Computational Science and Engineering using Python

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Lecture - 18
PDE Solver: Diffusion Equation in Spectral Method

So, here it is starting very important topic PDE solvers.

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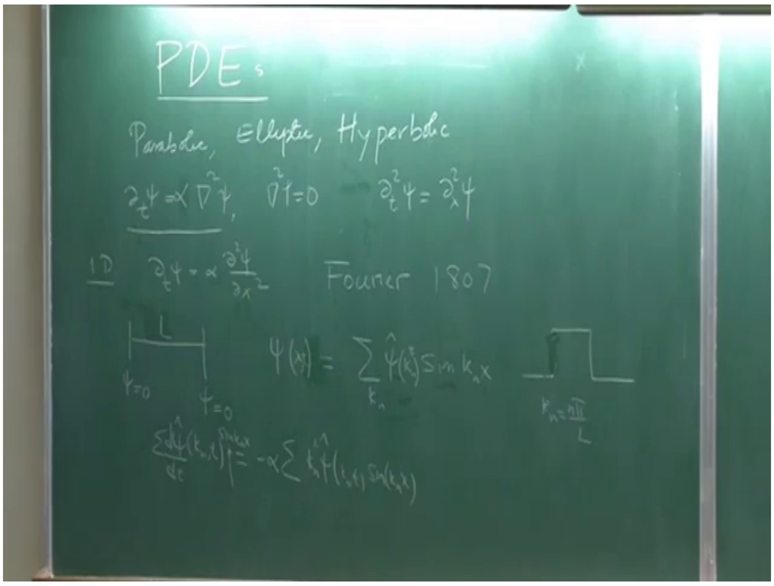

So, the three types; parabolic, elliptic and hyperbolic. So, this PDE classification is critical. So, parabolic I will give only examples, I will not do the math part of this. So, d by d t, this partial t is Laplace in style diffusion equation is full of parabolic. So, these are linear equation. We can also make it non-linear which I will do it later. Elliptic equation is example of elliptic equation. You have done this in your math course. So, example of elliptic equation for what?

No, wave is not elliptic. Wave is hyperbolic Laplace equation. So, this is elliptic and parabolic is hyperbolic. So, we do only these two classes. Not this class. I will do one. Well, I mean basically make a slight exclusion in it, but I will do these two. It is more complicated. So, let us look at first this equation how to solve it in 1 d. So, d t d psi, the D square psi d x square, you know how to solve this by what method.

Student: Separation of variables

Separation of variables then what? So, separation of variable will not really, well first who solved the equation. The first person to solve this equation, it was done by Fourier. Well, it is not separation of variable, but Fourier 18 on 7 and if the Fourier series, you solved in Fourier series. So, the idea is to expand. So, we will assume that I am solving in 1 d grade, where size 0 at both the ends. Please assume that. So, it is very similar to particle in a box or infinite potential. So, size is equal to 0.

So, if this is a case, then Fourier says this person is Fourier, he says that psi x can be expanded in terms of sin functions sin k n of x k n. I can expand in terms of Fourier series. So, this is what he told first. Not this is a very important theorem, he can use this function. Using this expansion, you can expand any function and in fact even discontinuous ones. So, well I am sure this function can also be written in terms of this. So, these are discontinuing at this point and this point. So, Fourier did not know the proof, but he postulated that this can be done and that is the reason why he was struggling. I mean nobody believed that time, yeah.

Student: Why discontinuous?

There is a discontinuity here at this point. There is a junk in the function. Therefore, yeah there is a discontinuous function. The derivatives does not exist. It has two values at this point, but it is a very important expansion. Now, using this let us try to solve this equation. So, what we do is, we will make, so this function of x and t. Now, x part I will, so one more point k n is n pi by l is a box size. So, this one I will make a function of time, this coefficient. So, x dependent and dependence are separated out. So, in some size it is less separational variable, but this way I am going to give the full solution.

Now, let us plug it in here. So, what do I get sum of? So, time derived lagged only on this. So, d by d t of k n t. So, right hand side will be minus alpha. So, if I take the double derivative, what will I get? I will get k n squared psi tilde k n. Now, I forgot I had to put a sin k and x here. So, I can take it to the left hand side and this gives us sum.

