Numerical Heat Transfer
(数值传热学)
Chapter 2 Discretization of Computational Domain and Governing Equations

Instructor Tao, Wen-Quan

Key Laboratory of Thermo-Fluid Science & Engineering
Int. Joint Research Laboratory of Thermal Science & Engineering
Xi'an Jiaotong University
Innovative Harbor of West China, Xian

2024-Sept-14

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 entire 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 (空间的) relationship between two neighboring nodes, the **influencing coefficients (影响系数)**, will be decided in the procedure of the 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

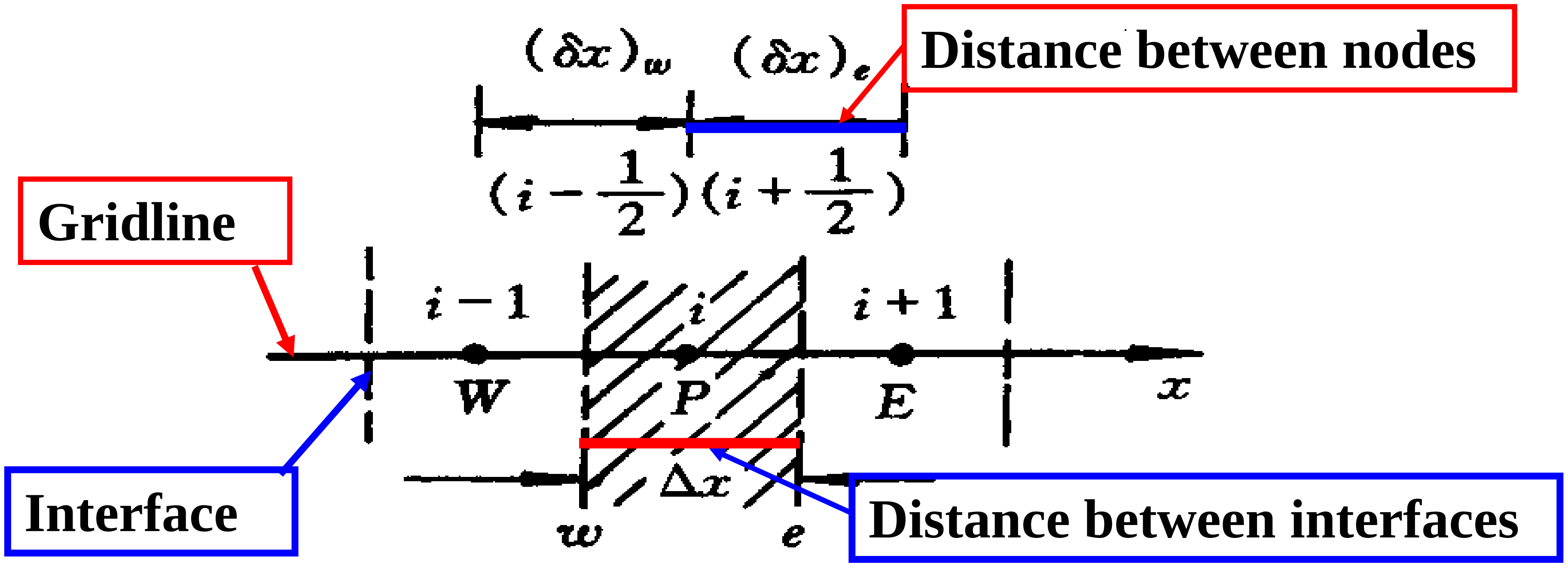
2.1.2 Expression of grid system (**网格系统表示**)

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

Distance between two nodes— δx

Distance between two interfaces— Δx

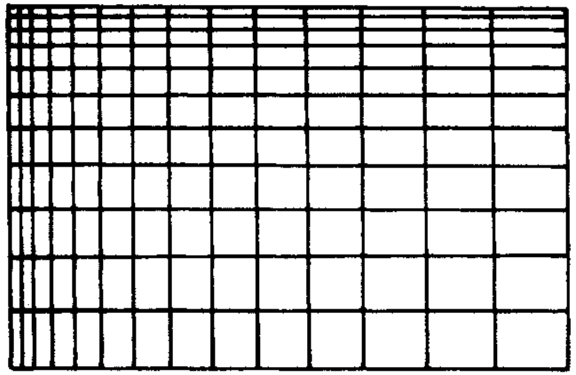
Interfaces by lower cases(小写字母) ***w*** and ***e*** .



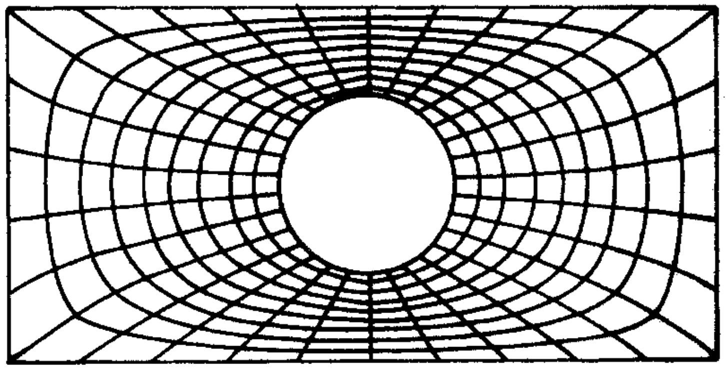
2.1.3 Introduction to different types of grid system and generation method

(1) **Structured grid (结构化网格)**: Node position layout（布置）is in order (有序的）, 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 **(存储)** of the relationship of neighboring nodes are the major work of grid generation.

