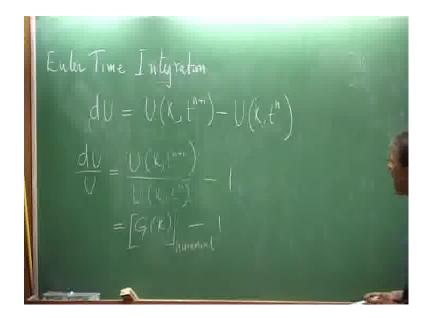
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What we could do is, we could define an amplification factor that I will call it as G of k; that is, for that quantity evaluated at the advance time by the predecessor; theoretically speaking this amplification factor ideally should be what? Ideally, it should be equal to, when delta t goes to zero, it should be 1. So, that is your theoretical estimate for this G of k. But, the moment you adapt a numerical method you would get the corresponding numerical amplification factor; so, this is a definition.

If I were to write G of k, exactly it should be equal to 1. We do not have any other option, but to do that. Please do understand that this exact estimate does not depend on the equation that you are studying; it is independent of what equation you are solving. It comes directly from its definition in the limit for vanishing time stamp, it should be there and it should be equal to 1.

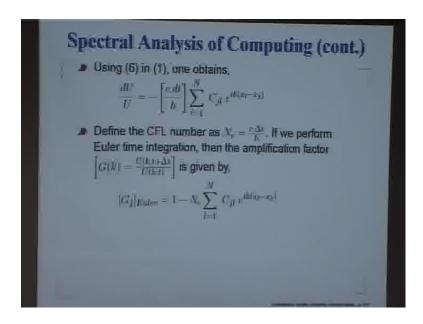
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Now, for example, we adapt say Euler Time Integration. If we do that what would we get? dU that we are writing, I will write it as U for that particular k, which we are looking at the advance time level minus U of k t power n. What we get is dU by U, it would be nothing but U of k plus one divided by U of k t of n, this of course will give you 1.

By definition, this is nothing but G of k. Now, this is the numerical estimate, because this estimate for G we are getting for this equation; it is an artifact of the method that we have chosen for time discretization. We have still not specified what the spatial discretization is; you can do it at your leisure. Choose a particular spatial discretization that will fix the coefficients of the C matrix and that you are going to get.

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Basically, if I adopt any spatial discretization, but adopt Euler time discretization for advancing the solution in time G of that would be this 1 minus this. What happens is then G is this expression. What you notice that it has a real and imaginary part. What you could do is you could look at its modulus. If you look at it modulus, what did you get? We should work it out; you will find out that it will be greater than 1.

What does it mean? Means that if I adopt Euler time integration for any explicit time advance or spatial discretization that corresponding numerical amplification factor is greater than 1. That means, with time, this quantity will keep on increasing, because that is the quotient. The numerator is greater than denominator, so it would mean that you have just looked at a method which is unstable.

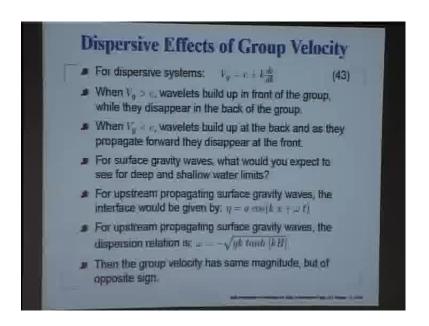
What was the property of this solution? The property of this solution was the amplitude should remain same, so that G should have been equal to 1. Theoretical estimate also says it should be equal to 1. The very fact that if it crosses the value of 1 implies this time discretization should be equal to unstable. This is what I actually mentioned in one of the lectures, we will show that not all space time discretization combination is amenable for solution. Here is an example, where you can see by this analysis method you could show that for any k this is going to be unstable.

This expression is a function of k, so for every k it is greater than 1. If you sum it over, Fourier-Laplace transform is a linear operation, so you can always superpose. You are going to see that it is going to be constant. I thought, I will just finish this part and explain to you what is analysis method that we started looking at yesterday. Now, I think we could go on with our discussion. If you have any doubts, we will have this as a discussion now.

Let us begin; any of you have any questions? Ankith, do you have any questions? Bipanshu.

