Introduction to Finite Volume Methods- I
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Lecture – 35
Gradient Calculation for Diffusion Equation-III

So welcome to this lecture of this Finite Volume Method and what we are discussing or rather we have discussed so far right now in to the business of doing the calculation for the gradient. And gradient calculation as we have seen in our previous lectures, we have two approaches; one is the using compact stencil another one is the extended stencil. And in the last lecture we have discussed the calculation procedure using the compact stencil.

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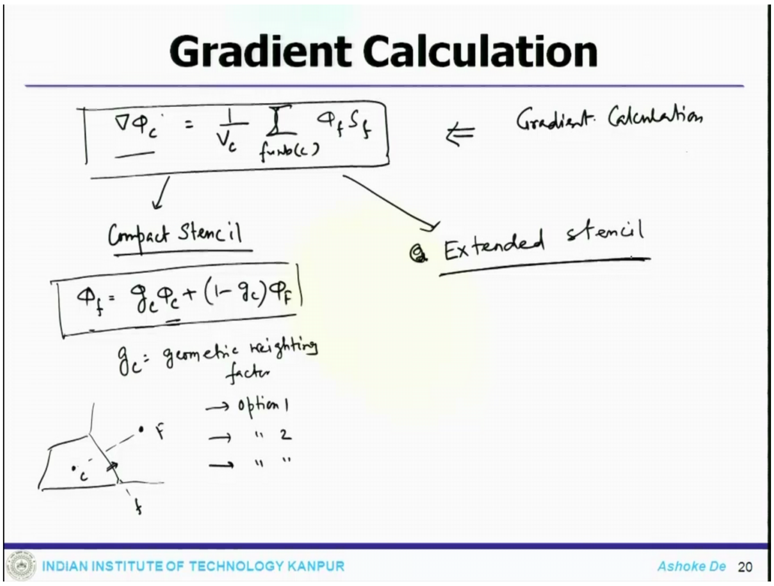

So, now you will move to that today on using the; so essentially what we are doing the gradient which is for a particular cell is represented as summation over all the phases and so this is what we are in to the business. So, essentially that is the gradient calculation that we are trying to do so, that is our objective. Now once you are trying to do this gradient calculation there are ways how we can do that. And specially when you move to the non orthogonal system you come across the cross diffusion term. So, gradient calculation becomes very important becomes very important in the sense that in the cross diffusion term cannot be evaluated using the nodal values.

Now how do you define your discretized stencil that leads to 2 approaches; one is the using some sort of a compact stencil and where what you do that you have a correction term for your flux or the surface flux which is like g c phi C minus 1 by g c phi F, where C is the particular element that 1 is concerned of calculating the. So, essentially if you quickly have a diagram like a particular cell this is C what we are interested and this is F and this is the connecting line between C and F so and this is the phase F.

So, calculation of the phase values which are interpolated using this formula and g c actually is nothing, but your geometric weighting factor. So, this and how to calculate the surflex flux phi F or the corrected flux and the g c for that there are different options. So, we have discussed three options option 1, option 2, and option 3.

So that is what we have essentially done till the last class. Now what we want to see using is the compact stencil we have looked at it. So, now, we want to look at is the extended stencil so; that means, which clearly give us an idea the cell which would be calculated it is not going to be connected with an immediate cell like this rather it would be connected with some other surroundings element.

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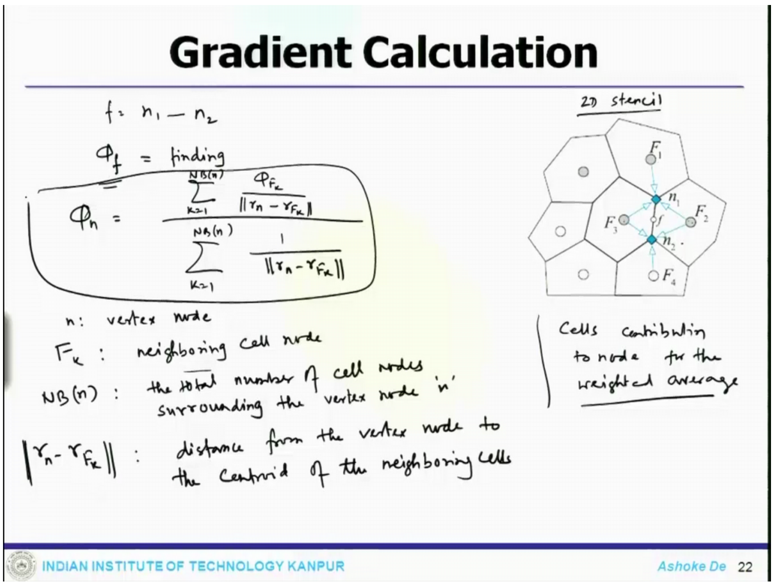

