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NEW NUMERICAL SCHEMES BASED ON A CRITERION FOR CONSTRUCTING ESSENTIALLY STABLE AND ACCURATE NUMERICAL SCHEMES FOR CONVECTION-DOMINATED EQUATIONS

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SUMMARY

In order to obtain stable and accurate numerical solutions for the convection-dominated steady transport equations, we propose a criterion for constructing numerical schemes for the convection term that the roots of the characteristic equation of the resulting difference equation have poles.

By imposing this criterion on the difference coefficients of the convection term, we construct two numerical schemes for the convection-dominated equations. One is based on polynomial differencing and the other on locally exact differencing.

The former scheme coincides with the QUICK scheme when the mesh Reynolds number (*Rm*) is $\frac{8}{3}$, which is the critical value for its stability, while it approaches the second-order upwind scheme as *Rm* goes to infinity. Hence the former scheme interpolates a stable scheme between the QUICK scheme at $Rm = \frac{8}{3}$ and the second-order upwind scheme at $Rm = \infty$. Numerical solutions with the present new schemes for the one-dimensional, linear, steady convection–diffusion equations showed good results.

KEYWORDS: finite difference method (FDM); computational fluid dynamics; transport equation; numerical stability; numerical oscillations; characteristic equation; LECUSSO scheme; QUICK scheme; LENS scheme

1. INTRODUCTION

When we construct numerical schemes, both good stability and accuracy of the numerical solutions are required. In this connection we have recently proposed a new finite variable difference method (FVDM)[1,2] in which a variable spatial difference instead of the conventional Δx is employed for the discretization of the convection term. The variable spatial difference is optimized from the viewpoint of numerical stability and accuracy. Namely, the optimum spatial difference is determined in terms of the mesh Reynolds number so that the variance of the numerical solutions is minimized under the condition that the roots of the resulting characteristic equation are to be non-negative to ensure numerical stability.

In our previous studies[1,2] the FVDM was applied to the LENS scheme[3] based on locally exact numerical differencing and to the QUICK scheme[4] based on polynomial differencing. The optimum spatial differences of these two schemes for the linear convection–diffusion equation were evaluated in terms of mesh Reynolds numbers up to 1000. By using this optimum spatial difference, the numerical accuracy of the convection–diffusion equations was increased greatly without spatial oscillations.

From our previous two papers[1,2] we can conclude that good stability and high accuracy of the numerical solutions at large mesh Reynolds numbers, i.e. values greater than about 10, are achieved simultaneously when the roots of the characteristic equation of the difference equation have poles.

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Based on this fact, we propose a criterion that the roots of the characteristic equation of the resulting difference equation have poles for constructing essentially stable and accurate numerical schemes for the convection-dominated equations.

By imposing this new criterion on the difference coefficients of the convection term, we construct new robust numerical schemes for the convection-dominated steady transport equations. These schemes are examined through numerical experiments.

2. MATHEMATICAL FORMULATION

2.1. Transport equation

We consider the one-dimensional, steady, linear convection–diffusion equation

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} - R\frac{\mathrm{d}\phi}{\mathrm{d}x} = 0, \tag{1}$$

where ϕ is the transported quantity and x denotes the Cartesian space co-ordinate. R is the ratio of the transport velocity v to a diffusion parameter ν such as the kinematic viscosity. Here we assume that v is positive and R is constant.

2.2. Difference formula

We approximate the convection term in (1) as

$$\frac{\mathrm{d}\phi}{\mathrm{d}x} = \frac{\phi_{i+1/2} - \phi_{i-1/2}}{\Delta x} \tag{2}$$

with Δx the uniform mesh size. Here $\phi_{i+1/2}$ and $\phi_{i-1/2}$ are the transported quantities at $x = x_i + \Delta x/2$ and $x = x_i - \Delta x/2$ respectively. These quantities are approximated for $v > 0$ by

$$\phi_{i+1/2} = a\phi_{i+1} + b\phi_i + c\phi_{i-1}, \tag{3a}$$

$$\phi_{i-1/2} = a'\phi_i + b'\phi_{i-1} + c'\phi_{i-2}. \tag{3b}$$

Since we are considering a uniform mesh size grid and a constant R, we set $a' = a$, $b' = b$ and $c' = c$.

