

Analysis and Modeling of Welding
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Lecture – 19
Numerical solutions to thermal field and fluid flow in welding - Part 2

Welcome to the part-2 of the lesson on numerical solutions to the thermal field and fluid flow in welding.

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Scope

- Control Volume Formulation (CVM) ✓
- Overview of the process is the aim
- Objective of numerical solution is to obtain thermal / velocity profiles at distinct locations across the weldment



We are choosing the control volume approach for the discussion on this numerical solutions, because it is the same method we have used to derive the governing equations. And the overview of the process that is the entire process of solving the numerical the equations discretizing and the algorithm that is used for solving the linearized equations, is the objective of this participant lesson. And we would go beyond what we have covered in the previous lesson and namely we will be able to take the additive term into account and also look at how the velocity field can be solved.

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Reference

- “Numerical heat transfer and fluid flow” – Suhas V. Patankar, Taylor & Francis, ISBN: 0891165223
- Indian edition of the book distributed by Ane Books, 4821, Parwana Bhawan, 1st Floor, 24 Ansari Road, Darya Ganj, Delhi 110002



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The reference remain is same as the first part of this lesson namely the book by Suhas V Patankar, book is title in Numerical heat transfer and fluid flow. And this book use is the terminology and the symbols for the various quantities is exactly the way, we are showing in this particular lesson and therefore, if you have this book handy then we can map on thus lecture with book. So, what you can understand further details that were not covered in this lesson for the book.

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Outline

- Governing equations
- Obtaining linear set of equations for 2D and 3D
- Solution schemes – line by line TDMA
- Discretization of Advection Term
- Interpolation schemes for advection term
- Programming issues for high computational cost
- Summary



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So, the outline as follows; we are going to start off by just quickly looking at the governing equations that we need to solve. This is a refresh your memory, from what we have discussed in the previous lesson. And then go beyond the only problem that we have discussed in the previous lesson; namely in this lesson, we will look at the 2D and the 3D geometries, and how the linearized set of equations would look like. And then when we want to apply the tri-diagonal matrix algorithm for 2D and 3D then what kind of an approach should be taken so that is what be going to discuss, and then how to discretize the advection term and whether or not the linear interpolation scheme.

That we have discussed would be valid here is going to be looked at and then in the end. We will wind up by making some comments on the high performance computing aspect of these simulations mainly, because when we go to three-dimensional problems then the computational time is quiet significant.

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Geometry aspects for welding

- Welding is usually in flat position and with the torch moving
- The direction of gravity, direction of motion of torch and the width of the weld pool are often mutually perpendicular
- Welding is necessarily a 3D transient problem

- Spot welding could perhaps be axisymmetric
- Continuous welding could be considered steady state in moving coordinate system
- Welding of similar materials could exploit use of mirror symmetry about the plane that contains depth of pool and direction of welding



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So, regarding the geometry aspects of welding I was structurally confused at this stage to say that the wave we are discussing the solution of these equations is not very different from any other discussion on the computational fluid dynamics course. For example, it is a same set of equations we are solving and the solution procedure is also the same.

However, there are some geometrical aspects that are peculiar for welding, because of which we want to discuss some of those things in this course and one thing I would like to say is most of the times the welding is done in a flat geometry. That is we have the vertically downward going the gravity direction, we have the torches velocity of the torch, which is normal to it; and the plate is actually extended in the direction that is normal to both of these.

In other words, most of the time the welding can be considered as a three-dimensional problem, and one may reduce this to two-dimensional only under very limited set of assumptions and usually it is three-dimensional problem. And in some limited situations such as in spot welding, where the torch is not moving, you may assume that the problem is asymmetric, so that you can solve perhaps just a 2D problem and get reasonable solutions, but then it is at least with three variables namely the x , y , r theta. For example, and the time because is a problem is transient nature.


In the case of continuous welding particularly of a dissimilar joining for example, this is necessarily four-dimensional namely it is all the three-dimension of the space and with time also the evolution of the thermal and velocity field is taking place. So, therefore, naturally a welding is a complex problem when comes to the numerical simulations.

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Generic form of the equations

$$\left[\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u \phi}{\partial x} + \frac{\partial \rho v \phi}{\partial y} + \frac{\partial \rho w \phi}{\partial z} \right] = \frac{\partial}{\partial x} \left(\Gamma_{\phi} \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma_{\phi} \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\Gamma_{\phi} \frac{\partial \phi}{\partial z} \right) + S_{\phi}$$

<i>Transient</i>	<i>Advection</i>	<i>Diffusive</i>	<i>Source term</i>
Thermal field	$\phi = C_p T$	$\Gamma_{\phi} = \frac{k}{C_p}$	$S_{\phi} = S_T$
The u component of velocity	$\phi = u$	$\Gamma_{\phi} = \mu$	$S_{\phi} = S_u$
The v component of velocity	$\phi = u \quad v$	$\Gamma_{\phi} = \mu$	$S_{\phi} = S_v$
The w component of velocity	$\phi = u \quad w$	$\Gamma_{\phi} = \mu$	$S_{\phi} = S_w$



So, the generic form of the equations is given here we have already seen these, but just quickly find out the meaning of these terms. Let me just choose the term here, so the first term is the transient term and the second term we looked at is the so called the advection term, the third set of terms is basically the diffusive term and the last one is basically the source term. So, with these four terms, then the equations are going to be similar for all the quantities are we want to solve for; however, we can see that when we go from the temperature field to the velocity components in the meaning of these terms can change slightly.

I have recognize this is small typo here this must be v on this must be w, otherwise rest are the things are same. So, what are these source terms is something that you could look up, we have discuss that in the previous lecture and this is same set of terms that go about to use now.

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Convention followed for subscripts

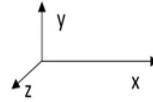
- East – West for $+x$ and $-x$



- North – South for $+y$ and $-y$



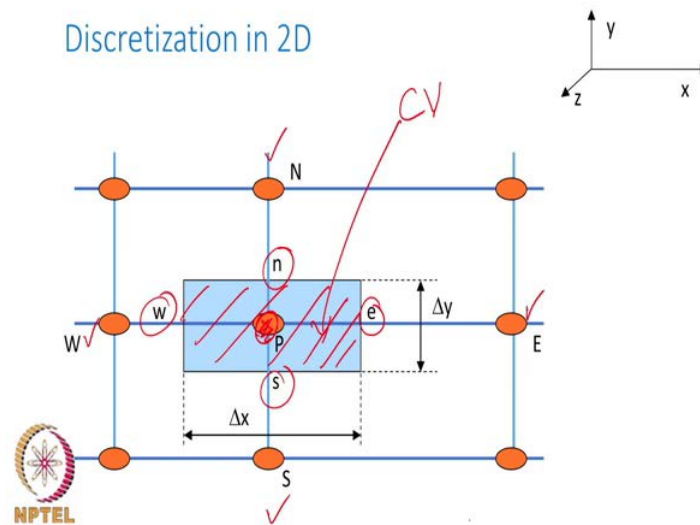
- Top – Bottom for $+z$ and $-z$



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This is convention that we must follow when we go from one dimension to three-dimensions and that is being shown here. We use the words east and west, when we are talking about the x direction. So, that when we talk about east which means we are in the plus x direction and when we say west we are in the minus x direction. Similarly for north south we have the y axis used for it and the words top and bottom are used for the z axis. So, the subscript like E, W, N, S, T and B are used represent basically the neighbors of any particular given location within the domain.

