Numerical Heat Transfer

(数值传热学)

Chapter 2 Discretization of Computational Domain and Governing Equations

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2.1 Grid Generation

2.1.1 Task, method and classification

1. Task of domain discretization

Discretizing the computational domain into a number of sub-domains which are not overlapped(重叠) and can completely cover the computational domain.

Four kinds of information can be obtained:

(1) Node（节点）:the position at which the values of dependent variables are solved;

(2) Control volume (CV,控制容积)：the minimum volume to which the conservation law is applied;

(3) Interface（界面）:boundary of two neighboring（相邻的）CVs.

(4) Grid lines（网格线）: Curves formed by connecting two neighboring nodes.

The spatial relationship between two neighboring nodes, the influencing coefficients, will be decided in the procedure of equation discretization.

2. Classification of domain discretization method

(1) According to node relationship: structured (结构化) vs. unstructured（非结构化）

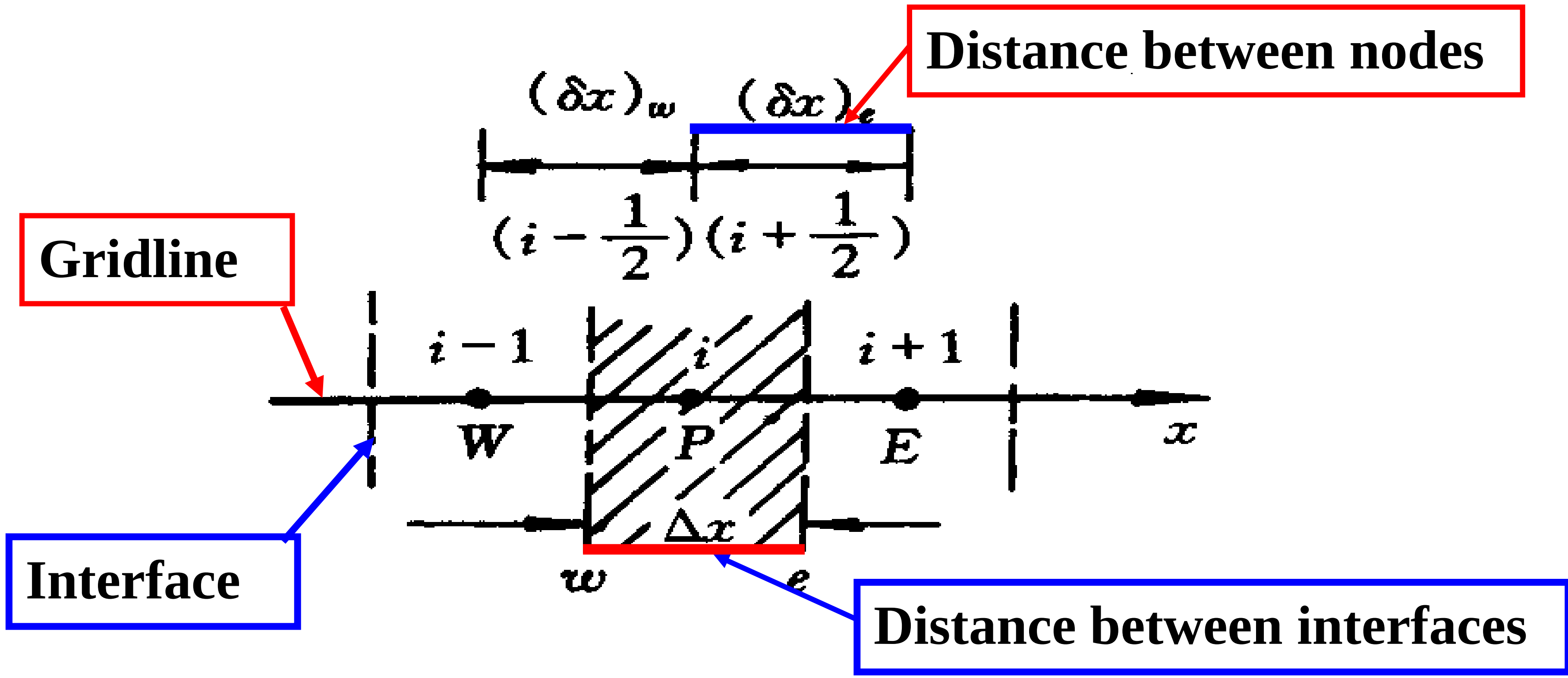
(2) According to node position: inner node vs. outer node

2.1.2 Expression of grid system (网格系统表示)

Grid line－solid line; Interface-dashed line（虚线）;

Distance between two nodes－ δx

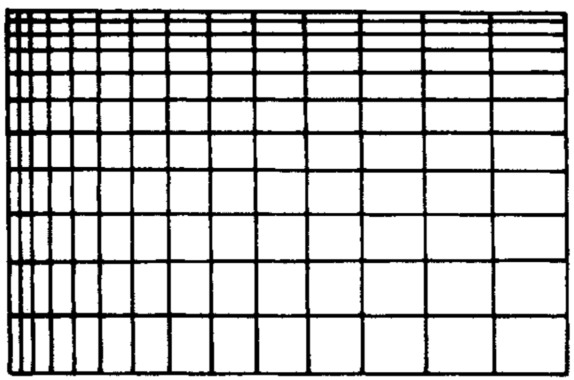
Distance between two interfaces－ Δx



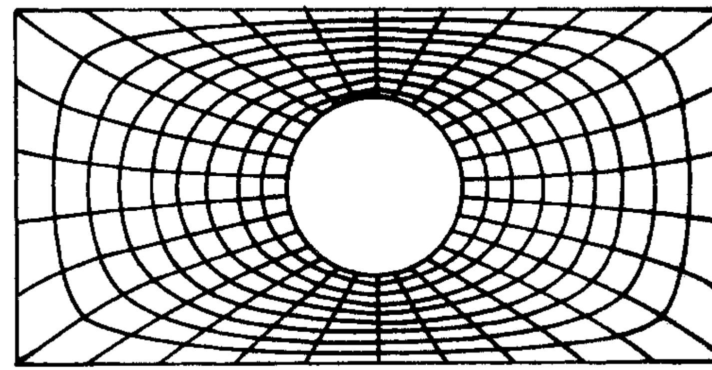
2.1.3 Introduction to different types of grid system and generation method

（1） Structured grid (结构化网格)：Node position layout（布置）is in order, and fixed for the entire domain.

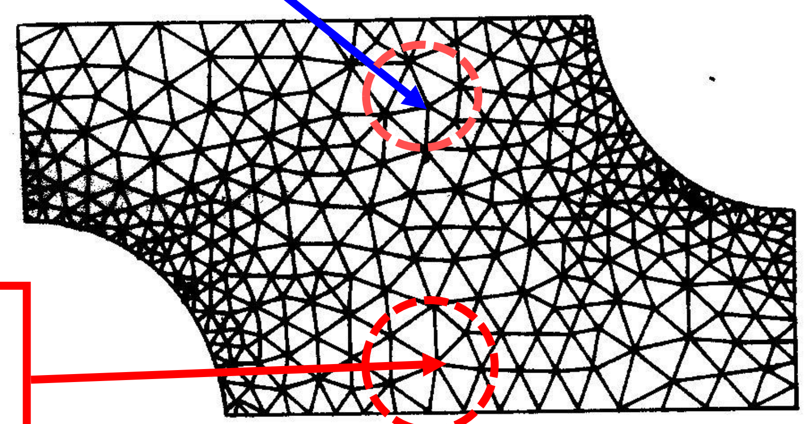
（2） Unstructured grid (非结构化网格)： Node position layout(布置) is in disorder, and may change from node to node. The generation and storage of the relationship of neighboring nodes are the major work of grid generation.



