Homework Assignment
Numerical solution of partial differential equations, I (Course 221)
Handed out: Tuesday, Oct 14, 2002, Due: Tuesday, Oct 28, 2003

4 Hyperbolic problems

4.1 Benefits and costs of extending precision

Follow the Taylor series expansion procedure to derive a

The Lax-Wendroff method for the simple advection equation

$$q_t + u\, q_x = 0 \tag{1}$$

with constant u can be derived by :

- using the Taylor series method to order $O(k^2)$, i.e.

$$q(t+k) = q + kq_t + \frac{k^2}{2} q_{tt}\,; \tag{2}$$

- using the advection equation to replace time derivatives with space derivatives

$$q(t+k) = q - ukq_x + (uk)^2 q_{xx}/2\,; \tag{3}$$

approximating the space derivatives with second order accurate finite difference approximations

$$q_x \simeq \frac{Q^n_{j+1} - Q^n_{j-1}}{2h}, \quad q_{xx} \simeq \frac{Q^n_{j+1} - 2Q^n_j + Q^n_{j-1}}{h^2}\,. \tag{4}$$

A $O(k^2, h^2)$ method is the result of this procedure.

From our study of ODE's of the form $y'(t) = f(t,y)$ we know that Runge-Kutta methods can obtain the same order of accuracy but avoid higher derivatives by evaluating f at various points between t and $t+k$. For instance we could seek that the ODE update

$$y(t+k) = y(t) + a_1 f(t,y) + a_2 f(t+\tau, y+\eta)$$

match the second-order accuracte Taylor series expansion by appropriate choices of a_1, a_2, τ, η.

Now suppose we seek to extend this approach to obtain a higher order formula, say fourth order. Then we would have to start from the $O(k^4)$ accurate series expansion

$$q(t+k) = q + kq_t + \frac{k^2}{2} q_{tt} + \frac{k^3}{6} q_{ttt} + \frac{k^4}{6} q_{tttt}$$

1. Carry out the series expansion for the proposed second-order accurate Runge-Kutta method and find appropriate choices for a_1, a_2, τ, η.
2. Show that there exists a choice of a_1, a_2, τ, η such that when the method is applied to the advection equation and $x-$derivatives that appear are approximated by central finite differences we recover the Lax-Wendroff method.
3. The advantage of the Runge-Kutta approach would be that we can organize the computation as a multi-stage method in which only first-order approximations of the derivative are required. Write an algorithm in this spirit and compare results with the Lax-Wendroff method.
4. Another advantage of the Runge-Kutta approach is that we can obtain higher order formulas that only use approximations of the first derivative at intermediate stages. Write an algorithm of this kind which employs a fourth order accurate Runge-Kutta method.
5. Bonus: Analyze the stability of the algorithm from question 4.

4.2 Solution

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The series expansion of the Runge-Kutta formula is

$$y(t+k) = y + (a_1 + a_2) f + a_2 \tau f_t + a_2 \eta f_y \tag{5}$$

and matching with the Taylor series expansion leads to

$$\begin{aligned} a_1 + a_2 &= k & (6)\\ a_2 \tau &= k^2/2 & (7)\\ a_2 \eta &= k^2 f/2 & (8) \end{aligned}$$

thus giving a one-parameter family of Runge-Kutta methods of $O(k^2)$. Let $\tau = \alpha k$ and we obtain

$$\begin{aligned} a_1 &= \frac{2\alpha - 1}{2\alpha} k,\ a_2 = \frac{1}{2\alpha} k & (9)\\ \tau &= \alpha k,\ \eta = \alpha k f & (10) \end{aligned}$$

leading to the Runge-Kutta formula

$$\begin{aligned} Y^{n+1} &= Y^n + c_1 K_1 + c_2 K_2 & (11)\\ c_1 &= \frac{2\alpha - 1}{2\alpha},\ c_2 = \frac{1}{2\alpha} & (12)\\ K_1 &= k\ f(t^n, Y^n) & (13)\\ K_2 &= k\ f(t^n + \alpha k, Y^n + \alpha K_1) & (14) \end{aligned}$$

Taking, for example, $\alpha = 1$ leads to $a_1 = a_2 = k/2$ leads to $\tau = k$ and $\eta = kf$ so the Runge-Kutta formula from this choice is

$$\begin{aligned} Y^{n+1} &= Y^n + \frac{1}{2}(K_1 + K_2) && (15) \\ K_1 &= k\ f(t^n, Y^n) && (16) \\ K_2 &= k\ f(t^n + k, Y^n + K_1) && (17) \end{aligned}$$

4.2.2 2 and 3

Now consider applying one of the formulas from the above family to the advection equation $q_t = -uq_x$. We need to approximate the x-derivative to obtain a system of ODE's and are given the hint to use centered derivatives so we obtain the generic ODE

$$\frac{dQ_j(t)}{dt} = -u\frac{Q_{j+\beta}(t) - Q_{j-\beta}(t)}{2\beta h} \tag{18}$$

