Computational Fluid Dynamics
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Lecture – 29
Properties of Numerical Schemes: Accuracy, Conservation property, Boundedness, Consistency, Stability and Convergence

In the last lecture we saw some of the concepts such as consistency and stability and convergence which are required for us to ensure a good solution, by way of ensuring that the equation that we are solving the discretized equation is a good approximation of the proper differential equation that we are trying to solve.

And also by ensuring that in the process of evolving time step by solving the discretized equation numerically using finite precision arithmetic, we are not compounding the errors which have been made in approximating the derivatives at different times and different space steps. We were looking at those concepts. So, as to get a proper understanding, of why the numerical solution seems to be behaving in so odd way for the simple problem that we considered earlier, this is the 1 dimensional linear convection equations.

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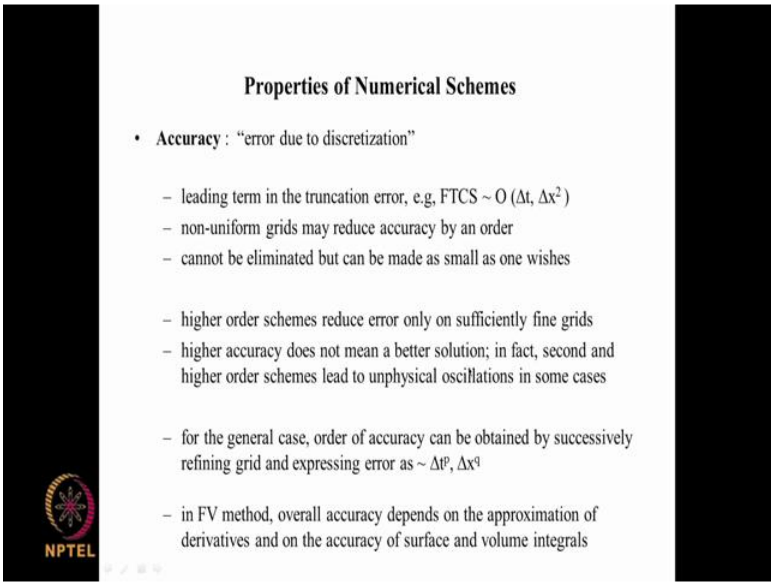

Apart from those we would also like to consider a few other properties, before we come back to the analysis of consistency and stability. Obviously, the first property that we think about for a numerical scheme is the order of accuracy. In fact, this is what we started with, and this when we say order of accuracy we mean error due to discretization and error due to approximation of the derivatives with finite difference approximations. So, this is essentially the truncation error and it is a order of the leading terms in the neglected Taylor series expansion.

So, the leading term in the Taylor series expansion for example, for the FTCS method is varies as delta t in the for the time derivative and for the special derivative for the 1D case the leading term has a, varies as delta x square. So, that we have first order in time and second order accurate in space kind of approximation for the FTCS numerical case for that particular 1D wave equation. We also noticed earlier that non uniform grids may reduce accuracy by an order of magnitude, because of the way we compute error in terms of delta x i and delta x i minus 1. Sometimes it is a difference between the 2 that comes into the picture, and when the difference is large then we effectively loose an order of magnitude. If they are of the order, if delta x i is very close delta x i minus 1, then the difference will be very small, but if the 2 are very large as in the case of sudden variation in the delta x, then the difference can be large and you could have, you could lose that where dependence on the delta x being very small at the point.

And we also made the mention that higher order schemes reduce error only on sufficiently fine grids, and higher accuracy does not mean a better solution, and we will see later on if you have second order or higher order schemes may these may lead to unphysical oscillations in some cases.

