Computational Science and Engineering using Python
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Lecture - 27
Summary

(Refer Time: 00:13) anything new today or I just want to talk. So, I will say little bit about where do you go from here, if you like programming, if you like numerical programming. And that is when advantage of python, with I tell in the beginning of the class which I hope you agree now that the programming time in large projects you doing small projects, but that two you can see if you wrote in C it you take you (Refer Time: 00:47) 5 times more times. You agree with that in especially there were large points also it matter.

Now, NASA has made a rule they are big project so of course they do bigger project; all space machines are driven mostly by well non-mostly in computing is the major part. So, they have large codes. So, to design a spacecraft the aerodynamic issues, there is the trajectory issues the huge simulations are done. Our ISRO, ISRO has new simulation. And NASA made they have understanding now there will do the prototyping in python; you understand what is prototype.

So, before we make the big aero plane you want to make a small aero plane right, because if you design a big aero plane then you make one you spend maybe a billion some hundred [FL] rupees now suddenly (Refer Time: 01:50) it does not work. So, it is waste money and manpower. So, one thing is to do make a small prototype. So, you do not be running on a big computers, but you run on a small computer. In fact, your PC and it works then you can design a bigger code.

So, these are what done to python.

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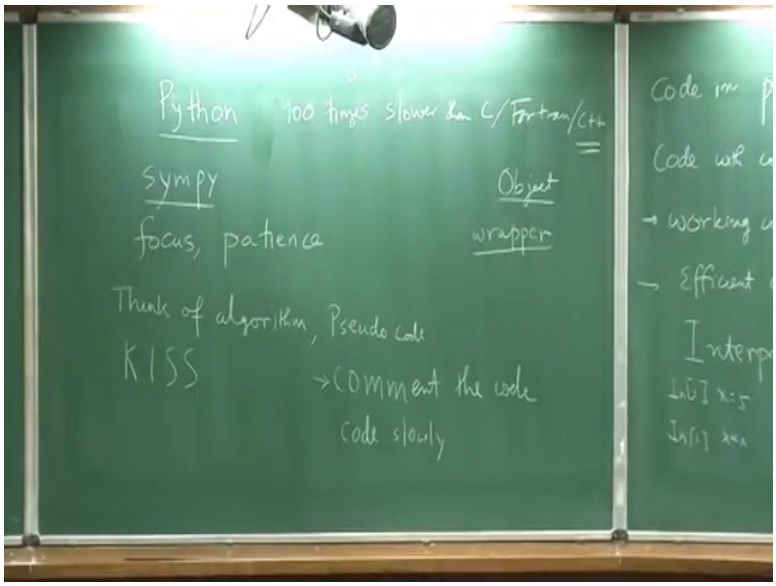

So, python is definitely good thing to learn, it will help you but use it, if you do not use it you will forget it. So, that is one reason I did not give many exercises which I should had, but you can use it for your courses like quantum mechanics now you can program to solve Schrodinger equation, you do not have to believe where is in the book. Sometimes what is there in the book is wrong including my own book I find that what I wrote was I just sketched it, but you really plot it you find that the depth of the potential value is so; much is it is tiny you know. So, you can see those plots will be better electrodynamic.

Once you visualize those electro fields he get a better field. Plotting is very useful. So, there is one problem I am not showing which gave in the last semester. The eight charge is sitting on the corner of the cube. So, equilibrium point is a middle center, but what is the potential; anybody remember- is quartic order, not x square. And that I could do it on a computer much easier rather than you tell a series. So, this one thing which I did not too much a sympy; sympy a is very powerful. And a lot of Jackson work which will do maybe already done doing right down next semester, right. Greedy Jackson books the electrodynamics one. So, you can do a sympy.

It requires bit of; so all this things require patience. So, again computing has put be patient, I was not so patient it brings you, you have to get the code working. And that requires focus and patience. So, this is main reason this write this word focus you are require and patience. Without this you cannot be more good programmer. So, most of the

time this after stated you know you write down you have to you have to say well I will you take a break and then you come back to the code again, ok.

So, you have to have these qualities. So, these about general program, so let me just a write few things for programming. I have written few steps. In fact, there are books written on it or in internet you find how to write good programs; there are bible written on those tough and then useful. So, I am just writing some condense version of those (Refer Time: 05:20) in one liners. And some of it hopefully you are practicing yourself right down.