2.3. Characteristic equation[5]

Discretizing the convection and diffusion terms in (1) with equation (2) and the second-order central scheme respectively, we have

$$(\phi_{i+1} - 2\phi_i + \phi_{i-1}) - Rm[(a\phi_{i+1} + b\phi_i + c\phi_{i-1}) - (a\phi_i + b\phi_{i-1} + c\phi_{i-2})] = 0, \tag{4}$$

with $Rm = R\Delta x$ (mesh Reynolds number). Rearranging the above equation yields the difference equation

$$A\phi_{i+1} + B\phi_i + C\phi_{i-1} + D\phi_{i-2} = 0, \tag{5}$$

where

$$A \equiv 1 - (Rm)a, \tag{6a}$$

$$B \equiv -[2 + Rm(b - a)], \tag{6b}$$

$$C \equiv 1 - Rm(c - b), \tag{6c}$$

$$D \equiv (Rm)c. \tag{6d}$$

Equation (5) has the exact solution

$$\phi_i = \alpha(\lambda_1)^i + \beta(\lambda_2)^i + \gamma(\lambda_3)^i, \tag{7}$$

where α, β and γ are constants determined by the boundary conditions. In (7), λ_1, λ_2 and λ_3 are the roots of the characteristic equation

$$A\lambda^3 + B\lambda^2 + C\lambda + D = 0. \tag{8}$$

From (6) we get the relation

$$A + B + C + D = 0. \tag{9}$$

Hence equation (8) has the root $\lambda_1 = 1$ and can be factorized as

$$(\lambda - 1)\{[1 - (Rm)a]\lambda^2 - [1 + Rm(1 - c - a)]\lambda - (Rm)c\} = 0. \tag{10}$$

From this equation we obtain the other two roots

$$\lambda_2 = \frac{1 + Rm(1 - c - a) + \sqrt{\Sigma}}{2[1 - (Rm)a]}, \tag{11a}$$

$$\lambda_3 = \frac{1 + Rm(1 - c - a) - \sqrt{\Sigma}}{2[1 - (Rm)a]}, \tag{11b}$$

where

$$\Sigma \equiv [1 + Rm(1 - c - a)]^2 + 4[1 - (Rm)a](Rm)c. \tag{12}$$

2.4. Optimizing condition

In Section 1 we set up a criterion that the roots of the characteristic equation of the difference equation have poles for constructing numerical schemes for the convection term of the convection-dominated steady transport equations. According to this criterion, the condition optimizing numerical schemes from the viewpoint of numerical stability and accuracy is given by

$$1 - (Rm)a = 0. \tag{13}$$

In our previous papers[1,2] the coefficient a depended on Rm and p, which is related to the variable spatial difference used in discretizing the convection term. In those papers we solved

$$1 - (Rm/2p)a(Rm, p) = 0, \tag{14}$$

given a value of Rm, and determined the optimum p in terms of Rm. However, in (2) and (3) we consider $p = ½$, which corresponds to the usual FDM. Accordingly, p is constant in (13) and equation (13) is easily solved as

$$a = 1/Rm. \tag{15}$$

Consequently, equation (15) is the condition optimizing numerical schemes from the viewpoint of stability and accuracy when $p = \frac{1}{2}$.

2.5. Determination of difference coefficients

Now we determine the difference coefficients (a, b, c) and construct optimized numerical schemes. In order to determine these three coefficients, we need two more conditions in addition to (15). Then we have two conceptions of numerical differencing as reviewed in Section 1. One is polynomial differencing and the other locally exact differencing. We construct two schemes according to these two different conceptions.

2.5.1. New Scheme 1 based on polynomial differencing. Expanding equation (3a) into a Taylor series with respect to the mesh point i yields

$$\phi_i + \frac{1}{2}\left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_i \Delta x + O(\Delta x^2) = a\left(\phi_i + \left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_i \Delta x + O(\Delta x^2)\right) + b\phi_i + c\left(\phi_i - \left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_i \Delta x + O(\Delta x^2)\right), \tag{16}$$

where $O(\Delta x^2)$ denotes the higher-order terms. By equating the zeroth- and first-order terms with respect to Δx on the left and right sides of (16), we obtain

$$a + b + c = 1, \tag{17}$$

$$a - c = \tfrac{1}{2}. \tag{18}$$

Equation (17) corresponds to the consistency condition that the right-side difference equation of (2) approaches the left-side differential equation as Δx goes to zero.

