Modeling Transport Phenomena of Microparticles
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Lecture - 37
Transport Equations, Part-II (Contd.)

We will continue our discussion with the numerical methods. So far we have talk about the numerical methods for boundary value problem, linear boundary value problem nonlinear and partial differential equations that is the re-transport equations. Now when we have an advection equation that means equation like these. This is the general transport equation because already we are seen the transport equations are governed by both advection and diffusion.

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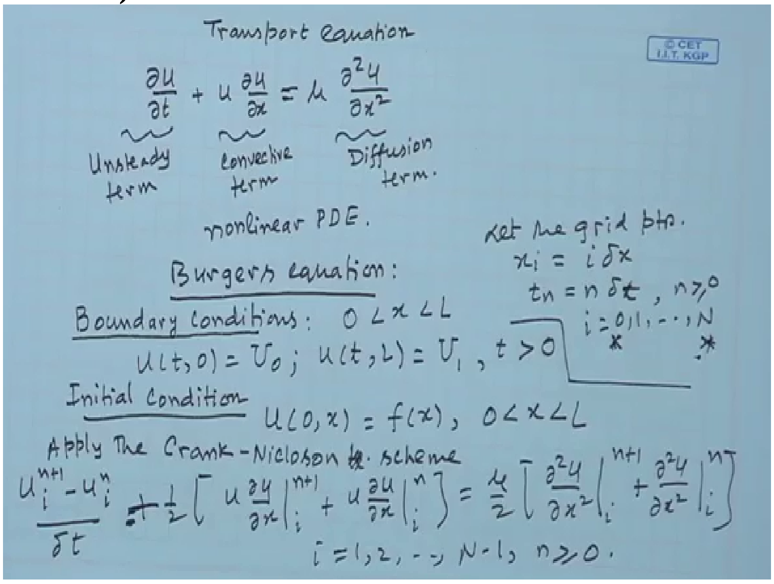

So the equation like this Del u, Del t + u, Del u, Del x = Mu Del 2 u, Del x 2. So this is the one we call as unsteady term and this one is the convective term and advective terms, Convective term due to the transport velocity as U. And this is the diffusion term. So this is the differential equation, partial differential equation we desire. Now the Partial differential equation is non-linear PDE. If I neglect this convective terms.

So this basically DE parabolic equation. Which we are already discussed about how to solves this. But if we do not have we cannot neglect, that mean it will be stopped. If Mu U, Del u, Del x, is significant, So that means the advective transport is not very negligible normally advection is refer to the heat transport. Here we can call as the convective transport. So the equation in the hold is called the Burger equation.

Now this Burger's equation is very famous. Because it has the property of many fluid transport problems. Like this model as the boundary layer situation. So that is the momentum equation and boundary layer approximation can be reduced to this form. So, that is why any numerical method can be validated by comparing with the burger's equation. Another difficulty is that these equations, In general we can say it is a parabolic type.

But these equations have the hyperbolic if this diffusion term is negligible. If this term becomes in negligible one. So in that case this is becoming an hyperbolic one. So this pose are boundary conditions this manner becomes this is the both an initial and as well as boundary conditions space PDE poles are there. So, this boundary conditions let us talk about the boundary is the X is very (0<x<L). So one boundaries t0 is equal to say some U0. And U TL is equal to U1 for T>0.

And this is the initial condition say U0X is FX for 0 less than X0 less than L. So this is the initial conditions and to boundary condition required because the second order derivative wall for the X. And the first order for the time. So apply the Crank-Nicloson Scheme are we can write this scheme. So we can write this Ui n+1 – Uin by Del t + half, because this half this U Del u Del x.

At basically Crank-Nicloson scheme is two time getting the we are integrating between n+1 in and using a rule two by this is Mu by 2 Del 2 U Dell x 2 and the n+1 i, and Del 2 U Del x 2 this is the x implicit part and this is the explicit part. So i Grid point say 1, 2, ..N-1 is greater than 0, Let us say the grid point xi = i Delta X. And tn = n Delta T, And i = 0, 1, 2…N. And any N is of course positive. So N greater than is equal to zero.