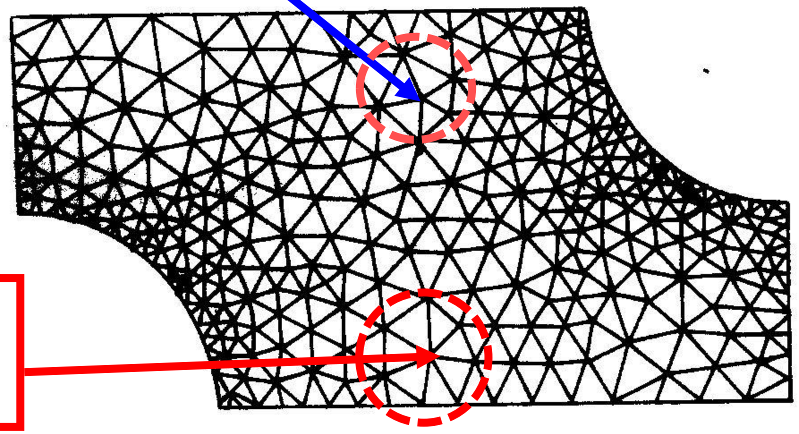


Structured （a）



Structured （b）

5 elements



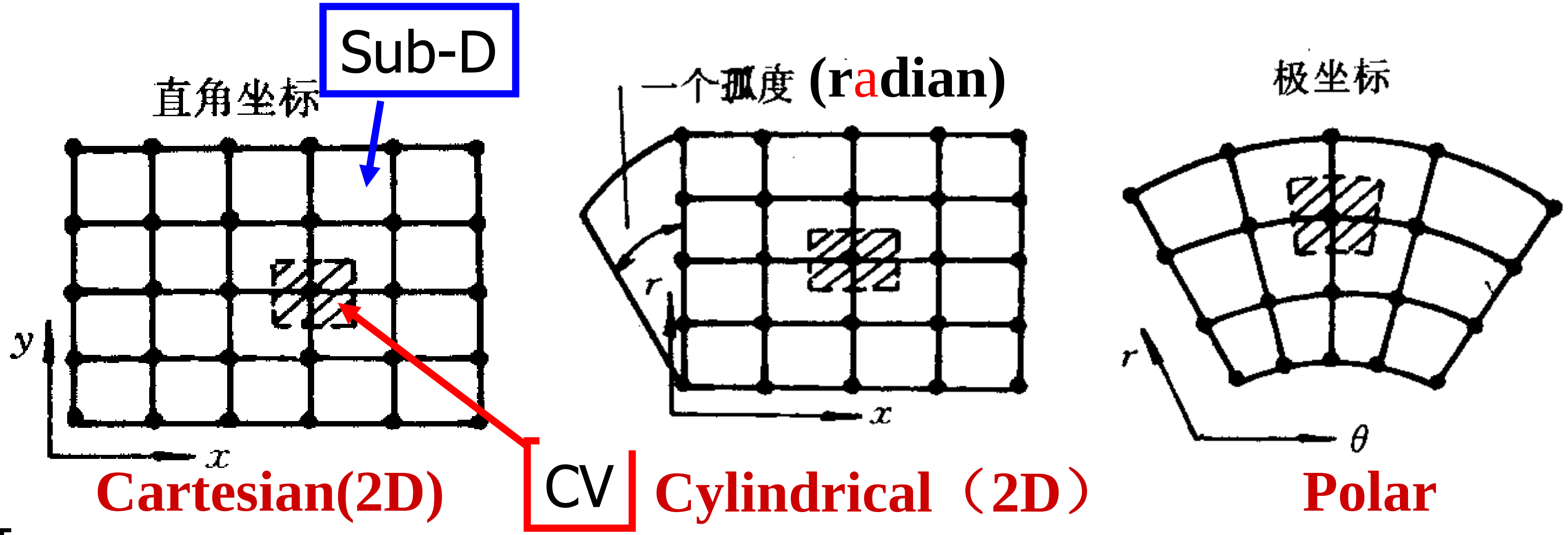
Un-structured

6 neighboring elements

Both structured and unstructured grid layout (节点布置) have two practices（实施）： outer node and inner node.

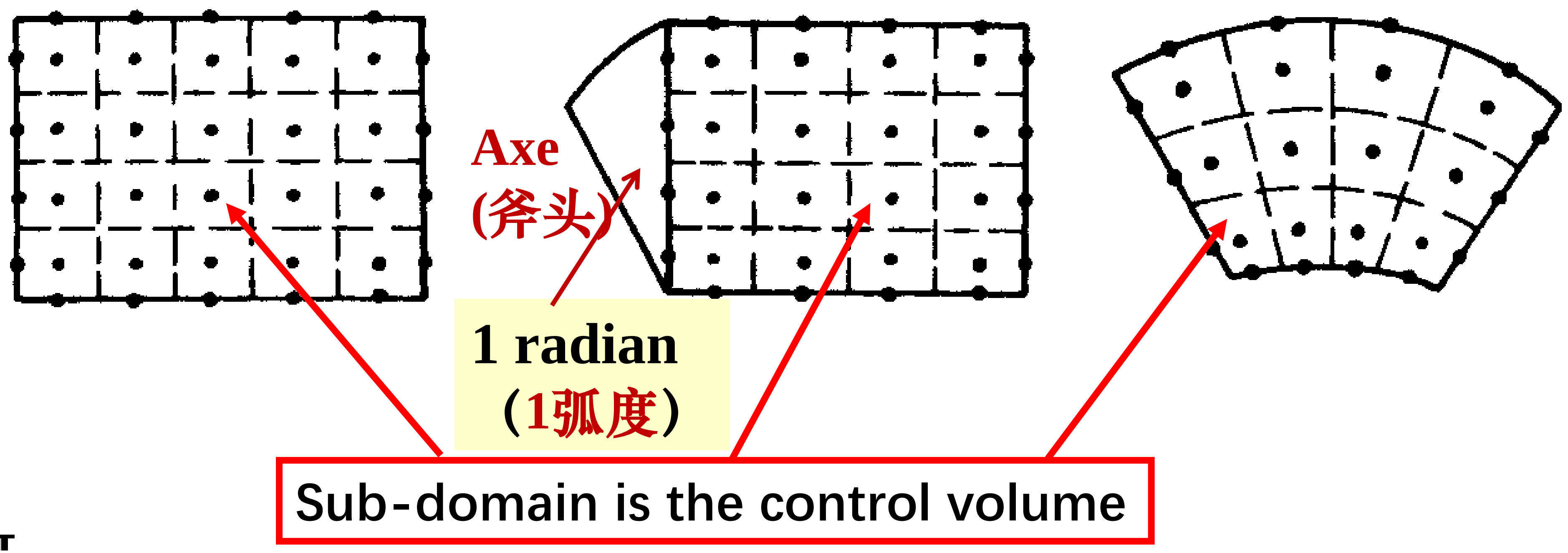
（3）Outer node and inner node for structured grid

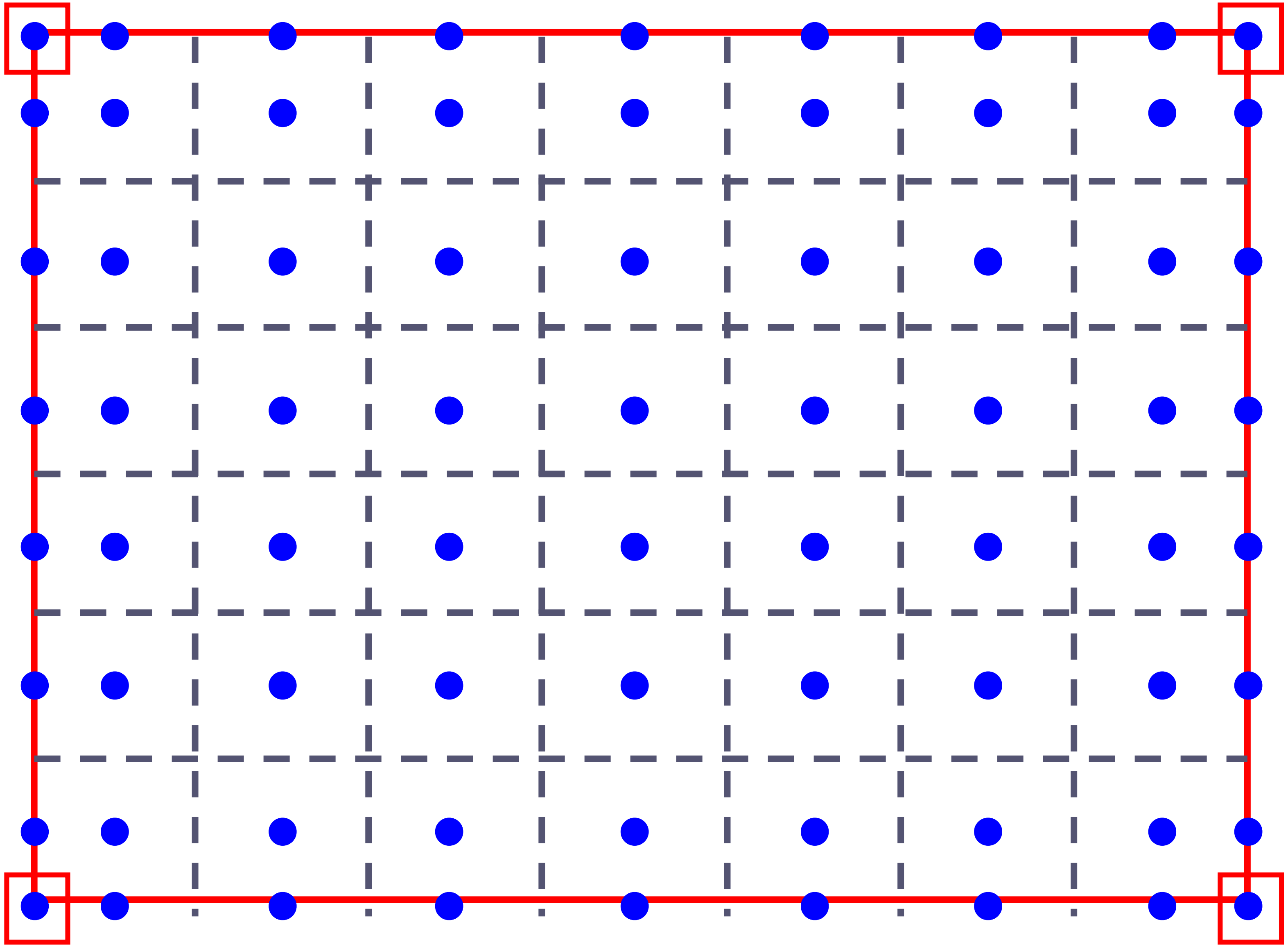
(a) Outer node method： Node is positioned at the vertex of a sub-domain(子区域的角顶)； The interface is between two nodes； Generating procedure： Node first and interface second---called **Practice A** (by Patankar) , or cell-vertex method (单元顶点法).



