

Computational Fluid Dynamics Using Finite Volume Method
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Lecture – 27

**Finite Volume Method for Diffusion Equation:
Steady diffusion in unstructured meshes Part 4**

Good morning. Let us get started. So, today we are going to discuss about the gradient calculation right because in the last lectures we saw that calculation of secondary gradient would actually mean that calculation of a face gradient right, that is what we kind of reduced in the last class.

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$(SG)_{\text{face}} \longrightarrow (\nabla\phi)_f \cdot e_{\xi}$

Gradient Calculation:

- 1) Secondary - gradient calc. requires
- 2) ∇p in N-S equations
- 3) Non-Newtonian model for viscosity
 ∇u

So, calculation of secondary gradient on the faces was reduced to the calculation of gradient of the scalar on the face right in the ξ direction right. So, this is a gradient on the face in the face normal direction that is what we wanted to calculate. If we can calculate this then the secondary gradient can be evaluated accordingly right.

So, today we are going to look at gradient calculation. So, one of the reasons to calculate gradients is of course, the it is requirement in the calculation of secondary gradient ok. So, secondary gradient calculation requires the gradients of the dependent variable on the faces, right. There are several other instances where the gradients of the dependent variable are required.

And, those are for example, let us say if we have if you are solving for complete Navier–Stokes equations right. Then we have we need to calculate what is the pressure gradient right. So, in the calculation of Navier–Stokes equations we have the pressure gradient term which is needs to be calculated.

Now, we also note that it is not just the gradient in the direction of the face that is required, but rather the gradient in all the directions right all the components of the gradient are required here all the i, j, k components are required not just in the direction of the face as is required by the secondary gradient ok.

Further let us say if you have a non-Newtonian model for your viscosity. So, if you have a non-Newtonian model for your viscosity, then we again would need gradients of velocities right because your gradients of velocities are required in the non-Newtonian coefficients that have to be calculated. So, as a result we need to calculate what are the gradients of the velocity right. Here u would be your phi right is required. Similarly, if you have let us say if you are solving for turbulent flows.

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4) Turbulent flows:
RANS model; K- ϵ model
production terms $\rightarrow \nabla \vec{u}$
LES model; Subgrid-scale stress
 τ_{ij}^{sgs} require $\nabla \vec{u}$
1) Gradient Theorem approach
Green-Gauss method
2) Least Squares method

Let us say if we have a statistical models and let us say something like a Reynolds-averaged Navier–Stokes model something like a K epsilon model or something like that then the production terms in these turbulence models would also require the calculation of the gradients ok. So, the gradient of the velocity vectors are required in evaluating the production terms of the RANS models.

And, further let us say if you have a large eddy simulation model something like a Smagorinsky model or so, then the sub grid scale stresses that we get that is the τ_{ij} the sub grid scale τ_{ij} superscript SGS would also require the filtered velocity gradients ok. So, which are the basically the dependent variables that, we are solving for ok. So, we would need gradients in any one of these instances or in all of these instances ok.

So, as a result we need to kind of seek a particular way or a method of calculating the gradients for the dependent variable ok. So, that is the motivation to kind of come up with a method that can calculate the gradients of the dependent variables.

So, there are several methods of course, to calculate the gradients, but we will only look at couple of standard methods and this is an ongoing area of research. So, they you will see research articles coming in with new methods to calculate the gradients which are more accurate and so on ok.

So, we will only look at 2 standard ways of calculating the gradient. The 1st one is the gradient theorem approach. This is also known as the Green–Gauss method and the other one we will look at is known as the least squares method or the least squares approach. These are 2 standard gradient calculation methods that are also available if you use any simulation software as well ok, fine.

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1) Gradient - Theorem Approach
Green-Gauss method

Closed volume that is enclosed by surfaces

$$\Delta V_0 \int_{\Delta V_0} \nabla \phi \, dV = \int_{CS} \phi \, \vec{dA}$$

Mean value approximation

$$\nabla \phi_0 \Delta V_0 = \sum_f \phi \vec{A}_f$$

The image shows a whiteboard with handwritten mathematical notes. The top part is titled '1) Gradient - Theorem Approach' and 'Green-Gauss method'. It describes a 'Closed volume that is enclosed by surfaces' and presents the equation $\Delta V_0 \int_{\Delta V_0} \nabla \phi \, dV = \int_{CS} \phi \, \vec{dA}$. Below this, it mentions 'Mean value approximation' and shows the equation $\nabla \phi_0 \Delta V_0 = \sum_f \phi \vec{A}_f$. The whiteboard is part of a video recording, with a small inset of a person in the bottom right corner.

Let us look at the gradient theorem approach or the Green–Gauss method ok. So, in this we kind of invoke the gradient theorem to calculate the gradient of the dependent variable ϕ ok. So, we have already seen the Gauss divergence theorem right in which we converted a volume integral into a surface integral for if you have a volume integral in the form of divergence of a vector right, then you could convert into a surface integral right.

But, gradient theorem is something different right. Gradient theorem is for gradient of a scalar integrated on a on a closed volume right let us say. So, we are considering a closed volume right that is enclosed by surfaces ok. These surfaces are enclosed it completely close the volume ok, there are no openings.

So, we consider a cell of to be of the same have to have the same property then if we have a closed volume ΔV_0 what would the gradient theorem say or the Green–Gauss theorem say. So, we have a ΔV_0 volume right, in this volume we want to calculate gradient of a scalar; ϕ is my scalar and dV would be the differential volume right. What would gradient theorem relate this gradient of the scalar to the surface integral as?

So, up till now we saw what is $\nabla \cdot \vec{\phi}$ right if we had $\nabla \cdot \vec{\phi}$ we wrote it as $\vec{\phi} \cdot \vec{dA}$ right or $\nabla \cdot \vec{\phi}$ right some kind of vector, right, in the Gauss divergence theorem.

But, now we are talking about gradient theorem right where ϕ is a scalar and the gradient of the scalar is what we are calculating in the volume of the cell right that is ΔV_0 , what would this be related to? This would be can be converted also into a surface integral right integration on the area integral over the control surface, what would be the quantity here? $\phi \vec{dA}$, is that correct? Is it correct dimensionally? What is on the left hand side?

Student: (Refer Time: 08:21).

You get a vector, right? Gradient of a scalar, what is on the right hand side? Right it is also a vector. You are adding the phi on essentially on the all the areas right ok. You are summing it up alright, now. If I assume that the gradient of the dependent variable ϕ is a constant in the entire cell, right. I am essentially making a mean value approximation.

