Computational Science and Engineering using Python
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Lecture – 17
Fourier Transform

Work on Fourier transforms. So, spectral method some of you are working on, you need some definition of Fourier transforms.

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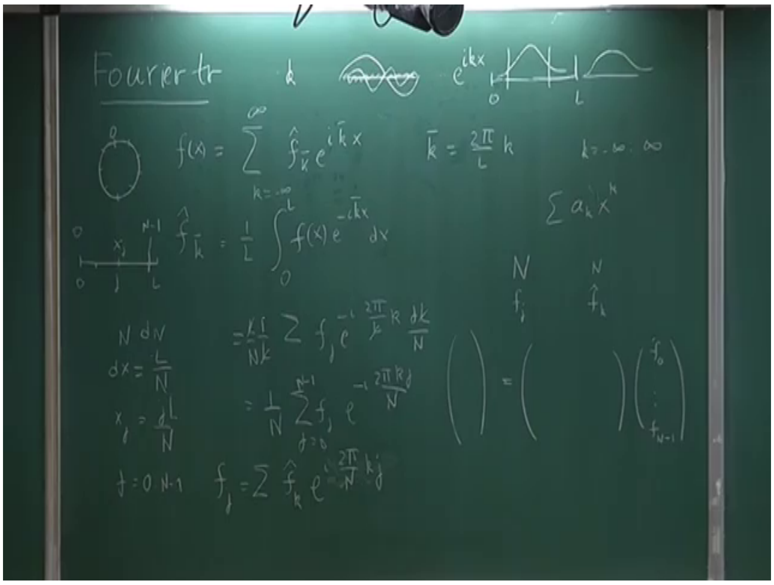

So, Fourier space is very important advantage that you can see different scales you understand scale no; I said, you have large, then I want to understand what happens at small scales. So, the idea even example which I give all quite often is that there are structures at the government level, right, the largest level, then the ministry level, then sub division level. So, there are different-different levels finally, you reach district village community.

So, these structures you cannot capture if you have real space; full real space, you can solve equations which are 1 billion or 1 trillion in variables, but it is possible to understand them at different-different levels. So, if they are physics; in fact, there are connections, it is not that they are not connected, but you can abstract what happens at that level, then different level, but Fourier transform makes you; let us; you do that. So, these are; so, when I have a numbers, then I have its properties at that scale. So, we have ace; this one, then this one any tiny. So, it tells you that what is a energy at that scale energy that scale, but if you are working real space you can say energy in real space will be energy here, energy here, energy here.

So, you can see in real space division; Kanpur temperature, Delhi temperature, but I want temperature at different scales you know. So, you want; what is a average temperature at 100 kilometre scale of 10th wave. So, that will come for Fourier transforms or else you will tell I want in 1 meter scale; if you measure it, you can get it by Fourier transforms. So, that is a very very powerful idea. In fact, this is really powerful idea; of course, mathematics is let us use to solve some equations, you should also understands what it means physically.

So, the definition of Fourier transform is. So, I given a function f x where I have assumed to be periodic. So, I am going to explain in terms of the e to the power i k x, but you can easily analyse in terms of sin k x and cos k x as well. So, if the function is periodic from 0 to L. So, you go back in this length value, then you can write this as Fourier transform f hat of k; k bar. Let me put k bar; k bar x. Now what is k bar? K bar is a wave number which is defined as 2 pi by L times k. So, k is a integer. So, that is why I put k bar. So, this is a factor and this you studied no; that is a wave number.

So, k will very range from minus infinity to plus infinity, right. So, that is the definition of wave number. So, this is due to Fourier; Fourier said this. So, you have to sum, but it goes from minus infinity to plus infinity. Now this series sum is quite weird series. In fact, lot of great people disbelieved it like Legendre did not believe it. Legendre Fourier; there were contemporaries 1800 after the French revolution was energy in trans and therein believed because this is not like Taylor series. Taylor series; we have sum a k x k and if its x is less than 1, then you can say, yes, series will converge, but what is guarantee that this series will converge. So, these are all mod 1. So, that was a major doubt, I mean mathematicians like we guys Lagrange was very powerful Laplace. So, it might; do not work. So, he published this in a book monogram; he is not published in the research paper, but later on, I mean where there were Fourier himself did not prove it, he did not prove the convergence.

So, this series does converge. So, the idea is that if I have finite number of terms N could be 100. So, convergence means that this N equal to 100, I get a representation of f of x not exactly f of x i proved 1 more term which will be better approximation that is what it means with convergence and it was proved by mathematician later Cauchy and; I think Cauchy proved this later, I mean that is mathematics of Fourier transform is very very useful and it is a very interesting math I can invert this very easily. So, f hat of k bar is 1 by L integral f x e i k x d x 0 to L and this is for real space; that means, x is continuous. It goes from 0 to L and k is infinite. Now in computer, I can never do this x to be continuous. It is not possible. So, idea is to de-criticize this x. So, I de-criticize them at N point. So, I can make a line with keeping in mind that this is same point is that we do not store the last point where that is same as a first point. So, I make N divisions. So, my delta x will be L by N and so what x j. So, index of the; or coordinate of the point j. So, its coordinate will be x j real value and that will be j times delta x.

