

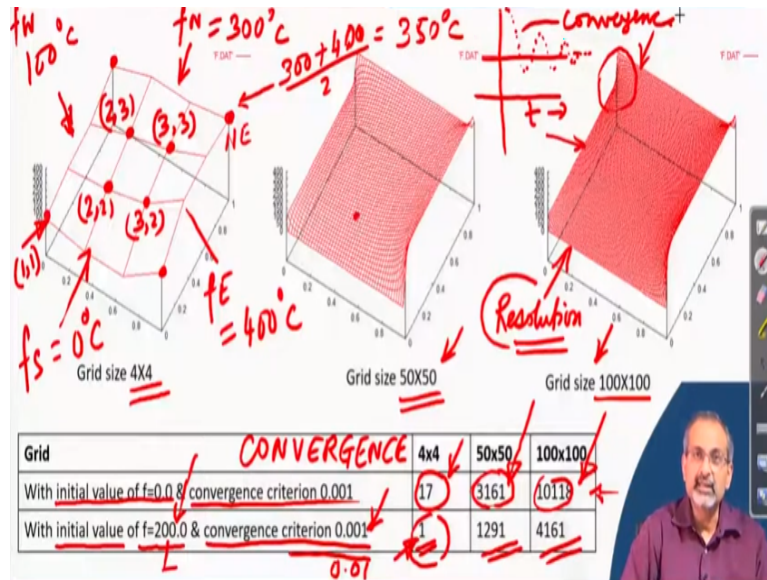
Introduction to CFD
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Module No # 04
Lecture No # 19

Numerical Solution of Steady State Heat Conduction (Elliptic PDE) (Cont'd)

In this lecture we will continue our discussion on elliptic partial differential equations.

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In the previous lecture we had tried to solve this problem of a square domain in which we had imposed 4 Dirichlet boundary conditions on the 4 sides of the domain. And then we had taken a 4 by 4 mesh including the boundary grid points and then try to discretized Laplace equation and solve it. So just for recollection we will try to remember what are the boundary values we have put on the left? And we have put a value of 100 degree centigrade.

So we marked it as fw and then on the north phase we have marked it as 300 degree centigrade on the east phase we had put 400 degree centigrade. And on the south phase it was 0 degree centigrade. And if you recall we had calculated an initial or guess value of 200 degree centigrade in the internal grid points. So since we marked this corner grid points as 1, 1 therefore this interior grid point are marked as 2, 2 3, 2 2, 3 and 3, 3 respectively.

And then we iteratively solve Laplace equation but fortunately the solution converges very rapidly and in the second iteration itself we found that we were getting the same values as in the first iteration that means the solution had already converged. And then we had briefly assessed what could be the measures for convergence. So either you base it on the difference in the functional value at each and every internal grid point where you are updating the value through an iterative approach.

Or you try to take a global measure by computing the RMS error in convergence. Now we recall that we had taken a 4 by 4 mesh including the boundary grid points now of course you can go about refining the mesh. And then you will get much more detailed variation of the function as it matches up with these boundary conditions which can be seen in a more refined mesh of 50 by 50 size. And therefore you can actually figure out that the discrete errors on a coarser mesh are much reduced on a finer mesh.

One issue which still remains is that at the corner points what are the values of the temperature we should be setting though in the computational stencil? That will not have any influence there should be some reasonable ways by which you estimate those values at the corners. Because for example at this corner which we can call as the north east corner; for example because it is sharing part of the northern phase and the eastern phase of the boundary.

You could estimate it by taking an arithmetic average of the values that you have set at the 4 boundaries. So, let us say you can set a condition of 350 degree centigrade at this corner point and that is precisely what has been done with. Similarly you can go about doing it at other corner points so that they are having an intermediate value between the sharing side temperatures. Again going back to finer mesh you can refine the mesh further and make it say 100 by 100 mesh.

And then you have still further increase in the resolution so this is what we call as resolution that means you are getting or capturing the finer details of the functional variation in the domain as we put in more and more grid points that is usually how it works? And then, ideally if your discretization is an accurate discretization and with the fairly good order of accuracy. Then as you put in more and more grid points you are essentially approaching the analytical solution.

So if you refine it further and further you will get finer details especially where the changes are rapid. So when you have changes in temperature at the boundaries there would be regions especially at the corner where the changes could be rapid and then a fine mesh should capture it later. So there is one part coming from the resolution aspect other part is that how much computing time would involve.

