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### **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 (网格生成) (Domain Discretization

## 2.2 Taylor Expansion and Polynomial Fitting (多项式拟合)for Equation Discretization

2.3 Control Volume (控制容积) and Heat Balance Methods for Equation Discretization



#### **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

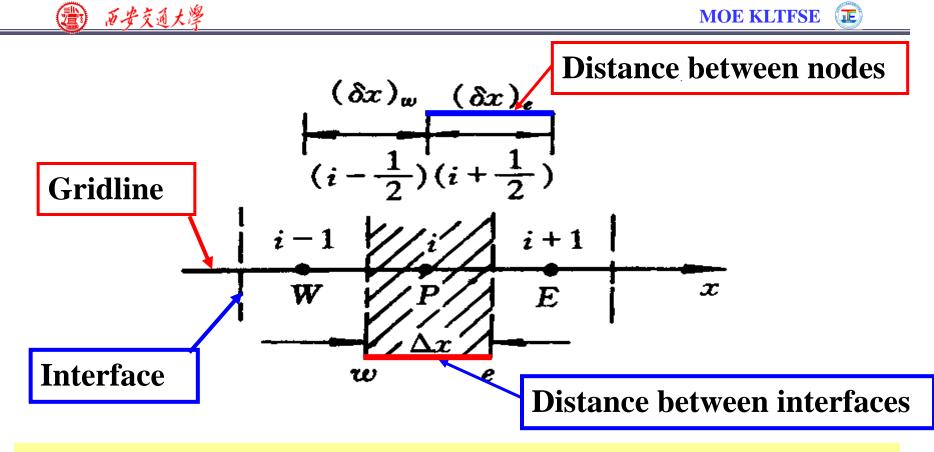
#### 1. Task of domain discretization

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 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**  $\delta x$
- Distance between two interfaces  $\Delta x$



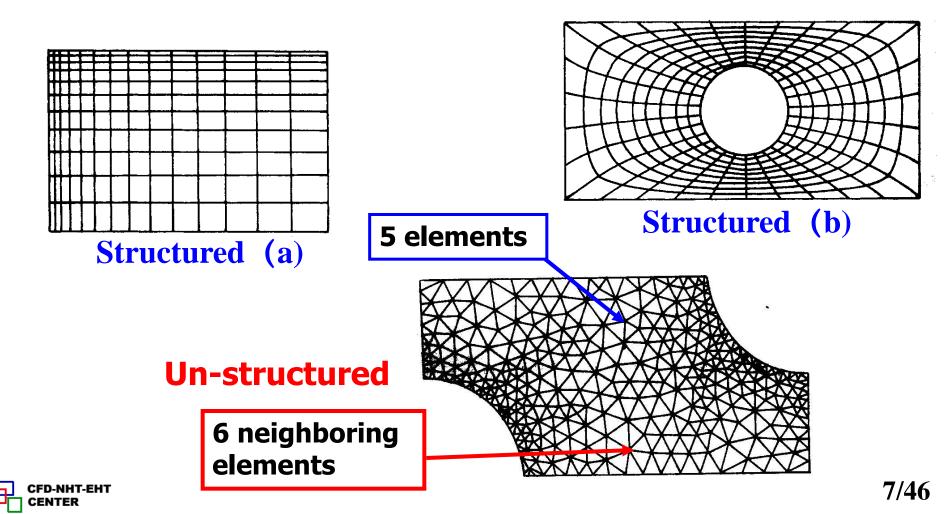
2.1.3 Introduction to different types of grid system and generation method

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

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(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.

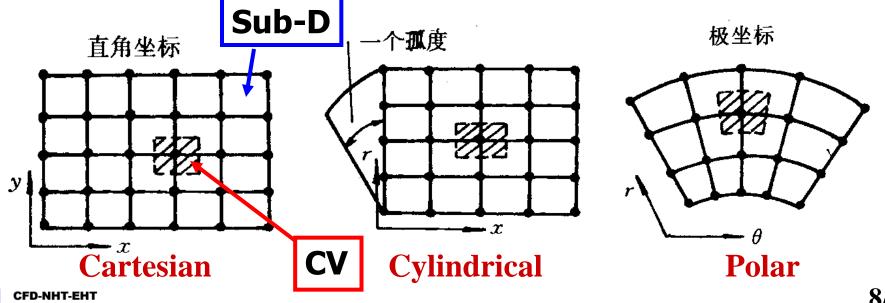




Both structured and unstructured grid layout (节 点布置) have two practices.