So, that will be L by N and I will make j vary from 0 to N minus 1. So, that k takes care; I will not have L. So, now, for I need to de-criticize it. So, this sum remains as this, but this sum will become this integral will become a sum. So, now, this is going to be a sum 1 by L now d x, I can take outside this is L by N f j power i. Now k is what is k; that is the definition k bar. Actually this is a k bar; k bar is 2 pi by L times k and x will be coming from here x j. So, I have to sum x j will be j L by n. So, integral become the sum no, this is you learnt from your calculus course. So, interestingly lot of things cancelled L cancels this L cancels. So, I get 1 over N sum f j j goes from 0 to N minus 1 exponential i 2 pi k j by. So, that is why I compute f hat k; this is a Fourier amplitude that is a complex number, this f; this is complex number.

Now, f x can also be complex I restrict most often discussing when f is real, but for Schrodinger equation psi is complex. So, you can use complex f. Now this is also some this k x k bar x will also be replaced since I am working with discrete x. So, this also will be replaced. So, let me write this f of x. Now this f of x will be f j. So, f j will be sum. This k f k k bar is it makes you same as index because this is a constant e to the power i k is 2 pi by L k and this is L by n. So, exactly same thing; this cancellation will happen. I made a sign here; you know this; this there minus sign here minus sign here and this is 2 pi by N k j. So, our notation is that for going from f k bar or f k to f x; I have plus sign and going from f x to f hat, I have minus sign that is our notation. Some books flip it, but that is how we follow this notation f hat k. Now, in this case, I have how many real variables, I mean how many real space variables; I should not say real variable; real space variable its f could be complex. So, there are N of them N f js;

Student: It should be N plus (Refer Time: 10:30)

No, I do not keep the last point because that is same as a first point. So, we keep 0 to N minus 1; so, which is somewhere here. So, how many Fourier variable must; there must be how many ks should be there? So, number of ks must be again N because this is a linear transformation; you can write this in terms of matrix; if it is a very interesting form. So, this becomes a matrix. This is f. Let us make f 0 f N minus 1. So, this must be also if you want one to one mapping of this to this; it also must be N variables. So, my f hat k should also be N of them that is a difference discrete Fourier transform will limit you to only N ks; not infinite ks.

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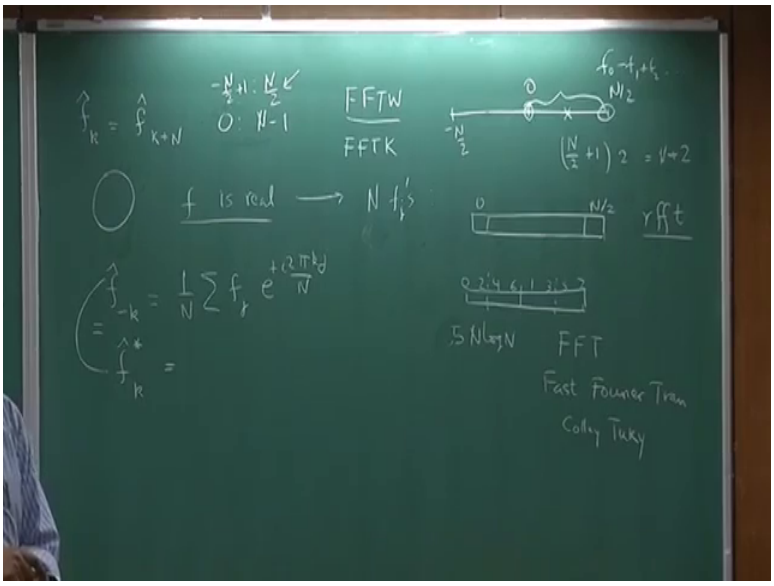

So, this will I can label. Now wait; there is one interesting property this definition we usually show that f hat k is same as f hat of k plus N, right. So, in this, if I add k to k plus N 2 pi j will come which is one. So, this is a property. So, I can choose my starting point any to any k. So, I can say my ks goes from 0 to N minus 1 for k or you can say minus N by 2 plus 1 2 N by 2. So, given f f 0 f js, I should be able to uniquely determine f ks f hat ks, otherwise Fourier transform will not be defined this is not a good definition. So, this is a linear transformation.