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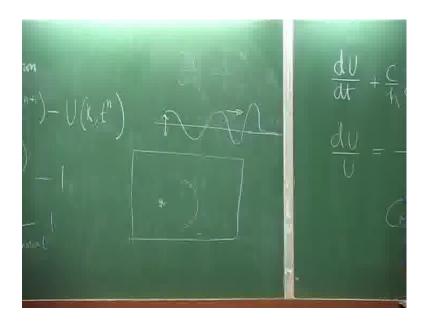
Let us go over to that part and see what we could do. Yes, this is what you are referring to right; these two bullets. Look, what is a phase speed? Does phase speed indicate movement of fluid particle in the direction of the wave propagation? No, because we have seen that for surface gravity wave the particles execute orbital motion. They could be either as circle or an ellipse; we have worked out the expression for that equation.

The particles by themselves do not move, however the phase speed indicates the relative positioning of the neighboring particles with respect to each other; that is, the phase difference.

So, the rate at which this phase difference changes is what we call as the phase speed, whereas we have noted the energy travels at the speed of group velocity. What is happening in this case is that let us say, do a third experiment. You drop say a stone in a pond, now what will happen? In this sum, you are giving a kind of a delta function excitation, it is very localized, so all case are excited.

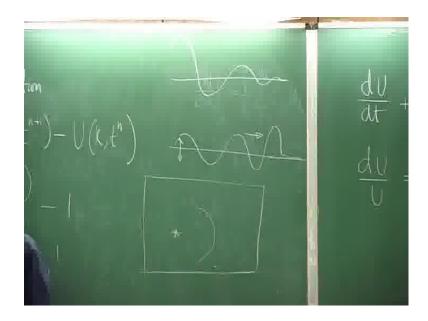
However, the analysis is for linearized framework, so we can build up. Let us look at one of the k; what it is doing? What did you say? The energy; for example, in the first part, the energy is able to outstrip the phase motion; that is what it means, right?

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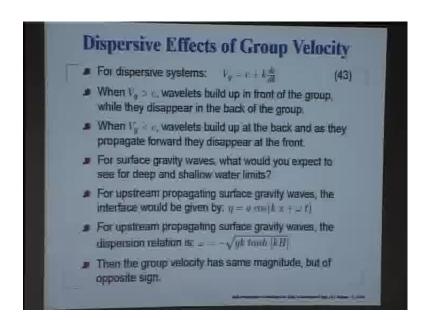
What you are going to see is that if I draw a side view, then this is where my excitation has occurred; the phase is lagging behind, whereas the energy is outstripping it. So, what happens? If I create a disturbance in a finite time I will see a wave front. What will happen here, as I go along, I will get a disturbance of this kind (Refer Slide Time: 17:25). So, amplitude builds up for the reason that energy is able to outstrip the phase, so that is where all the energy arises together.

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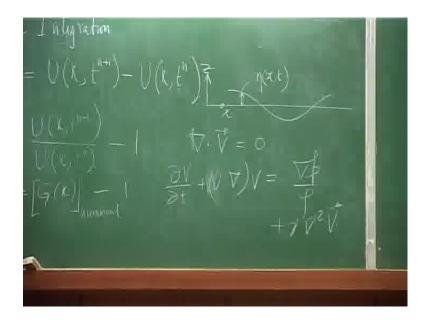
But, of course, it has a finite front, so it would end there. So, that is what it means in the first part. In the second part, of course, it is the other way round. If you have c greater than v g, then what will happen? You are going to see the energy will lag behind and you may see that situation would be something like this. So, I suppose that clarify this is not a very trivial concept. I mean group velocity is a very important concept, we should understand. I purposely chose this, because with respect to this mechanical system you can visualize what is happening.

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Are we referring to the interface equation? Ok.

It is really simple. Let us say, we have the undisturbed interface like this; that is flat. Now, I create a disturbance or I look at one of the harmonic, we will not look at everything taken together. So, this is my disturbed interface, I fix an axis system x and z like this. This interface description is what I am calling it as eta. So, that is going to be a function of x and tan; that is what we are saying. That is this z, so z equal to 0; so this is distance. Basically, we are parametrically defining the interface as equation 17.

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The particle at the interface, so it would not vary with time; of course, it will vary with time, because that is the way wave is un-relative.

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Which one? No.