I have kept mentioning it bit way in between, but let me just write it, but this is the last class. So, first is thing of algorithm first how to solve the problem. So, suppose you want to solve Schrodinger equation, so which scheme I will use, what is the problem? So, is it particle in some conical box or square box? So, think algorithm problem, do not start away right away start putting. So, think of the problem first. So, what algorithm, what times (Refer Time: 06:11) I had choose and keep it simple first. So, one thing which I have written is the first code should be simple code which works.

So, we have a v code and we use first Euler's scheme for it is easier to debug before. So, has a exact relations which some of you I ask them to energy conservation; that should work to one question decrease. We would demand more for professional code it should be better. And so we keep the codes simple. First I need to diagnose if this is an error. So, keep the code simple this is what I had said; remember what I said you want to say- what the full form of this?

Student: (Refer Time: 06:59).

Keep it simple stupid. Then after this algorithm you should make a pseudo code. A python is in fact very close to what you write in English, but do not worry about arrays and arrays syntax just write a pseudo code. You saw the code, but in English you had a loop n times within the loop I will do this. So, this is important. Now I think a before; because there will be errors if we just write without thinking. And your code will be bad code if you do not think about it in English or in Hindi also or in Tamil, we can loop; we have to think clearly. Programming is important if at one thing is I do fine let me just be slightly frank.

A people are not thinking clearly. Now, I find it more common your thought patterns are not clear thoughts; is a global phenomena that is my perception will I also probably do not think very clearly, but you should think clearly. I give the example of Einstein theory that is one of the simplest theory one can start when the assumptions are so simple. Anybody if you tell the common mans saying all physics are same for everybody you know, but of course this is the same; what to what to do after that.

So, I think it is important to think simple. And that is why I am quite against the culture where your thinking very complicate n dimensional phase and then they some from something and something and something which I do not know want name. because (Refer Time: 08:41) people. But just you are thinking complicated and this is incorrect most of the time. So, programming is very critical. If you quaint thing simple your code will not work. That is my; my code is too complicated, it will work sometime but do not want some other times. So, you have to keep simple that is very important for coding.

One thing I did not emphasize comment the code. I am not a good commenter, actually this something which is; I do not have my good practice myself, but commenting is important. Where I am in hurry so we do not commented, but next time we come back to the code I have to struggle what did I write; myself forget about that. So, when we write last code you should comment. So, code is submit I will like to see it is some comments, in the top what is the code suppose to do. And then standards at the top we have to write: when authors name, some licensing scheme. So, I can show you; well I am I do not have my code here well I mean I will not plug it in, but I can send you one file what is there in the top.

And for every function it is written what the function is suppose to do. What is the input parameter mean, what is the output of the function? So all that is; there is there standard ways to do it, which people have may written some kind of a practice. Actually is a common language you know so people accept that this word will have in a code.

Then code slowly, this is important. There is no prize for coding in 10 minutes; I mean it is not like (Refer Time: 10:41) you have to code slowly, ok.

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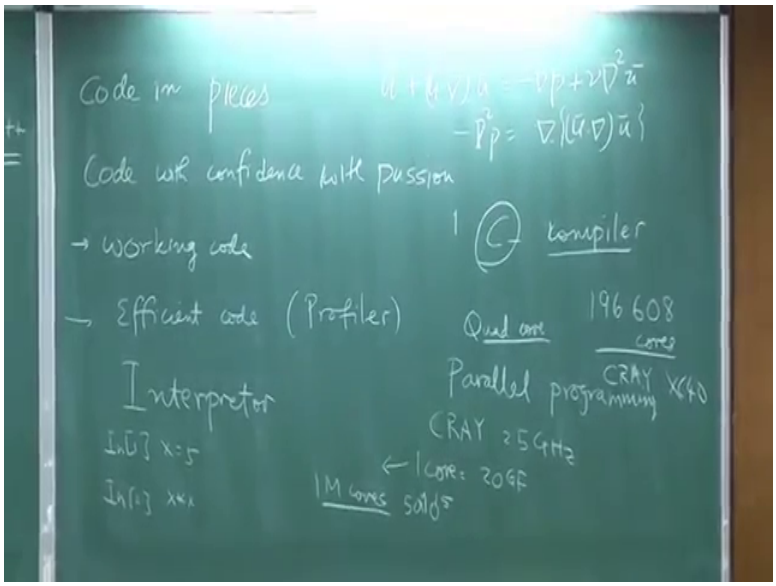


