Computational Fluid Dynamics Prof. Sreenivas Jayanti Department of Chemical Engineering Indian Institute of Technology, Madras Module No. # 03

Template for the numerical solution of the generic scalar transport equation Lecture No. # 10 Topics One sided high order accurate approximations Explicit and implicit formulations for the time derivatives

Before, we move on to the time derivatives, let us just write down second order accurate and higher order accurate derivatives. Not only for the first derivative, which we have already done, but also for the second derivative, which appears as a diffusion term.

So, let us just write these down. I will not, we will not derive this. But we will leave it as an exercise for the interested students .What we have discussed so far, will enable the interested student to derive this formulas.

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Second derivative , with respect to x at point i.It can be written using forward differencing as 1 by delta x square, 2 phi i ,minus 5 phi i plus 1, plus 4 phi i plus 2, minus phi i plus 3, plus 11 by 12, delta x square ,fourth derivative of 5 with respect to x at i .So ,this is an approximation .For the second derivative with respect to x at point I,

represented as a forward differencing. That is why, we have point i, i plus 1, i plus 2, i plus 3, appearing in this. This is a second derivative.

So, according to our conversion, p is equal to 2. We have a second order accurate value. So q is equal to 2. We have one sided differencing. So the number of points ,that are required ,are 2 plus 2 4, and we have 4 points, i plus 1, i plus 2, i plus 3 .And ,we could also see that the negatives and the positive coefficients , they cancel out each other .They have minus 1, minus 5 ,minus 1, that is minus 6 plus 2 plus 4 ,so it is plus 6. They cancel out, and what we also see here is the leading term in the truncated series ,and this defines the order of accuracy of the approximation .We can get ,what this leading term is ,by expanding each of these terms around point i .In terms of Taylor series expansion , we have to expand at least up to the fourth derivative .We have to return, in terms up to fourth derivatives ,and then multiply this expansion by 4, and this expansion by minus 5, this by minus 1 ,and put everything together . When we do that, we will be able to recover this. We will not derive this, in the class, but ,I leave it as an exercise, for the interested student .

So, this is a forward differencing formula. We can also write ,a backward differencing formula ,which looks very similar to this .Plus four i minus 2, minus i minus 3 ,and then leading error is, minus 11 by 12 delta x square. And here it is , plus 11 by 12 delta x square .This does not make ,any more accurate then this scheme, because both are nominally second order accurate terms . We expect that the contribution of this term will be small, when we have small delta x.

So, this is a backward differencing formula. Both of these, are for second derivative and for good measure, we can also write an approximation, which is fourth order accurate. Just to see what kind of structure, it has, we can write it like this. Plus 16 phi i plus 1, minus 30 phi I, plus 16 phi i minus 1, minus phi i minus 2, plus delta x to the power 4 by 90. This sixth derivative of phi, with respect to x evaluated at i.

So, this is we can see it is a fourth order approximation, because the leading term in the truncated series, is multiplied by delta x raise to the power 4. We can also see, that, we are evaluating the second derivate at point i . In order to do this, we have used points on, i minus 1 ,and i plus 1 ,and i plus 2 ,and i minus 2 .So, this is a central differencing formula ,which is fourth order accurate. So, that means that order of accuracy q, is equal

to four and second derivative. So, that is the number of points, required for a central differencing ,will be p plus q minus 1 that is 5, and we can see the 5 points, i plus 2, i plus 1, i, i minus 1, and i minus 2.

We can also check the coefficients, minus 30, minus 1 ,minus 1. So, that is minus 32 plus ,16 plus 16, plus 32 ,so again ,they cancel out .What we notice is ,that as we go to higher order accuracy, the size of the molecule increases. So in this particular case ,we are looking at i here ,i plus 1, i plus 2, i minus 1, and i minus 2. So ,instead of having just 3 points ,for a second order central differencing, we, now have 5 points ,for a fourth order central differencing. We can add 2 more points on either side .And, we can derive a sixth order accurate central differencing the coefficients, for which will be increasing in terms of magnitude.

When we are dealing with stream function velocity approach, sometimes we have to find approximations for a third derivative .And, we are dealing with Biharmonic equations, for example, something like creeping flow over a sphere. In such kind of conditions, we will have to deal with fourth order functions, fourth order derivatives.