These oscillations is property that we are going to discuss next, and in the general case the order of accuracy can be obtained by successively refining the grid and expressing error as varying with respect to delta t to the power p and delta x to the power q. So, if you have a numerical scheme and it is difficult to find analytically the order of accuracy and all that if you are looking at a not in terms of order of accuracy for a particular derivative, but for the solution. Then you could compute the solution on successively finer and finer grids and you take the finest grid as a best solution and then you can for each grid you can find the error in the value of your interest may be the heat transfer coefficient may be the net drag coefficient or whatever it is we express that the error in that as the difference between the value computed on the finest grid minus the value computed on the grid that you currently estimating, and if you then express that variation of error with delta t and delta x as in a power loss series then you could get effectively the exponents p and q, which will tell us as far as this particular variable is concerned what is the order of accuracy of this particular numerical scheme.

So, this is another way of estimating it in the properly done case, we expect the exponent values of p and q for example, 1 and 2 in this particular case to be the same as what we would get from a Taylor series expansion. In the case of already sufficiently fine grids and smoothly varying u or t and all that, and we also saw the finite volume method in the second example of flow in a triangular duct and there the order of accuracy depends not only on the approximation of the derivatives, but also on the evaluation of the surface and volume integrals.

There also some inaccuracies introduced, and usually that is of second order accuracy if you are looking at schemes which are third-order fourth-order and the things like that then we have to worry about how well you evaluate the surface and volume integrals. So, this is about the accuracy which is a property of a numerical scheme if you change the numerical scheme then the accuracy will change. And if you change delta t or delta x it will change if you change the way you define the derivatives then the numerical scheme changes and therefore, accuracy also may will change may change.

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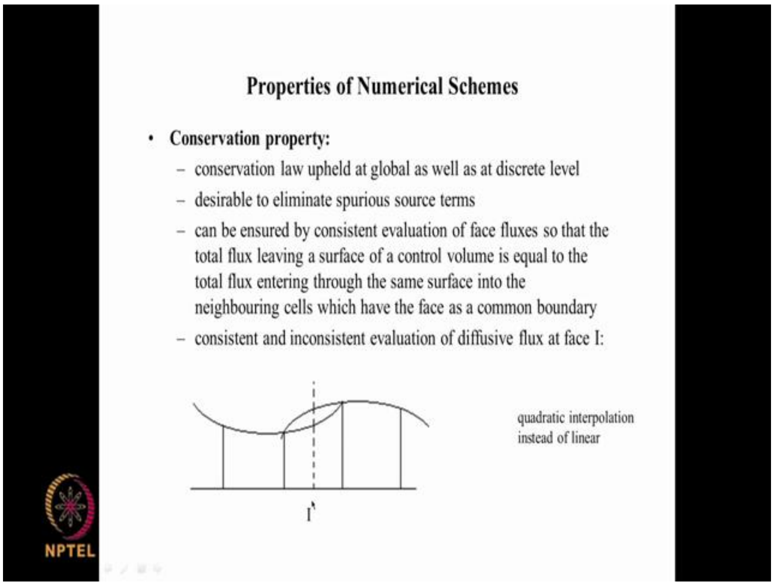

Another property which is also very important is a conservation property. This is something that comes especially in the case of finite volume methods, where we express the terms in the scalar transport equation in terms of fluxes. We have a convective flux and we have a diffusive flux, and the diffusive and convective fluxes are evaluated at the faces of these control volumes. For example, if you are looking at i being the point at which you want to evaluate the flux. Usually flux is in the case of convective flux it is determined by the velocity at which it is coming in and the value of the variable, but in the case of diffusive fluxes then for example; temperature gradient or the concentration gradient will tell us what is the heat flux and then mass flux respectively. So, if you are looking at a situation where you have point a node here and a node here a node here and a node here, and you have values of the function which will be let us say which are like this it is here decreases and then increases and then decreases in this way. And you need to evaluate the gradient at the point i.

so you could say that I evaluate the gradient using these 2 points, but you could also say in the case of for example, quadratic interpolation of quick scheme or you could evaluate the value of this using this point this, point this, point and up string points here. When you evaluate the flux here for this cell you could be using these points here and then this point. Now the point is that in each case when you do this interpolation you are fitting some algebraic polynomial function which is going through this 3 points for example, and based on this variation you evaluate the flux to be a certain value now for this control volume here if you make use of the same points you get you would get the same flux, but in order to evaluate the flux here.