So for looking at that you try to figure out that how many iterations are taken in order to reach the converge solutions. So we have the issue of convergence which is essentially the process of reaching the final steady state solution. So the intermediate values that we compute are essentially having no physical significance they are just lying on the path towards a converged and steady state result. But as we the refine the mesh more number of iterations is taken to reach it.

So, on a 4 by 4 mesh when you start with an initial value of the function as 0 and you set the convergence criteria to be 0.001 for each and every grid point to be satisfied. Then on a 4 by 4 mesh it would take 70 iterations. Again on a 50 by 50 mesh it will take 3161 and 100 by 100 mesh more than 10000 iterations to compute. Last time incidentally we had made an intelligent guess about the initial value we had taken an average of the boundary temperatures and set it as 200 degree centigrade.

Incidentally we just took 1 iteration to complete on a 50 by 50 mesh it would take 1291 iteration to converge. And on a 100 by 100 mesh it would take 4161 iterations to converge. So there are number of things that we can easily understand one is that in general a more refine mesh will involve more number of iterations still you reach the steady state. The initial guess value would have an impact on how many relations are actually needed before you reach a steady state solution.

And then the other thing is that how stiff is you convergence criteria so let us say if you had relax this criteria and made it lower. Let us say you made it 0.01 all these computations would take much less number of iteration. Of course you cannot go any lower than 1 but for the other cases it would take much less number of iterations in general. So the convergence criteria the initial guess and the grid size so these are the 3 things which have influenced the solution in a big way.

And again remember that when we reach convergence there is a certain path that the solution is actually taking which can be probably be monitored better, if you look at how the solution tended to behave at each and every grid point. So if you look at a specific grid point let us say this grid point and then you try to monitor how the solutions look like? Then you will see that initially the value of the function may be following a path like this and then oscillating about a certain value till it converges at large times towards a steady state value.

So, that could be the way the convergence is achieved so the convergence may take place through little bit of an oscillatory behavior till it actually studies out. There could be other ways or other paths also through which convergence may be achieved but the final intention is to reach and ensure that convergence is reached. So to sum up some of the learning's that we had through this activity we will try to recapitulate the main points once more.

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- ❑ The value $f_{i,j}$ is updated by averaging the neighbouring grid values- this is related to the physics of diffusion. The averaging operation is called as 'relaxation'.
- ❑ What we mean by convergence is reaching a 'zero' residual for all the discrete equations for internal grid points through an iterative procedure.

$$f_{i,j}^{k+1} - \frac{1}{4} [f_{i+1,j}^k + f_{i-1,j}^k + f_{i,j+1}^k + f_{i,j-1}^k] = R_{i,j} \quad \Delta x = \Delta y = \Delta$$

$\rightarrow 0 \in$

- ❑ As we iterate, we generate updated values of $f_{i,j}$. These intermediate values of $f_{i,j}$ which are produced in course of iterative calculations do not have any physical significance. The only distribution of $f_{i,j}$ that is physically significant is the equilibrium distribution which is reached at the end of the iterations.
- ❑ Convergence depends on boundary conditions. Usually purely Dirichlet BCs based problems converge more rapidly than mixed Dirichlet-Neumann BCs.
- ❑ Choice of initial conditions affects convergence.
- ❑ A refined mesh takes more computing time but gives better resolution.

So if you look at these points we can recall most of the experiences we now have from this solution. So the $f_{i,j}$ values they have been updated by averaging the neighboring grid values you remember that we were just summing up the neighboring grid values and multiplying them by a factor of 1 fourth to reach the value of $f_{i,j}$ the updated value of $f_{i,j}$ so this is essentially related to the physics of diffusion which is a moral by this governing equation Laplace equation.

And the averaging operation to reach the updated value of f_{ij} at a certain grid point is referred to as relaxation. When we talk about convergence in the context of Laplace equation elliptic equation in general we are essentially reaching a 0 residual or near 0 residual and that is the target that we have in terms of convergence. So when we lay down the discrete equation for all the internal grid points and we are trying to iterate the value of f_{ij} at each one of i 's and j 's of the internal points in an iterative manner.

Essentially what we are trying to do is we are trying to set this residual to 0 or to a very small epsilon before we stop the computations. So if you do this you get the residual that means what is left on the right hand side of the equation? Is it a perfect 0 or a very small number can we make it any smaller? And of course all these equations are working on the basis that the grid spacing along the 2 directions are equal.

So now onwards until and unless it is specify; we would in general assume that the grid spacing's along the different Cartesian directions are equal. So that just gives the convenience that the governing equation simplifies significantly. As we iterate we end up generating updating values of f_i and j and as we do that as we keep generating these updates these are all intermediate values of f_{ij} they are not the final or the equilibrium or the converged distribution of f_{ij} .