So, essentially this is the gradient theorem which relates gradient of a scalar integrate over the entire volume to be equal to some of the scalar multiplied by all the vector differential areas on the entire surface right, that is what the theorem says. Now, if I use a mean value

approximation and say that the $\nabla\phi$ at the cell centroid is a representative of the entire cell, right and $\nabla\phi$ remains a constant inside the particular cell that we are talking about ok.

Then I can how do then can I rewrite this integral into something else? Can I evaluate this integral? $\nabla\phi$ is constant wherever you go in the cell then what would be this integral?

Student: $\nabla\phi$.

$\nabla\phi$ times.

Student: (Refer Time: 09:40).

ΔV_0 , right. So, this would be $\nabla\phi$ times ΔV_0 and this is $\nabla\phi_0$, right essentially that is for the cell equals. Again if I use a mean value approximation right for the ϕ on the faces right let us say my control surface is made up of several areas several faces and all these faces are planar faces.

And, the value of the face of the ϕ on the face is basically taken as the face centroid value right if I do that can I replace this integral into a summation? Right this will be a summation \sum_f right and what would be this?

This would be $\phi \vec{A}_f$, right. This is $\phi \vec{A}_f$ summation f right here actually this control surface integration has 2 components one is integration over the little area other is sum of all these areas right for the ϕ times \vec{A}_f ok. So, this is the discrete form of the gradient theorem.

Now, do you see why it is useful to calculate why is this a method to calculate the gradients? You will see it right away because what are the inputs for this?

Student: ϕ .

ϕ is the input right which we already know from the previous iteration value or the current iterate value. Do we know \vec{A}_f ?

Student: Yes.

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The slide shows a handwritten equation in a blue box:
$$\int_{\Delta V_0} \nabla \phi \, dV = \int_{C_f} \phi \, dA$$

Below it, the text "Mean value approximation" is written. Underneath, another equation is written in a blue box:
$$\nabla \phi_0 \, \Delta V_0 = \sum_f \phi_f \vec{A}_f$$

The slide also features a small video inset of a man in a blue shirt in the bottom right corner.

We know areas; what about the cell volumes? We know and what do we need to calculate? $\nabla \phi$ right, we just need to calculate this $\nabla \phi$ of 0, right at the cell centroid that is as simple as that. Of course, we do not know phi exactly on the faces right that is one thing we do not know because phi is only stored at where?

Student: Cell centroid.

At the cell centroid. So, we need to kind of devise a way of calculating ϕ interpolate it to the faces from the cell values that we need to do ok.

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The slide shows a handwritten equation in a blue box:
$$\nabla \phi_0 = \frac{1}{\Delta V_0} \sum_f \phi_f \vec{A}_f$$

Below it, the text "Assume $\phi_f = (\phi_0 + \phi_1) / 2$ " is written. Below that is a diagram of a cell with a centroid C_0 and a face f . The diagram shows a vector $\vec{\Delta V}_0$ pointing from the centroid to the face, and a vector $\vec{\Delta x}_f$ pointing from the centroid to the face. The face is labeled f and has a normal vector \vec{A}_f pointing outwards. The cell is also labeled with ϕ_0 at the centroid.

The slide also features a small video inset of a man in a blue shirt in the bottom right corner.

But, if I rearrange this equation we can say grad phi for any cell can be calculated as $\frac{1}{\Delta V_0} \sum f_f \phi_f \vec{A}_f$ ok. Of course, we need to come up with an interpolation scheme to evaluate ϕ_f from the ϕ_0 and ϕ_1 values.

So, let me begin with a crude approximation ok. Let me assume that I would calculate my ϕ_f as an arithmetic average of the ϕ_0 and ϕ_1 values ok. Now, this is not correct, right. This is only correct if you have.

Student: (Refer Time: 12:15).

Uniform cells. If you do not have uniform cells this has to be replaced with a.

Student: (Refer Time: 12:20).

A linear interpolation right, need not be harmonic mean. It can be it mean it is not arithmetic mean, it will be a linear interpolation. You need to get a factor f right which is basically the distance between the face and the cell centroid p and $1 - f$ and so on, right. So, as of now I am assuming that it is just an arithmetic mean of the cell values we know that this is not correct if you have non uniform meshes ok.

But, what we will do is we will try to improve this ϕ_f little later in a different way ok. So, this is. So, I assume ϕ_f to be the cell centroid values average and now can I use this ϕ_f values in the equation above and calculate the gradients? Of course, I can calculate, right. If I do that then I am going to get $\nabla \phi$ at every cell that I have right.

So, if I have a cell bounded by 5 faces this will be summation of the $\phi_f \vec{A}_f$ on all the 5 faces right divided by the volume that will give me gradient and so on right. Then this way I can calculate what is the gradient of the dependent variable ϕ . Of course, we know that this is not quite correct, right.

So, what we do is we try to improve this by saying that if you look at the cells let me draw typical cell here. So, this is the face centroid let us say, this is the face centroid and this is the cell centroid. So, we are talking about C_0 and this is the face f this is our \vec{A}_f and this is my C_1 right, that is what I have and this is the face centroid ok. So, and these distances are not the same ok.

So, then what I would do is I would say I would draw a line connecting the cell centroid C_0 to the face centroid I would call it as $\overrightarrow{\Delta r_0}$, and I would call connect the cell centroid to the face centroid I would call it as $\overrightarrow{\Delta r_1}$ ok. These are 2 vectors that connect the cell centroids to the face centroids which can be done ok.

Now, can I use Taylor series expansion not in just 1D, but a general Taylor series and relate what is the value of ϕ_1 from ϕ_0 right. If it were a 1D we know that how to do it right essentially ϕ_e is ϕ_e was writ10 as how much ϕ_p or something right plus we wrote how.

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$$\phi_e = \phi_p + \left. \frac{\partial \phi}{\partial x} \right|_p (\Delta x) + \dots$$

$$\left\{ \begin{aligned} \phi_f &= \phi_0 + \nabla \phi_0 \cdot \overrightarrow{\Delta r_0} + \dots \\ \phi_f &= \phi_1 + \nabla \phi_1 \cdot \overrightarrow{\Delta r_1} + \dots \end{aligned} \right.$$

$$\phi_f = \frac{1}{2} \left\{ \left(\phi_0 + \nabla \phi_0 \cdot \overrightarrow{\Delta r_0} \right) + \left(\phi_1 + \nabla \phi_1 \cdot \overrightarrow{\Delta r_1} \right) \right\}$$

We wrote it as $\left. \frac{\partial \phi}{\partial x} \right|_p$ at p right times Δx right and so on, right. We could do it in a 1D expression or we had used $x - x_p$ right, if it were not the east face ok.

