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Module No. # 03 Template for the numerical solution of the generic scalar transport equation Lecture No. # 14 Topics Consistency and stability analysis of the unsteady diffusion equation Analysis for two -and three-dimensional cases

Stability of implicit schemes

The application of the Von Neumann stability analysis for the linear wave equation has shown us that we can determine the conditions of stability of a particular discretization scheme using the Von Neumann method.

If you are assuming a periodic boundary condition, and it has shown us, that, that ,typical kind of discretization schemes that we have, can have conditional stability or unconditional instability and that depends very much on the parameters, that, that are part of the equation itself.

Now, we will, before we go on to the generic scalar transport equation, we will try to use the same method to investigate the second part of the scalar transport equation. We have seen the hyperbolic nature reflected in the linear wave equation, in which, we could see that there is an expected movement with respect to time in a particular direction of the wave and that is the characteristic of the advection term or the hyperbolic nature of the equation, but we also have the diffusive nature of the equation that comes from the diffusion term on the right hand side of the of the equation.

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So, let us try to see the simple case of diffusion and one-dimensional diffusion with a constant diffusibility. So, we are considering the case - dou phi by dou t equal to d dou square phi by dou x square as the one dimensional unsteady diffusion equation and it can be a transient conduction equation for example and this can also be equivalent to the stokes first problem of infinite plate moving at a constant speed, suddenly set in to motion at constant speed, and it can be a mass transfer problem.

So, this kind of situation may arise and this is 1 half of the of the generic scalar transport equation, and let us see what are Von Neumann stability analysis says for a straight forward discretization of this equation.

When we say straightforward, when we have a first derivative in time, we normally prefer to have phi i n plus 1 minus phi i n by delta t; that is the forward in time, because we have the initial condition, so that is at n equal to 1, this known, and we want to get the value at n plus 1. So, this is the most straightforward discretization of the time dependent term, and here, we have, we can use central scheme which gives us a second order accuracy, so, phi i plus 1 n minus 2 phi i plus phi i minus 1. We evaluate everything at n making this an explicit scheme and this is divided by delta x square, and we know that this is first order accurate in time and second order accurate in space.

So, this is a straightforward FTCS discretization of the transient diffusion equation and which is first order in accurate in time and second order accurate in space, although this is accurate in the first order only in time. If you are looking at a steady state solution to this, then the first order accuracy does not matter and this gives us an a method of finding the steady state distribution of phi over x. So, in that case also it is to use a first order accurate time scheme.

But if you are interested in something like that or even if you are interested, in a, in a time transient, then we have to make sure that this scheme is stable. So, we can apply the Von Neumann stability method with it is limitation that we are considering only periodic boundary conditions, and of course, we have a linear equation here, so that is not that much of problem.

So, if we do this, then as we have described earlier, we have an exact equation and a numerical solution and we have, let us put this as D, and we have an exact solution to the discretized equation D_i i d i n and we have a computed solution N i n and the computed solution has the exact solution plus an error .We substitute this into this and we note that the exact solution d satisfies the discretized equation exactly and what will be left out is the error propagation equation, so, which will be error at n plus 1 divided minus error at n divided by delta t at ith space step is equal to d error at i plus 1 n minus 2 error at n error at i error at i minus 1 divided by delta x square.

So, this is the error propagation equation and we can as usual assume that error is distributed as an error at a particular time step is the spatial distribution is expressed in terms of Fourier series terms, Fourier series expansion and given the assumption of periodic boundary condition. We have finite number of these terms and we look at the evolution or the variation of the mth component of the Fourier series expansion from as the solution goes from n to n plus 1.

So, we are looking at an error of the form a n delta t j k m i delta x. So, the error at i n is expressed in terms like this. It should be i plus 1 delta x or i delta x, does not matter so very much.

So, this is the form that we are looking at for the error at nth time step and error at n plus 1 time step at the same location is therefore given as e a n plus 1 delta t e j k m i delta x, and if you were to compute from this the amplification factor which is the error at n plus 1 time step divided by error nth time step, this will be equal to exponential of a delta t, and therefore, the argument goes that if a turns out to be positive, then we have an increase in the, we can have the error increasing. In general, G is a complex number; therefore, we have to look at the magnitude of G, and therefore, determine whether it increases or not.

So, we make these substitutions here and then try to get an expression for the magnification factor. So, we can substitute this here, and since we have already done this, we, what we will be looking at is this whole thing with these substitution divided by e a n delta t exponential j k m i delta x.

