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Note

On the Optimal Time Step and Computational Efficiency of Difference Schemes for PDE

1. Derivation of an Optimal Time Step

We assume that we have an initial value problem for a partial differential equation $\partial u/\partial t = L(u)$ whose solution is $u(x, t)$. We denote the solution of a finite difference approximation to this equation by U_j^n which is an approximation to $u(x_j, t_n)$ where the $\{x_j\}$ are the mesh points and t_n represents the discrete time levels. We will assume that there is a power series expansion for the error in terms of the mesh spacing $h = \Delta x$ of the following form.

$$u(x_j, t_n) = U_j^n + h^q e(x_j, t_n, \lambda) + O(h^{q+1}). \tag{1}$$

The function $e(x, t, \lambda)$ is the solution of an associated differential equation [1]. Here $\lambda = k/h^{q/p}$ where $k = \Delta t$ and $h = \Delta x$ denote the time step and mesh increment. The integers q and p determine the order of accuracy in space and time. For a scheme with fourth-order accurate space differences and second-order accurate time differences, we would have $q = 4$ and $p = 2$. Note that we have chosen the asymptotic relation between k and h so that the spatial and temporal truncation error is balanced.

For example, consider the Crank–Nicolson scheme for the heat equation

$$\partial u/\partial t = (\partial^2 u/\partial x^2) + \rho, \tag{2}$$

where $u = u(x, t)$, $\rho = \rho(x, t)$, $0 \leqslant x \leqslant 1$, and $0 \leqslant t$. The initial-boundary conditions are

$$u(x, 0) = f(x), \qquad u(0, t) = g_0(t), \qquad u(1, t) = g_1(t).$$

The finite difference scheme is

$$U_j^{n+1} = U_j^n + (\mu/2)\, \Delta(U^{n+1} + U^n)_j + \Delta t\, \rho(x_j, t_n + \Delta t/2), \tag{3}$$

where $\mu = \Delta t/\Delta x^2$ and $\Delta U_j = U_{j+1} - 2U_j + U_{j-1}$, $x_j = j/J$. In the above difference scheme centered at $j = 1$, we replace $(U_0^{n+1} + U_0^n)/2$ by $g_0(t_n + \Delta t/2)$.

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A similar replacement is used at $j = J - 1$. An error expansion for the heat equation of the form given in Eq. (1) has been given by Keller [1]. If we simplify (2) by setting $\rho(x, t) \equiv g_0(t) \equiv g_1(t) \equiv 0$, then we can derive an expansion in the form of Eq. (1) for the Crank–Nicolson scheme (3). In this case we have

$$u(x_j, t_n) = U_j^n + h^2 e(x_j, t_n, \lambda) + O(h^4), \tag{4}$$

where the function $e(x, t, \lambda)$ is the solution of the following heat equation.

$$\begin{aligned} \partial e/\partial t &= (\partial^2 e/\partial x^2) + R(u); \\ R(u) &= -(1/12)\, u_{x^4} - (\lambda^2/8)\, u_{t^2x^2} + (\lambda^2/24)\, u_{t^3}; \\ e(x, 0) &\equiv e(0, t) \equiv e(1, t) \equiv 0; \\ \lambda &= k/h. \end{aligned}$$

The author is indebted to the reviewers for pointing out that this relation also holds for a problem with nonhomogeneous source term ρ and boundary conditions g. The method used to obtain this equation is explained by Keller [1]. In this case we have $\lambda = k/h^{q/p}$ with $p = q = 2$. If we had used a fourth-order approximation for $\partial^2/\partial x^2$ ($\Delta U = (-U_{j-2} + 16U_{j-1} - 30U_j + 16U_{j+1} - U_{j+2})/12h^2$), then we would have $\lambda = k/h^2$ (that is, $p = 2$ and $q = 4$).