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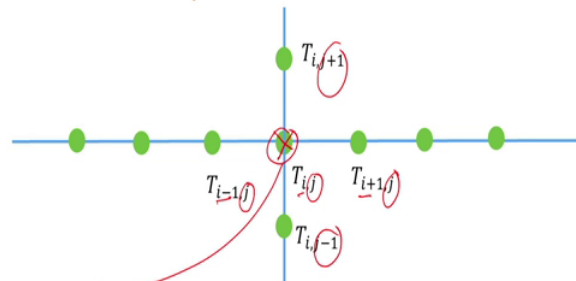


So, here is where we are showing you how the grids are laid out the rectangular reason. That you shown here which I am going to hatch, this region is basically the control volume we are talking about. So, the control volume phases are then label with small letters that is 'e' and 'w' and 'n' and 's'. So, these are the east, west, north and south phases of the control volume and then the locations where the parameters are specified with values are given with capital letters; that is these are a locations where there specified as a neighborhood locations and we are writing the discretize the equation at the location of the interest namely p.

So, p is the location of interest where we are writing the equation and if you choose to have the discretization such a way that the width of the control volume is different along x and y directions, then you would have delta x and delta y separately written and you could also have them different for different locations. That is as you move along x direction the width of the control volume can also be choose into change.

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Linear set of equations



$$a_{i,j}T_{i,j} = b_{i,j}T_{i+1,j} + c_{i,j}T_{i-1,j} + d_{i,j}T_{i,j-1} + e_{i,j}T_{i,j+1} + f_{i,j}$$

Equations are valid for locations from $i = 2$ to $i = N - 1$.



The values T_1 and T_N are given at the boundaries via the boundary conditions.

And we have seen in the previous lesson that when we discretized the equation, we saw that the one-dimensional problem has come with a linear set of equations. And in the case of two dimensions we are going to have the same set of linear set of equations, but with more terms. So, we can see them here that in one dimension you would have for example, only the - i index coming in. So, you would have only the - i coming in here, but in the case of two-dimensional, you also have the j index coming in here, and you could see that you have instead of two neighbors we are talking about basically four neighbors and when we are writing the equations for the variation of temperature at this location.

Then you would see that it is given in terms of the neighboring temperatures waited by factors which are basically in this equation given as $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, $e_{i,j}$ respectively for the four neighbors, and these are basically thermal conductivity taken with a ratio of the distances between the control volume phases. So, you could see that the linear set of equations are looking in a same pattern and these equations are then written for indexes of i and j going from 2 to n minus 1, where n is a total number of control volumes along each of the directions.

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Linear set of equations in 2D

$$a_p T_p = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b$$

Where

$$a_E = \frac{k_e \Delta y}{(\Delta x)_e} \quad a_W = \frac{k_w \Delta y}{(\Delta x)_w} \quad a_N = \frac{k_n \Delta x}{(\Delta y)_n} \quad a_S = \frac{k_s \Delta x}{(\Delta y)_s}$$

$$a_p^0 = \frac{\rho C_p \Delta x \Delta y}{\Delta t} \quad b = S_c \Delta x \Delta y + a_p^0 T_p^0$$



$$a_p = a_E + a_W + a_N + a_S + a_p^0 - S_p \Delta x \Delta y$$

S_p is -ve!

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And in the 2D we are writing the equations now with the same terminology as given in the Patankar's book. And you would see that the coefficient of having the same meaning as in the earlier slide. You see that the thermal conductivity is given here and then the distance between the control volume phases is given here, and you could see that so these are all basically giving you the weight factors by which the neighboring temperatures are going to be average doubt to get the temperature at any given location.

And you could also see that the four rules that we have set as to be valid for this particular approach that is also can be verified here. You could see that the equation written here is such that when the source term is not present, then the coefficient of the T_p is going to be some of coefficients of all the neighboring values. So, this is one of the four rules that we have discussed earlier, and also the fact that all the coefficient must be positive, and you can see that all the coefficients here these are all going to be positive. And we only need a question mark on this particular term. And we saw that S_p is always negative, because the source term linearization is generally to lead to temperature coefficient S_p as a negative.

So, you would also assure that the coefficient a_p will also be positive. So, like this we can verify that the discretization was done correctly and once these coefficients are

available then we have the linear set of equations ready two dimensions. In three-dimension it is a straight forward extension and they looked the same, where except for that the coefficients are going to have more terms that are coming in.

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Linear set of equations in 3D

$$a_p T_p = a_E T_E + a_W T_W + a_N T_N + a_S T_S + a_T T_T + a_B T_B + b$$

Where

$$a_E = \frac{k_e \Delta y \Delta z}{(\Delta x)_e} \quad a_N = \frac{k_n \Delta x \Delta z}{(\Delta y)_n} \quad a_B = \frac{k_b \Delta y \Delta x}{(\Delta z)_b}$$

$$a_W = \frac{k_w \Delta y \Delta z}{(\Delta x)_w} \quad a_S = \frac{k_s \Delta x \Delta z}{(\Delta y)_s} \quad a_T = \frac{k_t \Delta y \Delta x}{(\Delta z)_t}$$

$$a_p^0 = \frac{\rho C_p \Delta x \Delta y \Delta z}{\Delta t} \quad b = S_C \Delta x \Delta y \Delta z + a_p^0 T_p^0$$

$$a_p = a_E + a_W + a_N + a_S + a_T + a_B + a_p^0 - S_p \Delta x \Delta y \Delta z$$



Spin -ve!

So, you could see that you have more terms coming in, here there are two distances coming in otherwise it is a same coefficient as in 2D and here also you would see that the minus S p here and S p is negative, and therefore you would see the coefficients are all positive. And a p is then some of the coefficients of all the neighboring temperatures and that would also be valid when the source term is zero. So, you can see that its straight forward extension from one d to 2D and 3D may it comes to this kind of a an approach when you are using a regular grid structured grid in three dimensions in the control volume approach.

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Choice of solution method

- Direct solution involving matrix inversion – not practicable as the number of grids are often large. Eg., a 100x100 grid would need a matrix of size 10000x10000 to be inverted! This issue becomes more difficult for 3D simulations.
- Iterative solution – Tri-Diagonal Matrix Algorithm (TDMA) is preferred as the matrix of coefficients is sparse and memory efficient.



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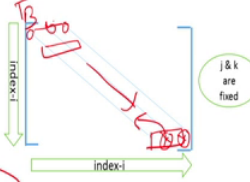
And one must then also now relook at the way of solving. We have mention that in 1D we could also perhaps think about inverting a matrix, which is going to be of size is square of the number of grids. So, if you have a 1D problem with 10 grids, then you basically have a matrix of size 100 by 100, but then out of these 10000 elements very few or non-zero, because you have got the matrix as tri-diagonal, which means that only three diagonal rows are having non-zero elements and rest of them may zero. So, therefore though one has the option of inverting the matrix for direct solution it is not a very efficient way of solving; however, in the case of 2D and 3D it becomes almost impossible to think of a direct solution.

