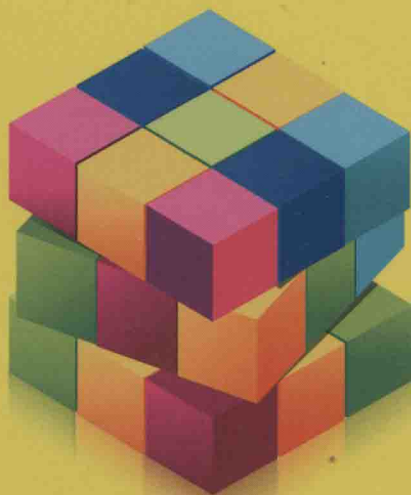


The Method of Order Reduction and Its Application to the Numerical Solutions of Partial Differential Equations

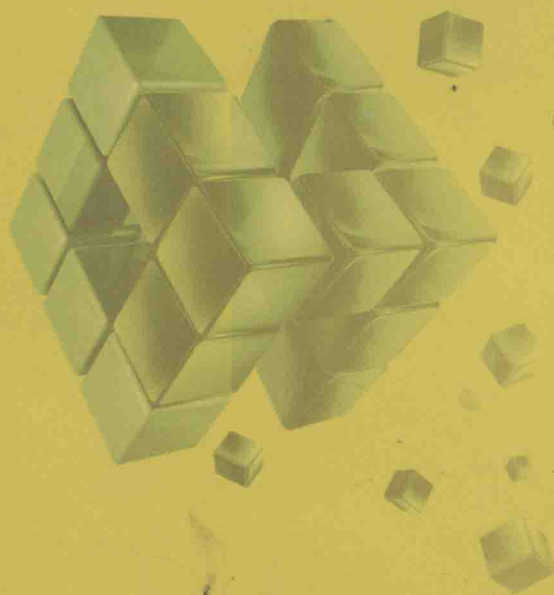
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Zhizhong Sun



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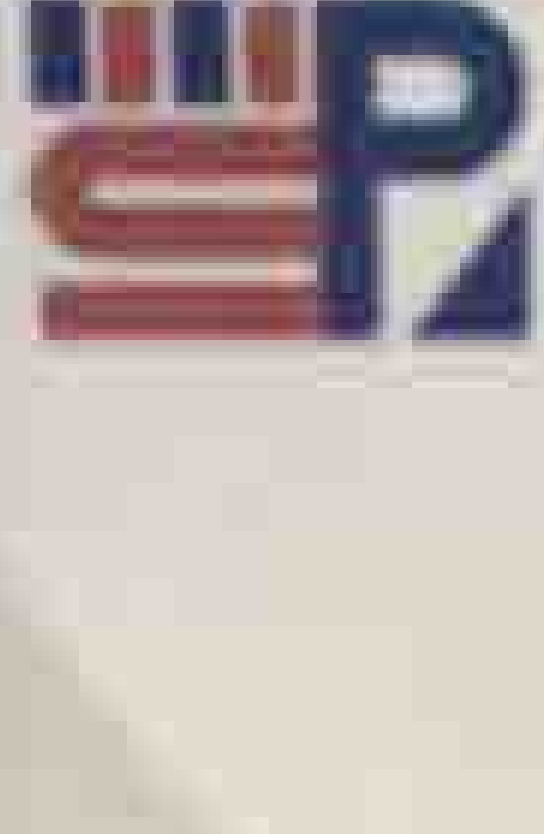