Structured （a）



Structured （b）

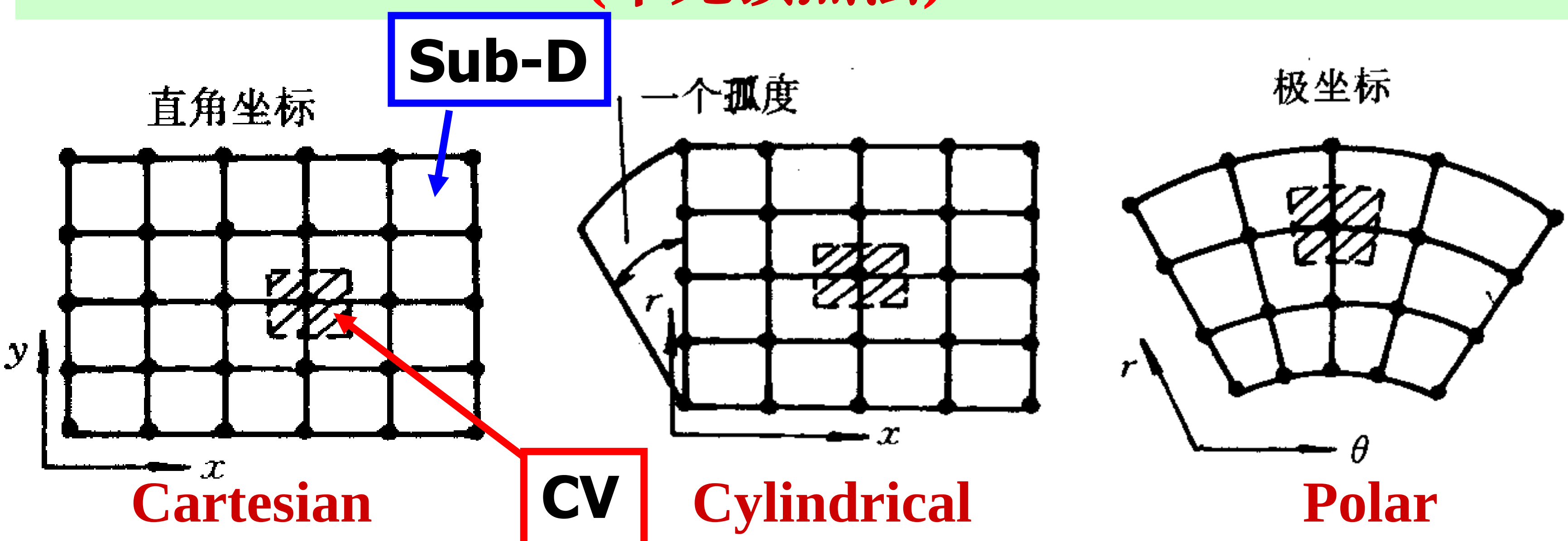


Un-structured

Both structured and unstructured grid layout (节点布置) have two practices.

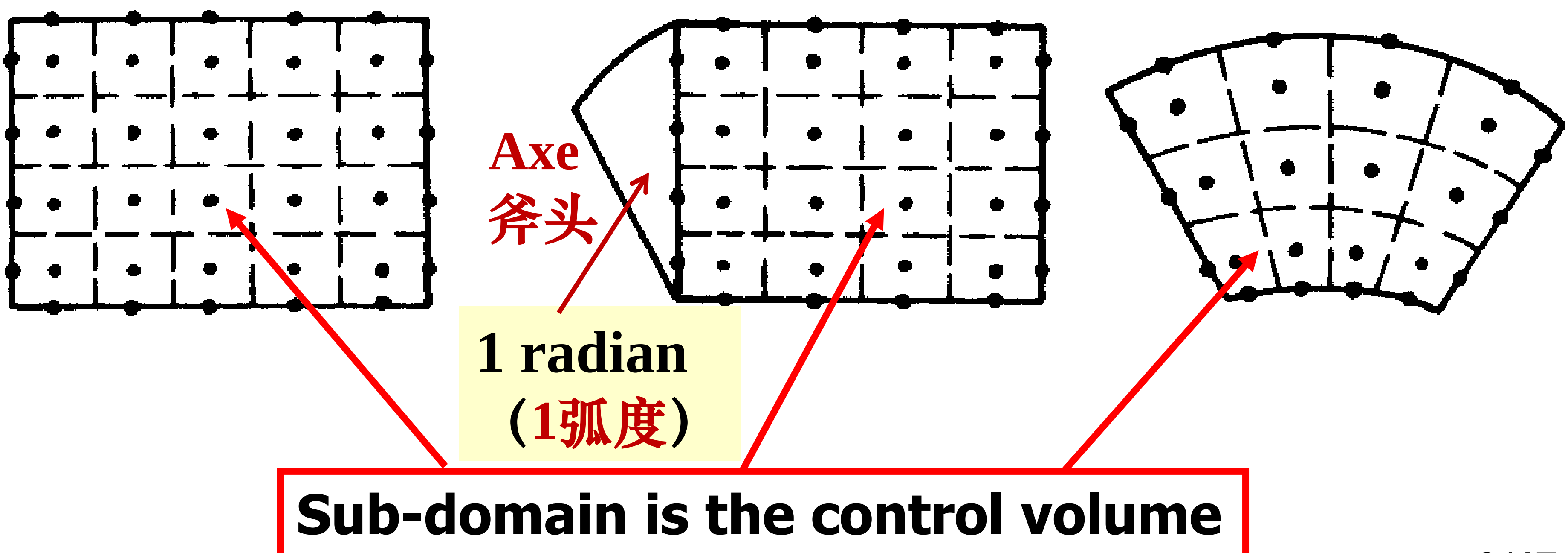
（3）Outer node and inner node for structured grid

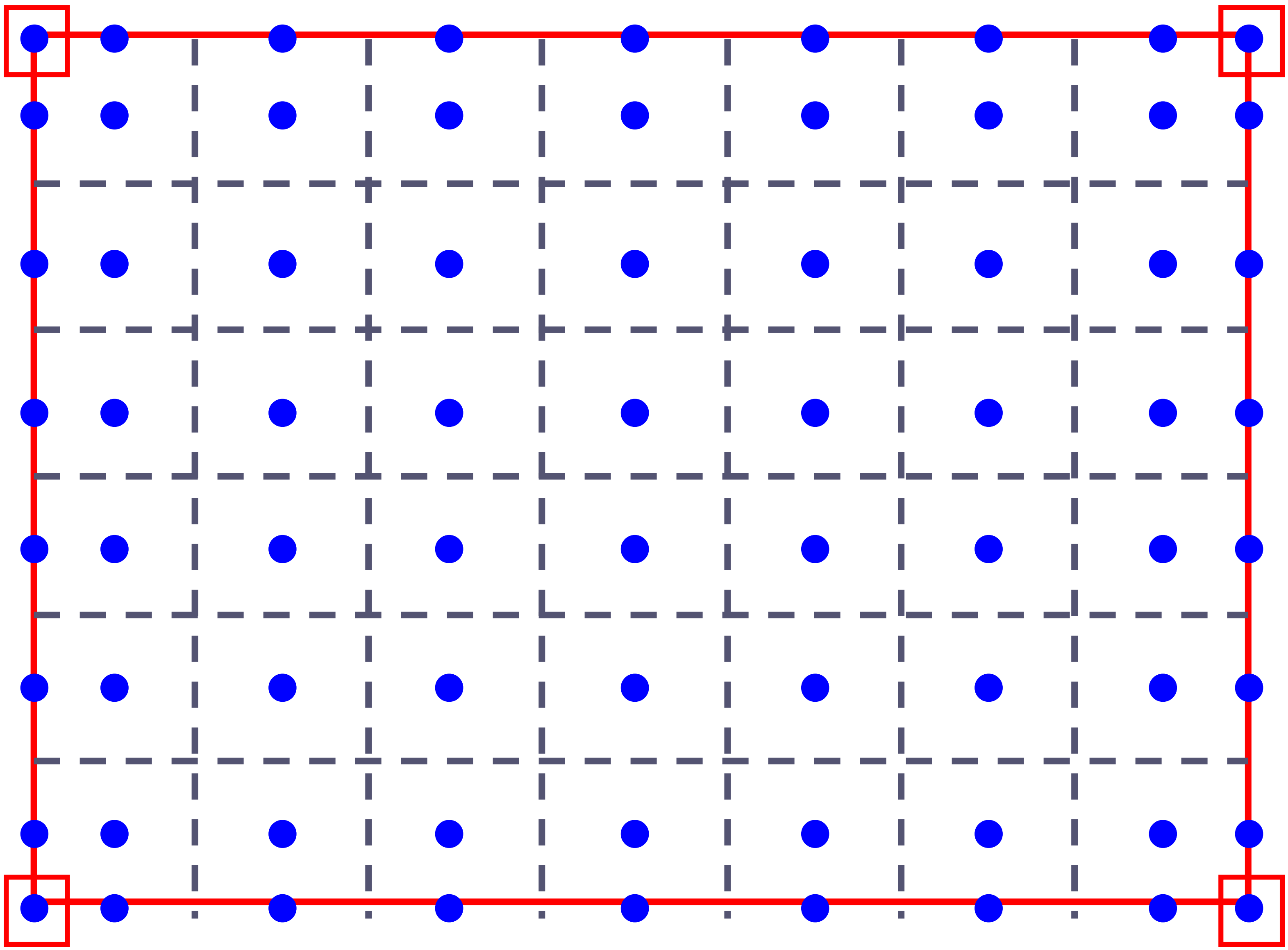
(a) Outer node method： Node is positioned at the vertex of a sub-domain(子区域的角顶)； The interface is between two nodes； Generating procedure： Node first and interface second---called Practice A， or cell-vertex method (单元顶点法).



