

Computational Fluid Dynamics
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Lecture - 32
Analysis of Generic 1-d scalar transport equation

We now know how to do the Von Neumann Stability analysis, and from which we have looked at how to evaluate the stability conditions for a one dimensional wave equation which is one part of the general scalar transport equation. Now we are going to look at the entire scalar transport equation, but for simplicity of analysis we will consider the one dimensional aspect only, one dimensional form only. And we will consider a linear version of this.

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Generic 1-d Scalar Transport Equation

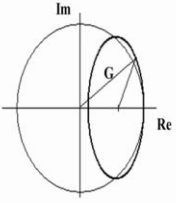
- No source terms, const property and constant given velocity:

$$\partial\phi/\partial t + u\partial\phi/\partial x = \Gamma/\rho \partial^2\phi/\partial x^2 \quad (1)$$
- FTCS Explicit scheme

$$(\phi_i^{n+1} - \phi_i^n) / \Delta t + u (\phi_{i+1}^n - \phi_{i-1}^n) / 2 \Delta x = \Gamma/\rho (\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n) / \Delta x^2$$
- Put $\beta = \Gamma \Delta t / (\rho \Delta x^2)$ and $\sigma = u \Delta t / \Delta x$ and rearrange to get

$$\phi_i^{n+1} = (\beta + \sigma/2) \phi_{i-1}^n + (1 - 2\beta) \phi_i^n + (\beta - \sigma/2) \phi_{i+1}^n$$
- Amplification factor

$$G = 1 + 2\beta [\cos(k_m \Delta x) - 1] - j \sigma \sin(k_m \Delta x)$$
- Stability: $\beta \leq 1/2$ and $\sigma^2 \leq 2\beta$



Here in equation 1 here, we have constant property, constant given velocity form of the one dimensional scalar transport equation which is given as $\partial\phi/\partial t + u \partial\phi/\partial x = \sigma/\rho \partial^2\phi/\partial x^2$. So, here is a scalar transport equation in one dimensional form in space sense, you have only $\partial\phi/\partial x$ here not $\partial\phi/\partial z$. We also have no source terms and we are taking the diffusivity here and the velocity here to be

constants, or this can be considered as linearized values of velocity and diffusivity in case there are changing with space and time.

So, this is linearized constant property one dimensional scalar transport equation. It is also known as the viscous burgers equation, and it has contribution to 5 variations coming both from the advective term which we have seen earlier and the diffusive term. In a way this is mimicking the basic transport equation that we are try to solve in a navier stokes equations.

Let us consider the simplest possible scheme for this, this FTCS explicit scheme therefore, we discretize the time derivative as a forward in time and the space derivatives $\frac{d\phi}{dx}$ here and $\frac{d^2\phi}{dx^2}$ using center scheme and we take the explicit form of this therefore, we write $\phi_i^{n+1} - \phi_i^n$ divide by Δt . And this is done using central scheme u is constant, so we write it as $u \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}$. This $\frac{d^2\phi}{dx^2}$ making it explicit method and this equal to $\frac{\gamma}{\rho}$ which is constant times a central difference explicit formula of this is $\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$.

So, this is a discretized form of the one dimensional constant property scalar transport equation including the convective derivative and the diffusive component terms in the governing equation. For simplicity we can put here you have Δt terms Δx and then you have u here. So, we have courant number term which is coming from the advection term part here. And then similarly Δt times $\frac{\gamma}{\rho}$ times divide by Δx^2 here. So, that gives rise to something like a diffusivity term which is coming here. So, we can put this as another non dimensional parameter β .

