Numerical Heat Transfer

(数值传热学)

Chapter 2 Discretization of Computational Domain and Governing Equations

Instructor Tao, Wen-Quan

CFD-NHT-EHT Center
Key Laboratory of Thermo-Fluid Science & Engineering
Xi’an Jiaotong University

Xi’an, 2016-Sept-19

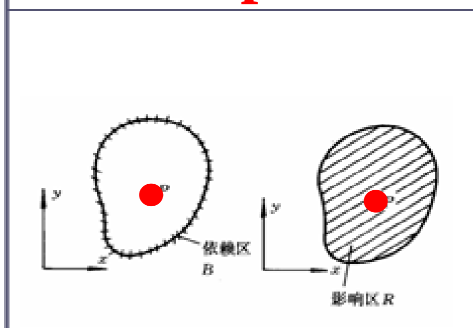
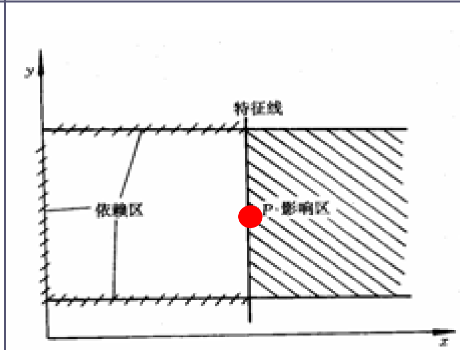
Brief review of 2016-09-14 lecture key points

1.Elliptic vs. parabolic PDF（Math viewpoing）

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

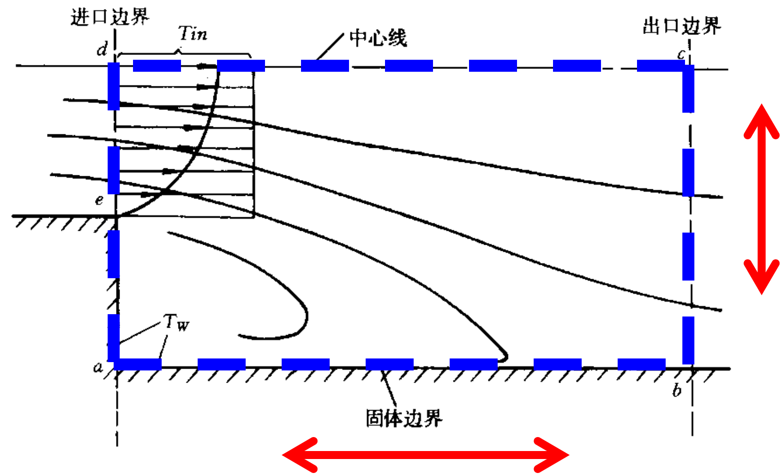
a, b, c, d, e, f can be function of x, y, ϕ

$b^2 - 4ac$ { Elliptic 椭圆型（回流型）; Parabolic 抛物型（边界层）

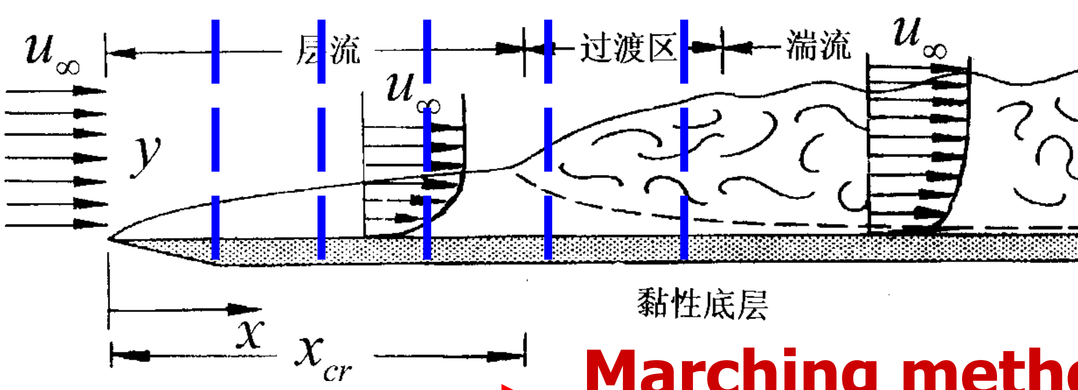
Elliptic	Parabolic
	

2. Relationship with numerical methods

（1）**Elliptic**： flow **with** recirculation（回流），solution should be conducted simultaneously for the whole domain;



（2）**Parabolic**： flow **without** recirculation， solution can be conducted by marching method, greatly saving computing memory and time!。



Marching method

3. 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.

4. Relationship with numerical solution

Discretization equations derived from conservative PDE **may guarantee** the conservation feature of the numerical solution. Conservation of physical quantity (mass, momentum, energy, etc) is usually required in engineering computation.

Contents

2.1 Grid Generation (Domain Discretization)

2.1.1 Task, method and classification of domain discretization

2.1.2 Expression of grid layout (布置)

2.1.3 Introduction to different methods of grid generation

2.1.4 Comparison between Practices A and B

2.1.5 Grid-independent （网格独立解）solution

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.

Five kinds of information can be obtained:

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

(2) Control volume (控制容积) :the minimum volume at 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.

(5) Spatial relationship between two neighboring nodes.

The influencing coefficients will be decided in the procedure of equation of discretization.

