Introduction to Finite Volume Methods-I
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Lecture – 34
Gradient Calculation for Diffusion Equation-II

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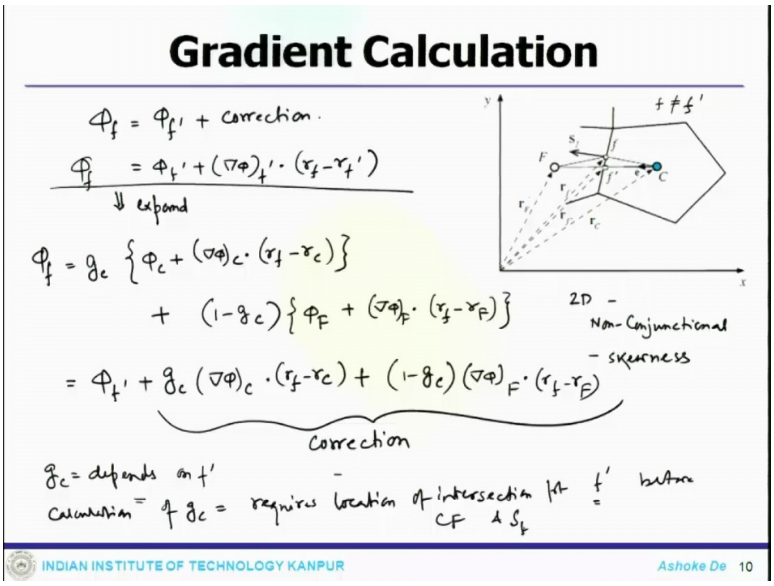

So, welcome to this particular lecture and will continue our discussion, what we have been doing so far. So, option 1, we can have multiple options.

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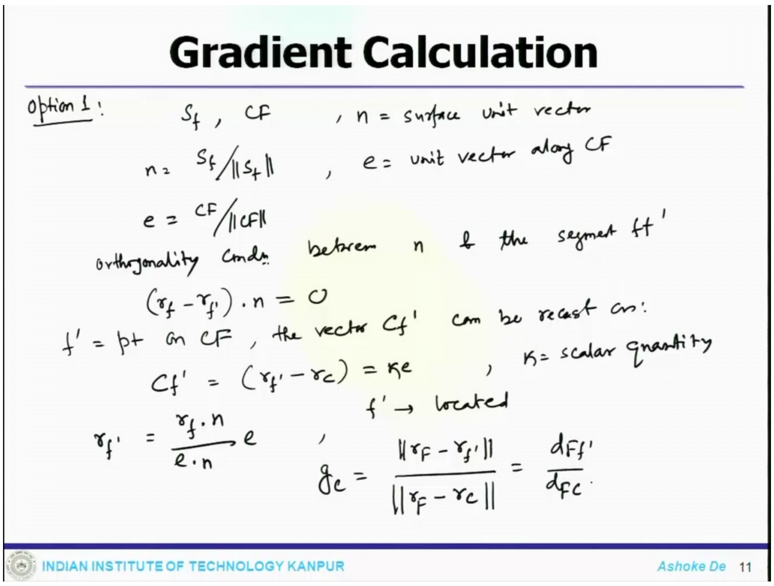

So, option 1, now you in this particular option what you can do? So, f prime you can take. So, if you consider this figure again, now if you consider this figure then we can calculate the f prime using the surface vector S f and the distance CF, where n you say the surface unit vector. Then, n can be calculated as S f divided by S f and e is the unit vector along CF which is also shown here, this is the e. So, once you say that e can be also calculated as CF divided by CF and now, you can find out the location of f prime by exploiting the orthogonality condition that exist between n.

So, the orthogonality condition between n and the segment f f prime. So, which is where if you look at it the n is the normal to the S f containing the segment f f prime. So, using that one can write that r f minus r f prime dot n equals to 0. So, since the f prime is the point on CF, the vector C f prime can be recast as capital C f prime that is a vector r f prime minus r c equals to Ke, where this K is a scalar quantity ok. Now, if you combine everything together r f prime becomes r f dot n divided by e dot n e.

