Notes on Finite Volume Method MME 9710

Max Le

December 18, 2021

Contents

1	CH.	APTER 1: INTRODUCTION	2
	1.1	Generic Conservation Equation	2
	1.2	Mass Conservation Equation	2
	1.3	Momentum Conservation Equation	2
	1.4	Energy Conservation Equation	3
	1.5	Discretization of the Generic Conservation Equation	3
	1.6	Main idea behind Discretization	4
	1.7	Determine Cell Centre + Face Integration Points	4
	1.8	Transient term	5
	1.9	Advection term	5
	1.10	Diffusion term	6
	1.11	Source term	6
	1.12	Linearization	6
2	CH.	APTER 2: STEADY DIFFUSION EQUATION	7
	2.1	Problem Definition	7
	2.2	Discretization	7
	2.3	Source Terms	10
	2.4	Discussion of Discretization Procedure	10
		2.4.1 Temperature Profile Assumptions	10
		2.4.2 Implementation of Linearization	10
		2.4.3 Properties of the Discrete Algebraic Equations	11

1 CHAPTER 1: INTRODUCTION

1.1 Generic Conservation Equation

Consider the following generic conservation equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) + \nabla \cdot \mathbf{J}_{\phi} = S_{\phi} \tag{1}$$

where the variables are defined as:

$\mathbf{Variable}$	Description
$\overline{\phi}$	Generic variable
t	Time
\mathbf{u}	Velocity vector
\mathbf{J}_{ϕ}	Diffusive flux of ϕ
S_{ϕ}	Volumetric source/sink of ϕ

1.2 Mass Conservation Equation

Setting $\phi = \rho$, where ρ is the density. Also, mass conservation of a continuous substance does not have diffusive flux $=> \mathbf{J}_{\rho} = 0$.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{u}\rho) = S_{\rho} \tag{2}$$

Notes:

• For incompressible, constant density flow:

$$-\frac{\partial \rho}{\partial t} = 0$$

$$- \nabla \cdot (\mathbf{u}\rho) = \rho \nabla \cdot \mathbf{u}$$

– Result in:
$$\nabla \cdot \mathbf{u} = \frac{S_{\rho}}{\rho}$$

– And if no source/sink => $\nabla \cdot \mathbf{u} = 0$

1.3 Momentum Conservation Equation

Setting $\phi = \rho \mathbf{u}$. Diffusive flux term $\mathbf{J}_{\mathbf{u}} = -\nabla \cdot \boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ is the fluid stress tensor.

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \sigma + S_{\mathbf{u}}$$
(3)

The stress tensor, σ can be expressed in terms of pressure (p) and viscous stress tensor (τ) and identity matrix, I:

$$\sigma = -p\mathbf{I} + \tau \tag{4}$$

After substituting, we get the following form of the momentum conservation equation:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + S_{\mathbf{u}}$$
 (5)

For incompressible Newtonian fluid, we can rewrite τ in terms of the dynamic viscosity, $\mu \tau = \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$. Thus, a momentum conservation equation for incompressible, Newtonian fluid, constant velocity:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + S_{\mathbf{u}}$$
 (6)

1.4 Energy Conservation Equation

Setting $\phi = \rho h$ with h being the specific enthalpy of a substance at a given state. Thus, the unit for ϕ is energy per unit volume. The diffusive flux is given by Fourier's law: $J = -k\nabla \mathbf{T}$ with k is the thermal conductivity.

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u}h) = \nabla \cdot (k\nabla \mathbf{T}) + S_h \tag{7}$$

If we assume:

- incompressible flow
- \bullet constant specific heat capacity, $h=c_p \mathbf{T}$
- constant thermophysical properties $(k \text{ and } \rho)$
- no source term

$$\frac{\partial(\mathbf{T})}{\partial t} + \nabla \cdot (\mathbf{u} \ \mathbf{T}) = \alpha \nabla^2 \mathbf{T}$$
 (8)

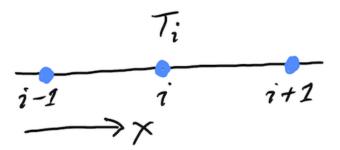
where $\alpha = \frac{k}{\rho c_p}$ is the thermal diffusivity.