Now here points are 0 are also two boundary points are 0 and N. So that why apart from the two boundary points 0 and N we need to compute in choice of in between 0 onwards very form the initial time t = 0. Now we want to write space discretisation.

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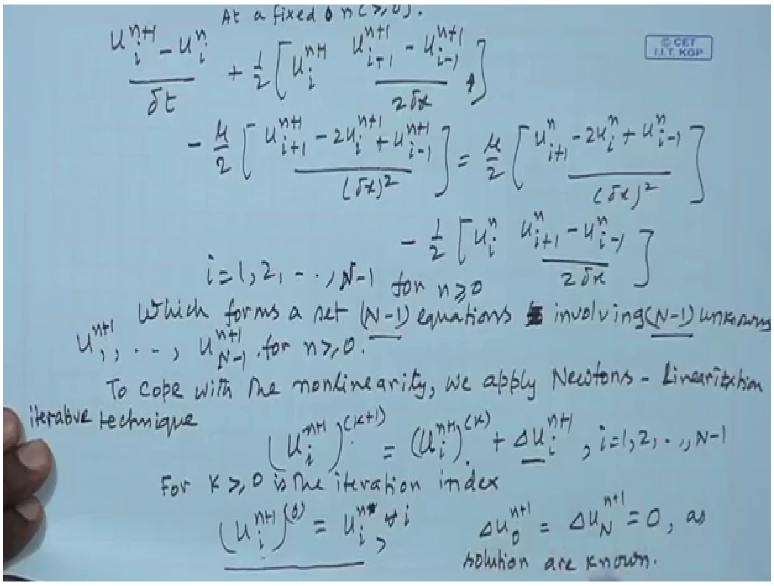

We get the full form as Un+1i – U in by Delta t + half Ui+1i Un+1 i+1 – Un+1 i-1 by 2 delta x. This is the x implicit term and you have the other so what we do the input of implicit term to this left side and explicit term which is known to the right side. So that means all in superscript n+1 comes to this i' th , n+1 and n+1 to the I + U n+1, i-1 by Delta x whole square. This is equal to Ui+1 – 2Ui+1n = Uin-1 by Delta x whole square.

So I = 1, 2…n-1 for the n greater than zero. So which form a set of (N-1) equations for involving same number of (N-1) unknowns? So U1n+1…,Un-1 for n greater than equal zero. So you have any that is have n greater than equal to zero for any fixed value of n. For because be going in the forward time so that means using the value of this solutions n = 0. N = 1 , n=2… like this time side step onwards. So we have difficulties contrasting equations unknowns, same number of equations and same number of unknowns.

To cope the non-linear, so what we do is we apply the non-linearity, we apply Newton's-linear equation technique. So before that let us write at a fixed in greater than equal to zero. Because we are fixing the time so that means from either from zero to first time set. Whatever solving for all i. So the solutions obtain by the Newton literation iteration technique. Because this iteration what we do the iteration technique is approximation of n+1 i at k+1 equal to Ui n+1 k + del Ui n+1.

This is the error, i = 1, 2, …N -1, then we substitute for k greater than equal to 0, is the iteration index, so what we do is we can take Un + 1 i greater than 0 very beginning is nothing but Un i, the previous time is, that is at the first iteration, 0th iteration level, to start with the iteration we can assume this, so at every iteration we are the Newton linearation technique what we do is we approximate the solution Un + 1 i at the k +1 iteration, we made the recurrensational by this way.

This is the error and we assume that this error are very small with square and higher order are negligible in addition we have Un +1 = Delta Un n +1 = 0, because at the two end points these are the two boundary points where solutions are as solutions is known over this two points, so what I do is know we substitute this Un +1 at i this form to here and drop all the values to square and higher order terms Del 2 u n + 1 i, and get equation which will be linear for Delta Un + 1 i.

