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A THIRD-ORDER COMPUTATIONAL METHOD FOR NUMERICAL FLUX TO GUARANTEE POSSITIVE DIFFERENCE COEFFICIENTS FOR ADVECTION-DIFFUSION EQUATIONS

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ABSTRACT

In CFD (Computational Fluid Dynamics), it is much concern to construct stable numerical schemes with higher-order accuracy because of a trend of trade-off relationships between numerical accuracy and stability.

Regarding the numerical stability, we have the positive coefficient condition, which guarantees the conditions related to the stability such as monotone property of the numerical scheme, monotonicity prerserving condition, maximum principle, TVD (Total Variation Diminishing) condition and boundedness condition.

The transport vector J associated with a quantity f in a flow field u with the diffusion phenomena is expressed as $J = \vec{u}f + (-\nu\nabla f)$, where the first term and the second term denote the advection and the diffusion, respectively. The conservation low for f is expressed as $\partial f / \partial t + div(J) = 0$, which corresponds to the advection-diffusion equation. The 1-D conservation equation is given by using the numerical fluxes $\phi^x_{i\pm1/2}$ as

$$\phi^x_{i\pm1/2} \equiv (J \cdot e^x) = u_{i\pm1/2} f_{i\pm1/2} + \left(-\nu \left.\frac{\partial f}{\partial x}\right|_{i\pm1/2} \right) \quad (1) \qquad f_i^{n+1} = f_i^n - \frac{\Delta t}{\Delta x}\left[\phi^x_{i+1/2} - \phi^x_{i-1/2}\right] \quad (2)$$

In the staggered grid with the velocity defined on the cell surface, the quantity f and its derivative are to be interpolated using f of the surrounding cells. Here we make derivation in case using 4 stencils to evaluate the numerical flux in one dimension.We expand $f_{i+k}\ (k = -1,0,1,2)$ with respect to the cell surface point (i+1/2) into the Taylor series. Taking a linear combination of the those Taylor expansion series with the multiplication of four parameters $(\alpha_+, \beta_+, \gamma_+, \delta_+)$ yields

$$\alpha_+ f^n_{i-1} + \beta_+ f^n_i + \lambda_+ f^n_{i+1} + \delta_+ f^n_{i+2} = (\alpha_+ + \beta_+ + \lambda_+ + \delta_+) f^n_{i+1/2} + (-3\alpha_+ - \beta_+ + \gamma_+ + 3\delta_+)\frac{\Delta x}{2}\left.\frac{\partial f}{\partial x}\right|_{i+1/2} +$$
$$\frac{1}{2!}\left(\left(\frac{3}{2}\right)^2\alpha_+ + \left(\frac{1}{2}\right)^2\beta_+ + \left(\frac{1}{2}\right)^2\gamma_+ + \left(\frac{3}{2}\right)^2\delta_+\right)\Delta x^2 \left.\frac{\partial^2 f}{\partial x^2}\right|_{i+1/2} + \frac{1}{3!}\left(-\left(\frac{3}{2}\right)^3\alpha_+ - \left(\frac{1}{2}\right)^3\beta_+ + \left(\frac{1}{2}\right)^3\gamma_+ + \left(\frac{3}{2}\right)^3\delta_+\right)\Delta x^3 \left.\frac{\partial^3 f}{\partial x^3}\right|_{i+1/2} + O(\Delta x^4) \quad (3)$$

Requiring that the right hand side of Eq.(3) may be consistent with the numerical flux $\phi_{i+1/2}$ within the third-order accuracy, we obtain

$$\alpha_+ + \beta_+ + \gamma_+ + \delta_+ = u_{i+1/2}\ , \qquad (-3\alpha_+ - \beta_+ + \gamma_+ + 3\delta_+)\frac{\Delta x}{2} = -\nu, \qquad \left(\frac{3}{2}\right)^2\alpha_+ + \left(\frac{1}{2}\right)^2\beta_+ + \left(\frac{1}{2}\right)^2\gamma_+ + \left(\frac{3}{2}\right)^2\delta_+ = 0 \qquad (4)$$

From those three equations, we obtain β_+, γ_+ with a free parameter α_+, which is to be determined from the stability condition and the requirement of minimum truncation errors. Thus we get

$$\phi^x_{i+1/2} = u_{i+1/2} f_{i+1/2} + \left(-\nu \left.\frac{\partial f}{\partial x}\right|_{i+1/2} \right) = \alpha_+ f^n_{i-1} + \beta_+ f^n_i + \gamma_+ f^n_{i+1} + \delta_+ f^n_{i+2} + O(\Delta x^3) \qquad (5)$$