(3) Outer node and inner node for structured grid

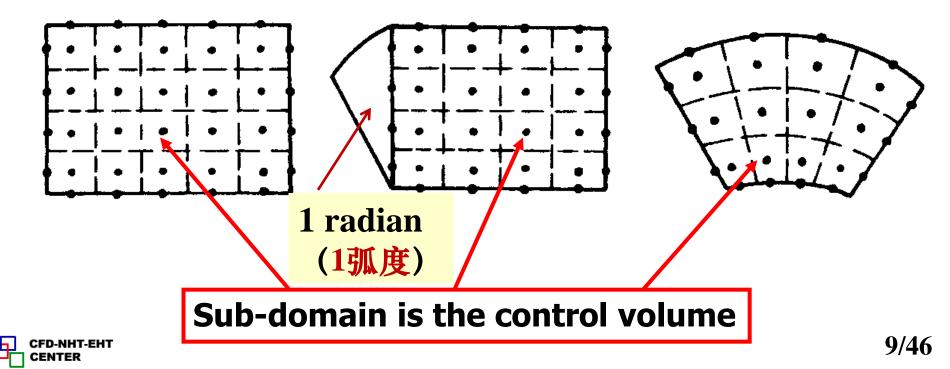
(a) Outer node method: Node is positioned at the vertex of a sub-domain(子区域的角顶); The interface is between two nodes; Generating procedure: Node first and interface second---called Practice A, or cell-vertex method (单元顶点法).



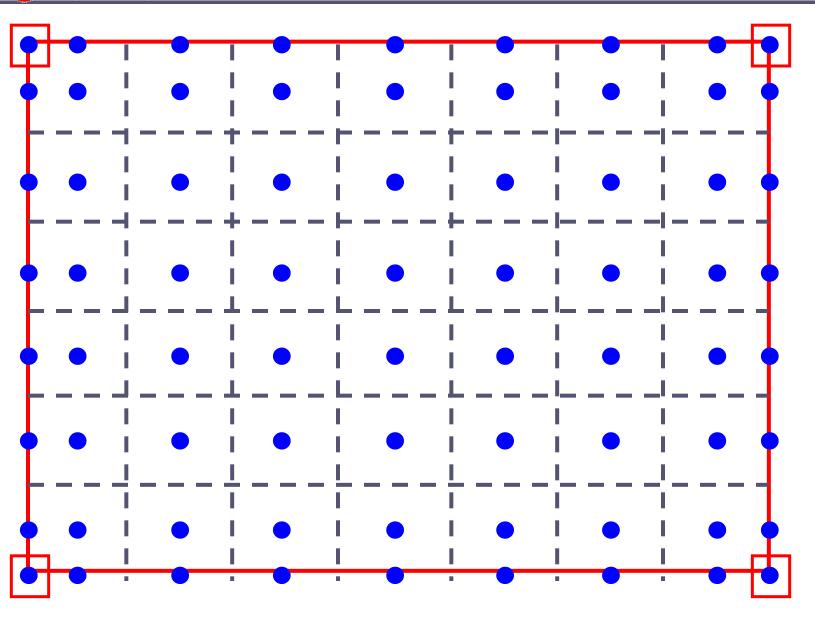


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(b) Inner node method: Node is positioned at the center of sub-domain; Sub-domain is identical to control volume; Generating procedure: Interface first ad node second, called Practice B, or cell-centered (单元中心法).



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#### **Generating procedure of Practice B**

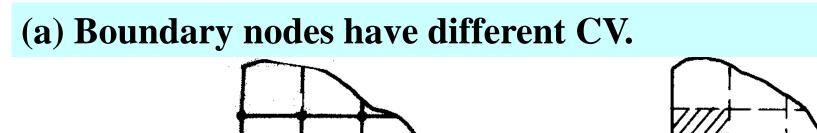




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#### 2.1.4 Comparison between Practices A and B

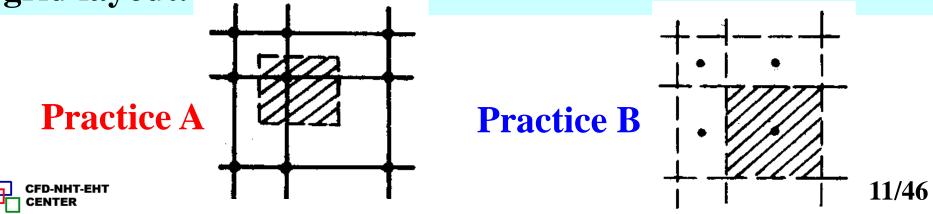


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Boundary point has half CV. Boundary poinnt has zero CV.