Similarly, can I use now I cannot use 1D because this is connecting $\overrightarrow{\Delta r_0}$ right which is a particular vector. So, can we use a general Taylor series and relate what is ϕ_f or evaluate what is ϕ_f purely from ϕ_0 values. So, I want to reconstruct phi on the faces from ϕ_0 , can I do that? Of course, we can do it right. So, we just expand this thing.

So, this will be in a similar sense ϕ_0 plus what would this be? It should be $\nabla \phi_0$ dotted with $\overrightarrow{\Delta r_0}$, is that correct? Essentially we get terms like $\left. \frac{\partial \phi}{\partial x} \right|_p$ times Δx plus $\left. \frac{\partial \phi}{\partial y} \right|_p$ times Δy plus

$\left. \frac{\partial \phi}{\partial z} \right|_p$ times Δz if it were 3D, right essentially that will be the dot product of the $\overrightarrow{\Delta r}$ with the 3-dimensional gradient ok.

Of course, if you want to do it a higher order terms you would have $\nabla^2 \phi_0$ and so on right which we are not writing here, fine ok. Then can we do the same thing can we reconstruct the ϕ_f from ϕ_1 ? Yes.

Student: (Refer Time: 16:40).

We can do that ok. So, what will that be? That would be ϕ_f equals ϕ_1 plus $\nabla \phi_1$ dotted with $\overrightarrow{\Delta r_1}$ plus higher order terms, is that correct? My I have chosen $\overrightarrow{\Delta r_0}$, $\overrightarrow{\Delta r_1}$ to always point to the phase centroid from the cell centroids ok. So, we do not have any confusion now can I now I have just computed what is $\nabla \phi$ at each and every cell right that is $\text{grad } \phi_0$ is calculated, $\nabla \phi_1$ is calculated. These are known, right.

And, the these vectors are also known from the mesh that we have created. Do we know the guess values for ϕ_0 , ϕ_1 ? We know these things right. So, now, can I calculate what is my improved value on the face as an average of these two? Right ok. So, that means, I can calculate my improved ϕ_f as ϕ_0 plus $\nabla \phi_0$ dotted with $\overrightarrow{\Delta r_0}$ plus ϕ_1 plus $\nabla \phi_1$ dotted with $\overrightarrow{\Delta r_0}$ right divided by 2 ok.

Now, this is not as crude as we had started off with, right? We started off with only the first terms in here right only we said ϕ_f equals ϕ_0 plus ϕ_1 by 2, but now we have an extra term here which is the second term in the Rayleigh series expansion. We have a little bit improvement compared to what we had started off with, right ok.

So, now the general algorithm is use this ϕ_f back in the equation back into this equation and calculate what is the improved cell centroid values ok. So, in the process we have set up an iterative scheme where we start off with a crude approximation for ϕ_f right, use that calculate the gradients. Use the gradients again to improve ϕ_f and then update the gradients right.

Now, this can go on for few iterations until we reach a converged gradient values ok, but generally you do not do more than couple of iterations, 2 to 3 iteration is sufficient. Why are we iterating here actually? What is the need for iterations here? Which term is actually making us to do this iteration?

Essentially the approximation for ϕ_f that is the truncating the terms in the Taylor series, that is what is making it ok. So, essentially couple of iterations is enough.

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2 to 3 iterations are sufficient

Gradient Theorem approach

- 1) $\phi_f = (\phi_0 + \phi_1) / 2$
- 2) $\nabla \phi = \frac{1}{\Delta V_0} \sum_f \phi_f \vec{A}_f$
- 3) Improve ϕ_f using

So, 2 to 3 iterations are sufficient that is what is done in the actual solvers if you look at. So, if I were to write a general algorithm for this, what would that be? That would be so, this is gradient theorem approach, what do we do? What is the first step in the algorithm?

You calculate you guess what is you evaluate what is ϕ_f from the existing ϕ_0 ϕ_1 using arithmetic average, right? What is the next step? Calculate what is gradients of phi this is gradient of phi at the cell centroids using ΔV_0 sigma f, $\phi_f \vec{A}_f$ right.

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3) improve ϕ_f using

$$\phi_f = \left(\phi_0 + \nabla \phi_0 \cdot \Delta \vec{r}_0 + \phi_1 + \nabla \phi_1 \cdot \Delta \vec{r}_1 \right) / 2$$

4) use updated ϕ_f and calc.
Go to step 2 and repeat.

Generic method and works on unstructured meshes.

Then once we have calculated gradients for all the cells improve ϕ_f using what? Using ϕ_f equals ϕ_0 plus $\nabla \phi_0$ dotted with $\Delta \vec{r}_1$ did we use $\Delta \vec{r}_1$ or $\Delta \vec{r}_0$? $\Delta \vec{r}_0$ plus ϕ_1 plus $\nabla \phi_1$ dot $\Delta \vec{r}_1$ divided by 2.

Now, use updated ϕ_f and calculate essentially go back to step 2 right that is basically go back to step 2 go to step 2 and repeat ok. Usually couple of iterations are sufficient to get a converge to grad phi fine, questions on this? Is it clear? Ok. So, if I give you some mesh with these area vectors that you can calculate and some phi values you can calculate what are the gradients using this approach right you can also code it up, fine alright.

So, this method is very generous generic method kind of works. It is a generic method and works on unstructured meshes ok. So, we do not need any special features here right it kind of works on general unstructured meshes alright, ok. Let us move on to the next method that is the least squares method. Any questions till now? Easy? Ok.

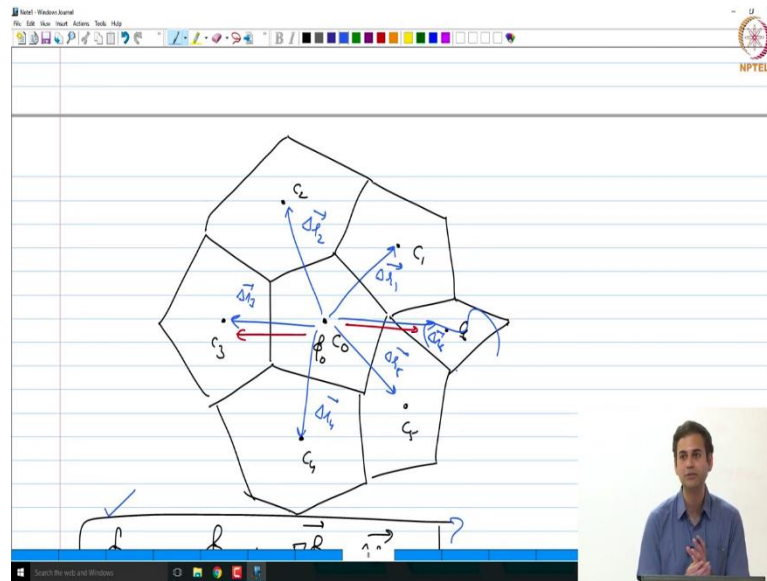
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2) Least Squares method :- obtain $\nabla\phi_0$ s/t
Reconstruct neighbouring cell value
from present cell value accurately.