Once we have Eq. (1) we can easily obtain an expression for the optimal time step. The method is an extension of that used by Douglas [2]. We let ϵ denote the maximum error in the interval $0 \leqslant t \leqslant T$. If we ignore the $O(h^{q+1})$ term in Eq. (1) we have

$$\epsilon = \max_{\substack{0 \leqslant x \leqslant 1 \\ 0 \leqslant t \leqslant T}} h^q \mid e(x, t, \lambda) \mid = h^q f(\lambda). \tag{5}$$

Next we assume that the cost of computing a solution is given by

$$C = TM_c/kh^d,$$

where M_c is a constant dependent on the difference scheme and the programming, T the length of the integration ($0 \leqslant t \leqslant T$) and d the dimension of the space over which the integration is taken. Our objective is to choose λ to minimize C for a given error ϵ. We have $\epsilon = h^q f(\lambda)$ and $k = \lambda h^{q/p}$, and therefore

$$C = (TM_c/\epsilon^\alpha)(f(\lambda))^\alpha/\lambda, \tag{6}$$

where $\alpha = d/q + 1/p$. The minimum is obtained where $dC/d\lambda = 0$, and thus we must solve the following equation to obtain the optimal value ($\bar{\lambda}$) of λ,

$$\bar{\lambda} = f(\bar{\lambda})/\alpha f'(\bar{\lambda}).$$

This yields the minimum of $(f(\lambda))^{\alpha}/\lambda$. Note that the optimum value of λ does not depend on the mesh spacing h or the error ϵ. We will assume that there are no stability restrictions on the time step, so that we are free to use the optimal time step.

2. Conclusion

From Eq. (6) we can obtain asymptotic estimates for the variation of C with ϵ. We have

$$C = K\epsilon^{-\alpha}, \tag{7}$$

where $K = TM_c(f(\bar{\lambda}))^{\alpha}/\bar{\lambda}$ depends on the difference scheme. To compare different schemes we can ignore K only if ϵ is very small. Since one seldom asks for small ϵ in practice, these comparisons are not too relevant. However, we will list the asymptotic behavior in Table I.

TABLE I

Asymptotic Variation of Cost C with Error ϵ[a]

d	p	q	C^{-1}
1	2	2	$\sim\epsilon$
1	2	4	$\sim\epsilon^{3/4}$
1	4	4	$\sim\epsilon^{1/2}$
3	2	2	$\sim\epsilon^{2}$
3	2	4	$\sim\epsilon^{5/4}$
3	4	4	$\sim\epsilon$

[a] $k = \lambda h^{q/p}$, d = dimension.

From these asymptotic estimates we are led to the following conclusions. In three dimensions a scheme which is fourth-order in space and second-order in time is quite effective; however, it is not effective in one dimension. A scheme which is fourth-order in both space and time is clearly much more effective in one dimension, as one would expect. Of course, we have here ignored the constant K in Eq. (7), which will be larger for the fourth-order scheme. These same results are obtained by Swartz and Wendroff [3], except they did not use quite as general an expression for the error (5) and considered only one-dimensional problems.

Note that the function $(f(\lambda))^\alpha/\lambda$ can be estimated without knowledge of the actual error $e(x, t, \lambda)$ (which would require knowledge of the exact solution). We can integrate to time $t = T$ using two different mesh spacings, but the same value of λ. Then we have

$$U_{j_1}^{n_1} - U_{j_2}^{n_2} = e(x_{j_1}, T, \lambda)(h_1{}^q - h_2{}^q).$$

Here we adjust the limits n_1 and n_2 so that $t_{n_1} = t_{n_2} = T$. To accomodate an arbitrary ratio of h_1/h_2, it may be necessary to adjust the value of Δt on the last time step so that $\lim t_{n_1} = T$ is reached. This should not affect the asymptotic estimate (4). Also we only compare at mesh indices j_1 and j_2 so that $j_1 h_1 = j_2 h_2$. Then we approximate $f(\lambda)$ by

$$\max_{j_1} | U_{j_1}^{n_1} - U_{j_2}^{n_2} |/| h_1{}^q - h_2{}^q | .$$

This provides an estimate of $f(\lambda)$ without knowledge of the exact solution.

3. An Example

We computed a test case using the Crank–Nicolson scheme (3) for the heat Eq. (2). We choose $\rho(x, t)$, $g_0(t)$, and $g_1(t)$ so that the solution $u(x, t)$ is given by

$$u(x, t) = \sin \pi(x - \pi t).$$

In Fig. 1 we show a graph of $f(\lambda)/\lambda$ and $f(\lambda)$ computed from

$$f(\lambda)/\lambda = \max_{1 \leqslant j \leqslant J-1} | e(x_j, 1, \lambda)/\lambda | .$$

Note that $\alpha = 1$ for this example.