Now you are using this point this point and this point. So, this polynomial function may be different from this polynomial function and therefore, when you evaluate the gradient here then you may get different value when you evaluate for this control volume and from the value that you got for evaluation as a gradient at the same place for this control volume. And what this means is that the flux which depends on the gradient is now different when it is seen by this control volume, as oppose to this control volume, but we know that if there is a flux here then the flux is going from this control volume and it is entering this control volume, or similarly if it is going in the other direction it is leaving this control volume and enters this control volume. So, the flux leaving the control volume, must enter the same quantity must enter the neighboring control volume.

So, this is what we call as consistent evaluation of flux that is, the flux at a particular location is evaluated consistently. When we consider the 2 cells which are on either side of the particular point either side of the particular face, if this is not the case when we do a flux balance on this then we say the flux at this point is this much at this surface is this much and the difference between these 2 is going to lead to the accumulation. When you come to this point here you have a flux here, which is not the same as a flux here, because you have used different set of points to evaluate the to interpolate the value of the gradient here and; that means, that the flux leaving this not all of that is coming into this. So, there is a loss of flux or may be more flux. Then what you evaluated as to the leaving here is coming into this.

So, that is that creates spurious source of flux in either case you do not have flux balance and that can give raise to problems. So, consistent evaluation of the fluxes at the faces of the control volumes is necessary in order to honor this conservation property. So, that is a conservation equation means that you have a conservation of angular momentum or linear momentum or total energy in a particular control volume. And in the process of evaluating that if you are generating spurious fluxes then you are not going to be able to satisfy that conservation property. So, the conservation property is lost at the discrete level.

There is an important a point when we evaluate gradients at faces at nodes and faces boundaries of the cell.

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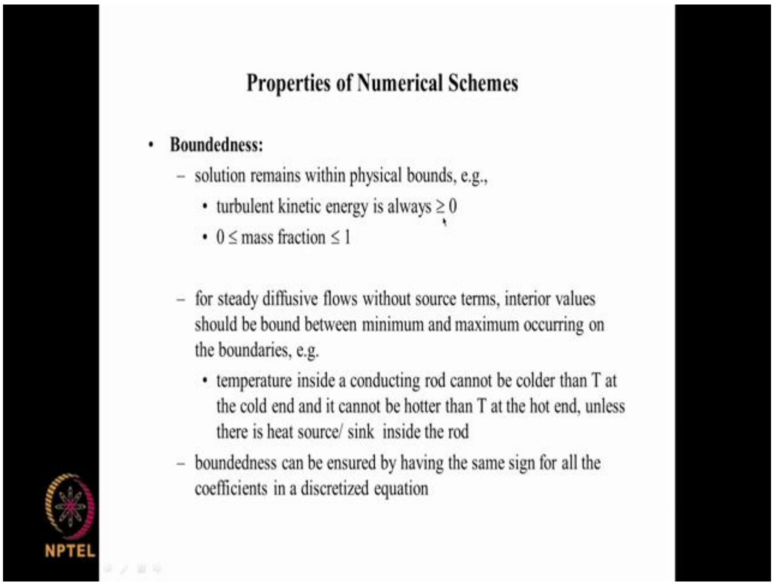

Another property that is very important from the practical point of view is the boundedness. For example, when you look at something like a mass fraction it has to be between 0 and 1 and when you look at a variable like temperature; obviously, negative temperature means nothing, mathematically it does not matter whether the temperature is negative or positive. It is only the value of temperature at this point compared to the value at of temperature at this point and the relative difference is what is going to make the flux temperature the heat flux. So, as far as the code is concerned, when you are evaluating the gradient it does not matter whether the temperature difference a is 100 minus 90 or minus 90 minus 80, but for us to say temperature is minus 90 absolute makes no sense because the absolute value temperature can be 0. In the Kelvin scale for example, similarly mass fraction cannot be negative turbulent kinetic energy which will see later on is always a positive quantity or it can at least be 0.