1.5 Discretization of the Generic Conservation Equation

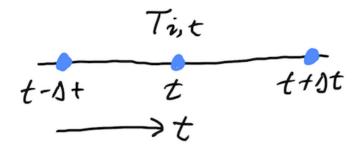
Our generic variable, ϕ is a function of of spatial and time: $\phi = \phi(\mathbf{x}, t)$, where $\mathbf{x} = (x, y, z)$. Note that spatial variable can be influenced "one way_" or "two way_", i.e.

- One way: changes in ϕ only occur due to change on one side of that location
- Two way: changes in ϕ occur due to changes on both side of that location.

For example, heat conduction in the image below at cell i is influenced by cell i-1 and i+1. Here, \mathbf{x} is a two way coordinate for heat conduction



Now consider transient heat convection/conduction. The temperature at any given time is influenced by existing conditions before that point **in time**. Here, **t** is a <u>one way</u> coordinate for transient heat conduction/convection



Recall our generic conservation equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) + \nabla \cdot \mathbf{J}_{\phi} = S_{\phi}$$

We consider the diffusion term or **elliptic PDE** : $\nabla \cdot \mathbf{J}_{\phi}$ to be <u>two-way in space</u> Likewise, the convection term or **parabolic PDE** : $\nabla \cdot (\mathbf{u}\phi)$ to be <u>one-way in space</u>

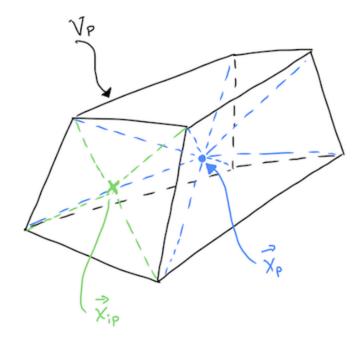
1.6 Main idea behind Discretization

Our goal is to:

• replace the PDEs' continuous solution with <u>discrete</u> solution, at <u>specific location</u> that approximates the continuous solution suitably.

For finite volume:

- domain is split into non overlapping finite regions that fill the domain
- the discrete point is at the centroid of each control volume with volume V_p , at position \mathbf{x}_p
- surround these cells, we have the "faces". At the center of these "faces", we have the integration point at position \mathbf{x}_{ip}
- the governing equations are then integrated over a control volume, where surface flux terms and volume source terms are balanced.



1.7 Determine Cell Centre + Face Integration Points

Cell centre => location of solution variables.

Points on face => fluxes are evaluated.

Consider a volume integral of a quantity ϕ , we may express this integral in discrete form as follow:

$$\int_{V} \phi dV \approx \phi_P V_P \tag{9}$$

where ϕ_P is the value of ϕ at some internal within V and V_P is total volume of the cell:

$$V_P = \int_V dV \tag{10}$$

To prove the above result, we expand ϕ in a Taylor series about the point P.

$$\phi \approx \phi_P + \nabla \phi_P(\mathbf{x} - \mathbf{x}_P) + \nabla^2 \phi_P(\mathbf{x} - \mathbf{x}_P)(\mathbf{x} - \mathbf{x}_P) + \dots O(\delta^3)$$
(11)

with δ being the characteristic grid spacing. Substitute this into our assumed expression for V_P :

$$\int_{V} \phi dV \approx \int_{V} [\phi_{P} + \nabla \phi_{P}(\mathbf{x} - \mathbf{x}_{P}) + \nabla^{2} \phi_{P}(\mathbf{x} - \mathbf{x}_{P})(\mathbf{x} - \mathbf{x}_{P}) + \dots O(\delta^{3})] dV$$
(12)

We note that ϕ_P and its derivatives are constants:

$$\int_{V} \phi dV \approx \phi_{P} dV + \nabla \phi_{P} \int_{V} (\mathbf{x} - \mathbf{x}_{P}) dV + \nabla^{2} \phi_{P} \int_{V} (\mathbf{x} - \mathbf{x}_{P}) (\mathbf{x} - \mathbf{x}_{P}) dV + \dots O(\delta^{3})$$
(13)

Because our \mathbf{x}_P point is at centroid, so $\int_V (\mathbf{x} - \mathbf{x}_P) dV = 0$. Likewise, the last term is also neglected, resulting in:

$$\int_{V} \phi dV \approx [\phi_V + O(\delta^2)] V_P \tag{14}$$

This means that there is a second order error when approximating the cell volume in this way. This is OK because the accuracy of the method is also second order.