Let us look at the second method that is the least squares method. Now, the idea in the least squares method is to reconstruct the neighboring value of ϕ , ok. So, essentially reconstruct neighboring cell value from the present cell value.

Now, how do you reconstruct this accurately gives you the value of the gradient, ok. So, we want to calculate what is ϕ at 1 cell 1 from ϕ_0 using certain gradient $\nabla\phi_0$ ok. Now, we want to calculate this evaluate this ϕ_1 as accurately as possible, then what would be my $\nabla\phi_0$, that is the idea ok. So, essentially evaluate or obtain $\nabla\phi_0$ such that you reconstruct neighboring cell value from present cell value accurately ok. Then, let us have look at a particular mesh configuration. Let me draw a mesh here.

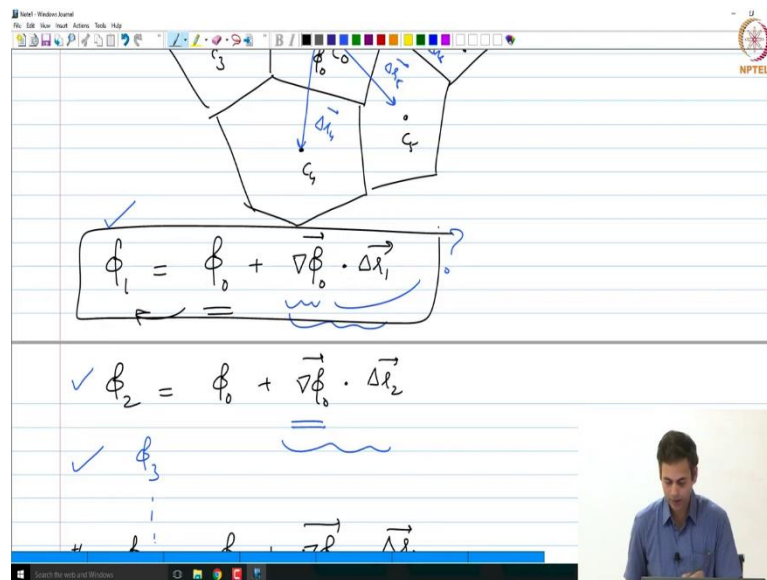
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I would use some mesh we have not seen till now something like this ok. So, we have a mesh here that need not necessarily have the same number of edges I created some mesh here, fine. So, let us call this as C_0 the value here would be ϕ_0 and let us call this as $C_1, C_2, C_3, C_4, C_5, C_6$ and so on right. This can be very different.

Now, I also want to draw some lines here that is basically we want to calculate what is ϕ_1 from ϕ_0 using the gradient at ϕ_0 right, that is what we want to do. So, let me connect C_0 and C_1 using 1 vector this is basically $\overrightarrow{\Delta r_0}$ or $\overrightarrow{\Delta r_1}$, ok. Let me call it $\overrightarrow{\Delta r_1}$ ok, can we obtain $\overrightarrow{\Delta r_1}$? We can right, we know the cell centroid values.

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So, if I were to calculate what is phi at 1 from phi at 0, how do I obtain this using general Taylor series? ϕ_1 equals ϕ_0 plus what do I need to know?

Student: Gradient.

Gradient at phi at cell centroid, this would be plus $\nabla \phi_0$ dotted with.

Student: Delta r 1.

Δr_1 , right? That is correct ok; that means, now Δr_1 definition is different from what we had before right, earlier Δr_1 was connecting the cell centroid C_1 to the face centroid here it is the distance or the vector connecting C_0 to C_1 right the cell centroid vector.

What about phi at 2? Can I obtain phi at 2 from ϕ_0 and the gradients? I can, right; phi at 2 would be phi 0 plus $\nabla \phi_0$ dot Δr_2 in which case I have to define what is Δr_2 as line connecting C_0 and C_2 right and so on and I would have $\Delta r_3, \Delta r_4, \Delta r_5$ and Δr_6 and so on as many number of neighbors I have.

Let us say if I have M neighbors, I would have to have M of these equations, but there is a problem that we can see right away, right. There is a problem in this approach ok, we will come to that problem.

So, essentially the idea is now how do I obtain this value, this is the unknown the $\nabla\phi_0$ such that I can accurately calculate not only ϕ_1 , but also ϕ_2 and also ϕ_3 , right and so on because all of these would use the same gradient at the cell center C_0 right.

So, I need to calculate $\nabla\phi_0$ as accurately as possible such that this gradient value at the cell centroid will give me or will help me reconstruct the neighboring cell values correctly in some sense, right ok.

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Mth equation: $\phi_j = \phi_0 + \nabla\phi_0 \cdot \Delta r_j$

M - equations

Two - dimensions

$$\vec{\nabla}\phi_0 = i \left. \frac{\partial\phi}{\partial x} \right|_0 + j \left. \frac{\partial\phi}{\partial y} \right|_0$$

That means, if I have let us say a j a neighbor ϕ_j would be what ϕ_0 plus $\nabla\phi_0$ dot $\vec{\Delta r}_j$, right and similarly, if I have m neighbours this would be the Mth equation right this would be the Mth equation if I have M cell neighbours right that share a face ok. That means, how many equations do I have? How many equation do I have?

Student: M.

M equations I have M equations alright. Now, what would be let us say I will consider a two-dimensional situation. We are talking about a calculate the gradients in two-dimensions ok, then what is my $\nabla\phi_0$? What is the definition for $\nabla\phi_0$? $i \left. \frac{\partial\phi}{\partial x} \right|_0 + j \left. \frac{\partial\phi}{\partial y} \right|_0$ at 0 right, this remains the same.