Cartesian(2D) **Cylindrical（2D）** **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 and node second, called **Practice B** (by Patankar) , or cell-centered method（单元中心法）.



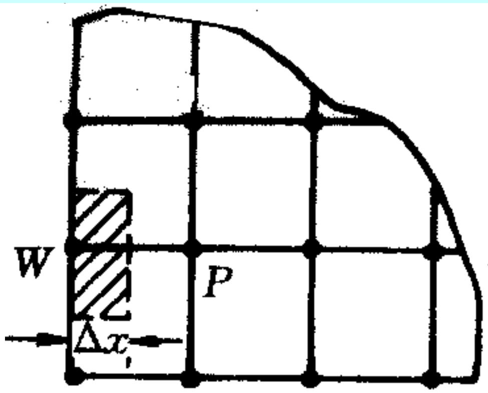


Generating procedure of Practice B

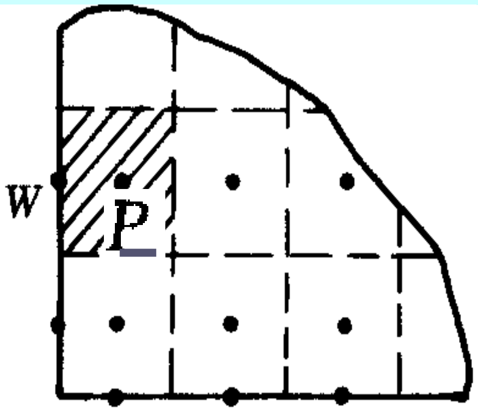
2.1.4 Comparison between Practices A and B

(a) Boundary nodes have different CV.

Practice A



Practice B

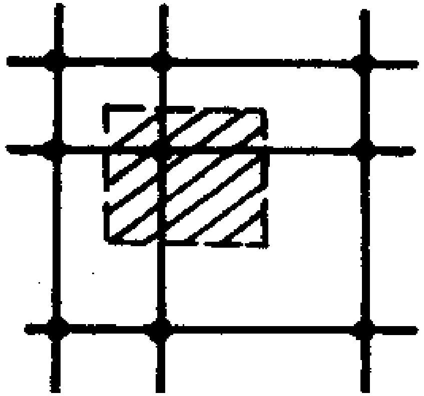


Boundary point has half CV.

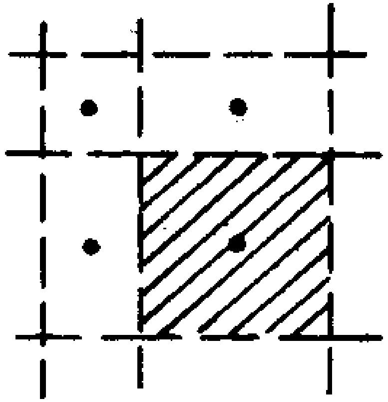
Boundary point has zero CV.

