

(4)西步交通大學

CENTER

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 2022-Sept-18

Contents

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. 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 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 $-\delta x$

Distance between two interfaces $-\Delta x$

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.

CENTER

(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.

:ENTER

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

(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 cellcentered method (单元中心法).

9/46

Generating procedure of Practice B

CENTER

2.1.4 Comparison between Practices A and B

CENTER

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

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.

(A) 万步交通大學

Γą

Heat Mass Transfer, 2007, 50:1163 -1175**CFD-NHT-EHT**

甴

CENTER

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 for derivatives of FD

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 the study of discretization methods.

2.2.2 Taylor expansion for FD form of derivatives

1. FD form of 1st order derivative

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

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

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

19/46 , $D_{i, n} = \frac{\phi(i + 1, n) - \phi(i, n)}{n} + O(\Delta x)$ *x* Δx $\partial \phi$ ϕ $(i+1,n) - \phi$ $=\frac{\gamma^{(i+1)(i)}\gamma^{(i)(i)(j)}}{i+O(\Delta)}$ ∂x^{∞} and Δ $O(\Delta x)$ is called truncation error (截断误差): $\big)_{i,n}$ *x* $\partial \pmb{\phi}$ \widehat{O} $(i + 1, n) - \phi(i, n)$ *x* $\phi(i+1,n) - \phi(i)$ Δ With $\Delta x \rightarrow 0$ replacing $\frac{\partial \phi}{\partial x}$, by Replacing analytical solution $\phi(i,n)$ by approximate will lead to an error $\leq K\Delta x$ 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**)** .

Forward difference: value ϕ_i^n , yields:

(向前差分)

1 $\big)_{i,n} \cong \frac{\sigma}{s} \big]_{i}^{n} = \frac{r_{i+1} - r_i}{s}, O(\Delta x)$ *n n* $\sum_{i,n} \geq \frac{\sigma \varphi}{c}$, $\sum_{i}^{n} = \frac{\varphi_{i+1} \varphi_{i}}{c}$, $O(\Delta x)$ α *x* Δx ϕ ϕ_{i+1} ϕ_{i+1} ϕ_{i} δ $\left. \begin{matrix} \partial \phi \ \end{matrix} \right\rangle \quad \left. \begin{matrix} \sim & \delta \phi \ \rrap{1}^n \end{matrix} \right\rangle \quad \left. \begin{matrix} \phi^n_{i+1} \end{matrix}$ \cong $\stackrel{\circ r}{\cong}$)ⁿ = $\stackrel{r_{l+1}}{\cong}$ $\stackrel{r_l}{\cong}$. $O(\Delta)$ $\partial x^{\frac{\gamma}{l},n}$ $\delta x^{\frac{\gamma}{l}}$ Δ

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

Stencil (格式图案) of FD expression

AD 万步交通大學

20/46

Table 2-2 in the textbook

CFD-NHT-EHT CENTER

甴

(A) 石步交通大學

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

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

(金) 万步交通大学

CFD-NHT-EHT

CENTER

Γą

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

2.2.3 Discretized form of 1-D model equation by FD

(A) 万步交通大學

凸

热流科学与工程

部重点实验室

 \bigoplus

CENTER

2. Explicit scheme of 1-D model equation

2.2.4 Polynomial fitting for derivatives of FD

Assuming a local profile (型线**) for the function (dependent variable) studied:** Originally (本来) the profile is to be found; here it is to be assumed!----Approximation made in the numerical method.

1. 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 x_0 , yields:

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

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

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

 ${\bf Set}$ the origin $\left({\pmb \bar{\mathbf{F}}}{\pmb \kappa}\right)$ at x_{0} *x* ,**yields:**

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

 $[\textbf{Exam.2-1}]$ **Known:** $T_{i,1}, T_{i,2}, T_{i,3}$ **Find:** wall heat flux expression in y-direction with 2nd-order accuracy. $\begin{array}{c}\n\cdot \cdot \cdot \\
\vdots \\
\vdots \\
\vdots \\
\vdots\n\end{array}$ **Solution:** Assuming a quadratic temp. function at $y=0$ $T(x, y) = a + by + cy^2$, $O(\Delta y^3)$ $T_{i,1} = a$, $T_{i,2} = a + b\Delta y + c\Delta y^2$, $T_{i,3} = a + 2b\Delta y + 4c\Delta y^2$ $b = \frac{-3T_{i,1} + 4T_{i,2} - T_i}{2}$ $3T_{_{i,1}} + 4T_{_{i,2}} - T_{_{i,3}}$ $-3I_{11}+4I_{12}-$ Yield: Compare with Table 2-2! $=$ $\frac{2\Delta}{\Delta}$ 2 *y* $=-\lambda \frac{\partial T}{\partial y}\Big|_{y=0} \approx -\lambda b = \frac{\lambda}{2\lambda y}(3T_{i,1} - 4T_{i,2} + T_{i,3})$ $\lambda \frac{\partial T}{\partial y} = -\lambda b =$ $q_b = -\lambda \frac{\partial T}{\partial y} = -\lambda b = \frac{\lambda}{2 \Delta y} (3T_{i,1} - 4T_{i,2} + T_{i})$ $\int_{y=0}^{\infty} \approx -\lambda b = \frac{\lambda}{2\lambda y} (3T_{i,1} - 4T_{i,2} + T_{i,3})$ ∂ *T* $\left(\frac{T}{y}\right)_{y=0} \approx -\lambda b = \frac{\lambda}{2\Delta y}$ Then: $q_b = -\lambda \frac{\partial I}{\partial y}$, $q_b = -\lambda \frac{\partial I}{\partial y}$ $= -\lambda b = \frac{\lambda}{2\Delta y} (3T_{i,1} - 4T_{i,2} + T_{i,3})$, $O(\Delta y^2)$ $\lambda_b = -\lambda \frac{\partial I}{\partial y}\bigg|_{y=0} \cong -\lambda b = \frac{\lambda}{2\Delta y} (3T_{i,1} - 4T_{i,2} + T_{i,3})$ 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 $(R + A)$ 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 $(\nightharpoonup \times \mathbb{R})$ shape function $(\nightharpoonup \times \mathbb{R})$ is to be solved; here it is to be assumed!----Approximation made

热流科学与工程 Ô

in the numerical simulation!