So, to do that let us look at these particular stencil so look at this 2D stencils. Now why we call it extended because there are F 1, F 2, F 3, F 4 this all are connected; so you can see the cells contributing to a particular node which is node for the weighted average. So, being said that you can see the node n 1 which is getting contribution since that node is common to 3 different elements like F 1, F 2, F 3. So, that gets the contribution from all 3 elements. Similarly if you look at the node n 2 the n 2 is getting contribution from all 3 elements like F 2, F 3, F 4 and connections between F is the phase between n 1 and n 2 or the connecting node between n 1 and n 2.

Now the what do I need to calculate is the value of phi F. So, what we are interested finding these value; finding the value of phi at the phase F which can be computed as the mean of the values and the vertices in n 1 and n 2. So, this essentially necessitate the estimation of the properties at the vertices. So, far we have been dealing with the system where we all concerned about the values which are available at the cell center.

Now here while you are trying to calculate this surface flux you need to get an information at the nodal point. So, the properties at a vertex node are calculated using this weighted average. So, this is some sort of a weighted average which is used, now how we take the weighted average because we take some sort of inverse distance function to calculate this kind of weighted average.

So, in that case when you calculate the phi n which can be expressed as the summation over k equals to 1 to NB n phi Fk divided by r n minus r F k. And denominator this is K equals to 1 to NB n 1 divided by r n minus r F k. So, here n stands for the vertex node, F k neighboring cell node cell node, NB n stands for the total number of cell nodes surrounding the vertex node so surrounding the vertex node. So essentially you get all this information and vertex node n and then we have a distance function r n minus r F k.

So, that stands for the distance from the vertex node to the centroid; centroid of the neighboring cells. So, that is what it gets you back. So, you have all the informations; you have the vertex node, you have the total number of nodes, you have the neighboring cell node then you have the distance from the vertex node to the center and then you can get some sort of a distance average distance calculation.

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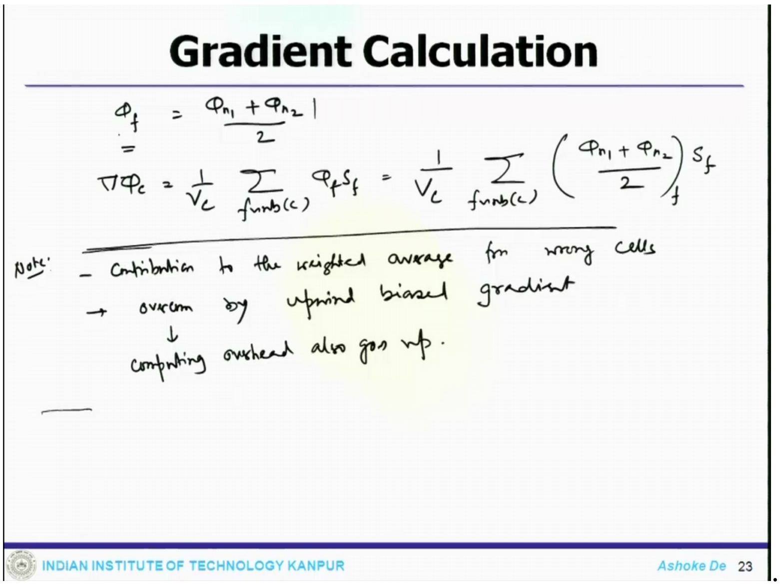

Once the phi and e at the vertices are found then at the phase you can find out the phi f as phi n 1 plus phi n 2 divided by 2. So using this sort of a inverse distance calculation at n 1 and n 2. We can find out and once you find out n 1 and n 2 the surface flux or the variable could be obtained using some sort of a arithmetic mean. And similarly the gradient could be calculated 1 by V c summation of F NB c phi f S f which is 1 by V c summation of then we get phi n 1 plus phi n 2 divided by 2 at f S f. So, when you go to 3D system the calculations are little bit involved, but it goes in the similar fashion.

