Introduction to Finite Volume Methods - I
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Lecture – 28
Calculation of Diffusivity

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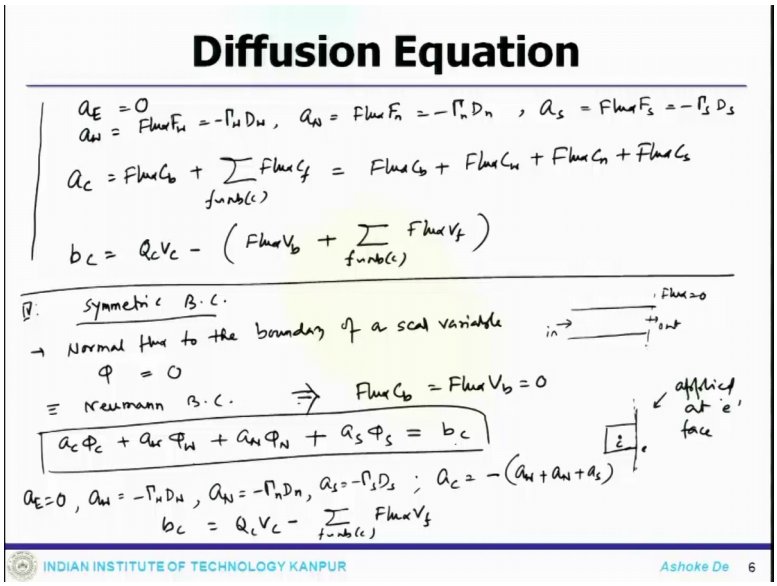

So, welcome to the lecture of this Finite Volume Method. Now another important parameter which comes into the picture is the calculation of diffusivity or rather interface diffusivity.

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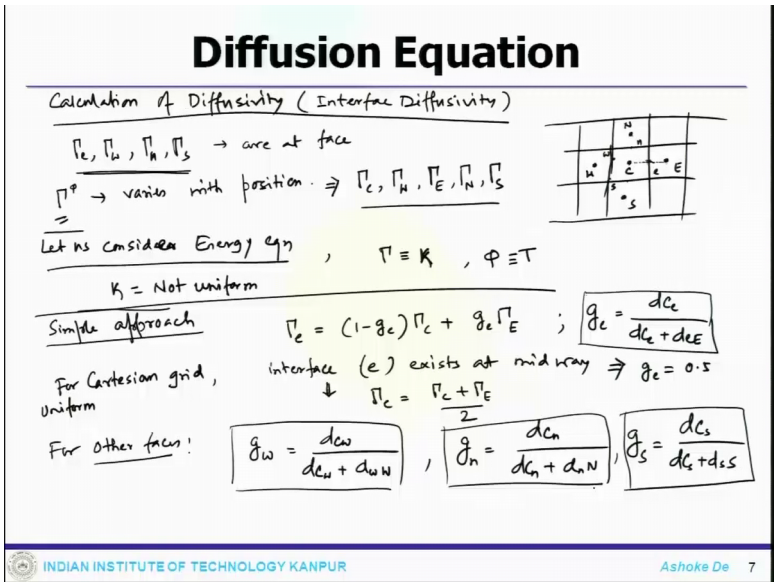

So, in our equation system or the discretized equation system, we have written these diffusive coefficients like gamma e, gamma w, gamma s, gamma n, gamma s, like that. So, these are actually the coefficients that belong to faces.

So, these diffusivity coefficients are at face. Now the thing is that we have certain information which are actually at the so if you again look at this cell corresponding stencils this is my C, this is my east, north, south, west and the faces like this W, S. Now it is important, when this gamma actually or gamma phi, it varies with position ok. And if it varies with position, which will let you to have at different different values of gamma at cell centre. So, you can have gamma C you can have gamma W, you can have gamma E, gamma N, gamma S.