**Practice B** 

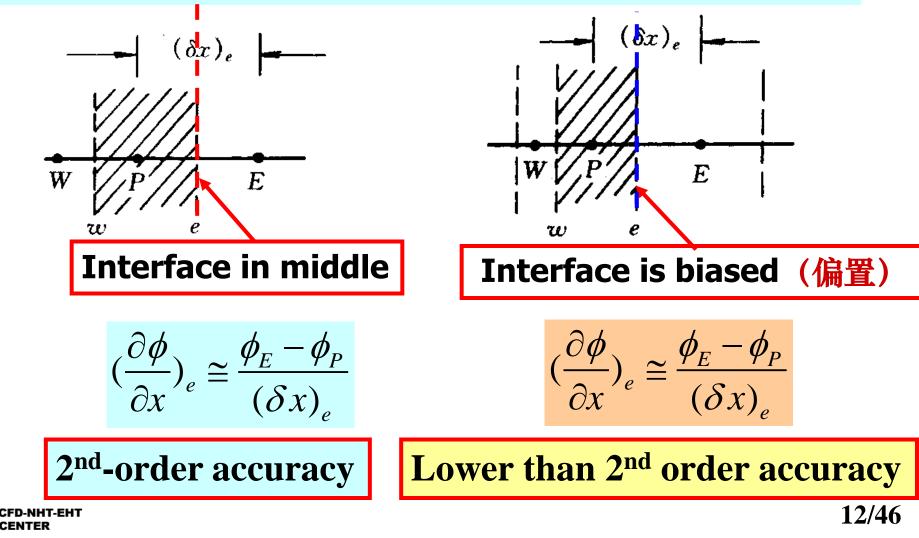
(b) Practice B is more feasible (适用) for non-uniform grid layout.





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

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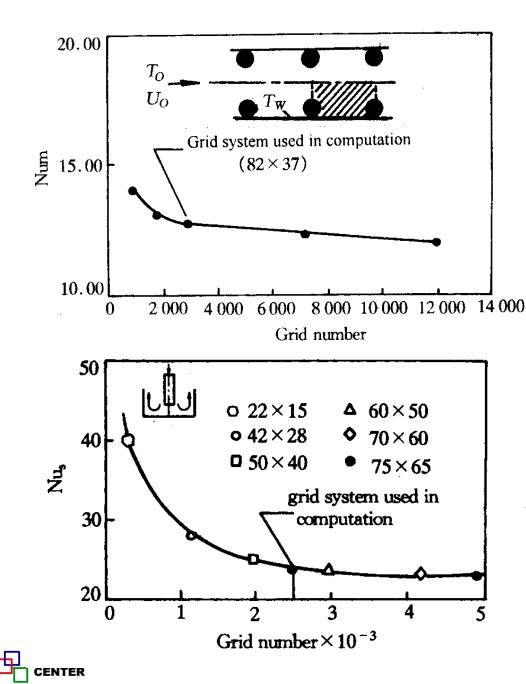
#### 2.1.5 Grid-independent solutions

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.