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So, let us just for the sake of completeness, let us write down a second order accurate formula. For the third derivative using central differencing ,minus 3 i plus 2,this is a first order accuracy. That is why, we have for a third derivative and 4 points means, that we can only get first order accuracy. If you want to go for fourth order accuracy, we need to

put one more point. So that is why ,instead of ,i plus 3, we also have i plus 4 ,plus 14 i plus 3, minus 24 i plus 2 ,plus 18 phi, i plus 1 ,minus 5 phi i ,plus 21 by 12 delta x square fifth derivative, with respect to x at i.

So, this implies a second order accuracy. For a third derivative, involving 5 points in the forward differencing, and in a backward differencing. It looks very similar phi .In this case, each coefficient is multiplied by 5 by minus 1. So this is, 5 phi i ,minus 18 i minus 1 ,24 i minus 2 ,minus 14 i minus 3 and, 3 i minus 4 with resulting accuracy like this.

And ,we can similarly write down a central differencing, minus 1 fourth delta x square .So this is a central differencing .Central differencing ,backward differencing and forward differencing ,each of second order accuracy, for a third derivative. Similarly ,we can write for any derivative .We can write finite difference approximation ,of given order of accuracy .By involving sufficient number of consecutive neighboring points, either on one side or on both the sides, and using forward differencing and backward differencing ,we can take account of the boundary points. Using central differencing, we can approximate for all the interior points, so that we can maintain using these kind of formulas uniform order. This must be delta x square .Here uniform order of discretization, or finite difference approximation, for a particular derivative throughout the fluid domain.

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So ,this enables us to take any derivative ,and then write a corresponding finite difference approximation .Thereby ,taking each derivative, that appears in the governing equation, and substituting with the corresponding expression, we will be able to convert ,a given partial differential equation ,at a particular point, i j , or i j k ,into a corresponding finite difference approximation, involving the values of the particular variable, at the grid notes at which we want to find out the values.

So, in that sense we will be able to convert using systematically, this finite difference approximations, at a given partial deferential equation ,at a particular point into an algebraic equation. So, we can do this, and we can do this even for a time derivative, even for a time derivative .When the time derivative occurs by itself, then it is no difference from any space derivative, that you have considered .

You can write, if you have a first derivative. You can write down the first order, second order, third order, whatever order of accuracy, and you can make it to the order of accuracy that you wish. But, when it comes in the governing equation, then we what we normally find is, that, we not only have the time derivatives, but we also have the space derivatives .For example, in this equation, we have rate of accumulation term here, which is a time derivative. The convection or the advection term, and the diffusion term are spatial derivatives, and the source term here, it may be an algebraic expression, or it may be a differential expression, or even a integrated expression. We do not know what it is, it can be different for different cases.

So, in the case, where s phi is just an algebraic expression, and we do not have either advection or diffusion. Then, the time derivative appears by itself and we can treat it exactly like any other derivative. But, when we have other differential terms ,coming either from the advection term or from the diffusion term ,or even from the source term ,then we are met with a choice.

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Let us ,illustrate this, with a very simple example of one dimensional case, with only a diffusion term, and no source term, and no advection term. So for that case ,we can write the equation as dou by dou t ,of rho phi, as being equal to ,dou by dou x ,of d dou phi, by dou x ,and assuming D phi ,is constant. For the sake of argument ,and assuming that that is equal to D. We can take we can take it out, and we can write it out as D dou square phi ,by dou x square and this is equal to . So this is an equation here, that is a part of the governing equation, for a special case ,of one dimensional flow without any advection.

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Now, if you want to discretize this ,using the formulas that we have done here .For example, we can make use of a central differencing formula here, and when when we come to a time derivative .Ok,let us do this space derivative, at i.It can be represented as, D times phi i plus 1, minus 2 phi i ,plus phi I minus 1, by delta x square .We are familiar with this .What about the time derivative? For a time derivative, just as we have an index i for x, and the index j for y, and k for z, we also need an index ,for the time step, time increment, and that is usually given the index n. And it is not given as a subscript, but as a superscript. Therefore, we normally write phi at x t, as phi at, this is discretized as, x I t n .This is represented as phi i as a subscript, and n as a superscript ,where t ,n as usual ,this is t n t naught ,plus n minus 1 times delta t

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So, just as we say that x i, is x naught plus i minus 1 times, delta x and, y j is y naught plus j, minus one times ,delta y. We also say, that t n is t naught, that is the initial starting point, plus n minus 1 times ,delta t. With this notation, and using the n here, indicating the n th step time, step as a superscript,we can write our forward differencing approximation ,for dou phi ,by dou t ,as rho phi, at n plus one minus, rho phi at n ,divided by delta t.