The reason being as also follows, if you what to choose a two-dimensional problem of hundred grid points along each direction, then we talking about a matrix of coefficient coming to 10000 by 10000. So, that would be a very huge matrix which is very difficult to invert, and when we go to three-dimensions you would be multiplying by another hundred. So, you are going to talk about a million grid points and then you have a matrix that is million by million in size and definitely direct solution is then not possible by inversion of a matrix. So, any iterative solver is only recommended.

So, tri-diagonal matrix algorithm them is basically a iterative process and therefore we are going to basically recommend to use a TDMA algorithm and the advantages are their it is memory efficient as well as it is also a computationally much, much faster.


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Solution using TDMA



- Tri-Diagonal Matrix Algorithm
- Start from the left boundary to forward-substitute to get $T_i = P_i T_{i+1} + Q_i$
- Express P_i and Q_i in terms of the coefficients as $P_i = \frac{b_i}{a_i - c_i P_{i-1}}$ and $Q_i = \frac{d_i + c_i Q_{i-1}}{a_i - c_i P_{i-1}}$
- At the boundaries we know that $P_1 = \frac{b_1}{a_1}$, $Q_1 = \frac{d_1}{a_1}$ and $T_N = Q_N$
- Use these recurring relations to obtain P_i and Q_i for $i = 2, 3, \dots, N$
- Set $T_N = Q_N$ and back substitute for $i = N - 1, N - 2, \dots, 3, 2, 1$.

$j=2$ loop
 $k=2$ loop
 $\rightarrow N-1$



Here is the algorithm we have already seen it in the previous lesson, but I am just showing you here to this refresh you are memory and we can see that we can write the algorithm as follows; we can see that on the top you have got the elements here and normally the first element is known, because it is from the boundary condition and then you have the inner condition outer condition.

So, have basically between these three you can evolve an equation that will have only two unknowns and that is a kind of equation that you are trying to write here and you can then solve for the one of the temperature. And then write the equation for the next two and like that you can keep going it is the last row and in the last row you already have one solution from the boundary and therefore you can evaluate one of the temperatures and which will you back substitute and then come back to solve all the temperatures.

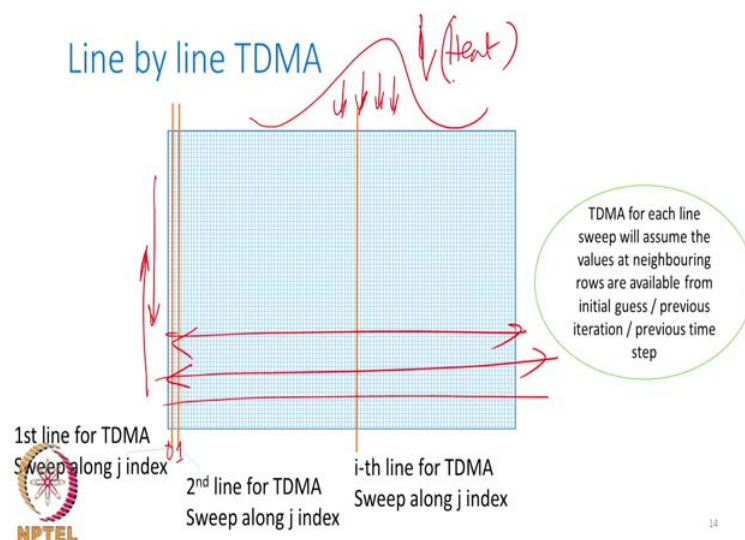
So, you basically have this idea of forward substituting. So, that you are equations are having only two unknowns and later on you are going a backward substitution. So, that

you can solve for the temperatures which will be coming out in the reverse direction, from n minus one to n minus two to up to two. And you can see that the way you are doing it is possible only when you have only one direction in which you are going to do the forward substitution and backward substitution.

Whereas, in the case of 2D problem and 3D problem, you do basically have two or three different directions in which unit to do this; so what is the modification of the algorithm that we are going to do? So, essentially what we are going to do is this following. So, we are going actually set the values of say j and k to be fixed let us take j is equal to two and k is equal to two and then you can then sweep i from 2 to n minus 1.

So, that way you can solve using TDMA when you have the values of temperatures in the second zero and second k row available then you can go ahead and do the TDMA iteration, and normally you always have the initial guess values available therefore one think go head and try this out without any problem. And with success iterations you are coming closer and closer to the solution. And therefore upon convergence you can say that the equation has been fully satisfied and this is actually illustrated by the following schematic.

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You can see that what we have done. Here is basically we are taking the line by line a TDMA, basically we are taking the first row and then solving the TDMA along the row and then we can then go to the next row and then solve it. So, like this row by row we can do is the solving and we can actually also change the directions. So, initially we can do forward substitution and backward substitution to get the values along these row and then later on you can get the next row and so on. Later if you like you can also change the direction of sweeping in this manner also, which direction should we choose first? That is governed by basically, what is the direction along reach the temperature is varying the fastest.

If you are going to sweep in the vertical direction you would do it, when let us say this is the domain when this is the heat that is coming in. So, if that is the heat that is coming in; then you know that temperatures are going from top to the bottom fastest, so if you going to iterate TDMA in the vertical direction first, then you are convergence is going to be slightly faster. So, this may line by line TDMA can be applied for 2D and it can be also extended to three dimensions.

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Solution method : Line by line TDMA

- Take initial conditions / previous iteration / previous time step values as initial guesses
- Fix values of the indices j & k and sweep the TDMA over the index i
- Change the direction of sweep over indices j and k successively
- Flip the direction of sweep over each index from forward to backward
- In 6 sweeps of TDMA, the first set of solution is available.
- Iterate such sets till convergence is achieved.



So, here we have just summarized the technique of solution of the linear set of equations. Initially we will have the initial conditions available or we will have the previous

iteration values available or previous time step values available. So, these are basically the initial guess values. So, once a initial guess values are available, when we will choose, pick values for j and k indices, and then sweep the TDMA algorithm over the index i, and then we will get the solution and then we can then shift the sweeping direction from i to j; that means, you can keep the values of index i and k constant in.

Then sweep along the index j, and then we can do it over the index k also and like that if you have totally six sweep of TDMA. Then you would have swept the solution process in all the three directions, in both forward and backward directions and therefore you would get basically a solution that is almost converged. So, you can actually check whether the converged is actually is achieved or not. Then choose to do one more set of six such sweeps of TDMA. So, line by line TDMA is the way to solve the linear set of equations to solve these equations in 2D and 3D.

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Convergence criterion

- Maximum residual compared to previous iteration within same time step to be less than a limit δ (say 10^{-3})

$$\max \left| \frac{T_i - T_i^*}{T_i} \right| \leq \delta$$

← previous iteration

- Limits can be different for different variables
 - Limits can be adapted as the solution emerges or welding progresses
- An upper limit for iterations to be set to avoid indefinite loops



So, how do you know that you are the solution is correct, in the sense it has converged the idea is has follows the star is basically to indicate this is to indicate the previous iteration. So, the idea is as follows, compare to the previous iteration in the current iteration how much is the relative change of the parameter. If that relative is less than a

particular amount of percentage, then you can say that the convergence has been achieved.

