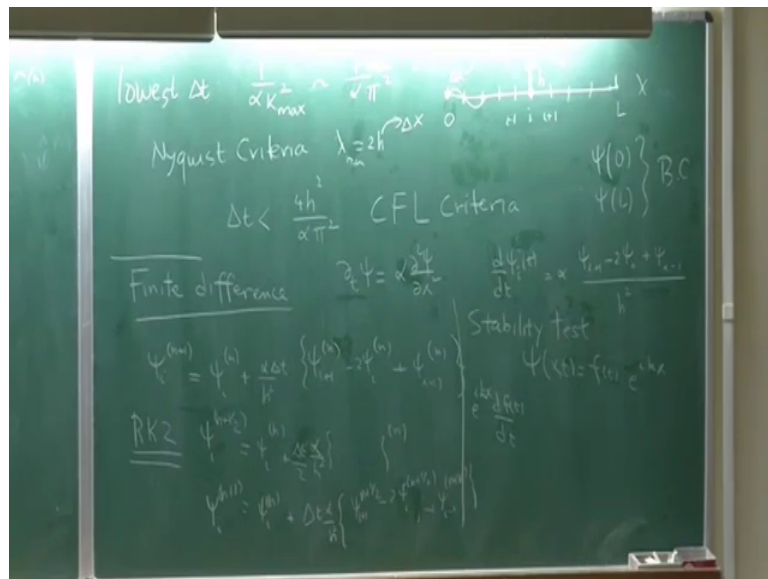


Computational Science and Engineering using Python
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Lecture – 19A
PDE Solver: Diffusion Equation using Finite Difference Method

So, now let us try to do this in real space.

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So, the new method I am going to describe now is called, so we will discretise in both real and time. So, if I had done over here, so this is my 0 this is my 1 right, so same equation let us just focus on same equation, and I have discretised it. So, let us convert this equation in finite difference form.

So, let us write it here, so the simplest scheme here, I will do this by central difference scheme double derivative, I will label them as $i-1$ i $i+1$. So, partial derivative at point i this point i , now I also have the time index, so let us say I am doing at time t . So, this is my variable its n this is time remember I had put a label this is for time index, so what I am trying to do here is that I convert this to again ODEs, but value the function at every time, so this is a time t let us just put time t . So, this becomes the ODE, I have focus on this point at time t , so I need to compute this right hand side double derivative with a value with a function at time t , so it will be α , what is the double derivative y

time by finite difference. So, $\psi_{i+1} - 2\psi_i + \psi_{i-1}$ by h^2 . So, this is my double derivative.

So, what do what have I done, I got ODEs, how many ODEs have I got equal to the number of points. So, this is makes to the n points, but you have to be careful or should I time step the function here and here should I time step it or not, what is the value of function at those I have holes 0, I should not time step the boundary values. So, these two I do not want to time step value and the function here and here where they are 0's. So, these are the boundary condition ψ at 0 ψ at l boundary, so do not time step, so do not add equation for that, but write equation for everything else, now how do i time step this usual technique, so ψ_i at $n+1$ equal to ψ_i at n plus Δt times this Euler explicit plus, so there is a minus sign no this is the plus sign plus sign plus α by h squared Δt . Now these are computed at n t , so I should be ψ_i $n+1$ plus 2 ψ_i not n by n , now in principle I have solved the problem, I have to just put in the computer and solve it.

Write them in you have to just instead of one ODE you have to solve ODEs for all the points except the boundaries, so this is a finite difference. Now what should your delta t and what should be your delta x. So, my spectral method gives you some prescription about delta t, so something should happen here, as well right I mean you can not one method say something other method some reflection should be appearing in the other in the method 2 as well. So, to figure it out let us try to put some trial solution; so trial solution, is I am going to try ψ of x t , so I am going to infinite I will put in this equation f t . So, this is to test stability. So, this is a standard technique. So, I am going to put this amplitude will it grow in time or will it sink in time or will it decrease in time. So, I need to try this. And I am going to plug it here. So, I hope there is enough space. So, let us just plug it in here. So, the time derivative will act only on this. So, $d F$ by $d t$ E to the power I k x . So, this is in fact, by the way this is general technique. So, you have to for stability and finite difference scheme this is what we try. I am trying to check the stability test ok.

So, let us just plug that in here. So, e to the power kx .