(()) (Conversation is not clear)

We have said df dt. This is basically we are following with the wave. So, this is the Eulerian description. So, if I follow with the wave then what happens? With respect to the observer, who is riding at this point; it will not see any change.

This is how you distinguish between Eulerian and Lagrangian description. When you are talking about a specific particle as such, then you are referring to Lagrangian description. But, if you all look positioning yourself at a particular station, then seeing what is happening to the whole fluid as such that is what you get as a Eulerian description.

What we are talking about, when we say df dt equal to 0, basically we are riding with the wave. So, if I am riding with the wave, I am not going to see any change with time.

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Which one?

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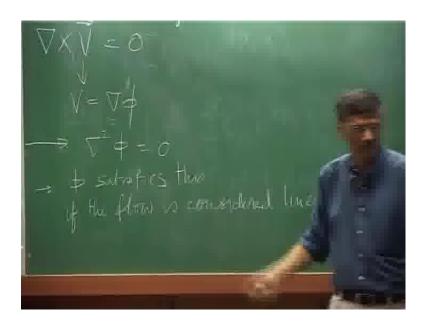
Surface Gravity Waves (cont.) Using (18) in (17a), we get $\frac{dE}{dt} + \nabla F \cdot \vec{V}_b = 0$ (19) If r denotes unit normal of the interface, then no-fluid through the interface requires: $(\vec{V} - \vec{V}_b) \cdot \vec{r} = 0$, where $\vec{r} = \nabla F/|\nabla F|$ and \vec{V} is the interface velocity. **s** Eqn. (19) simplifies to $\frac{\partial F}{\partial T} + \nabla F \cdot \vec{V} = 0$ (20)From (17), we get $\frac{\partial F}{\partial t} = \frac{\partial \eta}{\partial t} \& \nabla F = \eta_s t - \hat{k}$ where, η_{-} is the x-component of unit normal at the interface Eqn. (20) simplifies to $\frac{d\eta}{dt} + u\eta_0 - w = 0$ at $z = \eta$ (21)

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Because, this is all linearized analysis, you see your governing equation is a Navier-Stokes equation. From there, we have made an assumption that its flow is irrotational and we have also removed all the non-linearity. So, your equation - governing equation

was like this del dot v equal to 0, this was the continuity equation. Then we had written down v dot del of v equal to del p by rho plus gamma del square del. So, this is your equation - governing equation.

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Now, suppose I say the flow is irrotational, then what happens is I can say the velocity is 0; that means what? That means del cross V is equal to 0. So, this is your condition of irrotationality.

So, this will be 0 if I can write V is equal to gradient of a scalar. Then what happens to this equation? If I gave V is equal to grad phi that will give me this (Refer Slide Time: 23:10). If I linearized and substitute this, then you will see that this phi automatically satisfies this equation 2. So, this is an artifact of the assumption that we are making small amplitude disturbances, so we linearized the system. The moment I do that the governing equation instead of these two equations, simplifies to this; that is what we have done consistently. In all descriptions of surface gravity wave we have assumed it to be linearized.

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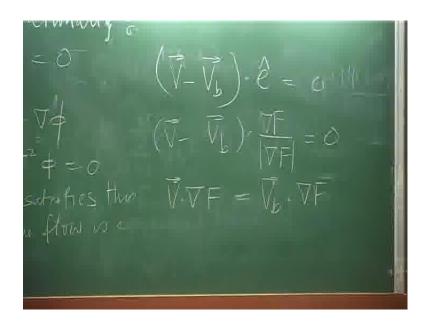
Yes

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How? You see here, V is equal to V b, so I have just simply replaced V b by V.

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On the interface they are same, not everywhere; that is what this boundary condition implies. See what I have done, you have to be careful here. What I have written here? At the interface, what is e? This is (Refer Slide Time: 25:00).

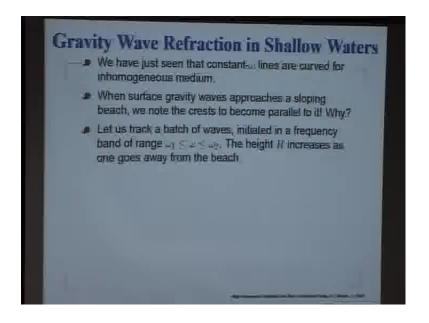
What happens is, of course, this can go away and it is the homogeneous. So, that would mean V dot grade F should be equal to V b dot grade F. I did not say V equal to V b; this is this vector product that is equal because of that boundary condition.