So, let us say if you took delta has ten to power of minus three we are talking about point one percent change. So, if the variable has come to change not more than 0.1 percent in iteration, you may chose not you iterate the any further. This basically you come to something like one Kelvin change in the temperature when the maximum temperature is about 1000 degree centigrade which means it is pretty good estimate because you experimentally the accuracy of the thermocouple or a perimeter is not better than 1 Kelvin when we come to temperatures above thousand Kelvin.

So, basically you can choose the cut off for the convergence criterion as you like something like minus three is generally practiced and you can choose. What is the maximum reschedule available in the entire domain, check whether it is within a particular threshold and if it is come then the number of iterations, you have done is the adequate we can stop iterating and move on to the next time step and that is how you can say that the convergence has been achieved.

These convergences should not be tested only against the convergence criterion mainly because sometimes it may happen that the choice of you are time step or the direction of sweeping etcetera may not be appropriate and therefore you may need much more number of iterations. So, instead of waiting for the convergence to come you may actually check whether the number of iterations you have done for the convergence is adequate. Let us say you can put an upper limit of 100 iterations. So, after 100 iterations if does not converge you would just stop and then come out after the loop and then check what has gone wrong so that we do not have the programs are going indefinitely in to the computing.

And sometimes these limits of convergence can also be adopted, what I mean by that is let us say if you take welding then doing the process of heating fluid flow is actually not happening, because there is no mold in pool yet. So, therefore, what you kind do is you can have a higher limits of convergence because only the temperature variable is going to be change later once the melt pool starts to form, you may have actually a very strict

convergence criterion. So, that the velocity profiles are accurate because they can change the thermal field significantly.

And once a weld pool is fully formed and the velocity profile is basically set, then again you can enhance the convergence criterion limit. So, that you are not very strict about the convergence mainly, because the velocities are not changing very much beyond some stage. So, like this you may adopt the convergence criteria as you go long, but at every such change you must also validate, whether what changes you are making is only for numerical speed up or is it also going to change the solution number significantly. And by validating these results against the experiments within the experimental errors, you can actually take a good decision to make the numeric reasonably faster.

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Measures to be taken to ensure convergence

- Start solution with the variable that changes fastest
- Start TDMA sweeps with the direction along which the variable changes most
In welding this would be the direction normal to the plane on which heat source is applied
- Consider lowering the time step
- Consider refining the control volumes if number of implicit iterations are too many for convergence
- Over-relaxation or under-relaxation

$$T_p = T_p^* + \alpha \left(\frac{\sum a_{nb} T_{nb} + b}{a_p} - T_p^* \right)$$



The relaxation parameter α to be chosen to ensure fastest convergence possible.

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And what are the measures that we can take to ensure convergence we have just discussed the few of those points, but I am summarizing all those points in slide. Here we can do basically by choosing to solve that variable which changes the fastest. So, among the variables that you are going to solve simultaneously, if you have temperature the three velocity vectors. Let us say even the composition variable then you can choose to start solution of that variable which changes the fastest.

Usually, little be the temperature which will this is mean rest of the flows therefore temperature can be used to solve the first at variable. Then whiles doing the TDMA sweep you can actually do the sweeping such a direction that that is the direction in which the variation is the fastest. In the case of temperature for example, in the direction normal to the plane on which the heat source is applied is the direction where the heat is actually flowing, that is a direction in which temperature is change in the fats test.

Therefore if you use the TDMA sweep in that direction first then you would come to a converged solution of the temperature fastest, so that is one more thing you can do. Sometimes you are convergence is not happening quick enough and lot of time is being wasted in the iterations then you may a want to considered lower in the time step. For example, if you take the time step to be half of what you have used you basically rend up in twice the computational time, because you would have two times the number of time steps that is required.

But then if it cuts down the iterations by more than 50 percent then surely you have save the time of computation. So, one can take a call on the time step variations also, and then control volume number of control volumes also can be refined. For example, if the grids are not fine enough in the region, where the variation of the parameters is happening very quickly then also would result in convergence being slow.

So, you may want to go back and see whether adequate number of grid point are available or adequate number of control volumes are available, in the location where the variation of the parameter is fast; namely for example, in the fusion zone and heat effected zone. For example, then go back to solve with refined set of grid points and you would see there the convergence would be again speed and up. There is another measure that one can do this is last measure and not recommend generally, but can be used numerically without causing any arch defect that is basically what is call the relaxation parameter.

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Measures to be taken to ensure convergence

- Start solution with the variable that changes fastest
- Start TDMA sweeps with the direction along which the variable changes most
In welding this would be the direction normal to the plane on which heat source is applied
- Consider lowering the time step
- Consider refining the control volumes if number of implicit iterations are too many for convergence
- Over-relaxation or under-relaxation

$$T_p = T_p^* + \alpha \left(\frac{\sum a_{nb} T_{nb} + b}{a_p} - T_p^* \right)$$

Handwritten annotations: A red circle around the term α with an arrow pointing to the value 0.7. A red arrow points from the term α to the term T_p in the denominator of the fraction. A red arrow points from the entire fraction term to the word "zero!" written in red.



The relaxation parameter α to be chosen to ensure fastest convergence possible.

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So, the relaxation parameter is basically this quantity, what it means is basically you have already seen that T_p is suppose to be equal to this quantity this is actually suppose to be T_p^* , but what we are doing is that we are looking at the difference between calculated T_p and the previous iteration T_p .

Then the difference is being added to the previous iteration with a scaling factor alpha, and this scaling factor alpha is it more than one or less than 1 would be calling by the name as over relaxation or under relaxation. So, let us seek under relaxation you have got 0.7 as we parameter alpha which means basically, if the temperature that particular location is suppose to change by 100 degrees then I will not change it more than 70 degrees at a time.

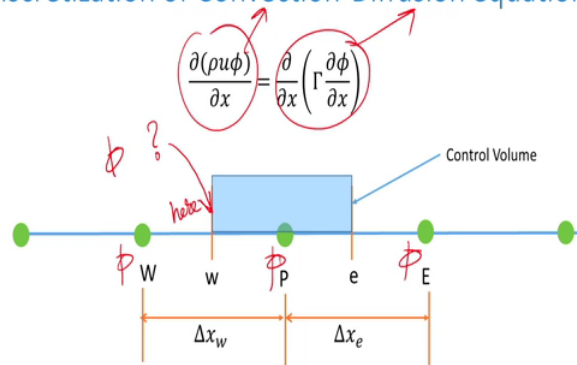
So, that over successive iterations in them, I am not changing it as much as a numerical solution is asking me to do. That, what I can slow down the changes and hope that the convergence is faster; what is the result of a relaxation parameter does it actually change the solution, actually not the reason being that when the convergence is completely achieved then this entire difference is 0, because T_p is suppose to equal to that. So, therefore upon convergence the factor after alpha is going to be 0. Therefore, there is no

change in the value of any temperature at any given location therefore under relaxation or over relaxation will not change the solution.

However, it will change the rate at which you approach the convergent solution in an accelerator manor or in a monotonous manor and whether it is going to be quicker or slower, and one may have to play with this parameter for a given problem to identify what is a best choice of this relaxation parameter alpha. These are all the various measures that one can do. So, that the convergence can be achieved fast in iterative solver such as line by line TDMA with alternative direction.

