Available at
http://pvamu.edu/aam
Appl. Appl. Math.
ISSN: 1932-9466

Vol. 4, Issue 2 (December 2009), pp. 263 – 272
(Previously, Vol. 4, No. 2)

Applications and Applied Mathematics:
An International Journal
(AAM)

Higher Order Difference Schemes for Heat Equation

Jianzhong Wang
Department of Mathematics and Statistics
Sam Houston State University
Huntsville, TX 77341 USA
mth_jxw@shsu.edu

Received: July 10, 2009; Accepted: October 15, 2009

Abstract

In this paper, we construct the explicit difference schemes for the heat equation with arbitrary high orders. We also show the validity of the new schemes by numerical simulations.

Keywords: Heat equation; explicit difference schemes; numerical solutions; high-order schemes

MSC (2000) No.: 65M06 65D25 35K05

1. Introduction

In this paper we study the construction of the explicit difference schemes for the 1-D heat equation

$$D_t u = cD_x^2 u, \tag{1}$$

where $u = u(x,t)$ is temperature, $c > 0$ is the heat conductivity, $D_t = \frac{\partial}{\partial t}$, and $D_x^2 = \frac{\partial^2}{\partial x^2}$. The operator form of (1) is

$$D_t = cD_x^2. \tag{2}$$

For a temperature function $u(x,t)$, let E_h $(h \in R)$ denote the spatial translation opera $E_h u(\cdot,t) = u(\cdot + h,t)$. We have $E_{kh} = E_h^k, k \in Z$. A Laurent polynomial of E_h :

$$A_h^{n,m} = \sum_{k=-m}^{n} a_k E_{kh}$$

is called a difference scheme of order $s \in N$ if

$$A_h^{n,m}\left(x^k\right) = 0, \quad k = 0, 1, \cdots, s-1.$$

A difference scheme of order 2 approximates D_x^2. Since the differential operator D_x^2 is self-conjugate, we are only interested in the symmetric difference scheme of order 2:

$$A_h^n = \sum_{k=0}^{n} a_k (E_{kh} + E_{-kh}), \quad \text{with } A_h^n(1) = 0 \text{ and } A_h^n(x) = 0. \tag{3}$$

For a temperature function u, we define the temporal difference operator Δ_t $(t > 0)$ by $\Delta_t u(x,\cdot) = u(x, t+\cdot) - u(x,\cdot)$. Thus, an explicit difference scheme for the heat equation (1) is

$$\frac{\Delta_t}{t} u = \frac{c}{h^2} A_h^n u. \tag{4}$$

Let $\lambda = \frac{ct}{h^2} > 0$ be the constant multiple of the ratio of the time-step to the square of the space-step (TSR). Then, $t = \frac{\lambda h^2}{c} (= O(h^2))$. A difference scheme (4) is said to have order $s \in N$ if

$$R(u) = \frac{\Delta_t}{t} u - \frac{c}{h^2} A_h^n u = O(h^s), \quad h \to 0.$$

Write

$$\delta_h^2 = E_h + E_{-h} - 2I, \tag{5}$$

where I is the identity operator. The simplest difference scheme for (1) is

$$\frac{\Delta_t}{t} u = \frac{c}{h^2} \delta_h^2 u, \tag{6}$$

which has order 2 and its stability condition is $\lambda \le \frac{1}{2}$ [Gerald Wheatley (1999), Richtmyer and Morton (1967)]. People are also interested in higher order difference schemes. In Qian et al. (2000), the authors proposed the following difference scheme of order 4:

$$\frac{\Delta_t}{t} u = \frac{c}{h^2} \delta_h^2 \left(I + \frac{6\lambda - 1}{12} \delta_h^2 \right) u, \tag{7}$$

and showed that when $\lambda \le \frac{2}{3}$ the scheme is stable. In this paper, we shall give a general formula for the construction of difference schemes for (1) with arbitrary orders and show the validity of the formula by numerical simulations.