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Preface

The method of order reduction has been developed on the basis of the well-known Keller's box scheme. It is an indirect method of constructing difference schemes for approximating the differential equations. First, some new variables are introduced for the reduction of the original problem into an equivalent system of lower order differential equations and a difference scheme is constructed for the latter. Then, the discrete variables are separated to obtain a difference scheme only containing the original variables. The aim of introducing the new variables is for the theoretical analysis of the difference scheme. The method is applicable to numerical approximations of the problems with derivative boundary conditions, mixed derivatives, discontinuous coefficients or inner boundaries, and the problems of high nonlinearity as well as the high coupled systems, etc. Now this method has been successfully applied to the numerical solutions for linear parabolic equations, linear hyperbolic equations, linear elliptic equations, heat equations with concentrated capacity, heat equations with nonlinear boundary conditions, nonlocal parabolic equations, diffusion-wave equations, wave equations with heat conduction, Timoshenko beam equations with boundary feedback, the Kuramoto-Tsuzuki equation, thermoplastic problems, thermoelastic problems, nonlinear parabolic systems, superthermal electron transport equations, oil deposit models, the Cahn-Hilliard equation, systems of parabolic and elliptic equations, etc. The resulting difference schemes usually have second order global accuracy in the maximum norm. Sometimes, with once extrapolation, the fourth order approximation in the maximum norm can be obtained. In addition, the difference scheme can be constructed on non-uniform grids which makes easy to refine the grids where the solution changes rapidly in order to reduce the amount of the computational work.

The problems we consider include linear equations vs. nonlinear equations, lower order differential equations vs. higher order differential equations, one differential equation vs. the system of differential equations, local differential equations vs. non-local differential equations, one-dimensional problems vs. multi-dimensional problems, problems in the fixed domain vs. problems in the variable domain, problems with classical boundary conditions vs. problems with nonclassical boundary conditions, problems in the bounded domain vs. problems in the unbounded domain, differential equations of integer order vs. differential equations of fractional order, real differential equations vs. complex differential equations.

The layout of this book is as follows. Chapter 1 provides a microcosm of the

method of order reduction via a two-point boundary value problem. Chapters 2, 3 and 4 are devoted, respectively, to the numerical solutions of linear parabolic, hyperbolic and elliptic equations by the method of order reduction. They are the core of the book. Chapters 5, 6 and 7 respectively consider the numerical approaches to the heat equation with an inner boundary condition, the heat equation with a nonlinear boundary condition and the nonlocal parabolic equation. Chapter 8 discusses the numerical approximation to a fractional diffusion-wave equation. The next five chapters are devoted to the numerical solutions of several coupled systems of differential equations. The numerical procedures for the heat equation and the Burgers equation in the unbounded domains are studied in Chapters 14, 15 and 16. Chapter 17 provides a numerical method for the superthermal electron transport equation, which is a degenerate and nonlocal evolutionary equation. The numerical solution to a model in oil deposit on a moving boundary is presented in Chapter 18. Chapter 19 deals with the numerical solution to the Cahn-Hilliard equation, which is a fourth order nonlinear evolutionary equation. The ADI and compact ADI methods for the multidimensional parabolic problems are discussed in Chapter 20. The numerical errors in the maximum norm are obtained. Chapter 21, the last chapter, is devoted to the numerical solution to the time-dependent Schrödinger equation in quantum mechanics.

This book is intended for graduate students and for researchers and specialists in the field of numerical simulation of partial differential equations. A desirable mathematical background for reading this book includes the basic knowledge of partial differential equations and the finite difference methods.

I would like to take this opportunity to thank my master advisors Prof. Yucheng Su and Prof. Qiguang Wu and PhD advisor Prof. Youlan Zhu for guidance in the field of numerical simulation of partial differential equations. I am grateful to Prof. Houde Han and Prof. Xiaonan Wu for their cooperation. I would also wish to thank my graduate students, Fule Li, Honglin Liao, Zhengsu Wan, Jialing Wang, Lingyun Zhang and Lei Zhao for their contribution to this book.

Most of the research work reported in this book has been completed with the support of the Natural Science Foundation of China (contract grant numbers 19801007 and 10471023, 10871044). The publication of this book is partly sponsored by the Publishing Foundation of Southeast University. However, it is very likely that there are still some errors in this book. I would greatly appreciate it if you could notify me of any mistakes found in the process of using the book and give me comments by sending e-mail to zzsun@seu.edu.cn.

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Chapter 1

The Method of Order Reduction

1.1 Introduction

The finite difference method is one of the most useful numerical methods for solving differential equations. The basic idea is to replace the differential equations approximately by a system of discrete difference equations. We regard the solution to the system of difference equations as the approximate solution of differential equations. In this chapter, we present some finite difference methods for a two-point boundary value problem of an ordinary differential equation and then introduce the method of order reduction.