Cartesian　　Cylindrical　　Polar

(b) Inner node method： Node is positioned at the center of sub-domain; Sub-domain is identical to control volume; Generating procedure: Interface first ad node second, called Practice B, or cell-centered （单元中心法）.



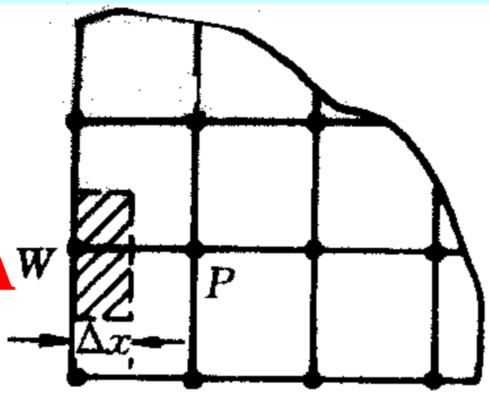


Generating procedure of Practice B

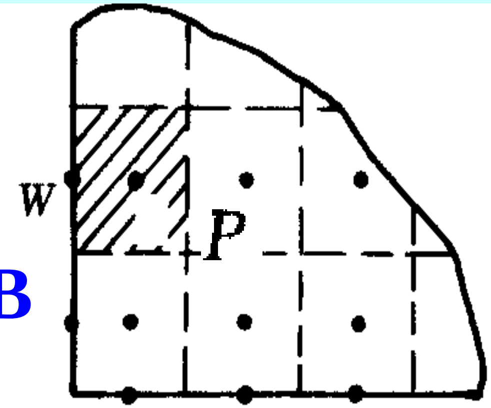
2.1.4 Comparison between Practices A and B

(a) Boundary nodes have different CV.

Practice A



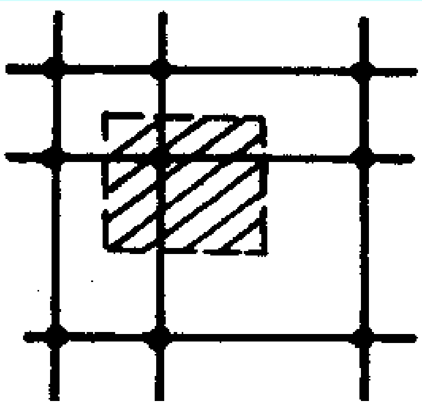
Practice B



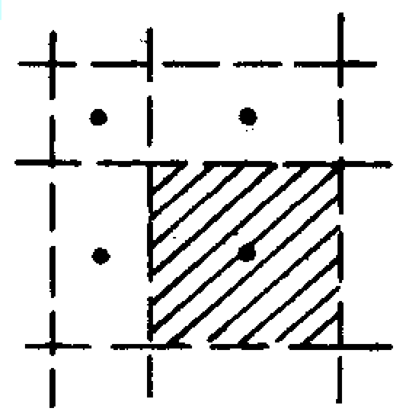
Boundary point has half CV. **Boundary point has zero CV.**

(b) Practice B is more feasible（适用） for non-uniform grid layout.

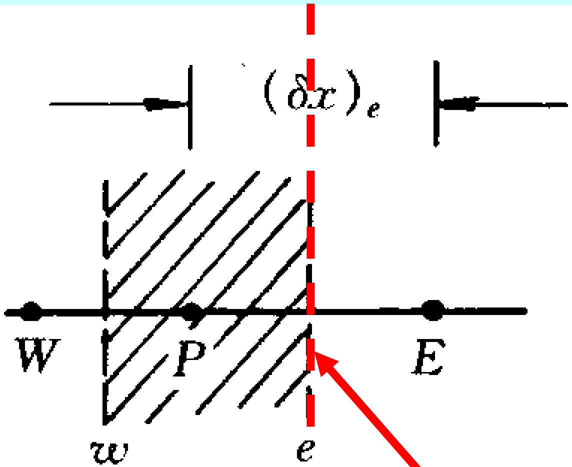
Practice A

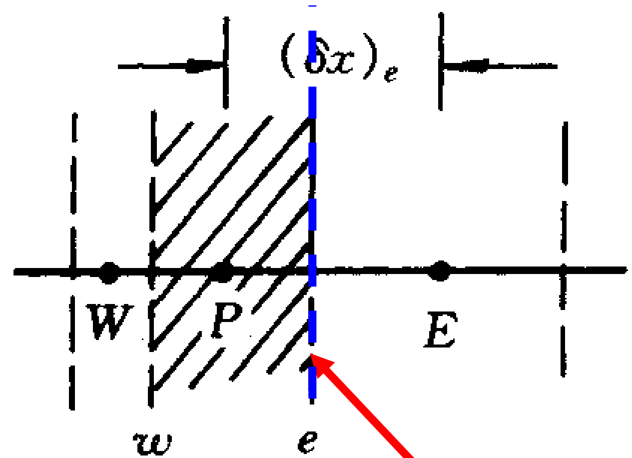


Practice B



(c) For non-uniform grid layout, Practice A can guarantee the discretization accuracy of interface derivatives （界面导数）.





Interface in middle

Interface is biased（偏置）

$$\left(\frac{\partial \phi}{\partial x}\right)_e \cong \frac{\phi_E - \phi_P}{(\delta x)_e}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_e \cong \frac{\phi_E - \phi_P}{(\delta x)_e}$$

2nd-order accuracy

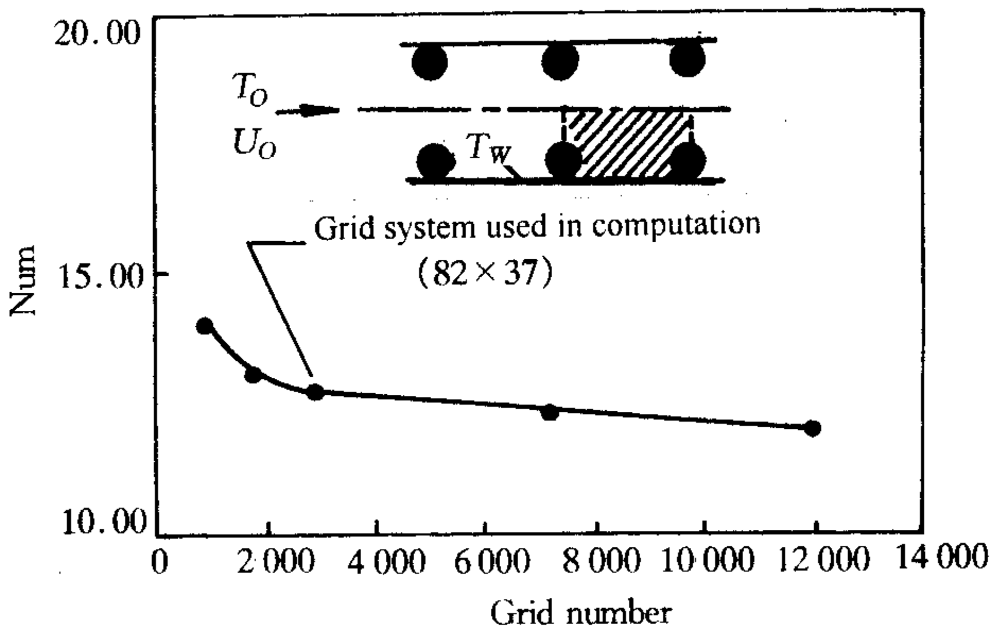
Lower than 2nd order accuracy

2.1.5 Grid-independent solutions

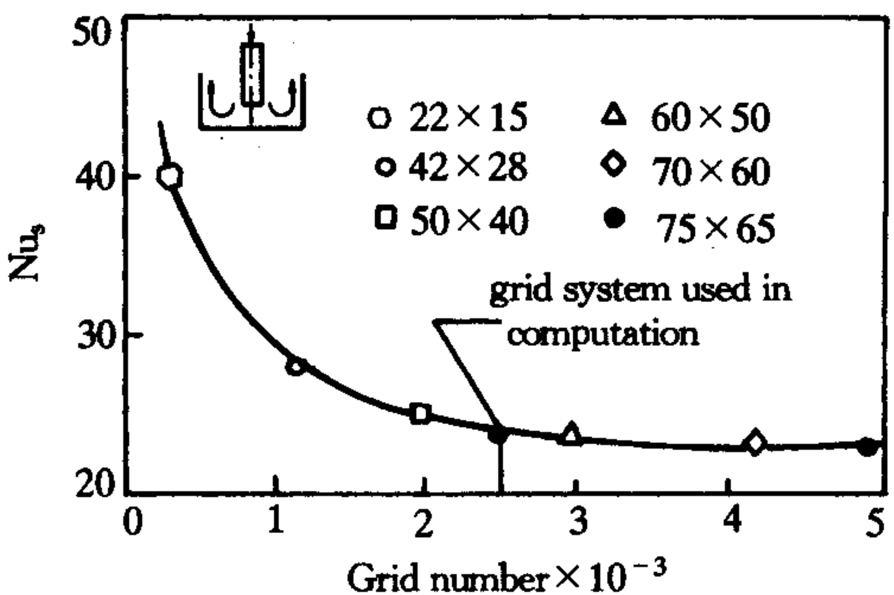
Grid generation is an iterative procedure（迭代过程）; Debugging (调试）and comparison are often needed. For a complicated geometry grid generation may take a major part of total computational time.

