Computational Fluid Dynamics

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Lecture No. # 16
Important Consequences of Discretization of Unsteady State Problems

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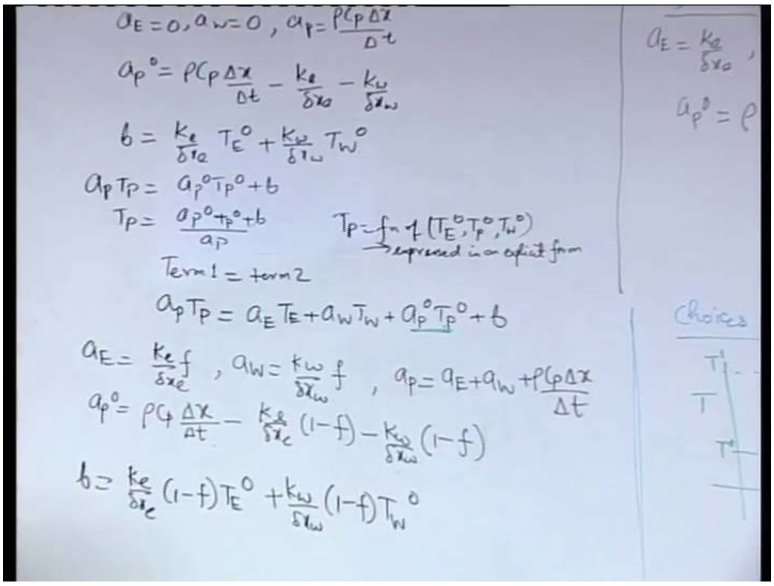

In our previous lecture, we were discussing about the finite volume discretisation of unsteady state diffusion problems. And we will take it up from there, if you relook into the derivations, you will find that we could derive the governing differential equation or rather, we could derive the discretized equation from the governing differential equation in a convenient form a p T p equal to a e T e plus a w T w plus a p naught T p naught plus b, where in the unsteady state problem, you have this additional neighboring term a p naught which takes care of the time neighbor.

Now, as we have seen that this coefficients of the discretized equations, they cannot have any arbitrary sign. We have seems four basic rules, and one of those rules is that all the coefficients must be of the same sign. Now, with different choices of the parameter f; if you recall that f equal to 0 was fully explicit scheme, f equal to 1 fully implicit scheme, and f equal to point 5, scant Nicholson's scheme. So, we will consider some limiting cases like f equal to 0 and f equal to 1 to begin with of course, we can test the case of f equal to 0 point 5 also, and see whether those cases are giving rise to all coefficients of same sign.

First look at the coefficients a E, aw, a p. You can see, that f is a positive fraction; k e is a thermal conductivity which is positive; delta x is positive. So, a E is positive similarly a w is positive; a p is positive, but you cannot tell anything about a p naught, until and unless you are specifying the value of the parameter f. So, let us consider the signs of a p naught and note that, we should have a p naught greater than 0. You can also put an equality with the sense, that it can be greater than or equal to 0; now, what happens with f equal to 0; f equal to 0 will give you a p naught is equal to rho C p delta x by delta t minus k e by delta x e minus k w by delta x w.

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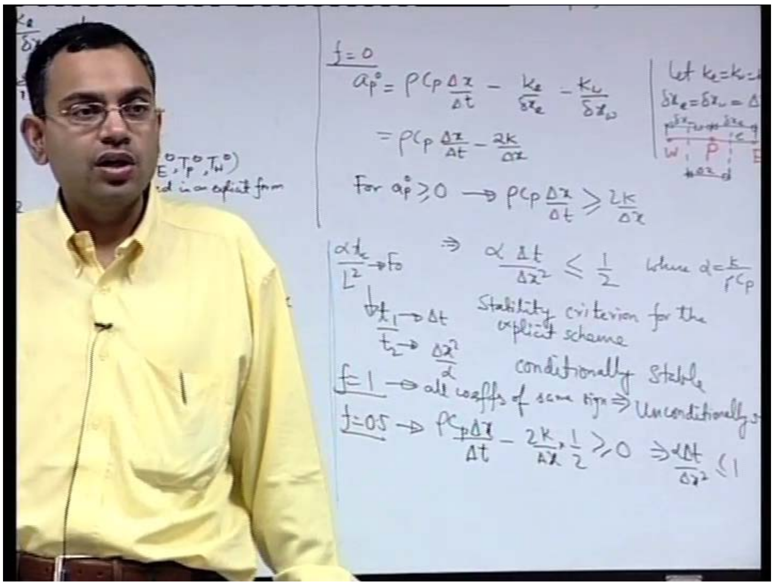

Now, for algebraic simplification, let us consider that k e and k w, all are same as a uniform thermal conductivity value of the material; the material has uniform thermal conductivity, and delta x e equal to delta x w equal to delta x. So, what it means is, if you have a grid layout, this is delta x; this is delta x e. This is true, when all the grid points are equidistant; then and if you have the grid point at mid way between the faces of the control volume, then you can have delta x e equal to delta x w equal to delta x, that is uniformly laid out grid points.