2. Classification of domain discretization

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

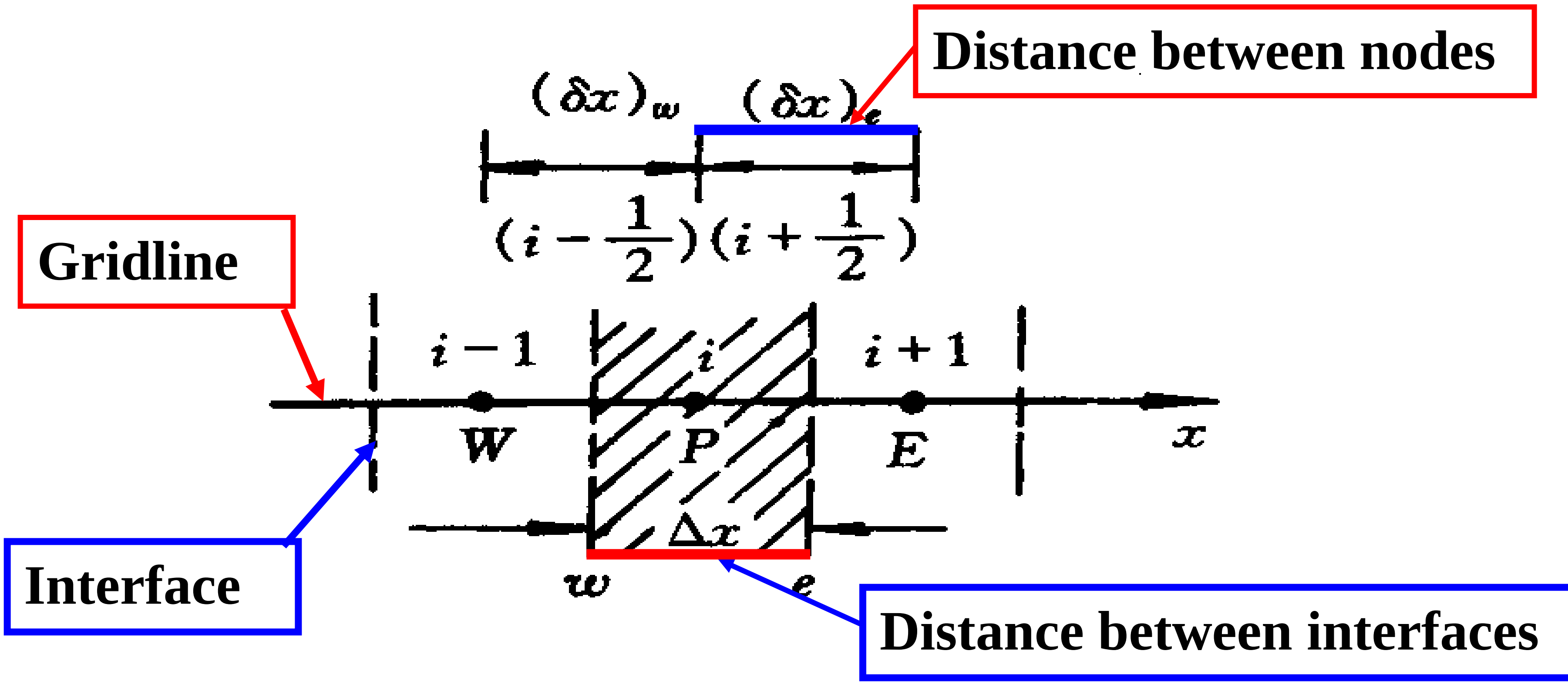
(2) According to node position: inner node vs. outer node

2.1.2 Expression of grid system

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

Distance between nodes－δx

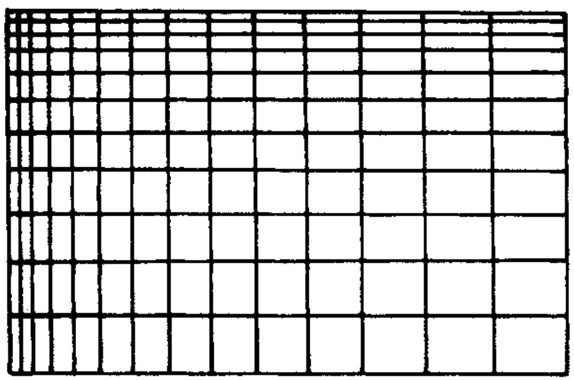
Distance between interfaces－Δx



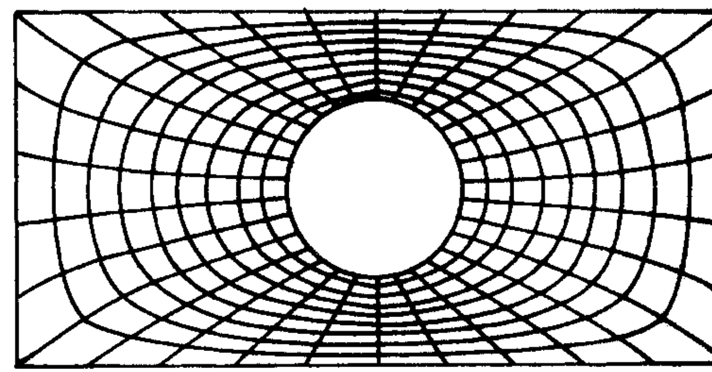
2.1.3 Introduction to different types of grid system and generation method

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

（2） **Unstructured grid（非结构化网格）**： Node position layout 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.