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

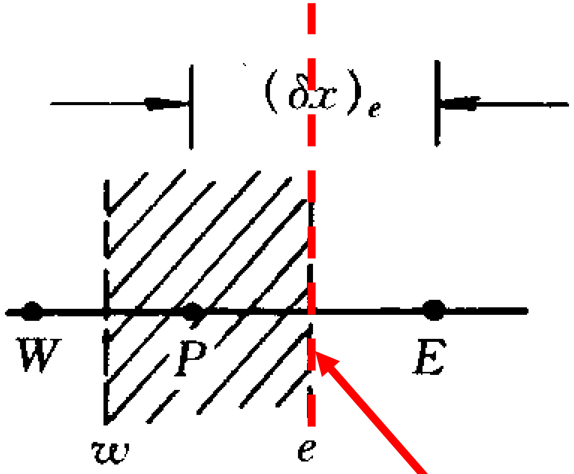
Practice A



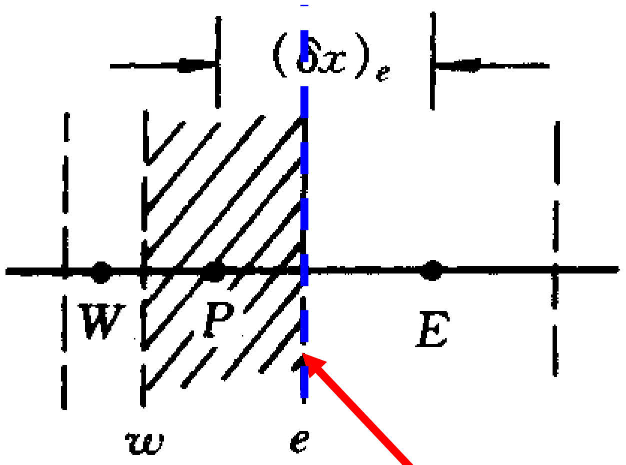
Practice B



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



Interface in middle



Interface is biased（偏置）

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

2nd-order accuracy

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

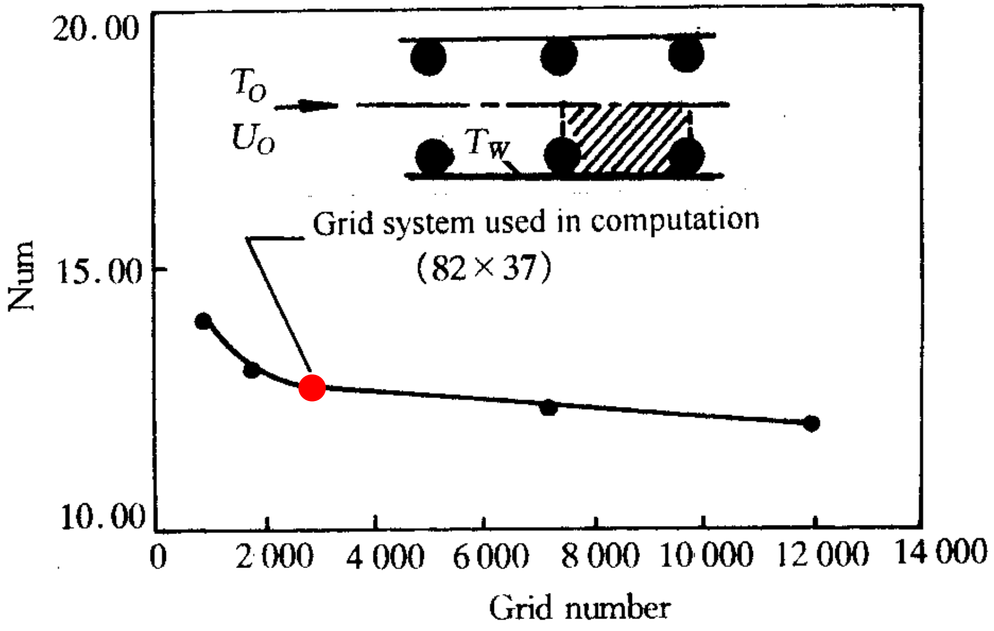
Lower than 2nd order accuracy

2.1.5 Grid-independent solutions

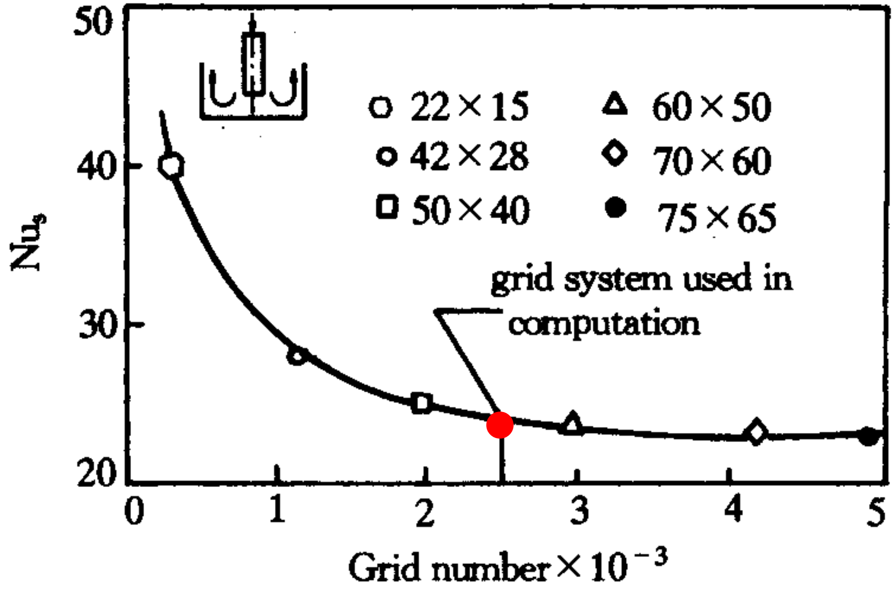
Grid generation is an iterative procedure（迭代过程）; Debugging (调试） and comparison are often needed. For a complicated geometry grid generation may take a major part of total computational time.

Grid generation techniques has been developed as a sub-field of numerical methods.

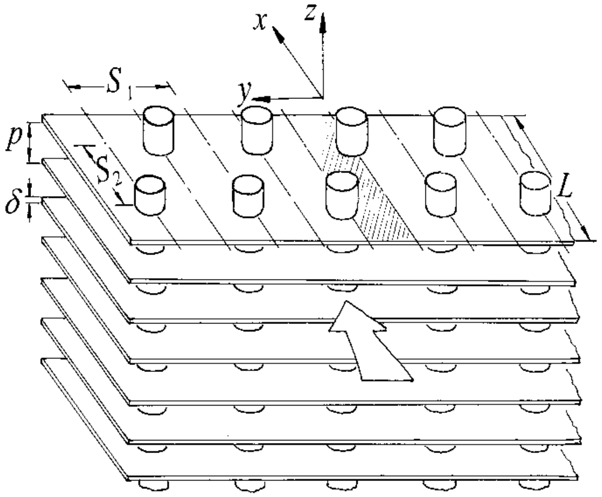
The appropriate grid fineness (细密程度) is such that the numerical solutions are nearly independent on the grid numbers. Such numerical solutions are called grid-independent solutions (网格独立解). They are required for publication of a paper.

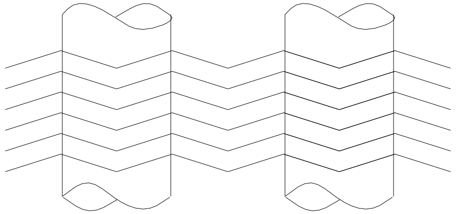


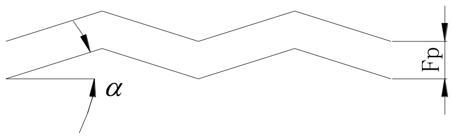
Int. Journal Heat & Fluid Flow, 1993, 14(3):246-253

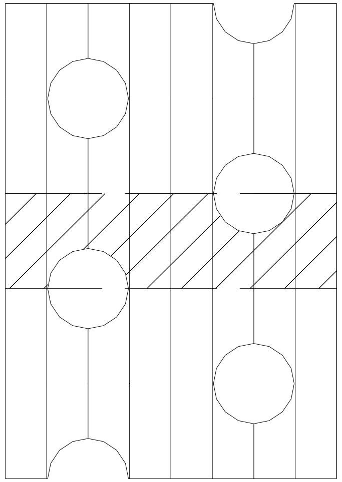


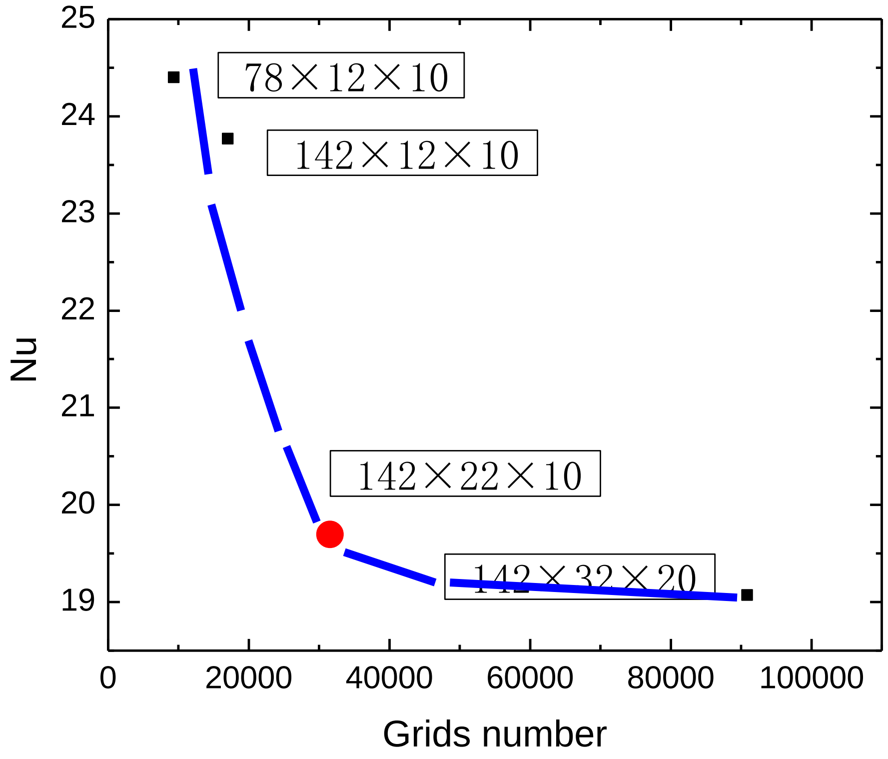
Int. Journal Numerical Methods in Fluids, 1998, 28: 1371-1387











