ME40064: Systems Modelling & Simulation
ME50344: Engineering Systems Simulation
Lecture 3

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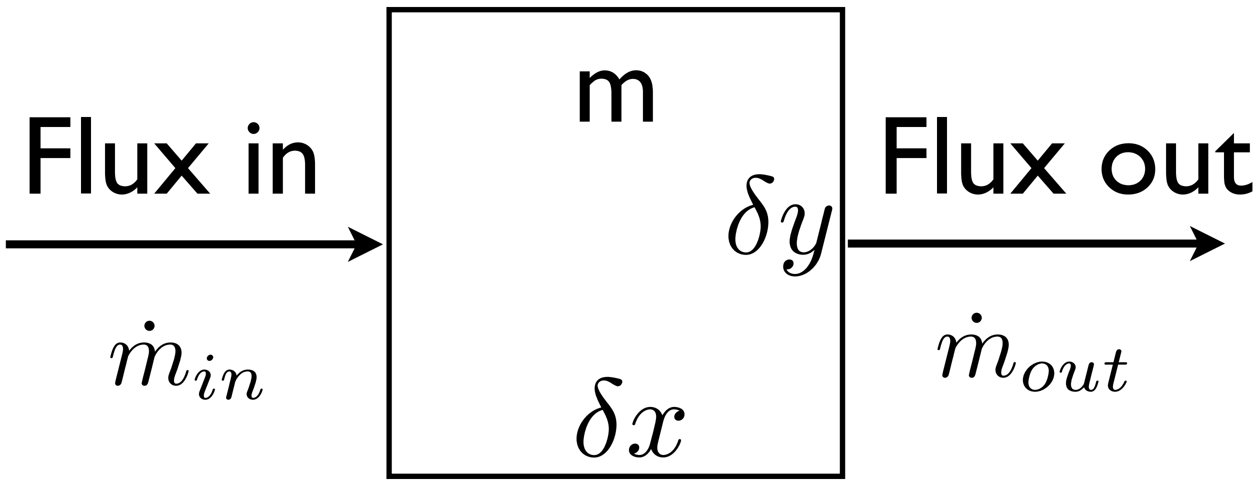
LECTURE 3
Overview Of Fem Course

1. Derive equations to be solved - Lecture 3
2. Define solution domain & generate finite element mesh - Lecture 4
3. Define the order of solution representation
    3.1. Linear solution - Lecture 4
    3.2. Quadratic solution - Lecture 10
4. Convert the equation into a form suitable for FEM (Galerkin weak form) - Lecture 5
5. Calculate each element's contribution (local matrix) to the equation
    5.1. Calculate by hand - Lecture 6
    5.2. Calculate numerically - Lecture 9
6. Create a matrix (global matrix) to contain all these element contributions for the entire mesh, to be solved as simultaneous equations - Lecture 7
7. Apply boundary conditions and solve the system of equations - Lecture 8
8. Determine numerical errors and test rate of convergence - Lecture 11
9. Derive the same method for transient equations - Lectures 12 & 13

LECTURE 3
PDES For Heat Transfer Modeling

- Able to derive the transient advection-diffusion-reaction equation
- Understand reasons for simplifying the model
- Possess a range of strategies for model simplification