Grid generation method has been developed as a sub-field of numerical solutions (Grid generation techniques).

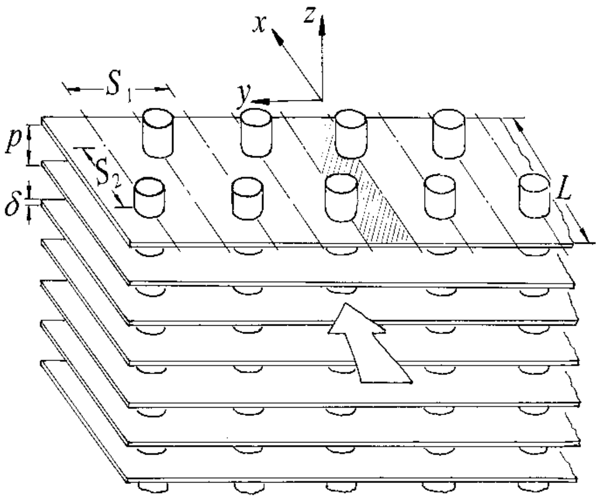
The appropriate grid fineness(细密程度) is such that the numerical solutions are nearly independent on the grid numbers. Such numerical solutions are called grid-independent solutions (网格独立解). This is required for publication of a paper.

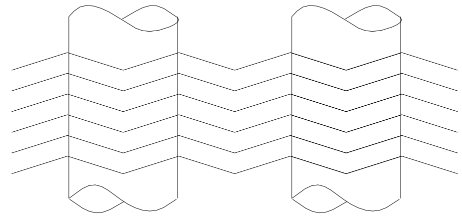


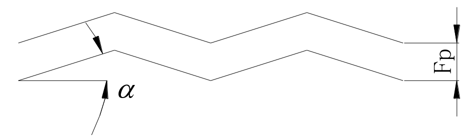
Int. Journal Heat & Fluid Flow, 1993, 14(3):246-253。

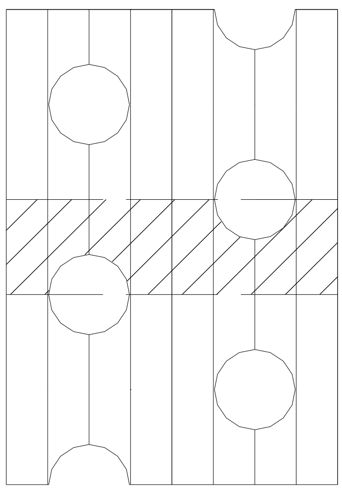


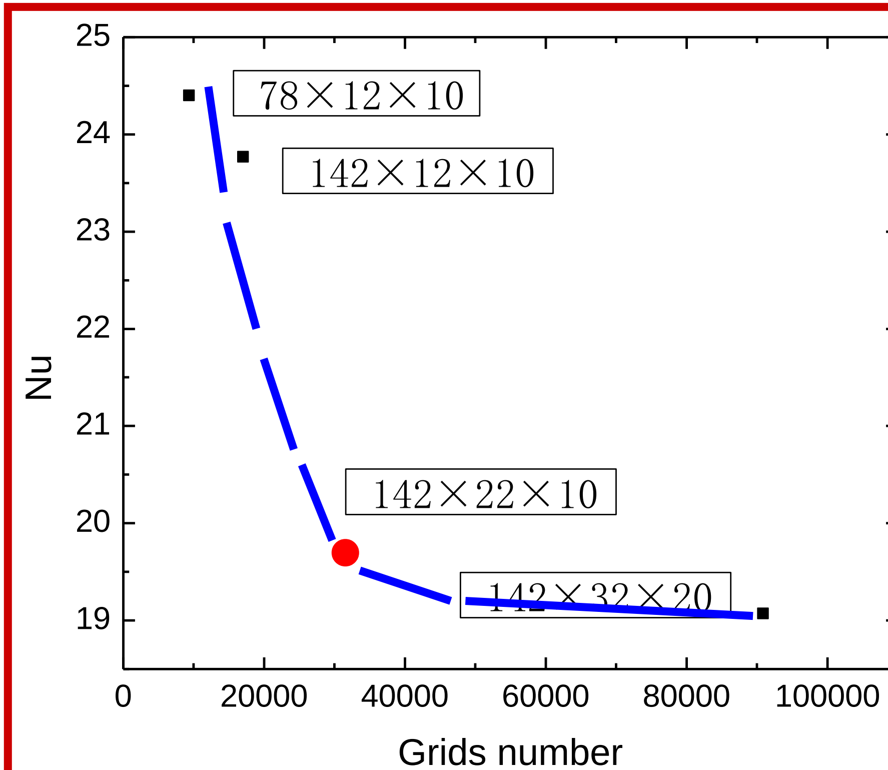
Int. Journal Numerical Methods in Fluids, 1998, 28: 1371-1387。











International Journal of Heat Mass Transfer, 2007, 50:1163-1175

2.2 Taylor Expansion and Polynomial Fitting for equation discretization

2.2.1 1-D model equation

2.2.2 Taylor expansion and polynomial fitting （多项式拟合）methods

2.2.3 FD form of 1-D model equation

2.2.4 FD form of polynomial fitting

2.2 Taylor Expansion and Polynomial Fitting for Equation discretization

2.2.1 1-D model equation（一维模型方程）

1-D model equation has four typical terms ：transient term, convection term, diffusion term and source term. It is specially designed for discussion of discretization methods.

Non-cons.

$$\frac{\partial(\rho\phi)}{\partial t}+\rho u\frac{\partial\phi}{\partial x}=\frac{\partial}{\partial x}(\Gamma\frac{\partial\phi}{\partial x}) + S_\phi$$

For FDM

Conserva -tive

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(\rho u\phi)}{\partial x}=\frac{\partial}{\partial x}(\Gamma\frac{\partial\phi}{\partial x})+S_\phi$$

For FVM

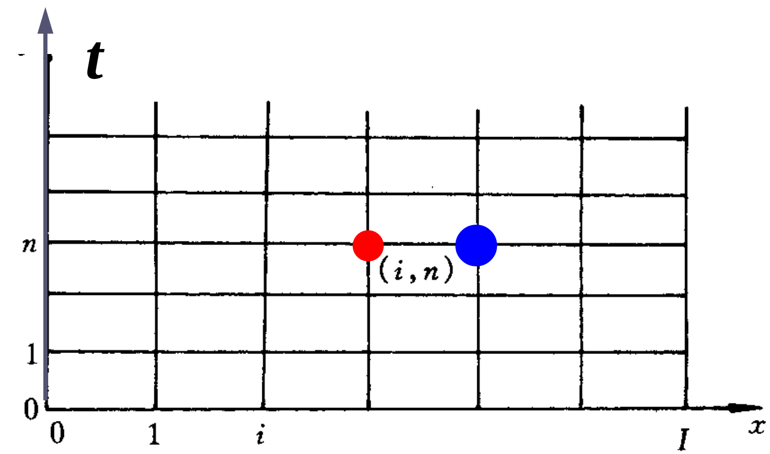
Trans **Conv.** **Diffus.** **Source**

Small but complete---"麻雀虽小，五脏俱全！"

2.2.2 Taylor expansion for FD form of derivatives

1. FD form of 1st order derivative

Expanding $\phi(x,t)$ at (i+1,n) with respect to (对于) point (i,n):



$$\phi(i+1,n)=\phi(i,n)+\frac{\partial\phi}{\partial x})_{i,n}\Delta x+\frac{\partial^2\phi}{\partial x^2})_{i,n}\frac{\Delta x^2}{2!}+.....$$

$$\frac{\partial\phi}{\partial x})_{i,n}=\frac{\phi(i+1,n)-\phi(i,n)}{\Delta x}-\frac{\Delta x}{2}(\frac{\partial^2\phi}{\partial x^2})_{i,n}+...$$

$$\frac{\partial \phi}{\partial x})_{i,n} = \frac{\phi(i+1,n) - \phi(i,n)}{\Delta x} + O(\Delta x)$$

$O(\Delta x)$ is called **truncation error （截断误差）：**

With $\Delta x \to 0$ **replacing** $\frac{\partial \phi}{\partial x})_{i,n}$ **by** $\frac{\phi(i+1,n) - \phi(i,n)}{\Delta x}$ **will lead to an error** $\le$ $K\Delta x$ **where K is independent of** Δx **----mathematical meaning of** $O(\Delta x)$