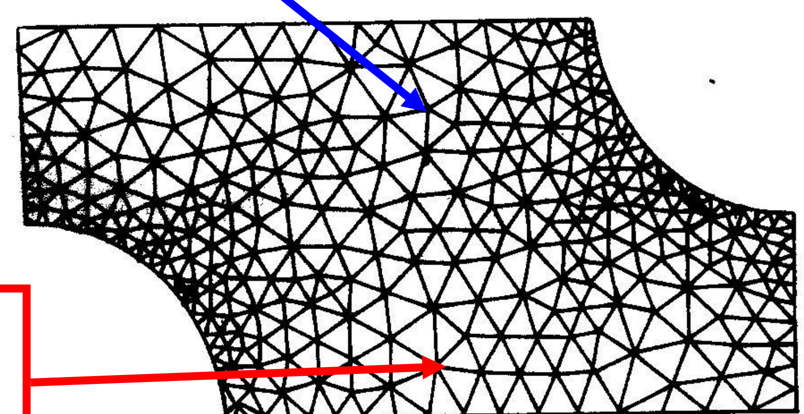


Structured （a）



Structured （b）

5 elements



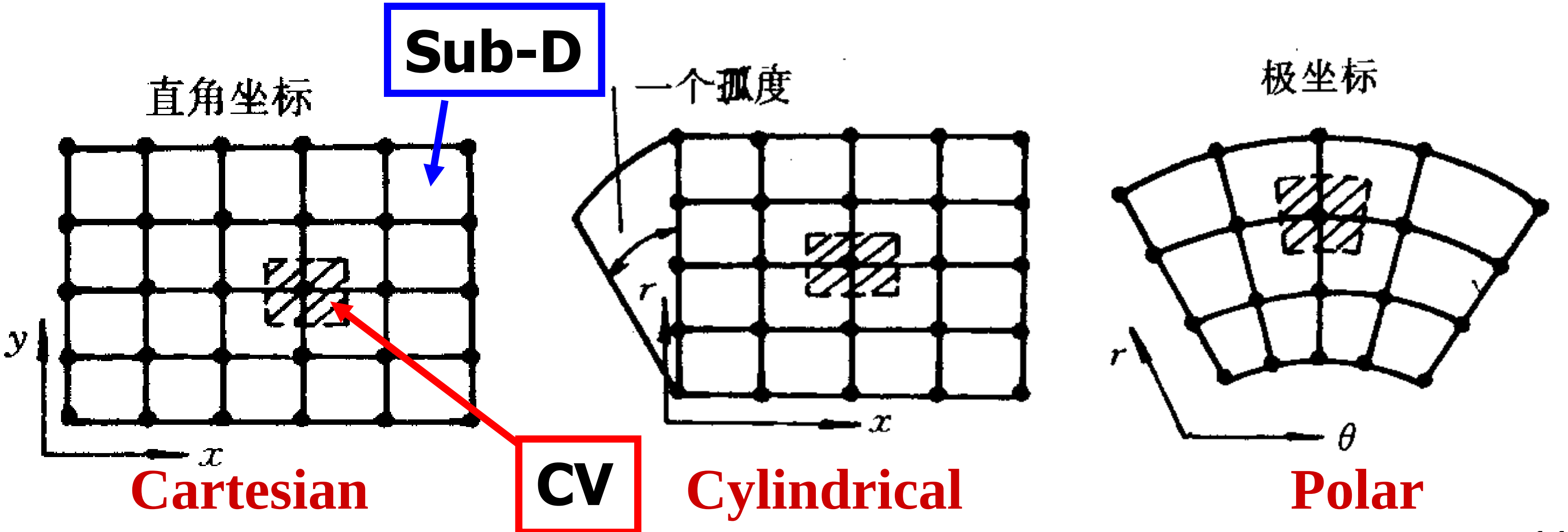
Un-structured

6 neighboring elements

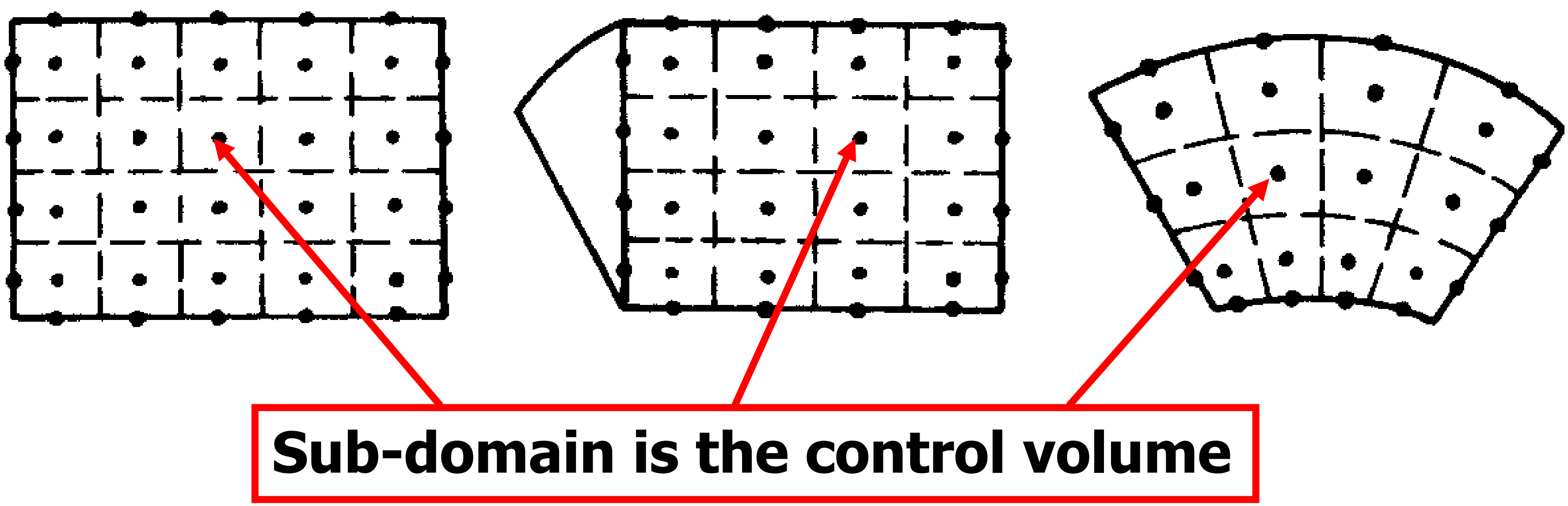
Both structured and unstructured grid layout (节点布置) have two practices.

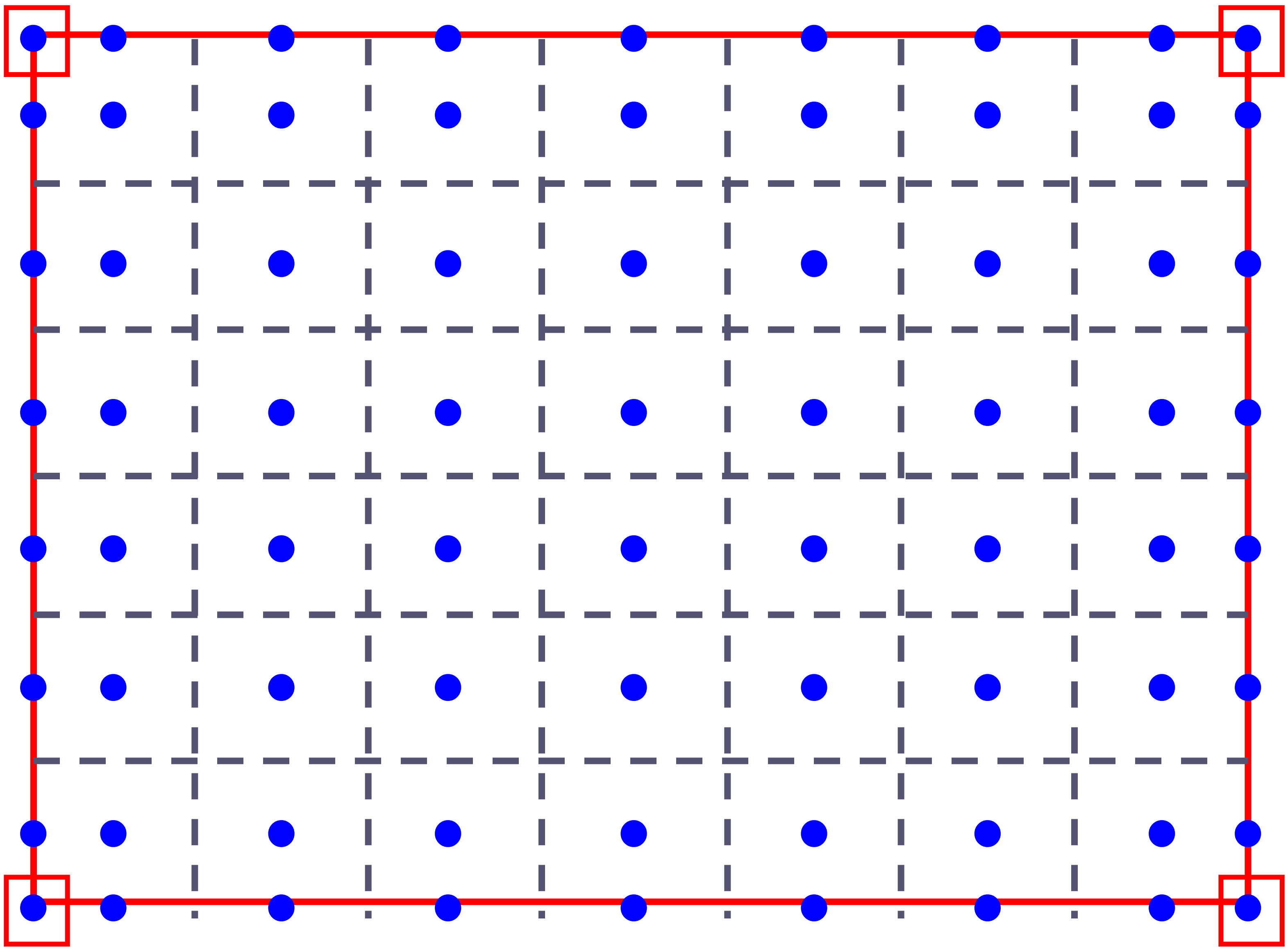
（3）Outer node and inner node for structured grid

(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).**



(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）.