CONTINUITY EQUATION
A Conceptual Explanation



$$\delta A = \delta x \delta y$$

Change in mass in control volume

$$\delta m = (\dot{m}_{in} - \dot{m}_{out})\,\delta t$$

Rate of change in mass in control volume

$$\frac{\delta m}{\delta t} = \dot{m}_{in} - \dot{m}_{out}$$

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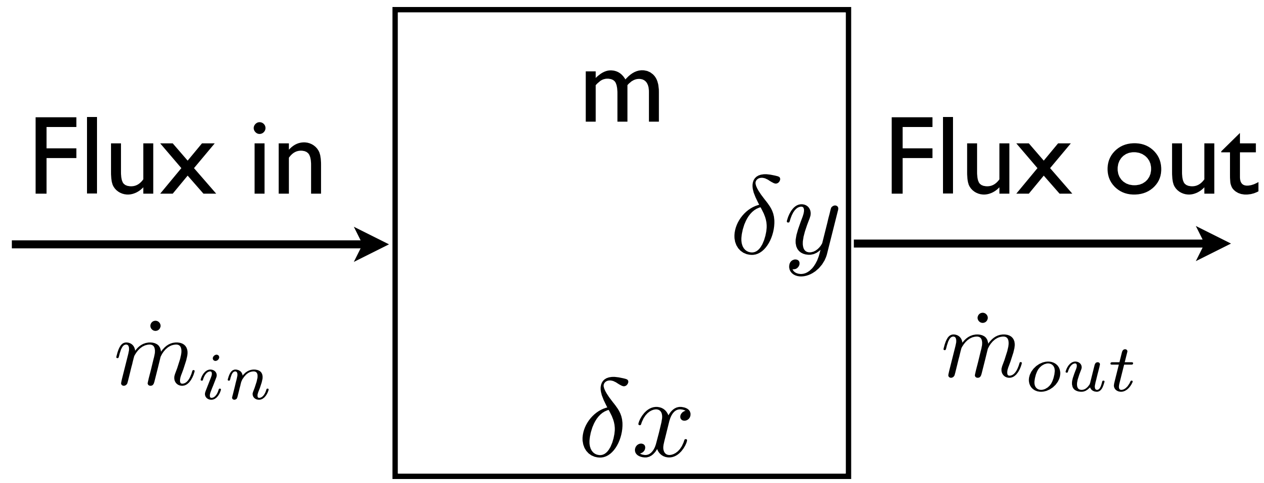
A Conceptual Explanation



$$\delta A = \delta x \delta y$$

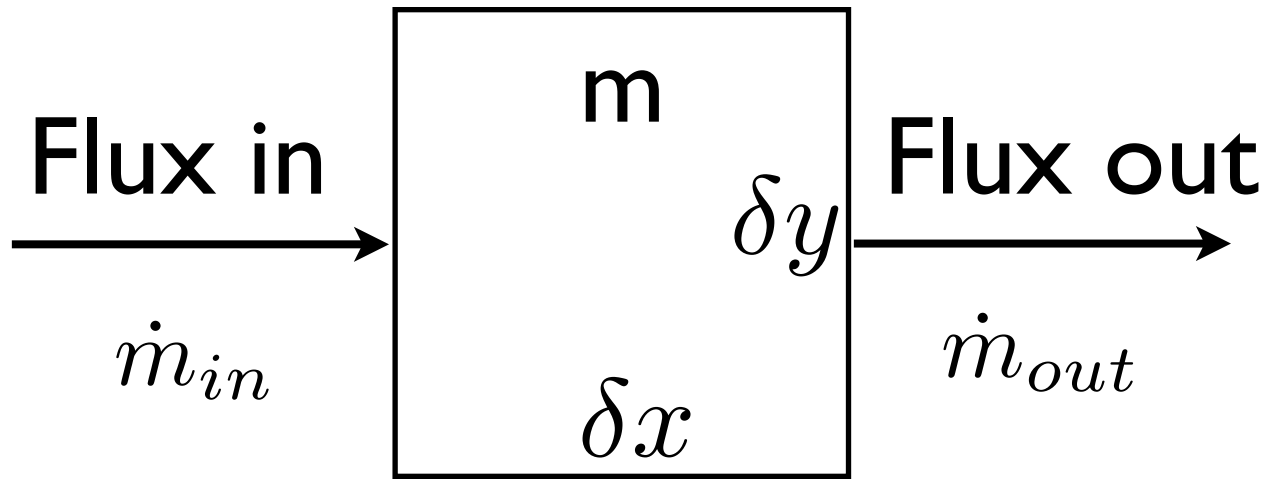
Concentration = mass/volume

$$\delta c = \delta m / \delta A \qquad \therefore \delta m = \delta c \delta x \delta y$$