And they essentially have no physical significance they are just lying on the path of convergence incidentally they are absolutely not relevant in terms of the physics. The only physically significant solution is the equilibrium distribution which you reach at the end of the iterative exercise. Convergence depends on boundary conditions usually when we deal with purely Dirichlet boundary conditions the problem converges faster.

Whereas if you have a mixed Dirichlet- Neumann boundary condition imposed on the boundary the convergence would in general be slower. Choice of initial condition is would also effect convergence and refining the mesh will add to the computing time and that will give better resolution of the physics. So these are some of the things which we already realized from the result as we saw in the previous slide. And just to reinforce the ideas we recapitulate it some of the facts that we already saw through the example demonstration.

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9x9 COEFFICIENT MATRIX

-4	1	0	1	0	0	0	0	0
1	-4	1	0	1	0	0	0	0
0	1	-4	0	0	1	0	0	0
1	0	0	-4	1	0	1	0	0
0	1	0	1	-4	1	0	1	0
0	0	1	0	1	-4	0	0	1
0	0	0	1	0	0	-4	1	0
0	0	0	0	1	0	1	-4	1
0	0	0	0	0	1	0	1	-4

5x5 Grid

(1,5)	(2,5)	(3,5)	(4,5)	(5,5)
(1,4)	(2,4)	(3,4)	(4,4)	(5,4)
(1,3)	(2,3)	(3,3)	(4,3)	(5,3)
(1,2)	(2,2)	(3,2)	(4,2)	(5,2)
(1,1)	(2,1)	(3,1)	(4,1)	(5,1)

Boundary Labels: S (South), W (West), N (North), E (East)

- Pentadiagonal system of equations. Can be solved by direct methods like Gauss elimination or Cramer's but they are extremely expensive
- Iterative methods of solution are quite efficient, however, strategies to accelerate convergence are required for minimizing the computational effort
- If the pentadiagonal problem can be represented as an equivalent problem involving tridiagonal system of equations then TDMA algorithm can be used, which is an efficient algorithm

This could time to look at the matrix representation of the problem that we have been handling. So earlier we had been used a 4 by 4 mesh incidentally here we are using a 5 by 5 mesh and we are still working with the square domain and you can make out that this is the south boundary this is the west this is north this is the east boundary. Now we have a fairly a comparatively larger number of points in the inner part of the domain earlier we have 4 points now we have 9 points.

Now if we were to write down the discretized governing equation for all this internal points going by point by point and developing all the equation the linear algebraic equations related to each points. And then lay them in a matrix form we would a matrix looking like this so if we just look at the first row of the matrix what it says is? -4 times $f_{2,2} + f_{3,2} +$ we skip 1 because it is coefficient is 0 here. So we go on to $f_{2,3}$ to 1 so that is $+f_{2,3}$ and then there are no non-zero entries any more on this row.

So none of the remaining f 's will figure here so that is equal to right hand side of that row which is equal to $-f_{1,2} - f_{2,1}$ so what is this equation? This equation is essentially representing the discrete form of Laplace equation for the grid point 2, 2. And what we have done is essentially is left the unknown values on the left hand side of this matrix equation, and send the known values of the function to the right hand side which are coming from the boundary point that is 1, 2 and 2, 1.

So actually can; get the functional value here on the right hand sides which are actually known to you from boundary conditions. Rest of the values are not known to you and they figure on the left hand side part of the matrix equation and the weightages are figuring in this matrix which we often called as the coefficient matrix. So since we have 9 times 9 inner points consider here we have a 9 by 9 matrix 9 rows and 9 columns here that is being multiplied by this column vector which contains the unknown the values of f corresponding to each grid point.

And then what you have on the right hand side are the known values which are coming from the boundary points. This is somewhat similar to what we saw when we were discussing about compact schemes earlier. However here we have a little more complicated structure of the coefficient matrix. In the sense, that here if you notice carefully the leading diagonal of this matrix has an entry of -4 all through.

And then there are 2 adjoining diagonals on the upper triangle and lower triangle and then another 2 at some distance and these 5 diagonals are non-zero entries. That is what gives you a pentadiagonal system of equations here. And it is not east to solve such a matrix equation very easily. So if you were to go for some direct methods like Cramer's rule for Gauss elimination. It could be quiet expensive and therefore that may not be an attractive proposal at all

Iterative methods of course we have discussed the point Jacobi method as well as the Gauss Seidel methods and they seems to be efficient. But we need to know strategies in order to make them more efficient and accelerate the convergence. So some of these strategies to accelerate convergence and minimize the computational cost would be discussed further. But iterative methods seems to work well if we at all want to solve this matrix equation through a more efficient manner then there are ways in which we can do it.