Now note that k +1 iteration already this is computed so wherever Un + 1 i (k) appears is assumed to be non quantity. This no longer a unknown say start with the k = 0 so that is the beauty of the neutral linearization technique. So what we did for the boundary value problem previously.

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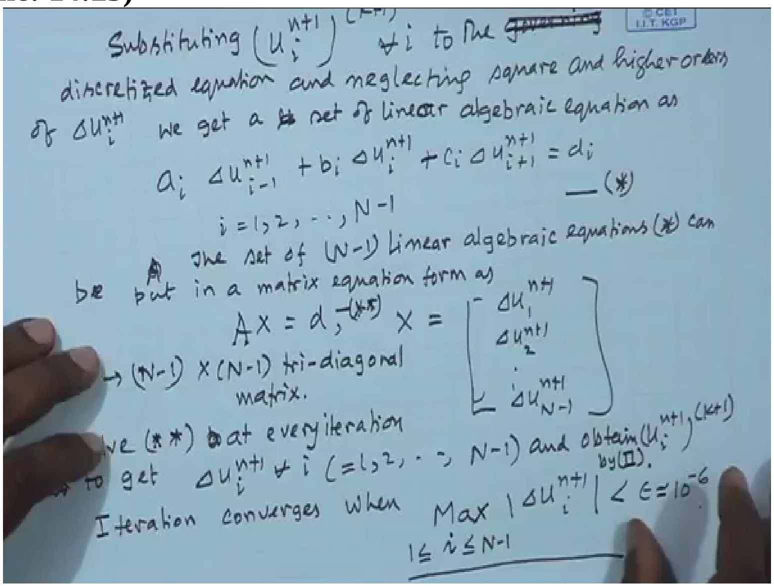

Substituting Ui n+1 whole k +1 + i to the governing equations, to the discretize equation and neglecting square and higher orders of Del 2 u n+ i, We get a set of linear algebraic equation as let us write in this way ai Del Ui-1 n+1+bi+ Del Ui+1+ n+1ci Del Ui+1 n+1 equal to di. Where i = 1, 2, N-1. So `these forms say tri-diagonal system. These set of equation let us call the, set of (N-1) linear algebraic equations.

(*) can be put in a matrix equation form can be expressed Ax = d, where X is equal to all these unknowns n + 1, n + 2 etc., and Delta Un + 1, n - 1 and A will be the (N-1) cross (N-1) tri-diagonal system matrix. So we can solve these systems let us call these double star (**) at every iteration to get Delta Un+1 i, for all i means 1, 2, n-1. So this iteration process once we get this, we go back here, modify as previously obtained.

Get the updated values; get the new values, then proceed further we go for k + 1 iteration process and so on. So iteration process converges when we pose this condition 1 less than equal to i less that equal N – 1. Delta Un+1 + i is less than Epsilon which can very, very small quantity something like 10 to power -6 so, this is iteration means the same process. So it will be repeated few number of times so till we get the convergence.

Here of course we assume that the iteration converge means when it can be stopped, that is assumed to be a reached a convergence is governed by this condition, so if we simply say the procedure is first we discretize this equation to this form and then substitute the Un+1 i at the k + 1 iteration level by this manner and then reduce this equation to a algebraic equation, linear algebraic equation of this form.

(*) star which is a linear equation form for Delta ui at the time level n + 1, that is why n+1 is shown, which forms a tri-diagonal system A(x) = d, solve this tri-diagonal system and get the X that is the Delta ui Un+1 i's, then go back to these equations and get this, let us call this equation we are referring several times, let us call this is one and this is two, so when you get the Delta U n+1 I, substitute here and get the modified value.

Obtain Un+1 k +1 by 2 by using relation or equation 2, so this the process repeated several number times, now whenever a process is repeated n numbers times, the there is a complication era is that whether can be stable, as we stated before if we have small number of error either we have incorporated truncation error or round of this error any other manner, so if that round of error or the error which is incorporated if it magnifies in the subsequent time.

So in that case this scheme is said to be unstable, but if you find that the error is reducing with as we proceed with the time, in that case this scheme is said to be stable either it is craned down or remained constant, now the Crank- Nicolson scheme as stated before.