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

2.2 Taylor Expansion Method for Equation Discretization in FD

2.2.1 1-D model equation

2.2.2 Taylor expansion method

2.2.3 FD form of discretized 1-D model equation

2.2 Taylor Expansion Method 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 the study of discretization methods.

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

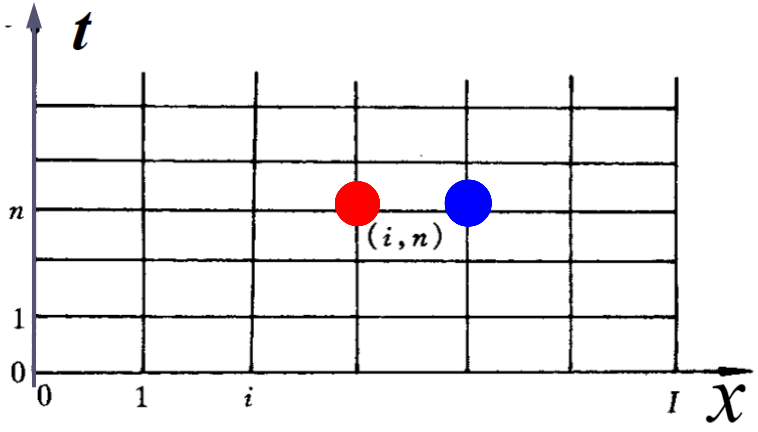
Trans **Conv.** **Diffus.** **Source**

Small but complete---"麻雀虽小，五脏俱全！"

2.2.2 Taylor expansion for FD 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)

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

Backward difference:
(向后差分)

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

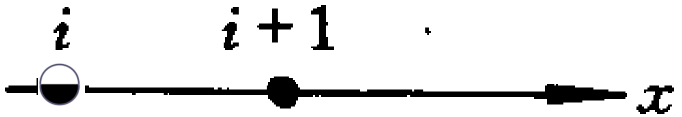
Central difference:
(中心差分)

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

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 node which is used in the construction of FD form

◒ For the node for which FD form is constructed and which is also used in the construction.

Table 2-2 in the textbook

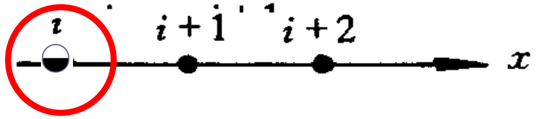
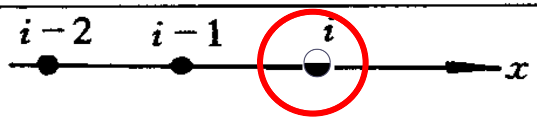
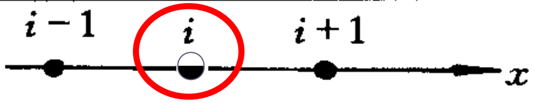
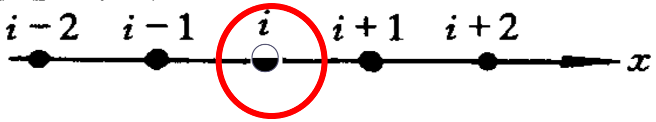
导数	差分表示式	格式图案	截差
$\left.\frac{\partial \phi}{\partial x}\right)_{i,n}$	$\frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$	$i+1$, x	$O(\Delta x)$
	$\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$	$i-1$, x	$O(\Delta x)$
	$\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}$	$i-1$, i, $i+1$, x	$O(\Delta x^2)$
	$\frac{-3\phi_i^n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

The stencil structure is biased.(偏置)

The stencil structure is symmetric, CD

The stencil structure is biased.(偏置)

The stencil structure is symmetric, CD

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

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

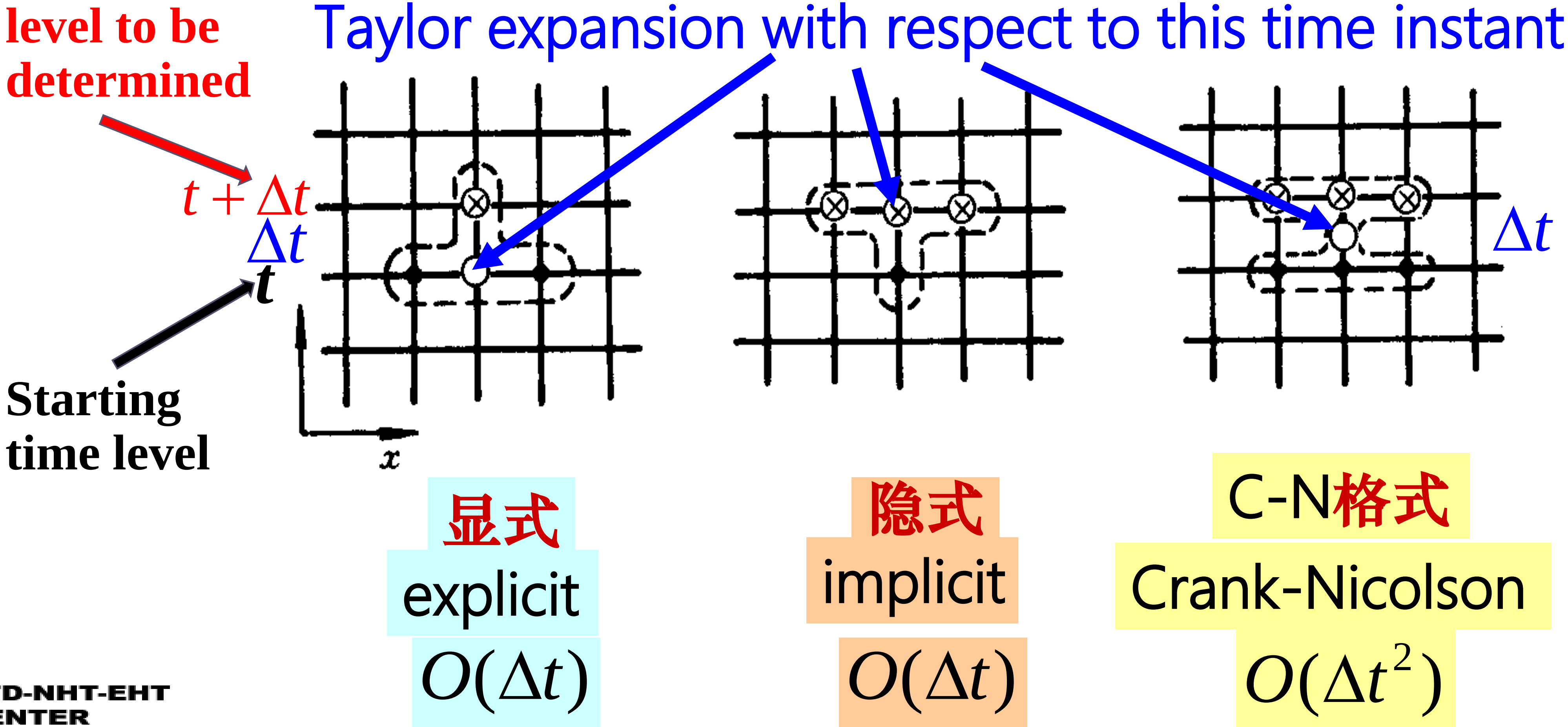
(1) Dimension (量纲) should be consistent(一致);

(2) For a uniform field any order of derivatives should be zero .

2.2.3 Discretized form of 1-D model equation by FD

For a unsteady problem, it is to be determined at which time level to calculate the spatial derivatives .