So, if that is the case, then we can write this one as rho C p. Now, what are the conditions for a p naught to be greater than 0 or greater than equal to 0? You must have rho C p delta x by delta t, greater than equal to 2k by delta x which implies alpha delta t by delta x square less than or equal to half, where alpha is the thermal diffusivity which is k by rho C p. In conduction heat transfer, alpha into some characteristic time by characteristic lane square is called as Fourier number. So, this is like a grid spacing, and time step size based Fourier number less than equal to half; this is called as a stability criteria. We will later on see that, what do you mean by stability here for the explicit scheme.

So, what we mean by stability criteria here or what do you mean by stability here? Now, when you are doing any numerical calculations, the calculations are susceptible to round of errors, because you may not be able to represent the number with limited decimal points as the correct number. So, there will be some approximate representation of the number, because of limited number of digits beyond the decimal point that you can use. Now, that is an error; with calculation, this error can propagate and can get amplified. So, if such round off error gets amplified, as the numerical solution proceeds, the corresponding scheme is considered to be, if it is inherent to the scheme itself, it is considered to be an unstable scheme.

Now, one of the key requirements of having a stable scheme is that, you should have a consequence of the scheme, that is physically consisted; that means, if all coefficients are of the same sign, then increasing the temperature at a particular point will ensure that temperature will be increased at all other neighboring points, but not decreased. So, that means, despite the perturbation being present, you will get physically meaning full solutions. We will look into a different mathematical angle of the stability, subsequently, but what we can see here from physical arguments, that we say that this scheme is stable. So, long as all coefficients of the differential, all coefficients of the descretized equation, algebraic descretized equation, they are of the same sign.

Now, what does these criteria effectively mean? So, you have we have derived a criteria. What will you do with these criteria, when you are working out a problem numerically? So, you have to be careful about your time step. What we in general intend to do to get a highly defined solution? We reduce the grid size spacing. So, when you reduce the grid size spacing by delta x by whatever, you can see that the corresponding time steps size also should be reduced, matching with this requirement. So, you cannot indiscriminately use a large time step size; the time step size is limited by the grid spacing. So, you can clearly see, that the this ratio is a ratio of 2 time scales; T1 and T2. What is T1? T 1 is delta t. And what is T2? Delta x square by alpha. What is delta x square by alpha? It is the characteristic time, over which a thermal disturbance propagates by thermal diffusion in a medium. So, alpha is, if you recall that it is thermal diffusivity. So, it is thermal conductivity relative to the rough into C p; that means, it is the ability of the material to conduct thermal energy relative to the storage ability of thermal energy; so, that means, when you have this alpha, this alpha is a characteristic is an is an indicator of how fast the thermal disturbance is able to propagate within a medium, relative to its storage capability, and if delta x is the corresponding length scale, that you are talking about, then what is the characteristic time, that takes the thermal disturbance to cover that link scale delta x is given by delta x square by alpha.

So now, what you are comparing is, how much is your time step size in resolution as compared to this characteristic time scale of the system. So, the system has a characteristic time scale of adjustment of thermal disturbance. So, e there is a thermal disturbance that is imposed on the system, and the system adjust to itself. So, it takes a time, characteristic time to adjust to itself. So, this is the characteristic time, that it takes to adjust to itself over a length of delta x. So now, what is the time step that you choose in comparison to that? Here it says that, the time step that you choose in comparison to that must be less than or equal to half of the characteristic time scale of the adjustment of the system with respect to the imposed disturbance.

So, you you you cannot indiscriminately use a large time step, but your time step size is restricted by the system’s ability to respond to a particular disturbance in thermal diffusion through thermal diffusion. So, this is the stability criteria and once there is a scheme which has a stability criteria; that means, you cannot indiscriminately use any large time step; you you have to use a restricted time step; then it is called as conditionally stable scheme; that means, the scheme will work, provided you use a time step size less than or equal to a particular constraint, that is determined from the discretized equation.