So, number of variables unknown must be same as I mean this is a matrix equation right. So, whatever is here should be here and determinant must be equal to one non zero and immediately you can check the determinant made of this i 2 pi N k. So, k will go to 0 to N minus one j will go to 0 to N minus 1, then define this transformation otherwise I cannot define this transformation this matrix will become some longer I mean there will not be N by N matrix. So, I want unique transformation from f j to f hat k and vice versa and that is possible only if this has N variables this has N variable that is property of linear equations after all I want the determinant to be non 0. So, this is all guaranteed because this determinant is non 0.

So, we use this notation, but. So, there is very famous library called FFTW the fastest Fourier transform in west, this is a parallel library we have developed another library called FFTK that is there is several property, I cannot do in this course. So, this is a parallel. So, you want to use in parallel library k for Kanpur that is what; we did not think a better name. So, this is for parallel library for using many processors. So, this I cannot teach in this course. So, FFTW has a very strong influence on the notation. So, they use this notation 0 N minus one you can always convert. So, you can using this property you can always convert, but in the today's class I will keep this in mind.

So, when you are working Fourier transform you have to be careful; what is wavelength number. So, the reason why we like to physically understand this if a wave number is property of the waves. So, it corresponds to wavelength which is L by N by 2 that is why that is why you should use that; now this is for 1 d Fourier's 1 d complex variables f x. Now I want to use only real variables like velocity is a real variable no if you solve for velocity in one of the projects you will get real variable for f if f is real if f is real then it has a some more interesting properties.

So, that is why it is quite easy to see in this equation no which equation f where is f hat k this; this equation f hat k. So, k and k bar are equivalent no by this multiplication. So, you can what about f hat of minus k. So, it will be one by N f j minus 2 pi minus minus we have plus k j by N, right what about complex conjugate of that equation. So, f hat of k star is in fact exactly same as this because f j is real. So, complex is the complex conjugate of this same as itself. So, it means that these 2 must be equal.

Student: Sir if k is real.

Yeah. So, I said if f is real. So, this property must be satisfied; that means, I do not need to store all the; so, if f is real, then how many variables I got. So, that counting is required no with when you do discrete transforms if f is real then all these guys will be real how many variables will be there N now please remember the complex has 2 numbers real and imaginary parts. So, this is N real numbers in my earlier definition I was assuming that N to be complex these are all complex. So, if this is real then this must be only N real odd numbers if I have more than that there is a problem N real numbers. So, they are not N complex numbers if f is real then N f js, but now I should have only N real numbers in the for f hat k.

Now I can easily show this property I will not believe on it, but you can just do this algebra because of this property this guy is going to be related to that; now this is a tricky part 0 to N by 2 and this is a minus N by 2. So, if I know this value let us say 3, then what is f of minus 3? Its complex conjugate of this if I do not want to store these if I do not store any of the left values your negatives are all connected. So, we do not store any of the left values we store only these.

Now, how many of them are there how many real numbers. So, 0 to N by 2 complex numbers. So, number of real numbers will be N by 2 plus 1; we have to count this as well times 2. So, that makes it N plus 2. So, it looks like there are N plus 2 real numbers for storing f hat k is that clear, but there is a contradiction right because I have only N real f js, but I have N plus 2 complex numbers now there must something some mistake I am making the mistake I am making is that the 2 values among these are purely real they are not complex and which ones are purely real f 0 is purely real why it is a average f 0 f hat 0. So, this becomes 1.So, the 0 component Fourier space is just the average of all f f js for. So, f is real f j is real then f 0 must.

So, f hat 0 must be real. So, this is real it also shows that this is also real it comes with plus minus sign this becomes a plus minus plus minus plus minus e to the power minus I pi j. So, this corresponds to f 0 minus f one plus f 2 plus minus. So, it comes with. So, both are real. So, now, it is everything is in order. So, indeed we have N by 2 complex numbers, but 2 of them are purely real. So, what is done in standard python library is that for real numbers we should use r f f t, I will demonstrate some examples we should use r FFT and r FFT is will give you. So, this for r is real. So, it assume that f is real f is real. Now there is no project in which you are doing spectral transforms for complex numbers.

So, we start with 0 and move up to N by two, but in the library all of they are chosen is complex numbers it is too much of a programming issue if you make some of them real some of them complex. So, all these numbers are complex throughout, but when you are doing the calculation you should keep in mind that these 2 are purely real. So, that is a thing you have to remember now this is for 1 d all story finished these are all called now I have just one more little point this is a math now how to do computer computation of this object, these 2 in computer.

Now nobody does this sum now this sum for every k how any sums are there I did I did mention that in the class last class these are all N operations right N multiplication f j multiplied by this complex number now I have to do this for every k. So, it will be N square operations, it is a huge for when N is large there is a very clever that instead of doing this we divide them to odd and even parts. So, if I have something like I want to do Fourier transform eight numbers; so, 0 to 8. So, idea is to make 0, 2, 4, 6 and 1, 3, 5, 7, you divide into this I will partial sum of this partial sum of this.

