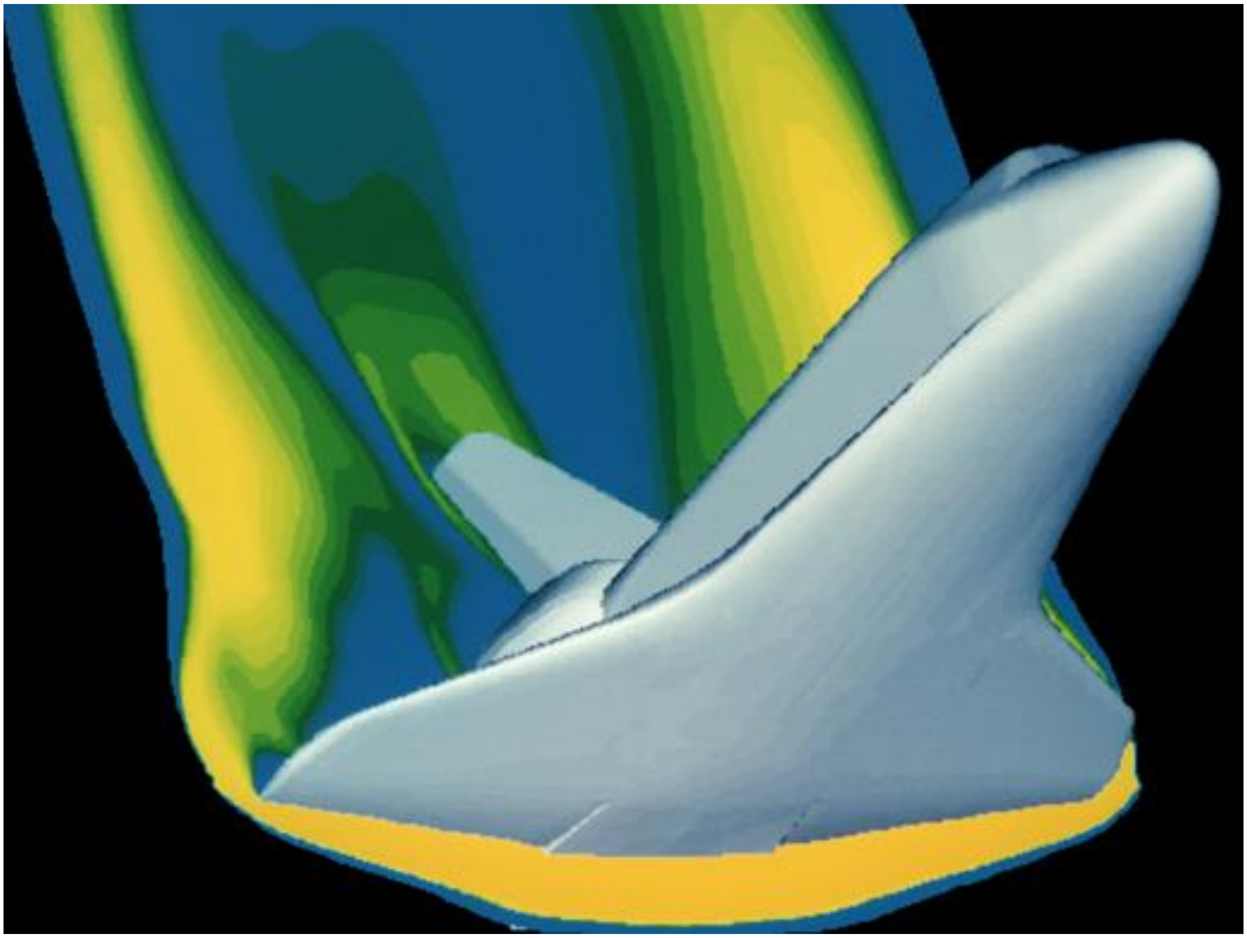


FLUIDS 4

CFD 1 – NUMERICAL METHODS IN SCIENCE AND ENGINEERING

This section looks at the solution of complex problems using numerical methods.

FLUIDS 4

CFD 1 – NUMERICAL METHODS IN SCIENCE AND ENGINEERING

OVERVIEW

In this section you will learn about:

- The general approach taken by popular numerical methods (the breakdown of a problem using a mesh or grid).
- The three main methods for doing this and their applications in science and engineering.
- The Finite Element Method (or Approach) – FEA/FEM
- The Finite Difference Method – FDM
- The Finite Volume Method – FVM
- You will also learn something of the basic operation of these, concentrating on FDM

ASSUMED KNOWLEDGE

In this subject it is assumed that you already have knowledge about the following topics:

- *A good knowledge of fluid parameters*
- *Incompressible flow including Bernoulli, Continuity, Reynold's Number and Thrust equations*
- *Compressible flows and shockwaves*
- *The basic ideas behind CFD and some practice of its use*

Cover image: "high velocity flow around space-shuttle on reentry" by NASA. Public domain, NASA terms and conditions (see page 16)

OBJECTIVE

The overall objective of this section is to learn about the three main numerical methods used in CFD, what they are used for and what their attributes are.