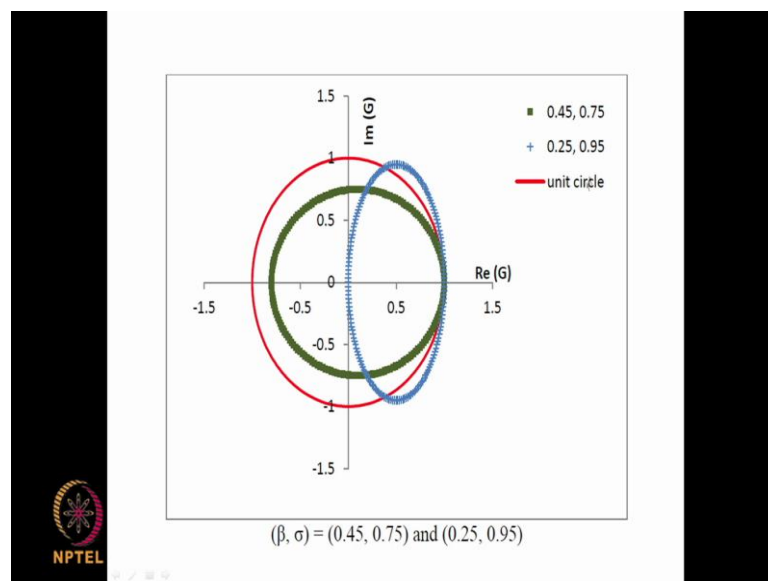
So, we put β equal to $\frac{\gamma \Delta t}{\rho \Delta x^2}$. So, just taking this Δt here and we put courant numbers σ equal to $\frac{u \Delta t}{\Delta x}$ and once you put this you can rewrite this as $\phi_i^{n+1} = \beta + \sigma \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2}$ you have $i-1$ coming from courant number here. And then you also have the β term contributing to this, so β plus when you take it to the right hand side you get

this has plus sigma by 2. And $1 - 2\beta \cos \phi + \beta^2 - \sigma^2$ again this is n here, n is missing.

And for this scheme we can go through the conventional one dimension stability analysis as we have seen just now, we can substitute d equal to $d + 1$ and then we can put $n + 1$, we can get the error evaluation equation and then we can investigate the n th wave component and we can get in amplification factor and that amplification factor looks like this. So, you have g equal to $1 + 2\beta \cos \phi - 1 - j\sigma \sin \phi$.

So, we can evaluate the variation of g for different values of ϕ because we know ϕ goes from 0 to π as the wave number goes from 0 up to capital m in discrete steps, for given value of σ and for a given value of β you have a computable value of g from this expression here because of the j term here this is an imaginary number. So, we can plot it on imaginary component here. And then, the real component here and we can get a value of g here as we change ϕ will be traversing down this route, down in this form here and as we change β and σ again the value of g changes.

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Now we can see what would happen for different values of beta and sigma here and here we are considering beta and sigma pairs to be having 0.45 and 0.75 and 0.25 and 0.95. So, the green one is the case where you have 0.45 of beta and 0.75 of sigma. If you consider just this scheme with only the advection term with zero diffusion term we have seen that FTCS explicit is unconditionally unstable. Similarly, if you neglect that advective component and if you just take the diffusive component here, and then we put $\frac{\partial \phi}{\partial t} = \frac{\sigma}{\rho} \frac{\partial^2 \phi}{\partial x^2}$ we can show through one stability analysis that that scheme will be unstable for beta greater than 0.5.

So, here we are considering the beta 0.45 and sigma 0.75 which is less than 1 and this is less than half here. So, for that value of Δx for different values of Δt you have an ellipse here which lies entirely in the unit circle of 1. That means, that this particular combination here is good, it is stable because if at no point we have Δt greater than 1. But if you take another set of values both of which satisfy the individual condition of beta less than 0.5 and sigma less than 1 here, you see that if you substitute these values in this expression for different values of Δx and then you draw the corresponding Δt here, you see that Δt is sometimes going beyond sigma equal to 1.

The true condition for this stability of this is not sigma less than 1 and beta less than half which are individually coming from these equations it is that $\sigma \Delta t^2$ should be less than 2 beta when these conditions are satisfied then we get stability. If it is not satisfied we get instability as we will see from here. So, this condition is satisfying that $\sigma \Delta t^2$ less than 2 beta, but this is not satisfying that condition here.

So, that is a kind of analysis we can write and what we can also see from here is that although the FTCS explicit scheme is unconditionally unstable for just the advection term, the presence of the diffusion term has made it conditionally stable it is now stable conditionally for $\sigma \Delta t^2$ less than two beta, and that is in that sense the addition of this term has made the scheme conditionally stable from unconditionally unstable.

