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Lecture - 25 Energy Transfers Fluid Simulations Dealiasing

In this lecture, I will give a brief intro on Fourier transfer, FFT. We will discuss how it is done. I think is it is interesting to discuss dealliasing. I will just briefly explain that. Now we will do discrete Fourier transform, both real space and Fourier space.

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Discrete Fourier transform (DFT)

$$\mathbf{u}(\mathbf{r},t) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k},t) \exp(i\mathbf{k} \cdot \mathbf{r})$$

Now, if you recall you know let us say x was a real, but k was discrete, but in simulation both x and k are discrete in computer, d for discrete and r for real. I will illustrate using 1D all these discussion.

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$$f(x) = \sum_{k} f(k) \exp(ikx) \quad f(k) = \frac{1}{L} \int dx f(x) \exp(-ikx)$$

$$dx = \frac{L}{N}$$

$$x_{j} = j L/N \qquad k = \frac{2\pi}{L} \overline{k}$$

$$\overline{k} = (-N/2 + 1) : (N/2)$$

$$kx = \frac{2\pi}{N} \overline{k}$$

For Fourier transformation see above figure. We have this 1D line, 0 to L a periodic. You do not save both the points to satisfy the periodic boundary condition. So, I have N points. See above figure for indices and discretization.

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$$f(x) = \sum_{k} f(k) \exp(ikx) \quad f(k) = \frac{1}{L} \int dx f(x) \exp(-ikx)$$

$$kx = \frac{2\pi}{N} \overline{k} j$$

$$\begin{cases} f(j) = \sum_{-N/2+1}^{N/2} f(\overline{k}) \exp\left(2\pi i \frac{\overline{k}j}{N}\right) & \text{Inverse} \end{cases}$$

$$f(\overline{k}) = \frac{1}{N} \sum_{0}^{N-1} f(j) \exp\left(-2\pi i \frac{\overline{k}j}{N}\right) & \text{Forward} \end{cases}$$

$$|k| = \frac{1}{N} \sum_{0}^{N-1} f(j) \exp\left(-2\pi i \frac{\overline{k}j}{N}\right) & \text{Forward} \end{cases}$$

Finally we get Fourier transform of f(x) as f(k). See above figure. This is called DFT Discrete Fourier Transform. This is also called forward transform and the opposite is called inverse Transform. There is a reasonably good manual called FFTW, Fastest Fourier Transform in West. If you look at their website you will find some more details.

As I said it will take given N point it will take N squared if I just do my ordinaries. This is

very expensive as this is sum as well as multiplication. So, the multiplication here of this

exponential and this of course, computing exponentially also it is done live it is not saved

in a data saved in array, exponentially is computed live and so, this is multiplication

component exponential and there is a sum.

So, how many sums and how many multiplications are there? So, for every j I need to

compute N times and there are N is. So, it becomes N squared in 1D and in 3D this is

easily generalizable. So, it is M, M is number of points.

Idea is to divide this in even and odd. This called divide and conquer, this is a British rule

recorded we divide and rule. So, divide this data into even and odd. So, not divide like left

right ok; so, even and odd and then again further keep dividing. So, you make a like a tree.

So, instead of doing this thing with equal, then you say you compute even odd even odd.

So, basically it is dividing literary. So, instead of doing it in one ways, then you just sort

of make a tree structure and solve in hierarchically.

So, this one idea which I am drawing myself in some different fields, let me just make a

remark. So, this is solving a problem by hierarchy scaling hierarchy. So, you do not solve

a problem in it at equal level. So, the thing is I like to say if you want to solve a country

problem countries problem you do not go to every house and solve the problem it will

solve at a in multi-scale level.

So, you have to make a policy at large at the country level, then district level, then state

well village level. So, you have to solve in a multi-step way. So, it is like divide and

conquer you do not do all of it in one shot, it just too bulky. So, divide even odd even odd

and it turns out it is done in N log N and this is the very powerful idea. So, this is was even

in mathematics.

