Chapter 1 - Introduction

Sections 1.1-2.4 (Versteeg)

ME 2256/MEMS 1256 - Applications of Computational Heat and Mass Transfer

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Student Learning Objectives

At the end of the lecture, students should be able to:

- Understand the basics of numerics applied to a system of partial differential equations:
  1. Discretization
  2. Basics of grid generation
  3. Solution to a set of algebraic equations
- Construct the governing constitutive equations (mass, momentum, energy)

Need for CFD

- Consider the heat conduction equation in 1D:

$$\alpha^2 \frac{d^2T}{dx^2} = \frac{dT}{dt}, \quad 0<x<L,\ t>0$$

- $T = T(x,t)$
- The thermal diffusivity, α is the thermal conductivity per the quantity of the density times the specific heat:

$$\alpha(T) = \frac{\lambda(T)}{\rho(T) C_P(T)}$$

- If the materials properties are invariant with respect to T, an analytic solution exists, if initial and boundary conditions are provided:

$$T(x,0) = f(x),\ 0<x<L$$

$$T(0,t) = A,\ T(L,t) = B,\ t>0$$

Need for CFD

- The is found via separation of variables and is expressed as a series solution:

$$T(x,t) = \sum_{n=1}^{\infty} c_n e^{-n^2\pi^2\alpha^2 t/L^2} \sin\frac{n\pi x}{L}$$

$$T(x,0) = \sum_{n=1}^{\infty} c_n \sin\frac{n\pi x}{L} dx$$

$$c_n = \frac{2}{L}\int_0^L f(x) \sin\frac{n\pi x}{L} dx$$

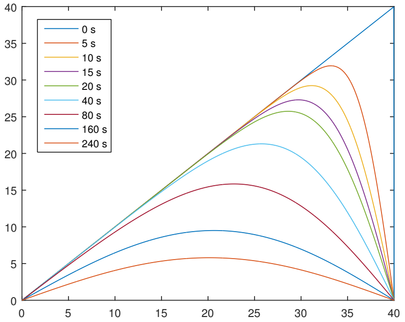
- This requires us to sum over a finite value of eigenvalues (n), but a solution is obtainable

Example #1

- Consider heat conduction within a rod that has a length of 40 [cm] whose ends at x=0 and x=L are kept at 0 °C for all t>0.
- Find the solution for $T(x, t)$, supposing α^2=1, with the initial condition T(x,0)=x for 0<x<40 and plot $T(x, t)$ versus x for t=5, 10, 15, 20, 40, 80, 160 and 240 seconds.
- See the MATLAB code titled "L1Ex1.m" posted on Canvas.

Example #1 Solution

- Thus:



- What happens when $\alpha=\alpha(T)$?

Numerics & Experiments

- The use of numerics does not supersede experiments on physical phenomena.
- Rather, numerics can be used to design experiments, while simultaneously reducing the number of experiments needed, to gain insight into a particular physics.
- Numerics can only be used as a predictive tool once the mathematical model and technique is validated against experimental data.
- The low computational costs of numerics is a major advantage over large-scale experiments, however, there are limitations.

Foundations of Numerics

- Considering the following equation:

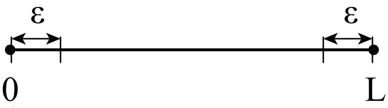
$$\frac{\partial^2 y}{\partial x^2} = f(x), \quad 0<x<L$$

- With the following boundary conditions:

$$\text{at } x = x_0,\ y = y_0$$

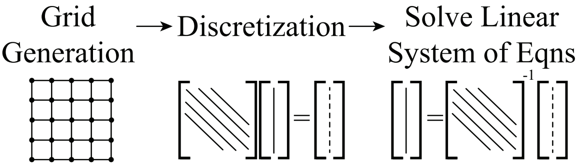
$$\text{at } x = L,\ y = y_L$$

- Differential equations are valid within the space of $[\varepsilon,\ L\text{-}\varepsilon]$, i.e. not valid on the boundary, where $\varepsilon \to 0$.