So, different terms contribute in different ways and the diffusion term is actually surprising some of the instability under certain conditions. So, what we have been able to establish from this analysis is that when we have a scalar transport equation, we can find

a conditional stable solution under certain conditions, under the condition of sigma square less than 2 beta. If this condition is satisfied we can get a stable scheme and we can also show that this scheme is consistent, so we can expect convergence with this thing. But with this FTCS explicit scheme for this equation here, there are some difficulties that are although we seem to be getting a stable solution.


(Refer Slide Time: 10:36)

Generic 1-d Scalar Transport Equation

- Oscillations are produced with FTCS explicit if $2 \leq Pe \leq \frac{2}{\sigma}$ where $Pe = \rho u \Delta x / \Gamma$ is the mesh Peclet number
- This loss of boundedness can be cured by
 - decreasing grid spacing so that $Pe < 2$ or by
 - using an "upwind" scheme for the convective term
- upwinding for convective term assuming $u > 0$ yields

$$(\phi_i^{n+1} - \phi_i^n) / \Delta t + u (\phi_i^n - \phi_{i-1}^n) / \Delta x = \Gamma / \rho (\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n) / \Delta x^2$$

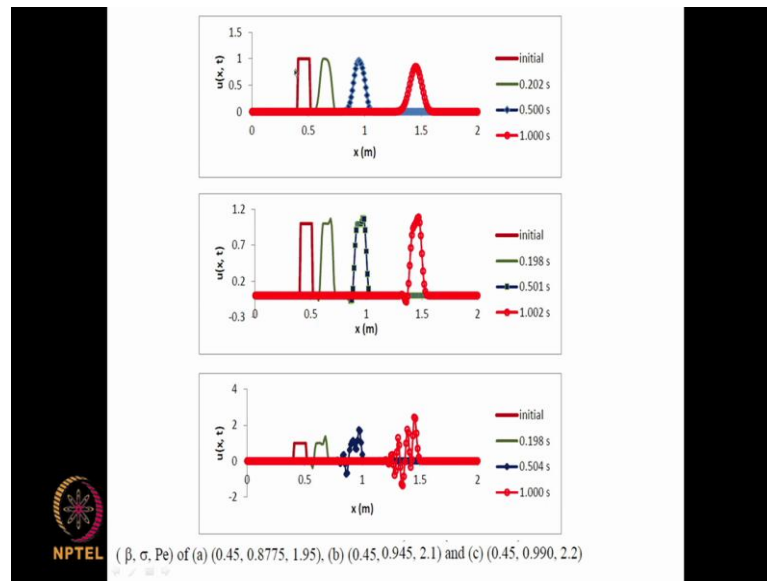
- or, $\phi_i^{n+1} = \beta \phi_{i-1}^n + (1-2\beta-\sigma) \phi_i^n + (\beta+\sigma) \phi_{i+1}^n$
- Stable, oscillation-free solution if $(2\beta + \sigma) < 1$
- Stability analysis becomes more complicated in 2- and 3-d, non-constant coefficients, non-uniform grids etc.



The solution itself can give us to oscillatory solution, oscillations and these oscillations are in the special direction not with the respect to temporal thing, under certain conditions that is if you define a Peclet number and mesh Peclet number as rho u delta x divide by sigma where sigma is diffusivity and u is obviously the velocity and rho is the density.

So, if certain values of Peclet number which lie between 2 by sigma will give raise to oscillations.

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So, that is what we can see here these are an initial square pulse lying between 0.4 and 0.5 at time equal to 0 with a value of 1 here and 0 otherwise, that is the initial condition. We are going to look at how this pulse is transmitted in the x direction at the velocity u while it is also diffusing. So, the evaluation of this square pulse is subject to this equation here. So, it will both be convected in the positive x direction and is also diffusing with a diffusivity of this.

Now, what kind of solution we get if we use the FTCS explicit scheme within the stability bounds. So, that particular scheme now has 3 parameters beta, sigma and Peclet number which a combination of these two here, and we are looking at the specific case of Peclet number being less than 2, greater than 2 and greater than 2 by sigma. So, we have said that if Peclet number is greater than 2 by sigma its unstable and if it is less than 2 we get a stable solution and if it somewhere in between it we get some special kind of character. And that is what we are looking here.

In this particular case we have beta as 0.45 and sigma as 0.8775. So, this these two values such by the condition of sigma square less than 2 beta and we also have a corresponding derived value of Peclet number as 1.95 and this also less than 2.