Now, we can add them and I will get this, but then instead of that I can also divide this further into 2 parts and. So, this is a recursive tree which is made and you basically if you know how to do for the even part and odd part and then compute the full part. So, this is called divide and conquer and using this one can do this in N log N. So, instead of N square, use N log N. In fact, the factor is 5 this FFTW people are trying to make even smaller more work, but it can be done. So, this five is Fourier factor and this algorithm is called FFT fast Fourier transform and this is Colley Tuky spelling I hope, I am right. So, I think this again comes from FFT. So, these are way back in 56 or something 1956. So, you do it this way and this fast that is why it is called fast instead of N square you do in N log N you can read this if you like on more details on that. So, this is for 1 d. Now we can do for 2 d. So, the 2 d data or 3 d data.

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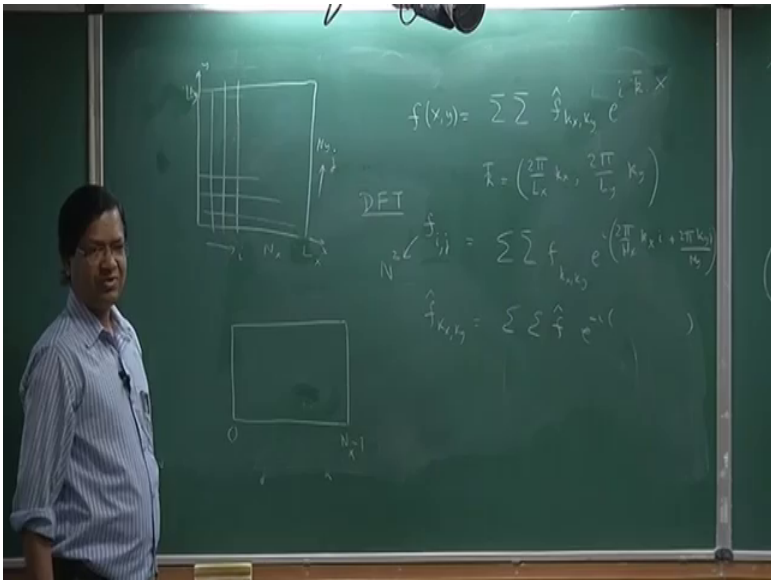

So, how do you do for 2 d and 3 d is that clear everything is clear for one d. So, I have 2 d real space data let us assume that we have real space data so for convenience, I will make it N square. So, this is x axis. So, you can think of plate on which you have electric potential or temperature of the plate now this is actually in real space this will be going from 0 to L, this is going from 0 to l, but when I have to work with computers, I will de-criticize this. So, I will only discrete things like this. So, for we can actually you can make it L x that is not a big problem L x L y. This is N x and N y. So, what is the definition of transforms? So, I will just work for 2 d. So, f x y is the 2 sums f hat of k x k y e to the power i k bar dot x bar or x not x bar, then what is k bar k bar is the vector whose components are 2 pi by L x times k x comma 2 pi L y k y k x and k y are integers, it is just a simple generalisation of 1 d to 2 d and I can invert it. So, inevitably 2 integrals. So, you can exactly generalise 1 d to 2 d; straight forward.

Now, how does; it will look like in terms of discrete transforms; so, x y will not be continuous anymore, it will be discrete. So, we call them f i j and there is one notation issue this I you will mix with this i. So, this (Refer Time: 26:19) of minus 1, but this is array index, nowadays standard followed in text books. So, this is f and now these are integers. So, k x, k y exponential i. Now again, following the same idea. So, L x by; so, this becomes 2 pi by N x k x j k k x times i is a index along this and this index along j plus 2 pi k y j by N y. So, this is a your this length. Now you can write down what is f hat k x k y. So, if in fact, is very similar f hat minus of this? So, there is a these are the definitions in this called I must assume this is called d f t discrete Fourier transform.

Now please note one important point that here length does not come into picture at all is there is no length here length is disappeared is a only function of N capital N now you saw you saw for you to think about how does a length come in a spectral method some of you are working spectral method how does length come into a linear equation Fourier transform is neutral on l. So, please think about it I will not tell you the answer now.

Now, here also L does not come it is off. Now the question is how do I store it. So, FFTW will spit out numbers and you have to make sense out of those numbers. So, the numbers will come out to be again I have to I assume to f is real. So, f is real then how many k x and k y will be there. So, this is let us assume that these are N squared number. So, now I will assume that N x equal to N y now this will be again should be N squared numbers again otherwise there will be a problem. So, how it is stored? So, this one is how it is stored in computer if this goes from 0 to N x N minus 1 or N x minus 1 along x direction.

