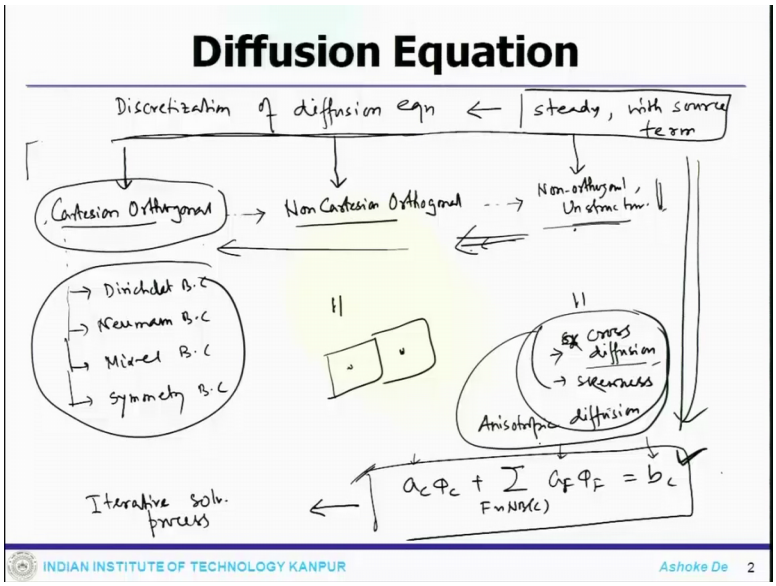
Introduction to Finite Volume Methods- I

Prof. Ashoke De
Department of Aerospace Engineering
Indian institute of Technology, Kanpur

Lecture – 33
Gradient Calculation for Diffusion Equation-I

(Refer Slide Time: 00:13)



So, welcome to the lecture of this Finite Volume Methods and we will start with a new topic on radiate calculations. And before moving there, let me just start with what we have done till the last lecture and if you recall this particular page, this is where we stopped. When we are talking about the diffusion system, we are talking about the discretization of the diffusion system, what we have considered steady state diffusion system with source term.

And then we started with Cartesian system Cartesian orthogonal moved to non-Cartesian orthogonal then non orthogonal unstructured system and in each of this respective system. We have taught about the discretized equation which actually looks like a equation of this nature, which is a same looking equation for all this different systems. What it differs is that, when we move to one to another system these coefficients will vary, and the contribution at the source term level that also changes and one important thing that you have come across that, when you deal with non orthogonal unstructured

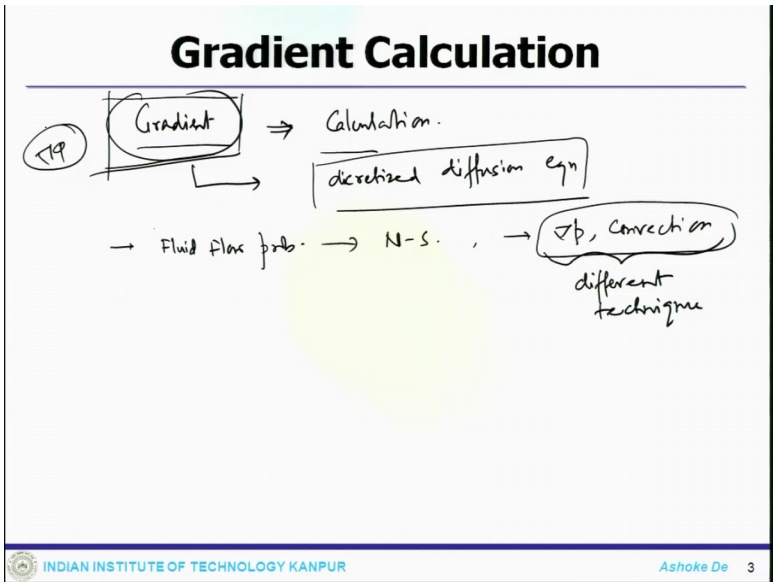
system. You come across 2 important quantity is the contribution due to cross diffusion term and which, actually leads to some sort of a difficulties in doing the calculation.

Because, the cross diffusion term if you recall it from our previous lectures cross diffusion terms you cannot calculate using the nodal values between the cells; that means, if you have the cells like this and using these nodal values. You cannot actually calculate the cross diffusion term and that happens, with the increasing and the cross diffusion term is actually increases with the increasing level of non-orthogonality.