Foundations of Numerics

- Thus, a solution to a differential equation is valid both inside the domain and on the boundaries.
- When creating a numerical solution there are three main building blocks:



- Grid generation is synonymous to meshing.
- Discretization is the contruction of the mathematical model representing the physics of the problems.

Numerical Solutions to Differential Equations

- There are two types of differential equations:
  1. Ordinary Differential Equations (ODEs).
  2. Partial Differential Equations (PDEs).
- There exist numerous techniques for solving 2^{nd} PDEs
  1. Finite difference $\rightarrow$ differentiation
  2. Finite element $\rightarrow$ integration
  3. Finite volume $\rightarrow$ differentiation+integration
  4. Spectral method
  5. Finite analytic

Numerical Solutions

- Properties of Numerical Solutions

1. Consistency - the extent to which the finite system of algebraic equations approximate the underlying PDE.
2. Stability - errors from any source are not permitted to grow in sequence of numerical procedures $\rightarrow$ applicable to marching algorithms.
3. Convergence - solution of algebraic expressions approaches true solution of PDE as mesh size tends to zero.

Numerical Solutions

- Types of variables:

1. Conserved - a quantity which is governed by some conservative relationship, e.g. mass, momentum, energy.
2. Primitive - variable that is not conserved, e.g. pressure, temperature, velocity.

Numerical Error

- Goal is to identify, quantify and control numerical error in calculations.
- Error is present in any approximation, regardless of the numerical techniques employed.
- When exact mathematical operators are replaced by the approximate algebraic expressions → Truncation Error (TE), for e.g.

$$\frac{dy}{dx} = f(x, y)$$

$$\frac{dy}{dx} \approx \frac{y_{i+1} - y_i}{\Delta x} + \text{H.O.T.}$$

- When exact numbers are represented as approximate numbers → Round-off Error (RE), for e.g π=3.14 vs. π=3.14159...

Numerical Error

- Let us consider a Taylor series expansion about a point i:

$$y_{i+1} = y_i + \left.\frac{\partial y}{\partial x}\right|_i \frac{\Delta x}{1!} + \left.\frac{\partial^2 y}{\partial x^2}\right|_i \frac{\Delta x^2}{2!} + \left.\frac{\partial^3 y}{\partial x^3}\right|_i + \frac{\Delta x^3}{3!} ...$$

- The derivative can be re-expressed as

$$\left.\frac{\partial y}{\partial x}\right|_i = \frac{y_{i+1} - y_i}{\Delta x} \underbrace{- \left.\frac{\partial^2 y}{\partial x^2}\right|_i \frac{\Delta x}{2} - \left.\frac{\partial^3 y}{\partial x^3}\right|_i + \frac{\Delta x^2}{6} ...}_{\text{H.O.T represents truncation error}}$$

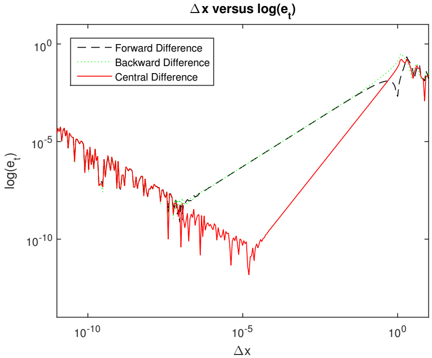
Example #2

- Consider the following expression:

$$\frac{\ln(\sin(x)^{\cos(x)})}{x^{1/3}}$$

- Approximate the derivative at x=792.93 using a forward, central and backward difference scheme. Find the optimum Δx and plot the error vs Δx.