Variation with spatial coordinate

Variation with time

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

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

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

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

(第) 西步交通大學

1. Transient term

Assuming the step-wise approximation for ϕ with space:

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

2. Convective term

Assuming the explicit step-wise approximation for ϕ with tim[e:](/)

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

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

Further, assuming linear-wise variation of ϕ with space

$$
\rho\left[\left(u\phi\right)^{t}_{e}-\left(u\phi\right)^{t}_{w}\right]\Delta t=\rho u\Delta t(\frac{\phi_{E}+\phi_{P}}{2}-\frac{\phi_{P}+\phi_{W}}{2})=\rho u\Delta t\frac{\phi_{E}-\phi_{W}}{2}\left(3\right)
$$

Superscript "t" is temporary(暂时) neglected!

x

 \widehat{O}

 $\partial \pmb{\phi}$

3. Diffusion term

Taking explicit step-wise variation of $\frac{1}{2}$ with time, yields:

 $\left[\left(\frac{\partial \varphi}{\partial t} \right)_{\rho} - \left(\frac{\partial \varphi}{\partial t} \right)_{w} \right] dt = \Gamma \left[\left(\frac{\partial \varphi}{\partial t} \right)_{\rho}^{t} - \left(\frac{\partial \varphi}{\partial t} \right)_{w}^{t} \right]$ t + Δt *t* $\ell \vee \forall$ t $e \sim 2$ W e ~ 2 ~ 2 ~ 2 ~ 2 \sim Further, assuming linear-wise variation of ϕ with space $dt = \prod_{i} \left(\frac{c_{i} \cdot r}{r_{i}}\right)^{t} - \left(\frac{c_{i} \cdot r}{r_{i}}\right)^{t} \Delta t$ *x ox ox ox ox* $\int_{0}^{t+\Delta t} [(\frac{\partial \phi}{\partial t}) - (\frac{\partial \phi}{\partial t})] dt = \prod_{i} (\frac{\partial \phi}{\partial t})^{t} - (\frac{\partial \phi}{\partial t})^{t} d\Delta$ $\int \left[\left(\frac{C\varphi}{\partial x} \right)_e - \left(\frac{C\varphi}{\partial x} \right)_w \right] dt = \Gamma \left[\left(\frac{C\varphi}{\partial x} \right)^t_e - \left(\frac{C}{\partial x} \right)^t_e \right]$

CENTER

$$
\Gamma[(\frac{\partial \phi}{\partial x})_e^t - (\frac{\partial \phi}{\partial x})_w^t] \Delta t = \Gamma \Delta t [\frac{\phi_E - \phi_P}{(\delta x)_e} - \frac{\phi_P - \phi_W}{(\delta x)_w}] \tag{4}
$$
\nUniform
grid
grid
of $\frac{\phi_E - 2\phi_P + \phi_W}{\Delta x}$ is temporary
neglected!

4. Source term

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

$$
\int_{t}^{t+\Delta t} \int_{w}^{e} S dx dt = \overline{S}^{t} (\Delta x)_{p} \Delta t
$$
 (5); \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 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

By selecting the profile of dependent variable ϕ with space, the discretization equation can be obtained. **If the same profiles as FVM are assumed, the final results are the same** the discretization equation can be obtained**. If the same profiles**

CFD-NHT-EHT

CENTER

software.

2.3.6 Comparisons of two ways

Home Work 2(**2022-2023**)

Please finish your homework independently(独立完成**) !!!**

Please hand in on Sept 27th

Problem 2-1

In the following non-linear equation of u , λ and ρc are constant, $\overline{}$

$$
\rho c_p u \frac{\partial u}{\partial x} = \lambda \frac{\partial^2 u}{\partial x^2}
$$

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

(第)西步交通大學

Problem 2-2

By using the control volume method , develop the discretized equation for the 3D steady heat conduction equation with spatially variable heat conductivity:

$$
\frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(\lambda \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z}(\lambda \frac{\partial T}{\partial z}) + S(x, y, z) = 0
$$

Problem 2-3

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

Problem 2-4

(4) 西步交通大學

size $\Delta x = h = 0.2$, evaluate the forward difference of its first-order Consider the function $f(x) = sin(10\pi x)$. By using a mesh derivative by following two expressions:

1)
$$
f_i = \frac{f_{i+1} - f_i}{h} + O(h);
$$
 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 solution[s.](/)

Problem 2-5

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:

Take h =0.5, 0.05 0.005, calculate d_1 , d_2 and their discretization errors. Draw a picture to show the variation trend of the discretization error with h.

Following textbook in English is available in our WeChat group: Versteeg H K, Malalsekera W. An introduction to computational fluid dynamics. The finite volume method. Essex: Longman Scientific & Technical,**2007**

Teaching PPT will be loaded on our WeChat Group

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