Any other questions

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Which one you are talking about?

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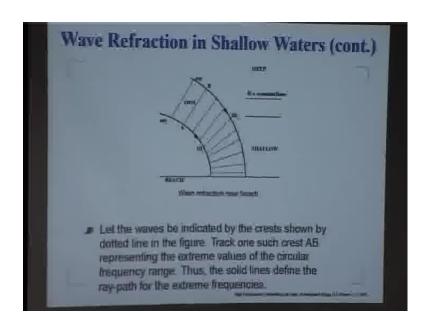


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Where we have talked about refraction?

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This example, how?

This is simple. You see what happens; you have the beach here and as you go across, the depth is increasing. So, if I now track a wave whose crest is given by this dotted line, then what happens? This end of the crest is at a deeper side compare to this. So, what happen? Because, it is on the deeper side, it will move at a faster speed.

If you look at the dispersion relation, then you can see omega by k will give you c. So, if omega is larger for this point compare to this point, c is larger for this point compare to this point. In a finite time, this may go from here to here. A shorter distance compare to a larger distance travelled by the point on the outside of the arc.

So, what happens? As time progresses, this points will outstrip in position due to this. So, what happens? Slowly this will start turning around. When you come close to the beach, of course, it has become very shallow and you will see that it has aligned itself perfectly parallel to the beach. Recall, we did discuss about the same thing, flow around an island. You would also see the same thing, the flow will always come towards island irrespective of whether you are looking at in the front side of the island or the backside of the island; the same phenomenon of wave refraction.

This comes about because of in homogeneity. See in optics we must have done it, where you have taken the density gradient causing the wave refraction. Here, what is happening? The height change is creating a change in the sea and that what is causing the crest to turn around, because of this, variable depth for a particular crest itself, one side is going at a smaller speed compared to the other and that turns it around.

Any questions from this side?

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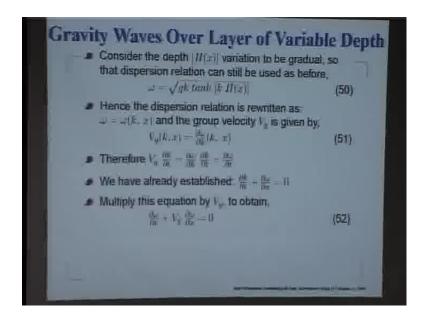
Yes

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Sure

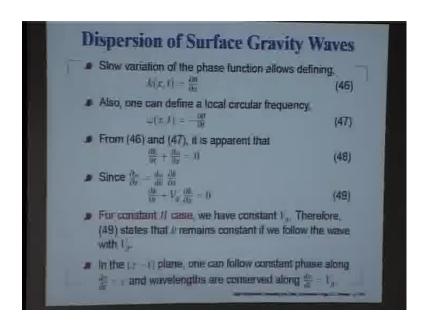
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Look at this. Well, I had it here. If I have h is constant, omega is this and then what will happen? I can calculate d omega by dk v g and that will remain constant.

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See what is happening, homogeneity is occurring, because h is changing with x and that is what is causing this thing to happen, but in the previous case where h is constant. You see the other possibility, what you are seeing there? For constant h case v g is constant. So, if you all looking at this scenario, if h are constant, omega is constant.

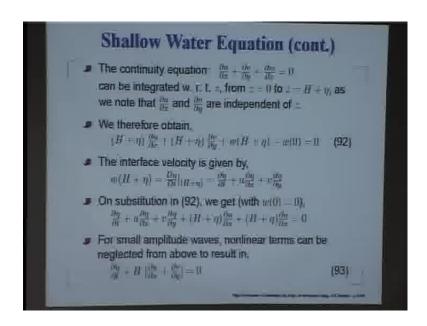
So, if I am tracking it k equal to constant line, then that corresponding c also will be constant. So c is constant, v g is constant, omega is constant and we are tracking k following this equation. This is that constant speed; that is what we are saying. If we want to look at the case for constant height, then what we would see, if we follow the wave, if we fix our gauge moving at a speed v g, we will be tracking a constant k.

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93 here, on this waves.