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$$\vec{\Delta r}_1 = \hat{i} \Delta x_1 + \hat{j} \Delta y_1$$

$$\vec{\nabla} \phi_0 \cdot \vec{\Delta r}_1 = \Delta x_1 \left. \frac{\partial \phi}{\partial x} \right|_0 + \Delta y_1 \left. \frac{\partial \phi}{\partial y} \right|_0$$

$$\left\{ \begin{array}{l} \Delta x_1 \left. \frac{\partial \phi}{\partial x} \right|_0 + \Delta y_1 \left. \frac{\partial \phi}{\partial y} \right|_0 = \phi_1 - \phi_0 \\ \Delta x_2 \left. \frac{\partial \phi}{\partial x} \right|_0 + \Delta y_2 \left. \frac{\partial \phi}{\partial y} \right|_0 = \phi_2 - \phi_0 \\ \vdots \\ \Delta x_M \left. \frac{\partial \phi}{\partial x} \right|_0 + \Delta y_M \left. \frac{\partial \phi}{\partial y} \right|_0 = \phi_M - \phi_0 \end{array} \right\}$$

What about $\vec{\Delta r}_0$? If you were to write it as a vector this would be $\hat{i}\Delta x_0 + \hat{j}\Delta y_0$ oh sorry we do not have $\vec{\Delta r}_0$ right we have $\vec{\Delta r}_1$. So, all these should be sub once alright. So, this is $\hat{i}\Delta x_1 + \hat{j}\Delta y_1$ right, what is Δx_1 ?

Student: (Refer Time: 29:21).

x_1 minus x_0 right, the x component distance between cell 1 and cell 0 fine. So, we have this. So, what is this product $\nabla \phi_0$ dot $\vec{\Delta r}_1$ that we have in each of these terms, right, we have we have this product here right, what would this be? This would be basically Δx_1 .

Student: (Refer Time: 29:48).

Sorry, $\Delta x_1 \left. \frac{\partial \phi}{\partial x} \right|_0$ plus.

Student: Delta.

$\Delta y_1 \left. \frac{\partial \phi}{\partial y} \right|_0$ right that is what we have; that means, I can rewrite this equation. If I send this ϕ_1 to the right hand side or ϕ_0 to the left hand side I can rewrite this equation this particular equation as what? As $\Delta x_1 \left. \frac{\partial \phi}{\partial x} \right|_0$ plus $\Delta y_1 \left. \frac{\partial \phi}{\partial y} \right|_0$ equals how much? ϕ_1 minus ϕ_0 right.

Similarly, I can write an equation for the second cell value that we reconstruct as $\Delta x_2 \frac{\partial \phi}{\partial x} \Big|_0$ plus $\Delta y_2 \frac{\partial \phi}{\partial y} \Big|_0$ equals ϕ_2 minus ϕ_0 alright and so on. $\Delta x_M \frac{\partial \phi}{\partial x} \Big|_0$ plus $\Delta y_M \frac{\partial \phi}{\partial y} \Big|_0$ equals ϕ_M minus ϕ_0 if we have M cells, right? Or this would be j for a particular jth cell ok.

Now, we have as many equations as we have number of neighbors, number of face neighbors ah, but what is the unknown in this?

Student: Phi.

Phi, is phi the unknown?

Student: (Refer Time: 31:18).

$\nabla \phi$ is the unknown right $\frac{\partial \phi}{\partial x} \Big|_0$ and $\frac{\partial \phi}{\partial y} \Big|_0$ at cell 0 right, this is the unknown. ϕ_1, ϕ_0 are known from the current iteration values and deltas are known as the from the mesh ok. So, these are all known. So, that means, if I were to write this in a matrix form, can I write it in a matrix form?

Student: Yes.

How many equations I have? M equations. So, how many rows should my matrix have?

Student: M rows.

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The image shows a whiteboard with handwritten mathematical equations. The main equation is:

$$\begin{bmatrix} \Delta x_1 & \Delta y_1 \\ \Delta x_2 & \Delta y_2 \\ \vdots & \vdots \\ \Delta x_M & \Delta y_M \end{bmatrix} \begin{bmatrix} \frac{\partial \phi}{\partial x} \Big|_0 \\ \frac{\partial \phi}{\partial y} \Big|_0 \end{bmatrix} = \begin{bmatrix} \phi_1 - \phi_0 \\ \phi_2 - \phi_0 \\ \vdots \\ \phi_M - \phi_0 \end{bmatrix}$$

Below the matrix, it is labeled A with dimensions $M \times 2$. The vector on the right is labeled b with dimensions $M \times 1$. The vector on the left is labeled x with dimensions 2×1 . Below the matrix, it says $M > 2$ and "Over-determined system".

M rows and what are the coefficients? $\Delta x_1, \Delta y_1, \Delta x_2, \Delta y_2$ and so on $\Delta x_M, \Delta y_M$. This is my matrix times what would be the other vector that I have? $\left. \frac{\partial \phi}{\partial x} \right|_0$ this should be a column vector or a row vector?

Student: Column vector.

Column vector. $\left. \frac{\partial \phi}{\partial y} \right|_0$ equals what would be on the right hand side?

Student: (Refer Time: 32:18).

ϕ_1 minus ϕ_0 , ϕ_2 minus ϕ_0 and so on; ϕ_M minus ϕ_0 , right. This is what I have right. I have a matrix equation which has M rows and how many columns? 2 columns this is an M by 2 matrix and I have an unknown vector here which is 2 columns sorry 2 rows and 1 column and then here I have M rows and 1 column ok. So, we have a M by 2, 2 by 1 and M by 1 vectors and matrices here.

In general, what is the in a two-dimensions what is the minimum cell neighbors I would have? What is the cell the smallest cell that you can take?

Student: (Refer Time: 33:02).

With minimum number of faces?

Student: 3.

3, right? It is a triangle right. So, in general M is the number of rows would be greater than 2 right, this is always greater than 2 right because you have at least 3 faces for a triangle ok. How many unknowns I have here?

Student: (Refer Time: 33:20).

2 unknowns; how many equations I have?

Student: M.

M equations; I have M equations and 2 unknowns, can I solve for the system?

Student: Yes.

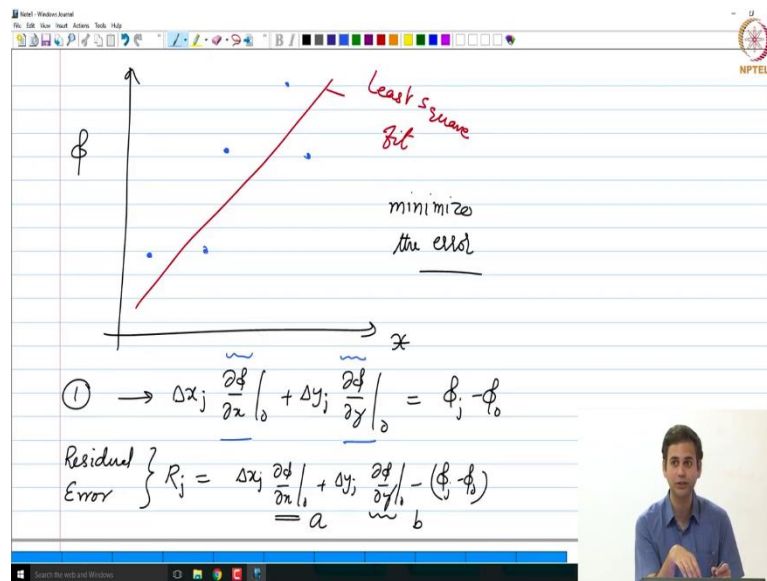
Uniquely, can I solve this? This you cannot solve right because if you use 2 equations you get a solution; you get 2 other equations, you get another solution. You cannot satisfy all these equations at once right; that means, this is a what type of a system?