2. Construction of Difference Schemes

We start our construction from the exponential expansion of Δ_t :

$$\Delta_t = \sum_{n=1}^{\infty} \frac{t^n D_t^n}{n!}.$$

Applying the heat equation (2) and recalling $\lambda = \frac{ct}{h^2}$, we have

$$\Delta_t = \sum_{n=1}^{\infty} \frac{\lambda^n h^{2n} D_x^{2n}}{n!}.$$

To illustrate our method, we first construct the difference schemes for (1) with order 2 and 4, respectively. The Taylor expansion of δ_h^2 in (5) is

$$\delta_h^2 = 2\left(\sum_{n=1}^{\infty} \frac{h^{2n} D_x^{2n}}{(2n)!}\right), \tag{8}$$

which yields

$$\begin{aligned}\frac{\Delta_t}{t} - \left(\frac{c}{h^2}\right)\delta_h^2 &= c\sum_{n=1}^{\infty}\left(\frac{\lambda^{n-1}}{n!} - \frac{2}{(2n)!}\right)h^{2(n-1)}D_x^{2n} \\ &= c\sum_{n=1}^{\infty}\left(\frac{\lambda^{n}}{(n+1)!} - \frac{2}{(2n+2)!}\right)h^{2n}D_x^{2(n+1)},\end{aligned}$$

i.e.,

$$\frac{\Delta_t}{t} - \left(\frac{c}{h^2}\right)\delta_h^2 = c\left(\frac{\lambda}{2} - \frac{1}{12}\right)h^2 D_x^4 + O\left(h^4\right). \tag{9}$$

The formula (9) shows that the simplest scheme (6) has order 2, and it achieves order 4 when $\lambda = \frac{1}{6}$.

To derive the difference scheme of order 4, we, replacing h in (8) by $2h$, derive the identity

$$\delta_{2h}^2 = \sum_{n=1}^{\infty} \frac{2^{2n+1} h^{2n} D_x^{2n}}{(2n)!}$$

and set the scheme to

$$\frac{\Delta_t}{t} = \frac{c}{h^2}(a\delta_h^2 + b\delta_{2h}^2), \tag{10}$$

where a and b are two real numbers to be determined. We have

$$\frac{\Delta_t}{t} - \frac{c}{h^2}(a\delta_h^2 + b\delta_{2h}^2) = c\sum_{k=1}^{\infty}\left(\frac{\lambda^{k-1}}{k!} - \frac{2}{(2k)!}(a+4^k b)\right)h^{2(k-1)}D_x^{2k}.$$

Let

$$\begin{cases} a+4b = & 1 \\ a+4^2 b = & 6\lambda. \end{cases} \tag{11}$$

Then,

$$\begin{aligned}\frac{\Delta_t}{t} - \frac{c}{h^2}(a\delta_h^2 + b\delta_{2h}^2) &= c\sum_{k=3}^{\infty}\left(\frac{\lambda^{k-1}}{k!} - \frac{2}{(2k)!}(a+4^k b)\right)h^{2(k-1)}D_x^{2k} \\ &= c\left(\frac{\lambda^2}{6} - \frac{1}{360}(a+64b)\right)h^4 D_x^6 + O\left(h^6\right).\end{aligned}$$

The solution of (11) is

$$\begin{cases} a = & \frac{4}{3} - 2\lambda \\ b = & -\frac{1}{12} + \frac{1}{2}\lambda. \end{cases}$$

Therefore, setting $a = \frac{4}{3} - 2\lambda$ and $b = -\frac{1}{12} + \frac{1}{2}\lambda,$ we have

$$\frac{\Delta_t}{t} - \frac{c}{h^2}(a\delta_h^2 + b\delta_{2h}^2) = c\left(\frac{\lambda^2}{6} - \frac{1}{12}\lambda + \frac{1}{90}\right)h^4 D_x^6 + O\left(h^6\right),$$

i.e., the difference scheme

$$\frac{\Delta_t}{t} = \frac{c}{h^2}\left(\frac{4}{3} - 2\lambda\right)\delta_h^2 + \frac{c}{h^2}\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)\delta_{2h}^2 \tag{12}$$

has order 4. By $\delta_{2h}^2 = \delta_h^2\delta_h^2 + 4\delta_h^2$, we have

$$\begin{aligned}&\frac{c}{h^2}\left(\frac{4}{3} - 2\lambda\right)\delta_h^2 + \frac{c}{h^2}\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)\delta_{2h}^2 \\ &\quad = \frac{c}{h^2}[\left(\frac{4}{3} - 2\lambda\right) + 4\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)]\delta_h^2 + \left(-\frac{1}{12} + \frac{1}{2}\lambda\right)(\delta_h^2)^2\end{aligned}$$

$$= \frac{c}{h^2}\delta_h^2\left(I + \frac{6\lambda - 1}{12}\delta_h^2\right),$$

which shows that the scheme (12) is the same as the scheme (7) obtained in Qian, et al. (2000). To obtain the stability condition for the scheme (12), we denote $E^t = I + \Delta_t$ and rewrite the scheme (12) to the form of

$$E^t = I + \lambda\left(\frac{4}{3} - 2\lambda\right)\delta_h^2 + \lambda\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)\delta_{2h}^2 = I + \lambda\delta_h^2 + \lambda\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)\left(\delta_h^2\right)^2. \tag{13}$$