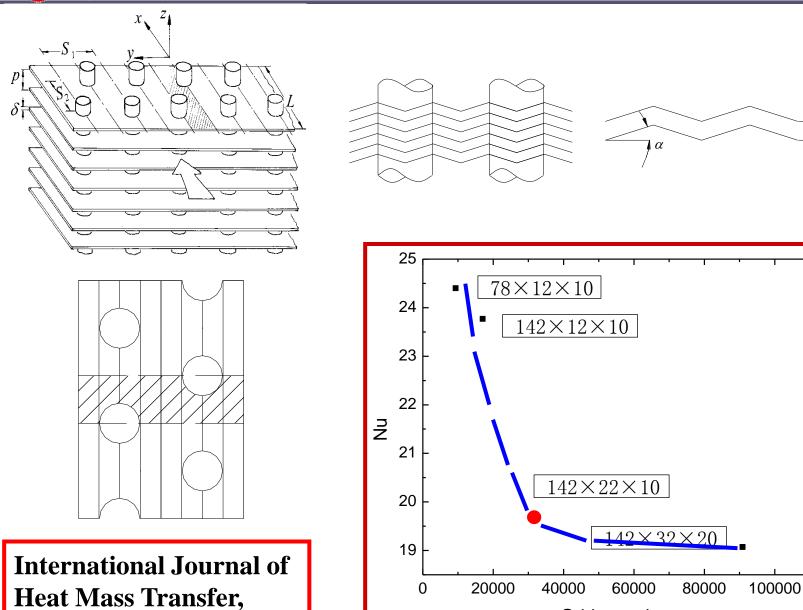
Int. Journal Heat & Fluid Flow, 1993, 14(3):246-253。

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





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Grids number

2007, 50:1163-1175





#### 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



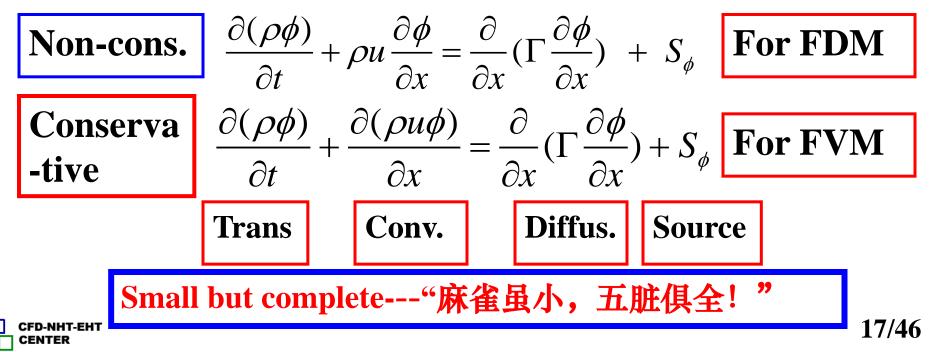


2.2 Taylor Expansion and Polynomial Fitting for Equation discretization

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2.2.1 1-D model equation (一维模型方程)

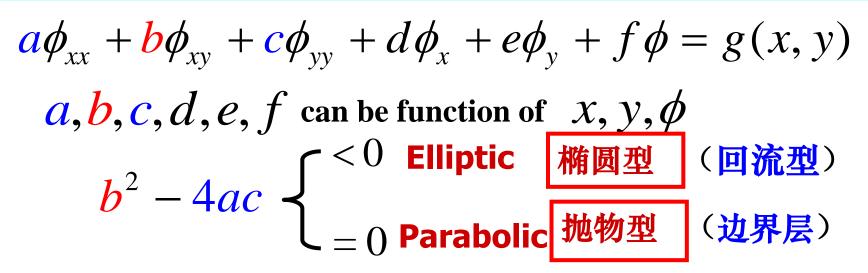
1-D model equation has four typical terms : transient term, convection term, diffusion term and source term. It is specially designed for discussion of discretization methods.

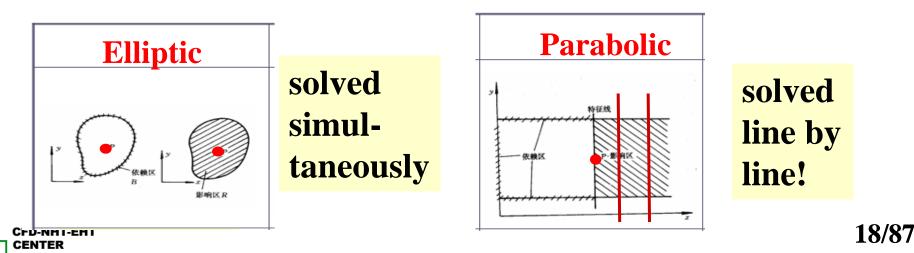




#### **Brief review of 2016-09-13 lecture key points**

**1.Elliptic vs. parabolic PDF (Math viewpoint)** 





- **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!
Conservative PDE may guarantee the conservation feature of the numerical solution.
Non-conservative PDE can not guarantee!