From (15), (17) and (18) we obtain

$$b = \tfrac{3}{2} - 2/Rm, \tag{19}$$

$$c = 1/Rm - \tfrac{1}{2}. \tag{20}$$

This new scheme ($a = 1/Rm$, $b = \frac{3}{2} - 2/Rm$, $c = 1/Rm - ½$) is simple in respect of its dependence on Rm and possesses interesting aspects. Namely, this scheme coincides with the QUICK scheme at $Rm = \frac{8}{3}$, which is the critical value to ensure a stable solution with the QUICK scheme. Moreover, as Rm goes to infinity, this scheme approaches the second-order upwind scheme, which is the same situation as in the case of the LENS scheme. Hence this new scheme interpolates a stable scheme between the QUICK scheme at $Rm = \frac{8}{3}$ and the second-order upwind scheme at $Rm = \infty$. Although this scheme was originally derived on the basis of Rm greater than about 10, it showed stable solutions of (1) at Rm greater than 1·0, but its accuracy was less than that of the QUICK scheme at Rm less than $\frac{8}{3}$, according to numerical experiments. Taking into consideration these situations, we construct a robust scheme applicable for all mesh Reynolds numbers by combining those two schemes as follows:

$$(\text{for } Rm \leqslant \tfrac{8}{3}) \quad \text{QUICK scheme}, \tag{21a}$$

$$(\text{for } Rm > \tfrac{8}{3}) \quad \text{New Scheme 1 given by (15), (19) and (20).} \tag{21b}$$

2.5.2. New Scheme 2 based on locally exact differencing. Equation (17) is a necessary condition for the resulting difference equation to converge to the convection term in (1) as Δx goes to zero. Next we get the third condition to determine the coefficients (a, b, c) based on locally exact differencing.

According to the conception of locally exact differencing,[3] we impose that equation (3) satisfy $\phi = \exp(\omega x)$, where ω is a non-zero root of the characteristic equation of the differential equation (*not* difference equation) we want to solve; in the case of (1), $\omega = R$. This imposition yields

$$\exp(\omega x_{i+1/2}) = a\exp(\omega x_{i+1}) + b\exp(\omega x_i) + c\exp(\omega x_{i-1}). \tag{22}$$

In the case of a uniform mesh size grid, equation (22) is equivalent to

$$\exp(\omega_{\mathrm{m}}/2) = a\exp(\omega_{\mathrm{m}}) + b + c\exp(-\omega_m), \tag{23}$$

where $\omega_{\mathrm{m}} = \omega\Delta x$.

From (15), (17) and (23) we obtain

$$b = \frac{(1 - 1/Rm)\exp(-2\omega_{\mathrm{m}}) - \exp(-\omega_{\mathrm{m}}/2) + 1/Rm}{\exp(-2\omega_{\mathrm{m}}) - \exp(-\omega_{\mathrm{m}})}, \tag{24}$$

$$c = \frac{\exp(-\omega_{\mathrm{m}}/2) - (1 - 1/Rm)\exp(-\omega_{\mathrm{m}}) - 1/Rm}{\exp(-2\omega_{\mathrm{m}}) - \exp(-\omega_{\mathrm{m}})}. \tag{25}$$

3. TEST CALCULATIONS AND DISCUSSION

We perform numerical experiments in a one-dimensional geometry with the uniform mesh size $\Delta x = \frac{1}{10}$, in which the total mesh number and the total computational length are 11 and 1 respectively. The boundary values at $x = 0$ and $x = 1$ are set to $\phi(0) = 1$ and $\phi(1) = 0$ respectively. This test calculation with a Dirichlet outflow boundary condition is a difficult problem since it generates a thin boundary layer near the exit ($x = 1$) as the mesh Reynolds number increases.

First we compare the exact solution with the numerical solutions for the convection–diffusion equation without source terms, equation (1). Table I presents a comparison of these solutions at $Rm = 100$. In this table the variance σ is defined as

$$\sigma \equiv \frac{1}{n}\sum_{i=1}^{n} [\phi_i - \phi_{\mathrm{e}}(x_i)]^2, \tag{26}$$

Table I. Comparison of numerical solutions with exact solution

I	Analytical	Original QUICK	New Scheme 1	New Scheme 2
1	1·000000	1·000000	1·000000	1·000000
2	1·000000	1·000000	1·000000	1·000000
3	1·000000	0·997522	1·000000	1·000000
4	1·000000	1·002680	1·000000	1·000000
5	1·000000	0·991089	1·000000	1·000000
6	1·000000	1·016990	1·000000	1·000000
7	1·000000	0·959083	1·000000	1·000000
8	1·000000	1·088540	1·000000	1·000000
9	1·000000	0·799156	1·000000	1·000000
10	1·000000	1·446040	1·000000	1·000000
11	0·000000	0·000000	0·000000	0·000000
Variance σ		$2{\cdot}26531 \times 10^{-2}$	$4{\cdot}48216 \times 10^{-33}$	$6{\cdot}14057 \times 10^{-31}$