Let $A(\omega)$ be representation of E^t in the Fourier domain. Then, by (13),

$$A(\omega) = 1 + 2\lambda\left(\cos h\omega - 1\right) + 4\lambda\left(-\frac{1}{12} + \frac{1}{2}\lambda\right)\left(\cos h\omega - 1\right)^2$$

$$= 1 - 4\lambda\sin^2\frac{h\omega}{2} + \lambda\left(8\lambda - \frac{4}{3}\right)\sin^4\frac{h\omega}{2}$$

The stability condition of the scheme (12) is $\max_{\omega\in R}\left|A(\omega)\right| \le 1,$ which leads the stability condition $\lambda \le \frac{2}{3}$.

We now develop the difference scheme for (1) with an arbitrary order. Assume that the difference scheme of order $2m$ has the form

$$\frac{\Delta_t}{t} = \frac{c}{h^2}\sum_{j=1}^{m} a_j\delta_{jh}^2, \tag{14}$$

where the coefficient vector $\mathbf{a} = [a_1, \cdots, a_m]^T$ is to be determined. Recall that

$$\frac{\Delta_t}{t} - \frac{c}{h^2}\sum_{k=1}^{m} a_k\delta_{kh}^2 = c\sum_{k=1}^{\infty}\left(\frac{\lambda^{k-1}}{k!} - \frac{2}{(2k)!}\sum_{j=1}^{m} j^{2k}a_j\right)h^{2(k-1)}D_x^{2k}.$$

In order to obtain a scheme of order $2m,$ the real numbers $a_1, \cdots, a_m$ have to satisfy

$$\sum_{j=1}^{m} j^{2k}a_j = \frac{(2k)!}{2k!}\lambda^{k-1}, \quad k = 1, \cdots, m. \tag{15}$$

Write

$$V_m = \begin{bmatrix} 1 & 4 & 9 & \cdots & m^2 \\ 1 & 4^2 & 9^2 & \cdots & m^4 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 4^m & 9^m & \cdots & m^{2m} \end{bmatrix}$$

and $\mathbf{b} = \left[1, 6\lambda, \cdots, \frac{(2m)!}{2m!}\lambda^{m-1}\right]^T$. The matrix form of Equation (15) is

$$V_m \mathbf{a} = \mathbf{b}.$$

Since the Vandermonde matrix V_m is invertible, Equation (15) has the unique solution

$$\mathbf{a} = \mathbf{V}_m^{-1}\mathbf{b}, \tag{16}$$

which yields

$$\frac{\Delta_t}{t} - \frac{c}{h^2}\sum_{k=1}^{m} a_k \delta_{kh}^2 = c\left(\frac{\lambda^m}{(m+1)!} - \frac{2}{(2m+2)!}\sum_{j=1}^{m} j^{2m+2} a_j\right) h^{2m} D_x^{2m+2} + O(h^{2m+2}),$$

i.e., the difference scheme (14) with *a* in (16) has order $2m$.

The scheme (14) can be rewritten to

$$E^t = I + \lambda \sum_{k=1}^{m} a_k \delta_{kh}^2. \tag{17}$$

Let $A(\omega)$ be representation of E^t in the Fourier domain. Then,

$$A(\omega) = 1 - 2\lambda \sum_{k=1}^{m} a_k \left(1 - \cos kh\omega\right)$$

and the stability condition of the scheme (14) is $\max_{\omega \in R} |A(\omega)| \le 1$. Therefore, a sufficient condition for the stability can be obtained by $a_k \ge 0, k = 1,, m,$ and $1 - 2\lambda \sum_{k=1}^{m} a_k \ge 0.$

As examples, we use (16) to derive the difference schemes of order 6 and 8, respectively.

Example 1.