The exponent (指数) of Δx **is called order of TE(截差的阶数)．Replacing analytical solution** $\phi(i,n)$ **by approximate value** ϕ_i^n **， yields:**

Forward difference：（向前差分）

$$\boxed{\frac{\partial \phi}{\partial x})_{i,n} \cong \frac{\delta \phi}{\delta x})_i^n = \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}, O(\Delta x)}$$

Backward difference:
(向后差分)

$$\left.\frac{\partial \phi}{\partial x}\right)_{i,n} \cong \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}, O(\Delta x)$$

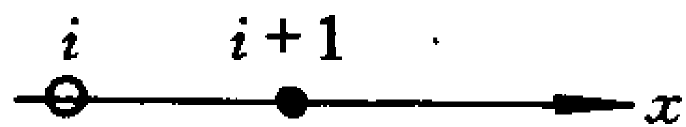
Central difference:
(中心差分)

$$\left.\frac{\partial \phi}{\partial x}\right)_{i,n} \cong \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}, O(\Delta x^2)$$

2. Different FD forms of 1st ad 2nd order derivatives

Stencil (格式图案) of FD expression

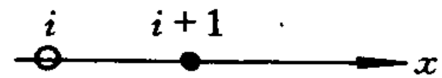
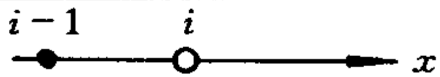
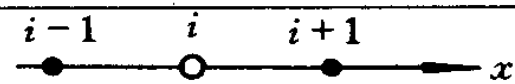
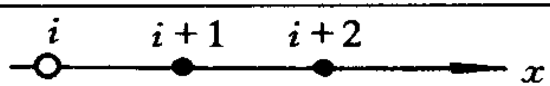
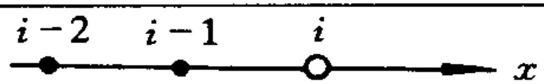
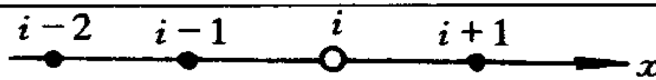
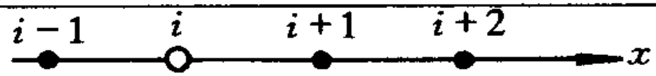
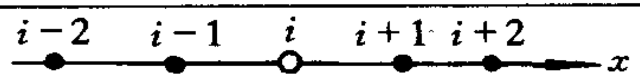
$$\frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$$

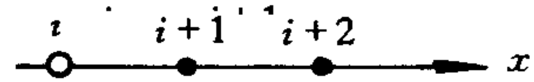
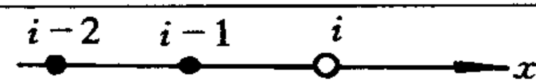
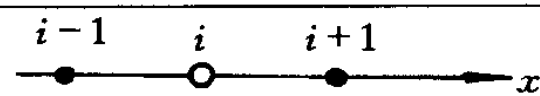
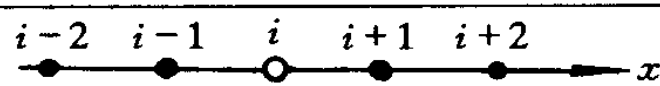


○ **For the node where FD form is constructed**

● **For nodes which are used in the construction**

Table 2 in the textbook

导数	差分表示式	格式图案	截差
$\left.\frac{\partial\phi}{\partial x}\right)_{i,n}$	$\frac{\phi_{i+1}^n-\phi_i^n}{\Delta x}$		$O(\Delta x)$
	$\frac{\phi_i^n-\phi_{i-1}^n}{\Delta x}$		$O(\Delta x)$
	$\frac{\phi_{i+1}^n-\phi_{i-1}^n}{2\Delta x}$		$O(\Delta x^2)$
	$\frac{-3\phi_i^n+4\phi_{i+1}^n-\phi_{i+2}^n}{2\Delta x}$		$O(\Delta x^2)$
	$\frac{3\phi_i^n-4\phi_{i-1}^n+\phi_{i-2}^n}{2\Delta x}$		$O(\Delta x^2)$
	$\frac{4\phi_{i+1}^n+6\phi_i^n-12\phi_{i-1}^n+2\phi_{i-2}^n}{12\Delta x}$		$O(\Delta x^3)$
	$\frac{-2\phi_{i+2}^n+12\phi_{i+1}^n-6\phi_i^n-4\phi_{i-1}^n}{12\Delta x}$		$O(\Delta x^3)$
	$\frac{\phi_{i-2}^n-8\phi_{i-1}^n+8\phi_{i+1}^n-\phi_{i+2}^n}{12\Delta x}$		$O(\Delta x^4)$

<table>
<tr><th>导数</th><th>差分表示式</th><th>格式图案</th><th>截差</th></tr>
<tr><td rowspan="4">$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,n}$</td><td>$\frac{\phi_i^n - 2\phi_{i+1}^n + \phi_{i+2}^n}{\Delta x^2}$</td><td></td><td>$O(\Delta x)$</td></tr>
<tr><td>$\frac{\phi_i^n - 2\phi_{i-1}^n + \phi_{i-2}^n}{\Delta x^2}$</td><td></td><td>$O(\Delta x)$</td></tr>
<tr><td>$\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$</td><td></td><td>$O(\Delta x^2)$</td></tr>
<tr><td>$(-\phi_{i-2}^n + 16\phi_{i-1}^n - 30\phi_i^n + 16\phi_{i+1}^n - \phi_{i+2}^n)/12\Delta x^2$</td><td></td><td>$O(\Delta x^4)$</td></tr>
</table>

Rule of thumb（大拇指原则） for judging correction of a FD form ：

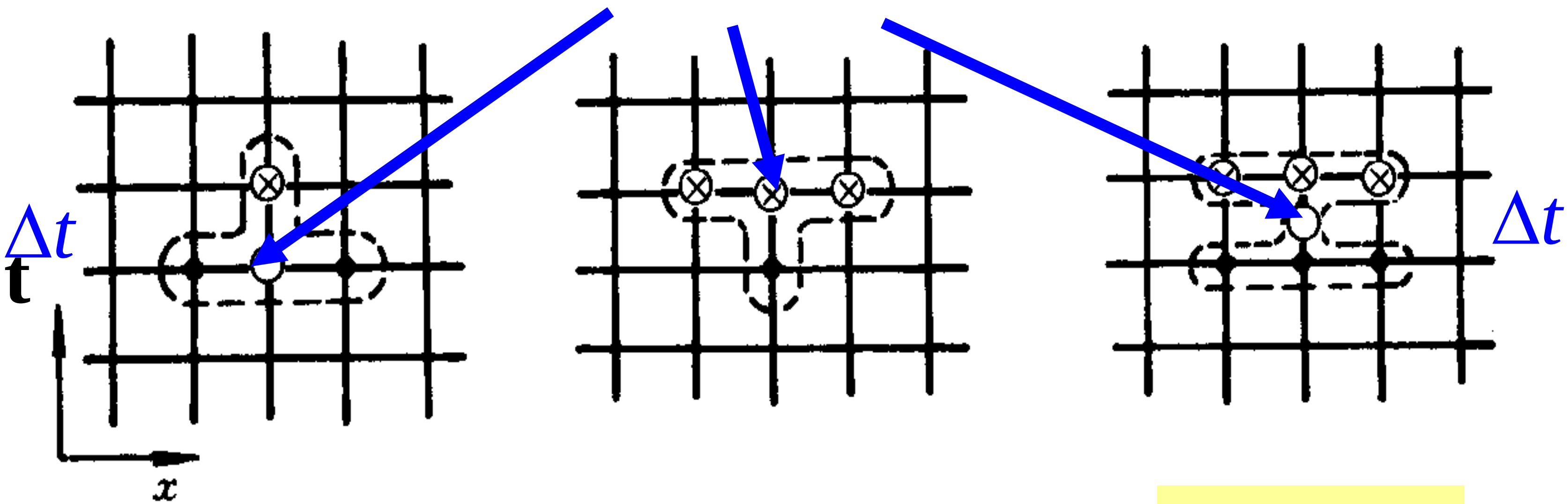
（1） Dimension (量纲) should be consistent(一致);

（2） Zero derivatives of any order for a uniform field.

