Modeling Transport Phenomena of Microparticles
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Lecture-36
Numeric Methods for Transport Equations, Part-II

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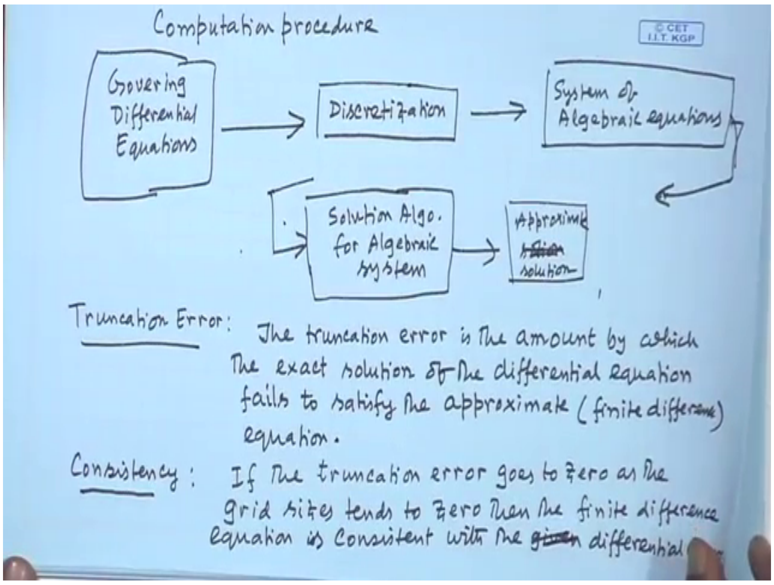

You can be put in a flowchart what is boundary value problem, all that is the you have the governing differential equations, which are discretize first so it goes discretizion procedure and then this is a system of algebraic equation, it need not be linear if it is a linear at them directly we can compute if it is a nonlinear boundary value problem, if not then we have to go for some solution algorithm.

I will go for algebraic system like Newton translation technique and all and then we get the approximate solution, this is basically so this is the procedure, this is the few steps we consider, now what are the difficulties of the order of approximation, now we can have first second and higher order and all which method will use and who guarantees that we have the solution whatever the solution.

And get it converts to the solution of the boundary value problem or the differential equations we are looking for, so now in order to compare the methods which the merits of the methods, we have to know the truncation error, so we define the truncation error which measures the accuracy of the method is the okay, is the amount by which the exact solution of the differential equation fails to satisfy the approximate.

Here it is finite difference equation or finite difference equation, now the global and local truncation error because here so for whatever we have done is the finite approximation is grid independent. So global and local truncation error here at the same, so it if is where is the way of the approximation out the difference scheme is depending on the grid we are choosing, in that case the truncation error will vary from grid to grid.

So that case we will have a local truncation error at global truncation error different, now consistency is a very important thing, so if the truncation error, if the truncation go to zero, as zero as the grid size, tends to zero then the finite difference equation or the approximate equation is said to be consistent with the given differential equation. I think even is not important word because according to that equation we get the approximate equation.

So if the truncation error goes to zero, if it is some constant value so this is not consistency, consistency is very important, Now one can show in all the situations whatever we have considered for the boundary value problem there one can find out that truncation error and consistency. The best way one finding the truncation error, what we did is?

