

# 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:

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

where the variables are defined as:

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

## 1.2 Mass Conservation Equation

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

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

**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  $\Rightarrow \nabla \cdot \mathbf{u} = 0$

## 1.3 Momentum Conservation Equation

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

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

The stress tensor,  $\sigma$  can be expressed in terms of pressure ( $p$ ) and viscous stress tensor ( $\tau$ ) and identity matrix,  $I$ :

$$\sigma = -p\mathbf{I} + \tau \quad (4)$$

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

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

For incompressible Newtonian fluid, we can rewrite  $\tau$  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:

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

## 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  $\phi$  is energy per unit volume. The diffusive flux is given by Fourier's law:  $J = -k\nabla T$  with  $k$  is the thermal conductivity.

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

If we assume:

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

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

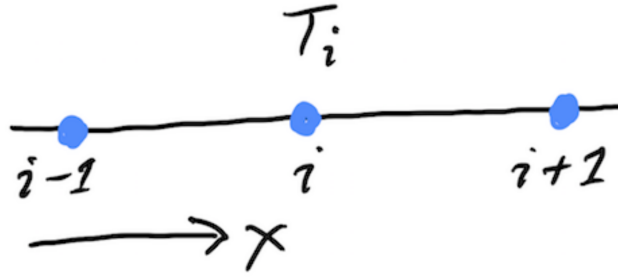
where  $\alpha = \frac{k}{\rho c_p}$  is the thermal diffusivity.

## 1.5 Discretization of the Generic Conservation Equation

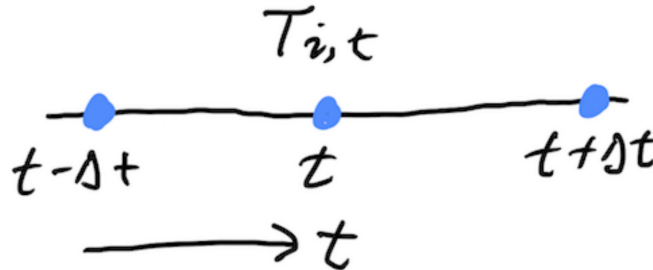
Our generic variable,  $\phi$  is a function of spatial and time:  $\phi = \phi(\mathbf{x}, t)$ , where  $\mathbf{x} = (x, y, z)$ . Note that spatial variable can be influenced "one way\_" or "two way\_", i.e.

- One way: changes in  $\phi$  only occur due to change on one side of that location
- Two way: changes in  $\phi$  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 one way 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 two-way in space

Likewise, the convection term or **parabolic PDE**:  $\nabla \cdot (\mathbf{u} \phi)$  to be one-way in space

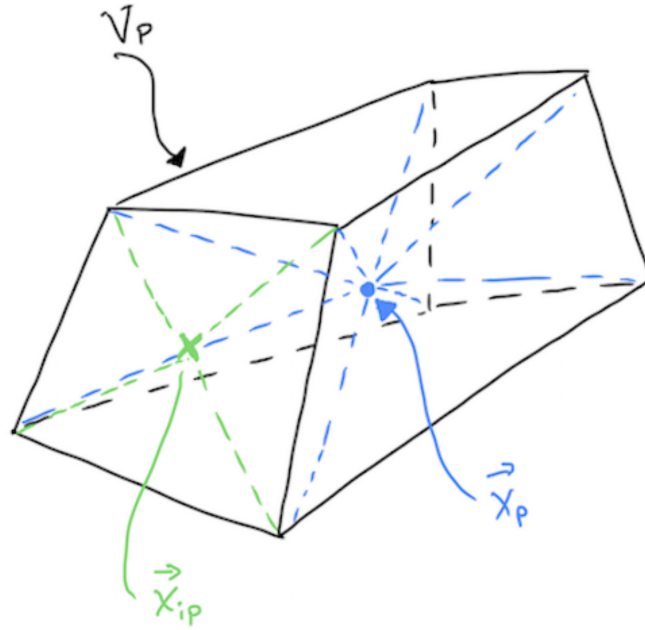
## 1.6 Main idea behind Discretization

Our goal is to:

- replace the PDEs' continuous solution with discrete solution, at specific location that approximates the continuous solution suitably.