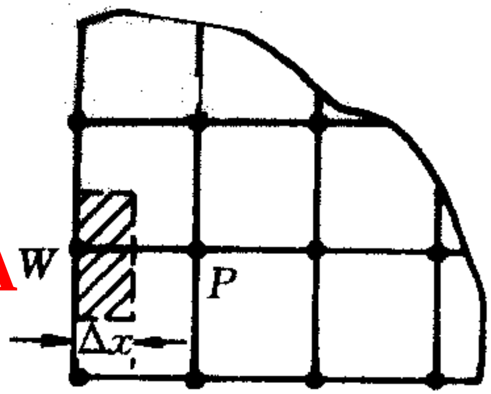


Generating procedure of Practice B

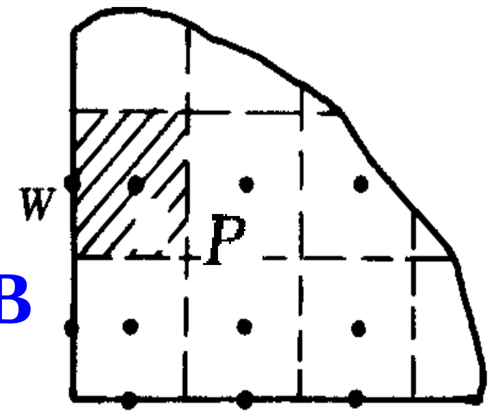
2.1.4 Comparison between Practices A and B

(a) Boundary nodes have different CV.

Practice A



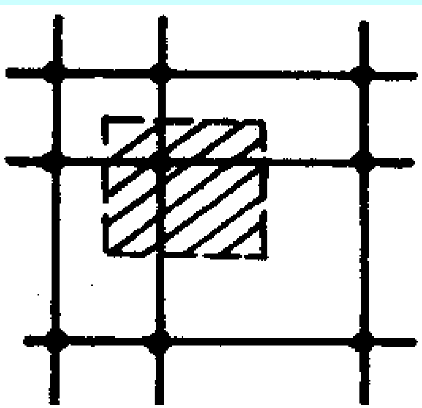
Practice B



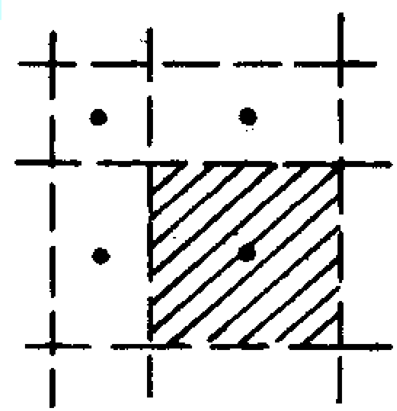
Boundary point has half CV. **Boundary poinnt has zero CV**