Let us, look into the case with f equal to 1; when f equal to 1, you can clearly see that these two minus signs go away, and a p naught is positive. So, all co-efficients are of same sign; that means it is unconditionally stable. So, what we have inferred out of this is, with any positive or advantageous effect, there is always a limitation; the explicit scheme, that is f equal to 0 had a positive or advantageous effect; that is, you could explicitly express the value of the variable in terms of the value of all the neighbors including the time neighbor, and calculate it on the basis of individual equations, rather than having to solve us. See connected system or coupled system of algebraic equations. So, solution of couple system of algebraic equations was not necessary for that scheme, but the cause that you have to pay is that, you have to use a time step size less than a critical one; you cannot use any large time step size.

On the other hand, for the fully implicit scheme, you can use any large time step size. Of course, if you want to capture a particular transient that is according within a particular time scale, you have to use the time scale less than that one, but that is for capturing the details, but at least to get a physically meaningful solution, you do not have to be bothered about the time step. On the other hand, the scheme has the disadvantage or rather limitation; if not a disadvantage, that you have to solve the coupled system of algebraic equations for the fully a implicit scheme. What about f equal to point 5, which is the Grant Nicholson's scheme.

So, if you consider the same case with all the thermal conductivities thermal conductivities throughout the domain being the same and uniformly spaced grids; then you have the stability criteria as rho C p delta x by delta t minus 2k by delta x into half, because f is equal to half. So, that will give you alpha delta t by delta x square, less than equal to 1. It is of course, a more relaxed requirement than the fully explicit scheme, but it still has a constraint.

So, this is also conditionally stable; sometimes in some literature, the Grant Nicholson's scheme is referred to as an a unconditionally stable scheme, but the notion that those literatures possibly use is not same as the concept that we are trying to invoke here; our idea is to see, that you get a physically meaningful solution. See, if we if the scheme is stable, that means, if there are oscillations in the numerical solution, because of round of errors; those oscillations will be dampened out, but even after the oscillations being dampened out, you may not get a physically realistic solution; the oscillations may get dampened out, and the solution may converse to something which is not physically meaningful.

So, here we are trying to go beyond mathematical stability requirement; mathematical stability requirement will just ensure that, the oscillations in the solution will die down. But once the oscillations die down, the that is the solution is converging to something. Is it converging to the physically acceptable solution that you are looking for? It need not always be. So, when you are considering the same sign of all the coefficients, you are ensuring that additional features also; that is, you are having the solutions converse to something which is physically meaningful. Now, so far we have discussed about the consequences of the discretization scheme from a finite volume discretization angle; now, we would also like to draw a parallel analogy with the finite default discretization of the time and the space coordinates.

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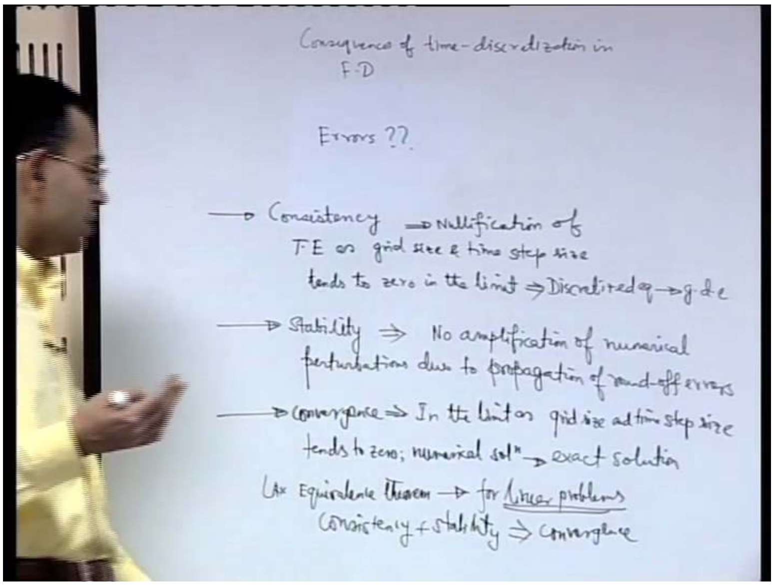

So, what we will try to do is, we will try to see the consequences of time discretization in Finite difference. We have briefly introduced the finite difference method earlier; and we will take it up from there; and see that how we can have different types of schemes which have different behavior; we have made one important remark earlier, that the Finite difference method is essentially an outcome of a Taylor series expansion of the derivative terms, in terms of algebraic differences; now, when you do that, you can do it of course, by truncating the Taylor series up to certain number of terms; when you do that, you will get some algebraic equations, but will those equations work or not in all cases; that is the matter of debate, and that is something that we would like to highlight on.

