Semiconductor Device Modelling and Simulation
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Lecture-51
Hydrodynamic Model (Contd.,)

Hello welcome to lecture number 51, we will continue our discussion on hydrodynamic model.

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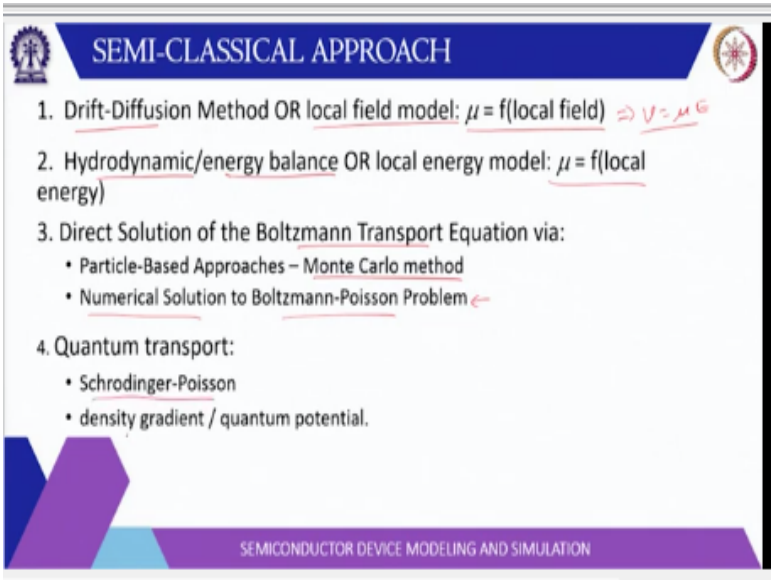

So, in this lecture we will cover the concept related to the relaxation times and the numerical schemes. Just a brief review that we have discussed the drift-diffusion model, so in that drift-diffusion model it was kind of equilibrium and it was a local field modular model. That means the mobility or the conduction parameter depended on the local electric field. So, velocity was mu times electric field.

Then of course to extend it we used field dependent mobility and we also used velocity saturation but further down the line if we want to go to higher electric field or a smaller dimension then there are phenomena like velocity oversoot**,** they can only be addressed by a higher order model called hydrodynamic model or energy balance model. So, here the velocity is not simply mu E but it depends on the energy.

Again that energy is local energy and electron is not equilibrium with the lattice, so electron temperature and lattice temperature are allowed to be different. Then there are direct solutions of Boltzmann transport equation, so one is Monte Carlo method and another is numerical solution to Boltzmann-Poisson equation. This is rarely used because it is very difficult in the sense there are 7 independent variables and it will take lot of time to calculate and solve this problem.

But for some one dimensional or some reduced state space, this can be used. Then of course there is another model called quantum transport, they are this Schrodinger and Poisson equations are solved or some kinds of density gradient or quantum potential methods are used, so this we will discuss in next week. So, let us continue our discussion on the hydrodynamic model.

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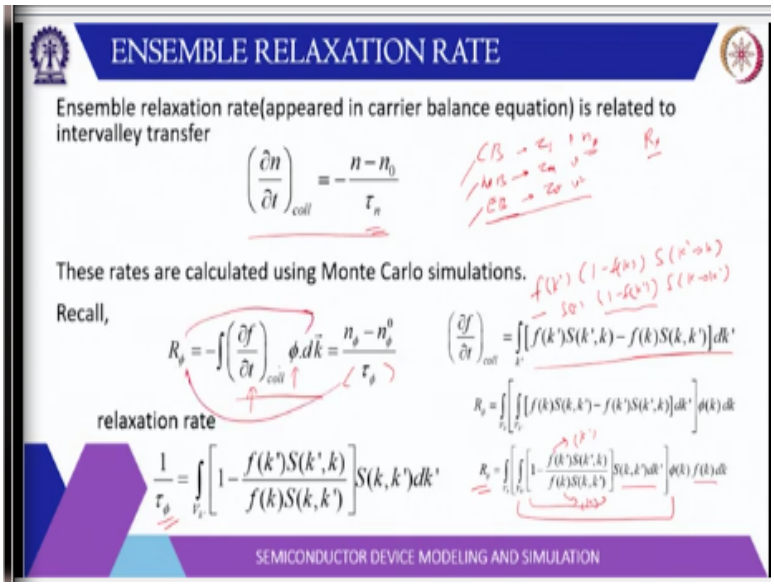

Now in hydrodynamic model we use relaxation time, so for this tau appears for all the 3 equations one is carrier balance equation other is momentum balance equation, another is energy balance equation. And then accordingly the name is different, this is momentum relaxation sometime this is energy relaxation time, this is tau f and this dn by dt collision is given by n - n naught by tau n.