Firstly, we list some formulae in common use. Suppose that $g(x)$ has an appropriately continuous derivatives in $[x_0 - 2h, x_0 + 2h]$. Then

$$g(x_0) = \frac{1}{2} [g(x_0 - h) + g(x_0 + h)] - \frac{h^2}{2} g''(\xi_0),$$
$$\xi_0 \in (x_0 - h, x_0 + h); \quad (1.1.1)$$

$$g'(x_0) = \frac{1}{h} [g(x_0 + h) - g(x_0)] - \frac{h}{2} g''(\xi_1), \quad \xi_1 \in (x_0, x_0 + h); \quad (1.1.2)$$

$$g'(x_0) = \frac{1}{h} [g(x_0) - g(x_0 - h)] + \frac{h}{2} g''(\xi_2), \quad \xi_2 \in (x_0 - h, x_0); \quad (1.1.3)$$

$$g'(x_0) = \frac{1}{h} \left[g\left(x_0 + \frac{h}{2}\right) - g\left(x_0 - \frac{h}{2}\right) \right] - \frac{h^2}{24} g'''(\xi_3),$$
$$\xi_3 \in \left(x_0 - \frac{h}{2}, x_0 + \frac{h}{2}\right); \quad (1.1.4)$$

$$g'(x_0) = \frac{1}{2h} [-g(x_0 + 2h) + 4g(x_0 + h) - 3g(x_0)] + \frac{h^2}{3} g'''(\xi_4),$$
$$\xi_4 \in (x_0, x_0 + 2h); \quad (1.1.5)$$

$$g'(x_0) = \frac{1}{2h} [3g(x_0) - 4g(x_0 - h) + g(x_0 - 2h)] + \frac{h^2}{3} g'''(\xi_5),$$
$$\xi_5 \in (x_0, x_0 - 2h); \quad (1.1.6)$$

$$g''(x_0) = \frac{1}{h^2} [g(x_0 + h) - 2g(x_0) + g(x_0 - h)] - \frac{h^2}{12} g^{(4)}(\xi_6),$$
$$\xi_6 \in (x_0 - h, x_0 + h). \quad (1.1.7)$$

Applying the Taylor expansion or the theory of polynomial interpolation, we can easily get (1.1.1)~(1.1.7).

Consider the following two-point boundary value problem:

$$-u'' + q(x)u = f(x), \quad a < x < b, \quad (1.1.8)$$

$$-u'(a) + \mu_0 u(a) = \alpha, \quad u'(b) + \mu_1 u(b) = \beta, \quad (1.1.9)$$

where $q(x) \geq 0$, $f(x)$ are two known functions, μ_0, μ_1, α and β are known constants. Suppose (1.1.8)~(1.1.9) have a solution $u(x) \in C^4[a, b]$.

Let us divide the interval $[a, b]$ into M equal parts and denote $h = (b - a)/M$, $x_i = a + ih$ ($0 \leq i \leq M$), $x_{i-\frac{1}{2}} = \frac{1}{2}(x_i + x_{i-1})$ ($1 \leq i \leq M$), $\Omega_h = \{x_i \mid 0 \leq i \leq M\}$ and $q_i = q(x_i)$, $f_i = f(x_i)$, $q_{i-\frac{1}{2}} = q(x_{i-\frac{1}{2}})$, $f_{i-\frac{1}{2}} = f(x_{i-\frac{1}{2}})$. Define the grid function

$$U = \{U_i \mid U_i = u(x_i), 0 \leq i \leq M\}.$$

If $v = \{v_i \mid 0 \leq i \leq M\}$ is a grid function on Ω_h , we denote

$$v_{i-\frac{1}{2}} = \frac{1}{2}(v_i + v_{i-1}), \quad \delta_x v_{i-\frac{1}{2}} = \frac{1}{h}(v_i - v_{i-1}), \quad \delta_x^2 v_i = \frac{1}{h}(\delta_x v_{i+\frac{1}{2}} - \delta_x v_{i-\frac{1}{2}}).$$

In this chapter, we present four difference methods for solving the problem (1.1.8)~(1.1.9) and make some numerical comparisons.