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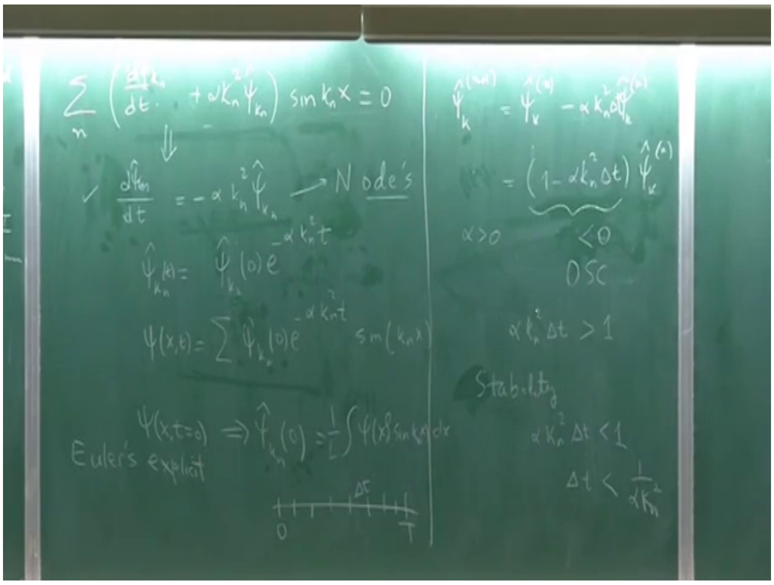

I can write like this, right. This is a notation. Psi n means here a nth for k n. So, this index n actually since we are going to use. So, we have to then, we just put k here, k n plus alpha k n squared psith of k n psi 0.

Now, what can I say about this?

Student: Zero

Should be 0 because these are independent basic function. So, if this to be 0 for all x implies that this quantity is 0. So, hat is a Fourier transform. So, I have converted my partial differential equation into ODE's. So, they have become ordinary differential equation and how many of them? It is infinite of them. So, n goes from bound to infinity for this case. So, infinity equation, but I have succeeded in converting into PDE ODE's. Now, in practice we do need infinite series. So, how do I cut it off. So, this is impossible to get infinite series in practical life.

So, how do I cut this off? So, there will be highest wavelength, highest wave number here. If somebody has to cut off right, there are fluctuation, but the fluctuation with highest wave number is up to that point only I need to go. So, there will be if I look at this time series, I will have something like this and like this, like this. So, there is a shortest wavelength and shortest wavelength corresponds to min k max which is l by no k max 2 pi pi by lambda min. I need to only sum up to that point. I do not need to go beyond it, ok.

Given the time series or somebody gives you the function, I have to just do this, find the lowest wavelength. So, this is set of NODE's and I can now use my techniques to solve this ODE's. In terms of this linear equation is the exact solution. What Fourier did, Fourier was not using a computer. So, this has a solution. What is the solution for this? K n equal to psi n e power to k t now, each of them can have exact solution.

So, what is my final solution? This t is my final solution of will be x t, but I am not done yet because I need to find out what this is. So, how do we compute this one? How will I compute this? This is t equal to 0. So, this has to be computed from the initial condition. So, I will give the initial condition psi x equal to 0 psi x t equal to 0. From this we compute, do the Fourier transform and that will give you, so this is solved. This is how Fourier solved it and it has exact solution, but I want to do numerically. This looks very simple equation, but figure out what are the issues for this problem and it will help you also to solve other more complicated problems, ok.

So, which method or else do the blindly simple method which is Euler. So, first let us do Euler. So, Euler method, Euler’s explicit this one. So, this will be, so I have n of them. For each of them I need to apply Euler. So, psi tilde I am going to put k. So, that is why I was afraid of this and n will conflict with my time stepping n. So, they are symbols. So, I am just going to say this is k for n. I am just specifying k is a wave number. So, n plus 1 equal to psi hat of k n, now this is a right hand side minus alpha k n square psi k n, this is spectral method, no. So, some of you have chose spectral method.

So, this is a Fourier transform. So, I can use this method to solve many differential equation PDEs. So, this is really the spectral. Spectral means I am making into different spectrum that prism spectrum. So, I have broken into different spectrum. So, these are equations for different wave numbers or different colours of light if you like. So, we are solving this. So, this will be 1 minus, no sorry I forgot delta t. No, it is a function of time now. So, you have two things. One is I have decretized in time and I decretized in wave number.

So, I start from t equal to 0, I go to t final, but let us assume that I have done uniform decretization in time. So, this is delta t. So, this must be delta t here, correct? All are explicit scheme, yes. So, this gives me minus k n square delta t psi hat of k now.

Student: Sir

Yeah

This one? So, given the initial condition, this is my solution, but I need to compute this right now. This is my temperature in Fourier space at t equal to 0 and how do I compute it? How do I find it? So, given the initial condition, I can find that, right. So, this is an initial value problem and solving this given the initial value. So, initial value I have to give you what is psi x at t equal to 0. So, first I know this I can do the Fourier transform to get this at t equal to 0. You can do it wrong. Should I write it or? So, your rule is inverse transform and that will give you psi k psi of this integral psi x sin something like this. There will be some factors 2 or something.