So, under these conditions we should be getting a stable solution and we also see this pulse at 0.2, 0.5, 1 second where it is and we can see it is being convected and we are getting a smooth solution. And part of the smooth solution is obviously from the diffusion. So, we can see that this square pulse which is like this is moving in the positive x direction and with a speed which is matching with the Δt variation and is also diffusing giving rise to that smooth and variation. So, it looks good.

But if you were to choose a different value of σ which still satisfies the $\sigma^2 < 2\beta$, this is satisfying the condition of $\sigma^2 < 2\beta$ that now the Peclet number is likely greater than 2, it is 2.1. And what we see here is a solution which is somewhat strange, it is beginning greater than 1, it is in a way anti diffusing. It should be beginnings smooth like this, but is beginning greater than 1 here and here it is less than 1, less than 0 here and greater than 1. So, it is giving rise to these, but it is not actually giving rise to any kind of unstable solution.

We can see a pulse which is still at the same location slightly more distorted than this case. So, it's stable, the variation is growing with time, but it is still growing it is still retaining that overall form that is expected and certainly something like this is not desirable because if u is actually representing some mass fraction then we are getting negative values of the mass fraction and that is undesirable. And we may be getting greater than 1 here and this solution is not physically acceptable.

A stable solution can give rise to this kind of unphysical solutions in certain cases and when we choose a different value of σ such that your Peclet number is greater than 2.2 we get unstable solution. And this is different from this only in the small change in σ here from 0.945 to 0.99 we change it. That also changes the Peclet number from 2.1 to 2.2 and we get like this is truly an unstable solution whereas this is not unstable solution. So, we can clearly see the difference here.

And small changes in the value of σ here violating that $\sigma^2 < 2\beta$ condition are giving rise to unstable solutions here. But as long as we maintain that $\sigma^2 < 2\beta$ solutions, we are getting good solution for Peclet number less than 2 and for Peclet number greater than 2, but less than 2 by σ we are getting

this undesirable solution here. In that sense this is not such a good thing and how to remove this undesirable solution, while retaining the stability even if we have stability here we still have a physically undesirable variation here and that is not acceptable. And this variation can be removed in two different ways here.

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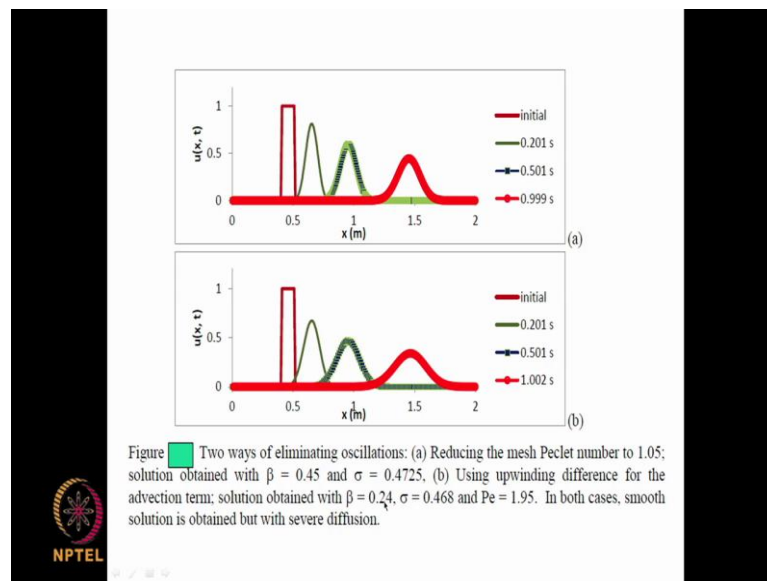


Figure 1 Two ways of eliminating oscillations: (a) Reducing the mesh Peclet number to 1.05; solution obtained with $\beta = 0.45$ and $\sigma = 0.4725$, (b) Using upwinding difference for the advection term; solution obtained with $\beta = 0.24$, $\sigma = 0.468$ and $Pe = 1.95$. In both cases, smooth solution is obtained but with severe diffusion.