1.2 First order off-center difference method

From (1.1.2), (1.1.3) and (1.1.7), we have

$$-\delta_x^2 U_i + q_i U_i = f_i - \frac{h^2}{12} u^{(4)}(\xi_i), \quad 1 \leq i \leq M-1, \quad (1.2.1)$$

$$-\delta_x U_{\frac{1}{2}} + \mu_0 U_0 = \alpha - \frac{h}{2} u''(\xi_0), \quad \delta_x U_{M-\frac{1}{2}} + \mu_1 U_M = \beta - \frac{h}{2} u''(\xi_M), \quad (1.2.2)$$

where

$$\xi_i \in (x_{i-1}, x_{i+1}), 1 \leq i \leq M-1; \quad \xi_0 \in (x_0, x_1); \quad \xi_M \in (x_{M-1}, x_M).$$

Omitting the small terms in the formulae above, we get the following difference scheme (denoted by Scheme I)

$$-\delta_x^2 u_i + q_i u_i = f_i, \quad 1 \leq i \leq M-1, \quad (1.2.3)$$

$$-\delta_x u_{\frac{1}{2}} + \mu_0 u_0 = \alpha, \quad \delta_x u_{M-\frac{1}{2}} + \mu_1 u_M = \beta. \quad (1.2.4)$$

The difference scheme (1.2.3)~(1.2.4) is a tridiagonal system of linear algebraic equations, which can be solved by the double sweep method (the Thomas method).

1.3 Second order off-center difference method

From (1.1.5)~(1.1.7), we have

$$-\delta_x^2 U_i + q_i U_i = f_i - \frac{h^2}{12} u^{(4)}(\xi_i), \quad 1 \leq i \leq M-1, \quad (1.3.1)$$

$$-\frac{1}{2h} (-U_2 + 4U_1 - 3U_0) + \mu_0 U_0 = \alpha + \frac{h^2}{3} u'''(\xi_0), \quad (1.3.2)$$

$$\frac{1}{2h} (3U_M - 4U_{M-1} + U_{M-2}) + \mu_1 U_M = \beta - \frac{h^2}{3} u'''(\xi_M), \quad (1.3.3)$$

where

$$\xi_i \in (x_{i-1}, x_{i+1}), 1 \leq i \leq M-1; \quad \xi_0 \in (x_0, x_2); \quad \xi_M \in (x_{M-2}, x_M).$$

Omitting the small terms in the formulae above, we have the following difference scheme

$$-\delta_x^2 u_i + q(x_i) u_i = f(x_i), \quad 1 \leq i \leq M-1, \quad (1.3.4)$$

$$-\frac{1}{2h} (-u_2 + 4u_1 - 3u_0) + \mu_0 u_0 = \alpha, \quad (1.3.5)$$

$$\frac{1}{2h} (3u_M - 4u_{M-1} + u_{M-2}) + \mu_1 u_M = \beta. \quad (1.3.6)$$

Eliminating u_2 in (1.3.5) by the equation (1.3.4) with $i = 1$ and eliminating u_{M-2} in (1.3.6) by the equation (1.3.4) with $i = M-1$, we obtain the following difference scheme (denoted by Scheme II)

$$-\delta_x^2 u_i + q_i u_i = f_i, \quad 1 \leq i \leq m-1, \quad (1.3.7)$$

$$-\delta_x u_{\frac{1}{2}} + \mu_0 u_0 + \frac{1}{2} h q_1 u_1 = \alpha + \frac{1}{2} h f_1, \quad (1.3.8)$$

$$\delta_x u_{M-\frac{1}{2}} + \mu_1 u_M + \frac{1}{2} h q_{M-1} u_{M-1} = \beta + \frac{1}{2} h f_{M-1}. \quad (1.3.9)$$

The difference scheme (1.3.7)~(1.3.9) is a tridiagonal system of linear algebraic equations, which can be solved by the double sweep method.