Then code in pieces. There is something I think some students are struggling. So, you mean one whole code to work, but it never happens; whole code never works, but part of the code will work. So, I can give you the example. So, Poisson solver for people who are doing incompressible fluid flows, right. So, remember I had; so we compute pressure by Poisson solver. Yes, the wedges of; so people who doing project they know that this important part, but fortunately Rishab has done this part which works. So, works does not mean that you can just plug it in, you are make sure that your input parameter as the same as the parameter to be used by the package.

So, if this code works then you know at least one part is working. So, you do not mean the building altogether, you make the first floor first, then second floor. So, its a design which people use all the time. So, you make pieces which work and then combine it. So, is very critical if you writing this big code and need not working, because your pieces are not working. And debugging is easy if each piece by piece you try to solve the problem. And we look so simple but this is very critical when you it comes with practice me do not adopted.

So, why functions are useful because each function it can tested, you put in the where argument and you should get then output if we does not work then it does not work you to debug that code that function. So, it is important to code in pieces and code with confidence and with passion. Now you cannot do half (Refer Time: 13:05); half (Refer

Time: 13:06) it do not work. So, you should do nice code, you should be proud of your code. And after this is done; so first code should be simple code. First get a working code: it could be simple in a sense it need not be efficient code we take longer time the Euler's scheme if it is not taking long time, but you test a small problem with the code which is not efficient.

After I remake the code efficient, after the code works it should make a efficient code. Now, efficient means some there are again techniques. So, you will be find which part of the code takes maximum time. There are tools now which can tell you which code takes longest (Refer Time: 14:00) profile this. Now this is; so the profilers which will profile the code then this function it is 80 percent of time, this function takes 20 percent time this function, this function takes 10 percent time, this function is basically just once it execute only once. Most of time will have loops 10000 times loop.

So, something equal ones you does not how to be feel you do not how to spend long days to playing that code which is use only once in the code. So, do not worry about that part because one which we takes longest in the code we should that part should be made efficient. The profiler will tell you this code is taking long time. Sometime you can time yourself. This function is taking longest time when you do it. For this code in (Refer Time: 14:46) solver the biggest part is Poisson solver which will take longest time, which we know from also just computation of order of complexity. Poisson solver is a longest, it takes longest time.

So, why I was being order n order n cube all that stuff, that is useful so which is taking longer time. And that that is what you should focus on optimizing, rest part you do not need to optimize at least in the first level. And we would like things like of library which is; sorry function which I have use more often that should be made a library. Like sin function you know it is a library of python to similarly Poisson solver could be a library of python.

If not python library it is your library. So, something which you use more often you make a library which python allows you and you have to do it. Now this is, I mean this all this practices for any language it is not for python is general programming practice. But I do want a make a remark that python is not a efficient language, by language itself it is not efficient the reason why it is not efficient is; why it is not efficient? Somebody

said it right is say interpreted language: so interpreter. So, what is interpreter? So, we say first in one have you put x equal to 5 then into then I say x star x trend x star x you know. So, I get the answer even short; it is like our mind when you I listen to you I try to understand word by word or sentence by sentence ok.

So, it is live execution. So, it execute this first then this then this. Now, I mean how does the computer first execute this. So, it converges in this language or rather will seeming less language into binary code- zeroes and one: it has to zeroes and one. And that zeroes and ones are executed in based on this transistors. So, you are this binary for this then there is a binary for this and then binary for that and so on. So, every line there is a binary executed.

Now, if I do one at a time then suppose somebody says it build one room, then another room, then another room, so you start building rooms in a lawn you know, related hazardous manner, we do not know the best design. However, if I write all of it is one short in C programming language from line 1 to line 100 is one code and the program is compiled. So, with the C programming language you compile it. So, this compiler- compile this code and that makes a executable one executable not like line by line executable. So, this is one binary is made for C of the whole package.