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Let us see, what we have there - Non-linear terms. So, non-linear terms are here, u del eta del x, v del eta del y, eta del u del x, eta del v del y. This is still wrong, I do not know why I have the old version; that is, your del v del y. So, all these product terms they are non-linear.

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Pardon

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Of course, it does so what we are analyzing here under the assumption of linearity. You do not need to make such assumption if you have enough resources and the methodologies. What we are trying to do is try to study a three dimensional flow field. As you can see here, it is a three dimensional flow field; we are making some small amplitude assumption that leads us this continuity equation to this equation. But, what is interesting as you have seen? Time and again we have seen, despite all these assumptions what we get as a solution; physically also we see that.

You recall that when we talk about that sinusoidal wave. You do see that happening in shallow water. Do you understand that all your questions are related to waves? I have created enough waves more of the thing, people say that in life never make - create waves that are disturbance, but starting a physical system we want to study the disturbances.

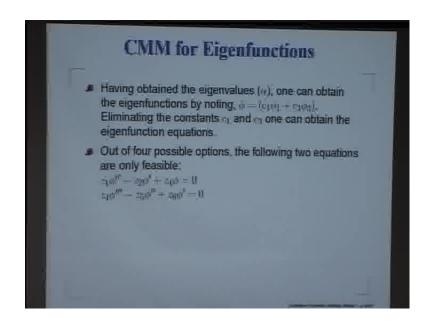
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Module 2 means ordinary differential equation what we had studied, let us try this.

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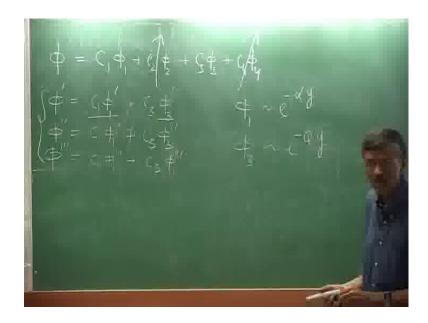
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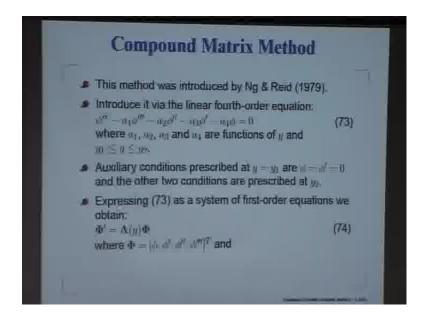
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I did not tell you. It is not very important, but since you asked I will explain. See what happened, we were looking at a fourth order system. We got the solution in terms of four fundamental modes. We wrote them as C 1 phi 1 plus C 2 phi 2 plus C 3 phi 3 plus C 4 phi 4.

What we noticed that this node along this node grows with height, so they are not physically admissible. So, we have this equation. We also have written down the governing equation phi; let me go to this generic form; look at 73.

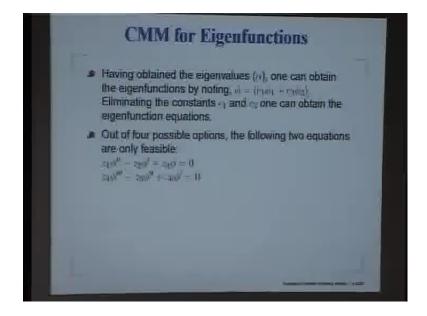
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So, that is what we do have; phi satisfying this differential equation. Now, what I could do is, I could write this phi prime equal to C 1 phi 1 prime plus C 3 phi 3 prime. Then, the same way, I could do the third derivative, I could write it like this.

Now, basically what we are trying to do is derive an equation for phi in terms of this compound matrix variable.

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What you need to do is this three equation plus 73, you have 4 equations. All you need to do is eliminate C 1 and C 3; two constants. So, we can do it in many possible ways, so that is what we get. We get actually four equations, out of those four equations I have written those two only, which are the correct ones; because, they satisfy the physical requirement the way we like it to be.

What you notice? Why they have to be like this? Because, this equation has two nodes phi 1 and phi 3, no wonder that we end up with an equation with second derivative, first derivative and the function.

So that you get those correct modes that you really are looking for. If you get those other two equations, you will see they will be of higher order, they will be third order equations.