The equations (1.3.8)~(1.3.9) can be written as

$$-\frac{2}{h} \left[\delta_x u_{\frac{1}{2}} - (\mu_0 u_0 - \alpha) \right] + q_1 u_1 = f_1, \quad (1.3.10)$$

$$-\frac{2}{h} \left[(\beta - \mu_1 u_M) - \delta_x u_{M-\frac{1}{2}} \right] + q_{M-1} u_{M-1} = f_{M-1}. \quad (1.3.11)$$

Similarly, from (1.3.1)~(1.3.3), we may obtain

$$-\frac{2}{h} \left[\delta_x U_{\frac{1}{2}} - (\mu_0 U_0 - \alpha) \right] + q_1 U_1 = f_1 + \frac{2h}{3} u'''(\xi_0) - \frac{h^2}{12} u^{(4)}(\xi_1), \quad (1.3.12)$$

$$\begin{aligned} & -\frac{2}{h} \left[(\beta - \mu_1 U_M) - \delta_x U_{M-\frac{1}{2}} \right] + q_{M-1} U_{M-1} \\ & = f_{M-1} - \frac{2h}{3} u'''(\xi_M) - \frac{h^2}{12} u^{(4)}(\xi_{M-1}). \end{aligned} \quad (1.3.13)$$

1.4 Method of fictitious domain

Suppose the solution $u(x)$ of (1.1.8)~(1.1.9) can be extended to the interval $[x_{-1}, x_{M+1}]$ and $u(x) \in C^4[x_{-1}, x_{M+1}]$, where $x_{-1} = x_0 - h, x_{M+1} = x_M + h$.

From (1.1.5), (1.1.6) and (1.1.7), we have

$$-\delta_x^2 U_i + q_i U_i = f_i - \frac{h^2}{12} u^{(4)}(\xi_i), \quad 0 \leq i \leq M, \quad (1.4.1)$$

$$-\frac{1}{2h} (U_1 - U_{-1}) + \mu_0 U_0 = \alpha - \frac{h^2}{6} u'''(\xi_{-1}), \quad (1.4.2)$$

$$\frac{1}{2h} (U_{M+1} - U_{M-1}) + \mu_1 U_M = \beta + \frac{h^2}{6} u'''(\xi_{M+1}), \quad (1.4.3)$$

where $\xi_i \in (x_{i-1}, x_{i+1}), 0 \leq i \leq M; \xi_{-1} \in (x_{-1}, x_1), \xi_{M+1} \in (x_{M-1}, x_{M+1})$. Omitting the small terms in the formulae above, we have the following difference scheme

$$-\delta_x^2 u_i + q_i u_i = f_i, \quad 0 \leq i \leq M, \quad (1.4.4)$$

$$-\frac{1}{2h} (u_1 - u_{-1}) + \mu_0 u_0 = \alpha, \quad (1.4.5)$$

$$\frac{1}{2h} (u_{M+1} - u_{M-1}) + \mu_1 u_M = \beta. \quad (1.4.6)$$

Eliminating u_{-1} in (1.4.5) by the equation (1.4.4) with $i = 0$ and eliminating u_{M+1} in (1.4.6) by equation (1.4.4) with $i = M$, we obtain (denoted by Scheme III)

$$-\delta_x^2 u_i + q_i u_i = f_i, \quad 1 \leq i \leq M-1, \quad (1.4.7)$$

$$-\delta_x u_{\frac{1}{2}} + \mu_0 u_0 + \frac{1}{2} h q_0 u_0 = \alpha + \frac{1}{2} h f_0, \quad (1.4.8)$$

$$\delta_x u_{M-\frac{1}{2}} + \mu_1 u_M + \frac{1}{2} h q_M u_M = \beta + \frac{1}{2} h f_M. \quad (1.4.9)$$

The equations (1.4.8) and (1.4.9) can be written as

$$-\frac{2}{h} \left[\delta_x u_{\frac{1}{2}} - (\mu_0 u_0 - \alpha) \right] + q_0 u_0 = f_0, \quad (1.4.10)$$

$$-\frac{2}{h} \left[(\beta - \mu_1 u_M) - \delta_x u_{M-\frac{1}{2}} \right] + q_M u_M = f_M. \quad (1.4.11)$$

The difference scheme (1.4.7)~(1.4.9) is a tridiagonal system of linear algebraic equations, which can be solved by the double sweep method.