So, we would specifically like to see that, what are the Errors associated in the Finite difference discretization or any Taylor series based discretization. To do that, we will consider certain terminologies; first we will consider the terminology consistency to appreciate the term consistency. So, consistency is a characteristic of a numerical scheme; we say that the scheme is consistent

So, what we mean by consistent is that, when we are discretizing a particular problem, we are representing the behavior that was supposed to be represented by a differential equation with some algebraic equation. So, the algebraic equation now has the responsibility of representing the behavior of the system which is differential equation in terms of its representation. So, there is a conflict there is a conflict, that the system behavior was suppose to be represented by a differential equation; now you are representing it by some algebraic equation. In the limit, as the grid spacing and the time step size spacing tends to 0.

If your algebraic equation mimics the behavior of the governing differential equation exactly, then we say that the scheme is consistent. So, when that is possible? It is possible only when the error incurred because of the discretization is nullified at very small grid size and very defined time step; and when you expect to expect that to happen? You expect that to happen, when the terms that you neglected in the Taylor series, turn out to be limiting small or 0, in the limit of small brick size and time step; and those that error associated with neglecting the terms in the Taylor series beyond a particular term; that type of error is known as truncation error.

So, truncation error is what? Truncation error. So, consistency essentially deals with nullification of truncation error, as the grid size and the time step in the limit tends to 0. So, nullification of truncation error as grid size and time step size tends to 0 in the limit which implies that, the discretized equation tends to behave same as the governing differential equation; the difference, because of negligence of certain terms in the Taylor series vanishes, because the corresponding terms tend to 0 as delta x delta t all tend to 0.

So, a scheme will be consistent, how do you test it? You can test it by checking the truncation error. So, the truncation error will have certain terms which will be functions of delta x and delta t; you put the limit as delta x tends to 0 and delta t tends to 0 separately; and see that when you consider them together, that is delta x tends to 0 and delta t tends to 0, the terms which contribute to the truncation error, the terms will tend to 0; then, as if your algebraic equation and the governing differential equation, they are behaving in the same way.

So, a scheme has to be consistent, and if it is not consistent, the corresponding inconsistency is because of non-nullification of the truncation error in in in this limit; that is a truncation error means; even if delta x and delta t are tending to 0. We have to remember that we are not checking the truncation error as a basis for finite size delta x and delta t, because we we can understand from common sense that, when delta x and delta t are finite size truncation error will remain, because we have truncated the Taylor series up to a finite number of terms; that is obvious, but when we truncate the Taylor series up to a finite number of term, but take the limit as delta x and delta t tends to 0, then at least and in that limiting condition, it should the truncation error should be 0. So, we are checking the consistency in the limiting condition of delta x and delta t tending to 0, and checking the Truncation Error has to be 0 at that condition

The next is stability; now, just like consistency talks about the truncation error, stability talks about the round of errors. So, when you have a number, e represented by a decimal system for example, you are using certain digits, number of digits, fixed number of digits beyond the decimal; that is based on the precession of the computer that you are using, but is not infinite precession; that means, you cannot use infinite numbers of digits. So, always there will be a error due to rounding off, and this error can propagate within the calculations, and they can amplify.

So, if the errors propagate, the round of errors propagate and then can amplify; so, the round of errors in a numerical scheme is like a physical perturbation. So, let us say that you you wanted to calculate a number 1 by 3, but you are truncating it; two are finite number of digits beyond the decimal. So, you get point 3 3 3 up to something. So, 1 by 3 was the actual thing that you desire for; and this is its representation; and the corresponding differences like a perturbation or disturbance to the calculation of numbers; and how strongly this perturbation propagates, because of by virtue of the numerical calculations is also a characteristic of the numerical scheme.

So, stability if the scheme is stable, then it says that, there is no amplification of numerical perturbations due to propagation of round of Errors. So, by ensuring consistency and stability, we are ensuring that the truncation error and the round off error are not creating an havoc to the numerical solution, and if that is ensured, then then for the linear problems then you can say the convergence is also ensured. So, the next important terminology is convergence; this is what is the ultimate goal for the numerical solution, and the concept of convergence is that, in the limit, as the grid spacing and the time step size spacing tends to 0, the numerical solution will tend to the exact solution; now, there is a very important theorem which is known as lapse equivalent theorem equivalent theorem which states that, I am not going to state the theorem in a very formal way, but which essentially means that, for linear problems, consistency plus stability if you can ensure these two, this will automatically ensure that there is convergence.