What will happen? This equation that we have, we have seen its property. In phi 1 goes as e to the power minus alpha y and phi 3 for the example that we have discussed of this; the decay with height. What you find that this equation, I can put those values of z 1, z 2 and z 4 for y large and then I can get a constant coefficient o d. I can calculate the Eigen values, you will be satisfied that those two fundamental modes are recovered.

What about this third order equation? Well, it is fairly be simple, because here you see one of the modes is the neutral mode, it is e to the power 0. So, what happens is, it has a neutral mode plus these two modes. Whereas, those other two equations, which I did not write, they are going to be unstable and they are spurious.

Any questions on this topic, how are you getting on with your assignment? Have you seriously started looking at it, if you are not you might be surprised this Saturday.

No, no I am Joking.

There is nothing to be. This is a very simple material; since you do not have questions, I assume that all of you have comprehended it absolutely clearly.

Yes Varun, any questions?

I must confess that I do not know your entire name, whoever comes and meets me I get to know the person. I know some of you, but not all of you. If you do not have any questions on o d, shall we go to any other?

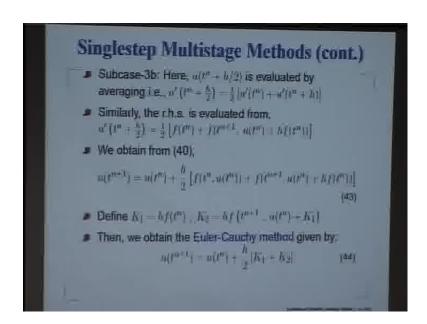
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Loudly I am short of hearing

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- (()) (Conversation is not clear)

Let us go over there and see. We were looking at second order methods not these.

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Yes,

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I do not get you completely.

(()) (Conversation is not clear)

Yes,

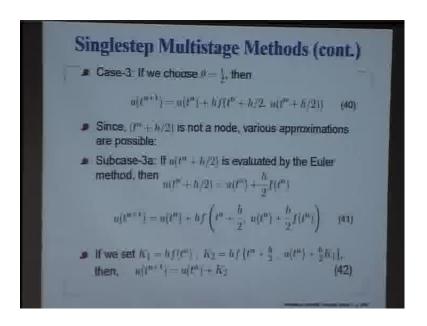
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Basically, you mean there is a typographic mistake, so there is a very strong possibility, because w 1, w 2 would be equal to half and half, so this h is wrong.

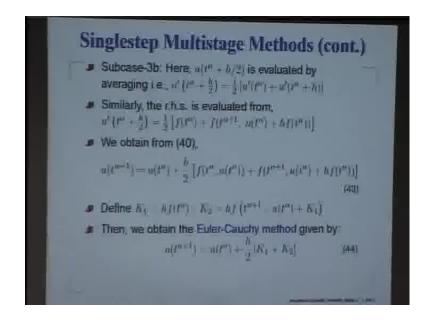
You are right.

Thank you

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Because, I think you can work it out from here and the solutions have been defined here, from 41. Then, we have set k 1 as this and k 2 as this, so this becomes simply equal to k 2 for this particular choice of theta equal to half. Next is, if we define - what are the possibilities of defining this? This is not a nodal point; this is a midway point. So, if I do it by averaging the values at t n and t n plus h, then we get this. Essentially, then what you are getting is this plus this into h into u prime, is in it? So, I suppose, this h should be there (Refer Slide Time: 40:53).

Now, what you are doing here is the quantity within the parentheses is this. So, k 1 and k 2 already has h, so we do not need an additional h outside. k 1, k 2 already has an h, so there is no problem. You can remove this h from this equation; it is indeed a typographic mistake.

Yes

(()) (Conversation is not clear)

Right

(()) (Conversation is not clear)

We did not do that.