Note: If our x_P does not lie at the centroid of the cell. The second term, $\int_V (\mathbf{x} - \mathbf{x}_P) dV$ does not go to zero, making our approximation to be 1st order, which is worse.

1.8 Transient term

Here we deal with the transient term, $\frac{\partial \phi}{t}$. Discretization of this term relies on:

- order of accuracy
- implicit vs explicit

The idea is to integrate this term over control volume V_P and some time step $\Delta t = t_1 - t_0$ to get the formula for the discretization.

$$\int_{t_0}^{t_1} \int_{V} \frac{\partial \phi}{\partial t} dV dt \approx (\phi V_P)^{t_1} - (\phi V_P)^{t_0}$$
(15)

1.9 Advection term

Here we deal with the advection term, $\nabla \cdot (\mathbf{u}\phi)$. Similar to the transient term, the formula for the discretization can be obtained by integrating over the control volume V_P . We also employ Gauss' theorem to convert volume integral to surface integral:

$$\int_{V} \nabla \cdot (\mathbf{u}\phi) dV = \int_{S} (\mathbf{u}\phi) \cdot \mathbf{n} dS \tag{16}$$

For the surface integral, we approximate by summing up over the faces surrounding the cell, each with area A_{ip} .

$$\int_{S} (\mathbf{u}\phi) \cdot \mathbf{n}_{ip} dS \approx \sum_{i=0}^{N_{ip}-1} \mathbf{u}_{ip} \cdot \mathbf{n}_{ip} \phi_{ip} A_{ip}$$
(17)

Note:

- using C program notation, so we sum from 0 till $N_{ip}-1$
- approximate \mathbf{u}_{ip} by many interpolation methods
- interpolating ϕ_{ip} carefully to obtain <u>stable</u> numerical method.

1.10 Diffusion term

Now, we deal with the diffusion term, $\nabla \cdot \mathbf{J}_{\phi}$. Similar to the advection term, we integrate over a control volume, then apply Gauss' theorem

$$\int_{V} \nabla \cdot \mathbf{J}_{\phi} dV = \int_{S} \mathbf{J}_{\phi} \cdot \mathbf{n} dS \tag{18}$$

Again, the surface integral is approximated as discrete sum over the faces surrounding the cell:

$$\int_{S} \mathbf{J}_{\phi} \cdot \mathbf{n} dS \approx \sum_{i=0}^{N_{ip}-1} \mathbf{J}_{\phi,ip} \cdot \mathbf{n}_{ip} \mathbf{A}_{ip}$$
(19)

where the flux, $\mathbf{J}_{\phi,ip}$ is interpolated from neighboring cell values.

1.11 Source term

Recall our source term: S_{ϕ} , we assume that the source term is <u>piecewise continuous</u>, with one specific value, S_{ϕ} , being represented by each cell. We can then write:

$$\int_{V} S_{\phi} dV \approx S_{\phi} V_{P} \tag{20}$$

Generally, the source term may depend on ϕ so linearization is needed to obtain <u>stable</u> numerical method.

1.12 Linearization

With regard to our last point about J_{ϕ} , the discretized terms depend non linearly on the solution. This non-linearity is caused by:

- source term depend non linearly on primitive variable, e.g. J_{ϕ} .
- non linearities in the governing equation, e.g. advection term $\nabla \cdot (\mathbf{u}\phi)$
- on non-orthogonal grid, gradient correction terms are needed <= these are non linear.

To linearize, we assume the governing PDE is represented by the following general differential operator

$$L(\phi^*) = 0 \tag{21}$$

where:

- ϕ^* = the continuous solution to the PDE
- Note that to solve a PDE using finite volume, the continuous solution ϕ^* is approximated by the discrete solution vector $\phi \in \mathbb{R}$ on N number of control volume. Our PDE is then integrated over each control volume and each term in the governing equation is approximated using the discrete solution ϕ
- Of course, the numerical solution will not satisfy the discretized equation exactly; rather we will have a residual, $\mathbf{r} \in \mathbb{R}^N$.