If we do not suppose that solution $u(x)$ of (1.1.8)~(1.1.9) can be extended to the interval $[x_{-1}, x_{M+1}]$, we can obtain the difference scheme (1.4.7)~(1.4.9) by the following method.

From

$$-u'(a) + \mu_0 u(a) = \alpha, \quad -u''(a) + q(a)u(a) = f(a),$$

we have

$$\begin{aligned}\delta_x U_{\frac{1}{2}} &= u'(a) + \frac{h}{2} u''(a) + \frac{h^2}{6} u'''(\xi_0) \\ &= \mu_0 U_0 - \alpha + \frac{h}{2} (q_0 U_0 - f_0) + \frac{h^2}{6} u'''(\xi_0),\end{aligned}$$

where $\xi_0 \in (x_0, x_1)$. From

$$u'(b) + \mu_1 u(b) = \beta, \quad -u''(b) + q(b)u(b) = f(b),$$

we have

$$\begin{aligned}\delta_x U_{M-\frac{1}{2}} &= u'(b) - \frac{h}{2} u''(b) + \frac{h^2}{6} u'''(\xi_M) \\ &= \beta - \mu_1 U_M + \frac{h}{2} (f_M - q_M U_M) + \frac{h^2}{6} u'''(\xi_M),\end{aligned}$$

where $\xi_M \in (x_{M-1}, x_M)$. Then

$$-\delta_x^2 U_i + q_i U_i = f_i - \frac{h^2}{12} u^{(4)}(\xi_i), \quad 1 \leq i \leq M-1, \quad (1.4.12)$$

$$-\delta_x U_{\frac{1}{2}} + \mu_0 U_0 + \frac{h}{2} q_0 U_0 = \alpha + \frac{h}{2} f_0 - \frac{h^2}{6} u'''(\xi_0), \quad (1.4.13)$$

$$\delta_x U_{M-\frac{1}{2}} + \mu_1 U_M + \frac{h}{2} q_M U_M = \beta + \frac{h}{2} f_M + \frac{h^2}{6} u'''(\xi_M). \quad (1.4.14)$$

Omitting the small terms of order $O(h^2)$ in the equations (1.4.12)~(1.4.14), we arrive at the difference scheme (1.4.7)~(1.4.9).

The equations (1.4.13)~(1.4.14) can be written as

$$-\frac{2}{h} \left[\delta_x U_{\frac{1}{2}} - (\mu_0 U_0 - \alpha) \right] + q_0 U_0 = f_0 - \frac{h}{3} u'''(\xi_0), \quad (1.4.15)$$

$$-\frac{2}{h} \left[(\beta - \mu_1 U_M) - \delta_x U_{M-\frac{1}{2}} \right] + q_M U_M = f_M + \frac{h}{3} u'''(\xi_M). \quad (1.4.16)$$

1.5 Method of order reduction

Let

$$v(x) = u'(x),$$

then (1.1.8)~(1.1.9) are equivalent to

$$-v' + q(x)u = f(x), \quad a < x < b, \quad (1.5.1)$$

$$-u' + v = 0, \quad a < x < b, \quad (1.5.2)$$

$$-v(a) + \mu_0 u(a) = \alpha, \quad v(b) + \mu_1 u(b) = \beta. \quad (1.5.3)$$

The problem (1.5.1)~(1.5.3) is a system of first order differential equations, in which the boundary conditions (1.5.3) do not include derivatives.