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Discretization of Convection-Diffusion equation



Now let us spent some time on the idea of convective diffusion equation and the how we can take care of the convective term, to discuss on the interpolation. Because this basically is the crux of the solution of the Navier-Stokes equation upon reduction to one dimension, it basically comes as convection diffusion equation. So, this is the convective term and this is the diffusion term. So, this equation if you want to discretize there is one particular aspect that we are going to do essentially the problem is as follows. So, pi is available at locations what you have specified.

We are asking question here, let us say I want to know what is the value of ϕ here, and normally in the previous discussion where we have looked at only the steady state or unsteady state heat conduction without the convection we were taking into account linear interpolation. However, when you have convection linear interpolation will not be valid that is what we are going to see in the movement.

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$$(\rho u \phi)_e - (\rho u \phi)_w = \left(\Gamma \frac{\partial \phi}{\partial x} \right)_e - \left(\Gamma \frac{\partial \phi}{\partial x} \right)_w$$

While ρ and ϕ are known at the centre of control volume, u is known at the faces of the control volume

How do we interpolate the value of ϕ at the interface in the presence of advection?

$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$

In the above equation, how do we estimate the values of the coefficients and the values of ϕ at the interface?



For compact notation, let us define: $F \equiv \rho u$ $D \equiv \frac{\Gamma}{\Delta x}$

The previous equations we are basically apply in the control volume approach to integrate over the control volumes. Therefore, you basically come up with this equation. So, this equation you come up, which basically tells you that up after integration you have the terms which are going to be evaluated at the phase centers of the control volume.

Then we can then look at how the values are going to be used. You see that naturally you have a need to evaluate the ϕ at the phase center, and you knew that ϕ is actually available only at the center of the control volumes. So, you have a requirement of interpolate in the value of ϕ at the location in between the locations, where it is been provided. Once you then gather the terms you again come to the same kind of a linear set of equation like this. But then you need to see how to interpolate and that discussion is then carried forward by using just two flat forms of these terms F and D , so that we can reduce the algebra.

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Interpolation of the advection term – 1/4

- Linear → leads to divergence if point-by-point solution is attempted when Scarborough criterion is not valid, typically for high Reynolds numbers.

$$a_E = D_e - \frac{F_e}{2} \quad a_W = D_w - \frac{F_w}{2} \quad a_P = a_E + a_W + (F_e - F_w)$$

This scheme leads to erroneous results when F_e or F_w are much larger than D_e or D_w .



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The first attempt to do is basically to take the simplest of the methods basically which is to say that we will use a linear interpolation. Now if you use a linear interpolation what happens is that you would encounter erroneous results, whenever there is some convection. In other words as the velocity is going a either plus direction or minus direction the value that you find which is average is either over estimated or under estimated.

You also see that there are four basic rules that are to be valid for the numerical solution will also be invalidated, because you would not have the all the coefficients to be positive for the linear set of equations. This can be then analyze and you can see that it is happening only when the Reynolds numbers is large, if you what to use for example, Gauss Seidel iteration method not the TDMA method, but Gauss Seidel method then there is a stability criterion for by the name Scarborough criterion. This also will be in valid.

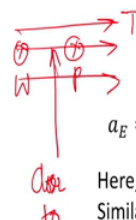
Essentially we can say that a linear interpolation method is going to be giving you erroneous results for high Reynolds numbers problems and also not going to be suitable for Gauss Seidel iteration and it will also invalidate some of the basic rules of this particular control around I am approach we are we have the coefficient to be all positive

etcetera. So, therefore linear method is going to be not recommended for interpolation in this solution of this equation.

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Interpolation of the advection term – 2/4

- Upwind scheme – convective term is calculated assuming the value of ϕ at the interface is equal to the value of ϕ at the grid point on the upwind side of the face.




$\phi_e = \phi_P$ if $F_e > 0$ $\phi_e = \phi_E$ if $F_e < 0$

$a_E = D_e + \llbracket -F_e, 0 \rrbracket$ $a_W = D_w + \llbracket F_w, 0 \rrbracket$ $a_P = a_E + a_W + (F_e - F_w)$

Here, the operator $\llbracket \]$ is to result the maximum of the arguments passed. Similar to the function `amax1` in Fortran.

This scheme remedies the issued faced by linear interpolation scheme.



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So, one method by which we can remedy some of these artifact that we come, because of linear interpolation is by using what is called then upwind scheme. The upwind scheme can be understood as follows essentially it is like this; let us take the flow to be in one particular direction. Let us take that, the variable that we are talking about is temperature and we look at two locations the location p and the location w.

The idea is as follows, if the velocity of the liquid is quite high when the temperature felt a particular location in between is closer to temperature at w, because this liquid its actually carrying the enthalpy from w all the way up to p and as it comes closer and closer to p then it would take away temperature that is changed by p, but then for most of the distance between w and p the temperature is going to be close to what has at w, which means that you could actually approximate that the value of temperature it any location between w and p to be that of w itself.

Such approximation is called upwind scheme, and this approximation can then be given mathematically by using this operator which basically is to say that what is the maximum

of these two values. So, whether are we taking the velocity effected with temperature from the left side or right side is depending upon the sign convection of the velocity. So, that is the reason why we have got these two expressions.

So, should be take the value from the east phase or west phase, but depends upon the direction of the flow, and upwind direction is what is being chosen as the values. So, which means that we are not at all averaging we are only taking the value from the previous neighbor. We are looking at the direction of the flow and peaking up the correct neighbor, for which we are going to take. This scheme has been successfully shown to remove the artifact that we are caused by the linear interpolation scheme. Therefore, this can be used if one wished to.

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Interpolation of the advection term – 3/4

- Exact solution / exponential – given that at $x = 0, \phi = \phi_0$ and at $x = L, \phi = \phi_L$, the exact solution would be

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp\left(\frac{Px}{L}\right) - 1}{\exp(P) - 1}$$

Here, P is Peclet number defined by $P \equiv \frac{\rho u L}{\Gamma}$

- Since exp function is involved, computation is expensive as this interpolation is needed for each control volume and at each iteration.



The third way is to actually solve analytically, what would be the value of temperature, when there is a flow that is induce. So, what kind of a problem has been solved to arrive at this solution? That problem is basically as follows if you have two walls and you have got temperatures T 1 and T 2. Then you have got flow in one direction then what would be the temperature at any location intermediate. So, this location this temperature at any intermediate location can be obtained as a deviation from the averaging between T 1 and T 2. That can be given as experimental function, and that has been solved name

analytically. This can be done by straightforward. And once this is available then you can use this relationship to find out what is the temperature here.

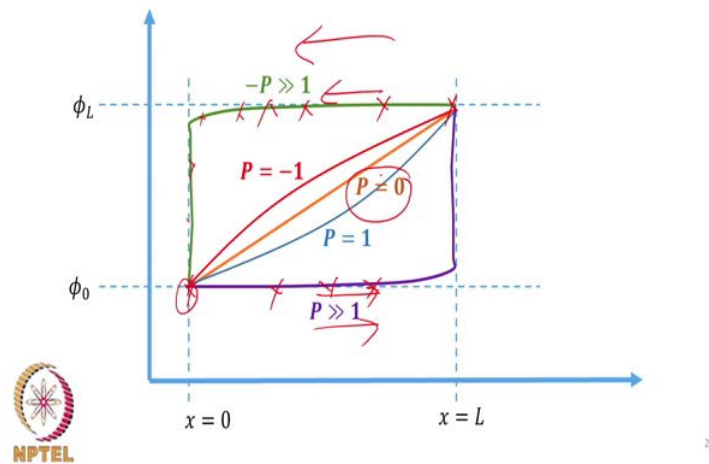
So, this can be then x . So, we can see that the analytical solution exact solution is actually exponential. Therefore you can see that naturally you should not be having a linear interpolation being meaningful at all, and exponential can be always approximated as a in upwind scheme in this following manner, if the temperature variation is like this, then the exponential variation is like this, then you can see that this value can be approximated as this value.