Let

$$\begin{cases} a_1 = \frac{3}{2} - \frac{13}{4}\lambda + \frac{5}{2}\lambda^2, \\ a_2 = -\frac{3}{20} + \lambda - \lambda^2, \\ a_3 = \frac{1}{90} - \frac{1}{12}\lambda + \frac{1}{6}\lambda^2, \end{cases}$$

which is the solution of the linear system

$$
\begin{aligned}
a_1 + 4a_2 + 9a_3 &= 1, \\
a_1 + 4^2 a_2 + 9^2 a_3 &= 6\lambda, \\
a_1 + 4^3 a_2 + 9^3 a_3 &= 60\lambda^2.
\end{aligned}
$$

Then, the difference scheme

$$\frac{\Delta_t}{t} = \frac{c}{h^2}(a_1\delta_h^2 + a_2\delta_{2h}^2 + a_3\delta_{3h}^2)$$

has order 6. We select λ in the following range

$$0.184\frac{1}{2} - \frac{1}{10}\sqrt{10} \le \lambda \le \frac{1}{2} + \frac{1}{10}\sqrt{10}0.816$$

so that a_1, a_2, a_3, and $[1 - 2\lambda(a_1 + a_2 + a_3)]$ are nonnegative, that ensures the stability of the scheme.

Example 2.

Let

$$
\begin{cases}
a_1 = \frac{8}{5} - \frac{61}{15}\lambda + \frac{29}{6}\lambda^2 - \frac{7}{3}\lambda^3, \\
a_2 = -\frac{1}{5} + \frac{169}{120}\lambda - \frac{13}{6}\lambda^2 + \frac{7}{6}\lambda^3, \\
a_3 = \frac{8}{315} - \frac{1}{5}\lambda + \frac{1}{2}\lambda^2 - \frac{1}{3}\lambda^3, \\
a_4 = -\frac{1}{560} + \frac{7}{480}\lambda - \frac{1}{24}\lambda^2 + \frac{1}{24}\lambda^3,
\end{cases}
$$

which is the solution of the linear system

$$
\begin{aligned}
a_1 + 4a_2 + 9a_3 + 16a_4 &= 1, \\
a_1 + 4^2 a_2 + 9^2 a_3 + 16^2 a_4 &= 6\lambda, \\
a_1 + 4^3 a_2 + 9^3 a_3 + 16^3 a_4 &= 60\lambda^2, \\
a_1 + 4^4 a_2 + 9^4 a_3 + 16^4 a_4 &= 840\lambda^3.
\end{aligned}
$$

Then, the difference scheme

$$\frac{\Delta_t}{t} = \frac{c}{h^2}(a_1\delta_h^2 + a_2\delta_{2h}^2 + a_3\delta_{3h}^2 + a_4\delta_{4h}^2)$$

has order 8. To ensure the stability of the scheme, we select λ in the range $[0.194, 0.955]$.

3. Numerical simulations

To validate our theoretical results, we show a numerical example in this section. For comparison, we set the same initial condition as in Qian, et al. (2000) for the heat equation (1):

$$u(x,0) = \sin(2k\pi x),$$

and seek for the unit-periodic (with respect to x) solution of (1). The exact solution is

$$u(x,t) = e^{-4ck^2\pi^2 t}\sin(2k\pi x).$$

To apply our schemes to the equation, we let $h > 0$ be the space-step and $\tau > 0$ be the time-step, where h is chosen such that $N = 1/h$ is an integer. The relation of τ and h is given by $\tau = \frac{\lambda h^2}{c}$, where λ is chosen from the range of the stability. Let $\hat{u}_m$ be the numerical solution obtained by the difference scheme of order $2m$. We measure the global error of the scheme at $t = n\tau$ by

$$E_m(t) = \sqrt{\frac{1}{N}\sum_{i=0}^{N}\left(\hat{u}_m(ih,t) - u(ih,t)\right)^2}$$

and show the pointwise error by the discrete function

$$Er_m(x,t) = \hat{u}_m(x,t) - u(x,t), \quad x = 0, h, 2h, \cdots, Nh.$$

As pointed out in Qian, et al. (2000), the maximal global error $E_m(t)$ is obtained at $t_0 = \frac{1}{4ck^2\pi^2}$, which is independent of schemes. Let $n_0 = \frac{t_0}{\tau}$, where $\tau = \frac{\lambda h^2}{c}$, which yields

$$n_0 = \text{round}\left(\frac{1}{4\lambda k^2\pi^2 h^2}\right).$$

Then, the maximal error is obtained after n_0 iterations of the schemes. In our numerical simulations, we set