So, once f prime is located you can once f prime is located, you can find out the so, the g c could be obtained like r capital F minus r f prime divided by r f minus r c which is d F f prime divided by d F C. So, that is how you can obtain the calculation and then, the calculation procedure one can write.

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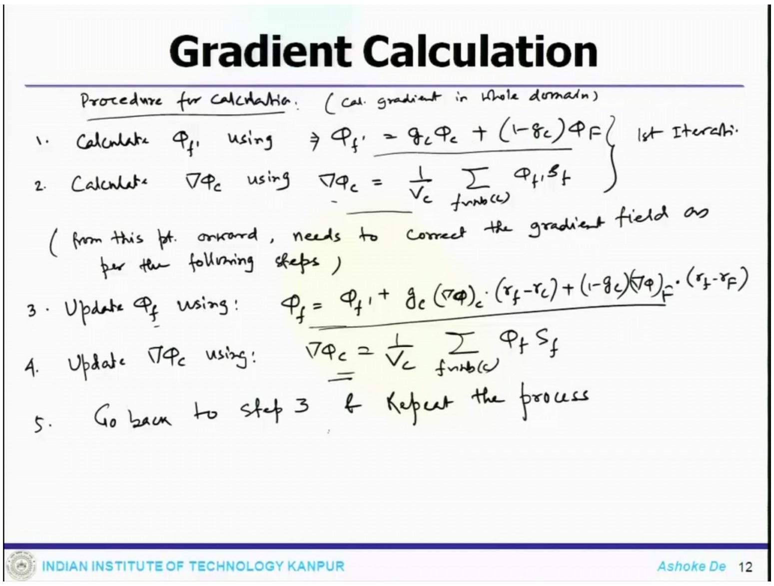

So, these are the procedure for calculation. What you do that so first iteration, you can compute the over whole domain and then, you follow the step. You first calculate phi f prime using phi f prime equals to g c phi c 1 minus g c phi F; second you calculate delta phi c using delta phi c equals to 1 by V c summation over all the phases phi f prime S f.

Now, from this point onwards, from this point onward one needs to; so, needs to correct the gradient field as per the following steps. So, once you reach up to this after that one needs to follow the other 3 steps. Like now you update phi f using phi f equals to phi f prime plus g c delta phi c dot r f minus r c plus 1 minus g c delta phi capital F dot r f minus r F.

Then, you update delta phi c using the equation like 1 by V c summation over the phases phi f S f. Then, you go back to step 3 and repeat the process. So, that is what you do. So, that is how you calculate. So, initially at the first iteration, you calculate the gradient field in complete domain. So, basically initially you calculate gradient in whole domain and then, you move along the along the calculation procedure and obtain the.

So, first you get this expression and calculate; then, you calculate the phi c using the neighboring phases and also the cell volume and after that you go on iteration to correct the field and how you do that? You do the corrections here, then again recalculate and go back and repeat this step. That is what you do in this particular option. So, that is option number 1.

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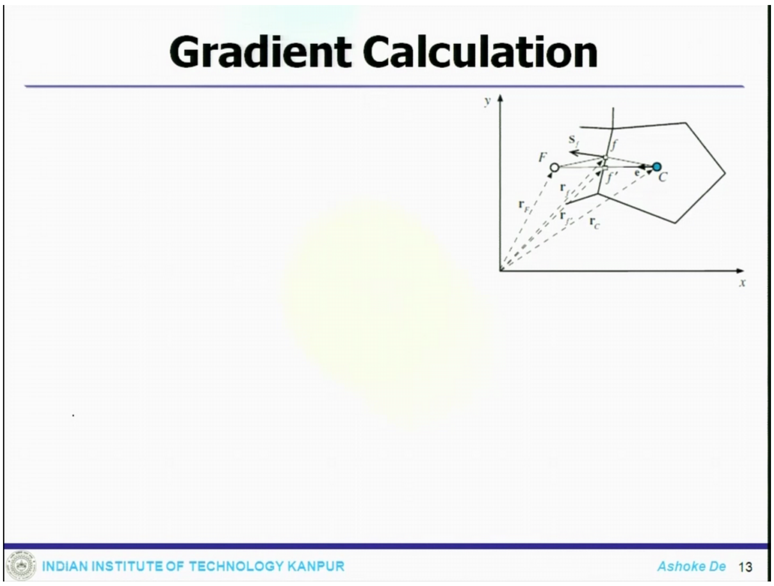

Now, we can consider another option which is called option 2.

