Lecture 2 - The Finite Volume Method

Sections 4.1-4.3 (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).

Transport Equation

- Recall the transport equation in vector form:

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

- $\phi \rightarrow$ conserved quantity;
- $\Gamma \rightarrow$ diffusion coefficient;
- $\rho \rightarrow$ density;
- We are interested in solving the diffusion term first.

Diffusion Equation

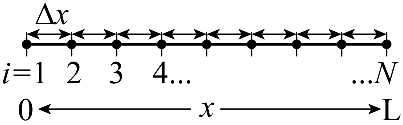
- The steady-state diffusion equation is expressed as:

$$\nabla \cdot (\Gamma \nabla \phi) = 0$$

- Let's take Γ as the thermal conductivity of the material (can be temperature dependent), and ϕ as temperature, T.
- There are two methods to solve this numerically:
  1. Finite Difference Method (FDM);
  2. Finite Volume Method (FVM).

Finite Difference Method

- We first must replace the physical, continuous domain of the problem with a mesh/grid.
- For instance, in 1D, if our domain is bounded between 0 and L, we would construct a grid of N points, separated by a distance Δx:



- Note, for FDM, it is preferable to have constant Δx, otherwise, the expressions for the derivatives becomes cumbersome using Lagrange polynomials.

1D Diffusion Equation

- The diffusion equation, in 1D, is expressed as:

$$\frac{\partial}{\partial x}\left(\lambda(T)\frac{\partial T}{\partial x}\right) = 0$$

- If λ=c:

$$\lambda\frac{\partial^2 T}{\partial x^2} = 0$$

- If $\lambda = f(T)$ (see slide 26):

$$\lambda(T)\frac{\partial^2 T}{\partial x^2} + \frac{\partial T}{\partial x}\frac{\partial \lambda(T)}{\partial x} = 0$$

- Either of these can be solved via the FDM - need to decide on a scheme.

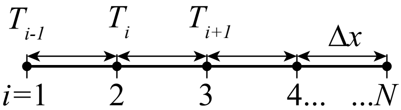
1D Diffusion Equation λ=c - FDM

- Consider the following:

$$\lambda \frac{\partial^2 T}{\partial x^2} = 0$$

- The second derivative can be approximated using a second order central difference scheme:

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} + O(\Delta x^2) = 0$$



1D Diffusion Equation λ=c - FDM

- Rearranging for T_i:

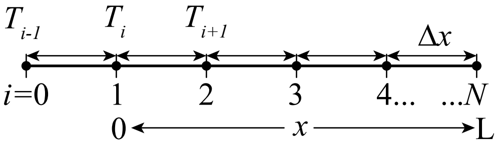
$$T_i = \frac{T_{i+1} + T_{i-1}}{2}$$

- This is valid in for $2 \leq i \leq N-1$, where i=1 and i=N are the boundary conditions.
- We see for a constant diffusion coefficient, and constant-temperature boundary conditions (Dirichlet), the steady-solution is trivial.

1D Diffusion Equation λ=c - FDM

- Now what happens if we have a Neumann boundary condition on the LHS?
- We can do a central difference expansion about $i = 1$:

$$q'' = -\lambda A \frac{\partial T}{\partial x} = -\lambda A \frac{T_2 - T_0}{2\Delta x}$$

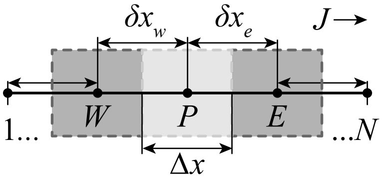


- Solving for T_0, i.e. the point on the boundary:

$$T_0 = T_2 + \frac{2\Delta x q''}{\lambda A}$$

1D Diffusion Equation - FVM

- As opposed to the FDM, we can look at what is happening within three discrete control volumes using a stencil:



- Recall J is our flux of a conserved variable; for a no flux condition:

$$\frac{dJ}{dx} = 0$$

- We can integrate this over the C.∀. centered at P, recognizing $J_e = J_w$.