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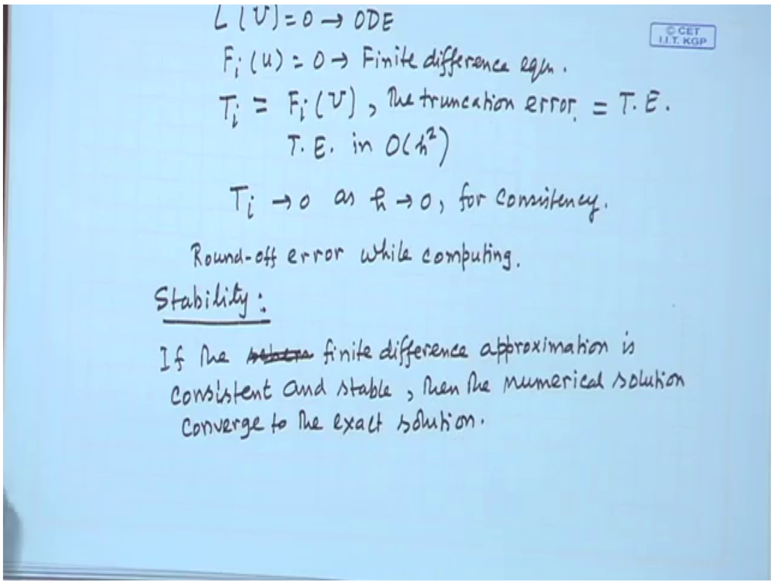

L(u) = 0 is the ODE and Fi(u) = 0 is the finite difference equation, so that the truncation error Ti is nothing but Fi(u) the truncation error. So now in the order of estimate of the truncation error is important so that means we have to write the truncation error at T E in order of h square for the central difference scheme and so on. So normally the truncation error should be expressed as a order of least power of h as mentioned before.

So Ti tends to 0, as a h tends to 0, for consistency apart from that this error, there is a another error when we implement this method numerical method as we described to solve in computer or say calculator and all so there will be a round off error will be, because there will be infinite digits and there will multiplication, division and all these things. So we have to chop out the infinite decimal place to finite decimal and all these things.

So there will be a round off error, that is the most important error while computing, so then another aspect occurs is the stability. Stability means that if some error is incorporated in the system at certain stage so either it may be a round off error or misinterpretation of the conditions given. So in that process a small amount of error, if it is incorporated now if you see that whether that error grows.

If the error grows as we progress in computation then it is called unstable and if the error remain same order case then it is a step okay. So stability of the scheme is very important, so now if the one can say that the scheme is here of course we did define so if the approximation is consistent and stable then the numerical solutions converge to the exact solution. So that much we can say.

Now here the stability particularly for this kind of direct method whatever we have considered, because here we are not repeating the process stability is not a very big issue in the sense that here the number of computations are limited, finite number of computation, finite number of steps are occurring. But if you have a situation where it is with a time integration, so large number of time stables to be followed.

So the same process has to be repeated several times, so in that process if somewhere around are occurring so that will go beyond bound, so in that case it is unstable situation. So next topic will quickly go through is the solution of partial differential equation.

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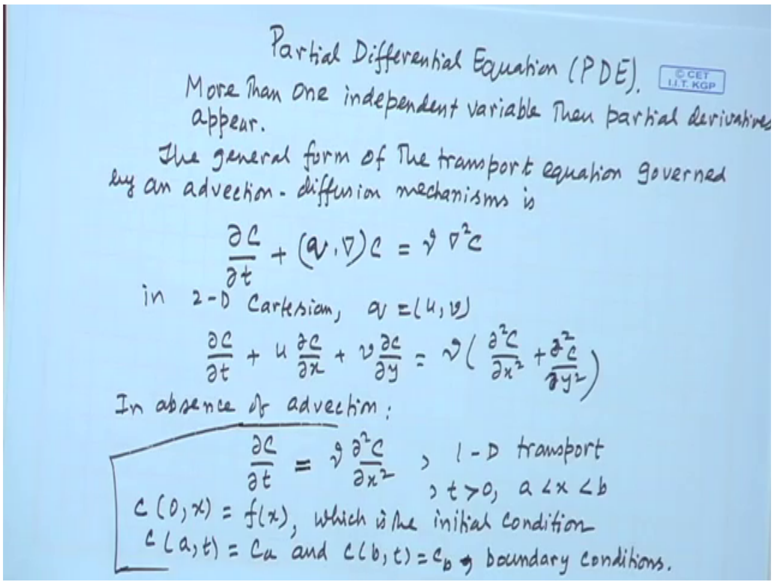

Now when variable are functions of more than one variables, more than one independent variable, so in that case we get a partial derivatives then partial derivative appears. Say you have come across already the transport equation, the general form of transport equation governed by advection diffusion mechanism of this form. This is C is the one transported by advection and diffusion, so this is advective term and this is diffusive terms.