Student: Over specified.

Over specified system, right. So, this is basically over determined or over constrained system for which we cannot you do not have unique solution right. Because, if we take 2 sets of equations you would get one solution which will satisfy only those 2 equations and not the other ones right.

So, this is nothing new to you because you have already come across such systems many a times, right. When you do an experiment you end up having.

(Refer Slide Time: 34:19)



Let us say if you are doing an experiment. You get some values here for the let us say phi and some x values you got some values here, right and you have to fit a essentially you have to find one equation one straight line that passes through all of these things, right? But, you cannot find one equation that passes through all of these things because you have too much data, right. What do you do in that case?

Student: (Refer Time: 34:48).

You would find a, you would kind of minimize the error the square of the error in an absolute sense square of the error minimize it and draw a line, right. Now, that line would it pass through any solution?

Student: (Refer Time: 35:01).

It would not it will not; it will not satisfy any of the points, right, but it will be in a sense it will have the least error possible right. So, essentially you would say I have calculated the equation, this is my equation right. So, this is my what do you call? Least square fit, right. This is the least square fit line which will not satisfy any of them, but it will have the least error if we consider one by one right.

In fact, that is what we have in the present situation, right. We have too much data and you have to calculate what is 2 components of the gradients right for the dependent variable. We just have to calculate $\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}$ from these M equations.

So, what we set out to do is we try to minimize this error and calculate what would be these gradients which will be in a least square sense reconstruct the neighbouring values accurately, ok. Is the method clear? What it is trying to do? We will do the remaining part of it the minimization of the error and so on alright ok. Questions on this part, till now?

So, essentially trying to minimize the error; error meaning from the line that we intend to fit between the data alright minimize the error ok. Questions? Ok, I want you to say something about this matrix.

So, essentially this matrix as it is cannot be solved right can you invert it and calculate no essentially you have you have you have to use any 2 equations and solve it right that is understood. Let us give the some names for this matrix. Let us call sorry, let us call this matrix as A and the gradient matrix as some g and this we would like to call it as this is from some delta of phi right. So, let us call it as some d, A, g. A is the coefficient matrix, g is the gradients, d is the delta of the phi ($\nabla \phi$) ok; that is what we have fine alright.

Let us can then move on to what do we do in this context? So, we have to reduce the error or minimize the error and the equation we are working with is basically $\Delta x_j \frac{\partial \phi}{\partial x} \Big|_0$ plus $\Delta y_j \frac{\partial \phi}{\partial y} \Big|_0$ equals ϕ_j minus ϕ_0 , alright, that is the equation we are working with.

Let us call this as say equation 1 ok. I can rewrite this equation as to calculate the residual or the error. So, what I mean is now if you know what is $\frac{\partial \phi}{\partial x} \Big|_0$ and $\frac{\partial \phi}{\partial y} \Big|_0$ at 0 correctly, you will this equation will be balanced right and if it is not the correct value then it will not be balanced.

There will be some error, right. ϕ_j minus ϕ_0 would be different from what you get on the left hand side right, depending on how well you calculate these guys right ok. So, what I do is I will define an error or a residual in the context of the in the context of computational methods you would call a residual as whatever is the difference between left and right hand sides in an equation, ok. So, or an error saying that the difference between the left side and the right side is my error at that cell or at that face ok.

So, I would like to call it as some residual R_j ; R_j is basically I bring the right hand side to left hand side. So, this will be $\Delta x_j \frac{\partial \phi}{\partial x} \Big|_0$ plus $\Delta y_j \frac{\partial \phi}{\partial y} \Big|_0$ minus ϕ_j minus ϕ_0 is my residual right. So, if I use 2 equations and calculate these gradients this residual would be 0 for those 2 cells right, but that is not what we are trying to do.

We are trying to calculate the gradients such that this R_j is minimized in a least square sense, fine; that means, of course, this is just one equation. We have M face neighbors.

(Refer Slide Time: 39:46)

The whiteboard content is as follows:

$$\text{Residual } \left. \begin{array}{l} \\ \text{Error} \end{array} \right\} R_j = \Delta x_j \frac{\partial \phi}{\partial x} \Big|_0 + \Delta y_j \frac{\partial \phi}{\partial y} \Big|_0 - (\phi_j - \phi_0)$$

Below this, the equations are simplified with labels 'a' and 'b' under the gradient terms:

$$R_j = \Delta x_j \frac{\partial \phi}{\partial x} \Big|_0 + \Delta y_j \frac{\partial \phi}{\partial y} \Big|_0 - (\phi_j - \phi_0)$$

$$R_j = a \Delta x_j + b \Delta y_j - (\phi_j - \phi_0)$$

The total residual R is then defined as the sum of the squares of the individual residuals:

$$R = \sum_{j=1}^M R_j^2$$

$$R = \sum_{j=1}^M \{ a \Delta x_j + b \Delta y_j - (\phi_j - \phi_0) \}^2$$

So, what would be the total residual R or the square of the residual R? I would like to call it as R_j square summed for all the j goes from 1 to M right. So, $\sum_{j=1}^M R_j^2$ would be my square of the error right, yes, ok. So, this is how much? This would be $\sum_{j=1}^M$ goes from 1 to M. Let me also write $\left. \frac{\partial \phi}{\partial x} \right|_0$ as some variable a $\left. \frac{\partial \phi}{\partial y} \right|_0$ as another variable b ok. A and b are the unknowns that we intend to get out of this problem ok.

So, this is a times Δx_j plus b times Δy_j minus ϕ_j minus ϕ_0 whole square is what we have to minimize right for this least square error, right. This error is now squared. We have to find the least value for that alright. How do you do least squares when you have 2 parameters?

Student: Differentiate the error.

Differentiate the error.

Student: (Refer Time: 41:04).

With respect to the unknown that you want, right. Unknowns that you want to calculate.

(Refer Slide Time: 41:10)

The image shows a digital whiteboard with the following handwritten equations:

$$\frac{\partial R}{\partial a} = 0; \sum_{j=1}^M 2(a\Delta x_j + b\Delta y_j - (\phi_j - \phi_0)) \Delta x_j = 0$$

$$\frac{\partial R}{\partial b} = 0; \sum_{j=1}^M 2(a\Delta x_j + b\Delta y_j - (\phi_j - \phi_0)) \Delta y_j = 0$$

A small video inset in the bottom right corner shows a man in a blue shirt speaking.