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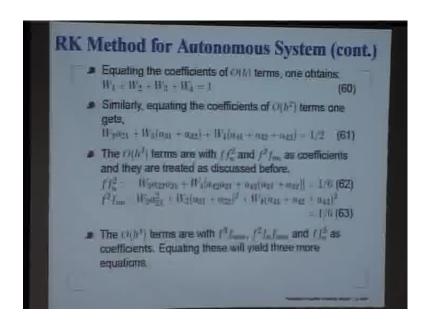
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Runge-Kutta Method for Autonomous System
     RK, method for the autonomous system: (in = fin)
         evaluates four slopes.
         K_1 = hf(u^\mu)
         R_2 = hf(u^n + u_{21}K_1)
                                                                   (58b)
         K_1 = hf(u^n + a_{31}K_1 + a_{32}K_2)
                                                                    (58c)
         K_1 = hf(u^n + a_{11}K_1 + a_{22}K_2 + a_{23}K_3)
                                                                   (58d)
         and u^{\mu\nu\lambda} = u^{\mu} + W_1K_1 + W_2K_2 + W_1K_3 + W_1K_4
                                                                   (58e)

These slopes are expanded next as:

          1 = \frac{K}{\hbar} = f(u^m) = a_{21}K_1f_0 + \frac{\log K(t^2)}{2}f_{00} + \frac{\log K(t^2)}{2}f_{000}
         K_2 = hf + h^2 a_{21} f f_0 + \frac{h}{2} a_{12}^{-2} f^2 f_{mn} + \frac{h}{4} a_{21}^{-1} f^{4} f_{mnn} (59)
         K_1 = hf + h^2(n_{11} + n_{32})ff_m + h^2(n_{21}n_{22})ff_m^2 +
                (un = un)2 [ Jm./2] = b1 ==== [2] Julian =
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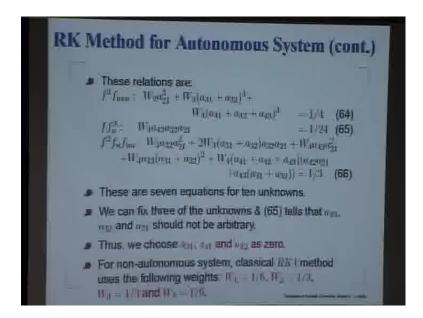


Let me make a confession. The confession is following; that it is too unwieldy. We have seen that when we went to RK 4 method, we restricted our self to an autonomous system. I just purposely removed time event to make things simpler. Despite that you have seen the type of complexity we ended up with. What happened was we ended up with seven equations and that is what we have written here.

So, this you get from equating the term of order h. Then, h square gives you this equation - single equation. Order h cube has two sets of terms, the coefficients of f u square and f

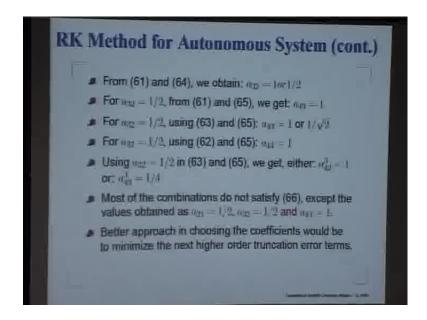
square f u u, so that gave us two equations. Then, when we went to h 4 terms we will have terms appearing with three combinations of functions depended on f. So this is one, the second and the third; this will give you another three.

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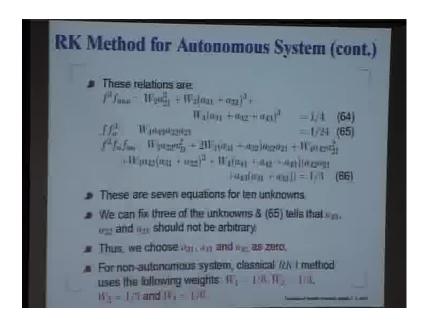
We have three from here, two from here and 1 plus 1; so those are seven equations. How many unknowns we have? We have ten, because we have this 4 weights w 1 to w 4 and all those coefficients a 2 1, a 3 1, a 3 2, then a 4 1, a 4 2 and a 4 3.

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How do we fix it, is that your question? The logical way, as I have said it is here. You look at the next higher order term, so that will be of h 5. You can see that you would have many more terms appearing there and that truncation error term has to be minimized by the choice.

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Numberless we have ten unknowns and seven equations. So, we have the freedom of choosing any three arbitrarily that is what we have done. In doing so, you need to be careful. One of the easiest ways of arbitrarily choosing this constant is set them equal to 0 that will simplify your calculations. But, I have warned you that please do not do this three, because they appear explicitly here. I do not want to violate any governing equation that is why I said that we do not choose a 4 3, a 3 2 or a 2 1 as 0; instead, whatever left of other three, we set it equal to 0 and that should minimize our calculations.