Now, these compilers are very smart and they can make a efficient code. Now suppose somebody says in this lawn I have to make a (Refer Time: 18:21) building you know then you already know what how to make a similar idea that it makes a optimize code. If it is a very lot of smart people are working on this even now. If has a program is involving that new programming language are being created or the old ones are being optimized different hardware, now new hardware comes and poor fellows are to go back and write object codes how to run things on this new processor.

Every time new processor comes you will get a new version of the compiler and. So, it is very important to know one of these languages; compiler language. So, this is not efficient, even though coding is faster, but execution is slower in python. In fact, this could be hundred times slower than C or FORTRAN. So, it is coding time is faster, but execution time is slower. Now, but I must also say that right now especially in the west so you have the trade off; trade off is whether good program or you spend time or I led the run code program run for more longer time.

This is not efficient then you had to run it for longer time. Now each of them cost money: the computer will cost money as a program will cost money. So, a good programmer cost money; you know good programmer will cost even in India good programmers are very rare, I mean that I do not rare being does not mean one person in the whole world, but there are a good programmer is not easy to get. So, basically you have to make a trade off, but you must I mean python ok.

So, what is done right now is that you write this python code, but the once which take longer time is written in C or you are look for a library with somewhere as written in C and you call them, and within you in this course but you can python can call FORTRAN library C library and do it, Java libraries. That means, a really python is like other snake which is slow moving, but it can eat anything and that is what (Refer Time: 21:05) it really can eat anything it can execute anything.

So, that is the advantage of this. So, what about my strong suggestion is that you should pick up another language you know if you want to program. So, I recommend C++. So, if you believe that (Refer Time: 21:25) you have good descent judgment then C++ it is a language. The advantage of C++ is that you can design big codes. So, either said you know you have to make this separate functions for each thing and then combine them.

Now, if your work is FORTRAN then combining these separate functions is not easy. So, you know what is object oriented language, how many if you done were the; he knows this one, but how many people speak today. So what is advantage of object oriented languages you (Refer Time: 22:12).

Student: (Refer Time: 22:13).

Ok, how why?

Student: Sir, I mean you can define objects for different purposes then call is objects.

Ok, is good, but I think. So, most programming language allow most in fact everybody allows structures. So, arrays in structure. So, you do not want to work with all this numbers you know array has certain advantages; you can how to access them, if I was more complicated data structure. Like IIT wholes institute will build as a data structure:

the student, there is a faculty, there is a staff, and there is a infrastructure. So, all this stuff are there. So, it is a data structure; so which we allowed in FORTRAN.

But C++ allow functions to work on this objects and that is part of the object. So, what you do with the data is also can be a package nicely in C++. So, C++ is thing is there objectives complete. So, within the object we have data as well as what to do with the data. So, we have certain basis function or we can write a library for which is self content. You can call those data as well as a print the data. So, for print the data it will part of the object or do FFT of the data its part of the object.

So, all that can be done and that is all C++ makes his each person independent and then you can combine them. And that is the advantage of C++. Java also has that feature, but Java has this slow language. In fact, there is nobody as far as I know works with scientific computing with Java; it is a slow. But of course, lot of will use FORTRAN. So, there will be a strong force for FORTRAN and we also struggle sometime that we have to there are things written in FORTRAN and you have to understand and you have to use it.

But I think the new thing is a python is going to rapid up. So, this is a new thing is called a python acts is a wrapper. Basically it's a, so this is a code and python will not know what is inside, but it what is about argument to send and the result to come out. So, that is a common practice; well not common yet but that is a very upcoming trend in computing that we use languages like this and then each piece you can call manipulate and do.

So the all this about in fact how to use the code programming, but it has out the programs or the problems you can solve with sequential code the one which you write is a tiny. So, all the code right now you written it run some single code. So, you might have heard of this quad core machine, right. So, like my laptop has two cores, but my python code will run only in one of them. But, suppose I want to use both of them or there are now machines with come it 10 codes; I mean it is like Ravan you know this 10 heads, but now you have to get all the 10 heads who work together. Well in Ravan head well. So, all this suppose to work together and not kill each you know so you have to you have to make them work together and achieve the task in one tenth the time. So, that is called parallel programming.