You could see that in the asymptotic path of the exponential you can always take the value to with end of the asymptotic, which means that t at this location x in the taken as T_1 itself and that is exactly the upwind scheme. So, in other words, you can say that the exact solution are exponential interpolation is basically a more general, and more correct form a compare to the upwind scheme. This can also be used. The only problem of using this in the interpolation scheme is because exponential function is an expensive computation. So, the computerize going to spend several cycles to compute the exponential value, if you are processor is not intelligent enough.

Therefore you would actually be wasting computational time calculating the exponential function again and again. This has to be done actually at every grid point, for every iteration of every time step, which means that it is going to be the function that is going to be used maximum in the entire computation. Therefore, one should avoid it if one can and there is reason why we have a hybrid interpolation that would be coming in the last part.

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Exact solution dependence on Peclet number



So, how are these various exponential solutions going to look like you can see that the variation from x to L is given by these various curves you can see that on the Peclet number is positive or negative, are you just show you the direction of the flow you can see that at the value is to be taken this is basically when the flow is this way. So, you can see that this value is valid for most of the distance and only when you come closer to the other point you start having the value of the location of the left hand side which means that when the Peclet number is large and negative then for the most of the time, you can actually take the right hand side value.

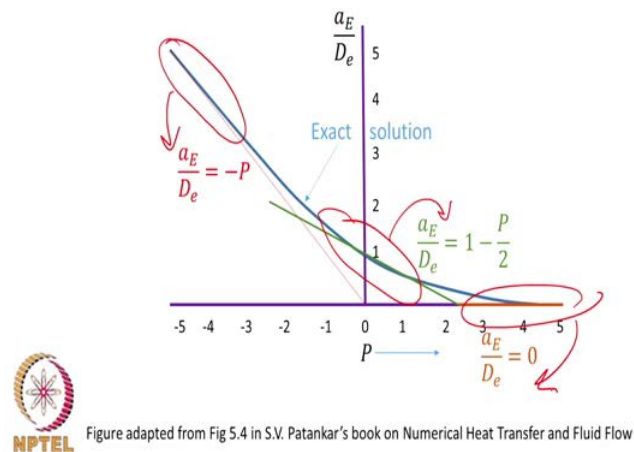
If the Peclet number is large and positive for most of the distance you can take the value from the left hand side. So, whether we take the left hand side or right hand side depends upon the direction of the flow which means that upwind scheme actually sort of prove in as a good approximation by this exact solution. What is the case under which linear solution linear approximation is valid, this is a special case only when the Peclet number is 0, which means that when the velocity is zero that is pure conduction.

So, only in a conduction problem you can take linear interpolation of the temperature values in between locations, otherwise you should not take linear interpolation you

should use one of these methods, where exponential illusion can be used or upwind can be used.

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Variation of coefficient a_E with scheme



Now, upwind scheme as we said has a problem of exponential promotion, which is expensive in a competition scenario. Therefore, we can choose a hybrid solution and hybrid solution can be there approximated in the following manner.

The exact solution is given by this curve, which is basically showing in the exponential variation. You can see that you can approximate the exponential part in some portion using a minus p value and in intermediate portion using this function and a later portion using this function. So, you can actually approximate the exponential function in three regimes by using a three parts of the function and this can be then used to save the computation that is to be done is using exponential function. So, this can be use as a hybrid scheme and that is what is given here.

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Interpolation of the advection term – 4/4

- Hybrid scheme – high-lateral-flux modification

$$\frac{a_E}{D_e} = \frac{P}{\exp(P) - 1}$$
$$a_E = \left[-F_e, D_e - \frac{F_e}{2}, 0 \right]$$
$$a_W = \left[F_w, D_w + \frac{F_w}{2}, 0 \right]$$
$$a_P = a_E + a_W + (F_e - F_w)$$



For $|P| < 10$, one can approximate the exponential function with a fifth power and save computation. The scheme will then be called as Power law scheme.

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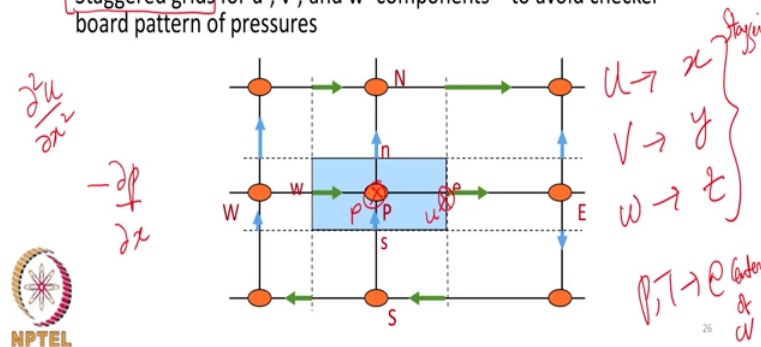
The hybrid scheme is basically choosing the three forms, you can see here. The three portions of the exponential function, which then can avoid having to calculate exponential at all and just by a simple algebraic manipulation of the two quantities d and f you can actually valid what are the coefficient.

Then once a coefficients are available the linear form of the equation is quit straight forward, which can then be used for the further processing for the calculation of the linear set of equations. So, this way you can actually see that the hybrid scheme is going to save computation time very close to being accurate and also avoids the artifacts that will come from the linear interpolation scheme. It is actually also found that when the Peclet number is less than 10, it actually saves a lot of effort in the computation.

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Location of variables

- Temperature and Pressure at the centre of the control volumes
- Velocities at the face-centres of the control volume
- Staggered grids for u-, v-, and w- components – to avoid checkerboard pattern of pressures



And where should be locate the variables this is again another discussion. The idea is as follows, if you have a checkerboard pattern of pressures then, because pressure term is coming in the naves of equations as just only single differential. You can see that you normally have this term, where as in the case of velocity is you have a double differential right. So, basically what a template is that you are going to have a center differencing where it comes to the velocities and you would have forward differencing when it comes to the pressures.

Therefore, you may have a situation where a checker board pattern of pressures may lead to low flow. That is absolutely not correct, because whenever the pressure is changing in the flow must be happening.

This kind of an artifact can be avoided by choosing to have the variables u and p located differently, that is the pressure can be located at the center of the control volume and you can be located at the faces. So, you can see that the pressure is located here. So, this is where the pressure is and u is located here. So, when you do these then upon interpolation etcetera then you would not have a situation of a checker board pattern being stabilized and one can look at more details of such artifacts coming from the book by pattern.