**End of review** 

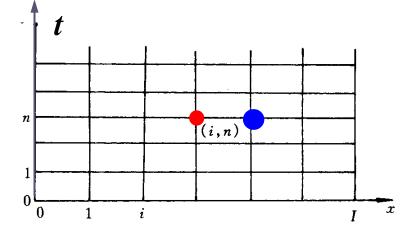




#### **2.2.2 Taylor expansion for FD of derivatives**

#### **1.** FD form of 1<sup>st</sup> order derivative

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



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

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

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

 $O(\Delta x)$  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  $\leq K\Delta x$  where K is in dependent of  $\Delta x$ 

The exponent(指数) of  $\Delta x$  is called order of TE(截差的阶 数). Replacing analytical solution  $\phi(i, n)$  by approximate value  $\phi$ , yields: Forward difference:  $\frac{\partial \phi}{\partial x}_{i,n} \cong \frac{\delta \phi}{\delta x}_{i}_{i}^{n} = \frac{\phi_{i+1}^{n} - \phi_{i}^{n}}{\Delta x}, O(\Delta x)$ (何前差分)



#### Backward difference: (向后差分)

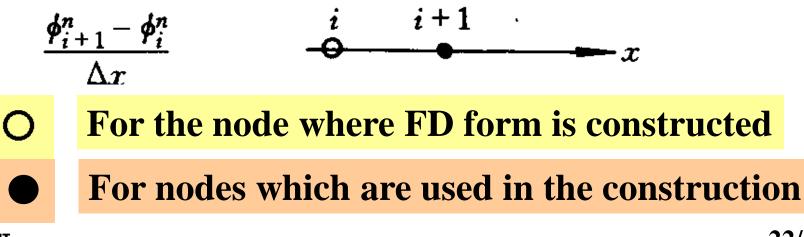
 $\left(\frac{\partial \phi}{\partial x}\right)_{i,n} \cong \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}, O(\Delta x)$ 

Central difference: (中心差分)

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

**2.** Different FD forms of 1<sup>st</sup> ad 2<sup>nd</sup> order derivatives

Stencil (格式图案) of FD expression





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导数	差分表示式	格式图案	截差
	$\frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$	i  i+1	$O(\Delta x$
	$\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$	i-1 $i$ $-1$ $x$	$O(\Delta x)$
	$\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}$	$\underbrace{\begin{array}{ccc} i-1 & i & i+1 \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \end{array}}_{x}$	$O(\Delta x$
9¢\	$\frac{-3\phi_i^n+4\phi_{i+1}^n-\phi_{i+2}^n}{2\Delta x}$	i  i+1  i+2	$O(\Delta x$
$\left(\frac{\partial \phi}{\partial x}\right)_{i,n}$	$\frac{3\phi_i^n - 4\phi_{i-1}^n + \phi_{i-2}^n}{2\Delta x}$	i-2 $i-1$ $i$	$O(\Delta x$
	$\frac{4\phi_{i+1}^n + 6\phi_i^n - 12\phi_{i-1}^n + 2\phi_{i-2}^n}{12\Delta x}$	$\frac{i-2}{2}  i-1 \qquad i \qquad i+1 \qquad \qquad$	$O(\Delta x$
	$\frac{-2\phi_{i+2}^{n}+12\phi_{i+1}^{n}-6\phi_{i}^{n}-4\phi_{i-1}^{n}}{12\Delta x}$	$\underbrace{\stackrel{i-1}{\bullet} \stackrel{i}{\bullet} \stackrel{i+1}{\bullet} \stackrel{i+2}{\bullet} x$	$O(\Delta x$
	$\frac{\phi_{i-2}^n - 8\phi_{i-1}^n + 8\phi_{i+1}^n - \phi_{i+2}^n}{12\Delta x}$	$\underbrace{\begin{array}{ccccc} i-2 & i-1 & i & i+1 & i+2 \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet$	Ο(Δ <i>x</i>