So, these are the kind of things that need to be honored, the value of the variables in this case the mass fraction and kinetic energy these are bounded to be in a certain limit and this case it is bounded to be greater than or equal to 0. You cannot it cannot be the negative, and here this is bound between 0 and 1, and this particular condition is not always satisfied especially, when you have i already mentioned earlier. When you are looking at using higher order schemes and we will come to that towards the end of this module will come back to that and we will see that in such a case in certain cases it is possible for the value of the variable to go beyond the bounds. In fact, we have seen that with the here.

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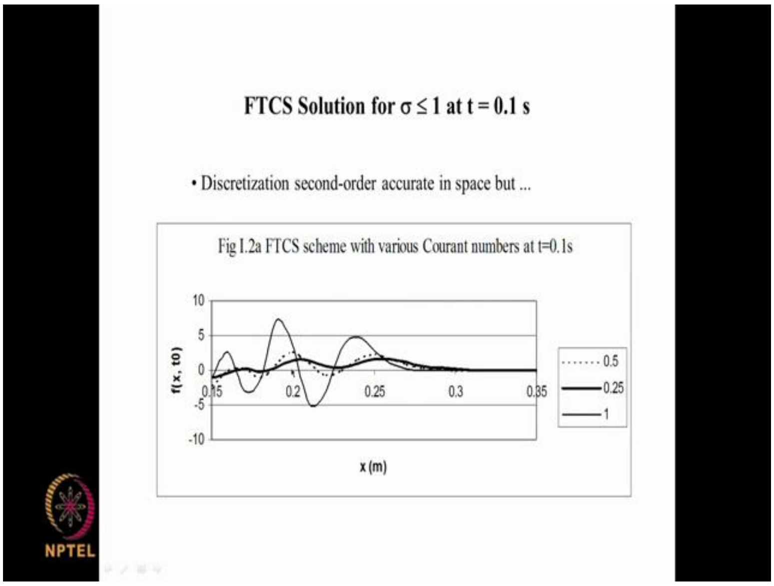

We have u which is supposed to be like square pulse here.

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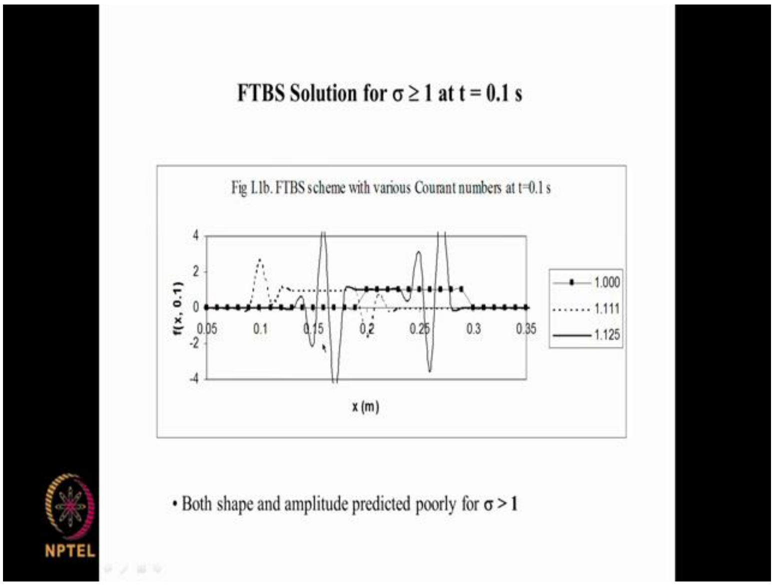

But it is becoming very low value negative value it should be between 0 and 1. So, those are the kind of things that may arise here, and also we have the condition a well known condition that for steady diffusive flows without source terms interior values should be bound between the minimum and maximum values occurring on the boundaries for example, temperature inside a conducting rod cannot be colder than the temperature at the cold end and it cannot be hotter than the temperature at the hot end. Unless you have some heat source or hot sink inside the rod. So, these kinds of things are some things that we expect the properties the boundedness or the property is something that needs to be honored and under certain cases it is possible to ensure boundedness and that we will see in later modules.

