Notes on Finite Volume Method MME 9710

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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:

Variable	Description
ϕ	Generic variable
t	Time
$\mathbf{u}$	Velocity vector
$\mathbf{J}_\phi$	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 $\Longrightarrow \mathbf{J}_\rho = 0$.

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

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 $\Longrightarrow \nabla \cdot \mathbf{u} = 0$

1.3   Momentum Conservation Equation

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

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

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:

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

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

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

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

- constant specific heat capacity, $h = c_p\mathbf{T}$

- constant thermophysical properties (k and ρ)

- no source term

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

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

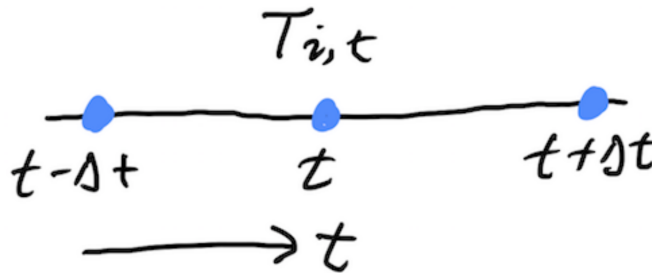## 1.5 Discretization of the Generic Conservation Equation

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 "$_{\text{one}}$ way_" or "$_{\text{two}}$ 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
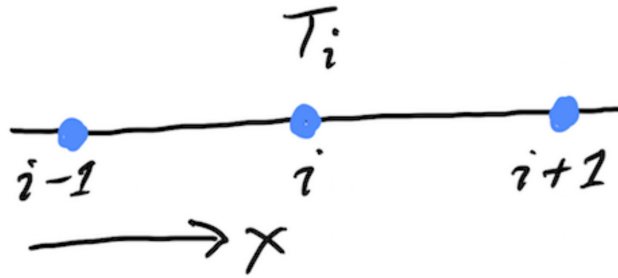
Now consider transient heat convection/conduction. The temperature at any given time is influenced by existing conditions before that point **in time**. Here, $\mathbf{t}$ is a one way coordinate for transient heat conduction/convection

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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** : $\boxed{\nabla \cdot \mathbf{J}_\phi}$ to be <u>two-way in space</u>

Likewise, the convection term or **parabolic PDE** : $\boxed{\nabla \cdot (\mathbf{u}\phi)}$ 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 <u>non overlapping finite</u> regions that fill the domain

- the discrete point is at the <u>centroid</u> 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.
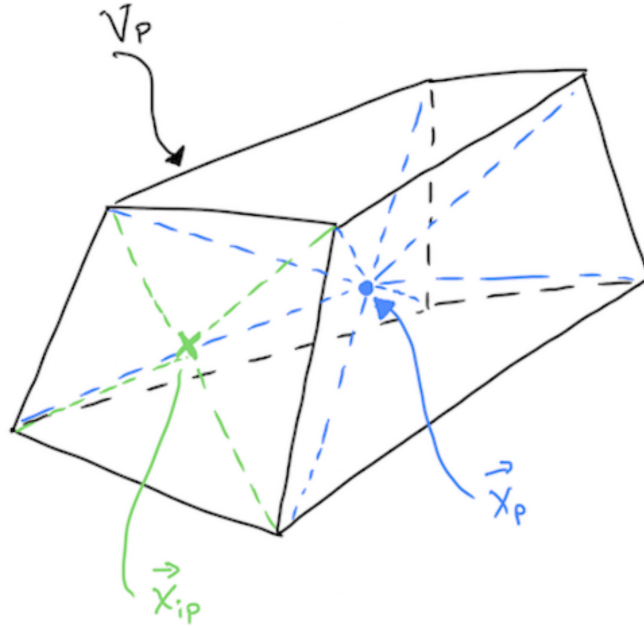
1.7   Determine Cell Centre + Face Integration Points

Cell centre => location of <u>solution</u> variables.
Points on <u>face</u> => <u>fluxes</u> 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.

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

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

$$\int_V \phi dV \approx \int_V [\phi_P + \nabla\phi_P(\mathbf{x} - \mathbf{x}_P) + \nabla^2\phi_P(\mathbf{x} - \mathbf{x}_P)(\mathbf{x} - \mathbf{x}_P) + ...O(\delta^3)]dV \tag{12}$$

We note that ϕ_P and its derivatives are constants:

$$\int_V \phi dV \approx \phi_P dV + \nabla\phi_P \int_V (\mathbf{x} - \mathbf{x}_P)dV + \nabla^2\phi_P \int_V (\mathbf{x} - \mathbf{x}_P)(\mathbf{x} - \mathbf{x}_P)dV + ...O(\delta^3) \tag{13}$$

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 $\mathbf{x}_P$} 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.

$$\int_{t_0}^{t_1} \int_V \frac{\partial\phi}{\partial t}dVdt \approx (\phi V_P)^{t_1} - (\phi V_P)^{t_0} \tag{15}$$

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}.