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This is what we have done earlier for the wave equation. We follow the same procedure and we know that this gives us exponential of a delta t after we divide by this, and this is nothing but epsilon i n; so, this is equal to 1, and here, this is the nth time step; so, this 1 cancels out; we have i plus one th space step. So, we will have one of this thing here - so, that is j k m delta x here it is just epsilon i n; so, this when divided by epsilon i n, this will be 1; so, minus 2, and here, we have i minus 1 times delta x here; so, that will give us exponential of minus j k m delta x divided by delta x square. So, this is the error equation and this is the magnification factor. So, we have g equal to this 1 goes on to the other side 1 plus the diffusibility times delta t by delta x square minus j k m delta x minus 2.

So, this is the magnification factor, and to help us with further manipulations, we put this whole thing as some beta here or let us call this as alpha, and this particular thing as phi; which is what we have been using earlier. Therefore, we can write this as and we also know that cosine phi is defined as by 2. Therefore, we see this as two times cosine phi minus 1.

So, we can write this g as 1 plus alpha times, 2 alpha times, and we notice that D is positive. So, this alpha here is always a positive quantity. We can just write this as, so, G is expressed in terms of this; so, that is equal to 1 minus 2 alpha times 1 minus cosine phi; just recognizing this 1 minus cosine phi is less than 1, and we can also write this as, we have sin square phi by 2 is equal to 1 minus cosine phi by 2.

So, we will have 1 minus cosine phi by 2 is 2 sin square phi by 2. So, that 2 and this 2 will go to 4. So, this is 1 minus 4 sin square phi by, sorry, sin square phi by 2. Now, the condition for stability is that modulus of G must be less than or equal to 1. So, we can consider this 1 minus 4, we have an alpha here, 4 alpha sin square alpha by phi by 2 must be less than or equal to 1.

We can immediately see that it is not always, this is not always satisfied for all values of alpha. For example, if alpha is 100, then definitely I can find some value of sin phi, for which, this value is going to be the magnitude is going to be greater than 1. So that this fact imposes readily an upper limit on the value of alpha, because let us say that sin phi by 2 is half; so, this is square of that is 1 quarter 1 quarter by 4 is 1. So, this becomes 1 minus alpha. So, if alpha is 3, then the absolute value of this will be 2 and it is not equal to 1.

So, the condition when we put it here in this way means that this condition is not satisfied for all values of alpha. So, that means that we have only conditional stability, so, it is not going to happen for all cases and we can find out what, for what, what should be the maximum value of alpha for which will have stability. We can consider two cases - when this is positive quantity and when this is negative quantity. So, if 1 minus 4 alpha sin square phi by 2 is greater than 0, so that is positive. So, that is possible only when you have very small values of alpha, so then, you have no problem, if, because this is alpha is positive and sin square is also positive.

So, if this is positive, then alpha is so small that this is less than 1. So, we do not have any problem, but if 1 minus 4 alpha sin square phi by 2 is less than 0. For example, this term is 100 and this term is 1.

So, this is minus 99. So, that is the case that we are considering here. Then in this particular case, we need to make sure that 1 minus 4 alpha, must be less than, must be greater than minus 1; that means that 4 alpha sin square phi by 2 is less than or equal to 2. We take this here and then cancel out negatives, then it becomes, the greater than becomes less than, and this implies because sin phi by 2 has a maximum value of 1 when phi is equal to pi. This means that alpha here must be less than or equal to two by 4 or less than or equal to half.

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So, the condition for stability of this particular scheme is that alpha which is the diffusibility times delta t by delta x square must be less than or equal to half. So, this shows that if delta t is too large, then we will not have stability making use of this particular scheme.

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So, in that sense, this is only conditionally stable, and what is the term that we are considering here? We are considering unsteady diffusion term. So, we have stability problem not only with wavelength transport which is the linear wave equation, which is the advective term of the generic scalar transport equation. Even the diffused term which is directionless, that is, which is in this particular case with constant diffusibility, we are looking at isotropic diffusibility. The diffusibility, which is same in which is going in all directions at effectively the same diffusibility factor here. Even under isotropic diffusion, directionless diffusion, we may have stability problems.

So, when we talk about the numerical solution of a governing equation, we can expect stability problem either from the linear wave equation the advection part or the diffusion part. So, we have to consider both of them together. Sometimes they counteract and then sometimes they abate each other and so on.

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So, we have to do a stability analysis for the entire thing, but before we leave this particular diffusion, - unsteady diffusion term - let us look at the Dufort Frankel scheme which we sighted as an example of inconsistent discretization, and at that time, we also said that it is unconditionally stable even though it is an explicit scheme.