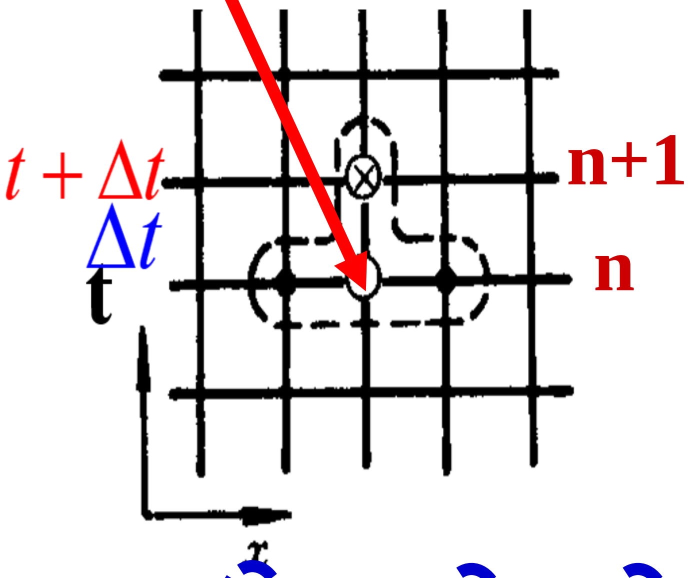
1. Time level at which spatial derivatives are discretized



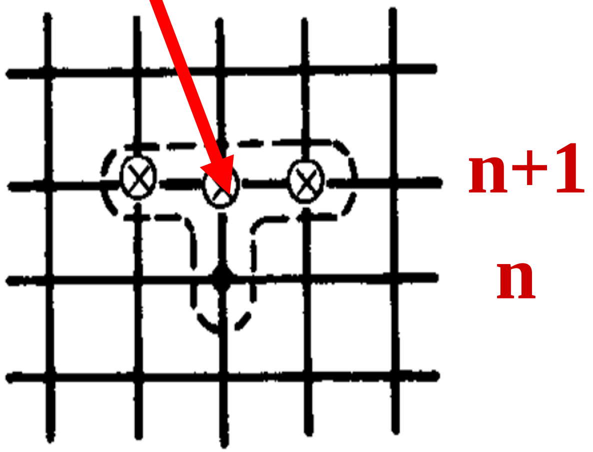
$$\frac{\partial T}{\partial t}=a\frac{\partial^2 T}{\partial x^2}:\ \frac{\partial T}{\partial t}\approx\frac{T_i^{n+1}-T_i^{n}}{\Delta t};$$

Three choices of time level for $\frac{\partial^2 T}{\partial x^2}$

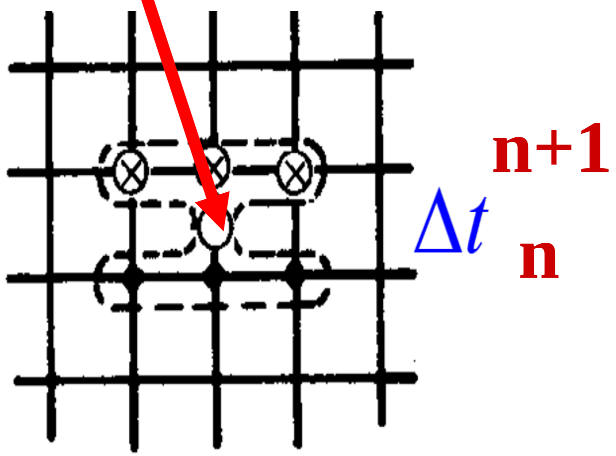
显式 explicit



隐式 implicit



C-N格式



$$\frac{\partial^2 T}{\partial x^2}\cong\frac{T_{i+1}^{n}-2T_i^{n}+T_{i-1}^{n}}{\Delta x^2}\qquad\frac{T_{i+1}^{n+1}-2T_i^{n+1}+T_{i-1}^{n+1}}{\Delta x^2}\qquad\frac{1}{2}\left(\frac{T_{i+1}^{n+1}-2T_i^{n+1}+T_{i-1}^{n+1}}{\Delta x^2}+\frac{T_{i+1}^{n}-2T_i^{n}+T_{i-1}^{n}}{\Delta x^2}\right)$$

2. Explicit scheme of 1-D model equation

Analytical form

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

HOT---Sum of higher order terms.

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

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) the conservative PDE over a CV

2. Selecting (选择) profiles for dependent variable (因变量) and its 1st –order derivative (一阶导数)

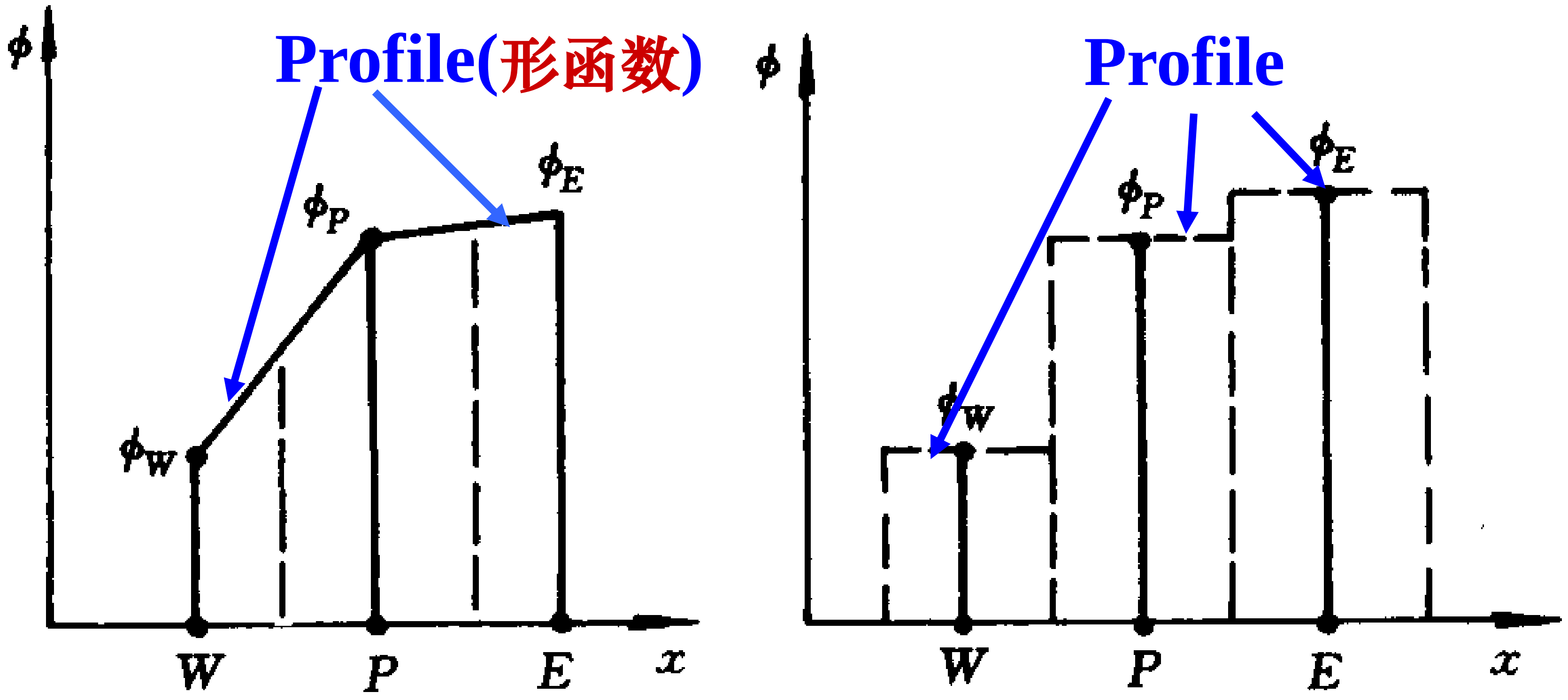
Profile is a local variation pattern of dependent variables with space coordinate, or with time.

3. Completing integral and rearranging algebraic equations

2.3.2 Two conventional profiles (shape function)

Originally (本来) shape function (形函数) is to be solved; here it is to be assumed!----Approximation made in the numerical simulation!