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So, when we take this in isolation, the time derivative evaluated, at the n th time step, can be expressed like this. The space derivative, dou square phi, by dou x square evaluated, at the i th space derivative can be written like this. Now let us put these two together, and then write the equation. So we have, and we can also take rho is equal to one ,and it is constant, so that we do not have to carry this all the time. So, we can write this as, phi n plus 1 ,minus phi n ,divided by delta t, equal to ,D phi i plus 1, minus 2 phi i plus phi i minus 1 ,divided by delta x square.We immediately feel, there is something ,that is missing in this. In the first case ,the space index is missing, and in the second case, the time index is missing.

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So, in a two dimensional case ,we obviously have for phi ,two indices phi i n. So , when we write an approximation for this ,we are not only writing at n at n th time , but also at the i th space location ,at the i th grid point. So we should put i here , and i here .So that we can put i here, and i here. Now what about the right hand side? So the right hand side is also evaluated ,at what time ?Because we are going from n th time, step to n plus, one time step. So we have a choice of evaluating this ,either at n th time step ,or at n plus one .So ,that is at the previous value or the current value, at the next time step, or somewhere

in between ,n plus half .So, let us just look at these three possibilities ,and let us evaluate this at n th time step.

We can also write this as, D of phi plus 1, n plus 1, minus 2 phi i f n plus 1 ,plus phi i minus 1 n plus 1 ,by delta x square. Or ,we can write this as, phi i plus 1 n plus half. So, which of them is correct? So in all the cases, the accuracy of the right hand side term ,is second order accurate in space .But the accuracy of the time derivative ,is determined by this ,and we can see that this is first order accurate.

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So ,the resulting approximation, can be first order accurate in time, and second order accurate is space .So between these two things, there is no difference in the overall accuracy. But, when we look at how to solve this equation, then there is a vast difference, between this approximation, and this approximation. Next just do that. For the time being, let us neglect this part, and let us see what we mean by solving this. We now have a 2 dimensional space, this is the x direction and this is the time direction . We are looking at phi, at several points, in the x direction and several points in the time direction .For example, if you say, that this is i here and this is n, this is n plus 1, and this is n minus 1, i minus 1, and i plus 1, and so on.

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So, this is reference point here .Now in order to solve this equation, obviously when you write an equation like this ,when you write an equation like this ,we can see ,that this is an initial value problem. In the sense ,that in order to complete specification of this problem ,not only requires a statement of this equation ,but also the boundary conditions ,at the two extremes of the x .So, that is x equal to zero, and x equal to 1. And also ,it requires the specification initial conditions, ok.

So, that means, that if you say that this, n equal to 1, is the initial condition. This is t naught then, all the values here, are specified. Not only that t, the boundary conditions are specified at, x equal to 0, and x equal to 1, for all times. Let us assume that these are constants. So, it is a dervish like condition, and it is invariant with time .So that means, that in this solution domain, this value at this extreme is specified, as a boundary condition for all time.

So, here we have the three boundaries are specified. And what we need to do is to get the points, in between and these are points that are that are unknown. And we want to get the values here .Now, we have this equation to solve, and let us consider the first case .We can write this a, 5 phi i n plus 1, is equal to, we take this, on to the other side. So, that is ,D delta t ,by delta x square times phi i plus 1 n ,minus 2 phi i n plus phi i ,minus 1 n plus phi i n.

So, this is the formula, that is available for us, to calculate the value of, phi i at n Th plus, one time step now. When you see, what is there on the right hand side, the diffusivity is specified ,as part of the specification in the problem .The delta t and delta x square ,are specified ,because we are specifying the grid spacing, in the time domain and the space domain .And for n equal to 1, that is at the initial condition,we know all these values .So that means ,since we know all these values now, we can make use of this template and apply it to find the value here. Because this is ,at n plus one at, so this is n equal to 1 ,this is n equal to 2 ,and this value will be i equal to 1 ,and i equal to 2 .So this can be computed ,as i equal to 2 ,n equal to 2 ,as i plus 1 ,so that is three value. This is known i value, at n Th time step, this is known, and i minus 1, this is known.