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$$f(x) = \sum_{k} f(k) \exp(ikx) \quad f(k) = \frac{1}{L} \int dx f(x) \exp(-ikx)$$

$$kx = \frac{2\pi}{N} \overline{k} j$$

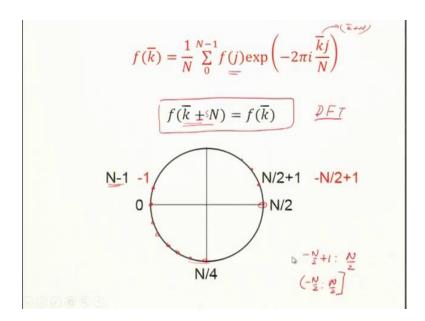
$$f(j) = \sum_{-N/2+1}^{N/2} f(\overline{k}) \exp\left(2\pi i \frac{\overline{k} j}{N}\right) \quad \text{Inverse}$$

$$f(\overline{k}) = \frac{1}{N} \sum_{0}^{N-1} f(j) \exp\left(-2\pi i \frac{\overline{k} j}{N}\right) \quad \text{Forward}$$

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That is how it is called dividing and once the data becomes small then you can do the Fourier transform on small data and then you go up. So, this is if you look at the we keep here find the detail. So, anyway we will not get into this, but this is done in N log N now FFT.

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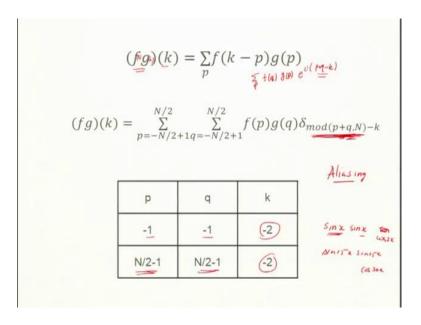
So, this what we need to compute f(k). So, these are another property of Fourier transform, this property of discrete Fourier transform DFT. See above figure. So, this is really important property. So, it is because of this properties nice to represent you know circle this is a followed in many textbooks. So, my data is starting from here and I just put them

is points on the circle. So, these N by 2 then this N by 2 plus 1, but by using this property N by 2 plus 1 is I just subtract N add or subtract know.

So, what if I subtract and what will I get? Minus N by 2 plus 1 so, these are points that N points what is this N minus 1. So, what is that N minus 1? Subtract means minus 1. So, all the negative ones were here all the positive ones are below if you like till N by 2, this point is N by 2. So, positive ones from 0 to N by 2 lower, lower, lower half and above part is negative is that clear?

But in for solving this problem it is important it is sometimes useful to think 0 to N minus 1 do not think negative positive. But for physics it is important to keep in mind that it is like that or we can write like this, this include you know square bracket means included left bracket means not included is that clear; so, this notation. Now, make life bit difficult for you. So, this called dealliasing problem. So, what is the problem first?

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The two functions f and g I multiply these in real space, see above figure, then do the Fourier transform. Now it is a convolution in 1D, there is no vector.

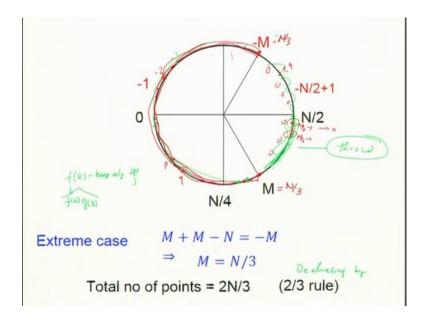
So, this is fine, but when I do discretization, then I do not have minus infinity to plus infinity I have minus N by 2 plus 1 to N by 2 that is where the problem is; where convolution will have error because of discretization. If I had infinite N then no problem

convolution will be exact, but because of convolution there is a chance of error and what is the chance of error.

This is a proof which I did in the class, see the figure. I get a delta function Kronecker delta function, δ . Because of this circular property p+q cannot be arbitrary large, k is bounded between -N/2 to +N/2.

So, is when I do the Fourier transform by discrete Fourier transform these what I will get; In the following picture it becomes clearer both p and q are going from $\frac{N}{2} + 1$ to N/2.