Apart from this conservation property boundedness and accuracy. When we are looking at the convergence.

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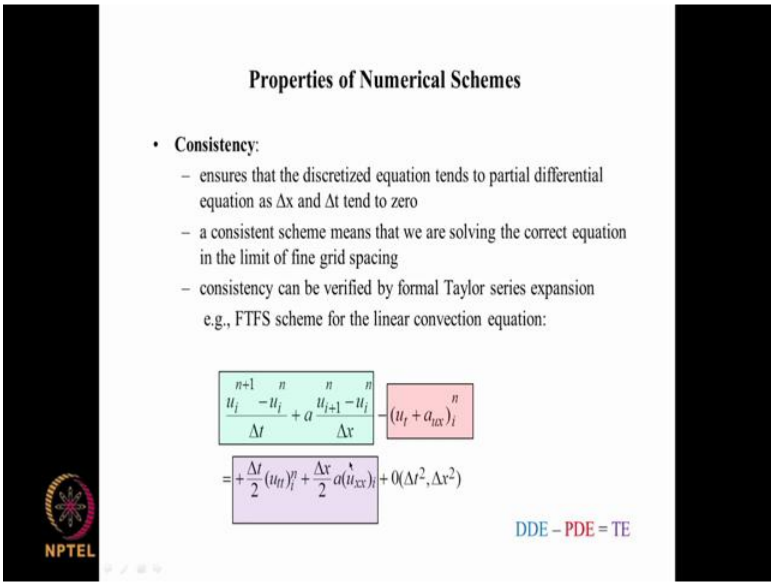

The goodness of the solution apart from those things, we have the consistency conditions and we also have the stability condition. So, and we mentioned that there is a powerful theorem of flux, which is applicable for linear initial value problems, well posed linear initial value of problems. Where if we can show that consistency is there, that is the discretized the equation is an accurate representation of the partial differential equation and if stability is there.

So, that is in the process of time marching, we are not accumulating and the small errors that are made at each time steps and at each space step. And these errors do not accumulate and render the problem unstable. So, if stability is there then we can have convergence. Convergence is guaranteed. So, in order for at least under the limit is of linear equations. If you can demonstrate consistency and stability then we can expect to get convergence and we have as we have seen if convergence is there, then we only need to make the grid spacing very, very small in order to generate a grid independent solution which we can confidently expect to agree with the exact solution of the partial difference equation. So, consistency is an important property from the point of the view of getting a proper solution, and consistency here ensures that the discretized equation tends to partial differential equation as delta x and delta t tend to 0.

So, if you have a discretized equation and a partial differential equation, the difference between the 2 is the truncation error. So, you can say PDE is equal to DDE plus the truncation error. So, if the truncation error goes to 0 then we can say that the DDE approaches PDE as delta x and delta t tend to 0. So, a consistent scheme means that we are solving the correct equation in the limit of very fine grid spacing in both delta x and delta t and delta y delta z as applicable.

So, this condition of consistency can be verified by formal Taylor series expansion for example, for the FTFS scheme for the linear convection equation which is dou u by dou t plus a dou u dou x, there is a mistake here a small mistake u should be here it is not a subscript now the evaluation of this PDE, this part of the PDE at i and n is made using the FTFS scheme in this way, that is u i n plus 1 minus u i n by delta t which makes it forward in time plus a times forward in space u i plus 1 minus u i divided by delta x both at n. So, this is an explicit FTFS scheme and this is for this scheme, for this equation being equal to 0. For this these 2 terms together the sum being equal to 0 for that PDE we have this as the corresponding discretized equation and the difference between the 2 is the truncation error which is delta t by 2 plus the second derivative of u at i and n plus delta x by 2 times a times second derivative of u at i and n plus other terms which are of higher order accuracy. So, this makes the whole scheme first order in time and first order in space ok.