TOPIC 1 – NUMERICAL METHODS IN ENGINEERING

There are three common numerical methods used in engineering to solve PDE type problems. Each one has its own advantages and disadvantages and tends to be used in particular niche areas. These three are shown in table 1 below along with their properties.

Method	Main applications	Advantages and disadvantages
Finite Element Analysis (FEA)	Mainly structural mechanics, also used in CFD, thermal modelling and magneto/electro-statics	Main structural mechanics method. Rather limited by the structure of the maths to problems which can be formulated in the same way as structural problems.
Finite Difference Method (FDM)	Electromagnetics, heat transfer, CFD and others.	Simplest and most general of the methods. Can be used to solve most types of PDE. Eclipsed in CFD now by FVM.
Finite Volume Method (FVM)	Mainly Computational Fluid Dynamics (CFD), but can be used in other applications	Allows unstructured grids and good representations of compressible flow (main CFD method).

Table 1, The three most common numerical methods used in advanced engineering problems.

Let's look at each of these methods one by one (FVM is too involved to consider in much detail, but an overview is given below).

TOPIC 2 – GENERAL PRINCIPLES AND IDEAS – USING FEA AS AN EXAMPLE

Since the Finite Element Method is mainly used in structural modelling, we'll consider it initially in this context here.

Stress, strain and deformations are easy to calculate for simple shapes and components – for example beams and shafts - but what about the complex shapes and structures that one might find in a real machine or structure? These are generally too complex to calculate simply by hand. The modern method of handling these issues is to use Finite Element Analysis (FEA) software.

The idea of this method and the others (FDM and FVM) is to break-down the structure to be analyzed into many small one, two or three dimensional blocks called *elements* as shown in figure 1, below:

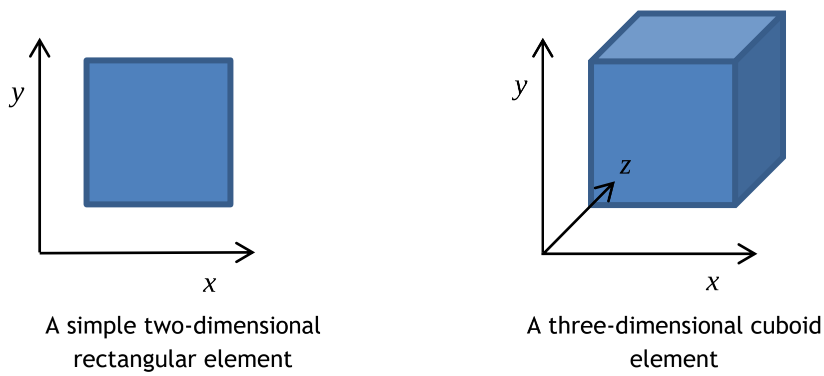


Figure 1, A complex structure can be broken down into simple elements such as these.

It is easy to write down the equations for one such simple unit – and not just if the element is surrounded by the host material, but also if one or more sides are exposed on a component edge. Rectangular elements are not the most often used, but are shown here as an illustration of the concept.

Now, if we split up a complex component into such simple units, we can analyze its behavior by working out all the single elements and then added them together to get the behavior of the whole thing.

Figure 2 shows an actual 3D component split up into cuboid type elements. The mapping of the *grid* or *mesh* of elements onto the object is called *meshing* and achieving a good mesh (with a fine resolution, in the important stress-prone areas) is key to the success of the FEA technique (and the others too, especially in CFD).

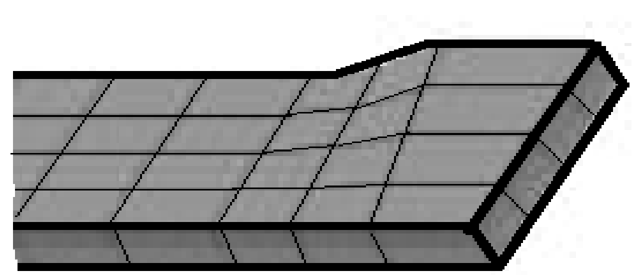


Figure 2, a complex component split into simple cuboid elements using a mesh.