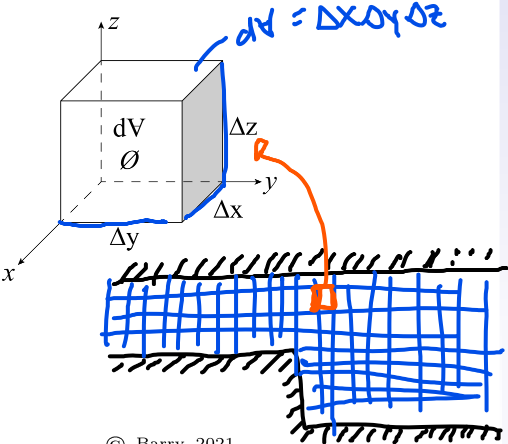
Example #2 Solution



- We see the second order accurate scheme minimizes error of the calculation.
- Note the slope of the first-order and second-order accurate schemes.

Derivation of General Transport Equation

- To illustrate the robustness of the finite-volume method, let's try to derive a generalized transport equation for an arbitrary conserved variable (ϕ)



Accumulation of ϕ

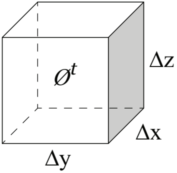
- Let us consider how a conserved variable, say energy per unit volume (specific ϕ), can change in the C.$\forall$. with respect to time
- Start Time $\rightarrow$ t
- End Time $\rightarrow$ $t + \partial t$

timestep

- ϕ at Start Time:

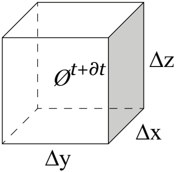
kg/m³

$$(\rho\phi)^t \underbrace{\Delta x \Delta y \Delta z}_{\partial\forall}$$



- ϕ at End Time:

$$(\rho\phi)^{t+\partial t} \underbrace{\Delta x \Delta y \Delta z}_{\partial\forall}$$



ϕ super - time, sub - spatial

- There are three mechanisms responsible for a change of ϕ in the C.$\forall$.

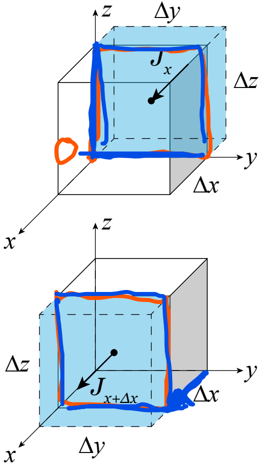
Flux of ϕ

- Let's define the rate of ϕ leaving a control surface as flux J
- In the positive x-direction, flux of ϕ entering C.∀. over ∂t:

$$(J_x)\underbrace{\Delta y \Delta z}_{dA}\Delta t$$

- In the positive x-direction, flux of ϕ exiting C.∀. over ∂t:

$$(J_{x+\Delta x})\underbrace{\Delta y \Delta z}_{dA}\Delta t$$



Flux of ϕ

- Likewise, in the y and z-directions, we have a flux of ϕ entering the C.∀. over ∂t:

$$(J_y)\Delta x \Delta z \Delta t$$

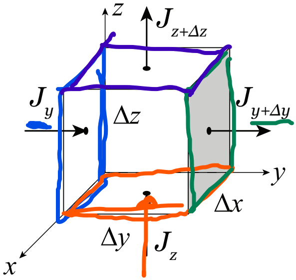
$$(J_z)\Delta x \Delta y \Delta t$$

- The flux of ϕ exiting the C.∀.:

$$(J_{y+\Delta y})\Delta x \Delta z \Delta t$$

$$(J_{z+\Delta z})\Delta x \Delta y \Delta t$$

Spatial location



Flux of ϕ

conserved quantity

- To determine the total flux of ϕ into or out of the C.∀., we sum like fluxes and combine terms:

$$(J_{x+\Delta x} - J_x)\Delta y \Delta z \Delta t + (J_{y+\Delta y} - J_y)\Delta x \Delta z \Delta t$$
$$+(J_{z+\Delta z} - J_z)\Delta x \Delta y \Delta t$$

out positive
in negative

- Recall the accumulation of ϕ within the C.∀. over some ∂t. Thus, the change of ϕ is expressed as:

$$\left[(\rho\phi)^{t+\Delta t} - (\rho\phi)^t\right]\Delta x \Delta y \Delta z$$

- We can relate the change of ϕ in the C.∀. over some time ∂t to the net flux of ϕ. For robustness, we also have to consider the generation of ϕ.