Now, if you examine this truncation error here, as delta x tends to 0; this 1 will tend to 0. Because you expect dou u by this dou square u u by dou x square at a specific point here, to have some finite value similarly the second derivative with respect to time this derivative here at a given point in space and time will have a finite value, and that value is a function of how u varies with t and x. So, we can expect that to have a finite value and as delta t tends to 0, as this becomes smaller the truncation error will become smaller because this is reducing to 0, and this is reducing to 0. So, as delta t and delta x tend to 0, in this particular case truncation error goes to 0. Therefore, the DDE approaches PDE the discretized, difference equation approaches the partial differential equation. Therefore, you would say that FTFS scheme is consistent in the limiting case of delta t delta x tending to 0 the discretized equation approaches the partial differential equation and therefore, it is consistent.

Now, what we notice here what we recall is that, the f t c f s scheme was a failure in terms of being able to reproduce the carrying forward in the x direction of the rectangular pulse. So, what this means is that consistency is not sufficient for us to deliver a correct solution, but it is a necessary condition. So, if you need to have this consistency and this is satisfied by this FTFS scheme which is otherwise not good, and you can go back to the FTBS scheme and FTCS scheme, and we can in each case we can find the truncation error for each of this and will find that in all the 3 cases, we have consistency. So, it may appear that consistency is a foregone conclusion. When we do this finite difference approximations, but that is not always true.

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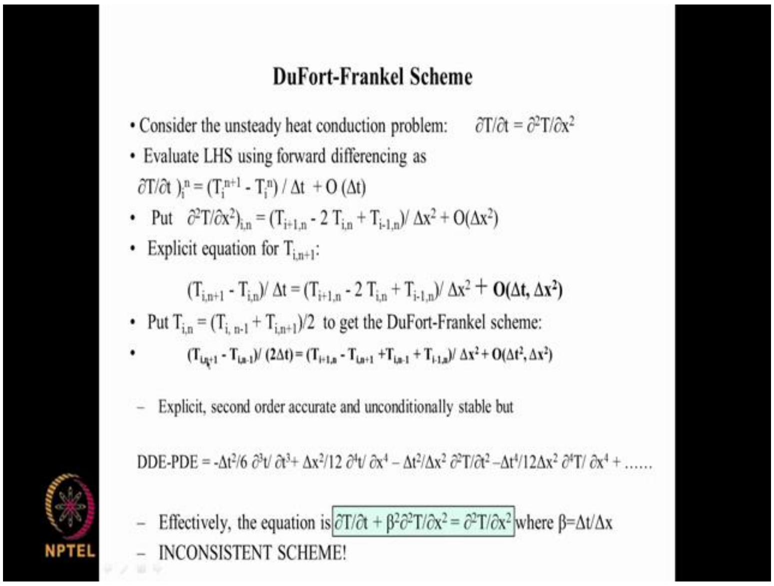

As we illustrate in the case of this Dufort Frankel scheme and consider this unsteady heat conduction problem, where you given by dou t by dou t equal to dou square t by dou x square. Where capital t is the temperature and small t is; obviously, the time and the thermal diffusivity alpha which comes here is taken to be 1, does not matter this is the partial differential equation, and we can use first order forward in time for dot t by dou n dot t at i n and it is given as t i n plus 1 minus t i n by delta t plus terms of the order of delta t the right hand side is evaluated explicitly using central difference scheme. So, you have it as dou square t by dou x square i n equal to t i plus 1 n minus 2 t i n plus t i minus 1 n divided by delta x square and other terms of the order of delta x square.

So, you can put these strings together to get an explicit equation for t i n plus 1 in this particular way and the resulting scheme is first order accurate in time and second order accurate in space because this is evaluated using a central difference scheme and this is evaluated using a forward difference scheme of first order. Now we can make a simple substitution here, we can say t i n is equal to t i n minus 1 plus t i n plus 1 by 2. So, that is the value of t i at time step n here is being taken as the average of the value of t i t at the same location i average of the previous time step and the next time step. That seems to be because we have that is a central difference. So, that is a second order approximation. So, that should be. So, if you substitute that expression into this then we get an equation of this particular form, and this is the equation by which we can evaluate t i n plus 1, and ah. So, what we see here is that on this side you have t i n plus 1, but that is at the same location here here you have t i plus 1, but this is at n and you have t i n minus one. So, the previous time step. So, this is known and t i minus 1 n. So, this is known here.