This approach allows the designer to check the stress, strain and deflection of very complex shapes - and many commercial programs are available which perform the analysis. The design approach adopted in many projects now has such simulation as a key part of the process as shown on the flow chart in figure 3.

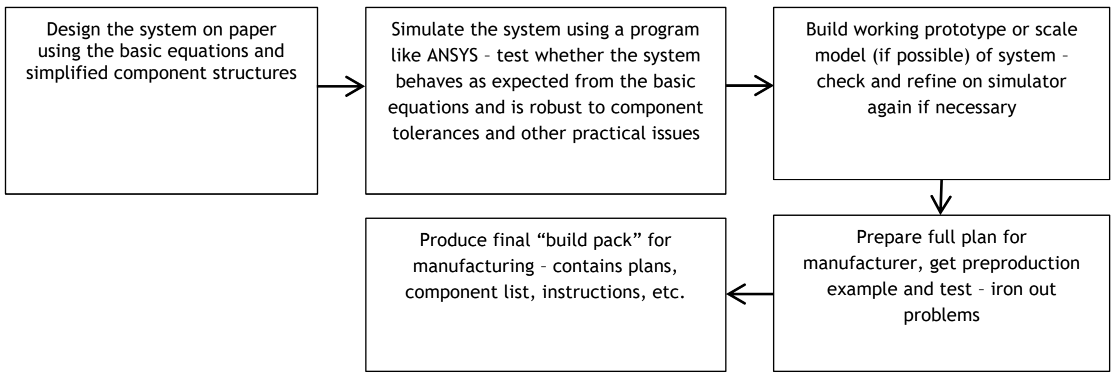


Figure 3, how simulation in a modern FEA/CFD simulator like ANSYS fits into the design cycle.

TOPIC 3 – HOW FEA WORKS

Consider a one dimensional bar of material in its elastic region as shown in figure 4. If we exert a force on this it will stretch and return to its original size when the force is removed – it obeys Hooke's law like a spring.

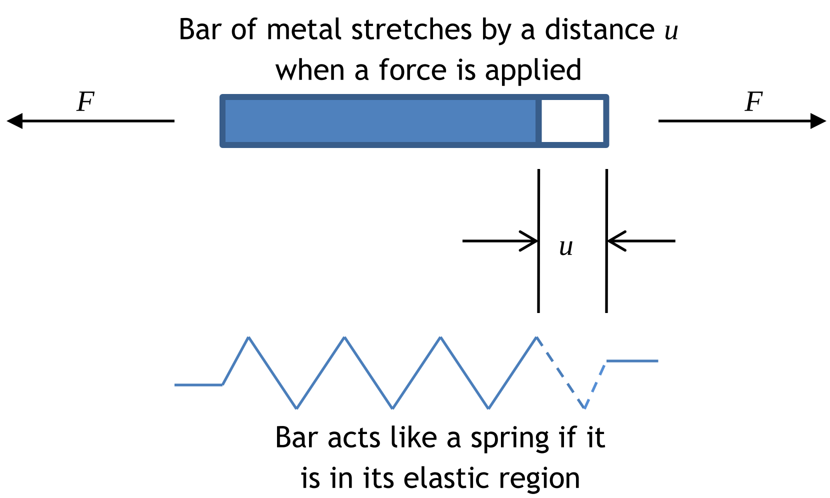


Figure 4, a simple bar in tension stretches elastically.

In the diagram, the original length of the bar is represented by the filled-in area and the extension caused by the applied force is shown unshaded. Likewise, the extension of the equivalent spring is shown as the dotted length.

The formula for this is shown below:

$$F = -ku$$

Where k is the spring's stiffness (given for a bar by AE/L, where A is cross-sectional area, E is Young's modulus and L is the original length).

The equation simply expresses the idea that the further you extend the spring the more force is required to pull it apart (or alternatively, the more force the spring exerts on your hands as it tries to return to its original position).

Therefore if we know the spring's stiffness we can calculate its deformation:

$$u = \frac{F}{-k}$$

From these relationships and the dimensions of the bar, we can also easily calculate stress and strain.

All this can be extended to two dimensions as shown in figure 5.