RTT: $\boxed{\left.\frac{dB}{dt}\right|_{sys}} = \frac{\delta}{\delta t}\int_{C.\forall} b\rho\, d\forall + \int_{C.S.} b\rho\, \vec{V}\cdot\hat{n}\, dA$

conserved

Internal Generation of ϕ

- We can also have ϕ generated within our control volume by some volumetric rate (S)
- Imagine examples of this:
  1. Energy - volumetric heat generation rate (q''')
  2. Species - chemical reaction rate (R)
  3. Momentum - the opposite of generation is dissipation, and friction or viscous dissipation is common in solids and fluids.
- Let's specify a general volumetric reaction rate:

$$S \Delta x \Delta y \Delta z \Delta t$$

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v}\right) = -\nabla P + \mu \nabla^2 \vec{v} - \rho \vec{g}$$

source sink source

Derivation of General Transport Equations

- Let's combine all our terms together:

solve for this

$$\underbrace{\left[(\rho\boxed{\phi})^{t+\Delta t} - (\rho\boxed{\phi})^{t}\right]\cancel{\Delta x}\cancel{\Delta y}\cancel{\Delta z}}_{\text{accumulation}} + \left(J_{x+\Delta x} - J_x\right)\cancel{\Delta y}\cancel{\Delta z}\cancel{\Delta t}$$

$$\underbrace{+\left(J_{y+\Delta y} - J_y\right)\cancel{\Delta x}\cancel{\Delta z}\cancel{\Delta t} + \left(J_{z+\Delta z} - J_z\right)\cancel{\Delta x}\cancel{\Delta y}\cancel{\Delta t}}_{\text{advection}}$$

$$= \underbrace{S\cancel{\Delta x}\cancel{\Delta y}\cancel{\Delta z}\cancel{\Delta t}}_{\text{generation}}$$

everything that can happen on and in dV

- Simplify by dividing all terms by $\Delta x \Delta y \Delta z \Delta t$

$$\frac{(\rho\phi)^{t+\Delta t} - (\rho\phi)^{t}}{\Delta t} + \frac{J_{x+\Delta x} - J_x}{\Delta x} + \frac{J_{y+\Delta y} - J_y}{\Delta y} + \ldots$$

$\frac{\partial}{\partial t}(\rho\phi)$

discretized variable!!

$$\ldots + \frac{J_{z+\Delta z} - J_z}{\Delta z} = S$$

Definition of Derivative

- Recall from your calculus classes the definition of the derivative:

Δt Δx

t t

$$\left.\frac{\partial y}{\partial x}\right|_x = \lim_{h \to 0} \frac{y(x+h) - y(x)}{h}$$

spatial

t Δt Δx

- This is applicable to both spatial and temporal terms. Let's do accumulation as an example:

$$\frac{(\rho\phi)^{t+\Delta t} - (\rho\phi)^t}{\Delta t} = \boxed{\frac{\partial}{\partial t}(\rho\phi)}$$

Simplified Transport Expression

- Doing this for each term in series yields:

$$\frac{\partial}{\partial t}(\rho\phi) + \boxed{\frac{\partial J_x}{\partial x}} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = S$$

used definition of a derivative

- What are the processes by which ϕ can be transported as J?

1. Advection - transfer of a conserved quantity by the flow of a fluid.
2. Diffusion - the movement of a conserved quantity through the imposition of a concentration gradient.