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So, let us just see what it was. So, in that particular Dufort Frankel modification of this FTCS scheme here, we made the approximation that this term here is written as phi i n plus 1 plus phi i n minus 1 by 2. So, this two will cancel out and we will have an equation which is phi i n plus 1 minus phi i n by delta t equal to d phi i plus 1 n and then we have plus phi; this is minus phi i n plus 1 plus phi i n minus 1 plus phi i minus 1 n which is what we have originally here divided by delta x square.

So, we have a discretization form of this, discretized form of this, and we can go through the same process of writing down the error equation and making these kind of substitutions and looking at the mth component of the of the error, and then, finally, we can find the magnification factor, amplification factor, and for the specific case of, for the case of Dufort Frankel scheme, we can show that the amplification factor G is given by 2 alpha cosine beta plus or minus square root of 1 minus 4 alpha square sin phi 1 plus 2 alpha.

So, this is amplification factor for the Dufort Frankel method for the same equation, for the same unsteady diffusion equation, and here, alpha is the same as what we have, that is, d delta t by 2 delta x square and phi is our k k m times delta x which takes values from 0 to pi.

So, are they conditions, in which, this can be greater than 1. If this is, if so, then it will be unstable. Are they conditions, in which, it will be less than 1 less than or equal to 1, then it will be stable.

So, we can investigate the stability of this. We can do it formally but we can also look at the specific form here, and we know that sin phi and cosine phi vary between minus 1 and plus 1, and from that we can just argue it out instead of, looking at, looking at formally. For example, we can consider the case where this term is predominant or first of all this term is very small compared to one, so, in such a case, alpha is very small so that this term will have only 1 here when this is equal to 0. So, you will have 1 plus 2 alpha times cosine phi divided by 1 plus 2 alpha more or less

So, in which case, we know that cos alpha is between minus 1 in the plus 1; so, that means that this is 1 plus 2 alpha times cosine phi over 1 plus alpha will be less than or equal to 1 at most. When cosine phi is equal to 0, then it will be plus 1 and especially because your alpha is very small compared to this.

When this term is, such that, this is predominant and this one is very small compared to this particular one. We have minus 4 alpha square sin phi and you can say that it has a maximum value of minus 4 alpha square. So, that becomes cosine phi, we have, yes, and two alpha here will come here, and so, even then we can show that this whole thing numerator has a value of two alpha, and here, 1 is very small compared to the 2 alpha because that is what $(())$ and we can say that this is always going to be less than or equal to 1.

We can do a formal analysis but we can show from those kind of arguments. We can see that the amplification factor is always less than or equal to 1 for all values of alpha and for phi varying between 0 and phi.

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So, this means that this is unconditionally stable which is very rare, and this unconditional stability is achieved by making a small change to the way that this particular term is evaluated and this evaluation is second order accurate, and therefore, it does not affect the overall accuracy of the scheme, but in the process, we have lost out on the consistency aspect.

So, we can see that using this particular way of dealing with the analysis, with the error analysis, stability analysis of a given discretization scheme. The Von Neumann method can give conditional stability or unconditional stability or unconditional un stability instability of a particular scheme as appropriate provided we have a linear equation with periodic boundary conditions.

Before we leave this particular analysis, let us just look at make it slightly more complicated and look at the case where we have not one dimension but we have two dimensions. So, we will looking at the case where we have dou phi by dou t is equal to alpha the diffusibility times dou square phi by dou x square plus dou square phi by dou y square. So, this is a two dimensional unsteady diffusion equation. So, compared to the this case, we are adding one more dimension. We note that in the general case, we will have three dimensions and this so that this is nothing unusual as for as the problems that we are dealing with are concerned.

So, we can see that the phi in this particular case will be a function of x y and t, and when upon discretization, we have phi given in terms of i j and n. Although we have, we would like to have from this phi as a function of $x \, y \, t$, in a c f d solution, we give only at discrete points i j and n; i and j representing the x and y directions, and n representing the time directional discretization, and we, therefore write this as phi i comma j as a subscript and n as a superscript. So, using that notation, we can again use the same f t c s scheme as what we have used here. Therefore, we can write this as phi i comma j n plus 1 minus phi comma j n divided by delta t equal to d times phi i plus 1 j n minus 2 phi i j n plus phi i minus j n divided by delta x square plus d times phi i comma j plus 1 n minus 2 phi i comma j plus phi i j minus 1 n divided by delta y square.

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So, this is the FTCS discretization of the two-dimensional form of the wave equation. With this discretization, we can go through the same procedure. We can look at numerical solution as the sum of an exact solution of the discretized equation plus an error. Except in this case, we do not have n i n but we have n i j n d i j n and epsilon i j n, and substituting this into the discretized equation, we will get an error equation and we can seek a solution for the error equation which is expressed in terms of a finite number of Fourier components. Assuming that we have periodicity in both x and y directions, and from that, we can get an error equation and then we can evaluate it. So, let us do that.