So, some 30 years back well from; so computers the digital computer came first in 1950s and this is a first one was really with radio valves you have not even seen that; it valves try (Refer Time: 27:06) of the civil conductors were started being used the chips key much later, but people who are after making more and more efficient chips. So, the big name was CRAY; CRAY was the company which was into making processor faster and faster, but then he reached the limit.

Now, this is simple quantum physics. So, what is the maximum clock speed one has achieved so far? Is 5 gigahertz I think I am not actually 4 is what heard about, but let us say 5 gigahertz. So, every computer has a clock speed know the electronic runs with a common clock it is like a heart of say computer and its synchronized, but somewhere it is a why 5; why not 50 it turns out the quantum interference starts playing. So, this I am not expert of this, but the quantum level phenomena starts disturbing the computation.

So, he cannot go above 5 gigahertz and how many transitions can be packed. So, now, these are electronic objects. So, the distance between two transistor it cannot go below angstrom; right I mean some is like 10 angstrom if you go closer than that then there will be all this wave functions will start colliding in overlapping in. So, there is a limit on how much can we pack. And that puts a constraint on how much; well more neurons you put in the brain we are suppose to be smarted.

So, that is what improve more and more transistor and you are suppose to making it more powerful. But the limit was reached and these chips cannot be faster than that. People are still working the trend pack more and more. So, it is called floating nanometer technology you know this is you might heard these are the buzzwords, but you should know this words if you want to do computing.

So, these are the dies you know. So, that when you nanometer, I do not fully know I mean, but these are the so that means packing more and more. Now, once you say well I have the chip is works only gives you this particular performance. So now, remember how much Giga flops can chip do right now; what processor? I gave this numbers anyone. So, 1 core presently gives 20 Giga flop. And that is easy to see, because it can do 8 operations per second. So, 2.5 gigahertz is typical; I think 2.5 into 8 is 20, ok.

So, that many operations can we do for (Refer Time: 30:19). So, each has limited number of computing power, but then you have combine them together and make a super

computer. Now, presently I did not mention in the class. There are 1 million cores have been assembled. So, that 1 million cores have been. So, there are ways to assemble them and it resists lot of power. Like full of Kanpur power it this one super computer will take. But it can do something like 50 time 10 power 15 Schrodinger power operation per second 50 paid of flop.

But now, of course the challenge is how to use as machine. How to write a program which will work on the whole machine and nobody has been able to run on the whole machine. We ran a code; well, we ran on one not this machine, but we ran a code on 196 (Refer Time: 31:25) emphasize this many codes. This means all of CRAY x into (Refer Time: 31:34) no sorry Cray XC 40. So, our code runs on the full machine. So, you required ask to work for 10 years, to optimize each part because is there any challenge that everything works together, ok.

So, how to write this codes you takes time and also need to learn you functions which will make this communications possible across nodes. So, this are new paradigm; I mean which I dint touch it at all, but this we do I well I teach this I taught last year, but this (Refer Time: 32:19) programming you know you have to it is not difficult, but some of it learn yourself. But if you want to do serious computing in any field: astrophysics, quantum physics you have to learn the parallel programming. The reason is obvious now because single core you can do only limited number of it has limited power this I told you this is like; I mean you can put 10 core that will be hundred Giga 200 Giga flop.

Now, you want to solve problem similar to whole earth; the climate of the whole earth. And the amount of grid which we want to put is in billions. So, the number of elements in the grid we packed in our code 64 billion points (Refer Time: 33:12) you can you really need to put more if you for climate bounding the challenges to make a grid which we look ridiculous, but the grid cannot go 3 kilometer by 3 kilometer grid. But once you make three kilometer grid you know how many data points are there along in each direction 20000 by 3 is 6000 each direct x war as z is the height atmosphere and that you like to put similar thousand in the height.

Now the height is, I mean the atmosphere is around it filling out that ionosphere. So, someway like 40 kilometer. Real activities in let us say 10 kilometer. So, 10 kilometers by 1000 gives you 0.1 kilometer 10 by 1000 is 0.01 kilometer which is 10 meter. But 10

meter is I mean like this, this full room above the room that is one point. Now that is not good because its lot of activity happens within that box. So, you want to pack even further, but that computers also are not so powerful.