So if two dimension 2D Cartesian, so q = uv, we get Del c Del t + u Del c Del x + v Del c Del y = Nu (Del 2 c Del x 2 + Del 2 c Del y 2, so we have come across this kind of equation in modeling the many transport phenomena in the previous lectures. Now suppose we first we consider the simplified situation, so in absence of advection there is the mechanism is pure diffusion, we get a equation Del c Del t = Nu Del 2 C Del x 2.

We consider only one dimension, 1 - d transport, so it is only governed by the diffusion mechanism. So say a condition has to be given for this is the time, so what I need to find out the a greater than 0 and x is varying between a to b, c(0, x) is something is given, say let us call effects, which is called the initial condition and the two boundary conditions are you say c(a, t) = ca and c(b, t) = cb.

So these are the boundary conditions, so this is my first we talked about how to handle, this is also called the heat flow equation where c is the temperature and the mechanism is governed by pure diffusion mechanisms. Nu is a constant divisibility in that case, so how you solve this.

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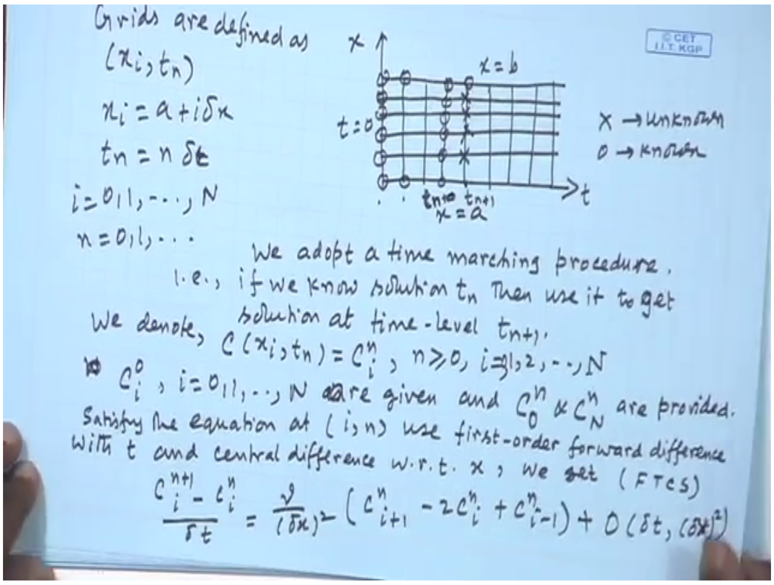

Now here the computational domain, or the domain where we are finding the solution, we need to find out the solution is a tx, t is the time, so this is the line t=0 and say x is varying from x = a and this is x = a and this line is x = b and this is t=0. So first as I said before that we have to construct the grids, so grids we define as say (xi, tn), xi = a + i Delta x and tn = n Delta t, i can vary from 0,1,2 up to capital N.

And N is vary from 0,1,2 semi infinite, so that means what you are doing is step size Delta t and these are the lines which x is varying, and this are the lines which t is varying. Now for conditions we have given, if I circle this, is the conditions are given, this is the initial condition and anytime this is the boundary condition. Now we adopt a time marching procedure, that is if we know solution at tn, time level tn.

And then use it to get solution at time level tn+1 so that means I suppose at certain stage I know the solution this is say tn+1, let us call this tn, I know the solution at all this level at this is tn+1, so this need to be updated. So denote, c(xi, tn) = cn i, so n is greater than equal to zero. And i varying from 1, 2, i can be zero also. Zero and n, so let us introduce 0, 0 and N are the boundary conditions.

So we need to find out so C0 i, i= 0, 1, N is there are given along with and any time levels Cn 0 and Cn capital N and are provided, these are the boundary condition. How to get the solution, so what we are presumed that we know the solution at N and we need to find out the solution at tn+1, so this is the level where we need to find out the cross, say unknown, 0 known.