For finite volume:

1. domain is split into non overlapping finite regions that fill the domain
2. the discrete point is at the centroid of each control volume with volume  $V_p$ , at position  $\mathbf{x}_p$
3. surround these cells, we have the "faces". At the center of these "faces", we have the integration point at position  $\mathbf{x}_{ip}$
4. 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  $\phi$ , we may express this integral in discrete form as follow:

$$\int_V \phi dV \approx \phi_P V_P \quad (9)$$

where  $\phi_P$  is the value of  $\phi$  at some internal within  $V$  and  $V_P$  is total volume of the cell:

$$V_P = \int_V dV \quad (10)$$

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

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

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

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

We note that  $\phi_P$  and its derivatives are constants:

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

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:

$$\int_V \phi dV \approx [\phi_P + O(\delta^2)] V_P \quad (14)$$

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,  $\frac{\partial \phi}{\partial t}$ . 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.

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

## 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:

$$\int_V \nabla \cdot (\mathbf{u}\phi) dV = \int_S (\mathbf{u}\phi) \cdot \mathbf{n} dS \quad (16)$$

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

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

**Note:**

- using C program notation, so we sum from 0 till  $N_{ip} - 1$
- approximate  $\mathbf{u}_{ip}$  by many interpolation methods
- interpolating  $\phi_{ip}$  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

$$\int_V \nabla \cdot \mathbf{J}_\phi dV = \int_S \mathbf{J}_\phi \cdot \mathbf{n} dS \quad (18)$$

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

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

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

### 1.11 Source term

Recall our source term:  $S_\phi$ , we assume that the source term is piecewise continuous, with one specific value,  $S_\phi$ , being represented by each cell. We can then write:

$$\int_V S_\phi dV \approx S_\phi V_P \quad (20)$$

Generally, the source term may depend on  $\phi$  so linearization is needed to obtain stable numerical method.

### 1.12 Linearization

With regard to our last point about  $J_\phi$ , 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.  $J_\phi$ .
- non linearities in the governing equation, e.g. advection term  $\nabla \cdot (\mathbf{u}\phi)$
- on non-orthogonal grid, gradient correction terms are needed  $\leq$  these are non linear.

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

$$L(\phi^*) = 0 \quad (21)$$

where:

- $\phi^*$  = the continuous solution to the PDE
- Note that to solve a PDE using finite volume, the continuous solution  $\phi^*$  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  $\phi$
- 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  $\phi_i$  at iteration  $i$ , and find the solution where  $r = 0$ :

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

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

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

We use this to update according to fix point iteration:

$$\phi = \phi_i + \Delta\phi_i \quad (24)$$

where:

$$\Delta\phi = (\phi - \phi_i) \quad (25)$$

and:

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

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:

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

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

$$a_P = \frac{\partial r_P}{\partial \phi_P} \quad (28)$$

$$a_{nb} = \frac{\partial r_P}{\partial \phi_{nb}} \quad (29)$$

## 2 CHAPTER 2: STEADY DIFFUSION EQUATION

### 2.1 Problem Definition

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

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

### 2.2 Discretization

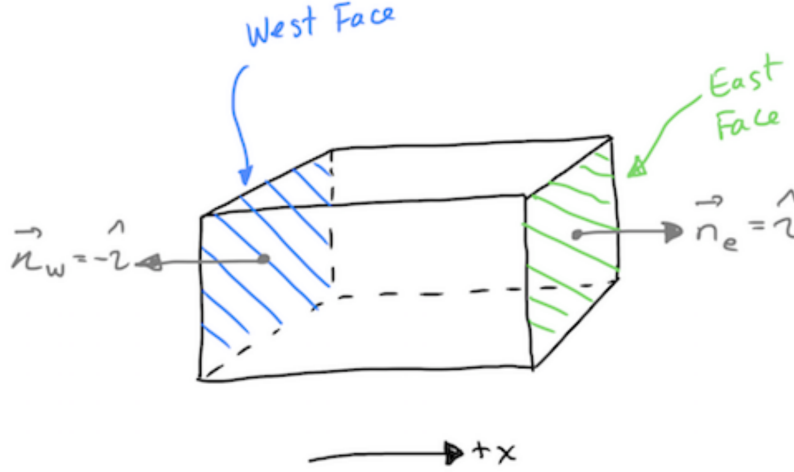
Recall our diffusion term can be discretized as:

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

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

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

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.

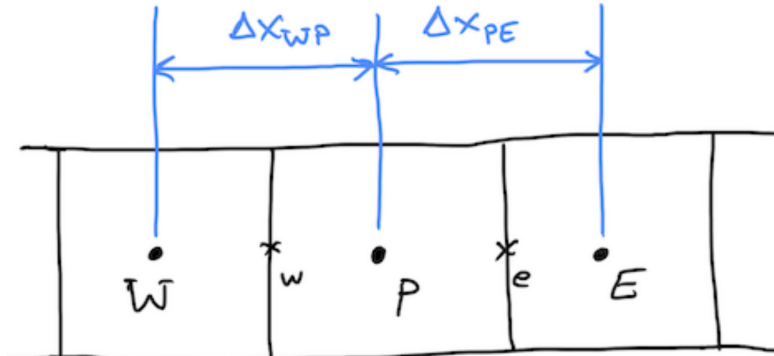
Thus,  $\nabla T \cdot \mathbf{n} = \nabla T \cdot \mathbf{i}$ .