So, consistency plus stability implies convergence, but very importantly only for linear problems; for non linear problems, consistency plus stability may not ensure may not ensure that there is convergence; one of the key reasons is that, for non-linear problems you could have multiple solutions. So, it is it is not automatic that for non-linear problems, consistency plus stability together will ensure that there is convergence. So, for non-linear problems what you do? Usually for non-linear problems, we test convergence in this way. We test the problem with a particular grid size and time step; then we go on reducing the grid size, and reducing the time step, and we come to a stage, when we see that, even if you reduce the size of the grid, even if you reduce the size of the time step, that is further refinement of the grid and refinement of the time step, the solution does not get refined any more.

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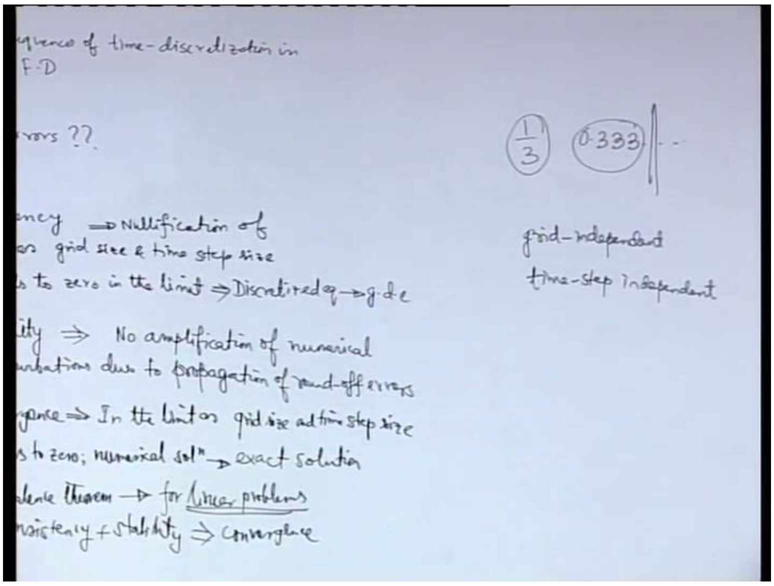

We say that the solution has become grid independent and time step independent.. So, a grid independence or time step independence study is what is required for a non-linear problem. If you just have a consistency and stability, that does not automatically ensure convergence for a non-linear problem, and when we will be doing the full solution of the Navier stokes equation, we should keep in mind that, because those non-linear equations, essentially consistency and stability will not just be enough; we have to check the grid independence and time step independence for solution of such problems.

So, we have now got of here idea of the sources of errors, that could be there in a discretization method, and in particular in reference to the Finite difference scheme. Now, let us look into certain examples of Finite difference schemes, and see that how do this Errors matter. So, we will consider Finite difference scheme for unsteady one dimensional unsteady diffusion type of problems. Just the corresponding cases on finite volume, we are studied the similar problems with Finite difference, now we will study.

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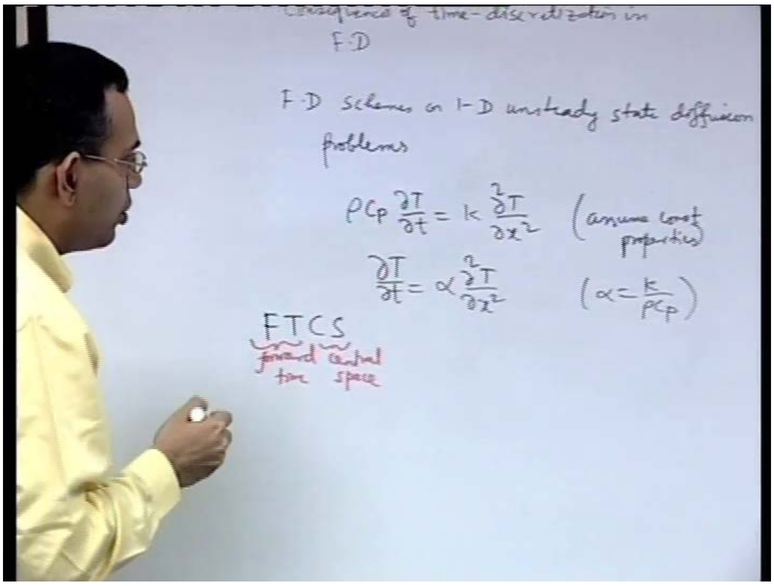

So, finite difference schemes on one dimensional unsteady state diffusion problems. So, the governing equation is this one, where we have assume a constant thermo physical property; that is density, specific heat and thermal conductivity all are constants. So, assume constant properties.