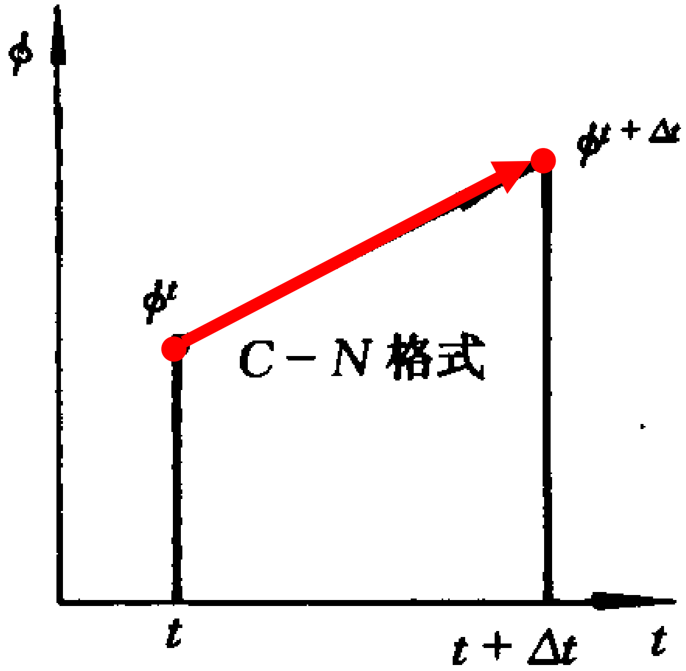
Variation with spatial coordinate

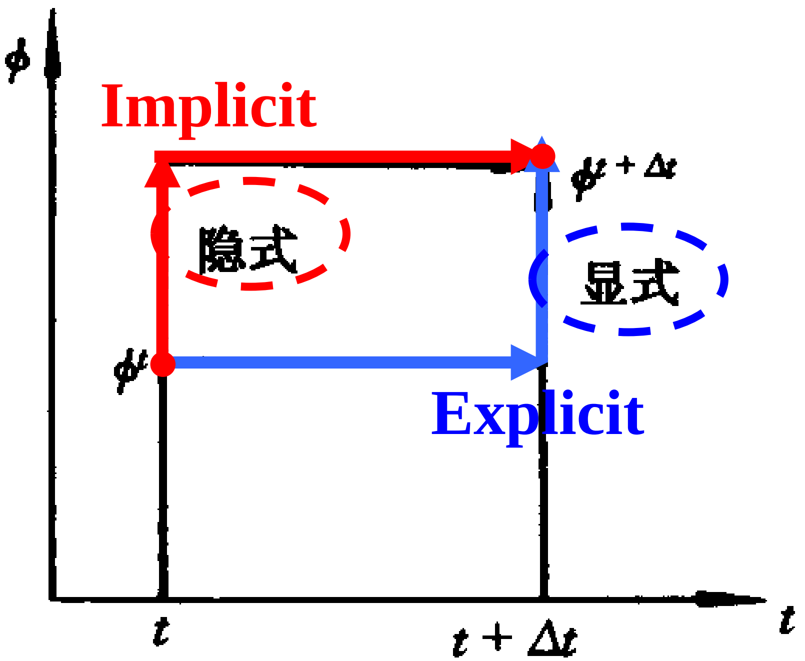


piece-wise linear　　step-wise approximation

分段线性　　阶梯逼近

Variation with time





piece-wise linear　　step-wise approximation

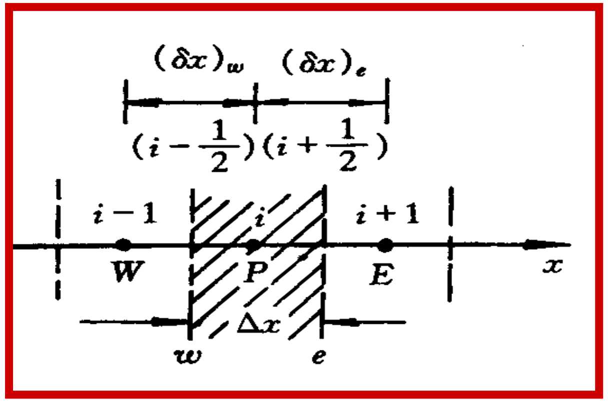
分段线性　　阶梯逼近

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

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

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

yields:



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

$$\Gamma\int_t^{t+\Delta t}\left[\left(\frac{\partial\phi}{\partial x}\right)_e-\left(\frac{\partial\phi}{\partial x}\right)_w\right]dt+\int_t^{t+\Delta t}\int_w^e S_\phi\,dxdt \quad (1)$$

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

1. Transient term

Assuming the step-wise approximation for ϕ with space:

$$\rho\int_{w}^{e}(\phi^{t+\Delta t}-\phi^{t})dx=\rho(\phi_P^{t+\Delta t}-\phi_P^{t})\Delta x \quad (2)$$

2. Convective term

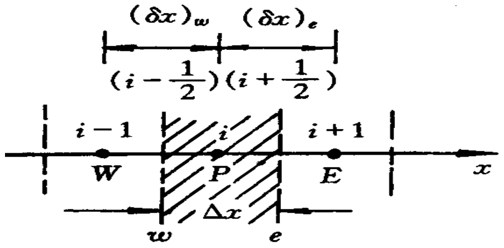
Assuming the explicit step-wise approximation for ϕ with time:

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

In the FVM simulation all information (u,v,p,t, properties) are stored at grids. The interface value should interpolated(插值) by node values.

Further, assuming linear-wise variation of ϕ with space

$$\rho[(u\phi)_e^t-(u\phi)_w^t]\Delta t=\rho u\Delta t(\frac{\phi_E+\phi_P}{2}-\frac{\phi_P+\phi_W}{2})=\rho u\Delta t\frac{\phi_E-\phi_W}{2} \quad (3)$$



Uniform grid

Superscript "t" is temporary(暂时) 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

$$\Gamma[(\frac{\partial \phi}{\partial x})_e^t - (\frac{\partial \phi}{\partial x})_w^t]\Delta t = \Gamma \Delta t[\frac{\phi_E - \phi_P}{(\delta x)_e} - \frac{\phi_P - \phi_W}{(\delta x)_w}] \quad (4)$$

Uniform grid →

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

Super-script "t" is temporary neglected!

4. Source term

Temporary assuming explicit step-wise with time and step-wise variation with space:

$$\int_t^{t+\Delta t}\int_w^e S dx dt = \overline{S}^t (\Delta x)_P \Delta t \quad (5); \quad \overline{S}$$ ---averaged one over space.

Substituting Eqs.(2),(3), (4) and (5) into Eq. (1), and dividing both sides by $\Delta t \Delta x$ for uniform grids, yielding:

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

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: with FDM being mathematically more rigorous (严格） and FVM being physically more meaningful（有意义）; 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 (目的) 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

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

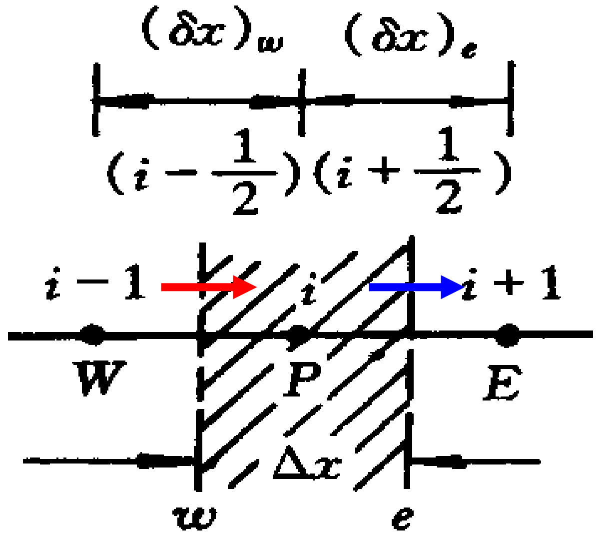
Writing down balance equation for Δx and Δt

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

Transient **Convection**

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

Diffusion **Source**



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

If the same profiles of the variable ϕ of FVM are assumed, the final results are the same:

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

The heat balance method is actually adopting the conservation law directly to a CV, and is very useful.