So, at elements or at the elemental level along it is centroid you will have a different values, which when this guy the diffusivity coefficient actually varies. And this happens when you have certain materials or non homogenous materials with the diffusivity coefficients are varying along the grid points. So, you have different term. The calculation of these flux, flux diffusivity will be would become important. And this would be much more clear let us consider the energy equation, let us consider energy equation ok. Once we consider the energy equation and which case the diffusion coefficient actually represents the thermal conductivity.

So, the gamma is essentially the thermal conductivity or kappa of the material. Now if that case phi is essentially denotes the temperature and the variation of the non uniformity conductivity; that means the kappa if it is not uniform. So if kappa is not uniform, then you have a problem. The reason is that for specially non homogenous material, this kappa could be varying. And once the kappa is varying then the conductivity at different location; that means, for a non homogenous material the kappa at this centre and kappa at this location or kappa at this location they are going to be different.

Once that is going to be different, then assuming a equivalent diffusivity is not going to get a exact solution. So, in that case you need to have proper estimation of this gamma at a particular cell interface. As long as they are homogenous there is no problem, but if it is not homogenous. So, one can actually think about a very simple approach or methodology how to estimate this. One simple is that one can using the value of gamma at cell centres C and E, one can get an estimate at face E by some sort of an arithmetic mean and one can write let us say gamma at interface e would be a contribution of gamma c plus g e gamma E.

So, if gamma c and gamma e is equivalent then there will be a equal contribution. Where the interpolate polation factor, g e could be calculated as a distances between the centroid from c and e. So, which could be written as d C e divided by d C e plus d e E so, that is how one can. Now for a Cartesian grid; for Cartesian grid if the interface is midway let us say uniform Cartesian grid, which we have considered so, for in our discretization formulation, then the interface then the interface e exists at midway. In that case the contribution of g e would be 0.5 or half. And gamma e could be computed as a arithmetic mean of essentially in that case gamma e is nothing, but gamma C plus gamma E divided by 2.

So, it is an essentially the arithmetic mean of that. So, similarly it just the east face that we are talking right now similarly for the other faces one can derive this expression. And if you derive that then for other faces the coefficients would look like the interpolation coefficient. Let say if it is at the west interface, then the g W would be d C w divided by d C w plus d w W.

In the north face it would be d C n divided by d C n plus d n N, and the south face it is d C s divided by d C s plus d s S. So, it takes care of the distance between this point and the distance between this point. So, distance from the cell centres C to the face E and from face E to face cell centre of E that is what it takes into consideration.

And similarly other faces distance between the centre C to the face west and from west face to W centre which will get you the coefficient of g w. And when you consider the north element it goes from C to north face north face to N. That will get you the interpolation coefficient for the north and from the south centre to south face and south face to centre of the S that will get you the coefficient for the south face. So, essentially it is sufficient to calculate coefficients at each surface points using the information you have at the element level. And sometimes one can use the volume interpolations also instead of this distance interpolation. So, it essentially takes care that thing, but there would be one this distance interpolation.

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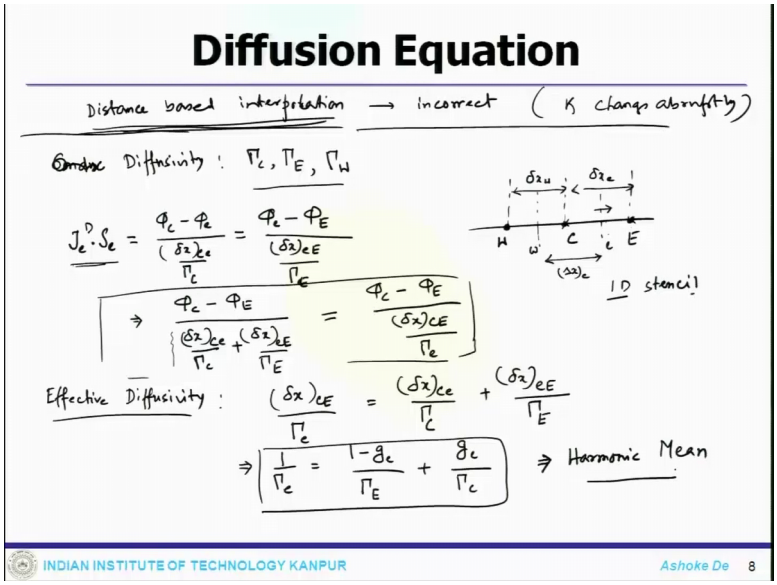