So, you can write where alpha is k by rho C p which is the thermal diffusivity which we discussed physically also; now, this prototype equation has a time component in it, and a space component in it. So, depending on the differencing scheme that we can use for the time and the space, there are different Finite difference schemes. So, if you recall that we had different types of finite different descretization like forward difference, backward difference, central difference like that. So, for example, we can use a forward difference sign for time, and central difference for space. So, that we call as FTCS; forward FT for forward time, and CS for central space so, forward time central space. So, let us write the corresponding Taylor series expansions. While doing, so what we will do is, we will use some notations that are common to Finite difference.

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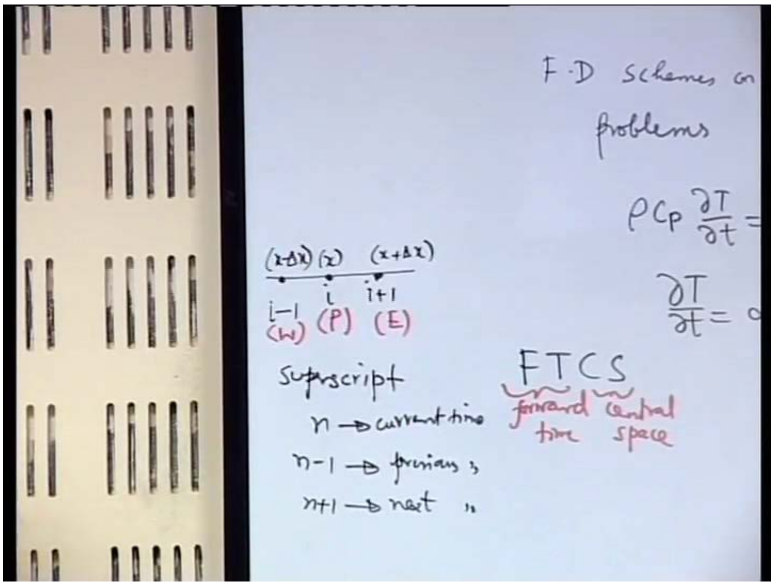

So, let us write the corresponding Taylor series expansions. While doing so, what we will do is, we will use some notations that are common to finite difference. What are these notations? We consider one grid point which is the grid point p that we were considering for the finite volume; the same we will use an index i; i plus 1 for e i minus 1 for w. So, just to give the analogy of the nomenclature; and super script n for current time; and n minus 1 for previous time; and n plus 1 next time .

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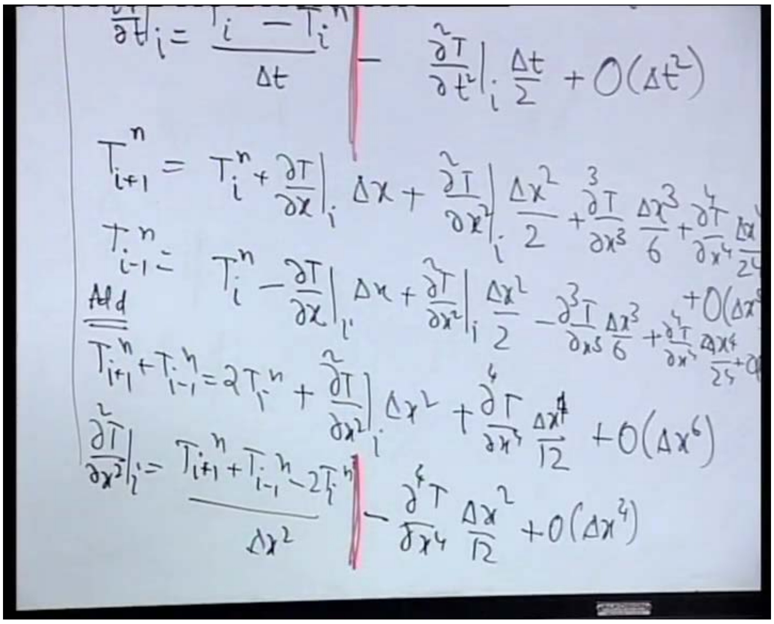

So, we can write Ti n plus 1. What is Ti n plus 1? This is T; at time t plus delta t actually, at the grid point i; that is at x;, i is x this is x plus delta x this is x minus delta x. So, Ti n plus 1 is equal to. So, we are writing keep in mind that we are writing T at time t plus delta t; we can write it in Terms of T at time t.