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:

$$\int_S \mathbf{J} \cdot \mathbf{n} dS \approx k \left. \frac{\partial T}{\partial x} \right|_w A_w - k \left. \frac{\partial T}{\partial x} \right|_e A_e \quad (33)$$

The diagram below shows the cell locations and the nomenclature for the distance between them, note how  $\Delta x$  is center-center



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

$$k \frac{\partial T}{\partial x} \Big|_w A_w - k \frac{\partial T}{\partial x} \Big|_e A_e = k \frac{T_P - T_W}{\Delta x_{WP}} A_w - k \frac{T_E - T_P}{\Delta x_{PE}} A_e \quad (34)$$

Our discretized source term is simply:

$$\int_V S dV \approx S_P V_P \quad (35)$$

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:

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

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

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

where:

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

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

$$D_e = \frac{k A_e}{\Delta x_{PE}} \quad (40)$$

$$D_w = \frac{k A_w}{\Delta x_{WP}} \quad (41)$$

Our cell residual equation is then:

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

The linearized coefficients are then calculated as:

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

$$a_W = \frac{\partial r_P}{\partial T_W} = -D_w \quad (44)$$

$$a_E = \frac{\partial r_P}{\partial T_E} = -D_e \quad (45)$$

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

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

$$a_P \delta T_P + a_W \delta T_W + a_E \delta T_E = -r_P \quad (47)$$

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

Equation for one cell

$$\begin{bmatrix} a_{P0} & a_{E0} & 0 & \dots & 0 \\ a_{W1} & a_{P1} & a_{E1} & \dots & 0 \\ 0 & a_{W2} & a_{P2} & a_{E2} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & \dots & 0 & a_{WN} & a_{PN} \end{bmatrix} \begin{Bmatrix} \delta T_0 \\ \delta T_1 \\ \delta T_2 \\ \vdots \\ \delta T_N \end{Bmatrix} = \begin{Bmatrix} -r_0 \\ -r_1 \\ \vdots \\ -r_N \end{Bmatrix}$$



**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:

$$\mathbf{Ax} = \mathbf{b} \quad (48)$$

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:

$$\mathbf{T} = \mathbf{T}_i + \delta\mathbf{T}_i \quad (49)$$

## 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:

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

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:

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

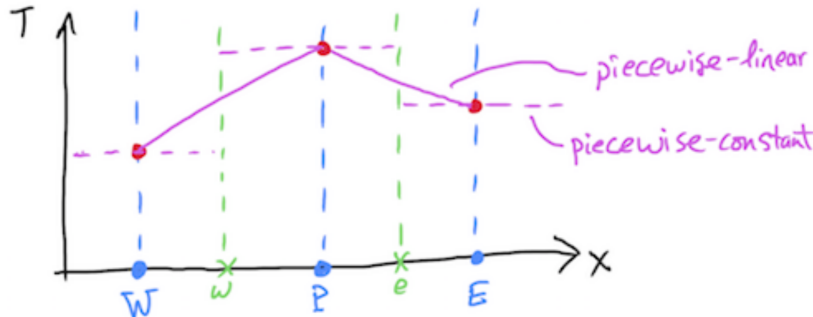
where:

- $\epsilon$  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 Patankar'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  $\rightarrow$  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

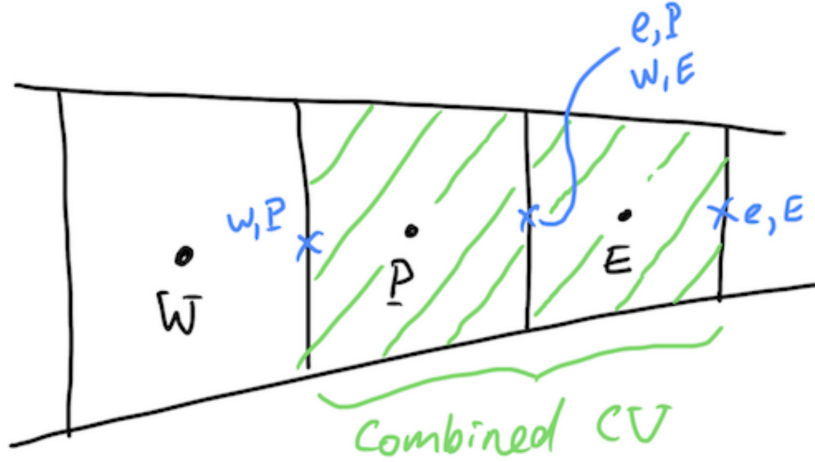
$$a_P \delta T_P + a_W \delta T_W + a_E \delta T_E = -r_P \quad (52)$$