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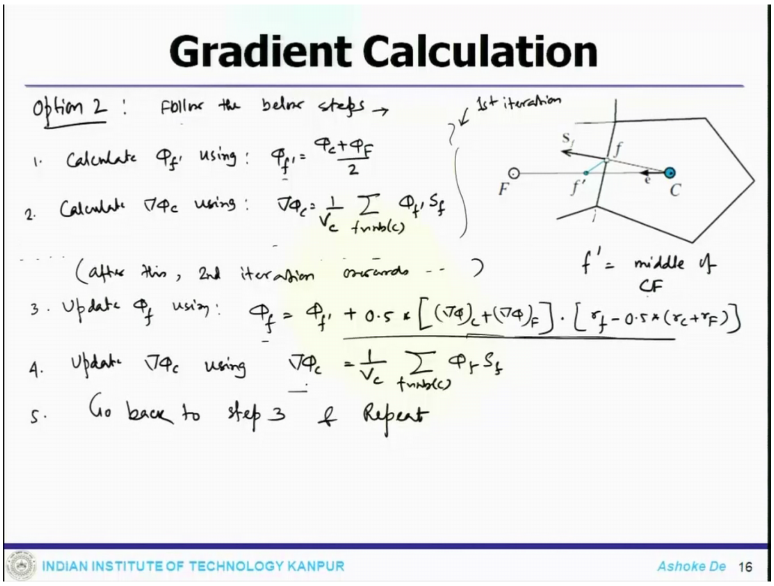

Let us say second option; option 2. Here, you look at this particular figure here is the cell center C and neighboring cell center F and f prime is essentially, here f prime is essentially at the middle of segment CF. So, it is in the 2 dimensional system and simpler system. So, the calculation of the gradient field over the domain, now you can follow different procedure and here small f is at the cell center a phase centered.

So, what you do again? You follow the below steps to get the calculation done. First step you calculate phi f prime using phi f prime equals to phi c plus phi F by 2. Second step, you calculate the phi c using standard procedure of 1 by V c summation over f which is across the all the phases, you get f prime S f. Now, that is what again in this case also at the first iteration you calculate the gradient in the whole domain and using like this. So, this is what you essentially do or these 2 steps you do at the first iteration.

Now, to correct this, now after this or second iteration onwards the correction takes place and how you correct the procedure. So, essentially the gradient that is corrected using this steps. So, now, you update phi f using the equation, phi f prime plus 0.5 in to delta phi c plus delta phi F dot r f minus 0.5 into r c plus r F.

So, that is a different expression that we used for option 1. Now, at the second level, you update delta phi c using delta phi c equals to 1 by V c, you loop over all the phases and get phi f S f. And finally, you what you do? You go back to step 3 and repeat the process. So, that is what you do in the second process, where you assume that f prime is lying in between the which is no more lying on the phase f. This is rather at the middle of this segment CF and show your correction factors are modified like this and using that current factor you can obtain the.