Now for any of these 3 equations we defined that n phi is the variable and this can be carrier condensation or the current density or the energy density. And then it is related to some flux, in flux, out flux and then generation recombination, so we had these equations. Now there was one

term called R phi that was basically kind of recombination due to scattering, so that means scattering takes out this carrier from the particular state.

And then R phi as df by dt due to collision times phi times dk. And if you recall phi was one for carrier balance equation it was related to velocity for momentum balance and it was related to velocity square or energy for energy balance equation. Then we wrote that R phi is n phi - n phi naught by tau phi. Now this tau 5 can be calculated, so if we substitute the expression for df by dt due to collision it can be done as f of k prime times 1 - f of k times scattering probability s k prime to k minus opposite of this process.

So, scattering from k to k prime, so k to that means there are available carries n k - f of k prime times s of k to k prime. Of course when if we assume that f of k or f of k prime is much smaller than 1 then this equation reduced to the form given below. So, f k prime, s k prime to k - f k times s k to k prime dk prime. Then we can take out f k and s k k prime, so f k, s k k prime and this is one factor, so which is some function of k prime, these are some function of k and this we integrate we can get R phi.

Now if we just extract out this integral we define that as a tau phi. And here the tau phi appears as the average value of tau phi. So, average value of tau phi can be described as n phi - n phi naught divided by R phi. So, you change the position, this goes to left and this goes to right.

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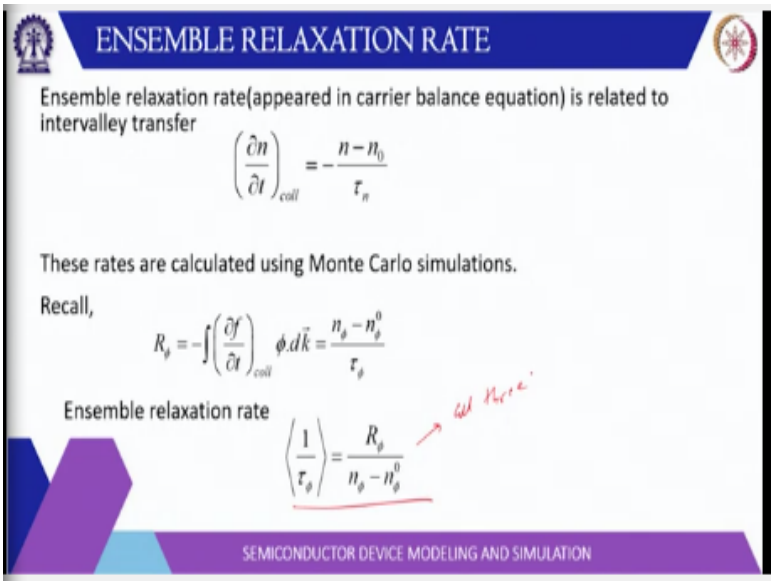

So, 1 over tau phi average value is R phi i n phi - n phi naught. Now this applies to all 3 equations, carrier balance, momentum balance, energy balance.

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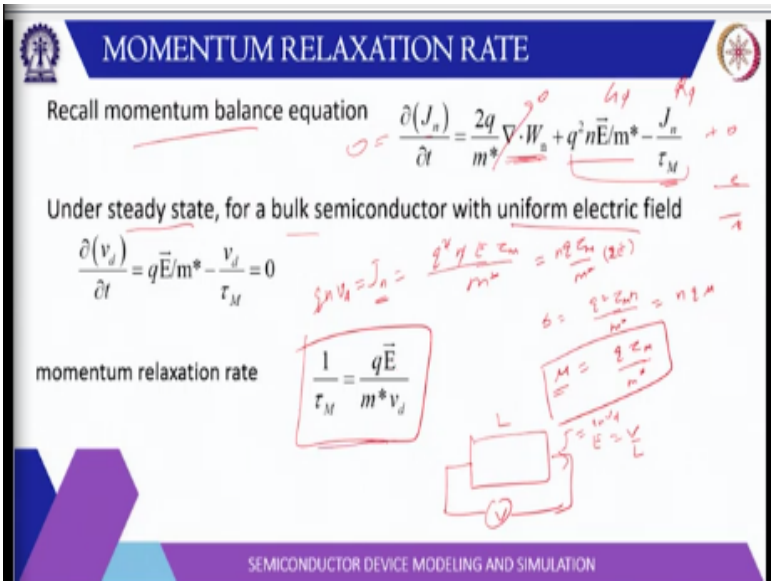

Now let us look at these equations individually. Now recall the momentum balance equation d J by dt, so this is basically coming from E m times drift velocity = 2q times this flux, so this is the gradient of energy density. So, flux of current density is the energy density, flux of the carrier density is the current density plus this is the scattering, due to the scattering, due to the electric field they will be scattered out to different momentum.