So, that is why the non orthogonal system brings some sort of an complexity in handling the process, but at the same time. The beauty of this particular discretization scheme or the method is that you deal with the similar set of expression. For all the note and these gets modified when you move down to the boundary note and the extra term that arises at the non orthogonal system, if you make them 0 you move towards this side. So, you can bring back your Cartesian orthogonal system. So, the whole idea is that from the programming point of view and also one thing that, we have to consider is the anisotropic diffusion coefficient. So, all these things if you make them simpler or assign certain values, it can get back you the simple Cartesian system.

So, the beauty of this discretization is that you can have a generic code which can be used for both Cartesian system orthogonal system and non-orthogonal system. When it be used for the orthogonal system, the extra term like cross diffusion term skewness approximation. All this should be made 0 that it is a special case and should be treated as an orthogonal system. And when the anisotropic diffusion values are assigned to one, this could be treated as isotropic diffusion. Now all this process while doing this diffusion discretization the one important quantity is the gradient.

(Refer Slide Time: 04:20)



So, gradient is another quantity, the calculation of gradient is also very important and why it is important because, the discretization of gradients of phi at cell center. And phases are any fundamental to construct the discretized set of diffusion equation. So, essentially the gradient is fundamental to any discretized diffusion equation.

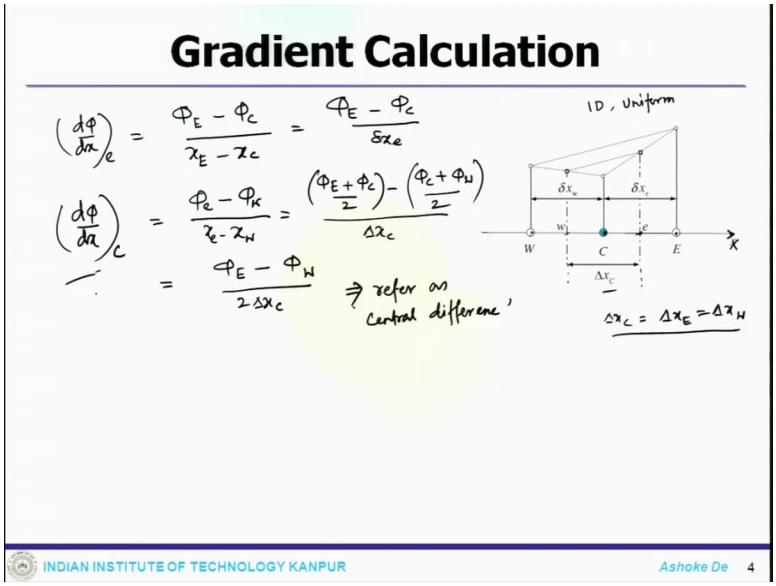
So, that is the important thing that you have so that is why now we move to the calculation of the gradient. And we look how or analyze how one can estimate this gradient for different kind of scenarios and how that helps to be used in a discretized diffusion equation. So, this is how we are moving and if you follow the things in a particular fashion, you can notice or one can notice that we are slowly building one step in a top of the other one so first, we have discuss general discretization.

Now, we have picked up a term by term discretization for that we have started with the diffusion system. Now the diffusion system requires one important quantity which to be calculated is the gradient. Now, in addition to that when you deal with the fluid flow problem, so, fluid flow problem means you will be dealing with navies stroke equation. That also requires some gradient calculation, in terms of pressure gradient, your convection term gradient. So, these are also there so, but these requires different technique for calculation. So, that is why it is not going to be discussed explicitly those pressure gradient term or convection gradient term, but essentially the normal gradient

calculation; that means, let us say del phi Calculation in a diffusion system that will start with.

So, to start with we first start with a 1Dimensional problem.

(Refer Slide Time: 06:58)