So, the resulting equation is explicit. We can show through a Taylor series expansion this actually second order accurate in time and second order accurate in space. So, we gained an order of accuracy in terms of with respect to time, and not only that we can also show that this is unconditionally stable.

So, we are satisfying even the stability condition which we will see in the next lecture, but if you look at the truncation error for this. So, that is the DDE minus PDE, then through Taylor series expansion, we can show that it is of this particular form where all the derivatives are evaluated at i and n, at the same x and t location. So, this if we notice here this is given as minus delta t square by 6 times the third-derivative with of capital t with respect to time plus delta x square by 12 times dou square t this is capital t here, with respect to space here plus delta t square by delta x square dou square t by dou t square minus delta t 4 by delta 12 x square, dou square dou t dou 4t by dou x 4 and on like this. Now if you look at this expression here as delta t tends to 0 this term will tend to 0 because this will be a constant and this this becomes smaller. Again this term here is becoming smaller and smaller where as this term will have a certain value and. So, this also goes to 0.

Now, if you look at this term here, this term will have a constant value dou square t by dou t square, but this term here is not going to 0 unless you keep delta you reduce delta t, but reduce delta x faster. For example, if you take a delta t of 0.1and delta x of 0.2 and then you reduce this by a factor of 2, reduce this by a factor of 2. Keep on reducing both in order to meet this consistency condition then this may become 0.0001 and this may become 0.0002, but the ratio may still be 1 by 2.

So, in that sense as delta t and delta x tend to 0 as a square here delta t square by delta x square it is not necessary that this term goes to very small value. So, that makes this one not going to 0, not necessarily going to 0. Whereas if you look at this term here, you have delta x square and this is delta t to the power 4 . So, as you keep reducing delta t and delta x together this term is going to smaller values faster because delta t to the power 4, than delta x square this term here. So, even though this is also delta t to the power of delta t by delta x like that is coming here this will be approaching 0, but not this one here. So, in the limiting case of delta t and delta x tending to 0 we have DDE minus PDE is not equal to 0, but it is equal to minus delta t by delta x whole square time dou square t by dou t square, and if you say delta t by delta x for given grid and time step is beta here then DDE minus PDE is actually minus beta square dou square t by dou t square. So, what we are actually solving is not this one, but dou t by dou t plus beta square dou square t dou x square equal to this should be dou t here equal to dou square t by dou x square here. So, in that sense, there we have it. So, this is the actual equation that is being solved a not this one. So, in that sense in the limiting case of delta t and delta x tends to 0 although we started out with this partial differential equation what we are actually solving using the dufort frankel scheme is this equation.

If you are using FTCS scheme which is this one will be effectively solving this because in that case this term will go to 0 this term will go to 0, but using Dufort Frankel scheme which we got by making this approximation here, we are getting into consistency problem. So, even though the Dufort Frankel scheme has other things which are to it is advantage in terms of unconditional stability for an explicit method and also second order accuracy with time with respect as opposed to first order accuracy here. Despite all the advantages it is inconsistent. So, this is in this way in consistency can creep in because of the assumptions that we make certain assumptions that we make, like this and it does not happen all the time, but in some cases because of the inter play between the time derivatives and space derivatives, you may get into this inconsistency here. So, we have to be careful about inconsistency and we can verify a given scheme we can verify the inconsistency by Taylor series expansion of a corresponding terms hence look at what is the truncation error, and examine whether the truncation error goes to 0 and whether each term of the leading truncation term of the truncation error goes to 0 as delta t delta x delta y tend to 0 independently.

So, in the next lecture we look at the stability problem.