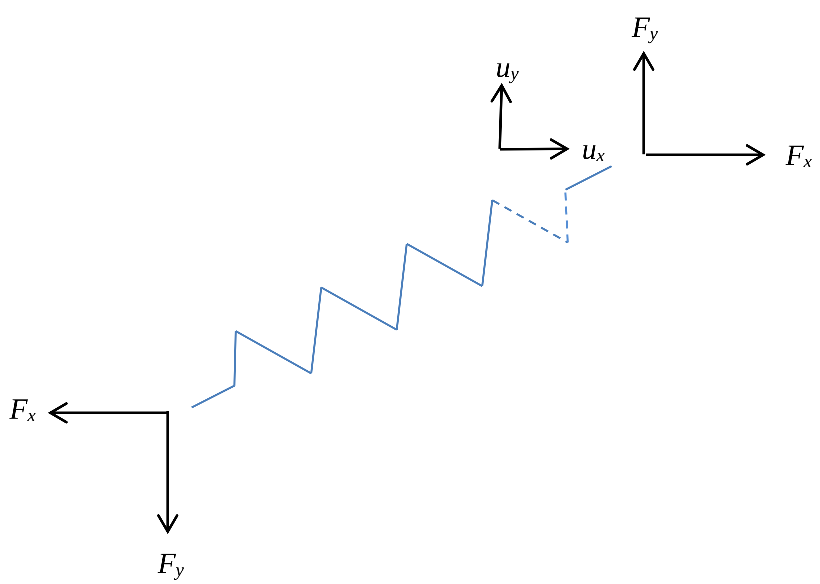


Figure 5, a spring (representing a bar) in two dimensions.

We could write out equations for all these components:

$$F_x = -k_x u_x$$
$$F_y = -k_y u_y$$

However at this point it might be easier to writing this in matrix form:

$$\begin{bmatrix} F_x \\ F_y \end{bmatrix} = \begin{bmatrix} -k_x & 0 \\ 0 & -k_y \end{bmatrix} \begin{bmatrix} u_x \\ u_y \end{bmatrix}$$

This can be written in shorthand like this:

$$\mathbf{F} = \mathbf{K}\mathbf{u}$$

Where the bold letters indicate that the variable referred to is a vector or matrix.

The $\mathbf{K}$ is called the stiffness matrix for the material. To work out the deformation $\mathbf{u}$ now means inverting the matrix $\mathbf{K}$:

$$\mathbf{u} = \mathbf{K}^{-1}\mathbf{F}$$

This idea can of-course be extended easily in the same way into three dimensions.

We can extend it to many springs in the same way as shown in figure 6.

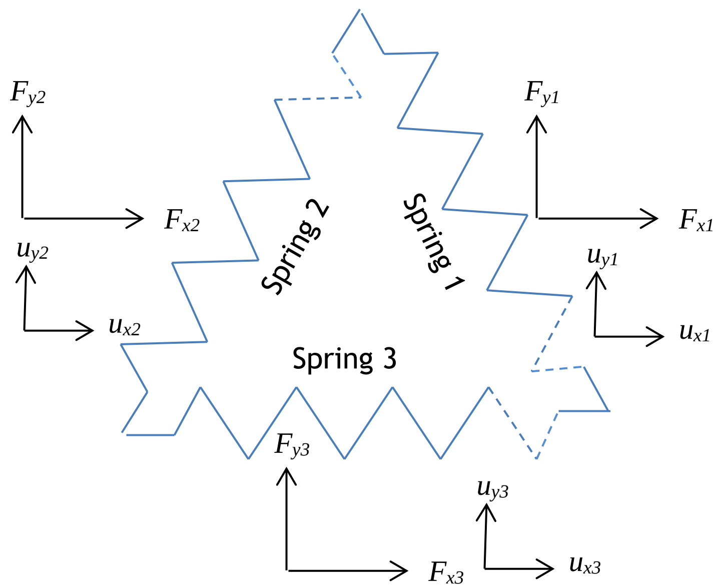


Figure 6, many springs (bars) can joined together to form a structure.

This is equivalent to chaining bars together to produce structures as shown in figure 7

Figure 7, two bars with different properties, forming a structure.

If the stiffness matrix of A is k_A and B is k_A:

$$k_A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \; and \; k_B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

The new total stiffness is k_T:

$$k_T = \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} + B_{11} & B_{12} \\ 0 & B_{21} & B_{22} \end{bmatrix}$$

And the matrices for large and complex structures can be built up in this way.

So, perhaps you can see that this is basically how a structure in FEA is formed (although the stiffness matrix would usually written down for a solid triangular element). The main computational overhead in the FEA is caused by inverting the stiffness matrix.