This is a distance based interpolation, it can have problem or rather it can be incorrect in some particular cases like that where or rather one can say that these distance based interpolation can lead to some sort of an incorrect results, when there is a sudden or abrupt change in conductivity. If kappa changes abruptly then this kind of distance based interpolation will have a problem.

So, in that case you need to have an alternative approach and sometime people use some sort of a instead of this arithmetic interpolation you use some sort of a different interpolation. So, to get that let us consider this one dimensional element. This is C this is west, this is east, and this will be the distances. So, this distance is delta xw, this distance is delta xe, and this is the west face, this is the east face and this is also delta xc. That means, that is the distance of that particular element ok. Now you have conductivity or the diffusivity or you can write the diffusivity gamma C, gamma E, and gamma W.

So, you have all this diffusivities which are stored at the centre of these elements. Now in this one dimensional analysis we are assuming there is a non homogeneity of the diffusivity. So, if there is a non homogeneity of the diffusivity one approach as we discussed one can do this kind of arithmetic interpolation, but this arithmetic interpolation may lead to some problem when there is a, I mean sudden changes or abrupt changes of diffusivity. So, what one can analyse looking at the diffusion equation, let us say at east face if write the equation from this simple 1D model this is the 1D stencil.

So, if you write that thing at that flux it is equivalent to writing phi c minus phi e divided by del x ce by gamma C. So, the diffusive flux at east face one can write that which is also equal to phi e minus phi capital E divided by del x e capital E by gamma E. Which is also equivalent to writing, phi c minus phi E between this cell and that cell divide by del x ce by gamma C plus del x eE by gamma E.

Which is also writing phi C minus phi E divided by del x cE by gamma e; that means, what we are trying to write here that at this particular interface the calculation of the east face flux. So, the east face flux one can represent using the information available at the cell centres C, using the available information at face E.

And then the distance which would used is this much which is delta x ce and gamma C or equivalently one can write the slope phi at this face E minus the cell centre value at E. But then, that case the distance which would be used is this much, which is e capital E and by gamma of this cell, which is also equal to or equivalent to writing phi C minus phi E by taking consideration of both the distances or some sort of a distance mean here in this particular terminology c e by gamma C, e E by gamma E. And the same

terminology if I use the flux value at cell centre of this, then it would be the distance of CE by gamma e at the flux level.

So, hence the effective conductivity or diffusivity whatever you call it effective diffusivity becomes del x by CE by gamma e del x CE; that means, the distance between this two cell centre equivalent to del x Ce small e by gamma c plus del x small e E by gamma E. So, if we look at this particular system or the expression from there one can write the effective conductivity is like that which is nothing, but writing 1 by gamma e equals to 1 minus g e by gamma E plus g e by gamma C ok.

Now, this essentially looks like an harmonic mean. So, the previous case which we have derived that was the arithmetic mean, but in this case this gives rise to the harmonic mean. So, if you look back this particular case was so the expression if you write down.