Now you can generalise this property for 2 d this for 1 d or in fact, any dimension f k, k f hat k is sorry; f hat star of k is f hat of minus k, k is a vectors, no, this is a these forms are vector why this is very similar to what do you do in solid state physics, right; you what is identical formulism if this is. In fact, the Fourier transforms also. So, I am sure you know about this, but for a minute to think little bit more about these stuff. So, if this is a case then do not want to store the negative k ys. So, in this space the lattice space I think its called I am not sure what it is called lattice space.

Student: Space lattice.

Space lattice; so, what is you should think like this. So, I will re-change it because of this again to this property you will work for each component no you just see that for each component. So, k x is equal to like this did works this one. So, actually what I am going to do is. So, this is not a convenient thing. So, you just store this by N x by 2 N minus N x by 2. Now if there is a wave number like this which is component k x this is k x and this is k y. Now this is k y and then there must be a number somewhere here which is minus k y and minus k x correct. So, do not store it because there is complex conjugate. So, we do not store anything which is negative k y.

So, basically cut off half of them and this goes from 0 to N y by 2, there is a bit of more variables here, but this detail I will not tell you if you are properly counting and all has to be done it must be same number of variables N squared here as well as N squared in real, but that is a detail which I will not discuss right now. So, we store only the upper half, there is a one group which is doing the project. So, for them I did mention them that reality condition this is called reality condition. So, I will I will not tell you exactly how to get N squared here, but there is one; part that if you have some variables here, let us say this one then there is a variable which is wave number k this will be minus k on the same line right this is k y 0. Now these 2 numbers must be complex conjugate of each other. So, this will tell you that you should not store these as well, but that is too much of a program he has if you do not want to store this; your array must be 2 d array proper dimension.

So, you store them, but you have to make sure that they are complex conjugate. So, this reality condition is a very important condition which must be imposed on the variables otherwise my temperature will not be real. So, same thing is done for 3 d. So, it is a clear how 2 d will. So, 2 d computer will give this in 3 d is going to be. So, so this k x and k y also will be like that. So, it is a cube, but you do not store again the bottom lower half you do not store it even in 3 d. So, we can do in Fourier transforms any dimension including four. So, I think in this class we probably need one and 2 d. So, homework will be based on 1 d and 2 d. So, let us see some examples.

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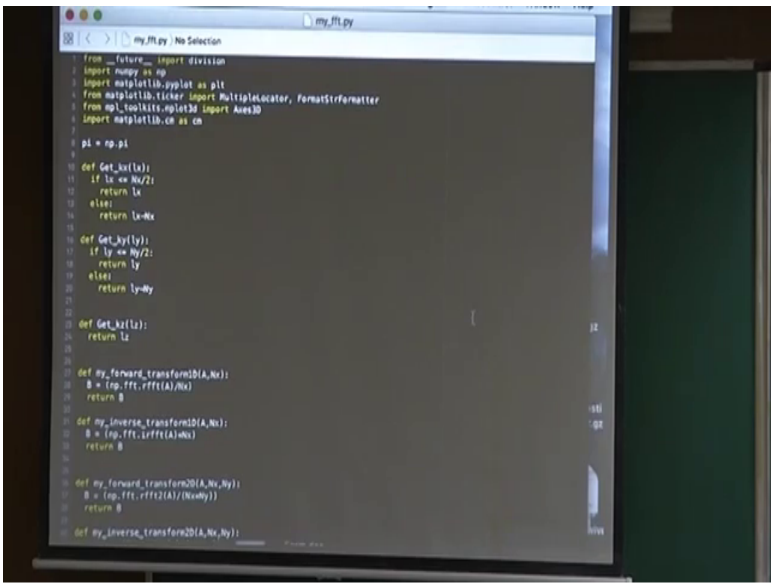

So, what was defined for this project for the; in this code, you will not come this side, still there are 10 minutes. So, our functions are part of N p num pi. So, FFT r FFT is what we will use r FFT is part of FFT library; FFT also has complex to complex definitions, but we will use only the real part r f f t. Now if you are doing Schrodinger equation, then you should do not use r f f t, we should use else some something else. So, 1 d transform this is syntax. So, I have to give an array a. So, he has made a nice function. So, forward transforms. So, you do not need to remember syntax. So, transforms given an array a which is 1 d array N size which give that it will return the Fourier transforms. So, this is a syntax.

N p dot FFT dot real FFT a a y N x. Now if you want to do. So, that is form forward transform and inverse transform inverse transform you just put I r FFT your i is sitting here.