And there you can also go across all the nodes or the vertex node and found out now in this particular approach the information from the wrong side of the cell also contributes to the weighted average. So, if you look at this picture it may be possible that the cells which are actually sitting on the wrong side they can also contribute to this weighted average to the converged variables. So, these can be overcome by using some sort of an up wind biased gradient and the higher order calculation based on the upwind biased gradients have both the memory over it.

So, essentially there could be some you can note contribution to the weighted average from wrong cells that is possible. If that happens it can be overcome by some upwind biased gradient calculation and if you use some sort of an higher upwind biased calculation the may computing overhead also goes up. So, the computing overhead also goes up. So, that is little bit involved and now if you move to 2D 3D that becomes bit tricky now. So, that is how one can use the compact stencil, and calculate the flux variable at the phase.

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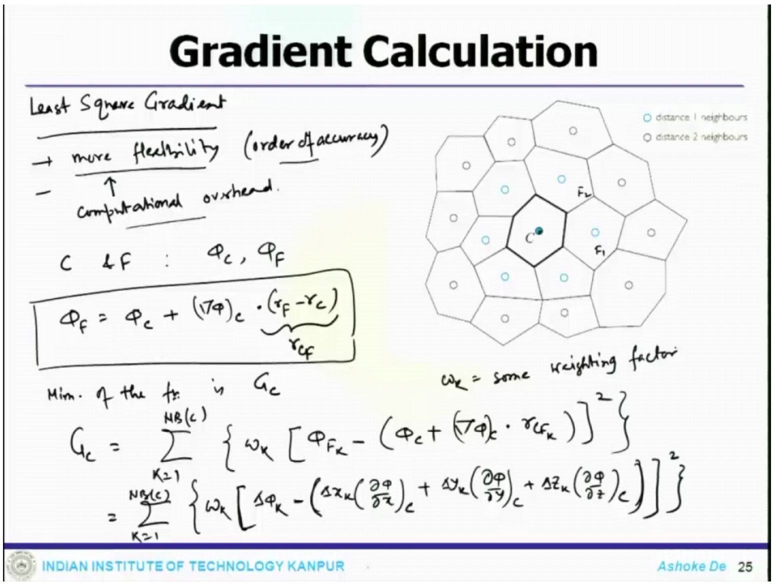

Now, we can move to another option is that least square gradient calculation so this is another option. And least square method it to it offer actually more flexibility. So, it offers more flexibility with the regard to the order of accuracy. So, order of accuracy is also slightly better or so order of accuracy is also slightly better or higher compared to other.

And in the least square measure what happens that divergent based gradient can be recovered as a special case. So that is one of the advantage of this least square method and the flexibility when we talk about the flexibility in brings some flexibility to a table it actually comes at certain cost.

So, as proper weighting is needed for the stencil terms the computation of weights at to some sort of an computational cost. So, this is getting hit by some sort of an computational overhead. So, once it offers you better flexibility or slightly better accuracy it also comes with some sort of an computational overhead.

So, it is not that straight forward that you can get everything together in your plate and get these things. So, let us look at these particular stencil and the change in the so, here the cell which are concerned cell is C and these are the all neighboring cell and then we can have an exchange between C and F. So, this could be F 1 F 2 like that and this we need to get the information of phi C phi F and all these. So, to calculate the gradient and So this width shows this schematic with the neighboring cells of this.

Now how do you obtain that phi F phi F it obtained at the using the value of phi C plus delta phi C dot r F minus r C; which is essentially the r CF. Now the thing is that unless the solution field is linear the cell gradient cannot be exert because C has more neighbors than the gradient vector has components. So, every time you get these calculation of the distance with the gradient vector now C has the new number of more neighbors. So, in least square method at gradient essentially is going to be computed by an optimization procedure.

So, you calculate this gradient by an optimization procedure. So, let us find the minimum of the function is G c and G c can be defined as summation K equals to 1 2 NB c weight factor w K phi F K minus phi C plus delta phi C dot r CF K so this is square. Now if I expand this one slightly more so I will get k equals to this I have this w K then I can write delta phi K minus delta x K del phi by del x at C so that is 1 component.