We expand the residual about the solution ϕ_i at iteration i, and find the solution where r=0:

$$\mathbf{r}(\phi_i) + \frac{\partial \mathbf{r}}{\partial \phi} \bigg|_{\phi_i} (\phi - \phi_i) = 0 \tag{22}$$

We define the **Jacobian of the residual vector** as:

$$\mathbf{J}(\phi) = \frac{\partial \mathbf{r}}{\partial \phi} \tag{23}$$

We use this to update according to fix point iteration:

$$\phi = \phi_i + \Delta \phi_i \tag{24}$$

where:

$$\Delta \phi = (\phi - \phi_i) \tag{25}$$

and:

$$\mathbf{J}(\phi_i)\Delta\phi = -\mathbf{r}(\phi_i) \tag{26}$$

The remaining unknowns are: the residual vector \mathbf{r} and Jacobian matrix $\mathbf{J}(\phi_i)$.

Note: we can express the linear system for a control volume P as:

$$a_P \delta \phi_P + \sum_{nb} a_{nb} \delta \phi_{nb} = -r_P \tag{27}$$

where nb is sum over all neighboring cells. The coefficients are defined as:

$$a_P = \frac{\partial r_P}{\partial \phi_P} \tag{28}$$

$$a_{nb} = \frac{\partial r_P}{\partial \phi_{nb}} \tag{29}$$

2 CHAPTER 2: STEADY DIFFUSION EQUATION

2.1 Problem Definition

We consider the solution of a steady, 1D heat diffusion equation

$$-k\nabla^2 T - S = 0 (30)$$

2.2 Discretization

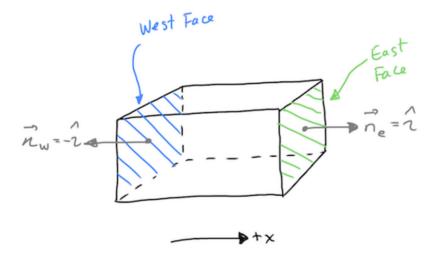
Recall our diffusion term can be discretized as:

$$\int_{S} \mathbf{J} \cdot \mathbf{n} dS \approx \sum_{i=0}^{N_{ip}-1} \mathbf{J}_{ip} \cdot \mathbf{n}_{ip} A_{ip}$$
(31)

Our flux **J** here is the diffusive flux, so: $\mathbf{J} = -k\nabla T$. Thus:

$$\int_{S} \mathbf{J} \cdot \mathbf{n} dS \approx -\sum_{i=0}^{N_{ip}-1} k_{ip} \nabla T_{ip} \cdot \mathbf{n}_{ip} A_{ip}$$
(32)

We assume constant thermal conductivity, $k_{ip} = k$. A 1D control volume, with West/East faces and unit vectors drawn, is shown below:



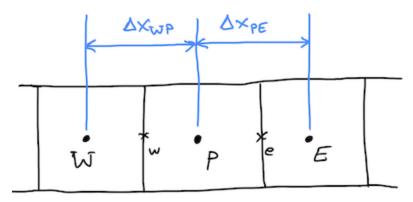
Since we are in 1D, our unit vector is in the i only.

Thus, $\nabla T \cdot \mathbf{n} = \nabla T \cdot \mathbf{i}$.

But,
$$\nabla T \cdot \mathbf{i} = \left\langle \frac{\partial T}{\partial x} \mathbf{i} + \frac{\partial T}{\partial y} \mathbf{j} + \frac{\partial T}{\partial z} \mathbf{k} \right\rangle \cdot \left\langle 1 \mathbf{i} + 0 \mathbf{j} + 0 \mathbf{k} \right\rangle = \frac{\partial T}{\partial x}$$
. With these points in mind, the discretization for the diffusion term is simplified to:

$$\int_{S} \mathbf{J} \cdot \mathbf{n} dS \approx k \left. \frac{\partial T}{\partial x} \right|_{w} A_{w} - k \left. \frac{\partial T}{\partial x} \right|_{e} A_{e} \tag{33}$$

The diagram below shows the cell locations and the nomenclature for the distance between them, note how Δx is center-center



We apply finite differences to the derivatives in the diffusion term, i.e.:

$$k \left. \frac{\partial T}{\partial x} \right|_{w} A_{w} - k \left. \frac{\partial T}{\partial x} \right|_{e} A_{e} = k \frac{T_{P} - T_{W}}{\Delta x_{WP}} A_{w} - k \frac{T_{E} - T_{P}}{\Delta x_{PE}} A_{e}$$
 (34)

Our discretized source term is simply:

$$\int_{V} SdV \approx S_{P}V_{P} \tag{35}$$

where S_P = value of source term within the cell, and V_P = cell volume.