But then we cannot handle the pentadiagonal problem very efficiently so can we represent this problem as an equivalent problem involving tri-diagonal system of equations. Because we have discussed earlier, that there is a tri-diagonal matrix algorithm which is efficient. And therefore the computing cost could be much lower and therefore that could be an attractive strategy to solve the problem by solving a system of linear algebraic equations.


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-4	1	0	1	0	0	0	0	0	0	$f_{2,2}$	$-f_{1,2} - f_{2,1} + S_{2,2}$
1	-4	1	0	1	0	0	0	0	0	$f_{3,2}$	$-f_{3,1} + S_{3,2}$
0	1	-4	0	0	1	0	0	0	0	$f_{4,2}$	$-f_{3,2} - f_{4,1} + f_{4,2}$
1	0	0	-4	1	0	1	0	0	0	$f_{2,3}$	$-f_{1,3} + S_{2,3}$
0	1	0	1	-4	1	0	1	0	0	$f_{3,3}$	$0 + S_{3,3}$
0	0	1	0	1	-4	0	0	1	0	$f_{4,3}$	$-f_{3,3} + S_{4,3}$
0	0	0	1	0	0	-4	1	0	0	$f_{2,4}$	$-f_{1,4} - f_{2,5} + S_{2,4}$
0	0	0	0	1	0	1	-4	1	0	$f_{3,4}$	$-f_{3,5} + S_{3,4}$
0	0	0	0	0	1	0	1	-4	-4	$f_{4,4}$	$-f_{3,4} - f_{4,5} + S_{4,4}$

Poisson equation formulation

$\nabla^2 f = S(x,y)$

compute at each grid point



If you were to write down the same matrix equation but this time you were looking at Poisson equation instead of Laplace equation. We had written down Poisson form in this way with a source term on right hand side right. So what you see is that in addition to the boundary values that we had obtained for the function we would additionally have a source term here. And the source term which is a function of x and y would then have to be computed at each grid point and added on to the right hand side.

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Jacobi iteration method

$$f_{i,j}^{k+1} = \frac{1}{4} [f_{i+1,j}^k + f_{i-1,j}^k + f_{i,j+1}^k + f_{i,j-1}^k]$$

Point Jacobi method. $\Delta x = \Delta y = \Delta$

Point Gauss Seidel iteration method


$$f_{i,j}^{k+1} = \frac{1}{4} [f_{i+1,j}^k + f_{i-1,j}^{k+1} + f_{i,j+1}^k + f_{i,j-1}^{k+1}]$$

accelerating convergence.

- Current values of f are used to compute the values at the neighboring points as soon as they are available. The formula works whether the domain is being swept row by row from bottom to top or column by column from left to right.
- This increases the convergence rate significantly over the Jacobi method.
- The method is convergent if largest elements are located in the main diagonal of the coefficient matrix

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|$$

And at least for one row

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|$$


Recalling some of the iterative methods that we have already discussed we have talked about the Jacobi iteration method. We have mostly used this technique in the numerical problem that we solved where we update the value of the function at a grid point ij. The updated value of iteration

is indicated by $k+1$ and that is done by taking values from the k th level iterations from the neighboring points.

So that was the Jacobi iteration method more precisely the point Jacobi method again we emphasize that $\Delta x = \Delta y = \Delta z$ this is inherently assumed, because that makes the formula much easier to represent. We also discussed about the point Gauss Seidel iteration method where we try to accelerate the convergence by making use of the latest available values of the function.

So by the time we reach the grid point ij we should have swept passed these grid points $i-1, j$ or $i, j-1$. And therefore we would be having the updated values already available at those grid points. And then using them on the right hand side of equation would actually accelerate the convergence significantly. So this is one of the strategies which can be used for accelerating convergence.

And this convergence rate increase could be quite significant over the Jacobi method or the point Jacobi method. Now as we apply these schemes we have to of course ensure something that the convergence is actually achieved. That means you are going to move towards a certain value of the function at each and every inner grid points asymptotically and you are not going to keep on oscillating perpetually or not ultimately reaching a steady state solution at all.