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

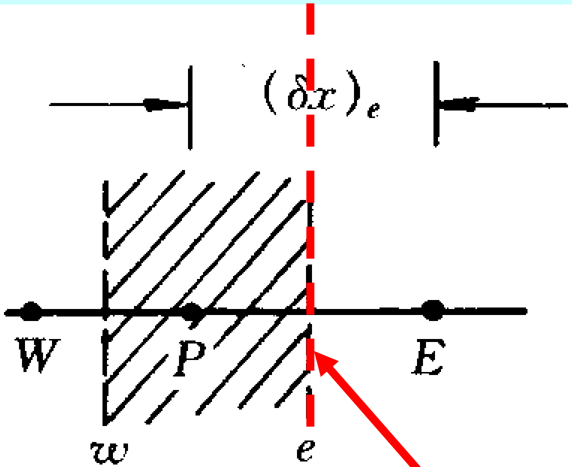
Practice A

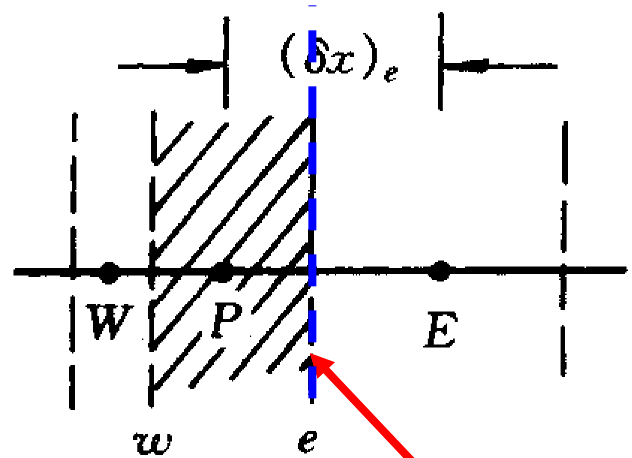


Practice B



(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

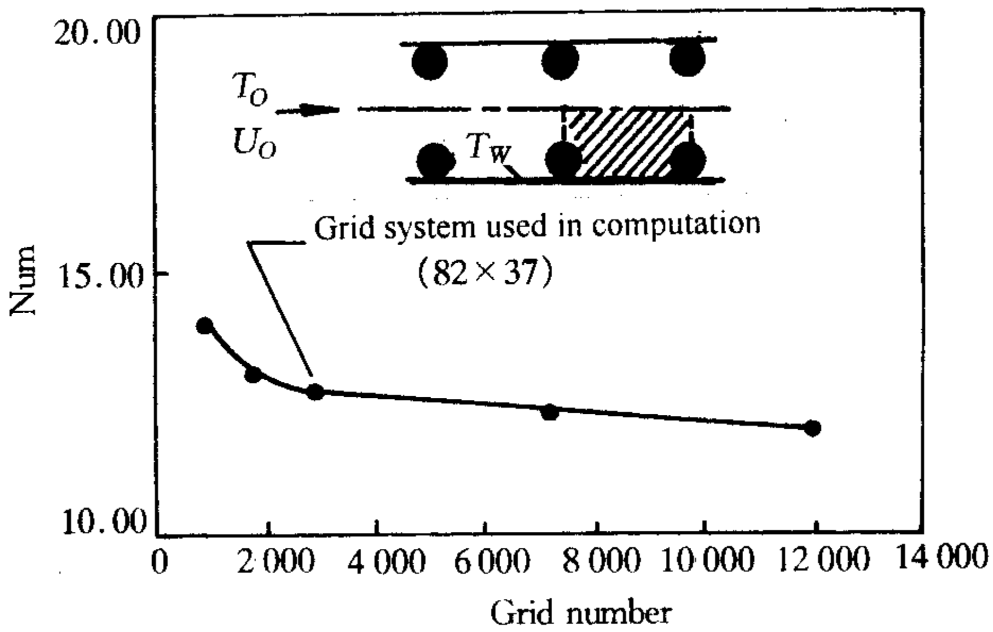
Lower than 2nd order accuracy

2.1.5 Grid-independent solutions

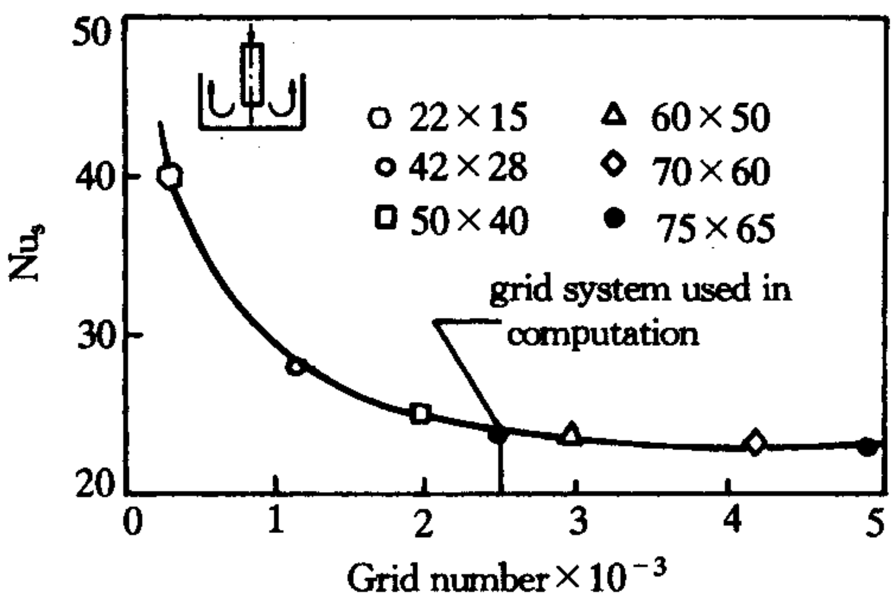
Grid generation is an iterative procedure（迭代过程）; Debugging (调试）and comparison are often needed. For a complicated geometry grid generation may take a major part of total computational time.

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

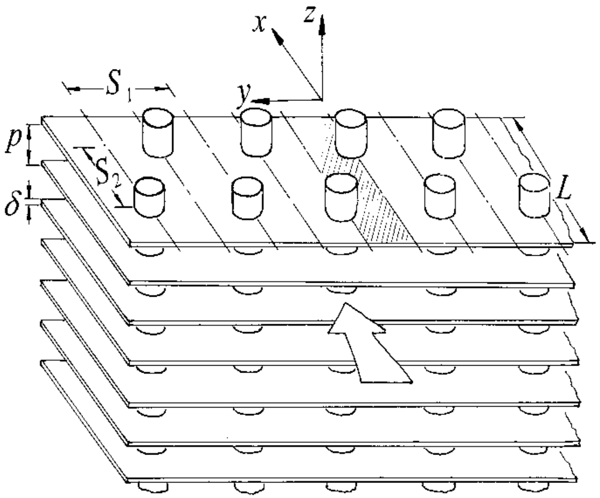
The appropriate grid fineness(细密程度) is such that the numerical solutions are nearly independent on the grid numbers. Such numerical solutions are called grid-independent solutions. This is required for publication of a paper.

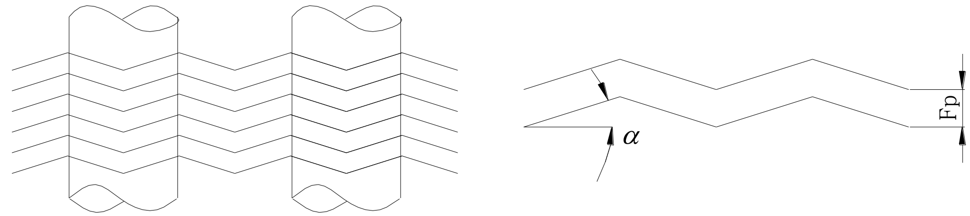


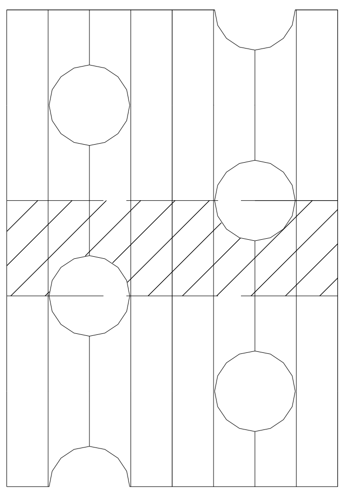
Int. Journal Heat & Fluid Flow, 1993, 14(3):246-253。

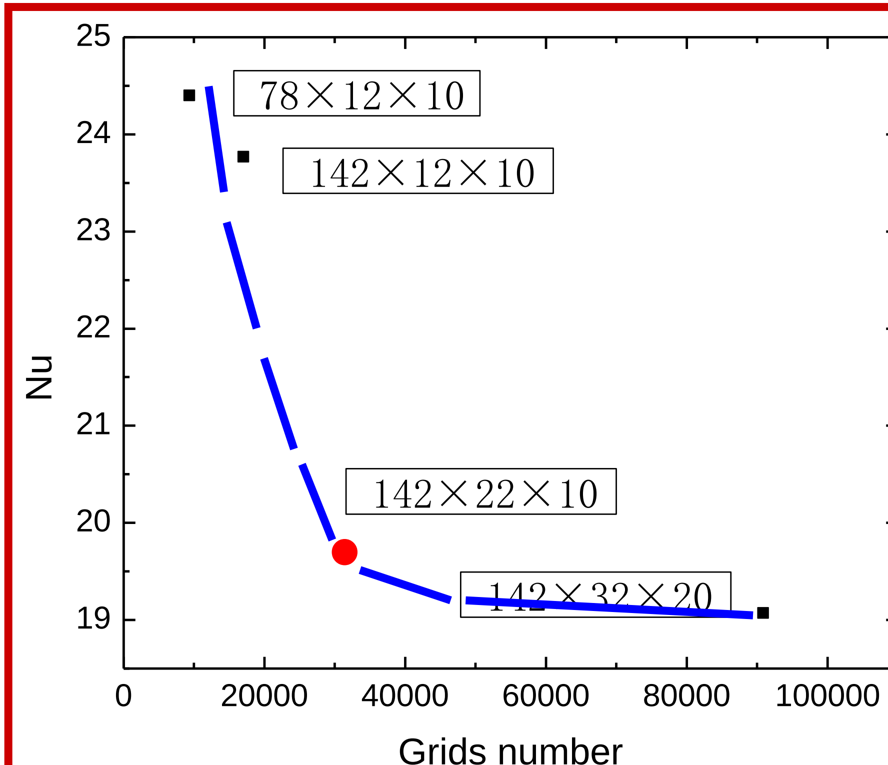


Int. Journal Numerical Methods in Fluids, 1998, 28: 1371-1387。









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

Conservative

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

For FVM

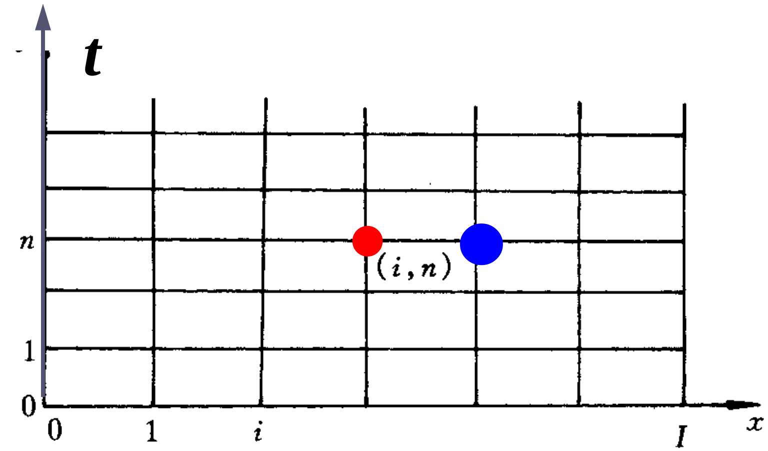
Trans **Conv.** **Diffus.** **Source**

Small but complete---“麻雀虽小，五脏俱全！”