So, that means, the we need to calculate what is $\frac{\partial R}{\partial a}$ and set it to 0 right and then $\frac{\partial R}{\partial b}$ and set it to 0 that is what we do. So, we already have the square of the error, we would calculate the least value by differentiating it minimum value ok. So, what would be these equations?

$\frac{\partial R}{\partial a}$ equals 0 what would this be? This would be summation would stay as it is right, you have a summation. This would be 2 times $a\Delta x_j$ plus $b\Delta y_j$ minus ϕ_j minus ϕ_0 times what.

Student: (Refer Time: 41:53).

Times Δx_j equals 0, what is the other equation? Sigma j equals 1 to M 2 times $a\Delta x_j$ plus $b\Delta y_j$ minus ϕ_j minus ϕ_0 times Δy_j equals 0, ok. So, we have 2 multiplying in every term. So, 2 can be thrown out alright. So, this can be taken away because it is there in every term in the summation ok.

Now, we got couple of equations. So, how many equations we have?

Student: 2.

2 equations because we have a summation for each equation ok. We have only 2 equations and how many unknowns we have?

Student: 2.

(Refer Slide Time: 42:49)

The whiteboard displays the following equations:

$$\sum_{j=1}^M a \Delta x_j^2 + b \Delta x_j \Delta y_j - (\phi_j - \phi_0) \Delta x_j = 0$$

$$\sum_{j=1}^M a \Delta x_j \Delta y_j + b \Delta y_j^2 - (\phi_j - \phi_0) \Delta y_j = 0$$

Below the summations, the terms are expanded as follows:

$$\Delta x_1^2 + \Delta x_1 \Delta y_1 + \Delta x_2^2 + \Delta x_2 \Delta y_2 + \dots$$

$$\Delta x_1 \Delta y_1 + \Delta y_1^2 + \Delta x_2 \Delta y_2 + \Delta y_2^2 + \dots$$

Only 2 unknowns ok. So, we have now reduced the problem you see right ok. This is basically sigma j equals 1 to M, how much would this be? This would be $a\Delta x_j$ square $b\Delta y_j$ minus ϕ_j minus ϕ_0 times Δx_j right equals 0. What is the other equation? Other equation is

sigma j equals 1 to M a Delta x_j Delta y_j plus b Delta y_j^2 minus phi_j minus phi_0 times Delta y_j equals 0 right, that is what we have ok.

We have 2 equations and 2 unknowns. Now, can I try to write this in a matrix form? I can ok. So, that would be we have these terms right. So, the kind of terms we have are basically if you look at if you look at the first equation, how does these terms look like? This will look like Delta x_1^2 right plus Delta x_1 Delta y_1 plus delta the from the for the first equation it will be Delta x_1^2 plus Delta x_1 Delta y_1 and then Delta x_2^2 plus Delta x_2 Delta y_2 and so on, right that is what we would get.

For the second equation you would get Delta x_1 Delta y_1 plus Delta y_1^2, right. This is what you would get right plus Delta x_2 Delta y_2 plus Delta y_2^2 of course, I have not writ10 a and b here, ok. I just wrote the coefficients for a and b and these are again multiplying with a and b.

Can I get this from the matrix we have?

(Refer Slide Time: 44:42)

So, we have a matrix what is the matrix A that we have? A is Delta x_1 Delta y_1 Delta x_2 Delta y_2 and so on Delta x_M Delta y_M right. This is an M by 2 matrix right. What would be if I were to write a transpose as Delta x_1 Delta y_1 Delta x_2 Delta y_2 and so on Delta x_M Delta y_M? This would be a 2 times M matrix right 2 by M matrix.

What would be A transpose times A? Would that give you these equations right?

(Refer Slide Time: 45:35)

$$\Delta x_1 \Delta y_1 + \Delta y_1^2 + \Delta x_2 \Delta y_2 + \Delta y_2^2 + \dots$$

$$A = \begin{pmatrix} \Delta x_1 & \Delta y_1 \\ \Delta x_2 & \Delta y_2 \\ \vdots & \vdots \\ \Delta x_M & \Delta y_M \end{pmatrix}_{M \times L} ; T = \begin{pmatrix} \Delta x_1 & \Delta x_2 & \dots & \Delta x_M \\ \Delta y_1 & \Delta y_2 & \dots & \Delta y_M \end{pmatrix}_{2 \times M}$$

$$A^T A = \begin{matrix} \Delta x_1^2 + \Delta x_2^2 + \dots + \Delta x_M^2 + \\ \Delta x_1 \Delta y_1 + \Delta x_2 \Delta y_2 + \dots + \Delta x_M \Delta y_M \end{matrix}$$

$$A^T A g =$$

So, that means, if I write this as A transpose A would be would be what? Essentially multiply this guy with this guy right, plus the second one plus the first one with the second column right that is your first row right A transpose A, would be what?

Student: (Refer Time: 45:54).

Do you see that you would get Δx_1^2 plus Δx_2^2 and so on Δx_M^2 plus the first row again multiplying the second column would give you $\Delta x_1 \Delta y_1$ $\Delta x_2 \Delta y_2$ and so on $\Delta x_M \Delta y_M$, do you see that? Do we get that? Yes or no? Yes, ok?

What about the second row? Second row would be this one multiplying the first column right that would be the mixed values $\Delta x_1 \Delta y_1$ and the plus the second row multiplying the second column, that would give you the delta y squares ok. So, I can write this of course, I have the a and b which are nothing, but just 2 values right which are the same for every term. So, I can put them as a column vector similar to what we had before.

(Refer Slide Time: 47:02)

$$\Delta \phi = \Delta x_1 \frac{\partial \phi}{\partial x_1} + \Delta x_2 \frac{\partial \phi}{\partial x_2} + \dots + \Delta x_n \frac{\partial \phi}{\partial x_n}$$

$$A^T A g = A^T d$$

$$\begin{matrix} 2 \times 2 & \downarrow & 2 \times 1 \\ \frac{\partial \phi}{\partial x} \Big|_0 & & \left\{ \begin{matrix} \Delta \phi_1 \\ \Delta \phi_2 \\ \vdots \\ \Delta \phi_n \end{matrix} \right\} \end{matrix}$$

$$\frac{\partial \phi}{\partial y} \Big|_0$$

I can rewrite these equations that we have essentially these 2 equations that we have as what? I can rewrite this as A transpose A times the gradient right that is basically gives you, what will be the size of the matrix A transpose A?

Student: (Refer Time: 47:13).