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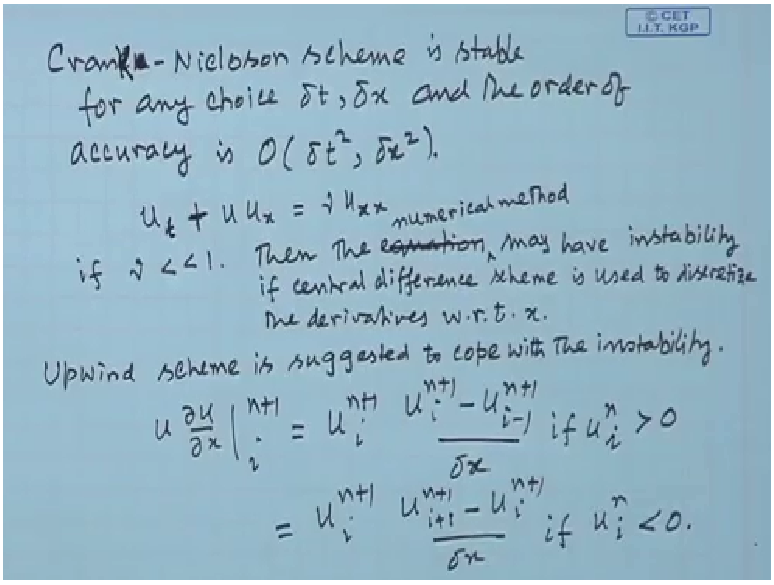

Crank-Nicolson scheme is stable for any choice Del t, Del x and truncation error the order of accuracy is 0 (Del t square, Del x square), now we have no difficulties, thing is we have situation we have considered this equation now if Nu is very, very small then in that case the equation is may become unstable if central difference scheme then the numerical solutions not equation, is used to discretize the derivates with respect to x.

For a hyperbolic equation is we use the central difference for x, there is FTCS time and central in x, so that becomes the unstable one. So that why this kind of situation we have to avoid, to avoid that this is called the Upwind scheme, so in a short form the Upwind scheme will be more useful for this and is suggested to cope with a instability, so Upwind what it does convince.

U Del u Del x at n+1 i is taken to be Un+1 i, Un+1 i - Un+1 i-1 by Delta x if Un i is greater than 0, and this taken to be Un+1 I that means backward difference of x, if the flow is in the forward direction and this is Un+1 i+1 - Un+1 I by Delta x if Un i less than 0, this is upwind, that is along the direction of the wind. So when the flow is coming forward from the backward directions, so at this point i, the flow is like this way so this is your Un i.

So you use the points which is backward of yours, so you are at i, so you take i-1, but when the flow, this is i and the flow is coming like this, so use the point the information is i+1, so that in part stability provided, if Nu is very, very, low so that means the deception is low, okay so if it only dominated by the hyperbolic term, so that is the advective term or convection effect is stronger, compared to the diffusion effect, then a upwind scheme is adjusted.

Otherwise if Nu is order 1, then Crank-Nicolson scheme is stable because there we used the both central difference scheme in the time in the X derivative, Now before stopping, so far what we have considered is that the space variable is a single variable so that means the variable of x only. Now we can have a situation by the transport equations we have already seen that you may have situation like.