2.2.3 Discretized form of 1-D model equation by FD

1. Time level at which spatial derivatives are determined

Taylor expansion with respect to this time level



显式 explicit $O(\Delta t)$

隐式 implicit $O(\Delta t)$

C-N格式 Crank-Nicolson $O(\Delta t^2)$

2. Explicit scheme of 1-D model equation

Analytical form

$$\rho\frac{\phi(i,n+1)-\phi(i,n)}{\Delta t}+\rho u\frac{\phi(i+1,n)-\phi(i-1,n)}{2\Delta x}=$$
$$\Gamma\frac{\phi(i+1,n)-2\phi(i,n)+\phi(i-1,n)}{\Delta x^2}+S(i,n)+HOT$$

Finite difference form

Explicit in space derivatives

$$\rho\frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}+\rho u\frac{\phi_{i+1}^n-\phi_{i-1}^n}{2\Delta x}=\Gamma\frac{\phi_{i+1}^n-2\phi_i^n+\phi_{i-1}^n}{\Delta x^2}+S_i^n,O(\Delta t,\Delta x^2)$$

Forward in time, (Δt)

Central in space, (Δx^2)

Central in space, (Δx^2)

TE. of FD equation $O(\Delta t,\Delta x^2)$

Forward time & central space--FTCS

Notes to Section 2.2

2.2.4 Polynomial fitting for FD of derivatives

Assuming a local profile (型线)for the function studied:

- **Local linear function－leading to 1st-order FD expressions**

$$\phi(x_0+\Delta x,t)\cong a+bx$$

Set the origin (原点) at x_0**， yields:**

$$\phi_i^n=a,\ \phi_{i+1}^n=a+b\Delta x,$$

$$\frac{\partial\phi}{\partial x}\cong b=\frac{\phi_{i+1}^n-a}{\Delta x}=\frac{\phi_{i+1}^n-\phi_i^n}{\Delta x}$$

2. Local quadratic function (二次函数) —leads to 2nd order FD expressions

$$\phi(x_0+\Delta x,t)\cong a+bx+cx^2$$

Set the origin (原点) at x_0, yields:

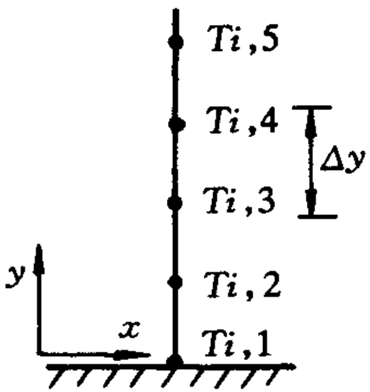
$$\phi_i^n=a,\quad \phi_{i+1}^n=a+b\Delta x+c\Delta x^2,\quad \phi_{i-1}^n=a-b\Delta x+c\Delta x^2$$

$$b=\frac{\phi_{i+1}^n-\phi_{i-1}^n}{2\Delta x},\qquad c=\frac{\phi_{i+1}^n-2\phi_i^n+\phi_{i-1}^n}{2\Delta x^2}$$

$$\frac{\partial\phi}{\partial x}\cong b=\frac{\phi_{i+1}^n-\phi_{i-1}^n}{2\Delta x},\qquad \frac{\partial^2\phi}{\partial x^2}\cong 2c=\frac{\phi_{i+1}^n-2\phi_i^n+\phi_{i-1}^n}{\Delta x^2},$$

3. Polynomial fitting used for treatment (处理) of B.C.

[Exam.2－1] **Known**: $T_{i,1}, T_{i,2}, T_{i,3}$



Find: **wall heat flux in y-direction with 2nd-order accuracy.**

Solution: **Assuming a quadratic temp. function at y＝0**

$$T(x,y) = a + by + cy^2, \quad O(\Delta y^3)$$

$$T_{i,1} = a,\ T_{i,2} = a + b\Delta y + c\Delta y^2, T_{i,3} = a + 2b\Delta y + 4c\Delta y^2$$

Yield:
$$b = \frac{-3T_{i,1} + 4T_{i,2} - T_{i,3}}{2\Delta y}$$

Then:
$$q_b = -\lambda \frac{\partial T}{\partial y})_{y=0} \cong \text{-}\lambda b = \frac{\lambda}{2\Delta y}(3T_{i,1} - 4T_{i,2} + T_{i,3}), O(\Delta y^2)$$

End of Notes

2.3 Control Volume and Heat Balance Methods for Equation Discretization

2.3.1 Procedures for implementing (实行） CV method

2.3.2 Two conventional profiles(型线）

2.3.3 Discretization of 1-D model eq. by CV method

2.3.4 Discussion on profile assumptions in FVM

2.3.5 Discretization equation by balance(平衡） method

2.3.6 Comparisons between two methods

2.3 Control Volume and Heat Balance Methods for Equation Discretization

2.3.1 Procedures for implementing CV method

1. Integrating (积分） conservative PDE over a CV

2. Selecting (选择) profiles for dependent variable (因变量) and its 1st derivative

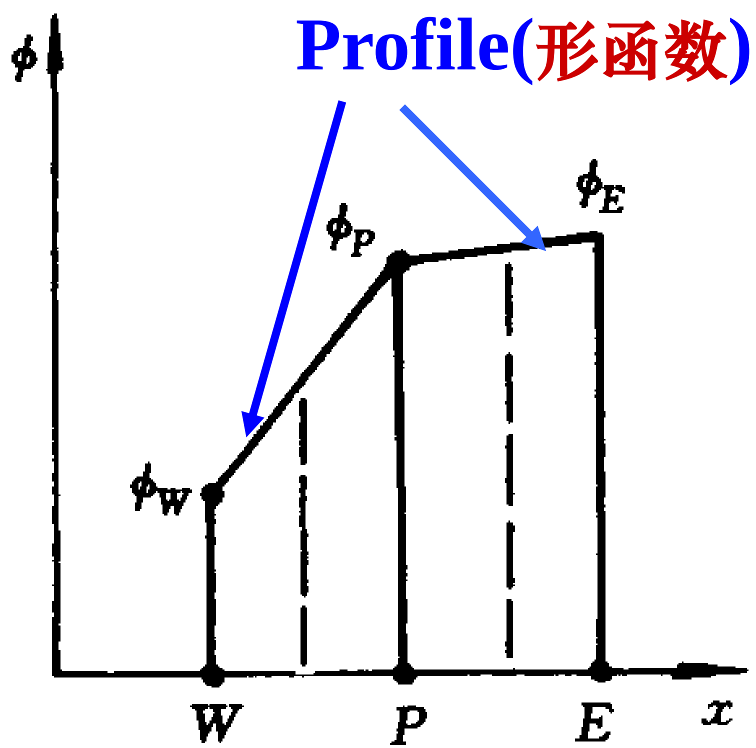
Profile is a local variation pattern of dependent variables with space coordinate.

3. Completing integral and rearranging algebraic equations

2.3.2 Two conventional profiles (shape function)

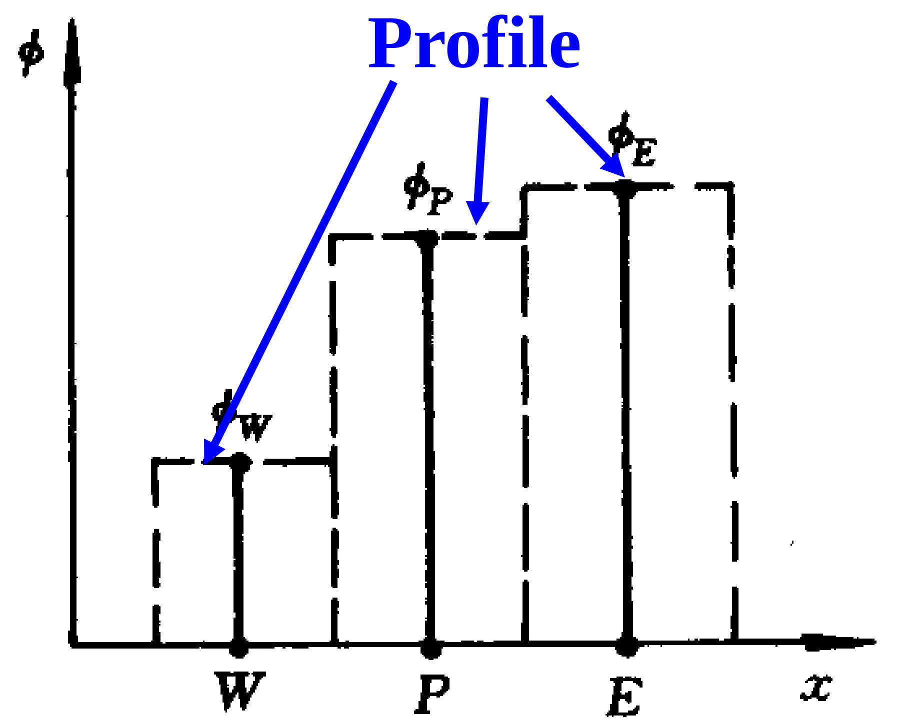
Originally (本来) shape profile (形函数） is to be solved; here it is to be assumed!