From (1.1.1) and (1.1.4), we have

$$-\delta_x V_{i-\frac{1}{2}} + q_{i-\frac{1}{2}} U_{i-\frac{1}{2}} = f_{i-\frac{1}{2}} + (r_1)_{i-\frac{1}{2}}, \quad 1 \leq i \leq M, \quad (1.5.4)$$

$$-\delta_x U_{i-\frac{1}{2}} + V_{i-\frac{1}{2}} = (r_2)_{i-\frac{1}{2}}, \quad 1 \leq i \leq M, \quad (1.5.5)$$

$$-V_0 + \mu_0 U_0 = \alpha, \quad V_M + \mu_1 U_M = \beta, \quad (1.5.6)$$

where

$$(r_1)_{i-\frac{1}{2}} = \left[-\frac{1}{24} v'''(\xi_{i-\frac{1}{2}}) + \frac{1}{8} q_{i-\frac{1}{2}} u''(\bar{\xi}_{i-\frac{1}{2}}) \right] h^2, \quad \xi_{i-\frac{1}{2}}, \bar{\xi}_{i-\frac{1}{2}} \in (x_{i-1}, x_i);$$

$$(r_2)_{i-\frac{1}{2}} = \left[-\frac{1}{24} u'''(\eta_{i-\frac{1}{2}}) + \frac{1}{8} v''(\bar{\eta}_{i-\frac{1}{2}}) \right] h^2, \quad \eta_{i-\frac{1}{2}}, \bar{\eta}_{i-\frac{1}{2}} \in (x_{i-1}, x_i).$$

Omitting the small terms in the formulae above, we construct, for (1.5.1)~(1.5.3), the following difference scheme

$$-\delta_x v_{i-\frac{1}{2}} + q_{i-\frac{1}{2}} u_{i-\frac{1}{2}} = f_{i-\frac{1}{2}}, \quad 1 \leq i \leq M, \quad (1.5.7)$$

$$-\delta_x u_{i-\frac{1}{2}} + v_{i-\frac{1}{2}} = 0, \quad 1 \leq i \leq M, \quad (1.5.8)$$

$$-v_0 + \mu_0 u_0 = \alpha, \quad v_M + \mu_1 u_M = \beta. \quad (1.5.9)$$

The difference scheme (1.5.7)~(1.5.9) is often called **box scheme**, which has the following three virtues: (1) the discretization of boundary conditions without any errors. (2) being suitable to construct difference scheme on nonequal grids. Actually, suppose $a = x_0 < x_1 < \cdots < x_{M-1} < x_M = b$ be a non-equidistant division of $[a, b]$. Let $h_i = x_i - x_{i-1}$, $\delta_x v_{i-\frac{1}{2}} = \frac{1}{h_i} (v_i - v_{i-1})$. Then we can also obtain the difference scheme as (1.5.7)~(1.5.9). (3) the difference scheme containing only the first order difference quotient, which makes the theoretical analysis easy.

Keller^[130] provided a method to solve difference scheme (1.5.7)~(1.5.9). Let

$$B_0 = \begin{pmatrix} \mu_0 & -1 \end{pmatrix}, \quad A_{M+1} = \begin{pmatrix} \mu_1 & 1 \end{pmatrix}; \quad W_i = \begin{pmatrix} u_i \\ v_i \end{pmatrix}, \quad 0 \leq i \leq M;$$

$$A_i = \begin{pmatrix} \frac{1}{2} h q_{i-\frac{1}{2}} & 1 \\ 1 & \frac{1}{2} h \end{pmatrix}, \quad B_i = \begin{pmatrix} \frac{1}{2} h q_{i-\frac{1}{2}} & -1 \\ -1 & \frac{1}{2} h \end{pmatrix}, \quad F_i = \begin{pmatrix} h f_{i-\frac{1}{2}} \\ 0 \end{pmatrix}, \quad 1 \leq i \leq M.$$

Then, (1.5.7)~(1.5.9) can be written as

$$\begin{pmatrix} B_0 & & & & & & \\ A_1 & B_1 & & & & & \\ & A_2 & B_2 & & & & \\ & & & \ddots & & & \\ & & & & A_{M-1} & B_{M-1} & \\ & & & & & A_M & B_M \\ & & & & & & A_{M+1} \end{pmatrix} \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ \vdots \\ W_{M-2} \\ W_{M-1} \\ W_M \end{pmatrix} = \begin{pmatrix} \alpha \\ F_1 \\ F_2 \\ \vdots \\ F_{M-1} \\ F_M \\ \beta \end{pmatrix}.$$