2.3.6 Discretization of boundary condition

First kind boundary condition can be directly adopted in the solution of the algebraic eqs. Numerical treatments of the 2nd and third kind boundary conditions will be presented in Chapter 3.

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 algebraic Eqs.	Not guaranteed	May be guaranteed

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

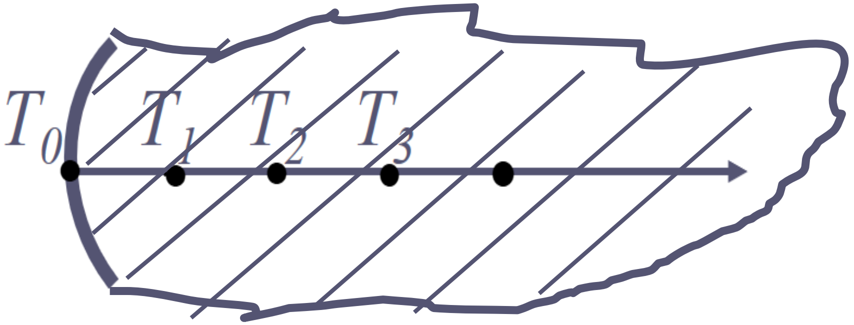
Home Work 2（2024-2025）

Please finish your homework independently !!!

Please hand in on Sept 23, 2024

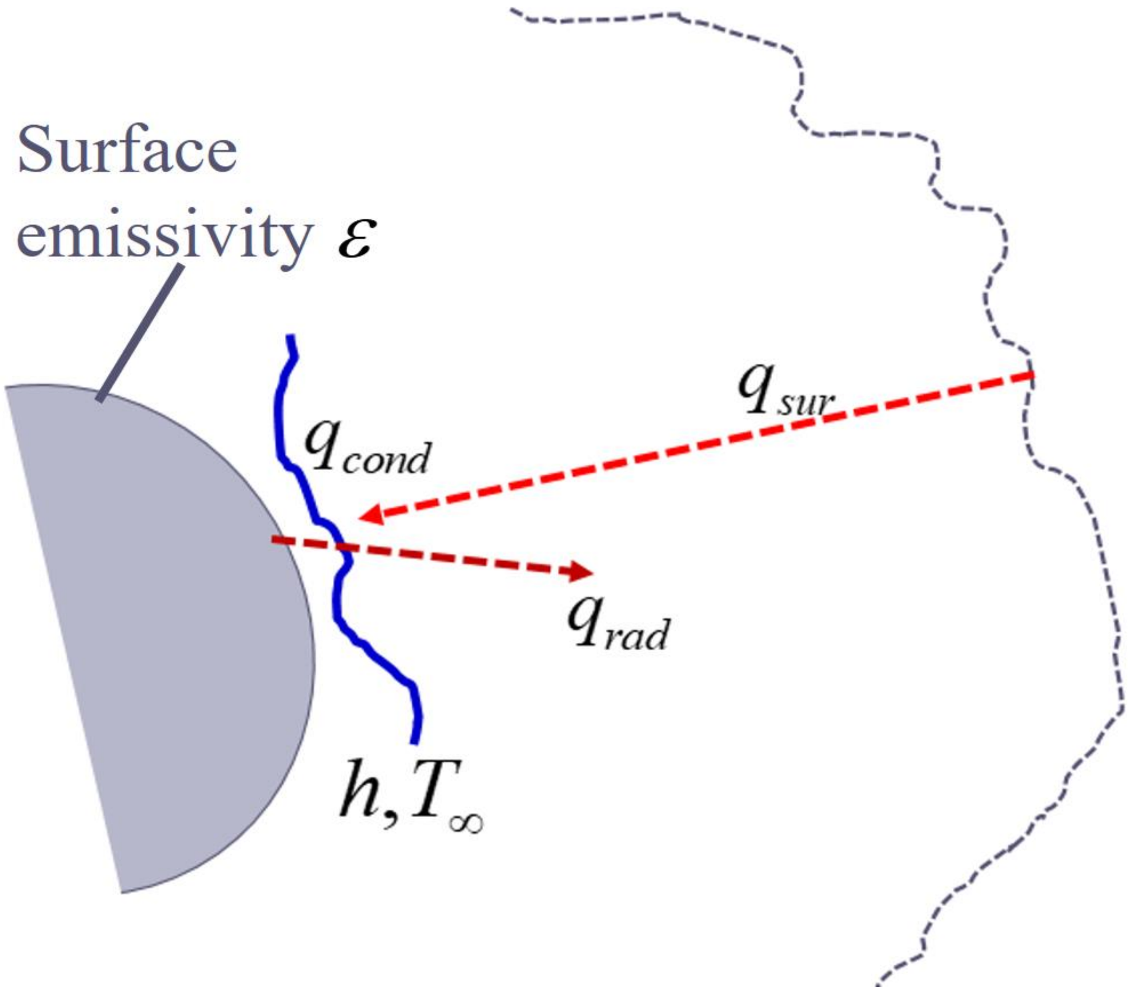
Problem 2-1

Let T_0 be the temperature on the solution boundary, T_1, T_2, T_3,… be the temperature along the positive x-direction. The grid size is uniform （Practice A）. Represent the boundary heat flux $q=-\lambda\left(\frac{\partial T}{\partial x}\right)_{x=0}$ with FD approximation of order of $O(\Delta x)$, $O(\Delta x^2)$ and $O(\Delta x^3)$.



Problem 2-2

As shown in the figure, a solid body surface is cooled by a fluid with temperature T_∞ and heat transfer coefficient *h*. The surface loses heat q_{rad} through radiation to nearby subjects. It also gains q_{sur} from remote surrounding radiation (q_{sur} is given) . Wright down the thermal boundary condition of the body surface .



Problem 2-3

Consider the function $f(x)=\sin(5\pi x)$. By using a mesh size $\Delta x = h = 0.2$, evaluate the forward difference of its first-order derivative by following two expressions:

$$1)\ f_i' = \frac{f_{i+1}-f_i}{h} + O(h); \quad 2)\ f_i' = \frac{1}{2h}(-3f_i + 4f_{i+1} - f_{i+2}) + O(h^2)$$

Compare the results obtained by FD with the exact solution. Explain the reason for the difference between the exact and numerical solutions.

Problem 2-4

When the space step of a FD expression of a function approaches zero , the errors between the FD expression and the function will also approach zero. For the function $f(x)=e^{-x}$ constructing the FD expressions for its 1st-order derivative as follows,

$$1)\ d_1 = \frac{e^{-(x+h)} - e^{-x}}{h} + O(h) --- \text{Forward difference}$$

$$2)\ d_2 = \frac{e^{-(x+h)} - e^{-(x-h)}}{2h} + O(h^2) ----\text{Central difference;}$$

Take h=0.5, 0.05 0.005, calculate d_1, d_2 and their discretization errors. Draw a log-log picture (for a fixed value of x) to show the variation trend of the discretization error of the two schemes with h and make some discussion.

Important words you will study in next lecture:

Please find the appropriate meanings for yourself

combustion	harmonic	dimensionless
generality	resistance	auxiliary
treatment	transient	scaling
multiply	inertia	supplement
linearize	meaningful	portfolio
linearization	guarantee	slope
arithmetic	reciprocal	lag
requirement	arc	convergence
		ensure

Teaching PPT will be loaded on our WeChat Group

本组网页地址：http://nht.xjtu.edu.cn 欢迎访问！

同舟共济渡彼岸！

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