TOPIC 4 – EXTENDING FEA TO OTHER APPLICATIONS

FEAs can be reformulated as a general solution approach to PDEs. However, they are particularly useful and successful in areas where the equations can be formulated similarly to that outlined above. Such applications include Electrostatics and Magnetics, Fluids (CFD) and Heat transfer. For example in conductive heat transfer, if $\boldsymbol{T}$ is a matrix of nodal temperatures, $\boldsymbol{K}$ is one of thermal conductivities (the equivalent of the stiffness matrix in the mechanics examples) and $\boldsymbol{Q}$ one of heat generators:

$$\boldsymbol{Q} = \boldsymbol{KT}$$

You should notice the similarity to the basic equation given for mechanical strain in the sections above. In fluids:

$$\boldsymbol{F} = \boldsymbol{K\varphi}$$

Here $\boldsymbol{F}$ is the matrix of forces on the fluid $\boldsymbol{K}$ is the equivalent of the stiffness matrix (essentially the fluid viscosity) and $\boldsymbol{\psi}$ is the “stream function” (the stream function is related to the velocity components of the fluid stream).

In general, you might notice that all these equations have the following form:

$$\boldsymbol{A} = \boldsymbol{P}\boldsymbol{B}$$

Where $\boldsymbol{A}$ is the input action applied to the system (like a force or a heat source), $\boldsymbol{B}$ is the resulting output behavior of the system (which is what we want to find in the end - like displacement, temperature or velocity) and $\boldsymbol{P}$ is the system properties (often material parameters) which relate the other two together. It is systems which can be expressed like this that FEAs are particularly adept at solving - and we do this by rearranging the equation using the inverted matrix $\boldsymbol{P}$:

$$\boldsymbol{B} = \boldsymbol{P}^{-1}\boldsymbol{A}$$

TOPIC 5 – HOW FDM WORKS

Of all the methods described in these notes, FDM is the most general and (arguably) the most powerful. It's one of the key tools in modern science and engineering and it can be applied, in some form, to solving almost all differential equations. It was the main CFD method before FVM became popular. For these reasons we will concentrate more effort into understanding it.

First of all, let's get the general idea.

Think back to what the derivative actually means – it's just the slope or gradient of a curve. So, if we were not concerned too much about accuracy, we could approximate the slope by the change in y divided by the change in x which is $\Delta y/\Delta x$, as shown in the diagram in figure 8.

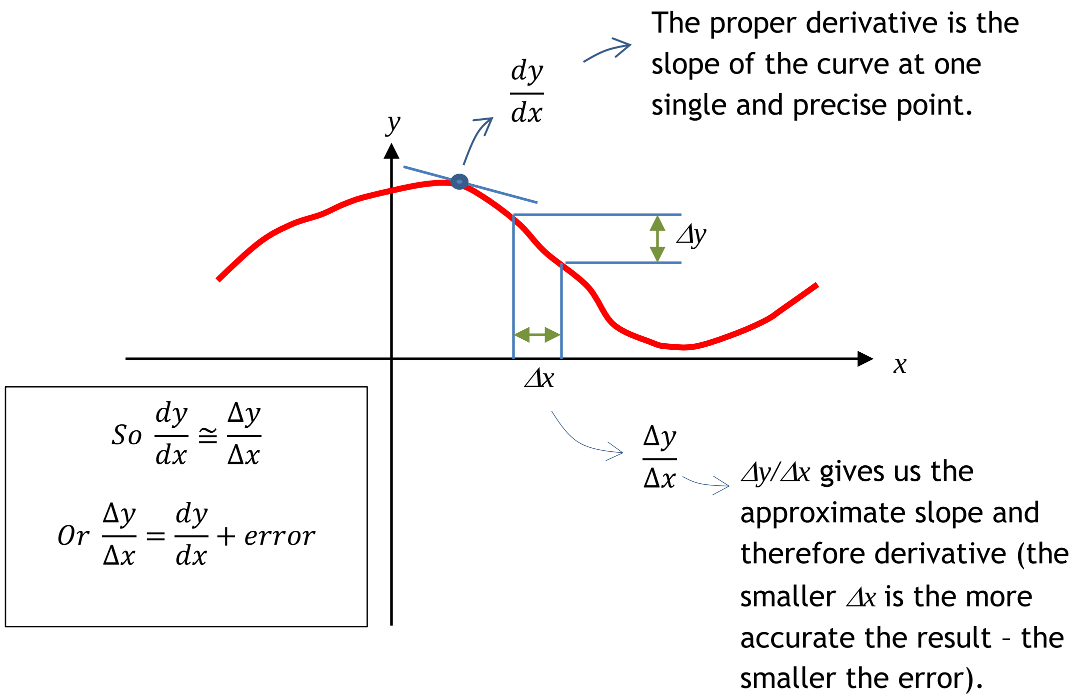


Figure 8, the derivative of a curve and its approximation - the difference function.