So this solutions are somehow update in other words I suppose start with n = 0 then and now I need to find out the t1. So if it satisfy the equation at the grid points, say words (i, n) used first order forward difference in t, with respect to t and central difference with respect to x. What you get this is also called the FTCS, so what you get is Cn + 1 i - Cn i by Delta T = Nu by Delta x whole square Cn i + 1 - 2 Cn i + Cn i – 1.

So obviously this one can so very easily is truncation error is first order time and second order in x. So from here we can write the unknown here directly.

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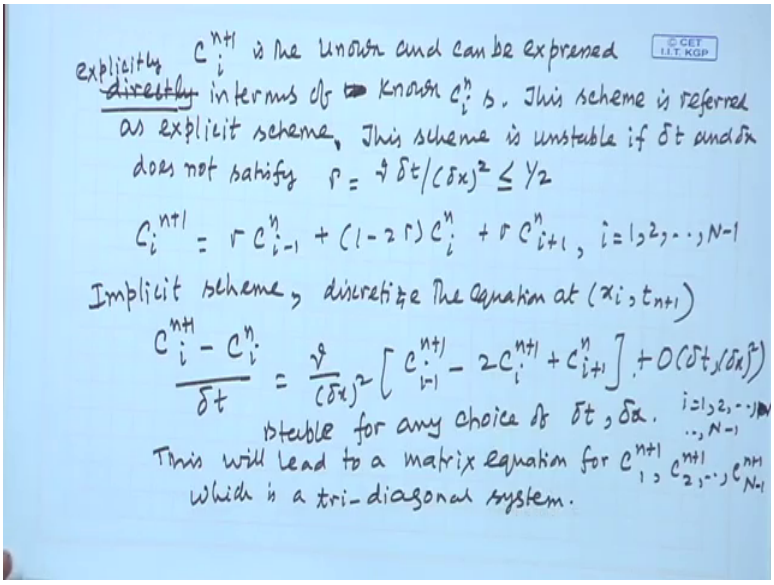

And can be expressed directly in terms of and known Cn i's should I call this scheme called is referred as explicitly, explicit scheme, directly or explicitly that is the better way instead of directly or can say the explicit, so that is explicit. Drawback of these explicit scheme, this scheme is unstable if Delta t and Delta x does not satisfy this condition, this is a parameter r = Delta t by Delta x whole square should not.

If it is does not satisfy this condition then it is unstable, so that is another bottleneck because you have to choose this Delta t very small compared to Delta x. So another advantage is another remedy but one advantage is that we can drive directly the Ci n + 1 in terms of all this Cin. So basically what we can do is we can write this Ci n + 1 = r Cn - 1 + (1 – 2r)Cn i + rCn i+1.

Now you vary i from 1, 2, etc., N - 1, you get the all set up values, but it is the drawback is unstable and first order in time. So then we go to the implicit scheme, so that means discretize equation at (xi, tn+1), so what I get Cn+1 i – Cn i by Delta t = Nu Delta x whole square Cn + 1 i - 2 Cn + 1 i + Cn i + 1, this is again order Delta T Delta x square but advantages that this is stable for any choice of Delta T and Delta X.

However if I vary i = 1, 2, n, we get this will lead to a matrix equation for Cn + 1, Cn + 2, etc., Cn + N, this is capital N and capital N -1 and so that is another and this matrix is a, which here tri-diagonal system. Now again this is a first order but advantages that it is a stable, so the most popular one above all this scheme is a Crank Nicolson scheme. So the Crank Nicolson scheme is so that is the most popular one.