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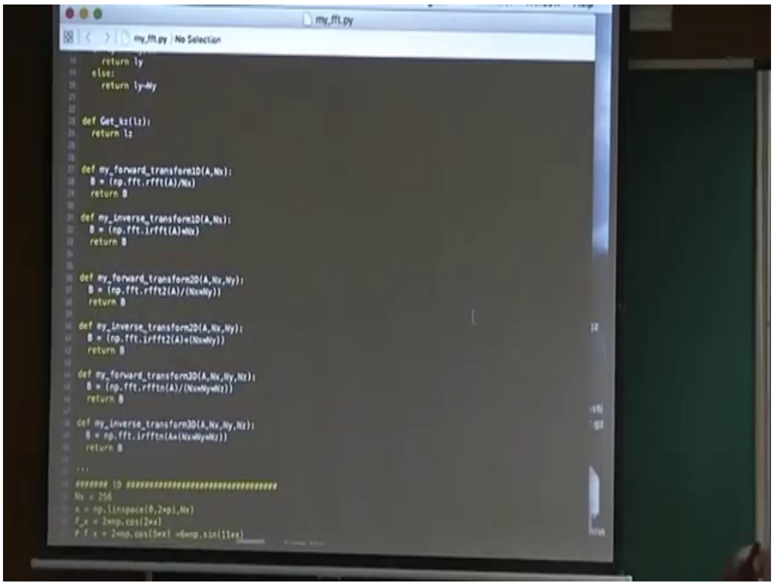

Now for 2 d; so, there is a i r f. So, there is a (Refer Time: 35:10) number 2 and for N d f f t, you have to put N; N means it could be free for. So, from the array A; if you figure out; what is an dimensional d of the matrix. So, if you want 3 d this is a transfer a, but well anyway. So, you can use this syntax. So, we divide by N because by definition there is a one by N sitting here.

So, if this following if I had to follow this notation one by n. So, this is how it is divided. So, python FFT does not divide by n, but we divide by N and here is multiplied by N x I think the definition is just reverse for what we do that is why it is multiplied by N x I am not hundred percent sure. So, this is our definition this will exactly give what I have done in the class; I think this part you do not need to worry about it this is for some other library. So, I will just show you one example how to call it and see the result.

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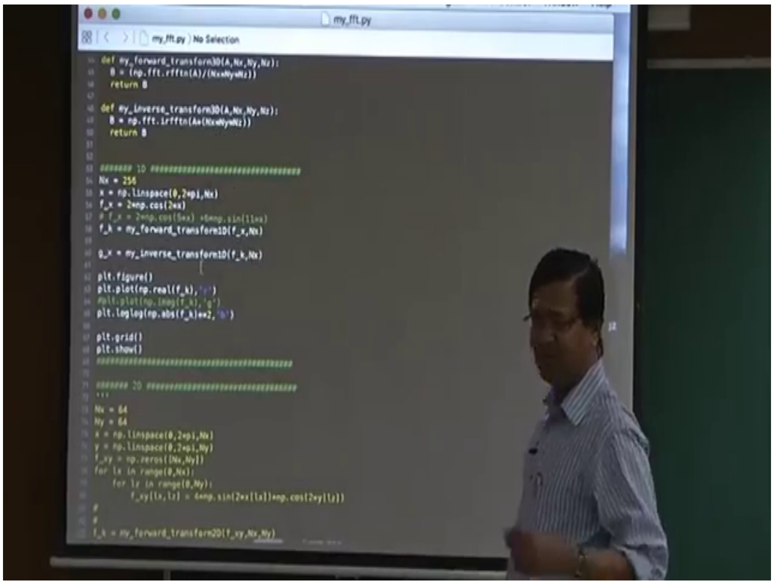

So, I am commenting these parts. So, 1 d, I have defined the size 256 and so my function is this. This is my function 2 2 cos 2 x. So, what is a wave number where it is non 0, it is 2 k equal to 2 L x is 2 pi. So, 2 pi 2 pi cancels. So, I see 2 pi is a box; many of the methods gives 2 pi is a box size; what is the advantage. So, 2 pi; 2 pi cancels and you get basically k integer wave numbers are integers 1, 2, 3, 4 like that. So, we got integers like that. So, I can; so, this is my f x, this is my x, I divide an N x stuff. In fact, we are not worrying too much about this because this is not we used in this course f k is Fourier transform. So, I just call this f x and N x, but this in turn is calling N p library num pi library, yeah;

Student: (Refer Time: 37:54)

What?

Student: L x is 2 pi;

L x is 2; I am choosing L x is 2 pi this is my L x.

Student: (Refer Time: 38:00)

L x is a figure of x, but as this my course should also for cos x. So, for any function; which is Fourier. So, I am my in box is 2 pi if for box 2 pi, this will be correspond to k equal to 2. Now this Fourier transform forward transform and my result is here f k, I can also get the energy this is called mod f k squared energy right the energy of the particular mode. So, this will give you like example I want temperature at that scale energy. So, this; this is a very commonly used function. So, let us run it.