Replacing dy/dx by $\Delta y/\Delta x$ in a differential equation makes it into a *difference equation*:

$$\frac{dy}{dx} + 5x = 3 \ \text{This is a differential equation}$$

$$\frac{\Delta y}{\Delta x} + 5x = 3 \ \text{This is the difference equation}$$

Replacing the differential equation by a difference version means that we can rearrange the equation and use it to iteratively work out the solution (the actual values of x and y), because:

$$x_{new} = x_{old} + \Delta x$$

And

$$y_{new} = y_{old} + \Delta y$$

Let's see how this works in practice.

Suppose we have a grid or mesh of points (where have we heard this before) across the range and domain of the graph. Let's call the points on the x axis i_n and those on the y axis j_n. This gives us the setup shown in figure 9 (this setup is actually for a function with two independent variables (a 2D function) - the equation above only has one (x), so could be represented by a simple line and just one index (i)).

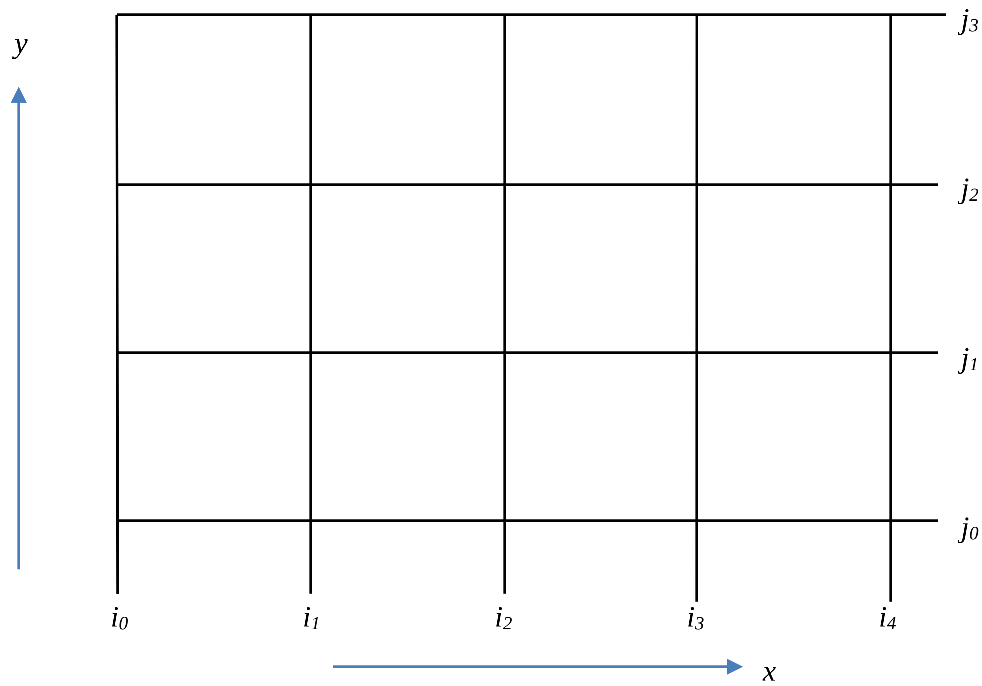


Figure 9, a two dimensional grid

So in this notation the last two equations would become (in 2D):

$$x_{i+1} = x_i + \Delta x$$

And

$$y_{j+1} = y_j + \Delta y$$

And if we know the conditions at the start (the initial and boundary conditions), then we can work out the rest of the points.

Let's do an example to see how this works. We'll take the previous equation and say that the initial conditions are $x_0 = 0$, $y_0 = 2$. Because there's only one dependent variable in our equation (y), we'll choose an incremental step size for x of $\Delta x = 0.1$ (rather than calculate it, as we'd have to do in 2D), we'll start by rearranging the previous equation:

$$\frac{\Delta y}{\Delta x} + 5x = 3$$

$$\therefore\ \Delta y = (3 - 5x)\Delta x$$

Let's work out the values for x_1 and y_1:

$$\Delta y = \big(3 - (5 \times 0)\big) \times 0.1 = 0.3$$

$$x_1 = 0 + 0.1 = 0.1$$

$$y_1 = 2 + (0.3) = 2.3$$

And using these values we could calculate x_2 and y_2.

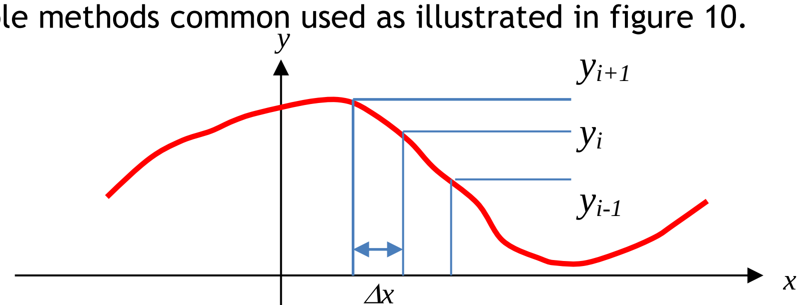
TASK 1

(a) Calculate x_2 and y_2 given the two points calculated above.