We have left the possibility of using different step sizes in the approximation of the x-derivative since this is also the case in the Lax-Wendroff method derivation from the Taylor series expansion where a step size of h is used in the first order derivative but a step size of $h/2$ is used for the second order x-derivative. Let us use this equation in the 1-parameter family of Runge-Kutta formulas indexed by α that we obtained above

$$\begin{aligned} Q_j^{n+1} &= Q_j^n + c_1 K_{1,j} + c_2 K_{2,j} && (19) \\ K_{1,j} &= k\left[-u\frac{Q^n_{j+\beta_1} - Q^n_{j-\beta_1}}{2\beta_1 h}\right] && (20) \\ K_{2,j} &= k\left[-u\frac{Q^n_{j+\beta_2} + K_{1,j+\beta_2} - Q^n_{j-\beta_2} - K_{1,j-\beta_2}}{2\beta_2 h}\right] && (21) \\ &= k\left[-u\frac{Q^n_{j+\beta_2} - \frac{uk}{2\beta_1 h}\left(Q^n_{j+\beta_1+\beta_2} - Q^n_{j-\beta_1+\beta_2}\right) - Q^n_{j-\beta_2} + \frac{uk}{2\beta_1 h}\left(Q^n_{j+\beta_1-\beta_2} - Q^n_{j-\beta_1-\beta_2}\right)}{2\beta_2 h}\right] && (22) \end{aligned}$$

Putting everything in one formula leads to

$$\begin{aligned} Q_j^{n+1} &= Q_j^n + \frac{2\alpha - 1}{2\alpha} k\left[-u\frac{Q^n_{j+\beta_1} - Q^n_{j-\beta_1}}{2\beta_1 h}\right] && (23) \\ &\quad + \frac{k}{2\alpha}\left[-u\frac{Q^n_{j+\beta_2} - \frac{uk}{2\beta_1 h}\left(Q^n_{j+\beta_1+\beta_2} - Q^n_{j-\beta_1+\beta_2}\right) - Q^n_{j-\beta_2} + \frac{uk}{2\beta_1 h}\left(Q^n_{j+\beta_1-\beta_2} - Q^n_{j-\beta_1-\beta_2}\right)}{2\beta_2 h}\right] && (24) \end{aligned}$$

and we now have to choose $\alpha, \beta_1, \beta_1', \beta_2$ such the above formula matches the Lax-Wendroff update

$$Q_j^{n+1} = Q_j^n - \frac{uk}{2h}(Q^n_{j+1} - Q^n_{j-1}) + \frac{1}{2}\left(\frac{uk}{h}\right)^2 (Q^n_{j+1} - 2Q^n_j + Q^n_{j-1}) \tag{25}$$

Let $\nu = uk/h$. We obtain

$$Q_j^n - \frac{\nu}{2}(Q_{j+1}^n - Q_{j-1}^n) + \frac{\nu^2}{2}\left(Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n\right) = \tag{26}$$

$$Q_j^n - \frac{\nu}{2}\left[\frac{2\alpha-1}{2\alpha}\frac{Q_{j+\beta_1}^n - Q_{j-\beta_1}^n}{2\beta_1} + \frac{1}{2\alpha}\frac{Q_{j+\beta_2}^n - Q_{j-\beta_2}^n}{2\beta_2}\right] \tag{27}$$

$$+ \frac{\nu^2}{8\alpha\beta_1\beta_2}\left[Q_{j+\beta_1+\beta_2} - Q_{j-\beta_1+\beta_2}^n - Q_{j+\beta_1-\beta_2}^n + Q_{j-\beta_1-\beta_2}^n\right] \tag{28}$$

and hit an impasse. It is clear from the second derivative approximation that we must have $\beta_1 = \beta_2$ so that the two terms with minus signs combine so we get $-2Q_j^n$. But $\beta_1 = \beta_2 = 1/2$ leads to a $Q_{j+1/2}^n, Q_{j-1/2}^n$ terms in the first derivative approximation while $\beta_1 = \beta_2 = 1$ leads to Q_{j+2}^n, Q_{j-2}^n terms in the second derivative. This is just an indication of the fact that the Lax-Wendroff method itself uses a somewhat inconsistent approximation of the derivatives (the main point of this exercise by the way) with a view to maintaining computational efficiency (i.e. not introduce more gridpoints than required). The inconsistency of the approach in Lax-Wendroff is not that bad since it does not affect the order of the method just the numerical constant appearing in the leading order truncation error. A consistent approach to discretizing spatial derivatives appearing in the Taylor series expansion would be to use the formula

$$Q_j^{n+1} = Q_j^n - \nu(Q_{j+1/2}^n - Q_{j-1/2}^n) + \frac{\nu^2}{2}\left(Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n\right) \tag{29}$$

but this is not done in the Lax-Wendroff algorithm because of the complication of storing values at half-index values. For the problem at hand the best approach is to use $\beta_1 = \beta_2 = 1/2$ and $\alpha = 1$ so that we maintain the over-all stencil width of the Lax-Wendroff method and use the approximation $Q_{j+1/2}^n = (Q_j^n + Q_{j+1}^n)/2$. This is essentially the technique used in the Lax-Wendroff method.

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If we want now to extend the above ideas to a fourth-order Runge-Kutta, say

$$K_1 = k\ f(t^n, Q^n) \tag{30}$$

$$K_2 = k\ f(t^n + k/2, Q^n + K_1/2) \tag{31}$$

$$K_3 = k\ f(t^n + k/2, Q^n + K_2/2) \tag{32}$$

$$K_4 = k\ f(t^n + k, Q^n + K_3) \tag{33}$$

$$Q^{n+1} = Q^n + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \tag{34}$$

we would just have to replace spatial derivatives at each stage using fourth-order accurate approximations of the x-derivative

$$(q_x)_j \simeq \frac{Q_{j-3/2} - 27Q_{j-1/2} + 27Q_{j+1/2} - Q_{j+3/2}}{24h} \tag{35}$$

This is what makes the Runge-Kutta type organization of the computation attractive. We don't have to explicitly compose these operations to obtain an overall update formula including all higher order derivatives that appear.