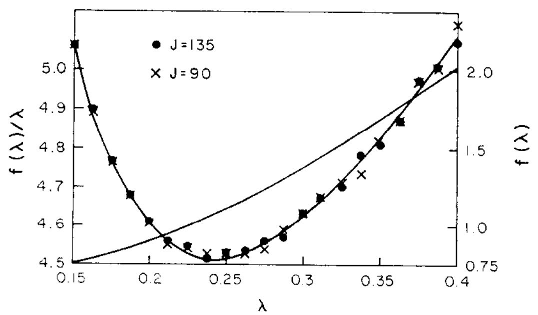

FIG. 1. $f(\lambda)/\lambda$ and $f(\lambda)$ vs λ. Computed from the exact error $e(x, t, \lambda)$.

In order to obtain a smooth curve we had to use a very large value of J. The points for $J = 90$ and $J = 135$ are plotted, and they show that $f(\lambda)/\lambda$ is not determined too well even at this resolution. The resolution required to evaluate $f(\lambda)$ may be highly problem-dependent. Note that the cost factor $(f(\lambda))^{\alpha}/\lambda$ is not highly sensitive to variation in λ, at least for this example. As λ varies from 0.15–0.4, the cost varies about 13 % from its minimum value. Once the values of $\bar{\lambda}$ and $f(\bar{\lambda})$ are known, then the values of h and k can be obtained from (5) and the definition of λ. The $f(\lambda)$ curve in Fig. 1 is obtained from the smoothed $f(\lambda)/\lambda$ curve.

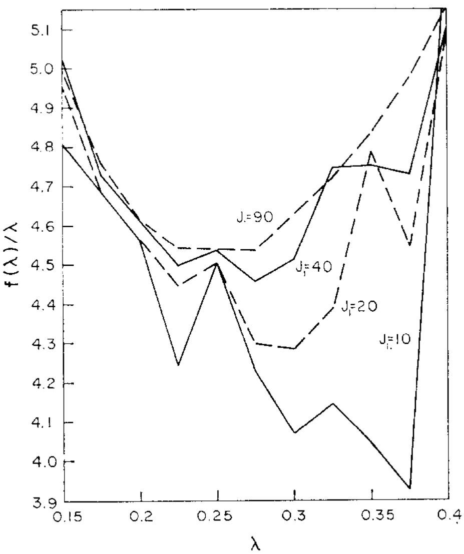

FIG. 2. $f(\lambda)/\lambda$ vs λ. Computed from $|U_{j_1}^{n_1} - U_{j_2}^{n_2}|/|h_1^q - h_2^q|$.

In Fig. 2 we show the results of an attempt to determine $f(\lambda)/\lambda$ by using the calculated solution only and not the error. Here we took $J_2 = 3J_1/2$ or $h_2 = 2h_1/3$. At a reasonable resolution, say $J_1 = 20$, the function $f(\lambda)/\lambda$ is not very well determined. This is probably because the asymptotic estimate is not very good. In Fig. 2 we connect the observed values and make no attempt to smooth the curves.

In Fig. 3 we plot the logarithm of the cost versus the logarithm of the error. To estimate the cost we used the expression $C = J\, T/\Delta t$. The slope of these lines ranges from 1.00–1.03. The error in determining the lines is perhaps 0.02 or 0.03. The points on the graph were determined using $J = 8$, 16, and 32. The variation in the error with J at fixed λ seems to be smoother than the variation in λ at fixed J.

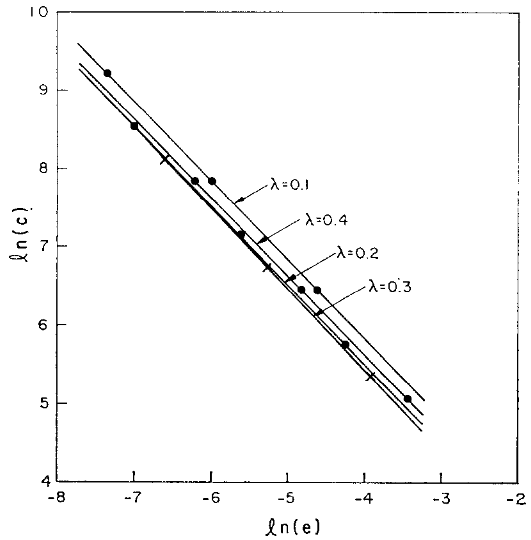

FIG. 3. Cost vs error. Logarithmic plot each obtained from the points at $J = 8, 16, 32$.

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