So, q square nE by m - J n y tau M, this system was called G phi this was the term was called R phi. And there is a generation recombination term but does not give any momentum the generation of electron whole pair or recombination, so that was 0. So, under steady state for a bulk semiconductor with uniform field, so this field is not varying with position. So, in steady state this has to be 0, so that means and this is uniform, so del w and by del r will be 0, so this term also goes to 0.

So, simply you can write J n = q square n tau times E by m, so this is J n = q square n E tau E tau m times m star. So, from this you can get tau or if you recall this is what? q tau m by m star times q E, so which is the force, so J = sigma E. So, sigma = q square tau by tau n by this is n is also there, n by m, this is sigma. And sigma is n q times mu, so mu is basically q tau m by m star, so in terms of momentum relaxation time tau m, mu is basically defined.

So, this is the expression and then of course if you just want to get the tau m from the current density you can use this expression, 1 over tau m is qE by m V d because this is q n times drift velocity, so 1 q 1 will cancel out here, so you have qE by m, so qE by m V d. So, momentum relaxation rate can be found out by applying a electric field some voltage here to a uniform piece of semiconductor of length L, so the electric field will be V by L and measure the current, what is the current here? So, that is q n times V d, so you can basically calculate the moment of relaxation time.

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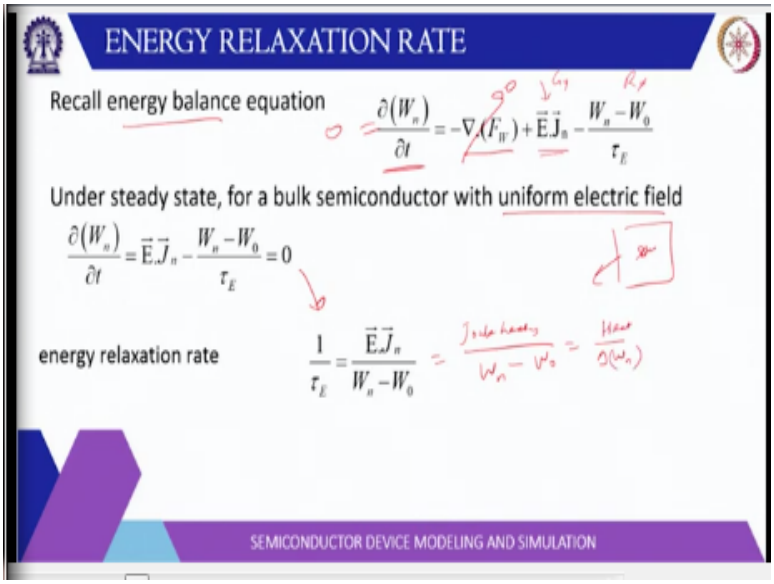

Similarly recall the energy balance equation, so this is the derivative of the energy density, then flux of the energy density and this is Joule heating E dot J which is basically the G phi term and this is R phi term. So, G phi generation that means it is the mechanism which is increasing the carriers with certain energy and this is the recombination mechanism which is taking away the carriers from that state to outside.

So, in steady state this will again be 0 and if a uniform electric field is applied and other things are uniform, so this can be assumed 0, so it simply tells that E dot J = W n - W naught by tau E. So, from this you can find tau E as E dot J y W n - W n naught, so this is basically Joule heating divided by energy density for modified distribution function minus energy density when there is no field, so there is a equilibrium energy density.

So, the change in the energy density basically, you can also write this as a change in the energy density with respect to the equilibrium case times the heat provided to the system.

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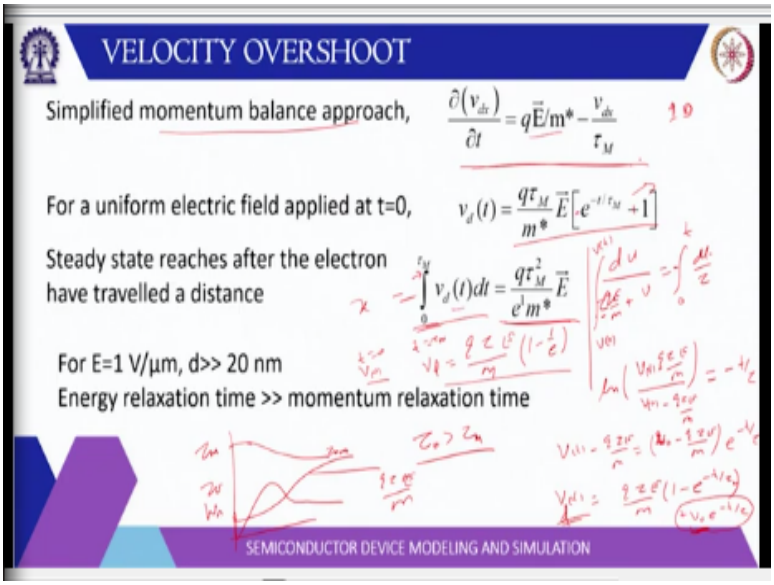

Now if you recall the phenomena of velocity overshoot we said that it can be explained using the hydrogen or dynamic model. So, whenever there is a possibility of velocity overshoot we tend to use this cytodynamic model. Now let us again go to the momentum balance equation and it is done for one dimension, just to illustrate the point let us assume this is one dimension. So, in one dimension dJ by dx is q n times v d, so we divided by q and everything.