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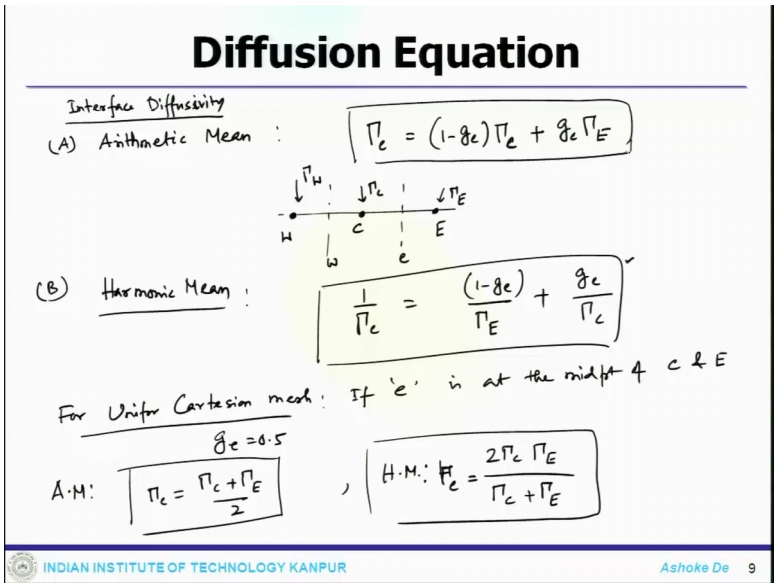

So, the interface diffusivity for interface diffusivity there are two option simpler option A, one can use some Arithmetic mean arithmetic mean expression which is essentially writing like gamma e equals to 1 minus g e gamma c plus g e gamma E where your elements are sitting C E west. So, this is the interface of e this is the interface of w and this guy will have gamma E, this guy will have gamma C, this guy will have gamma W.

So, at the east interface you can get the arithmetic mean like that, or one can write the second option which is the harmonic mean; that means, you write 1 by gamma e equals

to 1 minus g e by gamma E plus g e divided by gamma C. Now as long as there is not very much non homogeneity in the system then arithmetic means would yield the proper results, but if there is a non homogeneity and along with that the changes of the diffusivity is very sharp or abrupt across this cell interfaces, then one may choose to use this harmonic mean.

So, the message here is that so both the cases let us say for uniform Cartesian mesh if e is at the midpoint of C and E then g e would be 0.5 which will lead the arithmetic mean would be gamma e is gamma C plus gamma E by half or harmonic mean, it would be 2 gamma C gamma E divided by gamma C plus gamma E. So, in the harmonic mean gamma e is like that. So, this one can obtain if this interface lies in between element c and e and that is only possible when that sits there in the half way through. So, the message here is that so essentially the harmonic mean has some sort of a advantage over the arithmetic mean.

Now, you look at the applicability all these interface diffusivity calculation will be important once you have some non homogeneity in the diffusivity along the elements if there is non homogeneity. If the material is homogenous or the properties of the diffusivity along this across the cells they are homogenous then there is no requirement of consider this kind of surface inter, I mean the straightway linear interpolation at the surface would be handy. Now when there will be a non homogeneity essentially; that means, the gamma this gamma is varying from cell to cell; that means, this is a function of space. So, from one location to another location gamma varies.

So, f b cell element or the finite element they will have a different values of gamma that time one can adopt either of these two approaches either arithmetic mean or harmonic mean. Both of them should yield similar results, but being said that harmonic mean has some advantage over arithmetic mean or alternatively one can say when the harmonic mean is more preferred over arithmetic mean is the following. When your I mean no matter you have a non homogenous system and your diffusivity is changing in space top of that is across this cell interface let us say any of this interface e or w the change of this diffusivity is very abrupt or rather sharp; that means, between gamma C and gamma E or gamma W, gamma C there is a huge gradient which exists.

That kind of situation or the situation which arises those kind of condition or the problem. If you use arithmetic mean then it can lead to a some sort of a incorrect result. In those kind of situation, it is always preferred that you use the harmonic mean which can lead to better interpolation of the surface or interface diffusivity. So, these are the conditions were one should have to have the calculation of the surface diffusivity. And will stop here, today and carry forward from here in the next lecture.

Thank you.