So, then you have the close system; seven equations, seven unknowns you can solve it. But, this still does not minimize your error; a better approach would still be what we noted like what we did for RK 2.

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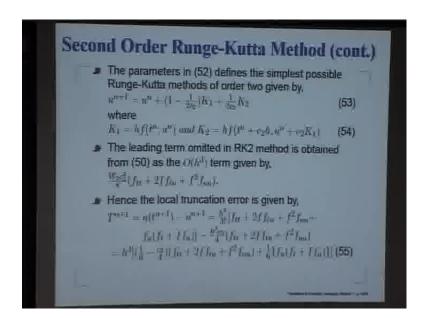
You are talking about error; error will appear in the next higher order, so that you will have to write order h 5 equations. There you would get many more equations; those

equations may make your system over determined. We already have seven equations. So, now if I write for order h 5, which you can try and do it. You will see probably, you will get another four or five equations in terms of all these ten unknowns. Now, then you have an over determined system, so you lose this.

What actually happen, I have looked at some of the texts. There are books written on Runge-Kutta method alone and I tried to consult one such expert. I said, look how did you get all these weights? In fact, in most of the books that I have given you as a reference, you will notice that instead of seven equations they talk about eight equations; that itself is a bit of a mystery. How they could generate an extra equation?

I am still waiting for that person to reply to me for last three months; apparently he is on summer vacation. May be next month he will come back and we will get to hear from him. But, there seems to be some conceptual problem there, because I do not see how you can get more than seven equations. You are absolutely right; the wave we did with RK 2 is the correct way of doing it.

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We looked at the truncation error term and then we said this part we can do much, because this depends on the problem definition that definition is determined by the f function. But, in this part we can play around by minimizing this part of the error that is what guided us in choosing c 2 equal to two-thirds.

You can do a similar thing, but I am not very sure that what we would get. It would be, take some, doing look at looking at it exactly, I have not done it, I must confess, but you can try and come back and tell rest of us what is the situation, when I write let us say the h 5 error term.

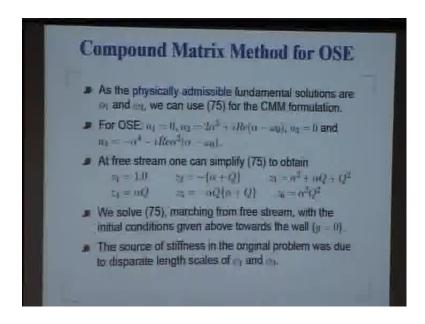
See here, it was simple, here only thing that came about is terms of c 2 and that helped us in freezing one of the constant that close the system. So, we are virtually coming to an end. If you do not have questions on any other topic we should be calling you today.

Monish any questions? I am seeing you frantically turning pages over pages.

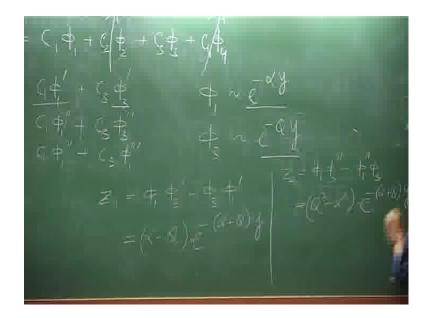
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In this; slide 60, is it

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How do we get this? This one's, if you recall Z 1 as this value, if I take phi, so we are looking at what is happening for large y; that is what the free stream means. So, y going to infinity, phi 1 looks like this, phi 3 looks like this. So, I can substitute this, what I get is, from here I will get alpha minus Q e to the power minus alpha plus Q into y, so that is Z 1. What about Z 2?

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Pardon

(()) (Conversation is not clear)

Hold on

Let me work it out. So, if I do it like this, I am going to get Q square minus alpha square e to the power minus alpha plus Q into y. Now, if you look at your governing equation they are homogeneous in Z. I have Z prime on the left hand side and right hand side I have terms only of Z and no constant additive term. What I could do is I could scale out a constant parameter. If I divide everything by this quantity then of course, Z 1 will become 1. As you can see, I show you that Z 2 will be this and same way you can work out the rest of them.

Didn't I do it on the blackboard? No, I did right? You missed.

Vijay, no questions, I am not asking you Jagmohan, because you have missed so many classes. I think there will be many questions for you that you will have to work yourself.

Shall we then stop here? Ok.