Del y K del phi by del y C plus del z K del phi by del z C so that is the term. And then you get the closer of this bracket which is going to be the square and closer of the other one. Where your w K is some weighting factor so using that you get this term now the other terms which are involved here.

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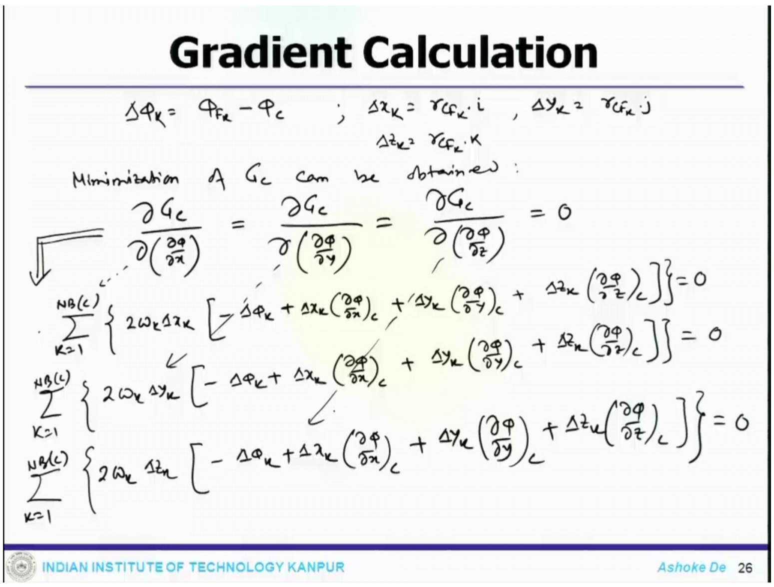

Delta phi K is phi F K minus phi C delta X K is r CF K dot i delta y K equals to r CF K dot j and delta z K is r CF K dot k so ijk. Now the minimization of this function can be obtained minimization of G c can be obtained by enforcing some condition. The condition is that del sel G c of del del phi by del x equals to del del G c of del of del phi by del y equals to del del j G c of del of del phi by del z these are all 0.

So, once you get this minimization function or the mathematics which will actually get you by some sort of an involved mathematical expression K 1 to NB c which will get you 2 w K delta x K minus delta phi k plus delta x K del phi by del x C delta y K del phi by del y C plus delta z K del phi by del z C which is 0 number one. So, that comes from the first expression second expression gets you back the similar expression, but it is on y K. So, it will be delta phi k plus delta x K del phi by del x C plus delta y K del phi by del y C plus delta z K del phi by del z.

So, that gets you the second one and the third condition will get you another condition or expression on delta z K. So, which is phi K del phi by del x C plus del phi by del y C. So, one can take the derivative of the previous expression and can obtain all this condition. So, you get from here you get all this three condition. So, each of them corresponding to the first one actually corresponding to these derivative, the second one corresponding to these derivative, third one corresponding to these derivative. So, you obtain this conditions which one can write in some sort of a matrix form.

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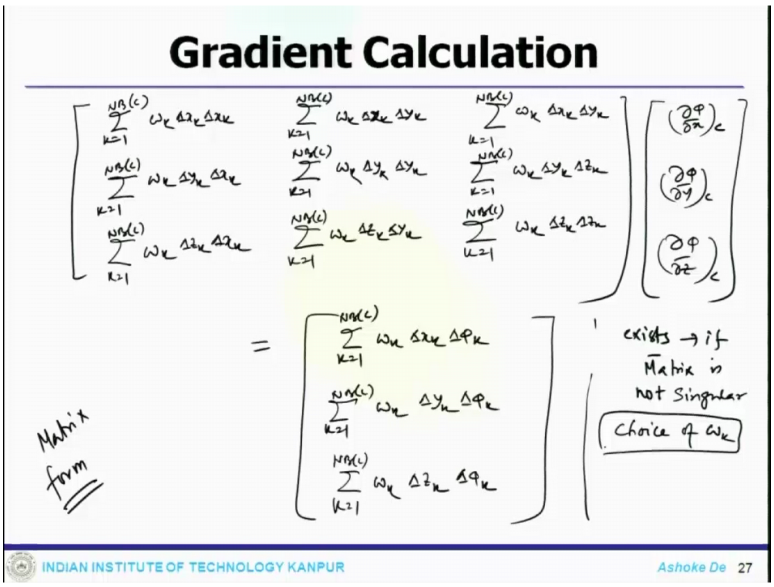