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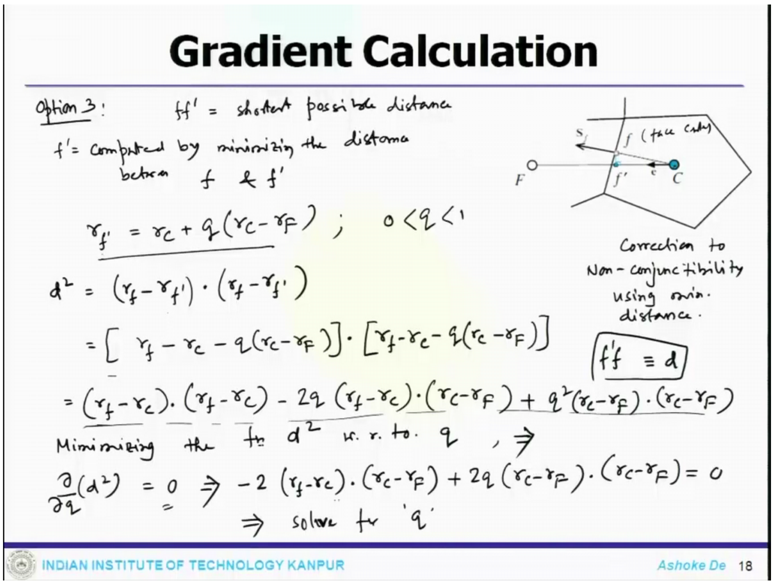

Now, third option which is option 3, where the you look at this figure again. Here, C and F which are again along this segment and the e is the direction, f is going to be the cells center, I mean centroid of this and what the way here basically it is a you can think about this is correction to non conjunctiblity using minimum distance. So that means, the position f prime is chosen such a fashion that f f prime is the shortest possible distance in 2 dimension. So, these leads to some sort of an more accurate competition of the gradient during first iteration. So, if this case f prime is computed by. So, f prime is now computed by minimizing the distance between f and f prime.

So, essentially this is a minimum distance kind of approach and the f prime is chosen such that f f prime, the small f and f prime this would be the shortest possible distance. So, to do that some minimization procedure is adopted; in general the vector r f prime is r c plus some factor q r c minus r f, where q lies between 0 to 1. Now, one would like to denote that distance f prime f equivalent to small d. So, if we do so, my d square is r f minus r f prime dot r f minus r f prime which is nothing but r f minus r c minus q r c r F dot r f minus r c minus q r c minus r F.

So, if I rewrite that it would be r f minus r c dot r f minus r c minus 2 q r f minus r c dot r c minus r F plus q square r c minus r f dot r c minus r f. Now what you want to do is the minimizing the function d square with respect to q. So, that gets you back that del del q of d square which is essentially 0 and that means, if you take the derivative of this with respect to q, you get back minus 2 r f minus r c dot r c minus r capital F plus 2 q r c minus r capital F dot r c minus r capital F which is 0. Now, if you solve q from here.

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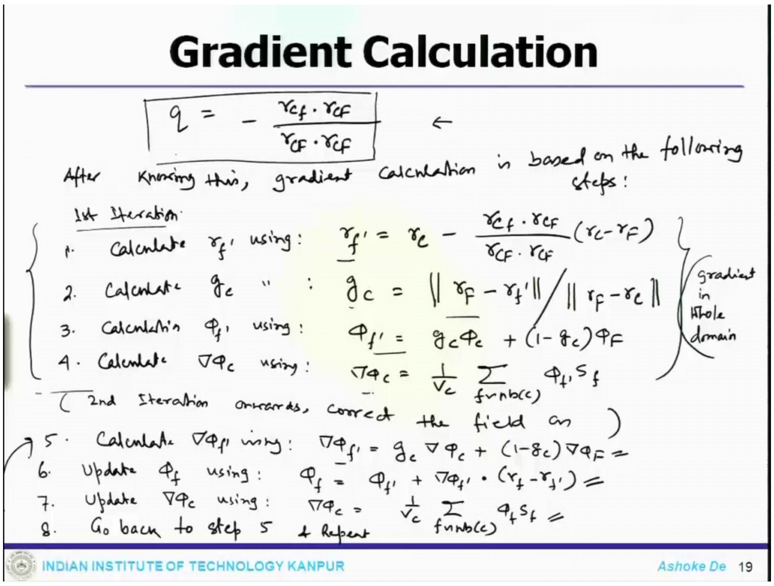

So, from here you solve for q and what we get back is that q equals to minus r capital CF dot rcf r CF dot r CF. So, if you know the q values. So, once you know so, basically you have to know this value, then the calculation of the gradient is follows. So, after knowing this gradient calculation is based on the following steps. So, again for the first iteration you calculate the gradient over whole domain and that is done like first you calculate r f prime using the equation r f prime equals to r C minus r cf dot r CF divided by r CF dot r CF in to r C minus r F and then, you calculate g c using g c equals to magnitude of r capital F minus r f prime divided by r F minus r capital C.