Components of Flux

1. Advection - conserved quantity transported by velocity field:

$$J_{\text{Advection}} = \rho\vec{V}\phi$$

2. Diffusion - conserved quantity transported through material from higher concentration to lower concentration:

$$\left\{\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right\}$$

$$J_{\text{Diffusion}} = -\Gamma\nabla\phi$$

diffusivity

3. The total flux is the net sum of the advection and diffusion across each control surface:

$$J_{\text{Total}} = J_{\text{Advection}} + J_{\text{Diffusion}} = \underbrace{\rho\vec{V}\phi - \Gamma\nabla\phi}$$

Expanding Flux advective term: $\rho \vec{v} \phi$

- Therefore, taking the spatial derivatives of the total flux J yields:

$$\frac{\partial J}{\partial x} = \frac{\partial}{\partial x}(\rho u \phi) - \frac{\partial}{\partial x}\left(\Gamma_x \frac{\partial \phi}{\partial x}\right)$$

$$\frac{\partial J}{\partial y} = \frac{\partial}{\partial y}(\rho v \phi) - \frac{\partial}{\partial y}\left(\Gamma_y \frac{\partial \phi}{\partial y}\right)$$

$$\frac{\partial J}{\partial z} = \frac{\partial}{\partial z}(\rho w \phi) - \frac{\partial}{\partial z}\left(\Gamma_z \frac{\partial \phi}{\partial z}\right)$$

$$\frac{\partial}{\partial x}\left(\rho u \phi - \frac{\partial}{\partial x}\left(\Gamma_x \frac{\partial \phi}{\partial x}\right)\right)$$

Transport Equation

- Substituting the expression for the total flux into the general transport equation:

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x}(\rho u\phi) + \frac{\partial}{\partial y}(\rho v\phi) + \frac{\partial}{\partial z}(\rho w\phi)$$
$$= \frac{\partial}{\partial x}\left(\Gamma_x \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma_y \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\Gamma_z \frac{\partial \phi}{\partial z}\right) + S$$

- If $\Gamma = \Gamma_x = \Gamma_y = \Gamma_z$, we have isotropic diffusion - the diffusion coefficient Γ is invariant with respect to which direction it is measure.

Transport Equation

- In vector form:

$$\underbrace{\frac{\partial}{\partial t}(\rho\phi)}_{\text{Accumulation}} + \underbrace{\nabla \cdot (\rho\vec{V}\phi)}_{\text{Advection}} = \underbrace{\nabla \cdot (\Gamma\nabla\phi)}_{\text{Diffusion}} + \underbrace{S}_{\text{Generation}}$$

- This is the General Scalar Transport Equation
- $\phi \rightarrow$ conserved quantity
- $\Gamma \rightarrow$ diffusion coefficient
- $\rho \rightarrow$ density
- $\vec{V} \rightarrow$ velocity

Continuity

- The continuity equation can be formed from the general scalar transport equation such that:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = S$$

- The continuity equation states that the rate of mass accumulating in a system must equal the rate of net mass influx.

Energy

- The general scalar transport equation can be formulated in terms of energy, which is expressed in terms of enthalpy, h. In vector form:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{V} h) = \nabla \cdot (\lambda \nabla T) + S_h$$

- Note the diffusion term is expressed in terms of temperature, T, which is not a conserved quantity. Can we transform the energy equation into the general scalar transport equation?

Energy

- From Thermodynamics, we can apply the following $dh = C_P dT$:

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \vec{V} h) = \nabla \cdot \left(\frac{\lambda}{C_P} \nabla h \right) + S_h$$

- Where we make the following transformations:
- ϕ=h
- Γ=λ / C_P
- S=S_h

Momentum

- Navier-Stokes (x-direction) for a Newtonian fluid:

$$\frac{\partial}{\partial t}\rho u + \nabla \cdot (\rho \vec{V} u) = \nabla \cdot (\mu \nabla u) - \frac{\partial P}{\partial x} + S_m$$

- Where we make the following transformations:
- $\phi = u$
- $\Gamma = \mu$
- $S = -\frac{\partial p}{\partial x} + S_m$
- Note: S will be a "dump" for all terms not diffusion, advection, or accumulation