So, it was q square M E by m, so now it is qE by m - v by tau n. Now if you solve this equation, this velocity overshoot is not a steady state phenomenon. So, this is basically we have to look at the evolution of this velocity as a function of time. So, now here we have equation d V by dt is qE by m - v by tau. So, if you solve it you can look like this, so it is dv by qE by m - V then tau = dt by tau.

So, I am dropping the subscript you can assume this tau is tau n and so on, if you integrate it for velocity it is starting from t = 0, so V at 0 and V at t this is 0 to t. So, you can also use minus sign here and this becomes plus and minus, so it becomes log of V - q tau E by m and limit is V 0 to v t. So, you can write v t here minus then V 0 - q tau E by m = - t by tau. So, if you further simplify it, so V t - q tau E by m = v 0 - q tau E by m times e to the power - t by tau.

So, you take antilog, so it is 1 s t by tau and this left side is the right side, so then it is a division here the denominator it becomes multiple here when it goes to right hand side. So, if you further

write it here, so V t = q tau E by m into 1 - e to the power - t by tau. And this term here +V 0 e to the power - t by tau and this becomes this is minus, this is plus. So, it should be plus, this should be minus. Now if you look here this sometime is appearing here, now this initial velocity is random velocity, so it is basically in all the directions.

So, this average will actually be 0, so if the electric field is in particular direction then you can write that the drift velocity in that particular direction is q tau E by m times 1 - e to the power - t by tau m, so this expression you will get. Now if you integrate up to tau m with tau m is the moment of relaxation time, so it will be basically at t = tau m this becomes 1 by E, so this will be q tau E by m times 1 - 1 by e, so e is around 2.78, so this will be your V d.

So, now this velocity is changing from V 0 at t = 0 to at t = tau m this is the velocity. And before it basically collide with some other scatter. Now during this time the distance traveled is integral V d dt, so that means you have to integrate it. So, then you will get basically if you integrate this e to the power one is t by tau, so this will be e to the power -t by tau times tau m. So, what you will get q tau square E by m.

So, this is the distance it has traveled till the time t = tau m. Now we know that tau e is larger than tau m, so energy relaxation time is more than the moment of relaxation time. So, that means up to this tau m, it has not gained the high energy, so it is scattering rate is still not that high, so that means the steady state velocity which is q tau by m will reach after certain time. Meanwhile it is still governed by scattering mechanisms corresponding to the previous state.

So, this tau m if you look into situation it will basically gradually go down and then tau e it will take longer time, so that the energy will basically increase after certain time. So, meanwhile it is actually still governed by this tau m then this is tau m infinity, so the velocity actually shows some kind of overshoot and it decays down. So, if we solve the equations corresponding to the momentum balance then of course that velocity overshoot is inbuilt in those equations.

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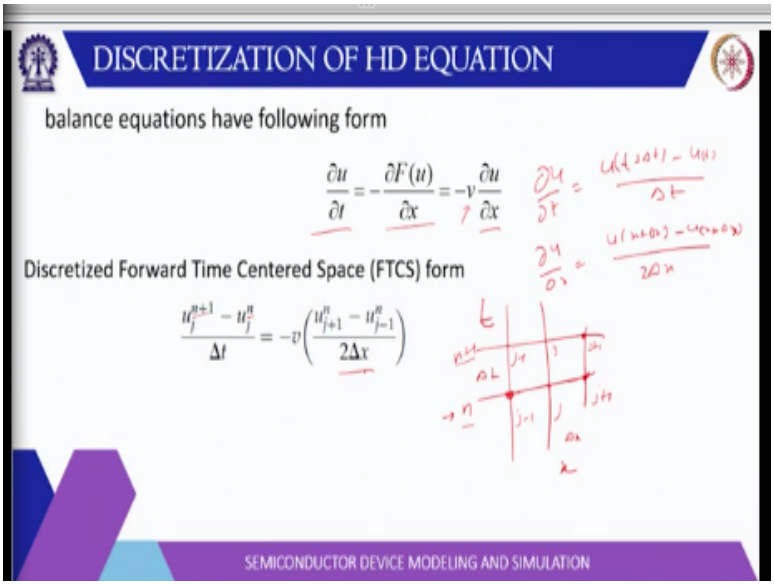

Now we will look at the discretization of hydrodynamic equations. So, when we discretize the solution has to be a stable solution means we should be able to solve it. So, if you consider general equation let us say du by dt = some dF by dx, so which will some coefficient times du by dx. So, if you discretize it, so this is basically du by dt is you can write du by dt is u of t + delta t - u of t divided by delta t, this is forward difference.