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Substituting the relevant, the exact discretized solution and the numerical solution and the error, we can arrive at that corresponding error propagation equation corresponding to the f t c s explicit discretization of the two-dimensional transient diffusion equation like this. Error at i j n plus 1 minus error at i j n, we can take the delta t on to that side, is equal to d delta t by delta x square of error at i plus 1 j n minus error at i j n minus 2 error at i j n plus error i minus 1 j n plus D delta t by delta y square of error at i j plus 1 n minus 2 error at i j n plus error at i j minus 1 n.

We can, as before, we can call this as, we have last time called it as alpha, because now we have x and y, we can call this as alpha x and alpha y here, and at this point, we seek the error at i j at nth times to be expressed as error component varying with times n j k m x i delta x j k m y j delta y, and we have to do something about this k here.

So, let us just keep in mind that this j and this j are different and we can write this whole thing as phi x and this whole thing as phi subscript y and immediately get rid of the confusion between this j which is square root of minus 1 and this j which is the space index, and we substitute this into this and divide the each term by this in order to get the magnification factor, and we note that epsilon i j n plus 1 divided by this is nothing but the amplification factor. So, we can write G minus 1 equal to alpha x times we have j phi x plus exponential of minus j phi x minus 2. That is what we get from this, and then, here, we have plus alpha y here; we have j phi y plus j minus phi y minus 2.

So, this part is similar to the case of one-dimensional part. Except that, we now have a term coming from alpha x and another term coming from alpha y. So, G the amplification factor is equal to 1 plus this whole thing, and just as before we can express, this as, this in terms of cosine functions of phi and then again in terms of sin square phi by 2 and this also in the same way as cosine phi y and then into sin square phi y by 2, and then come up with the thing that G is equal to 1 minus 4 alpha x sin square phi x by 2 minus 4 alpha y sin square phi y by 2 .

Now, for stability, this G must be less than or equal to 1; so, that means that this whole thing minus 4 alpha x sin square phi x by 2 minus 4 alpha y sin square phi y by 2 must be less than or equal to 1.

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Following a similar kind of argument like what we had, taking this whole thing as negative and positive. We can show that in this particular case, alpha delta t times 1 minus delta x square plus 1 by 1 by delta y square must be less than or equal to half. So, the condition for stability for a two-dimensional case is like, this and the same thing for a one-dimensional case was alpha delta t by delta x square is less than or equal to half. So, this one is for a 1 d case and this is for a two dimensional case.

What we see from this is that as you go from one dimensional case to the two dimensional case, the same scheme has got conditional stability but the delta t that is allowed is now less than what it was in the one dimensional case. Here, for example, if you say that delta t is half of, so that means that delta t must be less than or equal to delta x square by 2 alpha here, and in the case of 2 d, delta t must be less than or equal to, so we have to take it there, so this is 1 by 2 alpha times.

So, here, for the delta t 2 d, this is the condition, and if you, for example, took that delta x is equal to delta y, then, then this would imply that this should be this, then this cancels out and we will be left with 2 here. So, if delta x is equal to delta y, then delta 2 d implies this is 1 by less than 1 by 4 alpha, because you have two coming here. So that this delta t 1 d is less than delta t 1 d, and if you have three-dimensional case, the same thing $(()$ three-dimensional case will mean that delta t three-dimensional is more less than is less than delta t 1 d which is less than delta t 1 d.

For this particular simple case and what this shows is that this may not be very generally applicable and to what extent this is less will also depend on, for example the delta x and delta y, and we have also assumed, for example that alpha is the same in all directions, so this is isotropic; otherwise, we will have a different condition. So, it is more complicated when in a realistic case, but what we can see is as you go from one dimension to two dimensions, three dimensions, that the stability condition is no longer the same; it now changes. So, one has to do the stability analysis for that particular case also and see under what conditions we get stability.

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So, in this way, this particular method is applicable for any type of discretization scheme, and what we have seen is extension to two dimensions. We can also look at multistep methods and we can look at coupled equations and although we have not looked at the effect of boundary conditions. If one needs to put boundary conditions, then one needs to look at matrix type of method of stability analysis. So, those kind of complexities can also be considered, and in that sense, this method is able to detect stability.