Variation with spatial coordinate



piece-wise linear

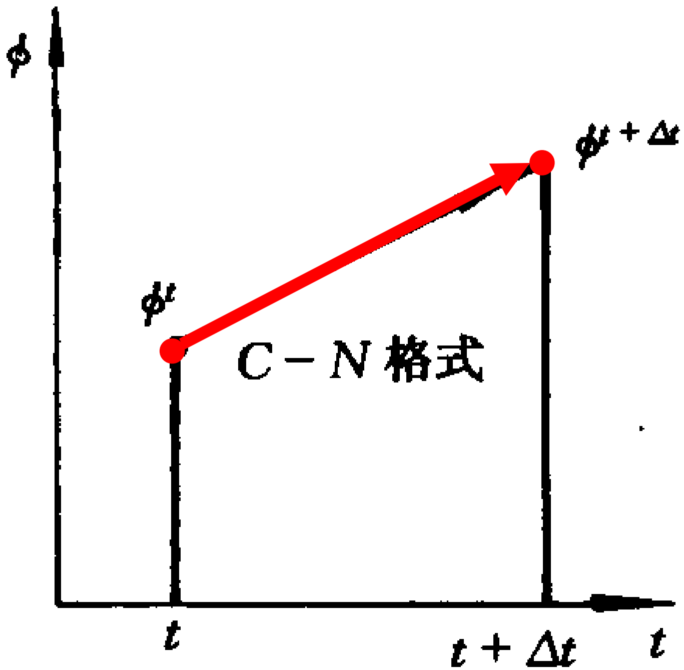
分段线性

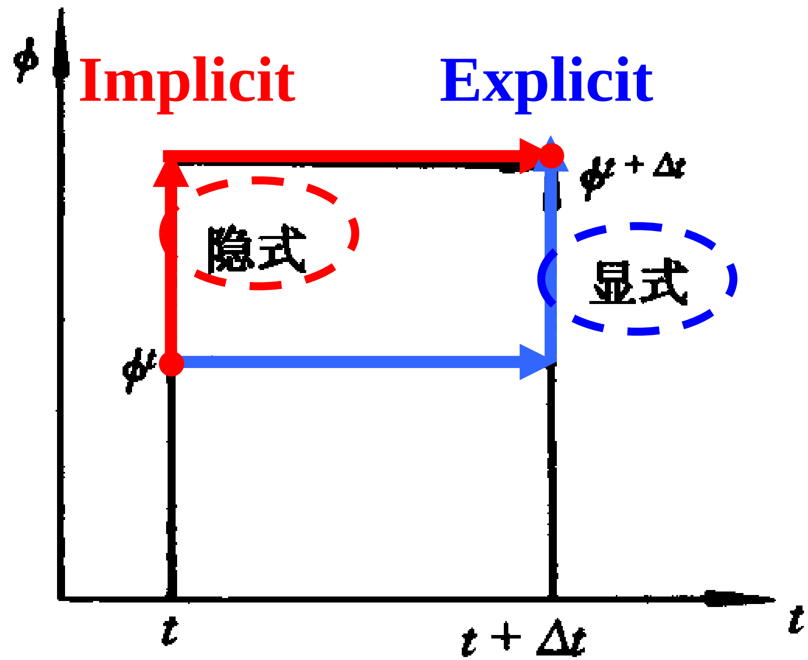


step-wise approximation

阶梯逼近

Variation with time





piece-wise linear　　step-wise approximation

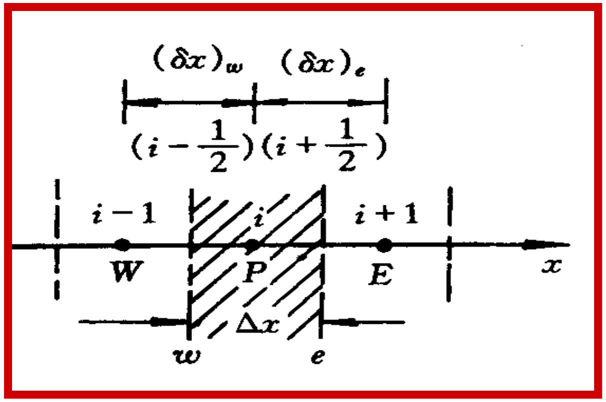
分段线性　　阶梯逼近

2.3.3 Discretization of 1-D model eq. by CV method

Integrating conservative GE over a CV within [t, $t+\Delta t$],

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(\rho u\phi)}{\partial x}=\frac{\partial}{\partial x}(\Gamma\frac{\partial\phi}{\partial x})+S_\phi$$

yields:



$$\rho\int_w^e(\phi^{t+\Delta t}-\phi^t)dx+\rho\int_t^{t+\Delta t}[(u\phi)_e-(u\phi)_w]dt=$$

$$\Gamma\int_t^{t+\Delta t}[(\frac{\partial\phi}{\partial x})_e-(\frac{\partial\phi}{\partial x})_w]dt+\int_t^{t+\Delta t}\int_w^e S_\phi dxdt$$

To complete the integraton we need the profiles of the dependent variable and its 1st derivative.

1. Transient term

Assuming the **step-wise** approximation for ϕ with space:

$$\rho\int_{w}^{e}(\phi^{t+\Delta t}-\phi^{t})dx=\rho(\phi_P^{t+\Delta t}-\phi_P^{t})\Delta x$$

2. Convective term

Assuming the **explicit step-wise** approximation for ϕ **with time:**

$$\rho\int_{t}^{t+\Delta t}[(u\phi)_e-(u\phi)_w]dt=\rho[(u\phi)_e^t-(u\phi)_w^t]\Delta t$$

Further, assuming linear-wise variation of ϕ with space

$$\rho[(u\phi)_e^t-(u\phi)_w^t]\Delta t = \rho u\Delta t(\frac{\phi_E+\phi_P}{2}-\frac{\phi_P+\phi_W}{2}) = \rho u\Delta t\frac{\phi_E-\phi_W}{2}$$

Uniform grid

Super-script "t" is temporary neglected!

3. Diffusion term

Taking explicit step-wise variation of $\frac{\partial\phi}{\partial x}$ with time, yields:

$$\Gamma\int_t^{t+\Delta t}[(\frac{\partial\phi}{\partial x})_e-(\frac{\partial\phi}{\partial x})_w]dt = \Gamma[(\frac{\partial\phi}{\partial x})_e^t-(\frac{\partial\phi}{\partial x})_w^t]\Delta t$$

Further, assuming linear-wise variation of ϕ with space

$$\Gamma[(\frac{\partial \phi}{\partial x})_e^t - (\frac{\partial \phi}{\partial x})_w^t]\Delta t = \Gamma \Delta t[\frac{\phi_E - \phi_P}{(\Delta x)_e} - \frac{\phi_P - \phi_W}{(\Delta x)_w}]$$

uniform $\rightarrow$

$$= \Gamma \Delta t \frac{\phi_E - 2\phi_P + \phi_W}{\Delta x}$$

Super-script "t" is temporary neglected!

4. Source term

Assuming explicit step wise with time and step-wise variation with space:

$$\int_t^{t+\Delta t}\int_w^e S dx dt = \overline{S}^t (\Delta x)_P \Delta t$$

$\overline{S}$ **---averaged one over space.**

Dividing both sides by $\Delta t \Delta x$

$$\rho \frac{\phi_P^{t+\Delta t} - \phi_P^t}{\Delta t} + \rho u \frac{\phi_E^t - \phi_W^t}{2\Delta x} =$$

$$\Gamma \frac{\phi_E^t - 2\phi_P^t + \phi_W^t}{\Delta x^2} + \overline{S}^t, O(\Delta t, \Delta x^2)$$

For the uniform grid system, the results are the same as that from Taylor expansion, which reads:

$$\rho \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \rho u \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} =$$

$$\Gamma \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + S_i^n, O(\Delta t, \Delta x^2)$$

FDM and FVM are a kind of brothers: they usually have the same TE and can help each other!

2.3.4 Discussion on profile assumptions in FVM

1. In FVM the only purpose of profile is **to derive the discretization equations**; Once they have been established, the function of profile is fulfilled (完成）.