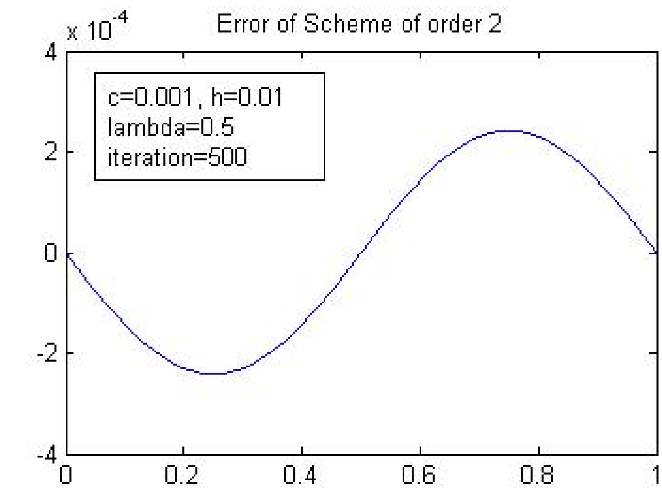
$$k = 1, c = 0.001, \lambda = 0.5, h = 0.01.$$

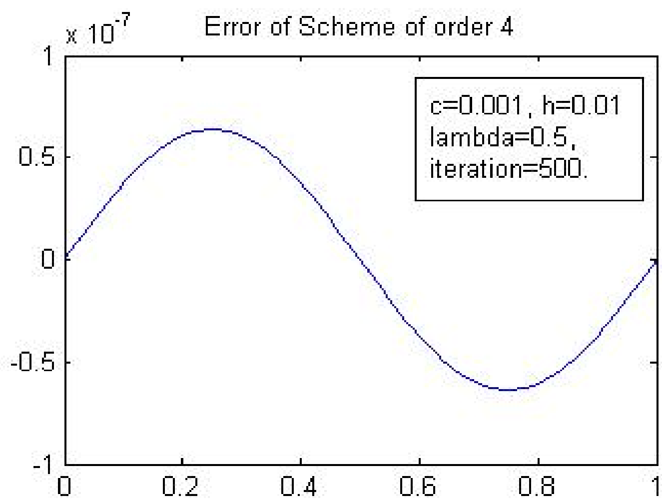
Then, the global maximal error is obtained after 500 iterations. The following table presents the maximal global errors for all schemes of order $2, 4, 6,$ and 8.

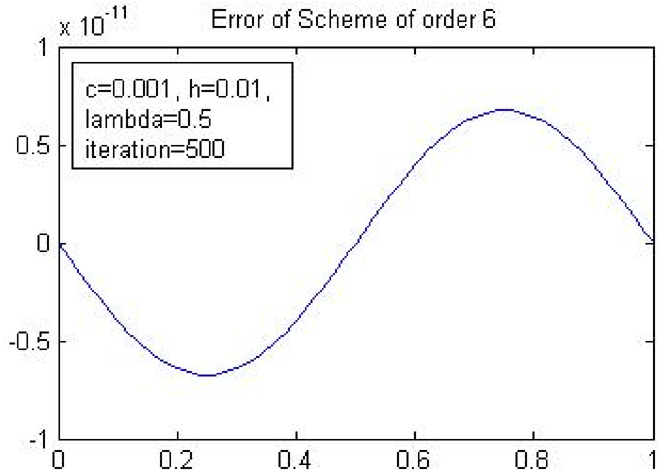
Order of scheme	2	4	6	8
Maximal global error	1.7042e-004	4.4859e-008	4.7456e-012	1.4156e-16

Remark: The maximal global error of the scheme of order 8 already comes up to the machine epsilon $2^{-64} = 2.2204e-16$.

The table shows that the numerical results match the theoretical results very well. The following figures show the pointwise errors of difference schemes of order $2, 4$, and 6 respectively.







Acknowledgement

The author would like to thank the editor and, especially, the reviewers for their valuable comments. The research is supported by NSF Grant of the United States, DMS-07-12925.

REFERENCES

Gerald, C. F. and Wheatley, P. Q. (1999). Applied Numerical Analysis, 6th ed., Addison Wesley.

Qian, Y., Chen, H., Zhang, R., and Chen, S. (2000). A new fourth order finite difference scheme for the heat equation. *Communications in Nonlinear Science and Numerical Simulation* **5**, 151–157.

Richtmyer, R. D. and Morton, K. W. (1967). Difference Methods for Initial-Value Problems, 2nd ed., Wiley, New York.