And then the physics: physics of the flow is also very non-linear and people do not understand how to model it. So, one thing is to how to core then secondly computer is only as smart as the programmer. So, I am not the big profounder of are the; big believer actually I am not a profounder, but I am not a believer of this artificial intelligent where people think that computer can rule the world.

Well, via computer humans wants rule the world that is my right. It is not the computer rule the world, but there are people who want to rule the world using computer I means the interns (Refer Time: 35:02) dependent on it, but then you can exploit it to control. Now this is one thing, but there is another thing which is coming up, again I wish to work on that field but I do not have time. But you should really think about quantum computing.

Now actually I will ask this question which I did ask the class which is I think very profound question; that in a hydrogen atom electron follow certain law and computes exactly where to be or electrons are not a particle. But the way the electron is computes what to do. Now how does it compute? If you believe that world is a computer. Now we have not think of the world, but I am just think of a electron only. Now how much resources does it have a single electron, how many memory does it have, how much computing power does it have. But it is precisely able to compute what he should do.

Now when I compute, suppose it has let see it has memory and the computing power like the super computer, but then I know every algorithm has an error, right this part you understood in the class. That whatever extremely used there will be error, unless due to symbolic computing. But this trajectory computing, this doing some trajectory computing or rather very function evolution. And if we evolution is exact now how can be it exact if it is a classical computation. Are you quantum computation the way we are thinking? So, it is computing but its speech, I mean I cannot really understand what it is doing.

But if you think in fact there are all the big (Refer Time: 37:06) think the like whole from you heard of this mathematic a whole from; the lot of arrogance someone some people I

mean I can say in this room another thing this whole word is a computer I mean how can it become fitter; if it is doing what so precisely and no computing seem can do so precisely. So, to do something and quantum computation can give you some clues how the world behave. In fact, that gives a different perspective. In that way we all work with (Refer Time: 37:38) and it compute that is correct, but this question is also important question; how does it know how to behave. I mean we believe neurons is doing all my work, but how does it work.

So this is one, and the other thing there is the biological computer for people have thing of using DNA, so you can make computers with that. Optical computer people are trying instead of using electrons is a pathway it is optics. So, that also I did not want. This is important I do thing that interiors down the line there will be a computer and you have to restart getting the new codes so that.

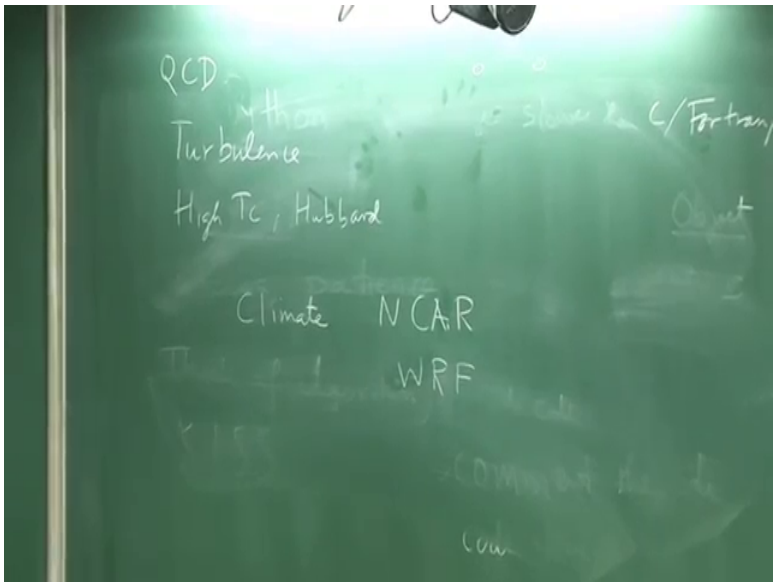
So, the problems which is a where, I did list lot of problems in the beginning of the class right I mean. So, some of you remember some of those forget then where you thought about a new topics which are use in computation. So, I will just list out few things. So, any questions on there; so kind of this is what are the paradigms. So, I mean this is where computing goes from first language to what you do in advance.

But normally we will do not offer courses. There are courses for parallel computing very rarely, nobody teaches in IIT. I taught in once, but I mean I cannot teach every time you know that is. So, you have to learn it yourself most of the time. And there is no course in this. But there will be introduction, but how to use this computer. At least in IIT I am not aware of (Refer Time: 39:45) ok.