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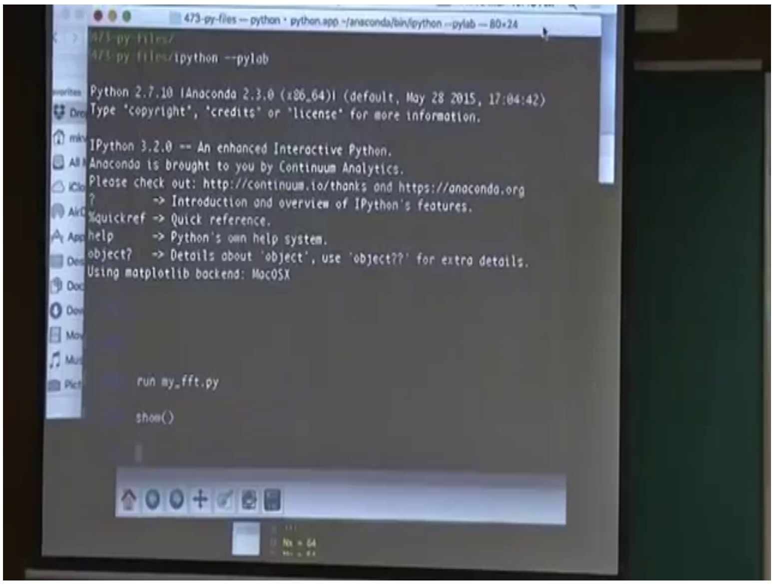

So, run my FFT. So, it has run now. So, I should why is it not showing. So, it is somewhere behind where is behind yeah.

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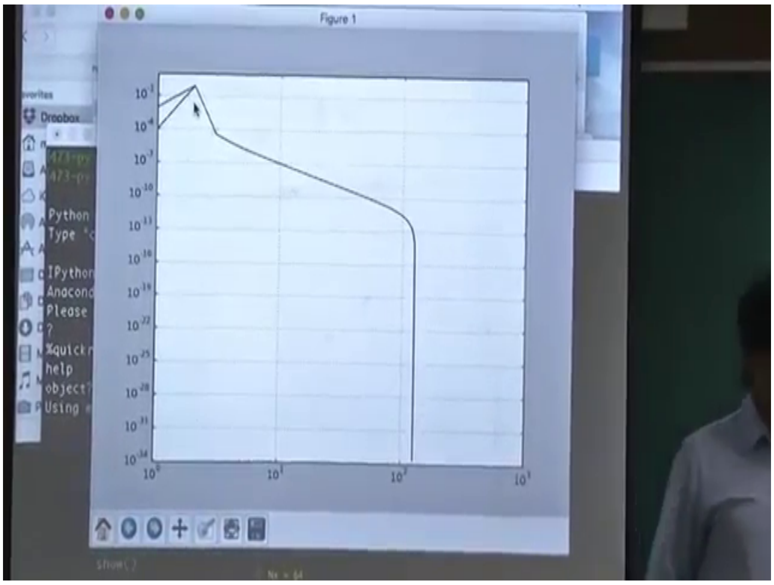

So, now you have to see this carefully, it is in log log plot. So, the 2 colours; let us just look at the (Refer Time: 39:48); red is my amplitude over the real part of the function f k is red no, this one and the energy is blue. So, these are the numbers I got now like it looks. So, I do not like the term y minus 34. In fact, the 2 time event this form this onward its 2 time. So, let us put a y limit. So, that I do not see all this stuff. So, one e minus e minus with respect to one e one minus tend to I know the answer is one, but let us put 2 this is my y limit where it looks slightly sensible no it was like.

So, my amplitude it is one it better be because its 2 cos k x, if you do the Fourier transform of 2 cos k x. So, let me just write these as well 2 cos k x lets put k is written as e to the power i k x minus I k x by 2. So, what is the amplitude no not 2; 2 is cancelled. So, amplitude is 1 and 1 for wave number k, it is 1 and wave number minus k; it is 1. So, these are real function. Now I am not storing please remember that this is not room is stored because of this notation and negative parts are not stored. So, my only non 0 is k equal to 2 Fourier mode. So, what do I get here?

So, k equal to 2 indeed is non 0. So, I have put k equal to 2 here 2. So, I get this infinite answer as 1, but I get do get some non 0 values here, these non 0 value tell me minus what since this is a DFT; discrete Fourier transform. There are always some error. So, this is one percent where this is an error energy is f square mode f squared. So, it is; so every mode. So, this has energy one this also has energy f 0 seems to have energy because again summing up no this is like summing up the stuff I feed well make one more remark have only do is to 256 points, if I use more points then it becomes better this will go down, but there is always some error in computer and it quickly goes to 0 discrete Fourier transform will not give exactly one for k equal to 2 and 0 elsewhere. So, is that? So, I can also make some complex functions. So, there is one function which where it went. So, this function which has combination of 5 and 11 x he needs x because x is stored here to define x we need x 5 times x. So, he is using; this x sorry.