So, we can write this as T i n. So, this is T plus delta t; this is t, and this is sorry this t minus delta t, and this is t. So, T i n plus 1 is equal to T i n plus, plus if we consider the higher order terms, that is of the order of delta tq. So, we can write minus plus of the order of delta t square; order does not get change with sign. So, it is just division by delta t makes it order of delta t square. So, if you now truncate the Taylor series up to this term, then this is the representation of the forward difference for the first ordered time derivative.

What about the second order special derivative? So, when you consider the special derivative, see, when we considered the time derivative, we kept the special position as constant i and change the time. So, here for the special derivative, we will fix the time; fix keep the time fixed, and vary the special coordinate. So, T i plus 1 n is equal T i n; we are not writing super script n everywhere, but it all are super script n; similarly, T i minus 1 n is T i n with a minus sign, now it will be. So, delta x become minus delta x, that is the only change. Now, if you add this 2Ti plus 1 n plus T i minus 1 n is equal to 2 T i n; then plus del square T del x square i into delta x square cube terms will go away; fourth order term will remain delta x4 by 12; then fifth order Terms will cancel. So, what will remain is of the order of delta x6, which one? which one

No, we have not yet divided by delta x square; this is alright; this is we have not divided this by delta x square. So, next step will be to divide both sides by delta x square, by delta x square minus delta x square by 12 plus of the order of delta x4. So, here also we will be truncating it up to this one which is the central difference scheme for the special second order special derivative. So, let us now substitute these expressions in the governing differential equation.

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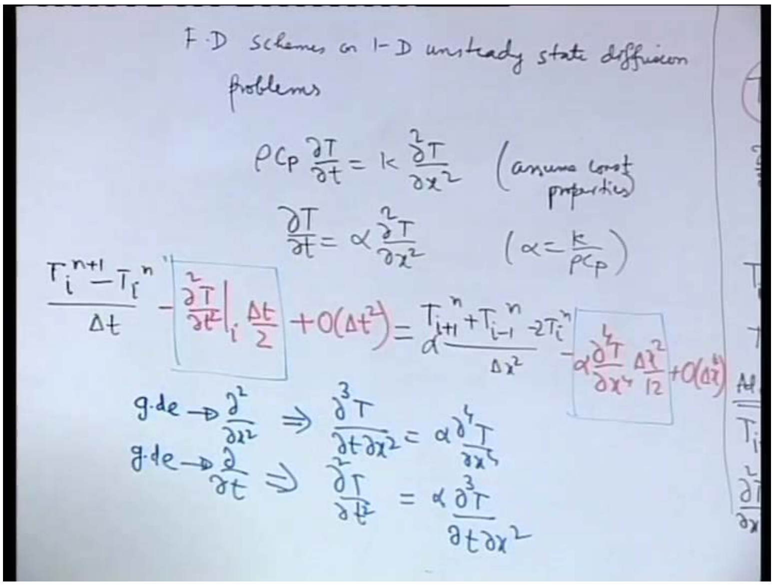

So, the time derivative Ti n plus 1 minus Ti n by delta t. minus Let us write it with the different color to indicate that, this is an Error Term minus de l4T del x4 delta x square by twelve plus of the order of delta x4. So, the terms that we have written with black color are the terms that are going to matter. There is alpha in the right hand side. So, let us multiply alpha, all the terms in this way. So, the terms that are going to matter for the descretized equation are the terms which are written in the black color, but the terms which are written in the red color are important because they can give rise to the understanding of the Errors, because of omission of those terms.

So, let us do that analysis; let us try to write; let us first consider interestingly, these 2 terms; this term and this Term, now this particular term; 4th order derivative of temperature with respect to x, that you can attain or that you can obtain by differentiating the governing differential equation, twice more with respect to x. So, governing differential equation, if you partially differentiate it twice more with respect to x, then what this will give? Similarly, you can differentiate the governing differential equation once with respect to time to get del square T, del T square.

So, governing differential equation, if you partially differentiate with respect to time, you will get… So, what we can conclude from here? We can find the relation between the first leading order term, because of truncation with respect of time discretization, and the first leading order term, because of the truncation with respect to the special discretization.