Substituting Eq.(5) into Eq.(2) yields the finite difference equation:

$$f_i^{n+1} = af^n_{i-2} + bf^n_{i-1} + cf^n_i + df^n_{i+1} + ef^n_{i+2}\ , \qquad (6)$$

$$a = \alpha^-, \quad b = -\alpha^+ - 3\alpha^- + \frac{3}{8}C_- + D, \quad c = 1 + 3\alpha^+ + 3\alpha^- - \frac{3}{8}C_+ + \frac{3}{4}C_- - 2D,$$

$$d = -3\alpha^+ - \alpha^- - \frac{3}{4}C_+ - \frac{1}{8}C_- + D, \qquad e = \alpha^+ + \frac{1}{8}C_+.$$

$$\alpha^+ \equiv \alpha_+(\Delta t/\Delta x), \quad \alpha^- \equiv \alpha_-(\Delta t/\Delta x), \qquad C_+ \equiv u_{i+1/2}\Delta t/\Delta x, \ C_- \equiv u_{i-1/2}\Delta t/\Delta x.$$

From the positive coefficients condition ($a>0$, $b>0$, $c>0$, $d>0$, $e>0$), we obtain

$$0 \le \alpha^- \le \frac{5}{32}C_- + \frac{3}{32}C_+ + \frac{1}{4}D\ , \qquad -\frac{1}{8}C_+ \le \alpha^+ \le -\frac{3}{32}C_- - \frac{9}{32}C_+ + \frac{1}{4}D. \qquad (7)$$

For the above inequalities to hold, the righthand side equations should be greater than the lefthand side equations. From this requirment, we obtain the stability conditions:

$$-\frac{3}{8}C_+ - \frac{5}{8}C_- \le D, \qquad \frac{5}{8}C_+ + \frac{3}{8}C_- \le D, \qquad 0 < D \le \frac{1}{2} - \frac{3}{8}C_+ + \frac{3}{8}C_-. \qquad (8)$$

From Inequalities(8), Δx and Δt are determined given $|u|_{max}$ and ν. Then the optimum values of (α^+, α^-) at local point $x_{i\pm 1/2}$ are to be determined so that the truncation errors may be minimum in the stability domain given by Eq.(7). Regarding time discretization, the second-order Runge-Kutta method is employed, which maintains the positivity of resultig difference coeeficients so long as the difference coefficients in each Euler step calculation are positive . We call this FLUX scheme.

Numerical experiments for the nonlinear Burgers equation: $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(\frac{1}{2}u^2) = \nu\frac{\partial^2 u}{\partial x^2}$ were performed with C_{max}=D=0.1. Figure 1 shows the comparison of numerical solution with the exact solution for initial shock distribution. Figures 2 and 3 show the numerical solutions with FLUX scheme for a shock formation problem (n=5000) and for an expansion wave (n=170), respectively.

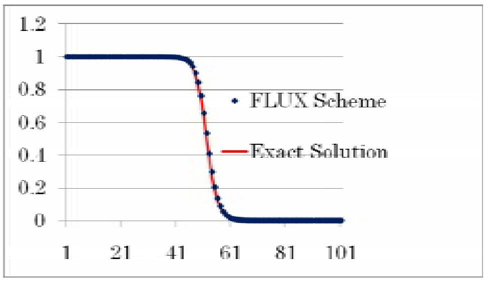

Fig.1 Comparison of solutions.

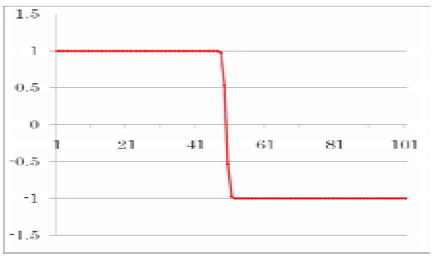

Fig.2 Solution for shock formation.

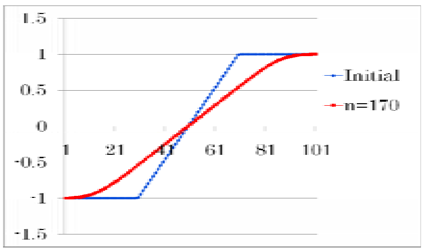

Fig.3 Solution for expansion wave.