Rate of change in mass in control volume

$$\frac{\delta c \delta x \delta y}{\delta t} = \dot{m}_{in} - \dot{m}_{out}$$

CONTINUITY EQUATION
A Conceptual Explanation



$$\delta A = \delta x \delta y$$

$$\frac{\delta c \delta x \delta y}{\delta t} = \dot{m}_{in} - \dot{m}_{out}$$

J = J_x**i**= flux of mass = mass per unit length (area) per unit time

$$\frac{\delta c \delta x \delta y}{\delta t} = J_x(x).\delta y - J_x(x + \delta x).\delta y$$

CONTINUITY EQUATION
A Conceptual Explanation

$$\frac{\delta c \delta x \delta y}{\delta t} = J_x(x).\delta y - J_x(x+\delta x).\delta y$$

$$\frac{\delta c \delta x \delta y}{\delta t} = -\left(J_x(x+\delta x).\delta y - J_x(x).\delta y\right)$$

Dividing by the lengths

$$\frac{\delta c}{\delta t} = -\frac{(J_x(x+\delta x) - J_x(x))}{\delta x}$$

CONTINUITY EQUATION
A Conceptual Explanation

$$\frac{\delta c}{\delta t} = -\frac{(J_x(x+\delta x) - J_x(x))}{\delta x}$$

As the deltas tend to zero

$$\frac{\partial c}{\partial t} = -\frac{\partial J_x}{\partial x}$$

The next step is to define the flux operator J

CONTINUITY EQUATION
A Conceptual Explanation

This law can be generalised to 3D

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

using the following definitions:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \qquad \mathbf{J} = J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k}$$

<u>Deriving this will be an exercise for Tutorial 2</u>

SCALAR TRANSPORT EQUATION
Fick's Law Of Diffusion

Fick's law of diffusion states that a quantity diffuses in proportion to the local concentration gradient

$$J_{diff} = -D\frac{\partial c}{\partial x}$$

where D is the diffusion coefficient

Note the minus sign, as flux is in opposite direction to the gradient

SCALAR TRANSPORT EQUATION
Fick's Law Of Diffusion

In general form this is written:

$$\mathbf{J}_{diff} = -\mathbf{D}\nabla c$$

where flux **J** is now a vector, and **D** is a tensor diffusion coefficient

SCALAR TRANSPORT EQUATION
Advective Flux

This accounts for the passive transport of a scalar quantity by a fluid velocity, **u**

$$\mathbf{J}_{advec} = \mathbf{u}c$$

Total flux is sum of advection & diffusion

$$\mathbf{J} = \mathbf{J}_{diff} + \mathbf{J}_{advec}$$

SCALAR TRANSPORT EQUATION
Source & Reaction Terms

Fluxes entering/leaving the domain not the only source of mass - it can be created/destroyed within e.g.

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J} = S$$

where S is a source (+ve) or sink (-ve) term, and is defined: mass/(volume * time)

SCALAR TRANSPORT EQUATION
Examples Of Source & Reaction Terms

Mass sources/sink e.g. a pollution source in environmental flows

$$S = f$$

Linear reaction-type sources/sinks

$$S = \lambda c$$

A linear reaction, where lambda is a constant, is a source term proportional to the concentration - commonly found in combustion type models (non-linear reactions are also possible but trickier to solve)

SCALAR TRANSPORT EQUATION
Advection-Diffusion-Reaction Equation

Putting terms all together gives transient advection-diffusion-reaction equation

$$\frac{\partial c}{\partial t} + \mathbf{u}.\nabla c = D\nabla^2 c + \lambda c + f$$