So, this value is now specified, in terms of these three values. You can see, i plus 1 i, and i minus 1, are coming in this at the previous time step .So this is known, so we can compute this.

Now, you go to the next one. Here, this is specified in terms of these three values. So this can be computed ,and we can march forward along the x axis ,and then get all these values ,all the way up ,to the end .Now you come here, at n equal to three, now n equal to three .At this particular point ,is specified in terms of these 3, and we know these 3, because we have already computed these .So this can be computed ,and so on like this, we can go all the way forward. So that means that using this formula here ,using this template for the calculation of the value of i th special point at n th plus one th time ,we can march forward in the x direction at a particular time step from, point i to i plus 1, to i plus 2, i plus 3 all the way up to the end .And once we finish the time step calculation, for all the spatial points at that particular time step ,we go to the next time step and then we again compute like this. So, we can march forward from point to point, in the spatial direction and then once we complete a particular row calculation. So that is for all the spatial points ,at a particular time, we go to the next step .So that way we can fill up all these unknowns, by marching forward in the x direction. And then once this is finished, we come back to the first point, and then we can do like this.

So, we can find all the unknowns by making use of this expression at each point. And ,so ,that is the characteristic of this particular solution, where we choose to evaluate the right hand side space derivative, in terms of the value at n .And ,so we can say ,that the value at n plus one at a particular space point, is expressed explicitly in terms of the values, at

the previous time steps .So this is called an explicit method, it is not implicit .And in the explicit method ,everything in the right hand side is known, and so the left hand side ,which is the value that you want at a particular point in terms of space and time ,can be computed explicitly and very easily in terms of the values that are already known.

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Now, if you come to the second method, here, we can write this as, phi i n plus 1. We do the same thing equal to D times delta t by delta x square times, phi i plus 1 n plus 1, minus 2 phi i n plus 1, plus phi i minus 1 n plus 1, plus phi i n.Now on the left hand side, we have phi i n plus 1, which is what we are looking for .On the right hand side also, we have phi i n plus 1, so we can bring this on to this side. We can write this as, 1 plus 2 delta t 2 D delta t by delta x square times, phi i n plus 1, is equal to D delta t by delta x square times, phi i n plus 1, plus phi i n.

So, now this is the formula, that we have to evaluate, phi i at n plus 1, in the second method. Now in the second method, we go back here and these are the points that we know .And if you want to compute this value here, that is i value at n plus 1, this is given in terms of phi i n, so that is this value here .Phi i plus 1 n plus 1, so that is this value here.And phi i minus 1 n plus 1, that is this value here .Let us just redraw this figure.

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So ,we have i equal to 1 2 3 4 ,and so on like this and n equal to 1 2 3 4 ,and so on like this .So if we consider this particular point, so we know ,that this is given as boundary condition. This is given as initial condition and this is given as boundary condition. So all these points are given as boundary conditions and are known to us .So if you look at this particular molecule, computational molecule which gives us a value of this. This is expressed in terms of phi i n, so this is this our n plus 1, and this is our i. So phi i n, is this one. So it is given in terms of that value ,and i minus 1 n plus 1, so that is in terms of this value .And i plus 1 n plus 1, in terms of this value.

So in order to compute this you need to know the previous time step value, which we know, and the left value and the right value .So can we march forward in time with this? It does not seem to be possible .Because, if you are marching to the right, then you know the left value. But you do not know the right value. You get to this point, only after computing this. But in order to compute this, you need to do this. If you march from the left to the right, then you know this .But you do not know this .But you do not know this.

So in that sense the value at this particular point cannot be explicitly calculated in terms of the values, which are coming in this equation So this is an implicit solution .So this is an implicit method for the evaluation of phi i at n plus 1. So in order to do this, we need to know the value of i plus 1 and i minus 1 at, and the n Th plus 1 Th times, the n in this particular case. We know either this or this but we do not know both of them.

So, in that sense you cannot simply directly independently evaluate i n plus 1. We need to couple it along with the evaluation that i plus 1 and i minus 1. So what we need to do is ,that we notice that the value here, is expressed in terms of the previous time step ,which is known and the 2 neighboring values at the same time step.