But at this movement, I would say that there is a case to use what is called a staggered grid, and staggered grid is in such a way that u is staggered along the x direction, v is staggered along the y direction and w is staggered along the z direction. This staggered and p and t are at the center of the $c.v.$ So, we can see that by locating in this manner you can avoid artifacts. That has been done in these schemes to ensure that the solution that you get is very accurate.

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Complexity of solution process

- Equations for T , u , v and w are interlinked.
- No explicit equation for p
- Solution should satisfy all equations simultaneously

Semi-Implicit Method for Pressure Linked Equations : SIMPLE Algorithm
proposed by Suhas V. Patankar



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And this also brings into one complexity that has been address by an algorithm that has been proposed by Patankar the complexity as follows you have the equations, which are written for temperature the u velocity, the v velocity and the w velocity. So, have basically a number of variables for which you have to solve. You also need to solve for pressure, but then there is no explicit equation available for pressure.

Therefore, when we have a difficulty in choosing, what is the order of solution that we can have and what kind of a guesses we can do for the pressures. How we can correct the effects of pressure on the velocities etcetera. So, this complex problem has been solved by an algorithm that is called as simple algorithm. Simple not has in the exact meaning, but it is acronym meaning for semi implicit method for pressure linked equations it has

been developed by Patankar. This has been very successfully used in fluid flow problems, where we are able to get solutions in a very reliable manner in an iterative manner.

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SIMPLE Algorithm

1. Guess the pressure field, usually zero for p^*
2. Solve the momentum equations to obtain guess values of velocities: u^*, v^*, w^*
3. Solve the continuity equation to obtain p'
4. Correct pressure field $p = p^* + p'$
5. Calculate the velocity corrections u', v', w'
6. Correct velocity field $u = u^* + u', v = v^* + v', w = w^* + w'$
7. Treat the corrected pressure p as a new guess p^* and go to step #2

Loop
till
Convergence



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And the algorithm itself is outlined here the idea is as follows initially we have to guess what is the pressure field because we do not have an explicit equation for pressures. So, we basically guess it has zero everywhere. Then we have the solution of momentum equations that we can use.

Once the momentum equations are available, then we can obtain what would be the changes in the pressure, because of these initial guess values of the momentums with other words it is basically the u^*, v^*, w^* ; once you have, then you can obtain what would be the change in the pressure. Then once you change the pressure, then you can also change how much is the correct required for the velocities. Then when you add those corrections to the initial guesses for the velocity, then you get the correct velocity and then you can iterate this again and again.

So, in other words you use this scheme this scheme of this as a loop till convergence. So, this loop of steps there has to be followed basically four steps guess the pressure, then get the first guess of the velocities, then correct the pressure, then, the correct velocities.

So, these steps can be then done again and again in an iterative manner. So, that all the four quantities namely the u , v , w and pressure are solved simultaneously and the convergence will then be obtained and we can check for that also. So, this algorithm them has been used successfully to calculate the flow field in various geometries and definitely in the fusion zone for weldments. It has been also used. And I can tell you that it has given accurate results and you could also then applied for any other welding scenario.

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Welding specific issues

- During welding : fusion zone forms \rightarrow flow in the liquid zone takes place \rightarrow fusion zone solidifies
- Time steps to be adapted to handle the phase change properly
- Initial stages of flow in the fusion zone critical
- Multiple driving forces for flow make the problem complex – strength of individual terms to be determined carefully
- Grid independence and time step independence on the final result are important
- Benchmark and validate results



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What are the welding specific issues that we discuss on the liquid flow the ideas as follows, during welding the fusion zone is not always present during the heating it actually forms and during the cooling it actually disappears. So, in other words the domain the region of the domain in which liquid flow is going to take place is going to actually appear and disappear during the solution, and this is not the same as any other CFD kind of an approach, where the liquid domain is always present.

Therefore one must take care of the take steps to ensure that the phase change has not been missed; that means, a control volume should not escape melting, and flowing the melt because of a wrong choice of the time step. So, ensure that time steps are very fine. So, that the liquid formation has been captured. So, that the liquid flow also has been

calculated properly and its effect on the temperature variation also has been done properly. So, initial stages of the flow development must be done very carefully, because they are going to effect the temperature variation.

There another complexity unlike in many of the CFD problems in welding, you have multiple driving forces acting simultaneously. So, you have basically complex fluid flow happening you have marangoni flow; you have the buoyancy flow solutal and thermal marangoni as well as solutal marangoni. You also have electromagnetic forces induced convection also taking place and I do that you also have the heat source having a pulse nature. So, you basically have fairly complex fluid flow happening in the weld pool and what is verse, you cannot actually visualize it directly during the welding process.

Because most of the time, the welding is at such a high temperature that the liquid pool is incandescent it is sending out so much light that it is very difficult to visualize it with camera techniques. Basically, you have a complex problem with very little validation. So, have it ensure that the solution procedure is as accurate as you would have it. And whenever we do the solutions, also ensure that the solutions are not depending upon the choice of the grids.

In other words, if you make the grids finer then the solution does not change and also with the time steps if you make the time step smaller then the solution does not change. So, these two does have to be done on the solution before we can call them as accurate and solved. We must always bench mark the results of these solutions with works done by others and we also should validate them with the experiments that we can do for thus problems that we are doing it ourselves.

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Programming

100 x 100 x 100

- Use arrays to store $\phi_i, a_p, a_w, a_e, a_t, a_b, a_n, a_s$ and b .
- If unsteady state is being solved for, store also a_p^0, T_i^0
- Determine initial (or guess) values of temperatures and property values
- Use subroutines or functions to evaluate boundary conditions and the TDMA solution
- One run of solver per variable for each time step
- Repeat the steps above for each time step & update time
- Write output every M time steps to visualize the temperature output
- Stop execution after all time steps are completed



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In the case of programming, there only few steps as an extension to 1D, we have basically multiple arrays has to be stored because it is a three-dimensional problem, we are looking at here. So, we will have as many arrays as a number of variables and also as many arrays as the number of coefficients for the neighbors.

In other words, we have for the three velocities, pressure and temperature and pressure correction, we have got about six variables out there, and then for the 5 neighbors, we have got 4 neighbors and one at the center for 2D, and 6 neighbors and one at the center, we have got 7 arrays for the coefficients. And if you are going to take a trans in problem, you will also have to store the arrays for the previous time step as well as previous iteration.

You basically have fairly large amount of memory foot print for these calculations, you have large number of arrays that will be stored. And each array will be n by m by x where these three n m and x are the dimensions in the three dimensions. So, which means that if the arrays going to be if you have for example, a three-dimension array which has grids of let us say 100, by 100, by 100 grid points then each of these array is going to have a million data point array have to be stored. You can see that very quickly

you would exhaust the memory of most of the current day work stations and one must also take care to save space as much as possible.

We must also write the various pieces of code of solutions separately. So, that we can manage the program better and we must have the solutions there are one run of solver per variable, which means that we will have if you are going to solve for temperatures and pressures and the velocity. You can see that first you solve the temperature and then you solve the simple algorithm; that means, the sequence of pressure correction, then the u star and then the pressure changes and then the u corrections.

In this loop you can do it and then after that you come to the composition solutions. So, you have a particular sequence of solving the equations and then you follow the sequence again and again to iterate. So, that all the equations are simultaneously solved for in a numerical manner.