Put everything on one side, we can form the residual equation for the cell \mathbf{P} as:

$$r_P = -k \frac{T_E - T_P}{\Delta x_{PE}} A_e + k \frac{T_P - T_W}{\Delta x_{WP}} A_w - S_P V_P$$
(36)

or expressing in terms of the diffusive fluxes, \mathbf{F}^d , through each face:

$$r_P = F_e^d - F_w^d - S_P V_P (37)$$

where:

$$F_e^d = -k \frac{T_E - T_P}{\Delta x_{PE}} A_e = -D_e (T_E - T_P)$$
(38)

$$F_w^d = -k \frac{T_P - T_W}{\Delta x_{WP}} A_w = -D_w (T_P - T_W)$$
(39)

$$D_e = \frac{kA_e}{\Delta x_{PE}} \tag{40}$$

$$D_e = \frac{kA_e}{\Delta x_{PE}}$$

$$D_w = \frac{kA_w}{\Delta x_{WP}}$$

$$(40)$$

Our cell residual equation is then:

$$r_P = D_w(T_P - T_W) - D_e(T_E - T_P) - S_P V_P$$
(42)

The linearized coefficients are then calculated as:

$$a_P = \frac{\partial r_P}{\partial T_P} = D_w + D_e - \frac{\partial S_P}{\partial T_P} V_P \tag{43}$$

$$a_W = \frac{\partial r_P}{\partial T_W} = -D_w \tag{44}$$

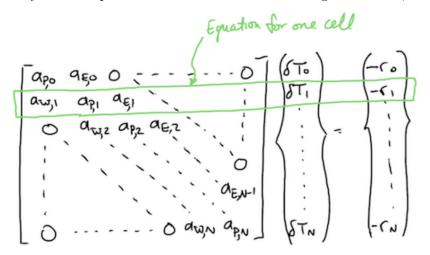
$$a_E = \frac{\partial r_P}{\partial T_E} = -D_e \tag{45}$$

Recall that we can form an algebraic system of equation for each control volume like this:

$$a_P \delta \phi_P + \sum_{nb} a_{nb} \delta \phi_{nb} = -r_P \tag{46}$$

$$a_P \delta T_P + a_W \delta T_W + a_E \delta T_E = -r_P \tag{47}$$

The above linear system of equations can be written as as tridiagonal matrix, like this:



Note: The first and last row only has 2 non zero elements each. This is because these are the left most/right most side and they are adjacent to the domain boundary. Therefore, special boundary conditions are needed to be set.

In matrix notation, we are solving:

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{48}$$

where **A** is the Jacobian matrix, $\mathbf{b} = -\mathbf{r}$ is the residual vector, $\mathbf{x} = \delta \mathbf{T}$ is the solution correction. At each current iteration i, the solution is updated according to:

$$\mathbf{T} = \mathbf{T}_i + \delta \mathbf{T}i \tag{49}$$

2.3 Source Terms

Our source term can have many forms, depending on the type of heat source. We will assume external convection and radiation exchange:

• For external convection:

$$\frac{S_{conv,P}}{V_P} = -hA_0(T_P - T_{\infty,c}) \tag{50}$$

where:

- -h is the convective coefficient.
- $-A_0$ is external surface area of the cell P.
- $-T_P$ is temperature at the centroid of cell P.
- $-T_{\infty,c}$ is the ambient temperature for the convection process.
- For radiation exchange:

$$\frac{S_{rad}}{V_P} = -\epsilon \sigma A_0 (T_P^4 - T_{\infty,r}^4) \tag{51}$$

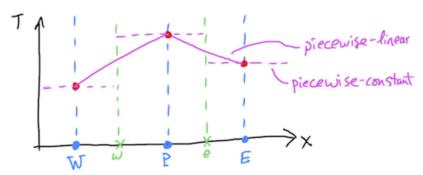
where:

- $-\epsilon$ is the surface emissivity.
- $-\sigma$ is the Stefan-Boltzmann constant.
- $-T_{\infty,r}$ is the surrounding temperature for radiation exchange.