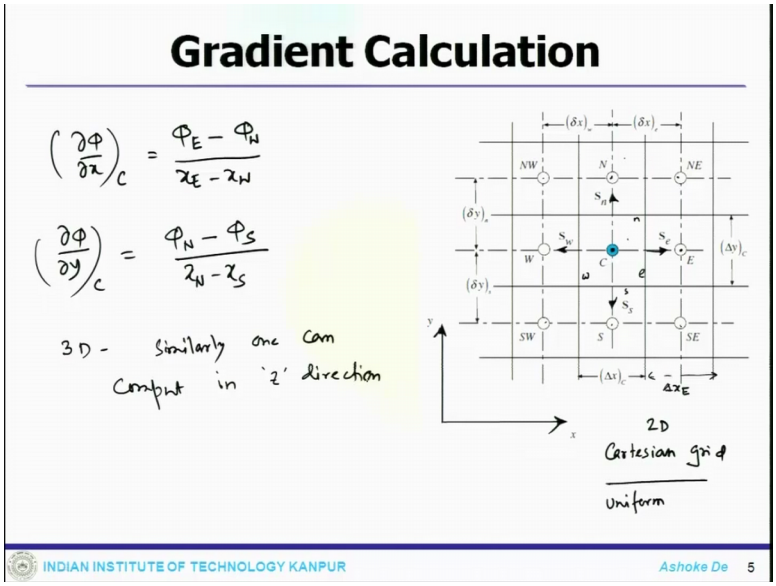
So, let us look at this 1Dimensional problem you have a cell here and this is the basically cell boundary. So, they are delta x E apart so the width of the cell width is delta x E. It is in the 1D and the east node is e and the west node is w. So, this is also one can think about 1D uniform; that means, delta x C equal delta x E it must be equal to delta x W. So, they are same. So, the cell width is kept same and as per our general convention the phase which is connecting the point C and E or the element C and E is small E. And this distance is delta x E and the connecting phases between west and C is small w. So, these are the notation and the direction is defined in x direction. So, what we want to calculate it that d phi by dx at the cell phase e.

So, that is what we are always interested in to calculate all these fluxes at the interphase. In order to do that, what we need to do we use the information from the cell values and this would be x C minus x C. So, one can write that is phi E minus phi C divided by del x E. So, can we so now, one can also write that d phi by dx at cell center c. So, this is the value which is at the centroid of that element c. How you can do that now previous calculation we have used the value at the cells center and calculated the value at flux phase E.

And similarly, one can find out at phase W. Now in the reverse calculation, qhat do? You want to do we want to use the information of this phases like e and west phases and try to calculate the derivative at centered c. So, which can be written as phi e minus phi w divided by x e minus x w which one can write that phi E plus phi C by 2, which is a basically again and linear interpolation between the information of C and E. And linear interpolation between C and west divided by delta x C. Because, these distance is delta x C which one can write phi E minus phi W divided by 2 delta x C.

So, this essentially means that they are of the central differences scheme; so, usually referred to as central difference scheme. So, this central difference which we now find out at cell center C we using the information of east node cell and the west value it is essentially one can refer as central difference and this is going to be the derivative of the first derivative using central difference scheme now for Cartesian grid in multiple dimension that derivatives can be also computed by applying the same principle. So now, if we move to Cartesian grid, the same derivatives can be applied using the similar principle in the respective coordinate system.

(Refer Slide Time: 11:39)



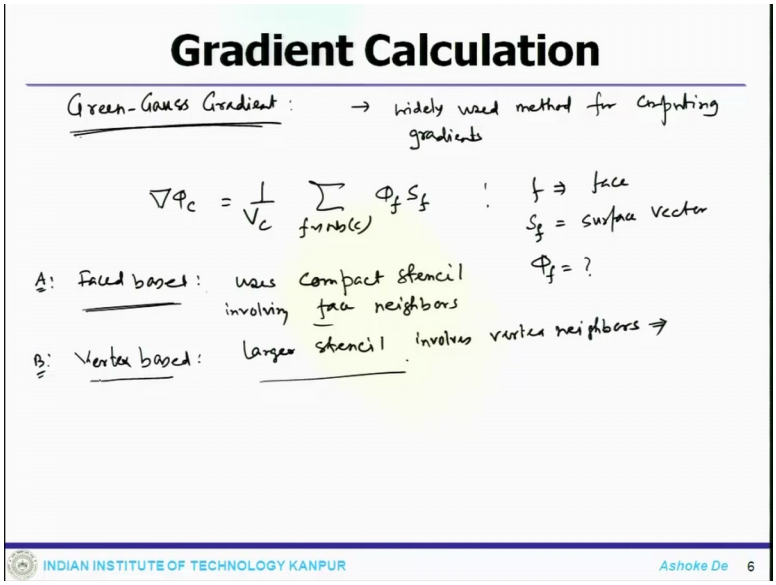
So now, let us consider this 2 dimensional this is a 2D Cartesian grid. So now, if you consider this 2D Cartesian grid and this is a very well known or familiar figure, that we have been using so far is a standard cell center C east node is E. So, this phase would be em north phase n, west phase w, south phase s. This are the cell vector or the surface

vector at E surface vector. At the north phase, surface vector at the west phase and surface vector at the south phase. And the other nodes like north east south east south west and north-west. And these are the respective cell distances in x and y direction again this is also uniform in each direction.