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,  $r_P \rightarrow 0$ :

$$a_P \delta T_P = -a_W \delta T_W - a_E \delta T_E \quad (53)$$

Now, suppose both  $T_P$  and  $T_E$  are perturbed. 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:

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

For the control volume  $E$ :

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

Adding these equations together gives:

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

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 fictitious force at the face, which is not reasonable. Therefore, our algebraic equation for control volume  $P$  and  $E$  becomes:

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

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:

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

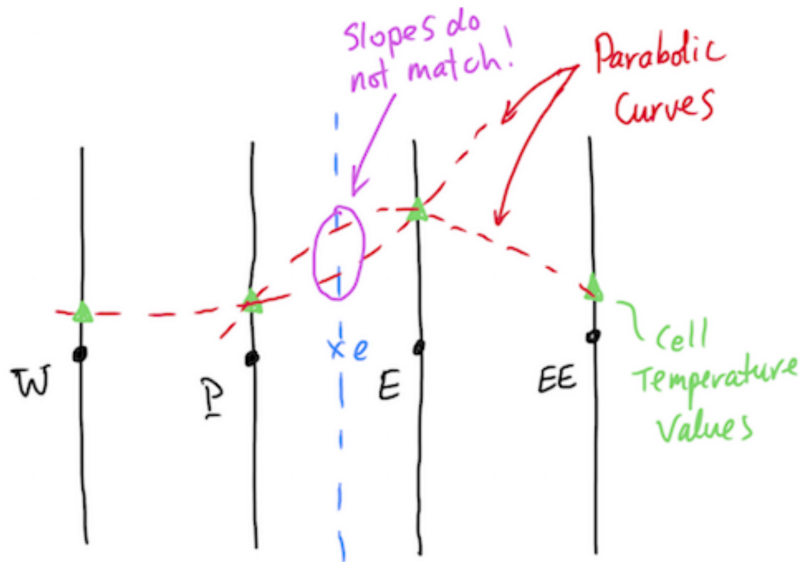
$$F_{w,E}^d = -k \frac{T_E - T_P}{\Delta x_{PE}} A_{w,E} \quad (59)$$

From the geometry 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:

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

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

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.



#### 2.4.4 Implementation: Python code

### 3 CHAPTER 3: TRANSIENT 1D HEAT DIFFUSION

#### 3.1 Problem Definition

In contrast to the steady case, here we are solving the following transient 1D heat diffusion equation

$$\frac{\partial(\rho c_p T)}{\partial t} = k \nabla^2 T + S \quad (62)$$

assuming constant  $\rho$  and  $c_p$

#### 3.2 Discretization

Integrating the governing equation through space and time yields:

$$\int_{t_0}^{t_1} \int_V \frac{(\partial \rho c_p T)}{\partial t} dt dV = \int_{t_0}^{t_1} \int_V k \nabla^2 T dt dV + \int_{t_0}^{t_1} \int_V S dt dV \quad (63)$$

By assuming a timestep  $\Delta t = t_1 - t_0$ , we also assume that the solution is stored at time levels  $t$  and later at  $t + \Delta t$ . Thus, we can assume various profiles for the integrands as functions of time. Here, we will examine the following:

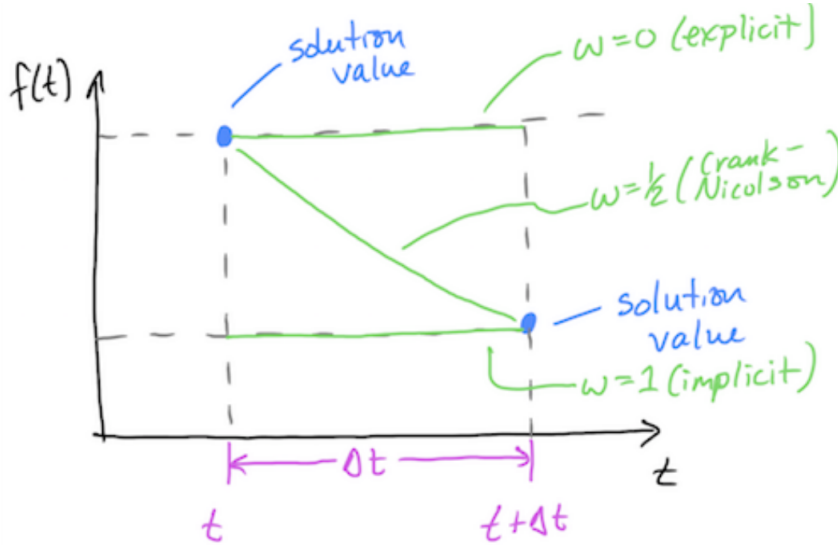
- **Fully explicit:** evaluate the integrands on RHS at initial time level,  $t_0 = t$ .
- **Fully implicit:** evaluate the integrands on RHS at final time level,  $t_1 = t_0 + \Delta t$
- **Crank Nicolson:** assume a linear profile of the RHS over the interval  $\Delta t$ .

For the LHS, we interchange the order of integration, which results in this, for a control volume  $\mathbf{P}$ :

$$\int_{t_0}^{t_1} \int_V \frac{(\partial \rho c_p T)}{\partial t} dt dV = (\rho c_p T_p)^{t+\Delta t} - (\rho c_p T_p)^t \quad (64)$$

Recall that for the steady case, the diffusive term is the difference in flux. Here, we add a weighting function  $w$  to control the assumed variation of the integrand over the timestep.

$$\int_{t_0}^{t_1} \int_V k \nabla^2 T dt dV = - [\omega (F_e^d)^{t+\Delta t} + (1-\omega)(F_e^d)^t] \Delta t + [\omega (F_w^d)^{t+\Delta t} + (1-\omega)(F_w^d)^t] \Delta t \quad (65)$$



Grouping the time levels together:

$$\int_{t_0}^{t_1} \int_V k \nabla^2 T dt dV = [\omega [F_w^d - F_e^d]^{t+\Delta t} \Delta t + (1-\omega) [F_w^d - F_e^d]^t \Delta t] \quad (66)$$

Assuming no source term,  $S = 0$ , constant properties and divide by  $\Delta t$ , our discretized equation becomes

$$\rho c_p \frac{T_P^{t+\Delta t} - T_P^t}{\Delta t} V_P = \omega [F_w^d - F_e^d]^{t+\Delta t} + (1 - \omega) [F_w^d - F_e^d]^t \quad (67)$$

#### Note

- fully implicit and fully explicit are *1st order* accurate in time.
- Crank-Nicolson are *2nd order* accurate in time.
  - but Crank-Nicolson are *less stable*, cause oscillations.
- Generally, explicit solutions do not require the solution of a system of equations. All diffusive fluxes are calculated using solution values from previous timestep
- Implicit requires solution of a linear system at current time step. The same is true for Crank-Nicolson, or any scheme where  $0 < \omega < 1$

### 3.3 Analysis of Explicit Scheme

Recall explicit scheme means  $\omega = 0$ . Our discretized equation becomes:

$$\rho c_p \frac{T_P^{t+\Delta t} - T_P^t}{\Delta t} V_P = [F_w^d - F_e^d]^t + \rho c_p \frac{T_P^t}{\Delta t} V_P \quad (68)$$

Recall that the fluxes can be defined as:

$$F_e^d = -k \frac{T_E - T_P}{\Delta x_{PE}} A_e = -D_e (T_E - T_P) \quad (69)$$

$$F_w^d = -k \frac{T_P - T_W}{\Delta x_{WP}} A_w = -D_w (T_P - T_W) \quad (70)$$

$$D_e = \frac{k A_e}{\Delta x_{PE}} \quad (71)$$

$$D_w = \frac{k A_w}{\Delta x_{WP}} \quad (72)$$

Thus, our explicit formulation becomes:

$$\rho c_p \frac{T_P^{t+\Delta t} - T_P^t}{\Delta t} V_P = D_e T_E^t + D_w T_W^t + \left( \frac{\rho c_p V_P}{\Delta t} - D_e - D_w \right) T_P^t \quad (73)$$

To get correct physical influence, the coefficient of  $T_P^t$  must be positive, to ensure  $\uparrow T_P^t$  leads to  $\uparrow T_P^{t+\Delta t}$ . Therefore, our timestep must be selected such that:

$$\frac{\rho c_p V_P}{\Delta t} \geq D_e + D_w$$

or

$$\Delta t \leq \frac{\rho c_p V_P}{D_e + D_w} = \frac{1}{\frac{D_e}{\rho c_p V_P} + \frac{D_w}{\rho c_p V_P}}$$