This equation will form the basis of Parts 1 & 2 of the module

SCALAR TRANSPORT EQUATION
Some Other Uses For This Equation

Mathematical finance
Black-Scholes equation

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$$

Incompressible fluid mechanics
Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla(\frac{p}{\rho}) + \nu\nabla^2\mathbf{u}$$

In silico medical Imaging
Contrast enhanced magnetic resonance imaging

Poroelastic advection-diffusion equation

$$\left.\frac{\partial(J\phi^f c^f)}{\partial t}\right|_{\mathbf{X}} + \nabla_{\mathbf{X}}\cdot[c^f\mathbf{W} - J\mathbf{F}^{-1}\phi^f D^f\mathbf{F}^{-T}\nabla_{\mathbf{X}}c^f] = JQ_{tot} + J\phi^f\phi^s\alpha(c^s - c^f)$$

Poroelastic diffusion equation

$$\left.\frac{\partial(J\phi^s c^s)}{\partial t}\right|_{\mathbf{X}} + \nabla_{\mathbf{X}}\cdot[-J\mathbf{F}^{-1}\phi^s D^s\mathbf{F}^{-T}\nabla_{\mathbf{X}}c^s] = -J\phi^f\phi^s\alpha(c^s - c^f)$$

AIMS OF MODEL SIMPLIFICATION
Less Is More

Why simplify your model?

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- reduce computational time

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Less Is More

Why simplify your model?

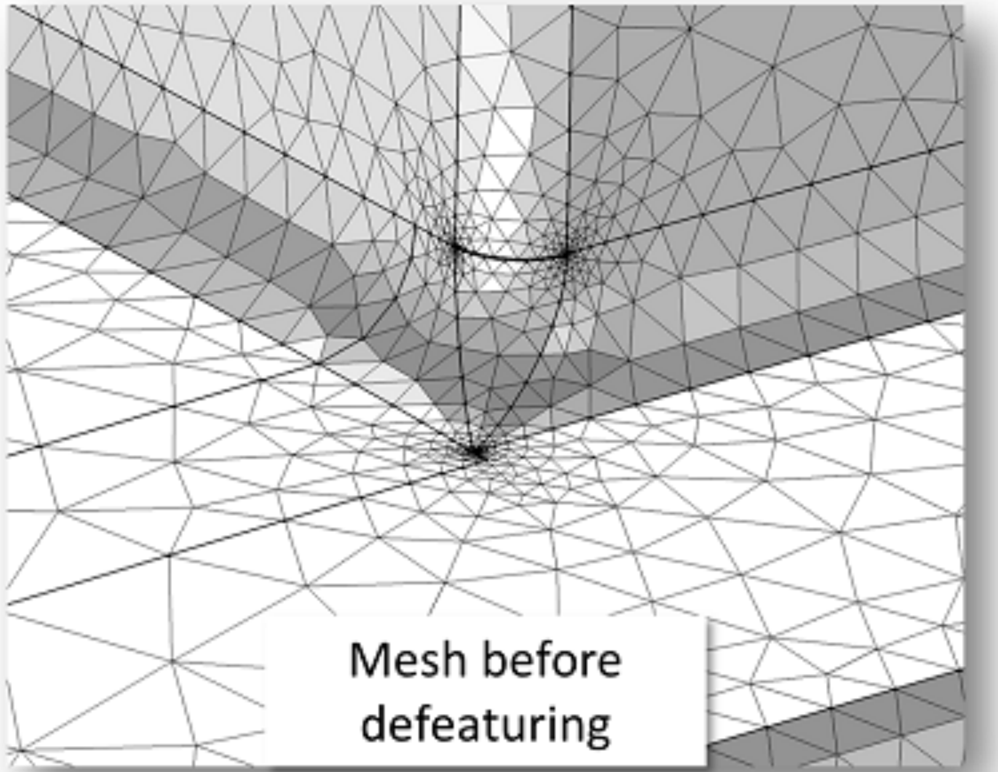
- reduce computational time
- reveal key model behaviours
- aid analysis of results
- allow for possibility of analytical solutions