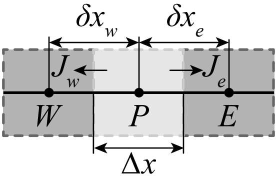
1D Diffusion Equation - FVM

- Integrating the diffusion term:

$$\int_{C.\forall.} \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right) = 0 \implies A_e \left(\Gamma \frac{\partial \phi}{\partial x}\right)\Bigg|_e = A_w \left(\Gamma \frac{\partial \phi}{\partial x}\right)\Bigg|_w$$

- Recalling from FDM, using a backward difference FD scheme:

$$\frac{\partial \phi}{\partial x} = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$



- In terms of cell-center values:

$$A_e \Gamma_e \left(\frac{\phi_E - \phi_P}{\delta x_e}\right) = A_w \Gamma_w \left(\frac{\phi_P - \phi_W}{\delta x_w}\right)$$

1D Diffusion Equation - FVM

- Expanding the expression for the backward difference of ϕ:

$$A_e \frac{\Gamma_e \phi_E}{\delta x_e} - A_e \frac{\Gamma_e \phi_P}{\delta x_e} = A_w \frac{\Gamma_w \phi_P}{\delta x_w} - A_w \frac{\Gamma_w \phi_W}{\delta x_w}$$

- Combining like ϕ:

$$\phi_P \left(A_w \frac{\Gamma_w}{\delta x_w} + A_e \frac{\Gamma_e}{\delta x_e} \right) = \phi_E \left(A_e \frac{\Gamma_e}{\delta x_e} \right) + \phi_W \left(A_w \frac{\Gamma_w}{\delta x_w} \right)$$

- We can specify coefficients to simplify the equation:

$$a_P = A_w \frac{\Gamma_w}{\delta x_w} + A_e \frac{\Gamma_e}{\delta x_e}; \quad a_W = A_w \frac{\Gamma_w}{\delta x_w}; \quad a_E = A_e \frac{\Gamma_e}{\delta x_e}$$

- Thus, the equation becomes:

$$a_P \phi_P = a_W \phi_W + a_E \phi_E = \sum a_{nb} \phi_{nb}$$

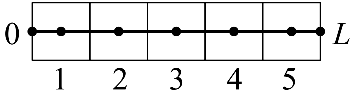
with $a_P = a_W + a_E$

Example #1

- Let us consider 1D conduction with the following:

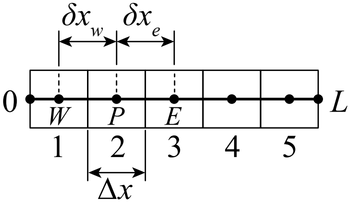
$$L = 1\,[\text{m}]$$
$$\Gamma = \lambda = 1\,[\text{W/m-K}]$$
$$\phi(0) = T(0) = 100\,[\text{K}]$$
$$\phi(L) = T(L) = 200\,[\text{K}]$$
$$A_e = A_w = A = 1\,[\text{m}^2]$$

- This is schematically shown as:



Example #1

- Denoting distances:



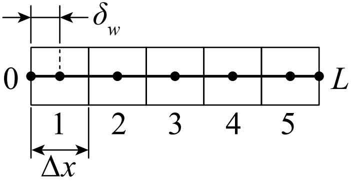
- Starting with the interior C.∀.s (2, 3 and 4):

$$\text{C.}\forall.\,2:\; a_P(2)T_2 - a_E(2)T_3 - a_W(2)T_1 = 0$$

$$\text{C.}\forall.\,3:\; a_P(3)T_3 - a_E(3)T_4 - a_W(3)T_2 = 0$$

$$\text{C.}\forall.\,4:\; a_P(4)T_4 - a_E(4)T_5 - a_W(4)T_3 = 0$$

Example #1



- At C.∀.1:

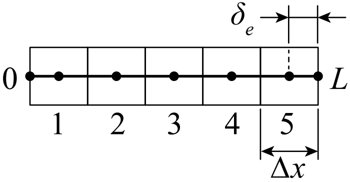
$$\text{C.}\forall.\,1:\; a_P(1)T_1 - a_E(1)T_2 - a_W(1)T_0 = 0$$