So, where will be non 0 what are the non 0 wave numbers for this Fourier amplitudes for this. So, which k?

Student: 5.

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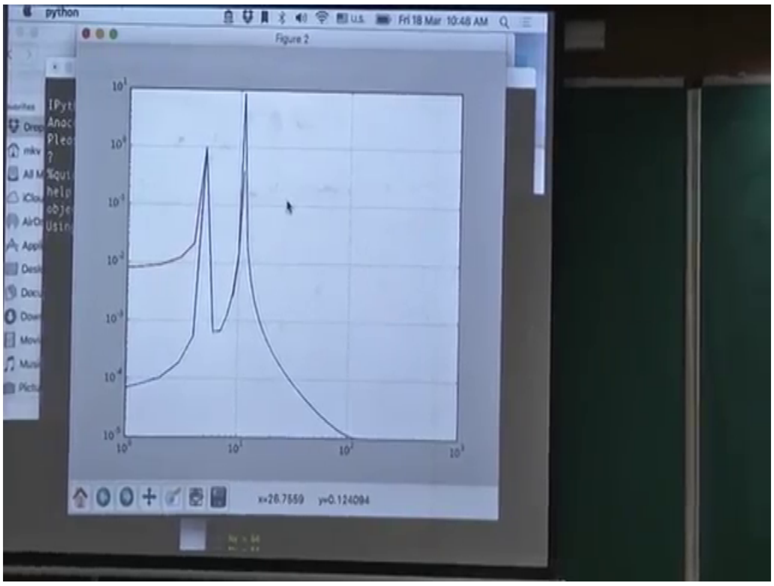

5 and 11 and amplitudes will be 2 or no 1; 1 because 2 will cancel; 1 and 3. So, 1 and 3; so, we run it. So, 1 and 3, sorry, 3 and 11, right; amplitude is 1 and 3, but the answer is for k equal to 5 and 11. So, this is 11 and this k equal to 5, 2, 3, 4, 5, 5 and energy is also following that. So, this 1 d; now we can also do for 2 d. So, 2 d program is; so, we setting up we are setting up here a cos sin 2 x cos 2 y, right. So, sin 2 x cos 2 y and we do 2 d Fourier transforms and is being stored in a is being shown as a p colour plot.

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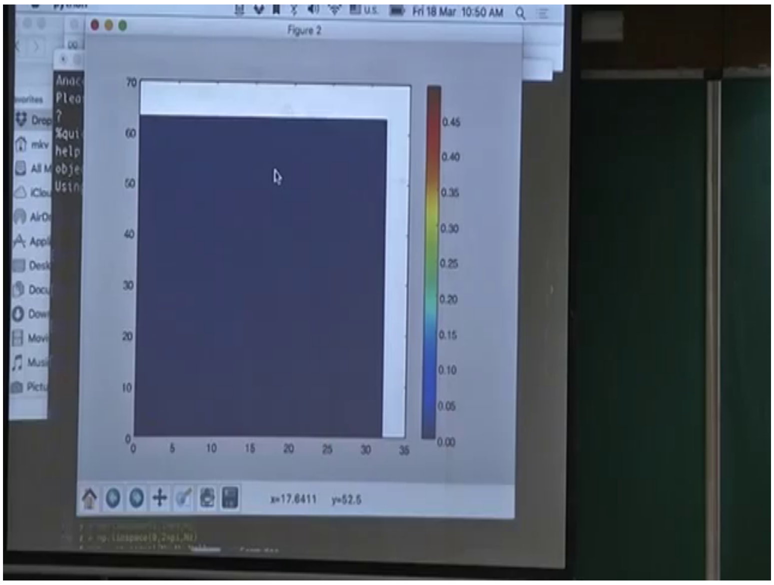

It also looks at the non 0 values. So, let us just do the colour plot. So, we are getting basically here. So, 2 comma 2 this is coming because of this is not correct this part is because of the reality condition and so on. So, 2 comma 2; this is 2 comma 2 not a good colour scheme, but it was cos 2 x sin 2 sin 2 y. So, please figure out what are the non 0 values; what are where is Fourier transform in non 0. So, you can follow the scheme you have to write in this exponentials.

So, for which k x and k y it is non 0, you can write sin is a product. So, this was energy this we put for energy. So, we can figure out which ones are non 0s. So, that part; please work out. So, I can tell you what is that f k no f k 2 comma 2 and this is a one of the non 0 values and it is a magnitude. This is a complex number. It is this number. So, you can always print which are the numbers which are non 0. So, it has. So, there is a 3 d example in this same code. So, that is about it Fourier transforms completed.