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Now, the dealiasing is quite easy to see. See the figures. sin x I think multiply by sin x, I get sin 2 x or sin square x cos 2 x know it gives you cos 2 x which is 1 plus 1 gives you 2 sin has plus minus 1. So, please bear with me on that part. But because of this property large wave numbers can also give us small wave number.

So, these are problem, if I have large wave numbers I am adding them, if I have sin 15 x sin 15 x will give you cos 30 x if 30 x there is no place to save then is going to come back by this by this rule is that clear. So, this called aliasing. So, this minus 2 has 2 possibilities. So, I get coming 2 names. So, one thing is coming contribution coming from minus 1 and minus 1 other one comes from this contribution.

So, to get a wave number to I just sin x and sin x i multiply, but somebody tells you that sin 15 x and sin 15 x, multiply gets sin 2 x then something is odd right something wrong I cannot multiply 2 large sin functions, but computer will give you that. There is a problem of DFT because of this rule. This called aliasing problem.

So, I have 2 wave numbers p and q add them I get somewhere here. So, they are small numbers 1 plus 1 gives you 2 no problem, but it becomes large then this going around happens if I take some number here N by 2 let us say N by 2 minus 1 N by 2 minus 1 that is what I was taking you know in the my previous table if I add them I will get N minus 2 which comes somewhere here minus 2.

So, minus 2 can be obtained by minus 1 plus minus 1 in convolution or it can also come from here if these modes are nonzero if they are present now that is the problem having 2 large wave numbers giving you a small wave number is not a desirable thing ok. So, what do I do? I make some of these 0 I demand that in fact, the demand is. So, I am going to make a circle I I could not do it in the computer only these are nonzero.

So, now, if it is 0 then multiply I will get 0. So, to what is the worst scenario? So, look if I take 2 large wave numbers add them I get large wave number.

So, I want to put a condition that I will get if I had them I get somewhere here it is a negative number, but somewhere here I am going to explain this in minute ok. So, these are condition and that gives you M is N/3. So, this I want to make is N/3.

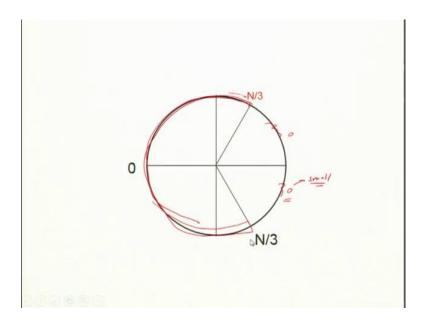
So, let me explain what it means. If I have my wave numbers somewhere here then if I add them I will be if I lie within this band lower band, I am fine because my I am going to keep only this wave numbers. So, when I add my k my result is valid result there is no aliasing problem. If I have somewhere if I my problem is if I have somewhere here then what happens? If the 2 of them lying somewhere here then add them adding them will give you it will come somewhere here, but these I am not keeping I am just throwing it out.

So, no problem this is you throw it out throw garbage your house is safe no problem. So, you throw that is garbage, but anything if we keep let us say p and q are here. So, we are lying inside this band no issues. But if I am here then of course, it will generate a k outside my range, but I will throw it out.

If I am come somewhere here then what happens? In fact, this is big and it comes somewhere here minus becomes big minus and that is like you add plus N to that it becomes positive. So, these again I throw. So, throw this part throw. So, I keep my data from minus N minus N by 3 to N by 3 then I am safe.

So, the idea is the following f full of k set keep only 2N/3, throw out the other things. Now from these you construct real space from here I construct the f(x) and g(x) multiply then again to the transform, but we keep only the data of 2 minus N by g 3 to N by 3 that is a reliable data. I will get nonzero amplitudes, but I do not keep it.

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So, just to summarize, you keep this data only here and these are the zeros before the before we going to real space, multiply and after the data is done you again throw them out ok. In our code we keep this data row after the transform these numbers are small typically well large wave numbers the amplitudes are small, they are not correct not accurate, but we keep the data for a spectrum calculations it gives a bigger range.

Thank you.