(b) This equation is solved analytically in the revision notes from the start of the course. Given that solution and the initial conditions given above, compare the values from the analytical solution and the difference equation.

So, we could iterate this over the whole grid (if the equation where two dimensional). If the x axis were time, this would be called a *time-marching* solution, although more generally (using any variable) it's called an *explicit* approach.

In fact to calculate the derivative as a difference from the graph there are actually three possible methods common used as illustrated in figure 10.



$$\frac{dy}{dx} \cong \frac{\Delta y}{\Delta x} = \frac{y_{i+1} - y_i}{\Delta x} \ (+error): \ \text{Forward difference method}$$

$$\frac{dy}{dx} \cong \frac{\Delta y}{\Delta x} = \frac{y_i - y_{i-1}}{\Delta x} \ (+error): \ \text{Backward difference method}$$

$$\frac{dy}{dx} \cong \frac{\Delta y}{\Delta x} = \frac{y_{i+1} - y_{i-1}}{2\Delta x} \ (+error): \ \text{Central difference method}$$

Figure 10, the three approximations to the first derivative.

Now, notice something interesting here. The equation we actually used in the calculation above was the backwards difference one (we calculated y_i knowing the previous (initial) value y_{i-1}). So we can actually write down the equivalent equation (which gives the same result) using the notation above:

$$\frac{dy}{dx} + 5x = 3$$

$$\Rightarrow \frac{y_i - y_{i-1}}{\Delta x} + 5x = 3$$

$$(3 - 5x)\Delta x = y_i - y_{i-1}$$

$$y_i = y_{i-1} + (3 - 5x)\Delta x$$

Which is exactly equivalent to what we had before.

TASK 2

Check you get the same answer as you got in task 1 using this formulation.

However, if we were to use the forward or central differences, we'd need to know the values at $i+1$ – but how could we? They haven't been calculated yet.

Well there is a way around this, we could write down an equation at every node (which will include these unknown terms) and solve them simultaneously. This can done using matrix methods (one simple way is using a method called Gaussian elimination).

This (simultaneous equation) approach is called the *implicit approach*. Now, you might be wondering to yourself, 'why bother with this when the explicit approach is so much simpler'. Well, the answer to this is that although it's much easier to implement, the explicit method only works well with the more straightforward equations (like Maxwell's equations and the heat transfer equation) – this is because it's less stable and predictable – but unfortunately the Navier-Stokes equations are exactly the complex type which need the stability of the implicit approach.

Finally, we can also write down similar approximations to those above for second order and higher derivatives – although in practice, second order is the highest we usually ever need. The second order central difference is:

$$\frac{d^2y}{dx^2} \cong \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2}$$

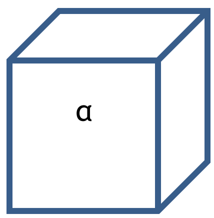
TOPIC 6 – HOW FVM WORKS

The Finite Volume Method (FVM) is the main method currently used in CFD solvers. This is mainly for two reasons:

- It allows the easier use of unstructured grids or meshes – very handy for fitting around awkward shapes.
- It captures flow discontinuities like shockwaves better than the other methods.

We only have time here to discuss the basic idea behind FVM and not the fine detail. It works particularly well in problems where some quantity can be visualized as "flowing".

The mesh in FVM forms elements of volume (in this case a volume α):



Now in a system where something flows – this might be mass, momentum or energy in a mechanical system or charge in an electrical one - we can represent this flowing quantity as a vector field $\boldsymbol{Q}$ which will be a function of space (and also time, but we'll consider that it's in steady-state here) $\boldsymbol{Q}\,(x, y, z)$. I'll call this $\boldsymbol{Q}(V)$ here ($\boldsymbol{Q}$ in space V) The amount of $\boldsymbol{Q}$ in the volume α is given by the volume integral:

$$\iiint_{\alpha} \boldsymbol{Q}(V)dV$$

If the amount of $\boldsymbol{Q}$ is increasing or decreasing within the volume, its divergence will be non-zero:

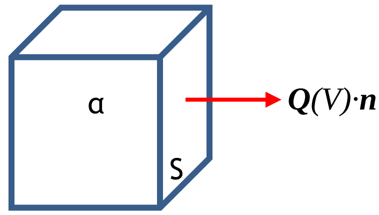
$$div\,\boldsymbol{Q}(V) = \nabla \cdot \boldsymbol{Q}(V)$$

Specifically, if the net content in the volume is increasing then the divergence will be negative and if it is decreasing them the divergence is positive.