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$$e^{ik(x+h)} - e^{ik(x-h)} = 2e^{ikx} \sin kh$$

$$\frac{e^{ik(x+h)} - 2e^{ikx} + e^{ik(x-h)})}{h^2} = \frac{2 \cos kh - 2}{h^2} f(x)$$

$$\frac{df}{dt} \approx \frac{4 \sin^2(kh/2)}{h^2} f(x)$$

$$f^{(n+1)} = f^{(n)} \left(1 + \frac{4 \sin^2(kh/2)}{h^2} \Delta t \right)$$

$$\Delta t \leq \frac{h^2}{4\alpha}$$

D f by d t equal to right hand side alpha; by h square. Now f will come out from this expression. Now these guys will be appearing here. So, f is coming out; now what will I get here. I get e to the power i k x plus h. So, this is psi i plus 1 this point so this is h this is x. So, this is f i plus 1. If your confused; please let me know right away that is fine; minus 2 I am going to put this here, i minus 1 f i k x minus h minus 2 i x. So, let us take it to i k x common both sides and that cancels. So, d f by d t is alpha by h square. Now this is going to be 2 cos x, 2 cos h. So, you got e to the power i k h plus e to the power minus i k h. So, that is 2 cos k h minus 2. So, e to the power minus i k x got cancelled and this is f here. So d f by d t looks like this. So, convert it to ODE that is and we know how to solve ODEs. Now does it tell you something about the stability now; d f by d t is this equation. So, what is the bound on this? So, this can become 2 right max is 2. So, max 2. So, I get 4 alpha by h square. So, this is bounded. So, make it minus 1, then you get minus 2. So, there is the modulus mod of this is max is 2.

So, for this case stability, so d f by d t for this one, this will tell you that Euler first order, Euler explicit, Euler is always first order for Euler explicit will be f n plus 1 equal to f n 1 minus 4 alpha. So, for this to be stable, when is this stable? I want this condition to be less than 1 order one; if it is bigger than 1 then there is a all hell will break loose. So, this quantity must be less than 1. So, that delta t so, delta t must be less h squared 4 alpha. So, the constants are different h squared by alpha is common, but here I get 4 by pi squared and here I get 1 by 4. So, the finite difference this analysis will tell you that system is

stable, when my Δt is less than this. So, given α and h ; I can estimate what is my Δt_{\min} and whatever you get for estimate you decrease even further down by factor may be for you I would say factor 10, just bring it down to factor 10 or at least factor 5 or that theory is; which is a good number? I mean will it will it equal to enough good enough or I should might divide by factor by some factor 2, factor 4, but for this course I will not deem to it we just say that this number by 10, it may be too tiny, but its I mean. So, your Δt must be this divide by factor.

So, this is a stability condition we need to do it for this scheme; Euler scheme. I would not so I will not recommend that you use this scheme I would say that you use Runge Kutta's second order. So, do you want to solve this equation? So, I can use Runge Kutta two complicated issues which started second order then I will also tell you that you can do some more clever ways. So, in terms of this system; let us do some more stuff then I will get back to finite details a bit more. So, how will you solve this Runge Kutta's second order this scheme this equation. So, I have converted it to this equation. So, what is the Runge Kutta's second order? So, ψ_i at mid so $n + \frac{1}{2}$ will be ψ_i at n plus α by h square all that at n . So, this will give the mid value Δt by 2. So, how good a midpoint? So, in function of time I take this I just focus on this one and I go to the midpoint in time. So, I am suppose to go to in time here Δt , but I go to this value. Then I say well I will now take finite steps ψ_{i+1} is ψ_i plus Δt α by h . So, I have these values now ψ is the midpoint. So, I should use them when compute the second derivative.

So, do not take this second derivative, but compute the second derivative from here which will be ψ_{i+1} plus $n + \frac{1}{2}$. So, this second Runge Kutta's second order yeah.

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Which which which.

Student: Sit that 4.

This one.

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Yes. So, put a minus sign that is. So, for large enough Δt these things as soon as it becomes negative like, what I have argued there the problem come. So, that tells you the condition for Δt ; precisely the same way. So, diffusion equation you had to solve by Runge Kutta's second order you will be reason be safe. Again Δt you just follow that criteria even for Runge Kutta's second order just use that criteria. You can do better, but its is safe. Now, what is a time increasing for Eulers scheme? Is this scheme. So, time increasing will be Δt square, here; for this first order in time this is Δt ts. So, error is of the order of Δt square error per step error Δt square and here Δt error is Δt cube. So, this is what we did before. So, Euler scheme error in Δt square and Runge Kutta's is second orderly accurate. So, error is Δt cube.

So, here the equation was a diffusion equation, we need to worry about stability as well as accuracy stability is critical. So, what we studied for differential equation ODE is we need to worry about it for PDEs as well.