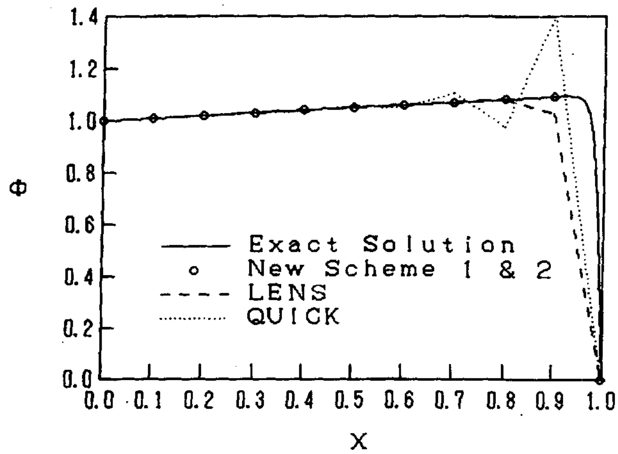

Figure 1. Comparison of numerical solutions with exact solution (case 1)

where ϕ_i and $\phi_e(x_i)$ represent the numerical solution and exact solution at mesh number i respectively. The present two schemes predict the exact solution quite well without oscillations; their variances are considered to be almost within round-off error.

Next we consider the transport equation with source terms such as

$$\frac{d^2\phi}{dx^2} - R\frac{d\phi}{dx} - S\phi + Q = 0, \tag{27}$$

where S and Q are the intensities of internal and external sources respectively and $Q = (x - 0{\cdot}5)^2$. We solve equation (27) under the same computational conditions that were used in the first test calculations. There exist two non-zero roots of its characteristic equation as follows:

$$\omega_1 = [R + \sqrt{(R^2 + 4S)}]/2, \tag{28a}$$

$$\omega_2 = [R - \sqrt{(R^2 + 4S)}]/2. \tag{28b}$$

Which of the roots ω_1 and ω_2 is better for ω in (22) depends mainly on S and weakly on Rm. In this experiment ω_1 is better at small absolute values of S while ω_2 is better at large absolute values of S. Here we consider two cases: $Rm = 10$ and $S = -10$ for case 1; $Rm = 100$ and $S = 1000$ for case 2. In case 1 we used $\omega = \omega_1$ while in case 2 we used $\omega = \omega_2$.

Comparisons of the numerical solutions with the analytical solution for cases 1 and 2 are shown in Figures 1 and 2 respectively together with the solutions by the QUICK and LENS schemes. The solutions with the two new schemes are almost the same. As already mentioned, the exact solution shows a thin boundary layer near the exit. We use a coarse mesh grid to make clear the difference between the exact and numerical solutions in this test calculation. Since no computational mesh points exist within the thin boundary layer, we cannot discuss the numerical accuracy in this layer. However, it is remarkable that the new schemes predict well the exact solution at the computational mesh points.

In the above test calculations a steep gradient of ϕ exists near the exit boundary, where ϕ just downstream from the steep gradient is not calculated but given as the boundary condition. There is a case where numerical instability may occur near downstream from the steep gradient of ϕ. Hence we solve equation (27) with strong internal absorptions in the almost half computational region, in which a steep gradient exists in the inner region. A comparison of the solutions with $S(x) = 0$ for $0 \leqslant x \leqslant 0{\cdot}55$ and $S(x) = 5000$ for $0{\cdot}55 < x \leqslant 1$ at $Rm = 50$ is shown in Figure 3. A comparison of the solutions with

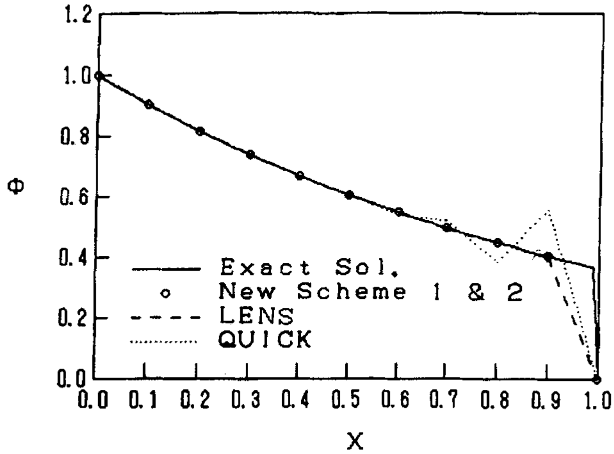

Figure 2. Comparison of numerical solutions with exact solution (case 2)