So we need to write down this equation for all the points, which are appearing in the same time step .And then for all these things , when you put them together you get an equation something like, a phi n plus 1, equal to b . So this we solve for phi n plus 1 for all i ,and after completing this .So that is we evaluate for all these points, and then we go to the next step .So the next step also ,we write down this computational molecule for each of these all the points ,appearing in the that particular time step. And then ,we solve them simultaneously .For example using gauss Seidel method ,if it is found to be convergent scheme ,then we can evaluate.

So we do row by row evaluation of this .So it is not possible to march forward from point to point as it is possible in the case of explicit method. We have to do a row by row calculation, in 2 dimensions and 3 dimensions .There will be more number of unknown's .So we need to calculate it in a coupled way, and we may have a large system of equations which we need to solve.

So, when we consider a time dependent term, to recap the time derivative itself does not pose any problem, it is just like any other derivative. But when it when it is combined with a spatial derivative ,then we have the possibility of either doing an evaluation purely in the explicit method, which is simple ,which allows us to hop from point to point in the 2 dimensional grid ,or the 3 dimensional grid or the 4 dimensional grid. Or we can do it in an implicit way ,by which requires us to do a row type of evaluation at each time step, in the case of one dimension, or a plane evaluation, in the case of 2 dimensions, and a 3 dimensional matrix evaluation ,in the case of 3 dimensions.

So this we have the possibility between an explicit method, which is simple and an implicit method, which is much more challenging, which requires more intricate programming. Because at each time, you have to you have to assemble all the constants of the matrix a, and all the elements of matrix b, and then we have to assemble this matrix equation, and solve it using any method, that we feel is appropriate.

We need to know and we need to keep in mind ,that although in 1 dimensions it becomes a small thing .When you consider a 3 dimensional case ,where you have phi i plus 1 n plus 1 ,and phi j plus 1 n plus 1 ,and phi k plus 1 n plus 1, you can be dealing with a large matrix .So all the difficulties, that we may have with the solution of large matrix equations ,will appear at each time step. So it is necessary for us, to find an efficient way of solving this kind of matrix equation .For a time dependent problem, the implicit method is ok.

So the choice of whether, we use an explicit method, or an implicit method is very deliberate .We have to choose either the explicit, or the implicit method. Question is, if the implicit method is so simple, why do an explicit method? It is a valid question. We will see in the next class. That it is not, as the choice is not as clear cut as that .That if we use an explicit method ,we can only go in very small time steps, if it is possible at all .Because we are making use of the previous values ,the previous values of the variables in order to estimate the space derivative here .

So that means that and if you take two larger time step, then these values might have changed ,in the meantime .So that means ,that the value that you are estimating ,the previous functional values ,may not be accurate. So that is why we are restricted to having only small time steps .Whereas in the case of the implicit method ,we are making use of the current values, in order to do the space derivatives.



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So, is the current estimate better than the old estimate? We cannot say, that we cannot say that this is more accurate. But what we know, is that the current derivative, based on the current estimates of the values, will not be violating the conservation law .Because both the left hand side and the right hand side are evaluated at the same time step n plus 1 the time step .So the kind of imbalance between 1 derivative which is which is evaluated at, n plus 1 and 1 another 1 which is evaluated at n, will not appear. And this kind of method, implicit method can tolerate even large time steps, without the solution becoming unstable.

We are anticipating what we will be discussing in future classes. So from that point that is why we say that the choice of whether we choose the explicit method or the implicit method is not as clear cut. And sometimes we may be forced to use an explicit method, because it is so simple to program. But sometimes, that may we may find that that restricts severely on the kind of delta t values, that we can choose .And in such a case, an implicit method will guarantee us a solution. But both are only first order accurate in time .So that means, that the approximation that we are making here, as forward differencing here, is only first order accurate. So that means, that the solution at different times is not very highly accurate ,for all the space derivatives we have considered .For example the second order accurate ,and fourth order accurate ,and fifth order accurate like that.