So, here we have two ways of eliminating these oscillations one is reducing the mesh Peclet number in such a way that its much less than that 2 by sigma value and here is a case where Peclet number has been reduced to 1.05. And the solution is obtained with the same beta value, but sigma is reduced to 0.4725, so that we have reduced Peclet value and at the same time almost 0.2, 0.5, 0.999, it is about one second. We now get an oscillation free solution.

And another way is to use upwind differencing scheme for the advection term. So, what is this upwind differencing scheme and upwind differencing means that the special derivative related to the advection term $\frac{du}{dx}$ is written as $\frac{\phi_i - \phi_{i-1}}{\Delta x}$, when you have $u > 0$. So, when u is greater than 0, this pulse is expected to move in this direction, when the pulse is moving in the positive x direction we use backward differencing for this for the $\frac{d\phi}{dx}$.

And when use negative, that it is expect to in this direction we make use of forward differencing for $\frac{d\phi}{dx}$ and we write this as $\frac{\phi_{i+1} - \phi_i}{\Delta x}$. So, depending on whether the pulse is whether u the velocity associated with the advection term is in the downstream direction or in the upstream direction we make use of the backward differencing or forward differencing.

So, essentially what this is saying is that the value here is coming from upstream direction, so it is in the direction of wind. In the direction of wind is the solution that is being brought in here. So, the difference between the previous term and this term is $\frac{\phi_i - \phi_{i-1}}{\Delta x}$ or $\frac{\phi_{i+1} - \phi_i}{\Delta x}$ therefore, this is first order accurate scheme. And in the other case it is a central differencing, therefore, this is second order accurate scheme.

Once you substitute this backward differencing scheme assuming u to be positive we get in the equation like this. So, the diffusion term is unchanged and the time derivative is unchanged it is only this one which is change from central differencing to backward differencing. So, we can call this as forward in time, backward in space, and central in space. So, FTCS kind of approximation with the backward in space for the advection term with positive u .

So, with this we can rewrite $\phi_{i,n+1}$ as $\beta \phi_{i-1,n} + (1 - 2\beta) \phi_{i,n} + \sigma \phi_{i+1,n}$. In this both β and σ are positive so that means, that this term has a positive value and this term has a positive value and we can do a stability analysis. And show that this particular scheme is stable for $2\beta + \sigma < 1$ so that means, that $2\beta + \sigma$ is always less than 1 for stability and once you substitute this, $1 - 2\beta - \sigma$ is also a positive quantity. So, you have $\phi_{i,n+1}$ is given as a positive coefficient times this plus another positive coefficient times this plus another coefficient positive coefficient times this.

So, when you have an expression like this where $\phi_{i,n+1}$ is given in terms of positive coefficients times the cell values like this, when all the coefficients are always positive we can be sure that we want get an oscillatory solution, where an oscillation

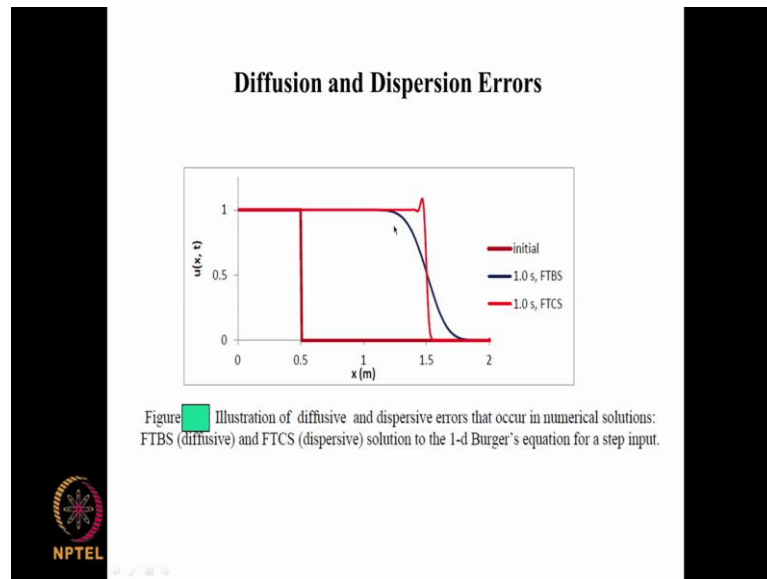
solution is not expected. So, we can get an oscillation free solution for 2β less than σ less than 2. So, that is what we are seeing here.