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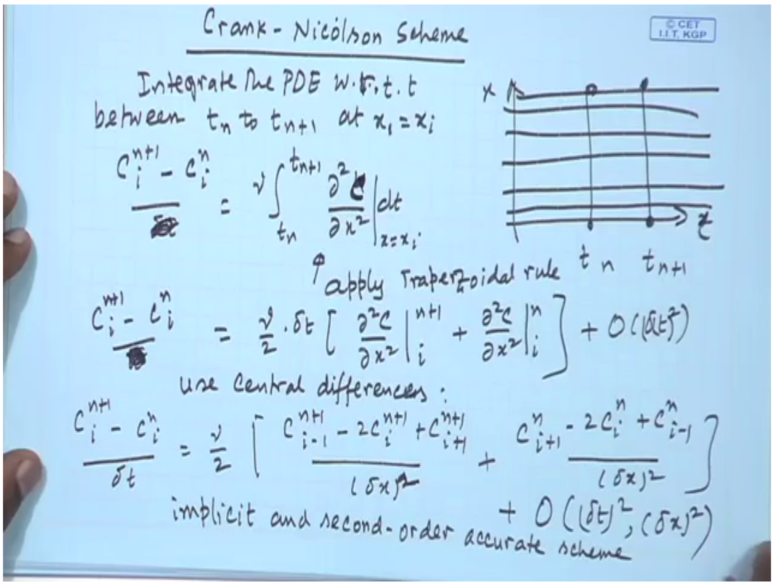

So here what I do is we have this is t, this is x, so you need to find out the solution say this is tn and this is tn+1, so we need to find out this solution using this tn, we need to find out the tn+1, what we do? Integrate the equation PDE with respect to t between tn to tn+1, so what I get is Cn + 1 i at grid point x = xi x, - Cn i by Delta t = Nu tn to tn+1 Del 2 c Del x2 dt, Hhre we have taken x = xi.

So here we apply trapezoidal rule, so if we apply trapezoidal rule this becomes Nu by 2 into Del t Del 2c Del x2 at n + 1 i + Del 2 c Del x 2 at n i because that is the average Delta t by 2 with the average values n + 1 and n. That is the, what is referred as the trapezoidal formula. Now you use Central difference scheme, differences so what I get we use central differences we get Cn + 1 i – Cn i by Delta t = I am sorry this Delta T should not appear here.

So this Nu by 2, no Delta t over here, so Nu by t, this Delta t now point there so Cn + 1 i - 1 - 2 Cn + 1i + Cn + 1 i + 1 by Delta x whole square + Cn i + 1 - 2 Cn i + Cn i - 1 by Delta x whole square. And these scheme because this is order Delta T square, so this is order Delta T square and here when I have taken the central difference scheme so these become order Delta T square, order Delta x whole square.

And also implicit so now if I, this is an implicit and second order accurate scheme. So this can be, this scheme can be written as we can express this schema as:

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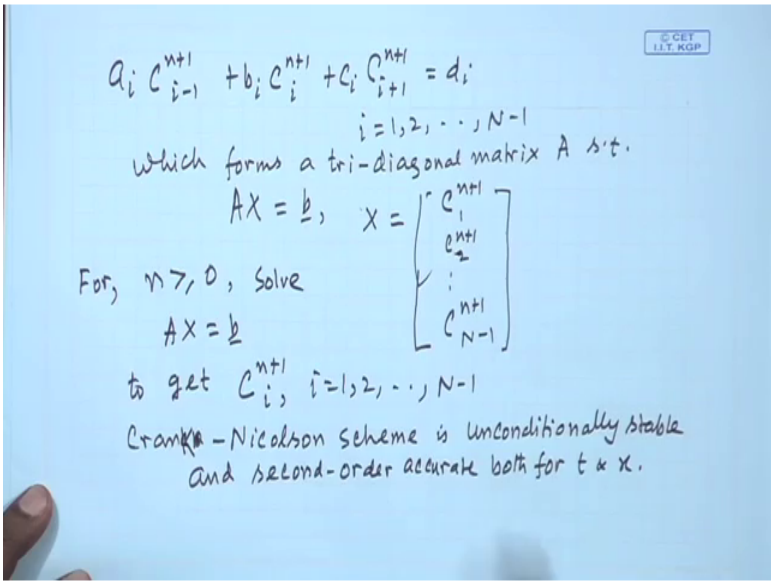

ai Cn + 1 i - 1 + bi Cn + 1 i + ci Cn + 1 i + 1 = di, for i = 1, 2, up to N - 1 which forms a tri-diagonal matrix equation. Matrix A such that Ax = B, say x at every time level this is unknown Cn+1,1, Cn+1,2 etc., up to Cn+1, N – 1, now if you solve this so is a tri-diagonal matrix. So every time level for n greater than equal to zero, for each n greater than equal to zero.