2.2.2 Taylor expansion for FD 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 in dependent of Δx

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 **, yields:**

Forward difference:

(向前差分)

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

Backward difference: (向前差分)

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

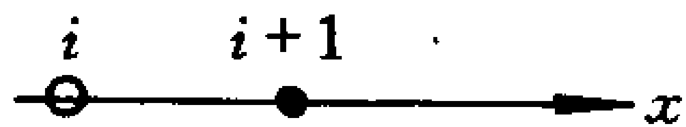
Central difference: (中心差分)

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

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

Stencil (格式图案) of FD expression

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

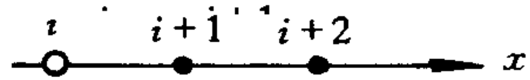
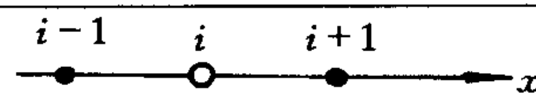
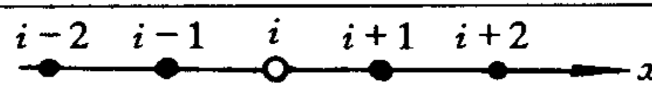


○ **For the node where FD form is constructed**

● **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
$\left.\frac{\partial \phi}{\partial x}\right)_{i,n}$	$\frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$	○ i ● $i+1$ → x	$O(\Delta x)$
	$\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$	● $i-1$ ○ i → x	$O(\Delta x)$
	$\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}$	● $i-1$ ○ i ● $i+1$ → x	$O(\Delta x^2)$
	$\frac{-3\phi_i^n + 4\phi_{i+1}^n - \phi_{i+2}^n}{2\Delta x}$	○ i ● $i+1$ ● $i+2$ → x	$O(\Delta x^2)$
	$\frac{3\phi_i^n - 4\phi_{i-1}^n + \phi_{i-2}^n}{2\Delta x}$	● $i-2$ ● $i-1$ ○ i → x	$O(\Delta x^2)$
	$\frac{4\phi_{i+1}^n + 6\phi_i^n - 12\phi_{i-1}^n + 2\phi_{i-2}^n}{12\Delta x}$	● $i-2$ ● $i-1$ ○ i ● $i+1$ → x	$O(\Delta x^3)$
	$\frac{-2\phi_{i+2}^n + 12\phi_{i+1}^n - 6\phi_i^n - 4\phi_{i-1}^n}{12\Delta x}$	● $i-1$ ○ i ● $i+1$ ● $i+2$ → x	$O(\Delta x^3)$
	$\frac{\phi_{i-2}^n - 8\phi_{i-1}^n + 8\phi_{i+1}^n - \phi_{i+2}^n}{12\Delta x}$	● $i-2$ ● $i-1$ ○ i ● $i+1$ ● $i+2$ → x	$O(\Delta x^4)$

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

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

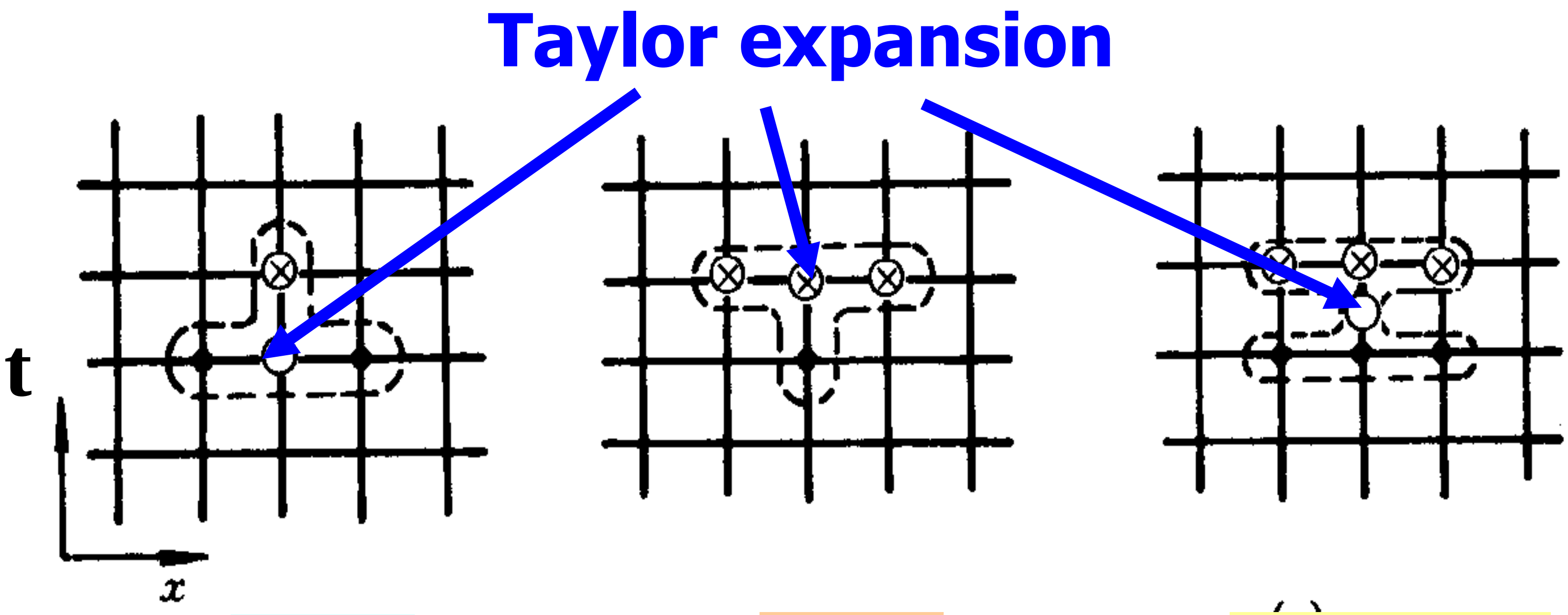
Rule of Thumb

(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

1. Time level at which spatial derivatives are determined



显式 explicit	隐式 implicit	C-N格式 Crank-Nicolson
$O(\Delta t)$	$O(\Delta t)$	$O(\Delta t^2)$