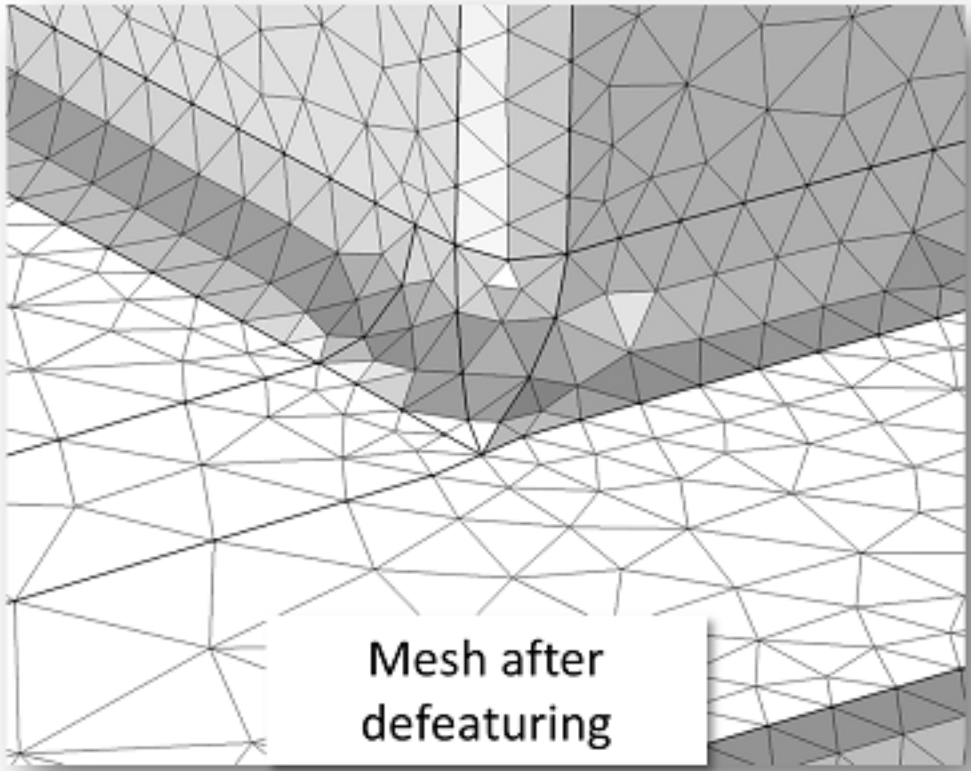
MODEL SIMPLIFICATION
Possible Approaches

- Geometric simplification
- Dimensional reduction
- Use of symmetry
- Simplification of model physics

GEOMETRIC SIMPLIFICATION

- De-featuring - common when taking CAD models into FEA/CFD codes





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- Approximation by canonical geometries
  - spheres, cylinders, cubes

USE OF SYMMETRY

- Can reduce computational run time by factor of 2 or more
- Reflectional symmetry e.g. a car, boat, airplane
- Rotational symmetry e.g. pipes, turbine engines

DIMENSIONAL REDUCTION

Through The Use Of Symmetry

- Examine material parameters & boundary conditions
- Look for a coordinate axis where solution won't vary due to this combination
- Remove that dimension from the model

MODEL SIMPLIFICATION

- Analyse the different terms in the equations
- Estimate magnitude of each
- Remove any that are an order of magnitude (or more) smaller

$$\frac{\partial c}{\partial t} + \mathbf{u}.\nabla c = D\nabla^2 c + f$$

MODEL SIMPLIFICATION

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- Estimate magnitude of each
- Remove any that are an order of magnitude (or more) smaller

$$\frac{\partial c}{\partial t} + \mathbf{u}.\nabla c = \cancel{D\nabla^2 c} + f$$

FURTHER READING

- Blog post about defeaturing & other topics related to FEM & CAD

  https://www.comsol.com/blogs/working-imported-cad-designs/