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

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

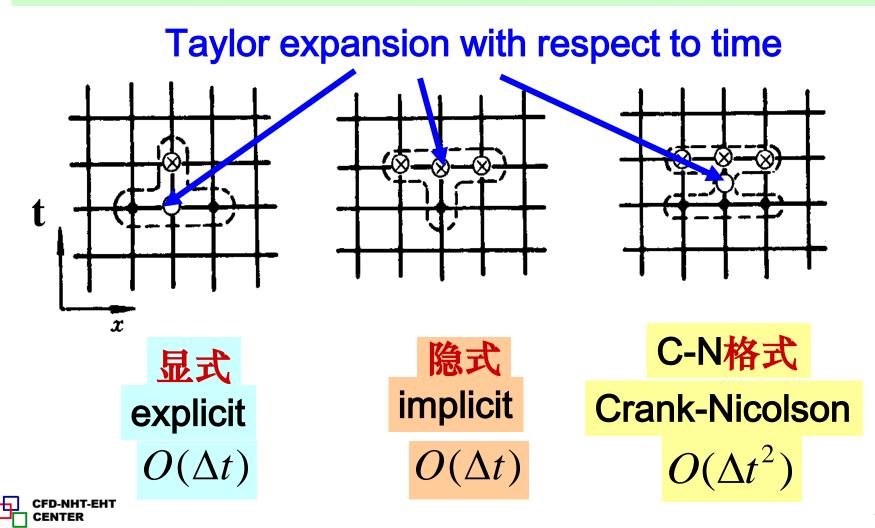
(1) Dimension (量纲) should be consistent(一致);

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



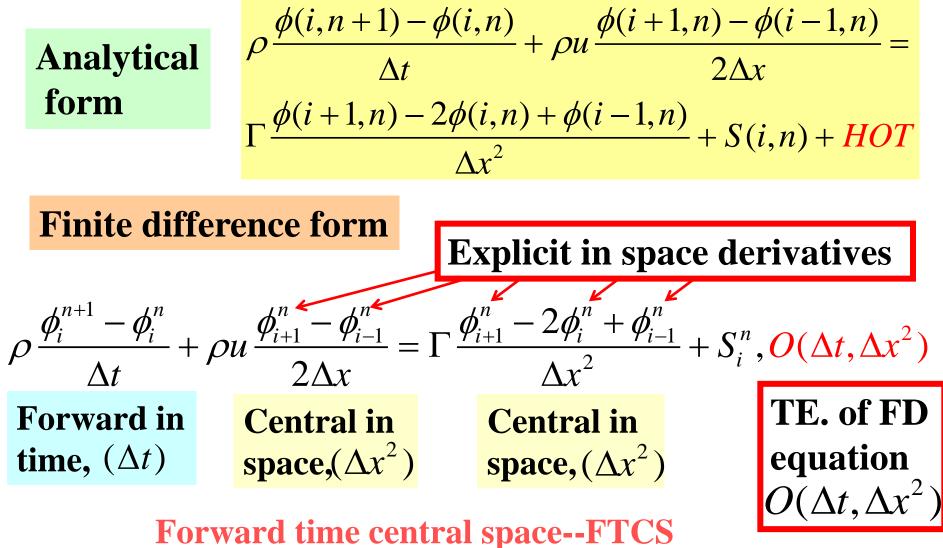
#### **2.2.3 Discretized form of 1-D model equation by FD**

1. Time level at which spatial derivatives are determined





#### **2.** Explicit scheme of 1-D model equation



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#### **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 1<sup>st</sup>-order FD expressions

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

Set the origin (原点) at  $X_0$ , yields:

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

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

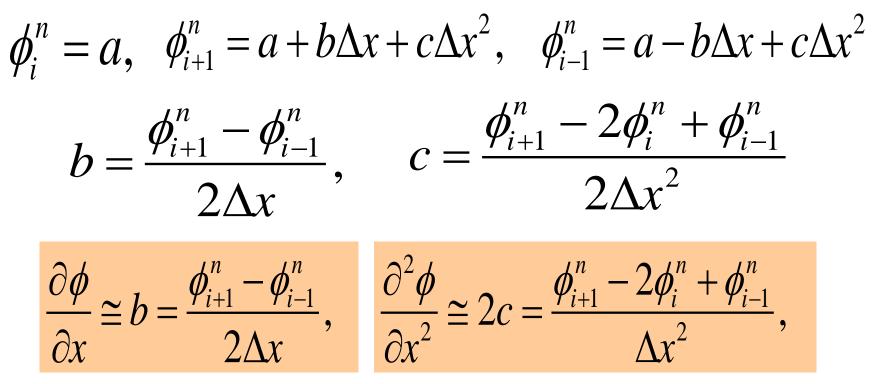




2. Local quadratic function (二次函数) —leads to 2<sup>nd</sup> order FD expressions

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

Set the origin (原点) at  $X_0$ , yields:



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#### **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 2<sup>nd</sup>order accuracy.
- **Solution**: Assuming a quadratic temp. function at y=0

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

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

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



#### **End of Notes**



Ti, 5

Ti,4

Ti.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 1<sup>st</sup> derivative

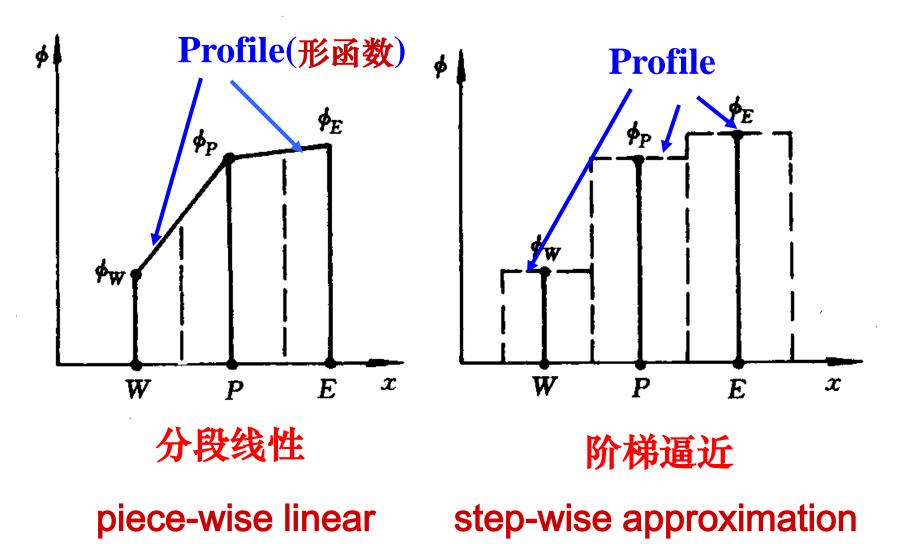
**Profile**—a local variation pattern of DV with space coordinate

**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!

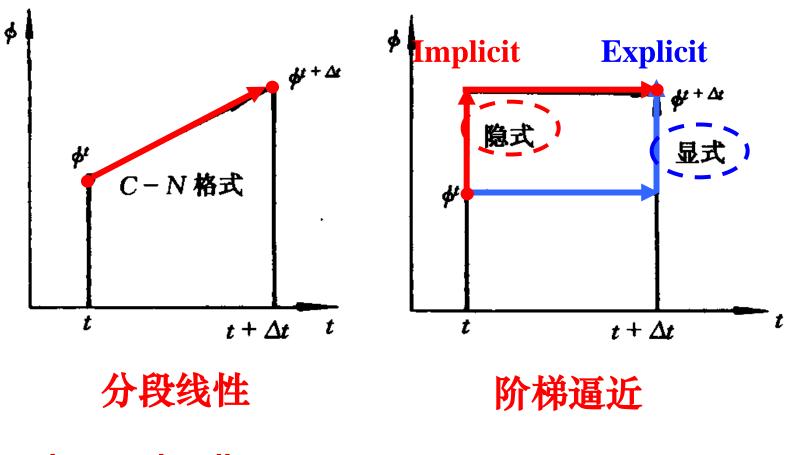
#### Variation with spatial coordinate



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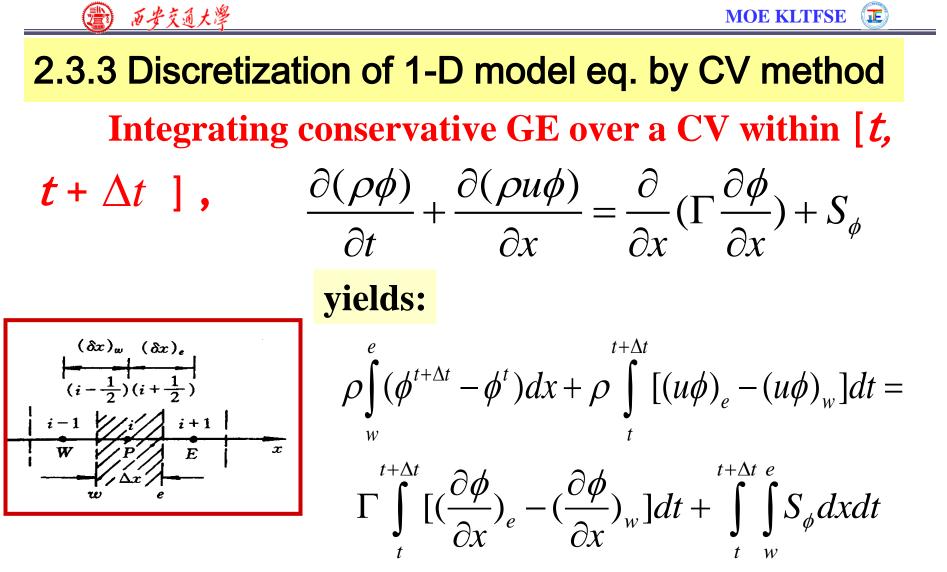
#### Variation with time