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

TE. of FD equation

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

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

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:

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

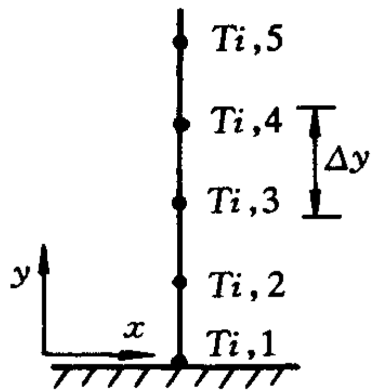
$$b=\frac{\phi_{i+1}^n-\phi_{i-1}^n}{2\Delta x},\qquad c=\frac{\phi_{i+1}^n-2\phi_i^n+\phi_{i-1}^n}{2\Delta x^2}$$

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

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

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:

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

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

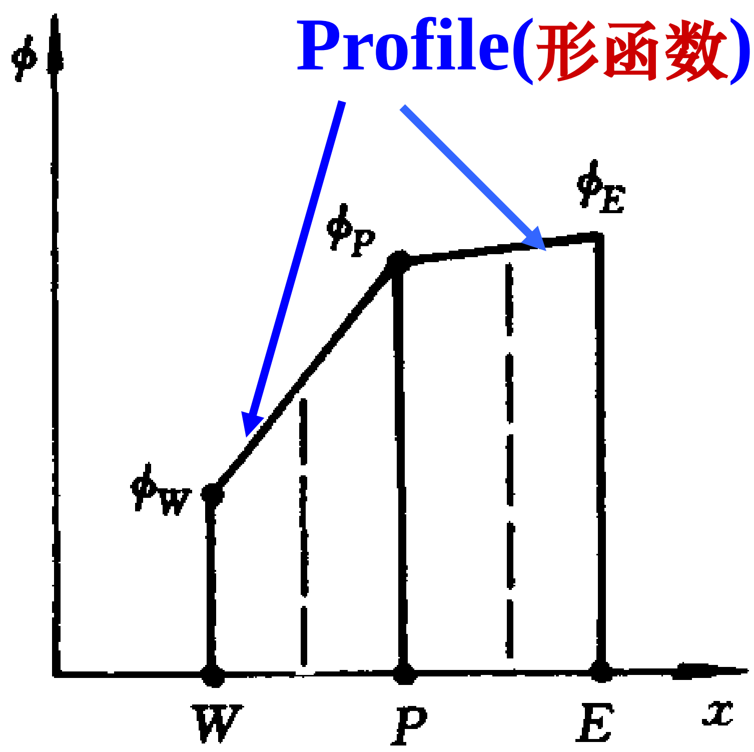
Profile－a local variation pattern of DV with space coordinate

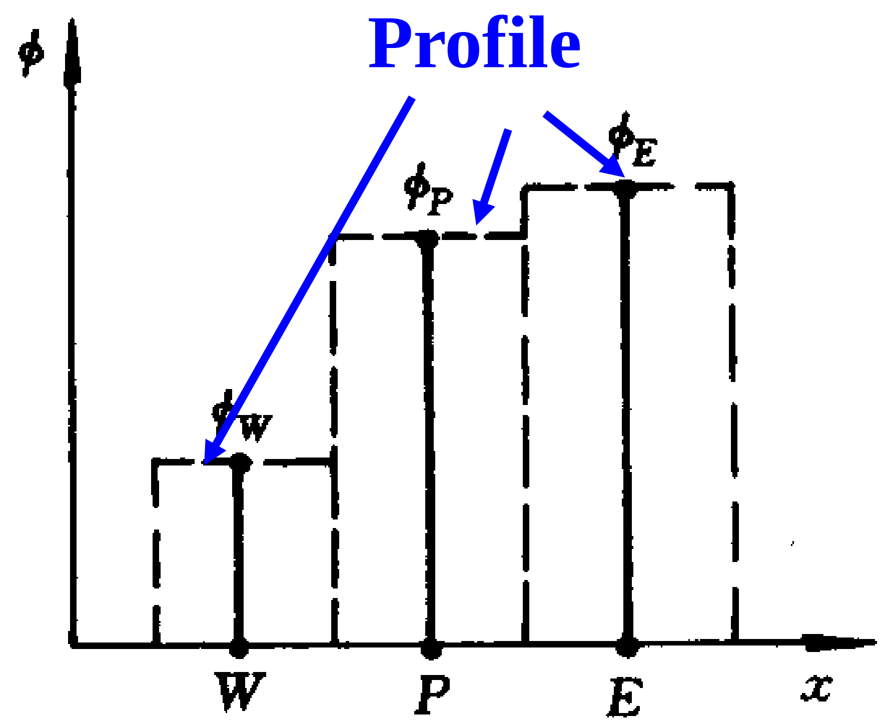
3. Completing integral and rearranging algebraic equations

2.3.2 Two conventional profiles (shape function)

Originally (本来) profile is to be solved; here it is to be Assumed!