Simplifying further, we assume  $V_P = A \Delta x$  where  $A$  is the cross-sectional area of the domain at  $P$ , and  $\Delta x$  is the grid spacing. Also assuming  $A_e, A_w \approx A$

$$\frac{D_e}{\rho c_p V_P} \approx \frac{\frac{k A_e}{\Delta x}}{\rho c_p A \Delta x} = \frac{k}{\rho c_p} \frac{1}{\Delta x^2} = \frac{\alpha}{\Delta x^2}$$

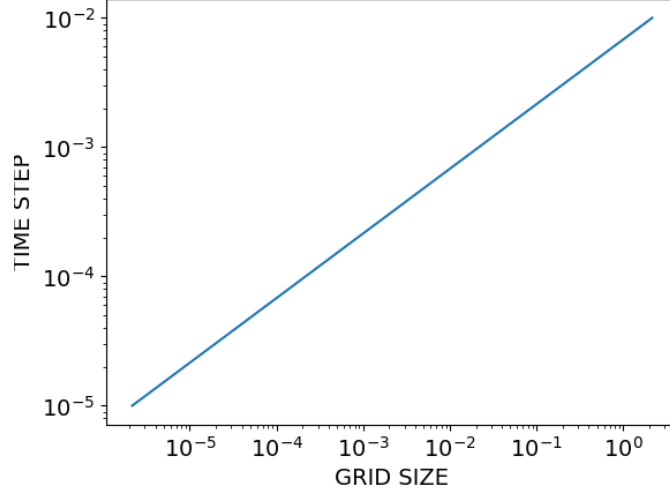
The quantity  $\frac{\Delta x^2}{\alpha}$  may be interpreted as the timescale associated with conduction through the face. For uniform grid,  $A_e = A_w = A$ , the timestep restriction is:

$$\Delta t \leq \frac{1}{\frac{\alpha}{\Delta x^2} + \frac{\alpha}{\Delta x^2}} = \frac{\Delta x^2}{2\alpha} \quad (74)$$

Note how our timestep is related to the square of the grid size, so the a fine grid will have a very small " $\Delta x^2$ ".

To study this, we consider an iron bar with  $\alpha = 23.1 \times 10^{-6} [m^2/s]$  at various grid sizes:

GRID SIZE [m]	TIME STEP [sec]
0.01	2.1645022
0.001	0.021645022
0.0001	2.1645022e-4
0.00001	2.1645022e-6



We can quickly see how the timestep restriction gets worse with increasing grid refinement. As a result, implicit methods are more commonly used in practice. Exception would be calculation of turbulent flow using direct numerical simulation (DNS). In this case, explicit method are a good choice because they are less expensive per timestep, since no linear system must be solved.

### 3.4 Analysis of Fully Implicit Scheme

Setting  $\omega = 1$  for implicit scheme. Our discretized equation becomes:

$$\rho c_p \frac{T_P^{t+\Delta t} - T_P^t}{\Delta t} V_P = [-D_w(T_P - T_W) + D_e(T_E - T_P)]^{t+\Delta t} \quad (75)$$

Drop the superscript  $t + \Delta t$  and denotes old value as "o", after rearranging, we have:

$$\left( \frac{\rho c_p V_P}{\Delta t} + D_w + D_e \right) T_P = D_w T_W + D_e T_E + \frac{\rho c_p V_P}{\Delta t} T_P^o \quad (76)$$

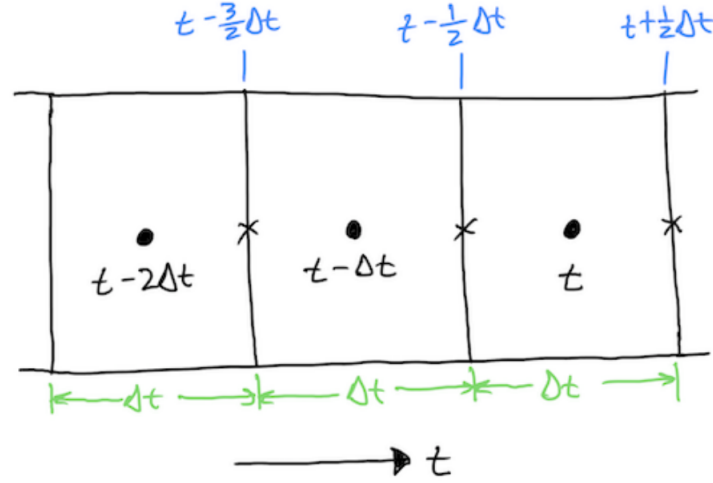
We can see that none of the coefficients can be come negative when written out this way. Still, we must ensure the timestep is small enough to resolve all transient phenomena. In contrast to this fully implicit scheme, the Crank-Nicholson scheme has no formal restriction on  $\Delta t$ , but still produces **oscillatory** at large  $\Delta t$ .