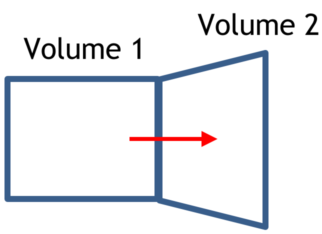
The divergence term so produced can be converted into a surface integral using the divergence theorem:

$$\iiint_{\alpha} \nabla \cdot \boldsymbol{Q}(V)dV = \oiint_{S} (\boldsymbol{Q}(V) \cdot \boldsymbol{n})dS$$

Giving us the fluxes into or out-off the volume surfaces:



And because the flux leaving the back face of a volume must be the same as that entering the front face of the next (even although they are different shapes), this gives us the starting point for the next volume and so on.



Which is why FVM allows such unstructured meshing.

TOPIC 7 – ISSUES WITH NUMERICAL METHODS

All the methods explained above have an error (they are inaccurate) - because they are approximations to the "real" (exact) equations. As the solution progresses it becomes less and less accurate – this must be taken into account when interpreting the results and factors of safety need to be used carefully in actual designs to mitigate the effect.

As discussed above, solutions can also be unstable (they can fluctuate wildly and unpredictably) - in which case the results are useless and will not bear any relationship to reality. Similarly, solutions can sometimes "blow-up" and become very large (or diminish to zero) and these are again completely inaccurate.

Sometimes such issues can be cured by changing the initial or boundary conditions or reducing the simulation step-size. However, simulation results should always be viewed cautiously and it is essential to perform simple hand calculations to confirm that the answers are in the correct "ball-park". Another useful method is to run a series of simulations with slightly different setups (topology, initial and boundary conditions and step sizes) and confirm that these all give similar results (or try the problem on a different simulator).

SUMMARY

- Although there are many numerical methods which can be used in science and engineering, three dominate - and these are: The Finite Element Method (or Analysis or Technique), FEA/FEM; The Finite Difference Method (FDM) and the Finite Volume Method (FVM).

- All numerical methods produce approximate solutions (they have an error) and can form divergent and/or unstable solutions (and these solutions are complete rubbish).

- FEAs are the main mechanical structures method and are particularly suited to problems which can be formulated in a similar way and yield relationships in the form ***A*** = ***P B***. Where ***A*** is the input applied to the system, ***B*** is the resulting output and ***P*** is the system properties which relate the other two together (these variables being vectors or matrices).

- FDM is the most flexible method and involves changing differential equations into difference equations and finding the solution by iterating these.

- There are two distinct ways of posing FDM problems – as an explicit formulation (which is simple but often unstable) or as an implicit formulation (which leads to complex simultaneous equations, but is usually stable).

- FVM is now the main CFD approach. It works by formulating an integral expression for the amount of substance in a volume, finding the divergence of this and using this to develop an expression for the flow through the walls of the volume element using the divergence theorem.

Note that this whole topic is complex subject at the forefront of science and engineering, and the approach we've gone through above is simplified in some respects (and methods differ somewhat depending on the nature of the problem to be solved) – if you want to know the full details, study the references below.

REFERENCES, OTHER MATERIAL AND BIBLIOGRAPHY

If you are interested in delving into FDM in more detail, there are two excellent (master's level) courses available on Youtube:

Lorena Barba of Boston University (CFD course)

Very good and thorough, but old fashioned course:

https://www.youtube.com/playlist?list=PL30F4C5ABCE62CB61

Raymond Rumpf of The University of Texas, El Paso (Maxwell's equations using FDM)

Similarly good, but thorough, course:

https://www.youtube.com/playlist?list=PLLYQF5WvJdJWoU9uEeWJ6-MRzDSziNnGt

There are also many other Youtube courses which I haven't had a chance to check.

Two particularly recommended CFD books are:

John D Anderson, Computational Fluid Dynamics: The basics with applications, McGraw-Hill, 1995 (several editions).

Jiyuan Tu, Guan-Heng Yeoh and Chaoqun Liu, Computational Fluid Dynamics: A practical approach, Butterworth-Heinemann (Elsevier), 2013 (2nd ed).

There are Wikipedia pages on all the techniques and these are excellent "jumping off points" for further study:

https://en.wikipedia.org/wiki/Finite_element_method

https://en.wikipedia.org/wiki/Finite_difference_method

https://en.wikipedia.org/wiki/Finite_volume_method

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