And similarly del u by del x is u of x + delta x - u of x divided by delta x, this is forward difference if you center difference then this -delta x divide by 2 delta x. Now that means your grid has to be in 2 dimensions, one is time and one is x, so let us say this is a grid here, so let us say t is n here and x is plus say j. So, this will be let us say this is J this is j - 1 and this is j + 1, so at t = n + 1, this is again j – 1, this is j, this is j + 1.

So, if you write this equation du by dt plus you are calculating at n, so du by dt will be n + 1 - n u of n + 1 - u n divided by delta t and this is delta t, or let us say this is delta x, so is equal to -V times u n j + 1 so this is u n at j + 1 - u n at this is a n j + 1 j - 1. So, along x direction basically divided by 2 delta x. Now if you want to find out the stability of this process, what is done basically?

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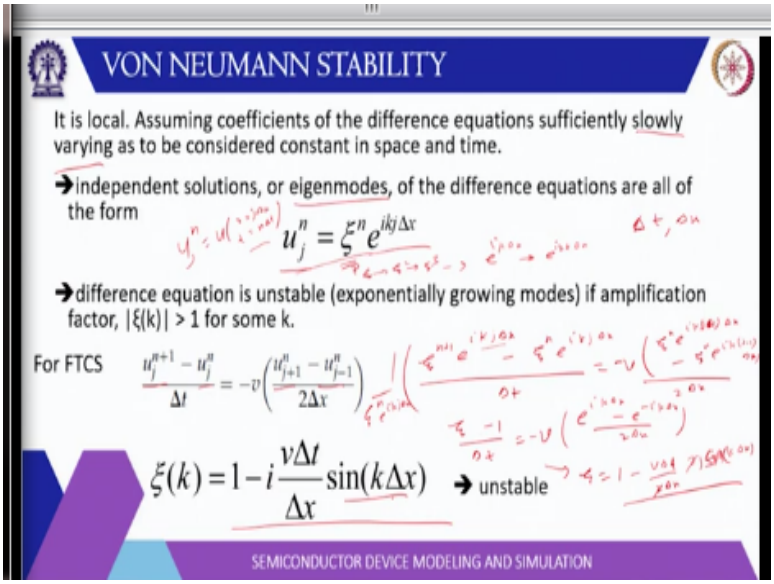

We assume that coefficient of the difference equation, so which is V here, so we assume that this coefficients are slowly varying, they are slowly varying. So, that means the advantage that if they are slowly varying then over the position the delta time delta t or over the space delta x they can be assumed constant. Otherwise if they are first varying then of course you cannot write equation like this, you have to include v or these coefficients also into account.

Now for this kind of equation generally Eigen mode solution is used and for any state variable u at position j x and n, so this u j n will be u at x = j delta x and t = n delta t. So, this will be Zeta type power n, so that means the error is increasing as Zeta. So, from n = 1 let us say error is Zeta first step, for second step it becomes Zeta square, for third step it becomes Zeta q and so on. And as far as delta x is concerned it is e to the power Iota k j delta x.

So, due to the space the error is changing like e to the power k delta x, first is the second e to the power 2k delta x and not this Iota. So, that means there is some phase change. So, if you substitute this one to the equation here what you will get? u j n + 1 will be Zeta to the power n + 1 e to the power Iota k j delta x - Zeta to the power n this is u j n e to the power Iota k j delta x divided by delta t = -v times u j + 1 n, so this is Zeta to the power n e to the power Iota k **j + 1** j + 1 delta x - Zeta to the power.

Again this is n e to the power Iota k this is j - 1 delta x divided by 2 delta x. Now Zeta to the power n is common, so it can be taken out, so you just have zeta here and e to the power Iota j k j delta x, this also common. So, we can divide whole equation by Zeta times Zeta to the power n times e to the power Iota k j delta x, so this will be simply Zeta - 1 by delta t = -v times e to the power Iota k delta x - e to the power - Iota k delta x divided by 2 delta x.

So, from this you can get Zeta = 1 if you take to write it becomes 1 - v delta t by 2 delta x, now this is e to the power j theta + e to the power - j theta is 2 cos theta, so this is 2 cos theta by 2 delta x. So, 2 cos theta becomes 2 cosine k delta x, this is 2 j minus this is minus, so it is becomes sine, so 2 j sine k delta x. So, then this 2 will cancel, so you have this expression here, 1 - Iota v delta t by delta x sine k delta x.