So, instead I tell quite often that again is a myth that you can solve with pen paper. Now whatever has been done, whatever could be solve with pen and paper I would not say all, but lot of it has been done. Now with pen and paper it just becomes reasonably impossible to solve every problem this is a big bottle neck. Now I do not mean to say that there are no smart people who can solve with pen and paper if possible, but where is not been fail in you will to solve those problems.

That means, there something inherently difficult in those problems. And which is making it problematic. Then every problem is just stuck like QCD. You know what is (Refer Time: 40:55) quantum.

(Refer Slide Time: 40:59)



In fact, the question (Refer Time: 40:01) lectures are that way very nice it tells you the problem in a simplest possible ways; is just give me the mass of the neutron from the first principle. So, if you think quantum mechanics can give the problem number and it try it.

Assuming the quack marks I mean assume the quack marks, but then derive neutron marks. I am not saying derive the quack marks too that is another problem, but assuming the quack marks you try to write QCD marks from such principle. The turns are even. So, this was a one thing of QCD. And I say nobody is able to do it. The reason is a non-linear, it is the nonlinearity is sitting in everywhere.

So, the equation which comes in (Refer Time: 41:53) is non-linear and that is what it is a same nonlinearity which is any turbulence I mean this is no different nonlinearity. One part has bit more complexity where the quantum mechanics play the big role in QCD. But it is a nonlinearity which is the problem, not the quantum part. So, in fact high Tc super conductor in the same problem. In fact, there are many problems in condensed by the physics which are again nonlinearity in the problem. So, this one example I mean it is called Hubbard model to these are quantum problems, but they are strongly cupping strong cupping.

So, very few things are exact solution. So, the only two problems are exactly solved is (Refer Time: 42:41) both classical in quantum an oscillator. I mean forget about particle

in a box that is the there also there is (Refer Time: 42:50), but non-trivial problems are these two both then classically and fundamentally, but then no third problem which has been solved analytically.

A helium atom is not solved analytically (Refer Time: 43:04) put the third object is the three body problem and three body problem is unsolved both classically and quantum mechanically. But unsolved does not mean there is another issue know what is meant by unsolved; does it mean I have only analytical fury that means unsolved. So, one mood have modify the questions I do I understand the problem. Does not mean I mean having some I understand somebody does not mean I saw somebody you know. You have understood the how the person behaves. Is that clear, so that is what you mean.

So, you understand how this turbulence problem behaves; does not mean I had this is the formula for turbulence. I think that is not very limited way of stating the problem. So, given this parameters I should be able to predict the feature, if you can do it that is understanding. I mean I have put say that is the modified way of the classical way of saying what is the understanding. So, that is way the extract can the way to do is computation it comes in a big way, ok.

So, I think is a important thing which I am saying it more boldly, but you have to understand that it is you have to do. And it is not solving in a simple one; I mean you have to do compile and you have to collaborate is impossible to write those big codes alone. So, you can visit the climate models this are the big activity in a; so National Central for Administrative Research this is the big website.

Now, I just want you to go and see any code which is being developed. So, they have lots of code, which does different things you know. So, one thing you ocean model, atmosphere model, but one this is a I like finite volume. So, they develop finite volume somebody is being spectral. And these code each of this will look at like WRF. So, this weather research forecast; now look at the number of people who are working on this. So, this is my just suggestion you just go and have a look there are hundred people working on this; hundred people. In fact, then another code I think I forget community climate model; I forget the name of that code I do not use that, but then WRF is hundred people.

Now, how to hundred people combine they write a code? But single person simply cannot I mean there I understand atmosphere, but I do not understand ocean. But you have to get those few people to write in such a way the code will come and in work. Now in India where is refer to write those step. So it is critical: I mean critical (Refer Time: 46:01) survival to do first criticize.

And that is why we do not have a climate code in India, can you imagine that people who pride the country which prides in software technology there is no single code, in fact hardly very few scientific codes. So, I mean these are things which you it will young and you should think of a new of fresh approach and learn you tools from this there is no other way. In fact, that is how you can survive otherwise if you do not I mean if you use start using stone edge (Refer Time: 46:35) I will come in the gun and shoot you; it is simple right.

So, that is what this phenomena. Here you are still using stone edge tools. Good, so I stop and go.