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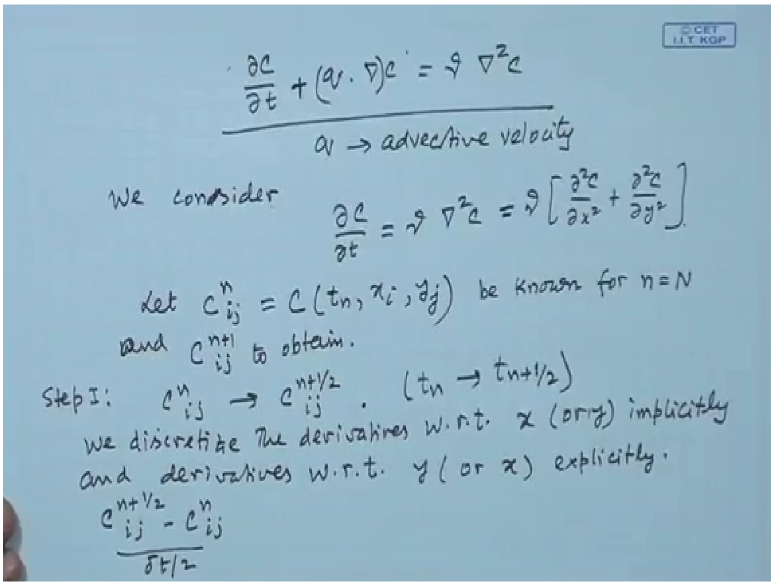

Del c Del t+(q dot Grad)c = say Nu Del 2 c, so this is again advection diffusion equations, this is the advection terms because there is fluid velocity, and solute transport and others at this is the diffusion now for simplicity q will be an advective velocity, q already know so for simplicity we can consider this situation we consider this equation now this is Nu Del 2c2 + Del x2 + Del 2C Del y2.

Two dimension we are not we can have also three dimension I just give one method of course this is a variation of the Crank-Nicolson scheme again this is like a parabolic vd it is a parabolic vd only thing is that it has a higher dimension that is both x and y are the variables in this case so what you have is that you want to compute the let Cn ij tnx = C (tn, xi, yj) okay.

So this is the point we are considering so let Cn ij be known for some n, n = N and C n+1 ij to obtain so this is our task, so here instead of going C n+1 as we do in the Crank-Nicolson scheme what I do is we go by two stay in the step 1 what I do is obtained there is Cn ij to a fictitious time step n+ of ij and so that means we are moving forward from n to n plus instead of so that means tn to tn plus.

Instead of jumping straight from n to n+1 here and the what do you do if we take it discretize the derivatives with respect to say x or y implicitly and derivatives with respect to y or x explicitly so what we were doing is here very simple Cn + half ij – Cn ij since it is a half time step so Delta t by 2 = Nu x is implicitly so that means this is the one to be kept at the current time level and this is the one is explicit that is previous available.

And then we use central difference so if a use central difference what it will look like so this is the one so it will look like let it be here, will be quickly we write.

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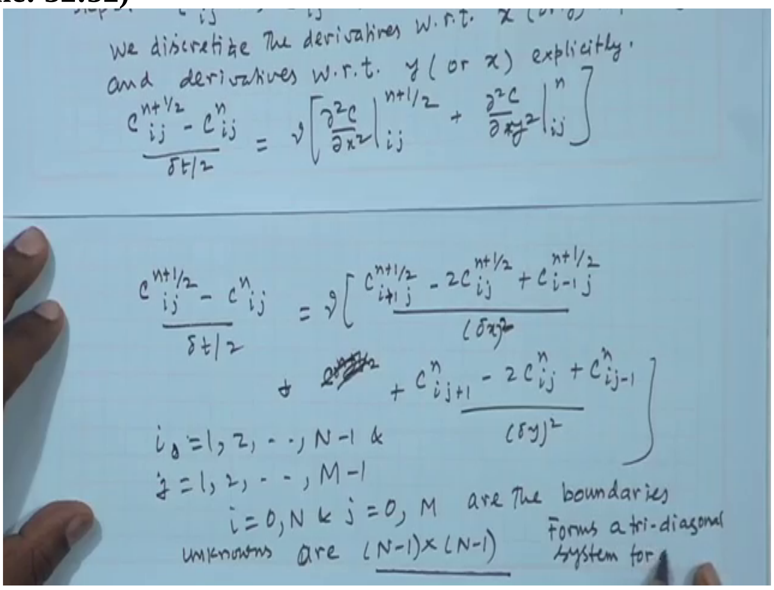

Cn + half ij - Cnj by Delta t by 2 = Nu Cn + half now I see this is a derivative just texted that means I is wearing j fixed so i + 1 - 2 Cn + 1 half ij + Cn + half i-1jby Delta x whole square + and sorry this is explicit so Cn ij+1 – 2Cn+1 ij + Cn ij -1 by Delta y whole square so because this is implicit fashion okay, so here inj, i is varying say from 1 to n -1 and j is from 1 to m-1 i=0 and i equal another boundary j=0 and j = m at the boundary.