Now this Zeta should be less than 1 for the numerical method to be stable, the magnitude of Zeta, so the magnitude of Zeta should be less than equal to 1. Now if you see here this is a real number, this is the imaginary number, so the magnitude will always be greater than 1. So, that means this FTCS discretization is unstable. So, how can we make it stable? So, there are different methods.

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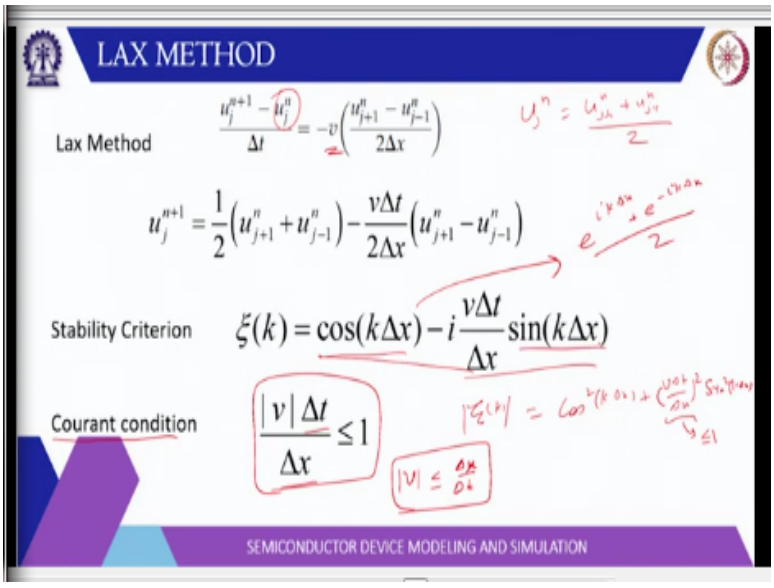

One simple solution is that you replace this u j n y average, so this is u at j + 1 + u at j - 1 divided by 2. So, if you do the similar analysis for this scenario, you will get now cos k delta x - Iota v

delta t by delta x sine k delta x. And if you calculate the magnitude of Zeta k will be cos square k delta x + v delta t by delta x square sine square k delta x. Now we know that cos square theta + sine square theta is always 1, so that means if this factor is less than equal to 1, this will always be less than equal to 1.

So, that means it will always be stable, so v delta t by delta x the magnitude is less than 1, that condition is called Courant condition. So, that means your discretization along time axis delta t or discretization along x axis delta x they are basically related. So, that means v the coefficient here on the right side is less than equal to delta x by delta t. Now we cannot orbitaly choose, we cannot make, so if you let us say make delta x very small, so this delta t very small then this condition is automatically satisfied.

But even that is not proper because there is something called phase error, so if you look at this criteria this cos k delta x + i Iota v delta t y delta x this cos k delta x can be written as e to the power Iota k delta x + e to the power -Iota k delta x divided by 2 and similarly sine k delta x.

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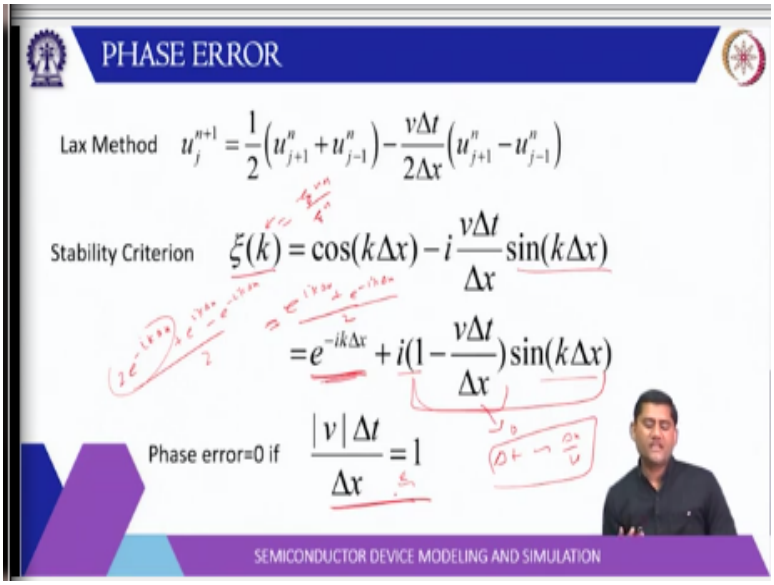

So, this is e to the power -Iota k delta x and this is sine k delta x, so this is e to the power Iota k delta x + e to the power - Iota k delta x divided by 2. If you look at this one, this is you can add and subtract -Iota delta k x, so it is 2 times e to the power -Iota k delta x + e to the power iota k delta x, so we have added 1 so let us subtract 1 e to the power -iota k delta x divided by 2. So,

this terms we take out is the first term and this e to the power Iota k delta x -e to the power -Iota k delta x is 2 Iota sine delta x divided by 2, so you have this Iota sine k delta x here.