So what assures convergence this is a very important issue which is essentially ensured by the nature of the coefficient matrix that we had looked at a few minutes back. So when you look at coefficient matrix entries you have to notice something that is. If the largest elements in a given row are located sorry so the first point is if the largest elements are located in the main diagonal of the coefficient matrix.

And additionally at least for 1 row you are ensuring that the main diagonal coefficient value is greater than the sum of all the magnitudes of the remaining elements in the same row. Then convergence will be achieved so first if we look back at the first row of the coefficient matrix that will probably give us a better idea. So we will try to look back at the coefficient matrix once more just to make sure that we are able to get the numbers properly.

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$$\begin{bmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -4 \end{bmatrix} \begin{bmatrix} f_{2,2} \\ f_{3,2} \\ f_{4,2} \\ f_{2,3} \\ f_{3,3} \\ f_{4,3} \\ f_{2,4} \\ f_{3,4} \\ f_{4,4} \end{bmatrix} = \begin{bmatrix} -f_{1,2} - f_{2,1} \\ -f_{3,1} \\ -f_{3,2} - f_{4,1} \\ -f_{1,3} \\ 0 \\ -f_{5,3} \\ -f_{1,4} - f_{2,5} \\ -f_{3,5} \\ -f_{3,4} - f_{4,5} \end{bmatrix}$$

(1,5) (2,5) (3,5) (4,5) (5,5)
 (1,4) (2,4) (3,4) (4,4) (5,4)
 (1,3) (2,3) (3,3) (4,3) (5,3)
 (1,2) (2,2) (3,2) (4,2) (5,2)
 (1,1) (2,1) (3,1) (4,1) (5,1)

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So we remember that the first row elements where in the diagonal we had a -4 and then the remaining non-zero entries where 1 over here and another over here. So if you look at the remaining location the remaining rows at all the rows the main diagonal element remains as -4. And in every other row if you notice if you go to the second row you have a 1 here and most are the rows have that the only exception is this row where you have some additional one's.

Where there could be more over here for example so you have 3 one's over here and a -4 here. So it varies between 2 one's in the first and that also is seen in the last row apart from the main diagonal entry. And then in the second row for example you have 3 one's in this row you have 4 one's. So they vary a little bit from row to row now the point is we are just trying to figure out that whether we are able to satisfy the convergence criteria, which is stated over here.

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Jacobi iteration method

$$f_{i,j}^{k+1} = \frac{1}{4} [f_{i+1,j}^k + f_{i-1,j}^k + f_{i,j+1}^k + f_{i,j-1}^k]$$

$$\Delta x = \Delta y = \Delta$$

Point Gauss Seidel iteration method

$$f_{i,j}^{k+1} = \frac{1}{4} [f_{i+1,j}^k + f_{i-1,j}^{k+1} + f_{i,j+1}^k + f_{i,j-1}^{k+1}]$$

- ❑ Current values of f are used to compute the values at the neighboring points as soon as they are available. The formula works whether the domain is being swept row by row from bottom to top or column by column from left to right.
- ❑ This increases the convergence rate significantly over the Jacobi method.
- ❑ The method is convergent if largest elements are located in the main diagonal of the coefficient matrix

$$|a_{ii}| \geq \sum_{j=1}^N |a_{ij}|$$

And at least for one row

$$|a_{ii}| > \sum_{j=1}^N |a_{ij}|$$

$$|-4| \geq |1| + |1|$$
$$4 = 4$$

So if you look this what it tries to say is that the main diagonal element the modulus of that is it greater than equal to the sum of the other entries in the same row that is what it tries to say. So in the first row for example you would actually do a calculation like this so what you have in the main diagonal is mode of -4 and that is actually happening to be greater than equal to the remaining.

So there were 2 one's so you are ensuring that 4 is greater than 2 here in this case and there was a middle row where there were 4 one's in the non-diagonal elements. So in that case it will exactly equal the diagonal element. And therefore in most of the rows you are able to ensure this greater than condition while in one of the middle rows you are able to get the equal to condition that means you are able to satisfy this condition.

And then what it says is that at least in one of the rows the diagonal element the mode of the diagonal element should exceed the sum of the non-diagonal element. Diagonal in the sense main diagonal and that is of course achieved say in the first row the last row, and many other intermediate rows where you have 3 one's and the -4 in the main diagonal. That means you have several such rows where you have even satisfied this condition.

So in general this method of convergence will work that means with the coefficient matrix that you have for this problem that will be suitable in converging the solution. So we have just cross

checked that whether the coefficient matrix entries will ensures convergence or not. We will discuss about more schemes to solve elliptic equations in later lectures thank you.