2. The selection criterion (准则） of profile is easy to be implemented and good numerical characteristics; **Consistency** (协调) among different terms **is not required.**

3. In FVM profile is indeed **the scheme（差分格式）**.

2.3.5 Discretization equation by balance method

Brief review of 2018-09-12 lecture key points

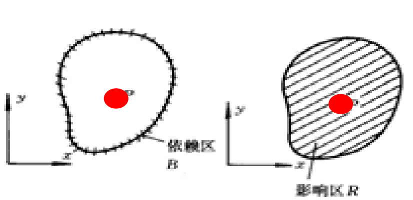
1.Elliptic vs. parabolic PDF（Math viewpoint）

$$a\phi_{xx} + b\phi_{xy} + c\phi_{yy} + d\phi_x + e\phi_y + f\phi = g(x,y)$$

a, b, c, d, e, f can be function of x, y, ϕ

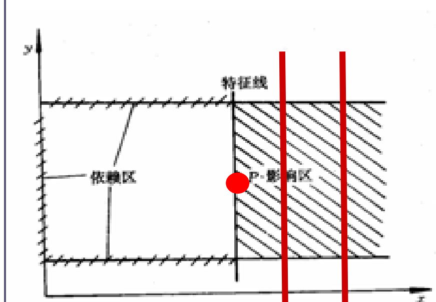
$$b^2 - 4ac \begin{cases} < 0 & \textbf{Elliptic} \quad \boxed{\text{椭圆型}} \ （\text{回流型}） \\ = 0 & \textbf{Parabolic} \quad \boxed{\text{抛物型}} \ （\text{边界层}） \end{cases}$$

Elliptic



solved simul-taneously

Parabolic



solved line by line!

2. Conservative vs. non-conservative (Physical VP)

Conservative： convective term is expressed by divergence form(散度形式).

Non-conservative： convective term is not expressed by divergence form.

3. Relationship with numerical solution

Elliptic: solved simultaneously for whole domain!

Parabolic: solved by marching forward method!

Discretization eqs. from conservative PDE may guarantee the conservation feature of the numerical solution.

Disc. eqs. from non-conservative PDE can not guarantee!

4. Procedures for implementing CV method

1) Integrating conservative PDE over a CV;

2) Selecting profiles for dependent variable and its 1st derivative;

3) Completing integral and rearranging algebraic equations

5. Two major profiles and their role

1) Two major profiles: piece-wise linear and step-wise;

2) The only purpose of profile is to derive discretization eqs. Consistency is not required.

3) Profile in space is actually the scheme for convection and diffusion terms, especially important for convection term.

4) Profile in time leads to explicit and implicit scheme in the determination of space derivatives.

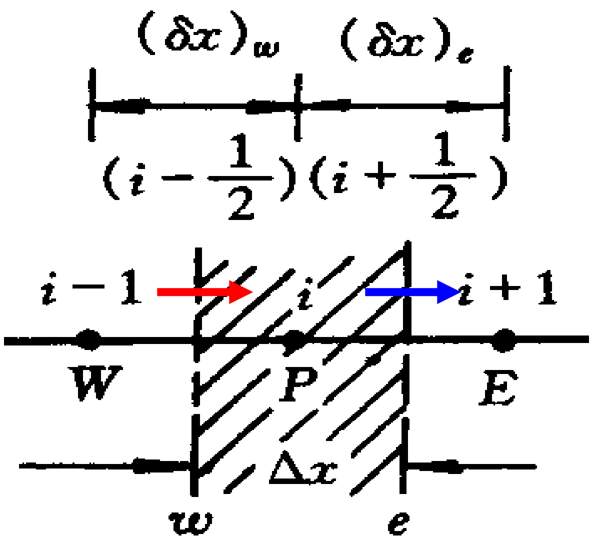
1. Major concept：Applying the conservative law directly to a CV, viewing the node as its representative (代表)

2. 1-D diffusion-convection problem with source term

Writing down balance equation for Δx and Δt

$$\underbrace{\rho(\phi_P^{t+\Delta t}-\phi_P^t)\Delta x}_{\text{Transient}}=\underbrace{\rho[(u\phi)_w^t-(u\phi)_e^t]\Delta t}_{\text{Convection}}$$

$$\underbrace{+[(\frac{\partial\phi}{\partial x})_e^t-(\frac{\partial\phi}{\partial x})_w^t]\Delta t}_{\text{Diffusion}}+\underbrace{\overline{S}^t\Delta x\Delta t}_{\text{Source}}$$



By selecting the profile of dependent variable ϕ with space, the discretization equation can be obtained.

2.3.6 Comparisons of two ways

Content	FDM	FVM
1. Error analysis	Easy	Not easy; via FDM
2. Physical concept	Not clear	Clear
3. Variable length step(变步长)	Not easy	Easy
4. Conservation feature of ABEs	Not guaranteed	May be guaranteed

FVM has been the 1st choice of most commercial software.

First Home Work

Homework of Chapter 1,2

Problem 1 was assigned in Chapter 1

2－3， 2－4， 2－5， 2－11

Please hand in on Sept.26, 2018

Please finish your homework independently !!!

Following textbook in English is available in our library:

Versteeg H K, Malalsekera W. An introduction to computational fluid dynamics. The finite volume method. Essex: Longman Scientific & Technical， 1995

Problem 2-3 **In the following non-linear equation of u, η is constant,**

$$u\frac{\partial u}{\partial x}=\eta\frac{\partial^2 u}{\partial x^2}$$

Obtain its conservation form and its discretization equation by the control volume integration method.

Problem 2-4

Using the control volume integration method discretize the 1-D heat conduction equation given below.

$$\frac{1}{r}\frac{1}{dr}\left(rk\frac{dT}{dr}\right)+S=0$$, where S is constant.

Also discretize the non-conservative form, as given below, of 1-D equation by using Taylor series expansion method.

$$k\frac{d^2T}{dr^2}+\frac{k}{r}\left(\frac{dT}{dr}\right)+S=0$$

Express the both results as: $a_P T_P = a_E T_E + a_W T_W + b$

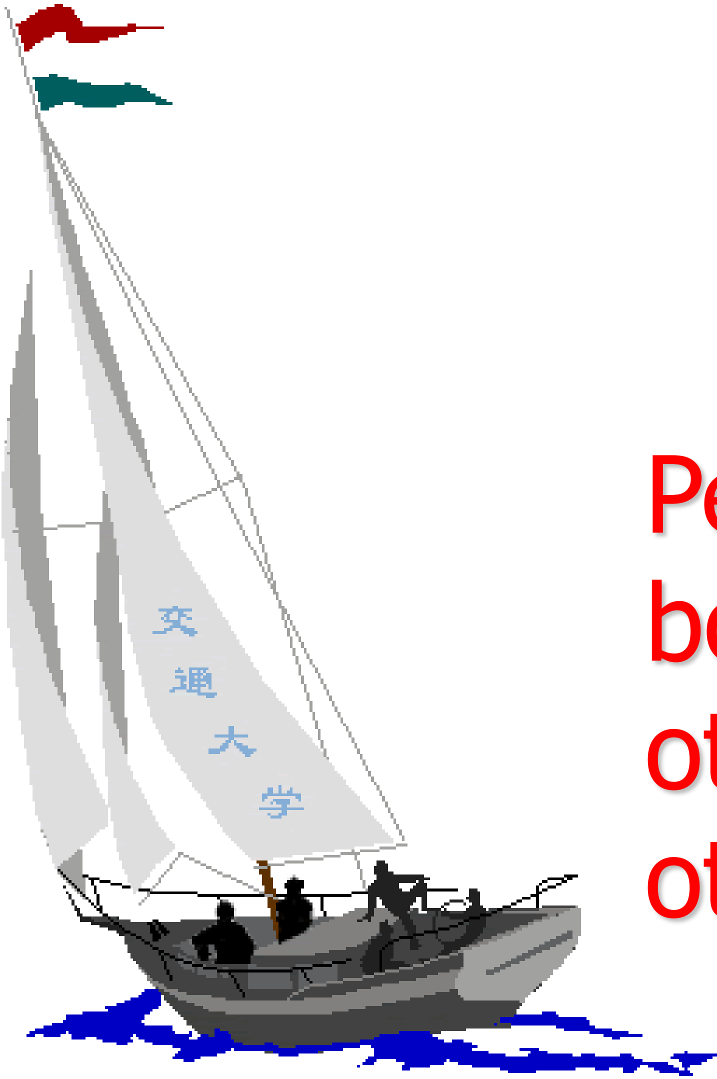
where 'b' is known but not contains T_P, T_E and T_W. Moreover, check for the case of constant properties and uniform grids that these two results are the same or not?

Problem 2-5 On a uniform grid system, adopt Taylor series expansion method to obtain the following FD form of $\dfrac{\partial^2\phi}{\partial x\partial y}$

$$\frac{\delta^2\phi}{\delta x\delta y}=\frac{\phi_{i+1,j+1}-\phi_{i+1,j-1}-\phi_{i-1,j+1}+\phi_{i-1,j-1}}{4\Delta x\Delta y}$$

Problem 2-11 **Derive following 3rd-order biased(偏) difference form for $\frac{\partial \phi}{\partial x}$:**

$$\frac{\delta \phi}{\delta x} = \frac{4\phi_{i+1} + 6\phi_i - 12\phi_{i-1} + 2\phi_{i-2}}{12\Delta x}$$



同舟共济
渡彼岸!

People in the same boat help each other to cross to the other bank, where....