So, now if you look at this one, this Iota k delta x is basically the phase that we want, this extra term is some kind of phase error. Now this term will be 0 if v delta t by delta x exactly 1. So, if this goes to 0 that means v delta t by delta x would be equal to 1. So, in that case phase error will be 0 otherwise phase error will keep building up from one step to next step because this is Zeta k, so here k is basically the step 1, 2, 3 and so on.

So, Zeta is basically Zeta n + 1 by Zeta n, so from one step to another step. So, this is controlling the phase error. So, the ideal situation is that that keep delta t = delta x by v and it is slightly less basically here. Because for the stability the condition is v delta t by delta x is less than equal to 1 and for phase error 0 it is equal to 1, so it should be slightly less than or equal to 1 basically. So, that phase error does not accumulate over the further step and the method is stable. Then there are different methods that are available which can be used.

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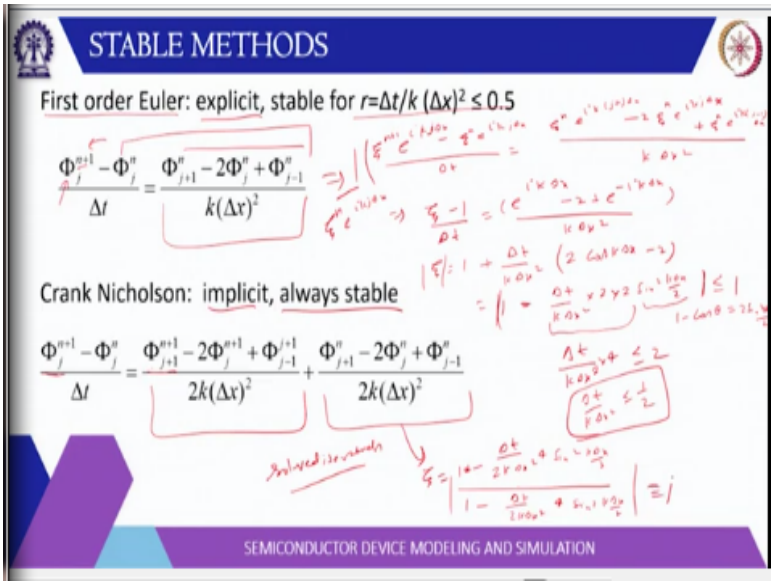

So, example of such a stable method is one is first order Euler method, so here also you can do the stability analysis. So, phi j n + 1 is Zeta to the power n + 1 e to the power Iota k j delta x - Zeta to the power n e to the power Iota k j delta x divided by delta t = Zeta to the power n e to the

power Iota k j + 1 delta x -2 Zeta to the power n e to the power Iota k j delta x + Zeta to the power n e to the power Iota k j - 1 delta x divided by k delta x square.

So, again you can divide whole thing by zeta times e to the power Iota k j delta x, so divided by Zeta to the power n e to the power Iota k j delta x, so what you will get here? This will be Zeta - 1 divided by delta t = e to the power Iota k delta x - 2 + e to the power - Iota k delta x divided by k delta x square. You further simplify it, so Zeta = 1 + delta t by k delta x square times this factor here, this numerator.

Now e to the power Iota k delta x + e to the power -Iota k delta x 2 cosine k delta x. So, it is 2 times cosine k delta x – 2, now cos theta - 1 is 2 sine square theta by 2. So, this is basically 1 delta t by k delta x square times 2, now cos theta - 1 is, so if you recall 1 - cos theta is 2 sine square theta by 2, so this plus replace with minus it was 2 sine square k delta x y 2. So, this is again Zeta if you take the magnitude of this Zeta and it has to be less than equal to 1.

So, now if you look at sine theta, now sine theta is always less than equal to 1, so the maximum value can be 1 here. So, for this mod to be less than 1, this coefficient here should be less than equal to 2. So, that means delta t by k delta x square times 4 should be less than equal to 2 because 1 - 2 will be 1, so it will be less than 2 basically. Now this is a positive number and so that means delta t by k delta x square should be less than equal to 1 by 2.

So, this is a condition, so this first order Euler is stable for if this condition is satisfied. Similarly these are basically explicit methods, now explicit methods are those where the nu value that means for t = n + 1 it does not depend on any of the value at n + 1, it all depends on the value at n. So, you know the value at n and you are calculating value at n + 1. But in implicit method what is done here this is basically averaged out over step n and step n + 1.