2.4 Discussion of Discretization Procedure

2.4.1 Temperature Profile Assumptions

When computing the diffusive fluxes through the faces, we assumed a **piecewise-linear profile** for the temperature. This ensures that the derivatives are defined at the integration points and provides consistency for flux at control-volume faces. For the source term, **piece-wise constant profile** is used, implying a single value of the source term in each cell. Note that for piece-wise constant profile, the derivatives are not defined at integration points, due to jump discontinuity. So if fluxes will be inconsistent if piecewise-constant profile is used for temperature.



2.4.2 Implementation of Linearization

In Patakar's method, the solution of the linear system **is** the solution for the variables at the control volume center.

In our method, the solution of the linear system is the **correction** to apply to the previous iteration of the solution.

The correction method is preferred because:

- at convergence, the solution for the correction goes to zero → zero a good initial guess for the linear solver.
- linear system involves the residual vector. In Patankar's, there are more work to calculate the residual vector.

2.4.3 Properties of the Discrete Algebraic Equations

Recall our algebraic equation for the linear system

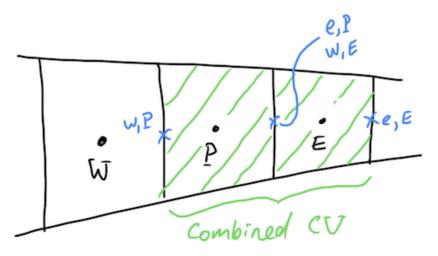
$$a_P \delta T_P + a_W \delta T_W + a_E \delta T_E = -r_P \tag{52}$$

In Rule 2, we require that $a_P > 0$ and $a_W, a_E < 0$. The reason for this is if we consider the case with no source, and the solution converge, $r_P \to 0$:

$$a_P \delta T_P = -a_W \delta T_W - a_E \delta T_E \tag{53}$$

Now, suppose both T_P and T_E are pertubed. If either of these temperatures were to rise, then T_P would also rise. Similarly, if either temperatures were to drop, T_P should also drop. Therefore, to ensure correct physical effect, if $a_P > 0$ then $a_W, a_E > 0$.

Consider the two cells (P and E) below:



At convergence, $r_P = 0$, the equation for the control volume P is:

$$F_{e,P}^d - F_{w,P}^d - S_P V_P = 0 (54)$$

For the control volume E:

$$F_{e,E}^d - F_{w,E}^d - S_E V_E = 0 (55)$$

Adding these equations together gives:

$$F_{e,P}^d - F_{w,P}^d + F_{e,E}^d - F_{w,E}^d - S_P V_P - S_E V_E = 0$$
(56)

Note that $F_{e,P}^d = F_{w,E}^d$ by continuity, i.e. the flux at cell P going eastward should be the same flux going from westward at cell E. If these are not equal, then it implies that there is a fictuous force at the face, which is not reasonable. Therefore, our algebraic equation for control volume P and E becomes:

$$F_{e,E}^d - F_{w,P}^d - S_P V_P - S_E V_E = 0 (57)$$

The above equation demonstrates integral conservation: a balance of the total source term within the combined control volume with the net diffusive flux from that same control volume. In addition, recall the definition of the diffusive flux:

$$F_{e,P}^d = -k \frac{T_E - T_P}{\Delta x_{PE}} A_{e,P} \tag{58}$$

$$F_{w,E}^d = -k \frac{T_E - T_P}{\Delta x_{PE}} A_{w,E} \tag{59}$$

From the gemeotry of the grid, $A_{e,P} = A_{w,E}$; therefore, it is in fact the two-point finite difference estimation of the derivative that cause the fluxes to be equal. This is also due to the piecewise-linear profile that we assume. If we assume a **parabolic profile** instead, there is no guarantee that the fluxes would be equal. Instead, we would have:

$$F_{e,P}^{d} = f(T_W, T_P, T_E) (60)$$

$$F_{w,E}^d = f(T_P, T_E, T_{EE}) (61)$$

This means that the flux through the common face depends on different temperature, so we cannot be sure that the derivative from either side is consistent.