Variation with spatial coordinate

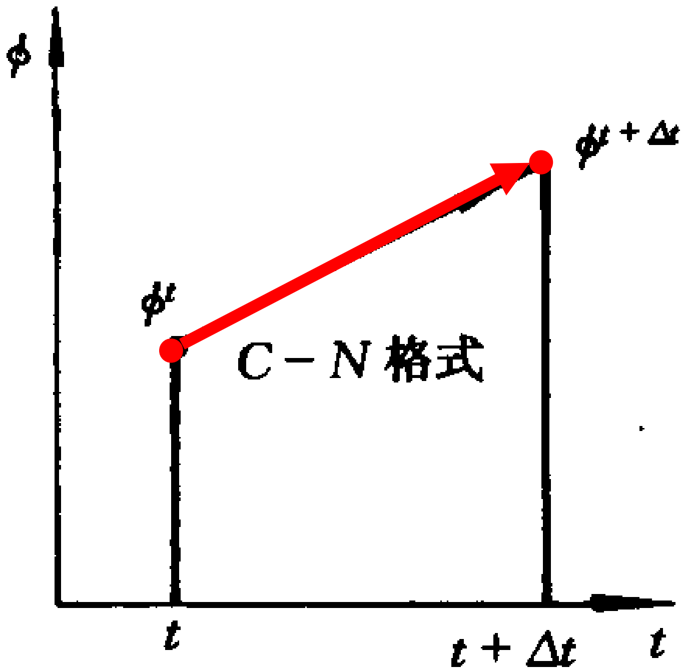


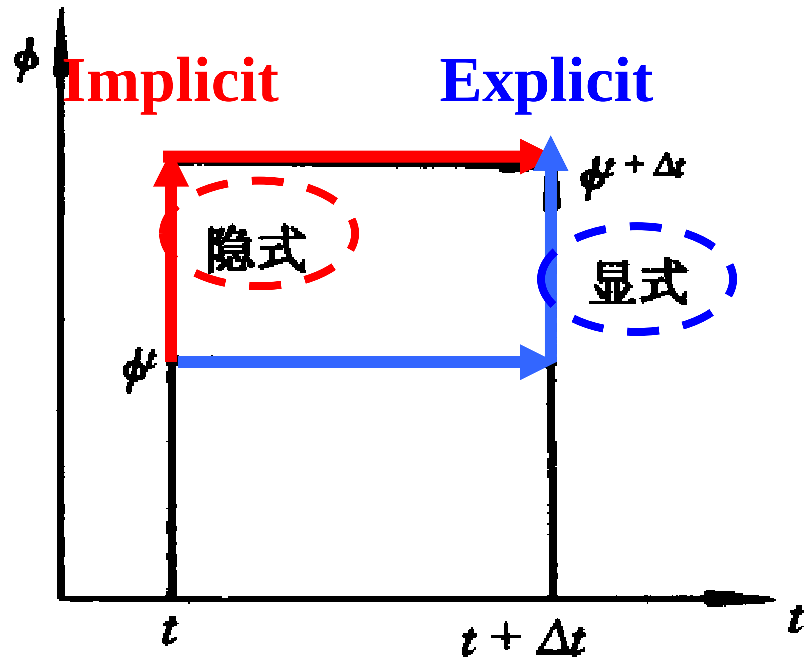


分段线性　　　　阶梯逼近

piece-wise linear　　**step-wise approximation**

Variation with time





分段线性 **阶梯逼近**

piece-wise linear **step-wise approximation**

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

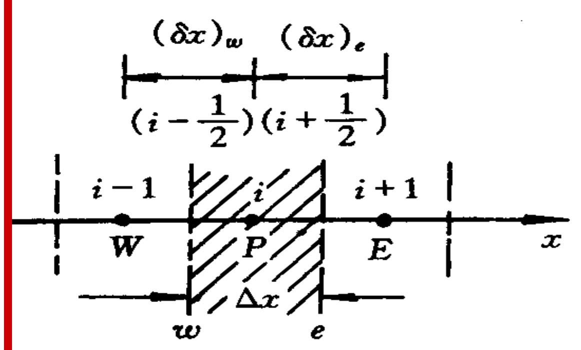
Integrating conservative GE over a CV within [*t*, *t* + Δ*t*],

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

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 integral 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

3. Diffusion term

Taking explicit step-wise variation with time for $\frac{\partial \phi}{\partial x}$

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

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 →

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

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:

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

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 are 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

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

2. 1-Ddiffusion-convection problem with ST

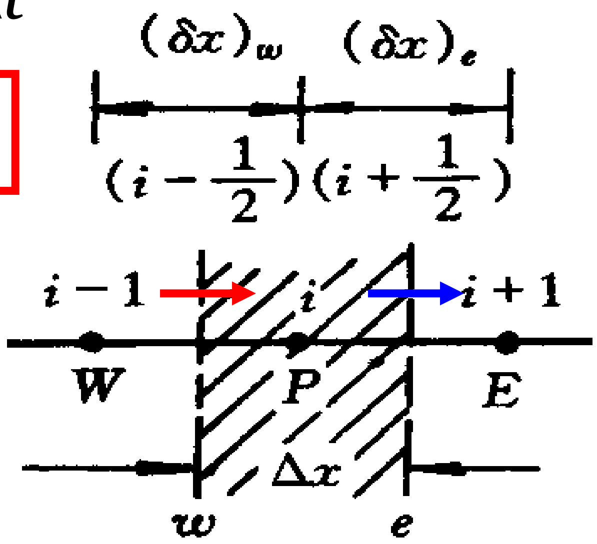
Writing down balance equation for Δx and Δt

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

Transient **Convection**

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

Diffusion **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 CSW.

First Home Work

1－7（补充不可压，常物性的条件）

2－4， 2－7， 2－9， 2－12

Please hand in on Oct.10, 2016

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 2-4

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 2-7

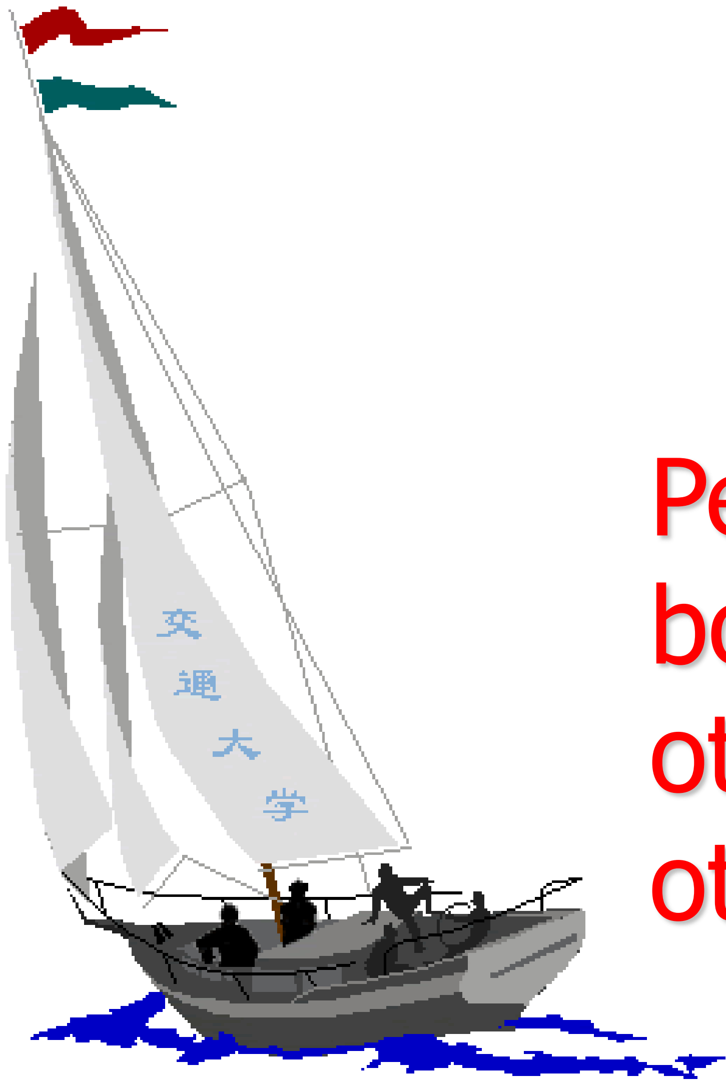
Derive the following equation and analyze the order of truncation error (Ref. Equation 2-7 in the text book).

$$T_{i,1}=\frac{1}{11}(18T_{i,2}-9T_{i,3}+2T_{i,4}+\frac{6\Delta y q_B}{\lambda})$$

Problem 2-9 **As shown in Fig. 2-11 (see page 45 of the textbook), grids 1,2,3,4 are uniformly distributed. The pressures at grids 1,2 and 3 are known. Derive the finite difference equation for the pressure gradient at the wall with 2nd order accuracy.**

Problem 2-12 **Derive the finite difference equation for the 2nd-order derivative , $\frac{\partial^2\phi}{\partial x^2}$, with fourth order accuracy.**

The English version of Problem 1-7 was given in the PPT of Chapter 1.



同舟共济
渡彼岸!

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