So, that delta x C or delta x E they must be equal. So, using now these particular things one can also look at the calculation of this first derivative at the cell center. So, this would be phi E minus phi W divided by x E minus x W and this is in this direction of x or x direction. Now, it is in that 2 dimensional system so we need to get an estimate in the other direction or the derivative in the other directions. So, the first derivative in the y direction would be phi n minus phi s divided by xN minus x S.

So, one can think now consider these 3 elements in 1 direction and similarly obtain the derivative at cell center, but now the derivative along this direction. So, that uses the information of north cell and the south cell. So, if this is quite state for what and if you have in 3 dimension similarly, one can compute in z direction. So, that would be quite straight forward and why that looks. So, straight forward it is a 2 dimensional uniform Cartesian system and; obviously, they are orthogonal to each other.

(Refer Slide Time: 14:39)



So once you do that now, we want to use the different techniques like one of the very famous technique is that green gauss gradient calculation. So that means, this is very or common or widely used methods for computing. So, it is widely used method for

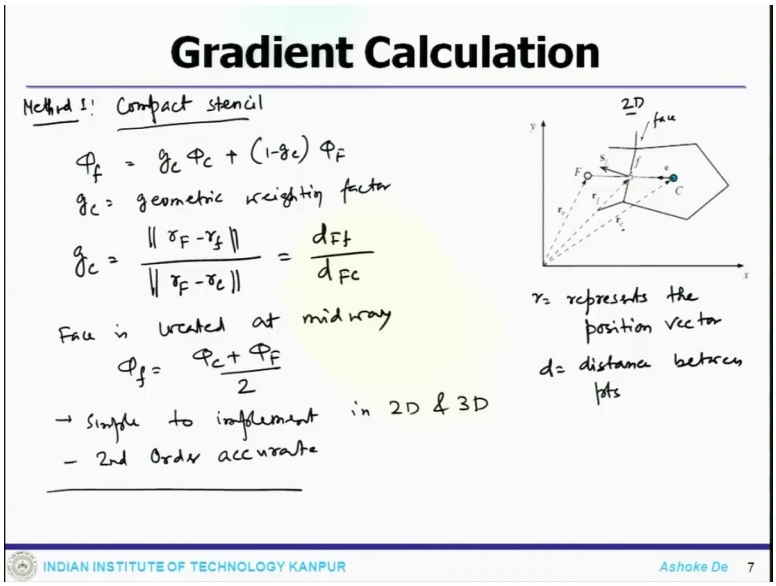
computing gradients; so, that essentially used in very commonly in CFD course. So, this has already been discussed while we are talking about the discretization of the diffusion system, but the final form of the equation. Now, we will discuss in details. Now, if you look at it the mathematical expression for that remains like the del VC of the VC summation over all the phases. And that would be phi f or phi f sa where, f stands for phase and s suffix f is the surface vector.

Now, the phase value phi f is still need to be calculated or some formula needs to be used to calculate the phase value. So, there are 2 approaches which are presented one is the phase based with a generally compacts stencil involving the phase neighbor.

So, one approach could be the phase based approach which actually uses some compact stencil involving phase neighbors. And the second option could be vertex based. So, that is another option one can use the vertex based that with larger stencil which actually involves the vertex neighbors. So, essentially in all these approaches you need to have the information from the neighbors. Sometimes it the phase neighbors, sometime is the vertex neighbor and also the number of cells in this extended stencil is about twice the one, which requires for the phase based.

So, the use of compact stencil that the phase based approach is quite attractive with implicit methods because, it leads to more compact job Jacobean matrices; however, this larger stencil that involves the vertex neighbors that being doing some more information into the reconstruction. And therefore, it is expected to be slightly more accurate. So, as soon as you say that it means whenever you use different kind of approach always it comes with some sort of advantages. Some sort of disadvantages now first thing that will start with is the calculation based on.

(Refer Slide Time: 18:38)