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But for time derivatives, we usually consider first order accurate, or may be second order accurate, and so on. Why is that? The reason is that, if you want to do higher order accurate approximations, for the time derivatives just like what we have here. We can see that a second order accurate expression ,for the third derivative will require four values .So that means ,that if you are writing a similarly an expression for the time derivative then, we need to store the values at n plus 2, n plus 1, n .Let me just put it in this 1. Here n plus 4, n plus 3, n plus 2, n plus 1, and n, so that means that we need to have the field values not only at n and may be n plus 1, but also at so many points .So that means that you cannot overwrite the values that you have computed in the current time step, with the previous time steps.

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So, that means that you have to store a large amount of data, in order to go from one time step to another time step .And we know that we are dealing with the large number of grid points, typically we are we may use a million grid points so that means that we need to have so many more millions of values variables that are needed to be stored. Not only that, in order to go from one time step to another time step, we need to recall these values. So this should be in an easily accessible memory, on a computer. Otherwise, you need to, you will be spending a lot of time in retrieving the data from your core memory and that will reduce the speed of computation .So from that point of view, we cannot afford to have highly accurate schemes for the time progression, because it requires us to store large number of data, which are otherwise, which may otherwise be not necessary.



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So that is why, we choose typically first order accurate, or second order accurate schemes in in time derivative. But in space derivatives ,we can go for more accuracy .Because these values are anyway known .So this this is these are the considerations ,that we have to keep in mind ,when we look at our governing equation ,and using a finite difference method ,for the discretization of the this particular equation..

So ,to summarize when we have an equation like this ,a partial differential equation, then we expand it to include all the terms, that are relevant .For example, in 2 dimensions ,there will be 2 terms here ,and 2 more terms here. In 3 dimensions, there will be 3 terms here, and 3 terms here. So each of them is a partial derivative .Wherever we have a partial derivative, then we substitute that partial derivative, with an equivalent finite difference approximation. Then we can assemble all the points together, and then come up with an overall expression for a discretized form of the governing equation.

So with this, we will be able to convert a given partial difference equation into an approximate form of a defined accuracy ,or of a chosen accuracy chosen by us, in terms of the derivatives involving the x direction ,y direction z direction and time direction. When we also look at the time derivative, we also make a choice between an explicit method, or an implicit method, or a combination of these methods.

So with using making these deliberate choices, we can convert a partial differential equation into an algebraic equation, which is valid, which is in approximation of the governing equation, at each discrete point in time and space. The form of this algebraic equation is such that the value of that particular variable, at that particular point in time and space is expressed in terms of the neighboring points .We need to do this approximation at all the grid notes that are of interest to us. Then as a result of this, we will be converting a single partial differential equation into 1 big set of algebraic equation, which can be written in a matrix form like a phi equal to b.

Sometimes, what we have is, we have we may have non-linear terms in which case, it will be a set of non-linear algebraic equations .In order to convert it to a matrix form, we may have to linearize it .We will look at some linearization techniques or considerations in linearization, so that a given partial differential equation can be converted into something like a phi equal to b which we can solve

So ,the summary is that we know now, how to take a partial differential equation and convert it into A phi equal to b.So we can claim ,that if you know how to solve this a phi equal to b .For example, using the gauss Seidel method ,which we have already addressed ,we should be able to say that now, we know how to solve that template equation .Unfortunately, the situation is not as straightforward and trivial as that there ,we have to look at more the properties ,of the discretized equations.

So the discretized equation being like this .To see under what conditions this discretization will guarantee us a solution, which is satisfactory ,we will see in the next class ,that it is not always ,that we will be able to get a satisfactory solution. Many cases, even the straightforward discretization, which looks on paper, may not give us a proper solution. It may, give us a totally unacceptable solution. So, we will look at the properties of the discretized solution .We will look at .We will do some analysis, to see under what conditions, we can expect to get a proper solution. Therefore based on this analysis, we will ultimately come up with a satisfactory way of discretizing a given partial differential equation, into and converting it into a set of a phi equal to b. We only know how to solve how to discretize a given partial differential equation.

Now what we want to see is, when we substitute the individual derivatives when you replace the individual derivatives with the finite equivalent, finite differential approximations, what kind of additional complications arise, by which some substitutions may not give us a proper solution. How to detect a priori even before attempting a solution ,how to say a priori ,that this particular combination of finite difference approximations with these terms, will give us a satisfactory solution .So that will be the essence of what we are going to discuss in the next classes.