And if you write in some sort of a matrix form this will look like summation K equals to 1 to NB c w K delta x K delta x K that is first term, k equals to 1 to NB c w K delta y K x K delta y K, third term K equals to 1 to NB c w K delta x K delta y K. So, that is what and the second term will contribute to w K delta y K x K. And similarly you get wk delta y K delta y K and the third one is K equals to 1 to NB c wk delta y K delta z K.

This is K equals to w K delta z K delta x K w K z K y K 1 2. And you get on the factor which is getting multiplied is that del phi by del C at C del phi by del y at C del phi by del z at C. Which is equal to my another vector which is K equal to 1 to NB c wk delta x K delta phi K. Similarly K equals to 1 to w K delta y K delta phi K K equals to 1 to NB c w K z K phi k so you got an essentially the matrix form. So, this is the matrix form of the previous equation.

Now how do you find out the solution to this particular equation so basically solution; obviously, the solution exists if the matrix is not if this matrix is not singular. So that means, this has a nice condition or it has to have a nonsingular system so that it can have. Then also the choice of w K so, that is another factor. So, choice of w K is also very important because that will essentially to some extend or rather partially contribute the convergence of this system. So, for example, if w K is chosen to be 1 for all the neighbors of C; then all neighboring points will have the same weight in computational of the gradient, irrespective of whether they are near or far from point c so that is one problem.

Actually points that are further from C will have a more important influences at the error function which will be more effective by their error. So, this is a very important or crucial element in this particular matrix because that has lot of impact. So, if you go back to this cell now since it is taking a neighboring cells information if for certain values of wk, it may have possibly have the farthest cell had has lot of influence on this approximation and that can lead to some sort of an error, or alternatively one can have some alternative choice for w K.

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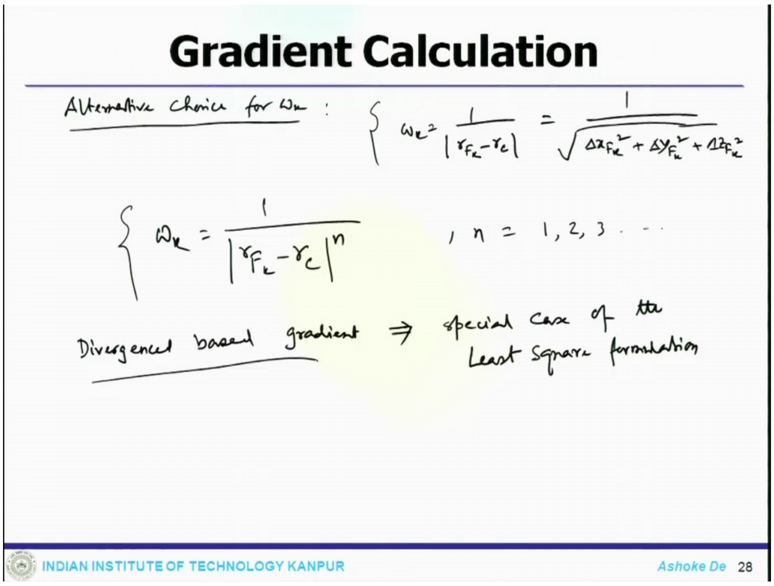

So, that one which some something which has been used and can be obtained is that w K could be some sort of a inverse distance function are F K minus r C which is going to be del x F K square del y F K square del z F K square. So, that way 1 can actually estimate the w K ok. So, other option is that 1 can also use w K as an inverse distance of power n where n could be 1 2 3 and so on so.

So, it is also possible not taking the direct inverse you can take an power of that inverse or with some kind of things. Now as mentioned the divergence based gradients is a special case of the least square formulation. So, one can show that so, what we have said that divergence based gradient is essentially a special case of the least square formulation. So, the formulation that we have for the least square approximation one can also obtain that divergence based gradient and we can see that. So,

Thank you; we will discuss our other things in the next lecture.