piece-wise linear step-wise approximation



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



#### **1.** Transient term

Assuming the step-wise approximation for  $\phi$  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  $\phi$  with time:

$$\rho \int_{w}^{t+\Delta t} [(u\phi)_{e} - (u\phi)_{w}]dt = \rho [(u\phi)_{e}^{t} - (u\phi)_{w}^{t}]\Delta t$$





with

#### Further, assuming linear-wise variation of $\phi$ 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

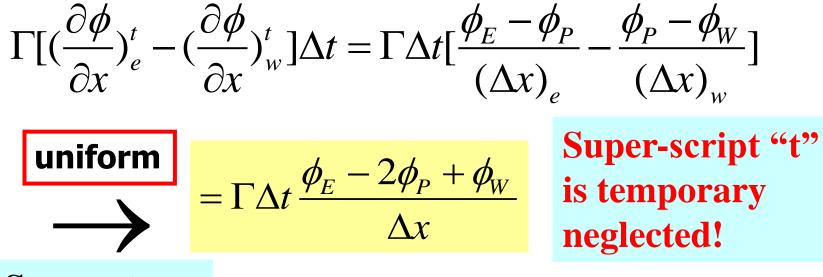
Taking explicit step-wise variation of time, yields:

$$\Gamma \int_{t}^{t+\Delta t} \left[ \left( \frac{\partial \phi}{\partial x} \right)_{e} - \left( \frac{\partial \phi}{\partial x} \right)_{w} \right] dt = \Gamma \left[ \left( \frac{\partial \phi}{\partial x} \right)_{e}^{t} - \left( \frac{\partial \phi}{\partial x} \right)_{w}^{t} \right] \Delta t$$

Further, assuming linear-wise variation of  $\phi$  with space







**4.** Source term

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

$$\int_{t}^{t+\Delta t} \int_{w}^{e} S dx dt = \overline{S}^{t} (\Delta x)_{P} \Delta t$$

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



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

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

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

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

FDM and FVM are a kind of brothers: both differences and common features exist 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)。

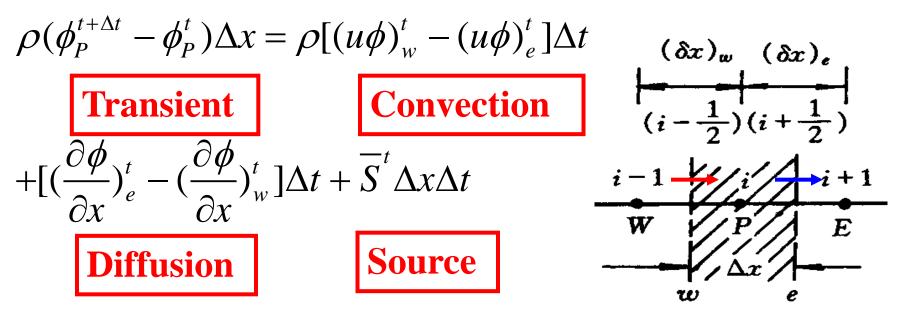
**2.3.5 Discretization equation by balance method** 





1. Major concept: Applying the conser. 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 $\Delta x$ and $\Delta t$



By selecting the profile of dependent variable  $\phi$  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 1<sup>st</sup> choice of most CSW.





#### **First Home Work**

## Homework of Chapter 1,2

**One problem assigned in Chapter 1** 

Please hand in on Sept.25, 2017

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





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

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



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