- T_0 is the temperature at the left boundary, but what is $a_W(1)$?

$$a_W = A_w\frac{\Gamma_w}{\delta x_w} = A\frac{\lambda_w}{\delta_w} = A\frac{\lambda_w}{\left(\dfrac{\Delta x}{2}\right)}$$

$$\implies a_W = A\frac{2\lambda_w}{\Delta x}$$

Example #1



- At C.∀.5:

$$\text{C.}\forall.5: \; a_P(5)T_5 - a_E(5)T_6 - a_W(5)T_4 = 0$$

- T_6 is the temperature at the right boundary, but what is $a_E(5)$?

$$a_E = A_e\frac{\Gamma_e}{\delta x_e} = A\frac{\lambda_e}{\delta_e} = A\frac{\lambda_e}{\left(\dfrac{\Delta x}{2}\right)}$$

$$\implies a_E = A\frac{2\lambda_E}{\Delta x}$$

Example #1

- We have the following system of equations:

$$\text{C.}\forall.\,1: \; a_P(1)T_1 - a_E(1)T_2 - a_W(1)T_0 = 0$$
$$\text{C.}\forall.\,2: \; a_P(2)T_2 - a_E(2)T_3 - a_W(2)T_1 = 0$$
$$\text{C.}\forall.\,3: \; a_P(3)T_3 - a_E(3)T_4 - a_W(3)T_2 = 0$$
$$\text{C.}\forall.\,4: \; a_P(4)T_4 - a_E(4)T_5 - a_W(4)T_3 = 0$$
$$\text{C.}\forall.\,5: \; a_P(5)T_5 - a_E(5)T_6 - a_W(5)T_4 = 0$$

- Assembly the system of equations, in matrix form:

$$\begin{bmatrix} a_P(1) & -a_E(1) & 0 & 0 & 0 \\ -a_W(2) & a_P(2) & -a_E(2) & 0 & 0 \\ 0 & -a_W(3) & a_P(3) & -a_E(3) & 0 \\ 0 & 0 & -a_W(4) & a_P(4) & -a_E(4) \\ 0 & 0 & 0 & -a_W(5) & a_P(5) \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} a_W(1)T_0 \\ 0 \\ 0 \\ 0 \\ a_E(5)T_6 \end{bmatrix}$$

- This can be solved via inversion, fixed-point iteration, row-reduction, etc., which will be covered in Lecture 4. See “L2Ex1.m” for the code.

Boundary Conditions

- Let's formulate a generalized discretization for 1D diffusion to include boundary conditions, denoted by the coefficient a_b and conserved quantity ϕ_b:

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

- Alternatively, if there is a flux boundary condition, denoted by q:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_b\phi_b + q$$

- If cell face not a boundary:

$$a_b = q = 0$$

- If boundaries are at C.∀., for a constant cell size:

$$a_b = A_b\frac{\Gamma_b}{\delta x_b} = A_b\frac{2\Gamma_b}{\Delta x}$$

Boundary Conditions

- There are two types of boundary conditions:

1. Dirichlet:

$$\phi_b = c \text{ i.e. given}$$

$$a_b\phi_b \text{ is known - move to RHS of eqn.}$$

2. Neumann:

$$+(\Gamma\nabla\phi)_B = q_{\text{b,given}}$$

$$J_b = q_{\text{b,given}} \text{ - move to RHS of eqn.}$$

Boundary Conditions

- To summarize:

$$-a_W\phi_W + a_P\phi_P - a_E\phi_E = \underbrace{a_b\phi_b}_{\text{Dirichlet}} + \underbrace{q_{b,\text{given}}A_b}_{\text{Neumann}}$$

- where:

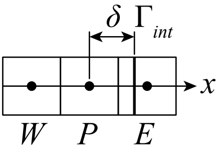
$$a_W = A_w\frac{\Gamma_w}{\delta x_w},\ a_E = A_e\frac{\Gamma_e}{\delta x_e},\ a_b = A_b\frac{2\Gamma_b}{\Delta x}$$

$$a_P = A_w\frac{\Gamma_w}{\delta x_w} + A_e\frac{\Gamma_e}{\delta x_e} + A_b\frac{2\Gamma_b}{\Delta x} = a_W + a_E + a_b$$

- Thus, you can make a more generalized code out of "L2Ex1.m" through the implementation of a_b.