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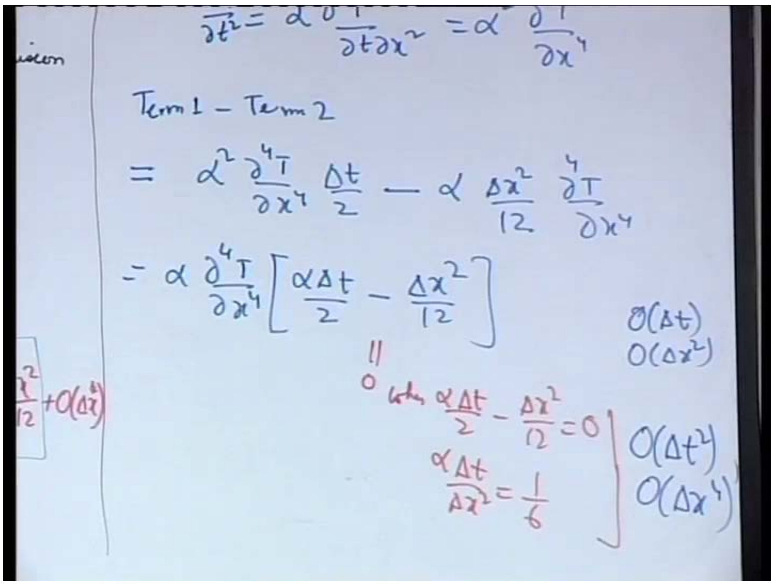

So, we can write, del square T, del T square is equal to alpha; del cube T, del T, del x square, that is equal to alpha square; del 4T, del x4, just check whether this is all right. So, if you compare this, let us call it Term 1 and let us call it Term 2. So, Term 1 minus Term 2 is what? Is equal to alpha square del 4T del x4 into delta t by 2 minus alpha delta x square by 12 del 4T del x4. So, if you take alpha del 4T, del x4 as common, then here you have alpha delta t by 2, minus delta x square by 12 in the bracket. So, you can see that if this term in the bracket is not equal to 0, then what is the order of accuracy of this discretization? Order of delta t is the Error for time, and order of delta x square for space.

So, first order in time and second order in space, but to understand what is that, but we have derived this particular term; now, if you see that, if this Term becomes 0, then it becomes the of the order of the delta t square for time and of the order of delta x4 for space because then these these are cancelled; when term 1 is equal to Term 2, this (( )) terms in the box in the 2 sides, they get cancelled. When do they get cancelled therefore? They get cancelled; this 0, when alpha delta t by 2 minus delta x square by 12 equal to 0; that means, alpha delta t by delta x square is equal to 1 by 6; of course, this is a possible choice.

So, 1 can make a choice of alpha delta t by delta x square equal to 1 by 6; then this term will become 0, and then it will be of the order of delta t square with respect to time and of the order of delta x4 with respect to space. So, this is about the temporal and special accuracy of the method. The next question comes, that is the scheme consistent number 1; number 2 is the scheme stable. So, we will try to give answers to these questions. In today's class, we will look into the consistency of the scheme, and in the subsequent lecture, we will look into the stability of the scheme. So, is it consistent? When we say that it is consistent? We say that it is consistent, when in the limit as delta t and delta x tends to 0; the truncation error tends to 0. So, what is the truncation error? The truncation error is represented by the rate color terms which are there in the 2 sides.

So, if you make delta t and delta x tends to 0; then, obviously, they will in the limit be tending to 0. So, something some expression which has directly been derived from the Taylor series, automatically ensures that the truncation error becomes 0, as delta t and delta x tends to 0, but if some how you want to temper the expressions that you get from Taylor series expansion; we will see there are certain schemes which attempt to do that; that they tend to temper the expression that you get from the Taylor series in an effort to achieve something more special, and in that way they can create problems with respect to consistency, but here it is simply an outcome of Taylor series based expansion of the derivative terms, and therefore, it it it is true that is a consistent scheme.

The next important point, that we will try to access in the next class is that whether the scheme is stable or not, and what we mean by a stability here is that, if you have a perturbation in some numerical values say of a temperature at a particular grid point, then thus that perturbation get amplified with time. So, as you proceed or merge ahead with time, remember these are all time merging schemes. So, as you merge a head with time, you you may see that those errors are propagating and the errors are therefore, getting amplified. So, we have to find out a mechanism, that will tell us mathematically whether the Error will get amplified or the Error will die down, and that we will take up in our next lecture. Thank you.