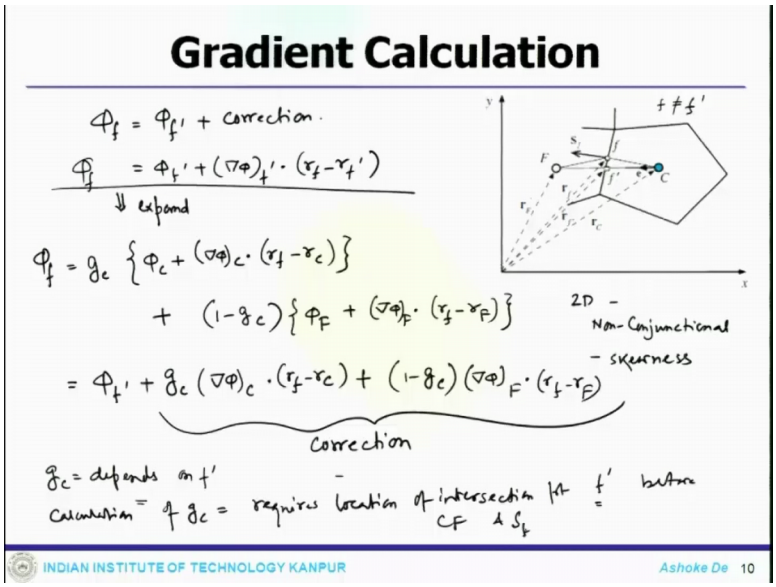
So, first method; so, the method one and method one is we use the method compact stencil and what is that. So, here is the picture of that it is again 2 dimensional and this is a phase which is connecting the points with the neighboring cell a and as usual the connecting line between C and F belongs to E and these are the from the reference frame the distance vectors for C is r C. Then, this F is r F the distance vector 2 capital F is R capital F and connecting point which touches the phase is small f and s f is the surface vector. Now, you need to calculate the phase value phi F and one simple approximation would be using g c phi C 1 minus g c phi F.

Where, again g c is the geometric weighting factor ok. So, once you use that information then what you get is that calculation of g c. So, that will become now magnitude of r F minus r small f divided by r capital F minus r C which is d FF because r F minus r F will give f F and r F minus r F will give the fC ok. So, r here is essentially represents the position vector and d is distance between points. So, that is what we get now if the phase is located at mid-way; that means, at the middle of that this phi F could be phi C plus phi F divided by 2. Now, this approach is quite simple to implement and top of that and simple to implement in 2D and 3D. And all operations which are involved are phase based not requiring any additional grid connectivity.

So, that way it is very straight forward and secondly, this is also second order accurate. So, the order of accuracy is also high now the other thing which is there that, when the

segment c F and phase s F intersects on point coincides with the centroid of the phase, but F does the second order accurate representation you can always obtain. Now, this condition is not usually satisfied with a general unstructured non orthogonal. So, this is not be easily satisfied for a general non orthogonal structured or unstructured system. So; that means, essentially if you have some skewness in the system whether in 2 dimensional or 3 dimensional this simple calculation would not happen.

(Refer Slide Time: 23:03)



And if you look at this particular 2 dimensional grid again, this is 2 dimensional phase 2D phase, but it is non conjunctional phase ok. So, ; that means, there are some level of skewness present in the grid which leads that that connection between C and F. That meets the cell centered of the concerned cell and the F they are passing through the phase at a point of intersection F prime and the C, which is touching the centroid of the phase at point F. So, there is a offset between F and F prime. So, F here not equals to F prime so and the surface vector is acting at F not F prime. So, there are multiple distance vectors which will turn out to be there one is capital r F r small f r F prime r C.

And this case now, your calculation would be like the correction time would be phi f which is equals to phi F prime plus some level of correction. So, that is what is required because now, F and F prime are not situated or located at the same point. So, once you have that direction you can expand that and get del phi dot r F minus r F prime now one can expand this one.

So, if you expand this one in more convincing form you can get at the phase value phi F equals to g c eq phi C plus delta phi C dot r F minus r C plus second component, which will come from 1 minus g c into phi F plus delta phi F dot r F minus r capital F. So, these are the 2 term which you get after invoking the correction due to skewness. So, once you do that what you finally, get is that that is equivalent to phi prime plus g c delta c dot r F minus r C plus 1 minus g c delta phi capital F dot r F minus capital F. So, this term which you look at it if you compare with this equation, which is phase value phi F. This is essentially the term which one can think about the correction term associated with this one.

Now, what happens here is that g c now, since g c strongly depends on F prime which indicates that the improved, estimation of the gradient can be obtained through some iterative process. Because this is now cannot be evaluated in a algebraic fashion. So, that is why there is a dependency on location of F prime. So, at each iteration the average value at phase is computed using gradient which is calculated in the previous iteration. So, these phase values are then used to compute the new estimate of the gradients.

So, if you do enough number of successive iterations and then which can actually can cause some oscillations and usually not more than 2 iterations are performed because of this. So, what it requires the calculation of g c which requires, the requires location of intersection point intersection point of F prime between c F and s F. So, now that is what it requires so essentially the calculation of g c which, requires locating the intersection point F prime between c F and of ss F for that purpose, now you need couple of options. So, thank you will discuss our other things in the next lecture.