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So, but what we have seen so far is only that we have conditional stability or instability. Now, can we improved upon the stability? Can we make, can we make this better than, can we have a higher time step? Because there is nothing that tells us, this analysis tells us beyond the fact that it is condition is stable. Other any schemes that are unconditionally stable. So, we have seen that cases like Dufort Frankel are unconditionally stable, but they are very rare and there is also we have a problem with consistency.

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So, in that sense, we are limited in progressing in that direction, but we have another possibility that instead of evaluating the right hand side in an explicit way, instead of doing it as an FTCS explicit, suppose we make the evaluation implicit, then what would happen? So, if we had implicit discretization, then what can we say about the stability?

One of the things we know about implicit method is that implicit method is more complicated to solve than the explicit method. So, that is why we would like to have an explicit method, but most explicit methods suffer from either from total un instability or only conditional stability. So, if we can achieve unconditional stability or if you can get a relaxed more relaxed condition on the delta t, then an implicit discretization would be desirable because it would allow us to have larger time steps, and so, for that we can forgive the extra computation that is necessary to get the implicit solution at every time step.

So, if the delta t limitation in an implicit method is a relaxed wherever we can have larger time steps. Then even an implicit method which requires more computations for solution at a particular time step. Even that kind of solution method may become more advantageous than an explicit method.

So, how can we, how can we look at the stability of the implicit method? Can we use this? And the obvious answer is yes, it can be used and it can be done in exactly the same way and the results are also very surprising in the sense that the methods which have proved unconditionally unstable can also become stable if we make them implicit.

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So, let us just look at one specific case as an example and the rest will be given left as an exercise for the reader or the listener or the viewer to evaluate. So, let us go back to the simple equation. So, this is our linear convection equation and we can write in FTCS explicit form as phi i n plus 1 minus phi i n by delta t plus u times phi i plus 1 n minus phi i minus 1 n by 2 delta x is equal to 0. Using the Von Neumann method, we can write down the error equation and then we can go through the derivation, and we can show that the amplification factor in this particular case is 1 minus 1 minus j sigma phi j is as usual square root minus 1, and therefore, we can consider this G star which is 1 plus j sigma phi and we can get the square of the amplitude factor, square of the magnification factor as G G star.

So, this is 1 minus j square sigma square phi square, and since j square is minus 1, so this equal to 1 plus sigma square phi square. So, this is for FTCS explicit and we can see that for any value, any non-zero value of sigma and sigma has to be anywhere positive. We can see that this is greater than magnitude is greater than 1, and therefore, this is unconditionally unstable. Now, let us see what we get if we make this explicit.

So, we can consider FTCS implicit form, in which case, we can write this as phi i n plus 1 minus phi i n by delta t plus u times phi i plus 1 n plus 1 because you want to evaluate this derivative at n plus 1 time step. Which is what you mean by implicit two delta x is equal to 0.

So, we can write down the error equation as delta t plus u by 2 delta x error at i plus 1 n plus 1 minus error at i minus 1 n plus 1 equal to 0, and we substitute as usual the error at i n varies as, e a delta t, e a n delta t j k delta x i and we consider the mth component here and then we substitute that we get n plus 1 divided by n we divide the whole thing by epsilon i n so that this gives us G G minus 1 by delta t plus u by 2 delta x. Here we have G coming from this n plus 1, and we will have i plus 1 here, so that gives us e j k m delta x minus, again we have n plus 1, so we have G times exponential of minus j k m delta x equal to 0. So, we can write down from this that g is equal to we take it to this side 1 minus u sigma u delta t by delta x is the courant number and we take the G out and e j phi minus e j.

So, we can write like this and we can show that g is 1 by 1 plus j sigma phi, and this, because of this, this is modulus of G is always less than or equal to 1. So, this means that this is unconditionally stable. Therefore, by going from just FTCS explicit to implicit, the scheme which is unconditionally unstable has become unconditionally stable.

And in this way, we can make we can improve upon the stability of a particular scheme without compromising on the accuracy or the consistency of that particular scheme.

But we have to see whether a stable solution is going to acceptable. Just as we have seen that a consistent scheme may not be sufficient for accuracy like FTFS and FTCS were both consistent but we did not get an acceptable solution. We will also, it may also be that purely stable scheme, may not be proper, may not give us a proper solution. So, we, before we go on to the discretization of the generic scalar transport equation using either an explicit method or implicit method finding out all the stability and all that. We have to consider what we mean by stability here and we have to look into the physical interpretation of this, and on the basis of that, we have to go forward and try to come up with a template for the generic scalar transport equation which gives us ultimately a satisfactory solution.

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We have now looked at consistency and stability. We will finally look at the interpretation of stability so as to come up with and link it with the well posedness of the problem, and finally, therefore, come up with a solution method.