$S(x)=0$ for $0 \leqslant x \leqslant 0{\cdot}55$ and $S(x)=10^6$ for $0{\cdot}55 < x \leqslant 1$ at $Rm=50$ is shown in Figure 4. In these figures NS1 and NS2 denote New Scheme 1 and New Scheme 2 respectively. The solutions with these two schemes were almost the same. The numerical solutions in Figure 4 are in good agreement with the exact solution at the mesh points.

4. CONCLUSIONS

From our previous studies on a new finite variable difference method (FVDM) we concluded that good stability and high accuracy of the numerical solutions for the steady transport equations at large mesh Reynolds numbers, i.e. values greater than about 10, are achieved simultaneously when a root of the characteristic equation of the difference equation approaches its asymptote. Based on this fact, we proposed a criterion for constructing numerical schemes for the convection term of the convection-

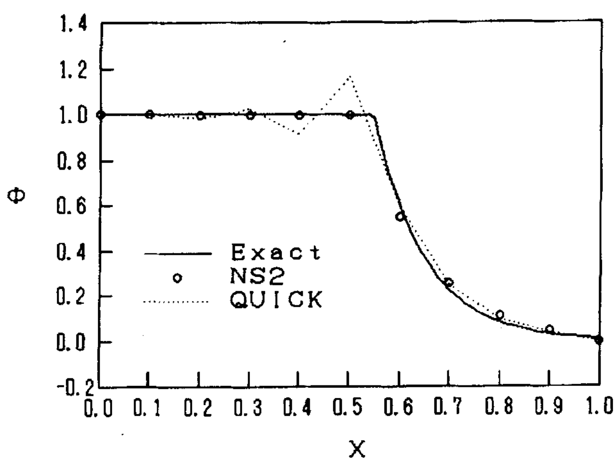

Figure 3. Comparison of numerical solutions with exact solution for $Rm=50$ and $S(x)=5000$ $(0{\cdot}55 < x \leqslant 1)$

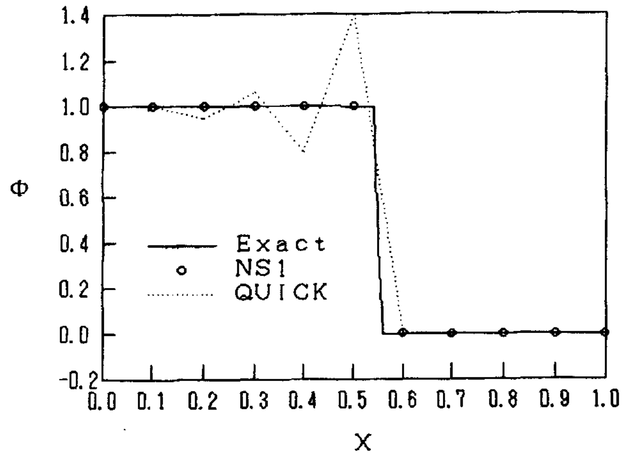

Figure 4. Comparison of numerical solutions with exact solution for $Rm = 50$ and $S(x) = 10^6$ $(0{\cdot}55 < x \leqslant 1)$

dominated transport equations that the roots of the characteristic equation of the resulting difference equation have poles.

By imposing this criterion on the difference coefficients of the convection term, we constructed two numerical schemes based on polynomial differencing and local exact differencing. The former is simple in respect to its dependence on Rm and coincides with the QUICK scheme at $Rm = \frac{8}{3}$, which is the critical value to ensure stable solutions with the QUICK scheme. Moreover, as Rm goes to infinity, this scheme approaches the second-order upwind scheme. Hence this new scheme interpolates a stable scheme between the QUICK scheme at $Rm = \frac{8}{3}$ and the second-order upwind scheme at $Rm = \infty$. Finally, we proposed a scheme applicable for all mesh Reynolds numbers by combining the present new scheme with the QUICK scheme at $Rm = \frac{8}{3}$.

Numerical solutions with these new schemes for the steady, linear convection–diffusion equations showed good results.

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