So, that is an inversion now. So, this might coming from Euler scheme, the problem will come. So, alpha positive for differential equation, the things are fine. This will converge or for alpha positive, this quantity is real. So, my psi k is n plus 1 will decrease like it decreases here. Now, there can be a problem if my delta t is too large. So, what can happen if this quantity becomes minus 2 minus 1. Ig as soon as this quantity becomes less than 0, then there is a problem.

So, I want this function to be positive. If this is positive, but as soon as this becomes less than 0, then there is a oscillation and the real solution does not have oscillation. This is monotonically decreasing. So, this creates oscillations and when does the oscillation starts? When alpha k n squared delta t greater than 1, so, for my well behaved nature, this is stability. That means, I do not want this oscillation. This is very similar to oscillations we were getting for unstable solution.

It is supposed to monotonically go down to 0, but it is oscillating now. So, for stability I require that this condition should not happen. So, I require that alpha k n squared delta t must be less than 1. So, delta t must be less than 1 by alpha k n squared. This is critical. So, when you do the project, you have to keep this in mind. Now, what is k n? So, k n as

I said look for every k n, I have a delta t. So, what is the worst delta t? The lowest delta t for it say every equation has a delta t correspondingly.

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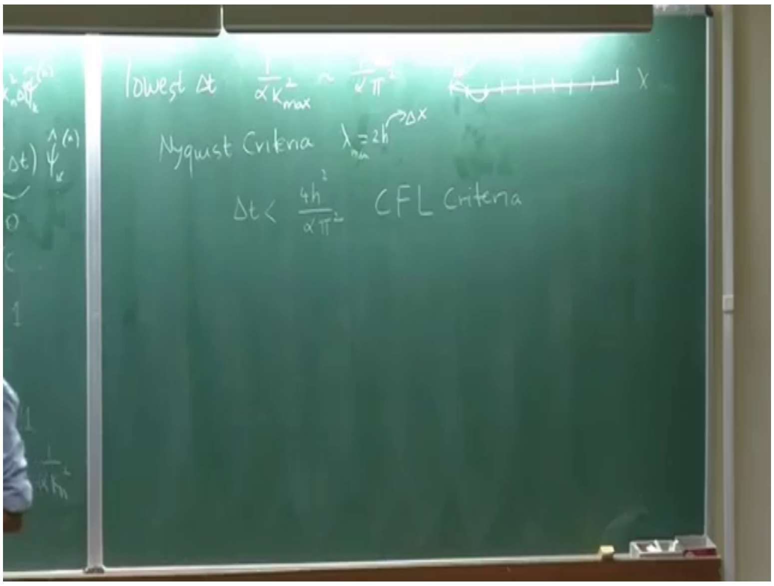

So, lowest delta t will be 1 by alpha k max squared. So, what is k max? So, there will be 1 by pi by pi squared lambda min lambda min, ok.

So, I am going to go now to the finite difference. So, there is a spectral. So, we can also estimate what lambda min is. So, we have a grid. So, now in real space now just so far I was in Fourier space. This quantity is all in Fourier space, but you look at the real space data. So, this is x. So, we got this is delta x. So, this will be h, you call it h, real space separation h. So, this is called Nyquist criterion. In depth I will not describe that.

So, Nyquist criteria, so lambda according to that lambda should be here the wavelength. So, the lowest wavelength should cover 2 h. So, that is a nyquisted area. So, lambda equal to 2 h. So, the criteria tells you physically that given the time series if I want to resolve it using Fourier transforms or I have to resolve it not necessarily Fourier transform, even by finite difference scheme, so the lowest wavelength should contain two points 2 h. So, suppose there is a single coming from the radio station, I want to filter it. I want to analyse the time series. So, what should be my spacing of delta x? So, my delta x must be, that is delta x. Delta must be lambda by 2 lambda min by 2.

So, this gives, this is your relationship between delta min and h. So, my delta t if I use this I get. So, lambda mean will be 4 h squared alpha pi square. So, I am just substituting this. So, from this I am getting a clue what should be my delta t for postulation solver and what should be my delta x. This is very critical for all the projects, but be very clear what should my delta x and what should be my delta t. If you do not choose it, the code will blow up. It oscillates, it will misbehave, it will work and this is called CFL criteria. So, now what should be my delta x and what should be my delta t? Now, this is how you solve diffusion equation in spectral method.