Solved Ax = b, to get Cn+1 i, for i = 1, 2, up to N - 1 so it to start the procedure, to start for the initial condition the given value of whatever the initial conditions as given and we proceed in that direction. Another thing is that so this Crank-Nicolson scheme is unconditionally stable because it is explicit, no implicit stable and second order accurate both for t and x.

So these are the advantages why the Crank-Nicolson scheme is the most popular numerical scheme to solve this if transport equation.

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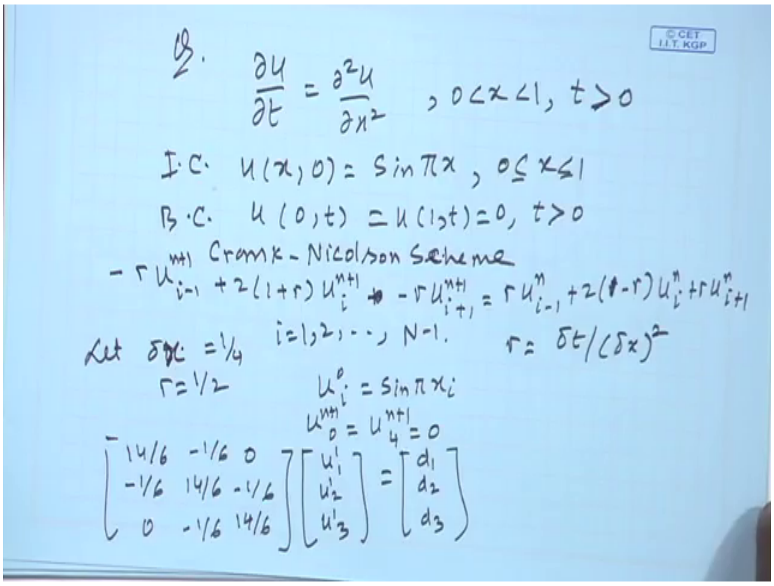

So this question Del u Del t = Del 2 u Del x2, u(x, 0) is the initial condition Sin Phi x, 0 less that x less than 1, t greater than zero, and u (0, t) this is the I.C and this is the B.C. Bpoundary condition, u(0, t) = u(1, t) = 0, this is for t greater than 0, 0 less or equal to x less than equal to 1. So if I write the Crank-Nicolson scheme corresponding to this Un + 1 i - 1 + 2 into (1 + r) Un + 1 i – r Un i – 1 + 2 into (1 – r) Un i + r Un i + 1.

Where i = 1, 2, etc., up to N – 1, r = here it is Nu is 1, so Delta t by Delta x whole square, so if I choose Delta x if I choose as 1 by 4 and r = 1 by 2 let this one, so initial conditions are U0i = Sin Phi xi and what you have is Un + 1 0 = Un + 1 4 = 0. So you get a system always as the, A comes out to be shown by 14 by 6, - 1 by 6, 0, -1 by 6, 14 by 6, -1 by 6, 0, - 1 by 6, 14 by 6.

This is the first step u1,1 u1,2 u1,3 and something like d1, d2, d3, which ones we solve this so I get the u1, u2, u3 at the time level 1. With that time level 1 and the boundary condition we go to the next time level and repeat the process till the desired time step we required to find out. So the next one will briefly talked about the solution of higher dimension equation, so that means U can be a function of X Y and also the convective transport is also taken care, so that will be discussed in the next subsequent lecture thank you.