Interfacial Diffusivity

- Lastly, how do we determine the diffusivity at the interface? One method is linear interpolation (i.e. arithmetic mean):



$$\Gamma_{int} = \delta\Gamma_E + (1-\delta)\Gamma_P$$

- where:

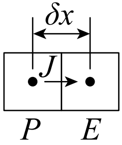
$$\delta = \frac{x - x_P}{x_E - x_P} \qquad \begin{aligned} x = x_P,\ \delta = 0 &\implies \Gamma_P \\ x = x_E,\ \delta = 1 &\implies \Gamma_E \end{aligned}$$

- At the midpoint:

$$\delta = 0.5 \implies \Gamma_{int} = \frac{\Gamma_E + \Gamma_P}{2}$$

Interfacial Diffusivity

- Now what happens when two materials exists on opposite sides of the interface?



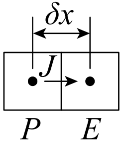
- Let's assume λ_E=0, i.e. a perfect insulator. Using linear interpolation:

$$\lambda_{int} = \frac{\lambda_P + \lambda_E}{2} = 0.5\lambda_P$$

- This leads to flux entering said perfect insulator, which means linear interpolation is incorrect.

Interfacial Diffusivity

- Let's try to formulate an interface diffusivity on the basis of flux conservation (composite slab):



$$J = -\lambda_{int}\frac{\partial T}{\partial x} = \frac{\lambda_{int}(T_E - T_P)}{\delta x_e}$$

$$\implies J = \frac{T_E - T_P}{\dfrac{1-\delta}{\lambda_P} + \dfrac{\delta}{\lambda_P}}$$

- Let's define the denominator as the effective diffusivity:

$$\lambda_{int} = \left[\frac{1-\delta}{\lambda_P} + \frac{\delta}{\lambda_E}\right]^{-1}$$

Interfacial Diffusivity

- Assuming the interface is equidistant from both C.∀. centroids (i.e. $\delta = 0.5$):

$$\lambda_{int} = \left[\frac{0.5}{\lambda_P} + \frac{0.5}{\lambda_E}\right]^{-1}$$

$$\lambda_{int} = \frac{2\lambda_P\lambda_E}{\lambda_P + \lambda_E}$$

- Let's check for consistency:

$$\lambda_E \to 0 \text{ or } \lambda_P \to 0 \implies J = 0$$

Interfacial Diffusivity

- Considering the other extreme case of $\lambda_P \to \infty$:

$$\frac{2\lambda_P\lambda_E}{\lambda_P + \lambda_E} \to \frac{2\lambda_P\lambda_E}{\lambda_P\left(1 + \frac{\lambda_E}{\lambda_P}\right)} \to \frac{2\lambda_E}{1 + \frac{\lambda_E}{\lambda_P}}$$

- This implies that the interface diffusivity tends to:

$$\lambda_{int} = 2\lambda_E$$

- This would mean that the rate of diffusion is limited by the least diffusive material.
- Note: the harmonic average always yields a value less than that determined by the arithmetic average.

1D Diffusion Equation $\lambda = f(T)$ - FDM

- Consider the following

$$\lambda(T)\frac{\partial^2 T}{\partial x^2} + \frac{\partial T}{\partial x}\frac{\partial \lambda(T)}{\partial x} = 0$$

- Using a second-order central differencing scheme:

$$\lambda_i\left(\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}\right) + \left(\frac{T_{i+1} - T_{i-1}}{2\Delta x}\right)\left(\frac{\lambda_{i+1} - \lambda_{i-1}}{2\Delta x}\right)$$

$$... = 0$$

- Rearranging for T_i:

$$T_i = \frac{T_{i+1} - T_{i-1}}{2} + \frac{(T_{i+1} - T_{i-1})(\lambda_{i+1} - \lambda_{i-1})}{8\lambda_i}$$