2 by 2 because we have 2 by M by 2 this will be 2 by 2. So, this will be a 2 by 2 matrix and what is g ? $\frac{\partial \phi}{\partial x} \Big|_0$ and $\frac{\partial \phi}{\partial y} \Big|_0$, this is 2 cross 1 equals, what is on the right hand side?

Student: A transpose.

This is ϕ_0 minus ϕ_0 times Δx_j , right. So, you are multiplying $\Delta \phi$ with Δx and this in the second equation you are multiplying $\Delta \phi$ with Δy and you are summing it, right. So, what would that be?

Student: A transpose.

A transpose times.

Student: Phi.

So, if I were to here if I were to write partial phi just the phi this is basically phi what values go here?

Student: (Refer Time: 48:05).

ϕ_j minus ϕ_0 right is what goes in here. So, this is basically ϕ_1 minus ϕ_0 ϕ_2 minus ϕ_0 and so on ϕ_j minus ϕ_0 , right. Each of them multiplying with 2 rows will give you the 2 equations, do you see? Ok. So, this is nothing, but our d or A transpose times d right that is your $\Delta\phi$. This is your $\Delta\phi_1$ $\Delta\phi_2$ and so on $\Delta\phi_M$ which is basically ϕ_1 minus ϕ_0 , ϕ_2 minus ϕ_0 and so on.

Now, what is the size of this equations here this matrix here? 2 by 2 matrix 2 by 1 and then we have.

Student: 2 by 1.

2 by 1 right. So, this is basically a 2 by 2 matrix that is all, right. So, and what do we need to do? We need to have we will have such a system, only one system for the entire mesh or will it be different for different cells?

Student: (Refer Time: 49:13).

It will be different for different cells right. So, essentially you will have one 2 by 2 such system for every cell in the mesh right, you would calculate that and then let us say if you have a fixed mesh the mesh is not changing, what will be the matrix A ? Will that be will that remain the same always?

Student: Yes.

The mesh is not changing, A only depends on Δx and Δy .

Student: Yes.

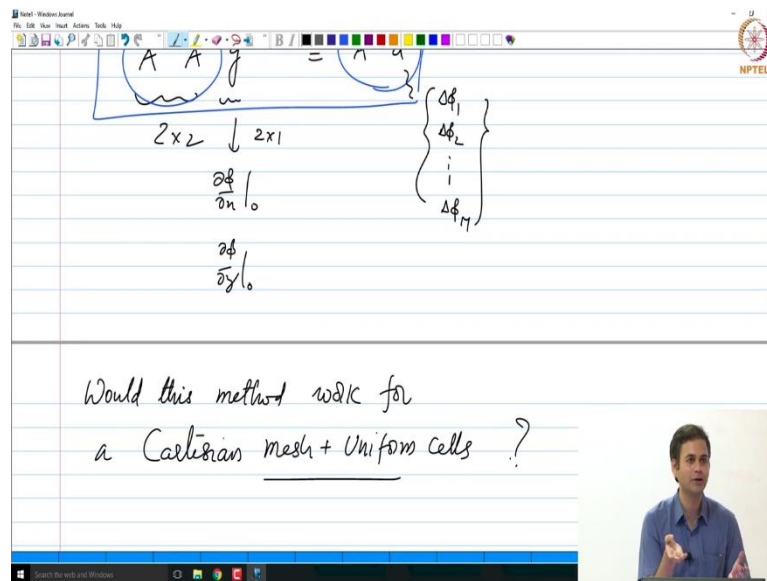
Right. So, can you pre calculate A transpose A and store it?

Student: Yes.

Yes you can. So, you do not have to do this all the time. So, this can be pre calculated right ah. Right hand side needs to be updated as your ϕ changes right and you need to calculate what is gradient, ok. So, in fact, you can even pre calculate what is A transpose A is inverse as well right because it just 2 by 2 system, right.

Does not matter how many faces you have, it is always a 2 by 2 system. So, you can calculate this and calculate it is inverse and calculate what is the gradient values right; that means, for every cell you just go and solve the system once and get the gradient values fine. And, the g thus obtained would satisfy none of these equations. It will satisfy only these equations in a least square equations ok. So, that is the essence of the least squares method ok. Questions?

(Refer Slide Time: 51:01)



Now, what would happen will this actually work for a let us say a structured rectangular mesh? Would it actually work? Would this method work for let us say a Cartesian mesh that is also uniform? Will it actually work for Cartesian structured or it will only work for unstructured? It should work for Cartesian structure, it is not a surprise.

But, then what will happen if you have a Cartesian structured mesh which is also uniform? What will happen to this matrix A ? What about Δx_1 Δx_2 ?

Student: (Refer Time: 51:42).

All are the same, then what will happen to the matrix A ?

Student: (Refer Time: 51:48).

Then, what will happen to A transpose A ?

Student: Drawn in vertical?

Would it become singular?

Student: Yes.

Then you said it will work for Cartesian structure, right? Now, we just saying that it is it will become singular, there is a catch here. What is the catch? They are not the same because.

Student: (Refer Time: 52:07).

No, the way we have drawn the vectors are all different what will be Δx_2 what will be Δx_1 and Δy_1 ?

Student: (Refer Time: 52:15).

They would point in the opposite direction. So, Δx_2 would be minus of Δx_1 if you have let us say Cartesian mesh, right, in which case the rows are not the same right. You would have let us say Δx_1 is 2 you would have 2 and Δy_1 is 0 let us say the cells are in the along the x axis, we would have 2 0 and the other one would be minus 2 0 right and so on.

As a result when you take $A^T A$ you would end up with a identity matrix, right. You have 1 0 minus 1 0 and so on, you would end up with an identity matrix with a uniform cell size that is Δx right and that is why it would work, right.

So, do not get confused this Δx is not just is not always it is basically defined in a way that it connects the current cell centroid to the neighbouring cell centroids ok. Do not use the your own definition of Δx here, fine. So, that is important here fine, that is the case it will work for anything.

Yes?

Student: Sir, Δx a term we will be considering only face neighbours, right?

Only the face neighbours, yes. I think I have drawn I have not drawn it nicely. Actually this cell is little complicated this is not there. But, the thing is, I mean this cell is not there we are only considering the face neighbors.

The figure is drawn little complicated, but in this context you may have to use the vertex neighbour also because this is it is because we are not using a lead interpolation between

the faces as such. So, it can you can still consider this thing right you can still be left over there. It is just that the other cells are not drawn in a similar way, right. Other questions? So, it will work for regular structured, Cartesian, uniform, non-uniform, everything unstructured and so on ok, fine, alright ok. I am going to stop here. See you guys in the next lecture.

Thank you.