So i= 0,N, and j=0,M at the boundaries, so a fixed N half which is not to be find out so i unknown are n - 1 into m - 1 number of unknowns and the same number of equations because if I vary i= n-1, j=1 to n-1 so we get the same number of unknowns and we get a so variable are who superscript n+ half so at this number of equations at this number of unknowns and important thing is forms a tri-diagonal system.

How for a fixed j, that means what are you doing if I kept j fix and vary i so this is formed okay.

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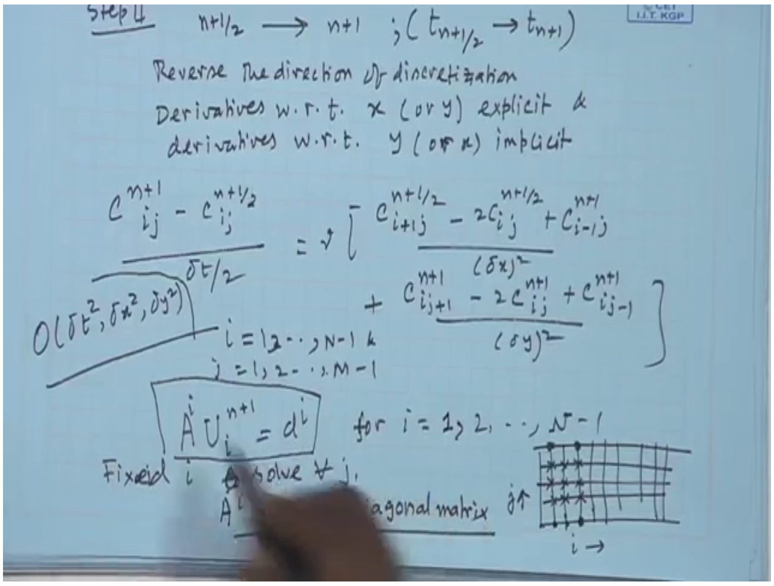

So I just say the big step 2, to so step 2 to what we do that processor got CN + half ij, here n+half to n+1, so that means tn + half to tn+1 so again we reverse the direction so that means that is why this is a alternating direction reverse the direction of discretisation that is to say derivatives if we have taken X was the implicit so now it will be derivatives with respect to x or y here it is explicit and derivatives with respect to y or x implicit.

So what I get Cn+1 ij – Cn+ half ij by Delta t by 2equal to one can write this way same manner so Nu Cn + half this is explicit i+1j – 2Cn+ half ij + Cn+1 i-1j by Delta x whole square + Cn + 1 ij+1 + 2Cn + ij + Cn + ij-1 by Delta y whole square, so ij, i is from 1,2 n-1 and j = 1,2 n-1 every step we get it so this is AUn + 1 = di for I = 1,2 n-1.

What I do is here fixed I, solve for all j so here so that means you have if I do in a pictorial form say the grids so this is the i is along this direction is varying, so this is i, so this is j, what you are doing is these are the boundaries so for fixed value of i wish all for all j, so that means now we are compute for all j.

Once that means we start with from here to fixed i, i=1, so its all for all j, once it is done then i=2, solve for all j and every time we get it tri-diagonal system like this way is Ai is tri-diagonal matrix so this is the beauty of the KDI scheme where we get it tri-diagonal system at every time step so only thing is that we have to repeat this procedure to solve the tri-diagonal matrix for n - 1 types for depending on the i, occurrence, so that it.

That is the way and the order of accuracy is again Delta T square Delta x square Delta y square because this is nothing but a variation of the Crank-Nicolson scheme so this is a second order accurate in both time and space variables okay so that it about the numerical scheme thank you.