This has to be done for every time step and each time step has to be done and updated with the time. So, that we can see how many time steps you have done, whether the time is up to say that the stimulation is completed. At any number of m number of steps you can say that I will put my output and then you can then use that output to visualize the temperature velocity fluid etcetera. So, this is overall scheme by which you do the programming to simulate the weld pool temperature and velocity profile evolution.

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Practices

- Use of FORTRAN, C or C++ is typical for these programmes. Higher level languages such as Python, Matlab® etc., may not be suitable due to high computational cost.
- Initial values including grid spaces are usually read from a file
- Output files are first written out as asci or binary files and then used for post-processing using a graph plotting software such as Tecplot®, Matlab®, Paraview etc.

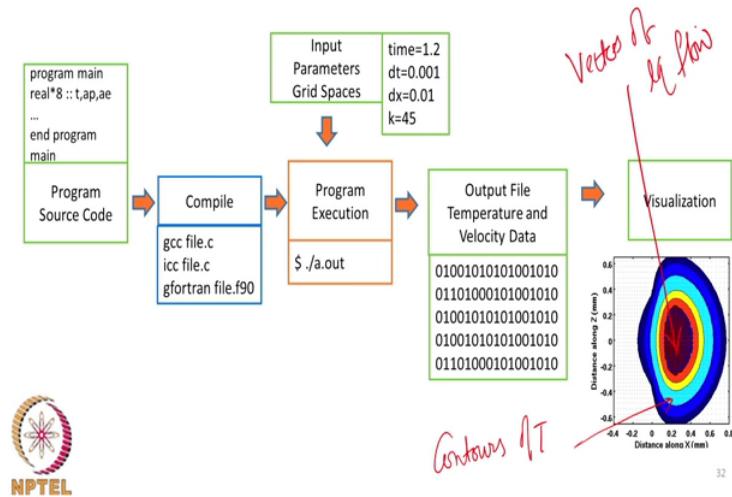


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What are the various ways of doing it this is the same as what we have discussed in one day basically you can write the programs in FORTRAN C or C++ a normally, because of the complexity as well as because of the speed required for the computations. One does not write a MATLAB program or a Python program, to solve these equations in three dimensions a low-level language such as FORTRAN or C can be used. So, that you can make the program one as fast as you can; however, with accelerator today you can run them in a high level language such as Python or MATLAB also.

Usually the input values have to be read from the files. So, you must have file - input output also taking care. So, would have visually the grids basins and the parameter values coming in from a file input. The output will then be written in a binary format usually, because files are quit big, and then they are then post processed using a graph plotting such as Tecplot or MATLAB or ParaView etcetera.

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These are overall the scheme this is how it is going on basically, you have the equations then, we have discretize them, we have got a liner set of equations then, we took care to ensure that the interpolation scheme is done properly taking the advection terms to account and hybrid scheme is used. So, that we do not have too much of computational expense done and then they are then solved using a TDMA algorithm.

Algorithm is a programmed in the programming language such as FORTRAN or C, and then that program is then compiled to create an executable. Then executable is run and then you get the output, and then output is visualized in software to produce a output which you can view. Such as this for example, you can see that in this situation you have got these contours temperature and you also have basically vectors of the liquid flow. So, you can then combine and then see how the weld pool is going to evolve and look at how the output is going to give you more learning about the process. So, this is the overall scheme by which you are doing.

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Programming issues for high computational cost

- A 3D transient run could often be with 10^6 grids and 10^3 time steps
- Each time step involves multiple iterations for convergence
- Simulations are memory intensive as well as cpu intensive
- Parallel programming is the way forward
- Domain decomposition could be adopted
- Single Instruction Multiple Data (SIMD) paradigm suits the problem
- Message Passing Interface (MPI) libraries available as a standard



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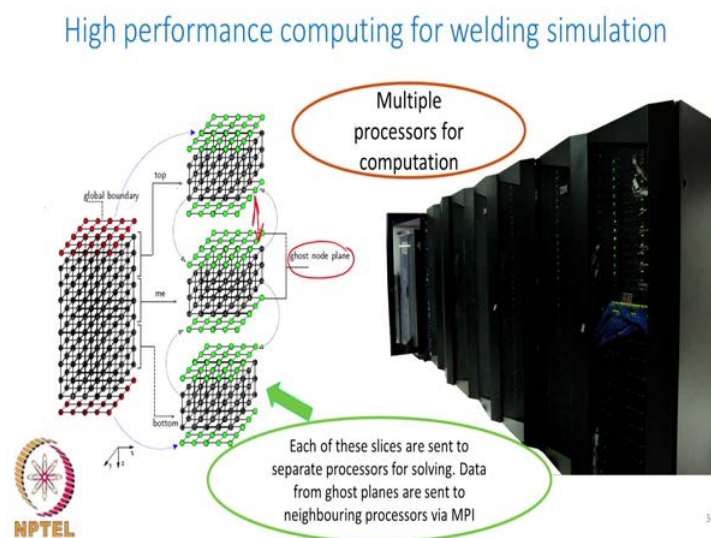
At this juncture, I would also bring one last concept in namely the high computational cost. As you can see that in a 3D transient run you could easily have a put a million grids are more and you would have a thousand time steps are mode. So, where is you starts seeing that you have to solve the equations about ten to the power of nine times over in every location and every time steps. So, it accommodated very huge computational cost, and we are talking about several hours or even base of computation they can depend upon the problem.

Each time step can then involve multiple iterations for convergence. They are also me memory intensive as well as CPU intensive. So, therefore one good approach would be to make the program as a parallel program, so, that you can make the computation faster.

Whenever we do it in parallel method you basically have two ways of doing it, one is what is called as the multiple instruction method, where you send different pieces of go to the different computers you can solve. For example, pressure equation in one computer, velocity equation in one computer, temperature equation in another etcetera that is one way, but does not recommend the reason been the we do have a algorithm, which has actually mixes and matches the solution what recommend is actually multiple data single instruction can define approach.

Which is SIMD approach and that requires you to use demand competence the composition to split the data across a processors and that can be done. How do we send the data across to other processors there is a standard available which is called as a MPI library message passing interface library, using that you can actually the write a program, whereby you can send parts of the array to other computers to compute and then collate the data after the computation over. So, that we can mix all the data and write the output file. So, this is an approach that is required whenever you want to do large problems.

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What I have said is illustrated here if you take the data as a 3D array of grid points on, which we are going to do the salvation there you can actually. For example, split in to three parts and then send them to three different computers. Then make those solutions and mix and match. So, you have already seen from the TDMA algorithm as well as from the linear set of equations we need the data from the neighboring notes. So, whenever you take slice of array and sent to one computer the neighboring notes data has to come from the another computers which is neighbor.

So, you basically have what are called ghost notes, which are basically these ghost node place basically replications. So, the same array will be available in both the computers, so that the data is replicated and this data replication is taken care by MPI and that way

you can actually handle this particular problem quite neatly to compute across multiple processors and make (Refer Time: 52:17) simulation reasonably faster.

With that, we come to the end of the second part of the lesson on numerical solutions. And we would then follow it by looking at actual solutions of temperature and velocity field to give you an idea of what kind of output is possible. And we would do that as a set of slides in a third part later on that I will close this lesson.

Thank you.