### 3.5 Derivation of Second Order Implicit Scheme

#### 3.5.1 General idea

We consider integration over a special **space-time control volume**, with:

- the time faces being located at  $t - \Delta t/2, t + \Delta t/2$
- the solution values are stored at  $t, t - \Delta t, t - 2\Delta t \dots$ .



By using the space-time control volume, the RHS of the discretized equation evaluated at time  $t$ , can be considered as a representative of the entire timesweep. The advantages are:

- we do not need to assume a profile in time, e.g. piecewise constant for fully implicit/explicit, piecewise linear for Crank-Nicholson.
- no need to store old flux value
- interpolation depends on the face values:
  - if piecewise constant  $\rightarrow$  1st order scheme
  - if piecewise linear  $\rightarrow$  2nd order scheme

### 3.5.2 Derivation

Integrate the governing equation over the space-time control volume

$$\int_{t-\Delta t/2}^{t+\Delta t/2} \int_V \frac{(\partial \rho c_p T)}{\partial t} dt dV = \int_{t-\Delta t/2}^{t+\Delta t/2} \int_V k \nabla^2 T dt dV + \int_{t-\Delta t/2}^{t+\Delta t/2} \int_V S dt dV \quad (77)$$

Resulting in:

$$(\rho c_p T_P V_P)^{t+\Delta t/2} - (\rho c_p T_P V_P)^{t-\Delta t/2} = [F_w^d - F_e^d]^t \Delta t + S_P^t \Delta t V_P \quad (78)$$

Divide by  $\Delta t$ , express the diffusive fluxes in terms of  $D_w$  and  $D_e$ , dropping superscripts  $t$  for current time:

$$\frac{(\rho c_p T_P V_P)^{t+\Delta t/2} - (\rho c_p T_P V_P)^{t-\Delta t/2}}{\Delta t} = -D_w(T_P - T_W) + D_e(T_E - T_P) + S_P V_P \quad (79)$$

LHS is known, for RHS  $\rightarrow$  need to specify values for times  $t - \Delta t/2$  and  $t + \Delta t/2$

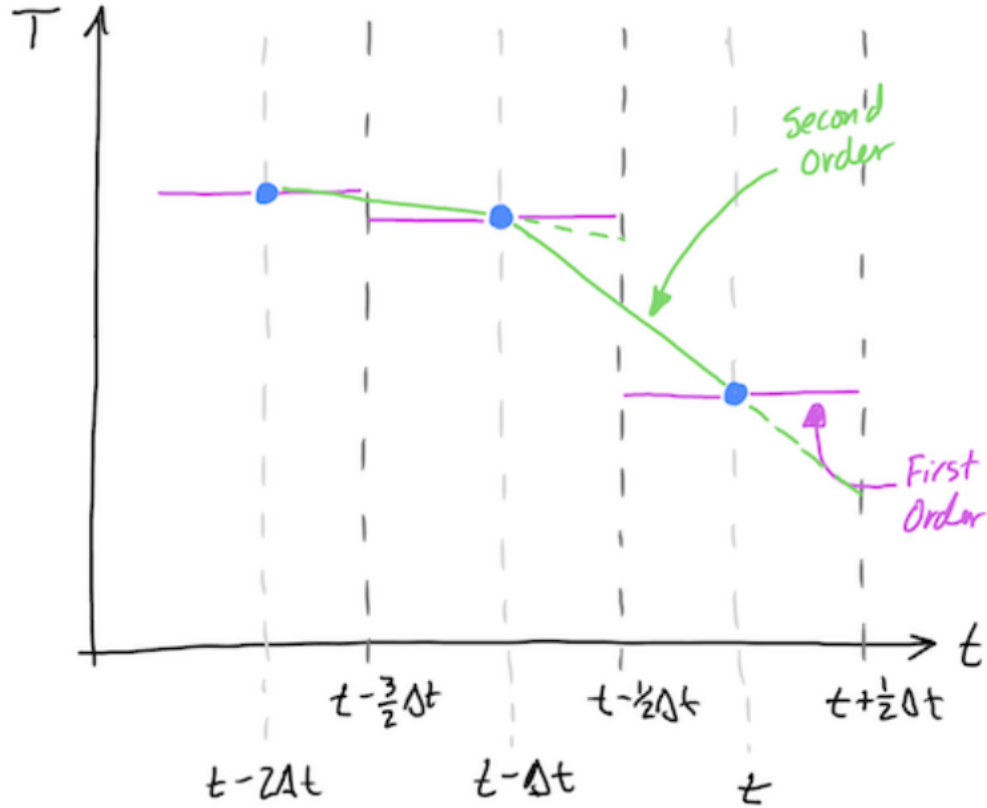
- 1st order time integration scheme We assume a **piecewise constant** distribution over each timestep between the face values, resulting in:

$$\begin{aligned} T_P^{t-\Delta t/2} &= T_P^{t-\Delta t} \\ T_P^{t+\Delta t/2} &= T_P^t \end{aligned}$$

- 2nd order time integration scheme We assume a **piecewise linear** distribution over each timestep between the face values, resulting in:

$$\begin{aligned} T_P^{t-\Delta t/2} &= T_P^{t-\Delta t} + \frac{1}{2}(T_P^{t-\Delta t} - T_P^{t-2\Delta t}) \\ T_P^{t+\Delta t/2} &= T_P^t + \frac{1}{2}(T_P^t - T_P^{t-\Delta t}) \end{aligned}$$

This is achieved by doing backward interpolation and then forward interpolation on the face values. The schematic below shows these interpolations:



Substituting these relations to the integrated governing equation's LHS:

– For 1st order scheme:

$$\frac{(\rho c_p T_P V_P)^{t+\Delta t/2} - (\rho c_p T_P V_P)^{t-\Delta t/2}}{\Delta t} = \rho c_p V_P \frac{T_P - T_P^o}{\Delta t} \quad (80)$$

Note:

- \* the superscript for current time is dropped, and superscript for  $t - \Delta t$  is replaced by  $\underline{o}$  for "old value".
- \* also that this is exactly the same as the result for the fully implicit scheme.

– For 2nd order scheme:

$$\frac{(\rho c_p T_P V_P)^{t+\Delta t/2} - (\rho c_p T_P V_P)^{t-\Delta t/2}}{\Delta t} = \rho c_p V_P \frac{T_P + \frac{1}{2}(T_P - T_P^o) - T_P^o - \frac{1}{2}(T_P^o - T_P^{oo})}{\Delta t}$$

or a more simplified version...

$$\frac{(\rho c_p T_P V_P)^{t+\Delta t/2} - (\rho c_p T_P V_P)^{t-\Delta t/2}}{\Delta t} = \rho c_p V_P \frac{\frac{3}{2}T_P - 2T_P^o + \frac{1}{2}T_P^{oo}}{\Delta t} \quad (81)$$

Note:

- \* superscript  $\underline{oo}$  is used for time value  $t - 2\Delta t$ .
- \* unlike Crank-Nicholson's, flux values at previous timestep **do not need to be solved**. Instead, only temperature values at the **previous two time step** need to be retained.

### 3.5.3 Other Transient Discretization Schemes

Some higher order schemes are also used such as:

- Adams-Bashforth (explicit)
- Adams-Moulton (implicit)
- Runge-Kutta (implicit or explicit)



### 3.5.4 Linearization

Recall the cell residual for steady conduction:

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

where  $D_e = \frac{kA_e}{\Delta x_{PE}}$ , and  $D_w = \frac{kA_w}{\Delta x_{WP}}$ . If we apply 1st order implicit to the transient term:

$$r_P = \rho c_p V_P \frac{T_P - T_P^o}{\Delta t} D_w(T_P - T_W) - D_e(T_E - T_P) - S_P V_P$$

This makes the linearization coefficients to be as follow:

$$\begin{aligned} a_P &= \frac{\partial r_P}{\partial T_P} = \frac{\rho c_p V_P}{\Delta t} + D_w + D_e - \frac{\partial S_P}{\partial T_P} V_P \\ a_W &= \frac{\partial r_P}{\partial T_W} = -D_w \\ a_E &= \frac{\partial r_P}{\partial T_E} = -D_e \end{aligned}$$

Similar to before, we can form an algebraic equation for each control volume like this:

$$a_P \delta T_P + a_W \delta T_W + a_E \delta T_E = -r_P \quad (82)$$

If we apply 2nd order implicit temporal scheme instead, then  $a_P$  term would look like this:

$$a_P = \frac{\partial r_P}{\partial T_P} = \frac{3}{2} \frac{\rho c_p V_P}{\Delta t} + D_w + D_e - \frac{\partial S_P}{\partial T_P} V_P$$