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

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 stable 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:

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

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:

- $\phi^* =$ 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 $r = 0$:

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

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

$$-k\nabla^2 T - S = 0 \tag{30}$$
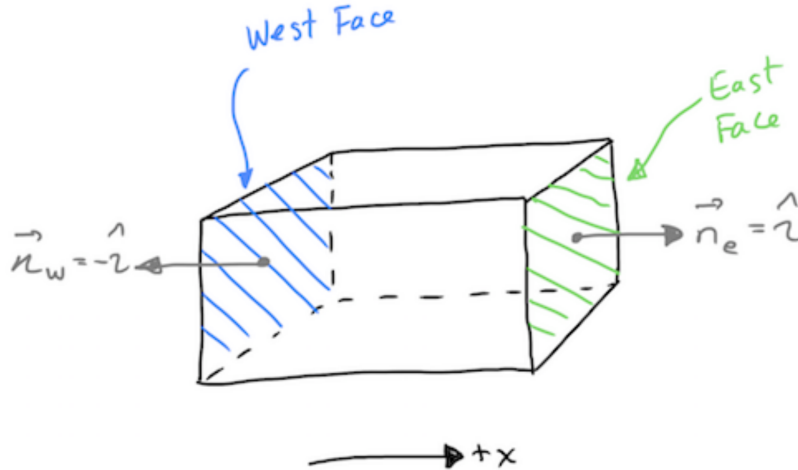
2.2 Discretization

Recall our diffusion term can be discretized as:

$$\int_S \mathbf{J} \cdot \mathbf{n} dS \approx \sum_{i=0}^{N_{ip}-1} \mathbf{J}_{ip} \cdot \mathbf{n}_{ip} A_{ip} \tag{31}$$

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

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

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

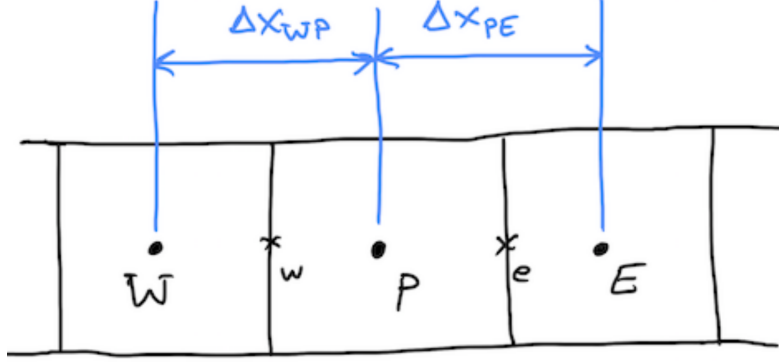Since we are in 1D, our unit vector is in the $\mathbf{i}$ only.

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

But, $\nabla T \cdot \mathbf{i} = \left\langle \frac{\partial T}{\partial x}\mathbf{i} + \frac{\partial T}{\partial y}\mathbf{j} + \frac{\partial T}{\partial z}\mathbf{k} \right\rangle \cdot \langle 1\mathbf{i} + 0\mathbf{j} + 0\mathbf{k} \rangle = \frac{\partial T}{\partial x}$.

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 <u>finite differences</u> to the derivatives in the diffusion term, i.e.:

$$k\left.\frac{\partial T}{\partial x}\right|_w A_w - k\left.\frac{\partial T}{\partial x}\right|_e A_e = k\frac{T_P - T_W}{\Delta x_{WP}}A_w - k\frac{T_E - T_P}{\Delta x_{PE}}A_e \tag{34}$$

Our discretized source term is simply:

$$\int_V S\, dV \approx S_P V_P \tag{35}$$

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

Put everything on one side, we can form the <u>residual equation</u> for the cell **P** as:

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

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

$$r_P = F_e^d - F_w^d - S_P V_P \tag{37}$$

where:

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

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

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

$$D_w = \frac{kA_w}{\Delta x_{WP}} \tag{41}$$

Our cell residual equation is then:

$$r_P = D_w(T_P - T_W) - D_e(T_E - T_P) - S_P V_P \tag{42}$$

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:

$$\mathbf{Ax} = \mathbf{b} \tag{48}$$

where $\mathbf{A}$ 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:

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