So, if you see here this is step n and this is step n + 1. So, that means to calculate n + 1 you need the information of n + 1, so that means these are solved iteratively. And if you do the similar analysis you will find that this is always stable. So, in fact I worked out the expression that comes out some quadratic here Zeta actually comes out 1 - delta t by 2k delta x square times 4

sine square k delta x by 2 divided by 1 - delta t by 2k delta x square times 4 sine square k delta x by 2, this is what works out, so this is always 1.

So, this term actually similar term is coming for n and n + 1, so that is why when it goes to left it adds up here and then it comes denominator here. So, if you analyze you will get this is always a stable.

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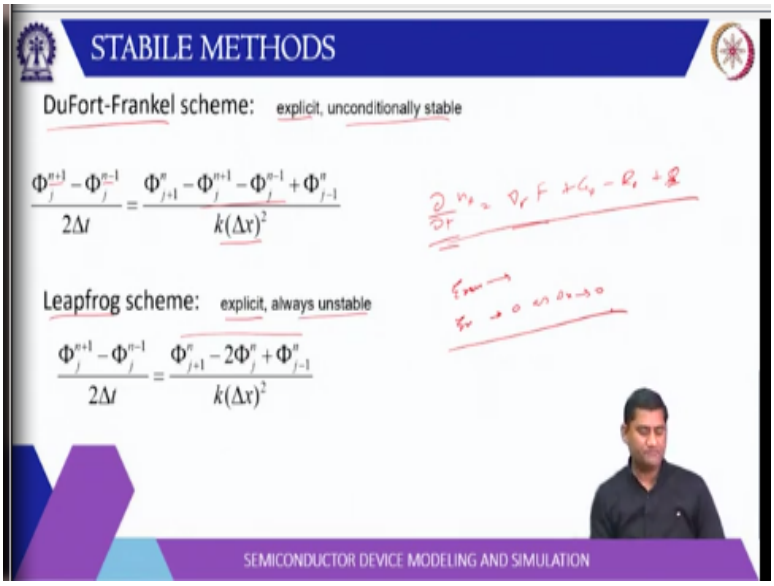

There are other method also which are stable methods one is Dufort-Frankel scheme. Here if you see this left side is the time derivative but it is centered one, central defense method basically. So, n + 1 - n - 1 and the right side is this divided by k delta x square, so it is phi n j + 1 phi n j - 1 - 2 phi j n, so this is also explicit and it is also unconditionally stable. Another one is a Leapfrog scheme which is explicit but it is always unstable that also you can analyze.

So, the left side is central difference but the right side is the central difference is only taken at step n, so there are different methods. Now those methods which are unstable by some change they can be made stable also. So, when we are going to solve the particular equations because in hydrodynamic models we have del by del t of this n phi. Then we have this del r of the flux + G phi - R phi and plus there are generation recombination term corresponding.

So, this is a d by dt here and there is a d by dx here also or d by d R here also. So, this has to be discretized in such a way that the numerical scheme is stable. Now there are fundamentally 2 criteria for stability that error should not increase with every approximation and this error should go to 0 as delta x tend to 0 or delta t tend to 0. So, with this criteria and numerical scheme we should be able to solve a given set of equations corresponding to the hydrodynamic model.

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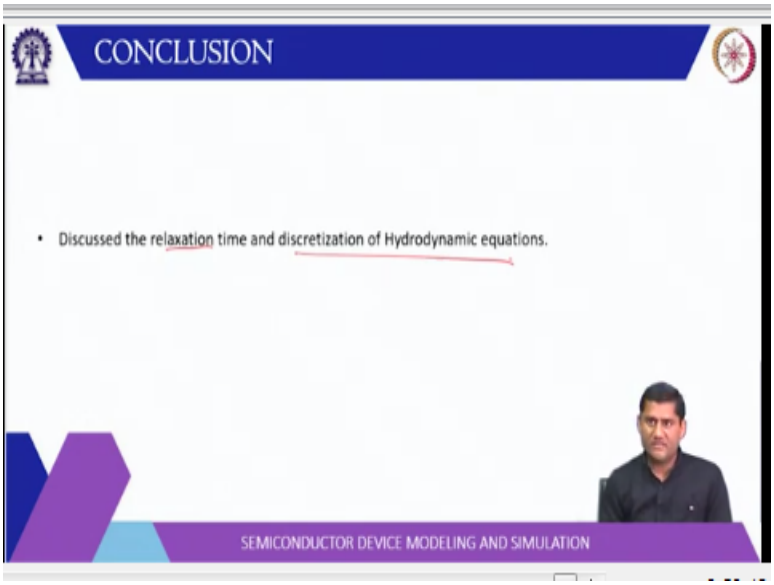

So, in this lecture we have discussed of the relaxation time and the discretization of hydrodynamic equation. Next class we will consider the Monte Carlo method, thank you very much.