So, in the first iteration, you calculate the gradient field in complete domain; but before doing that one has to get this calculation of this q value which is very much essential and once you know that, after that we will follow the steps. So, now, you get g c; then obviously, the next step will be very obvious the calculation of phi prime which is using the standard equation g c phi c plus 1 minus g c phi F. So, then the fourth one would be you calculate delta phi c using the cell volume and the summation over all the phases phi f prime S f. Now up to this which you need to calculate at the first iteration. So, in the first iteration, you do the calculation and obtain the gradient in complete domain.

So, essentially this will get you gradient in whole domain. Once you get that, now second iteration onward you can correct the field. So, second iteration onwards correct the field as 5, you calculate delta phi f prime using delta phi f prime equals to g c delta phi c plus 1 minus g c delta phi F. Then, you update phi f using phi f equals to phi f prime plus delta phi f prime dot r f minus r f prime. So, that will update the phase value. Then, the 7th step, you update your delta phi c using the equation of V c summation of all the phases which goes of phi f S f. Then finally, you can go back to step 8 and repeat the procedure.

So, essentially go back to step 5 and repeat. So, that is how you do in this particular case. So, this is quite in the sense it leads to an accurate computational so, if let be re-iterate the whole thing quickly. So, option 1, we have done the calculation which is based on essentially in option 1, we do the calculation by finding the exact intersection of f prime. So, there you first in the first iteration these are all done in the first iteration. So, you calculate the phi f prime and then, you complete domain you get phi c and then, second point onwards you update the phase filed by this correction procedure update the phi c and repeat. So, this gives you some sort of an accuracy.

Then, option 2, it is finding the this f prime is assumed to be in the middle of CF and once you do that, then what you do? In the first iteration, you calculate the correction of the phase value using the cell information of the C and F. Then, get the complete information in the domain and name second points onwards or second iteration onwards, you update phi f the phase value using this kind of expression, then update the gradient of the cell and then go back. But the one which is most accurate is option 3, where you use some sort of an minimization procedure of the distance; that means, your f prime lies in between the segment of C and F and the distance between f which is the phase center value.

So, the distance between f and f prime should be the shortest possible distance and that is the process or the mechanism which is adopted for this correction in this non conjunctibility using this minimum distance procedure. So, how do I find out the f prime? F prime you have to find out the distance between f and f prime by finding some sort of a or optimizing the minimum distance procedure.

So, what you define first the radius vector of r f prime is r c plus some factor q which lies between 0 to 1 and the bit distance between r C minus r F. So, it is a simple definition of your distance vector which includes the distance between the diameter of this plus some factor weighting factor and the distance between this, which is defined here and then, you say this particular distance f and f prime which is defined as a small d that is the representation of that and we want to see the distance square. So, that becomes essentially the drought product between r f minus r f prime and the dot products once you put this r f prime expression back here, this leads to this particular expression.

So, now, since you want to minimize the distance between r F and f prime or the vector between or distance between f and f prime. So, you taken derivative with respect to this q; q is the weighting factor or some factor which is used for the segments C and F. So, if you take the derivative and for the minimization of that is distance it is 0. So, once you take derivative of this expression that allows you to get this and after solving that you get the value of q which is very important to know that distance factor. Now once you know the q, then you can actually process the steps or follow the steps to find out the gradient.

So, first iteration which will actually allow you to calculate the gradient in whole domain; you first calculate the r F distance vector using q and r c. Then, you calculate the g c which is like this, then calculate r q f prime and then, finally, delta c for whole domain. Then, second iteration onwards you actually update calculate delta f prime with this expression, then calculate the phase value; then, you update your delta phi c and you go back to step 5 and repeat. So, this is how you do the gradient calculation in different options for compact stencils and will discuss in the next lecture for the extended stencil.

Thank you.