In this particular case 0.468 and 0.24 is β under this and we have a Peclet number almost close to 2. So, we have the condition of $\sigma + 2\beta$ being less than 1, just about less than 1.468 plus two times, as 0.48, it is about 0.95. So, it is slightly less than 1. So, we can expect a stable solution with this and that is what we are actually got. We are getting stable solution which is moving forward which is also diffusing. So, we can suppress these kind of on stable oscillations that we getting here under undesirable oscillations under stable conditions can be eliminated by either reducing the Peclet number, mesh Peclet number or by using upwinding differencing.

In both cases we are getting solution, but even here we can see that the solution is not exactly the same at one second, this seems be much more diffusive than this. And when you compare this with the previous solution here this seems to be better than this scheme here because the solution that we are getting at one second, that is 0 all they up to this and then pulse and then again 0 here.

If you want to compare this with this thing here, the pulse is about the same location the peak is about the same. But it is diffused over a larger x value here, and this is diffused even over even larger value and you can see that corresponding the peak value is less than 0.5, it is slightly more than 0.5 and here its much closer to 1. So, you have much more diffusion in this case, in this case. We are gaining on stability and smooth solution at the cost of increased diffusion.

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This is something that we have with numerical schemes. With numerical schemes we have what is known as diffusion error and dispersion error. Diffusion error is, for example, in this particular case, this is a pulse which should have come to at 1.5 meters per second. It should have come at and be a sharp step down exactly like this. But a diffusive solution actually gives you a smooth solution like this. Instead of being a sharp step down, it is diffused over a much larger length. In this case, all the way from 1.3 to 1.7, it has a non-zero value. It has less than 1 value. A dispersive solution produces these oscillations like here. We can see small waviness that is there, and this waviness may increase as it goes backwards here with time as it's moving forward here. So, this is a characteristic dispersion error.

Numerical errors are of the diffusion type or the dispersion type or a combination of both, and this is something that we should keep in mind. If you want to reduce the dispersion error, then we could be introducing this diffusive error, and that is what we are seeing here. We wanted to reduce this dispersion error here, and in the process we tried reducing the mesh Peclet number, we got more diffusion. And we tried upwinding differencing to eliminate the oscillations, and then we got even more diffusive things.

So, we have to balance the amount of stability to reduce dispersion errors with the additional diffusivity that may be introducing, and this is where in order to capture these sharp gradients that are common in compressible flows at high speeds under supersonic conditions like in shock waves you have these kinds of gradients. In order to capture this gradient well we need to have better differencing schemes than highly diffusive FTBS scheme or dispersive FTCS schemes. And people are come up with concept of a total variation dimension TVD schemes, and ENO essentially non oscillatory schemes like that to get a solution which is as close to a square pulse as possible for this type of thing.

In which there is very little diffusion and no dispersion. So, it is an essentially non oscillator solution with very little diffusivity much less than what we get with the simple upwinding approach or with this highly diffusive approach that we are seeing here. So, the idea there is to see under what conditions a dispersion solution is produced and how much diffusion we can add we need to add in order to suppress that oscillation there. So, it is a targeted and metered amount of diffusivity is put in there.

With those kind of things it is possible to get a solution which looks almost like this square pulse or like any other expected shape without introducing too much of diffusion dispersion error. But that is not part of the course here this is only an introductory course. It is discussed in books like the Book by Harsh, is one such book which discusses this TVD schemes extensively and that will be of interest to people dealing with comprehensive flows and where shocks may be expected. In general subsonic flows inside internal bodies probably we do not get these sharp gradients and we do not to have go for such schemes.

We can probably deal with second order scheme and we can get fairly accurate resolution of the gradient for us to estimate the heat fluxes and all those things. What we would like to mention at this point is that when we have first order scheme, we can have huge diffusion we can have large amount of diffusion and that is way it is preferred to have second order schemes. Second order schemes introduce a dispersion error and if that dispersion error is likely to be affecting the solution we have to care to minimize it.

So, that is about diffusion dispersion errors and about the basic ideas as to how we can get a satisfactory solution for a one dimensional scalar transport equation. So, we have got a template for consistent, stable and oscillation free solution. With this scheme we can go in for the solution of Navier-stokes equation and that is what we are going to do in the next module.