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PERTURBATIONAL FINITE DIFFERENCE SCHEME OF CONVECTION-DIFFUSION EQUATION*

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ABSTRACT: The Perturbational Finite Difference (PFD) method is a kind of high-order-accurate compact difference method, But its idea is different from the normal compact method and the multi-nodes method. This method can get a Perturbational Exact Numerical Solution (PENS) scheme for locally linearlized Convection-Diffusion (CD) equation. The PENS scheme is similar to the Finite Analytical (FA) scheme and Exact Difference Solution (EDS) scheme, which are all exponential schemes, but PENS scheme is simpler and uses only 3, 5 and 7 nodes for 1-, 2- and 3-dimensional problems, respectively. The various approximate schemes of PENS scheme are also called Perturbational-High-order-accurate Difference (PHD) scheme. The PHD schemes can be got by expanding the exponential terms in the PENS scheme into power series of grid Renold number, and they are all upwind schemes and remain the concise structure form of first-order upwind scheme. For 1-dimensional (1-D) CD equation and 2-D incompressible Navier-Stokes equation, their PENS and PHD schemes were constituted in this paper, they all gave highly accurate results for the numerical examples of three 1-D CD equations and an incompressible 2-D flow in a square cavity.

KEY WORDS: perturbational finite difference method, convection-diffusion equation, perturbational exact nemerical solution scheme, perturbational high-order-accurate difference scheme

1. INTRODUCTION

As the rapid development of computers and continuing accumulation of computational experience, computational fluid dynamics has got great evolutions, and many highly efficient numerical methods were put forward. The Perturbational Finite Difference (PFD) method[1] is a kind of high order accurate compact difference method but its idea is different from the normal compact method[2]. The PFD method has two basic points. Firstly, derivatives are approximated by direct difference, i. e. the first-order derivative is approximated by forward, backward or central difference and the second order derivative is approximated by a second-order central difference; secondly, in the premise of keeping both the structure form and the node-number of first-order upwind difference scheme, the accuracy of perturbational difference scheme is raised by modifying the contributions of diffusion quantities at upstream and downstream nodes. We can deduce the PFD scheme in two steps. First step, the convective coefficient and source term are expanded into power series of grid-size (Δx) (here, for simplicity, 1-D problem is considered). Second step, the coefficients of $\Delta x^m (m \geqslant 1, 2)$ are determined by using the relationship between first-order-derivative and second-order-derivative given in the Convection-Diffusion (CD) equation, and by adopting recurrence method to remove the truncated error terms in the modified differential equation of the perturbational scheme, we can work out all the coefficients of the power series. Perturbational Exact Numerical Solution (PENS) scheme can be got in the case that the convective coefficient and source term are constants in grid interval (x_{i-1}, x_{i+1}), i. e. make a locally linearlized approximation. PENS scheme's approximate schemes with various accuracy can be got by expanding the exponential term in the PENS scheme into the power series of grid Reynolds number. For convenience, these approximate schemes are called Perturbational-High-order-accurate Difference (PHD) schemes. We can choose to use the PENS or its PHD schemes according to computational experience and the characteristics problems. For example, the present research shows that the PENS scheme can lead to relatively precise results for constant-coefficient 1-D CD equation, but the PHD scheme has higher resolution for the 1-D Burgers problem containing an abrupt change. The PENS scheme is similar with the Finite Analytical (FA) method[4, 5] and the Exact Difference Solution (EDS) scheme[5], which are all exponential schemes, but the PENS scheme has notable advantages: it uses less nodes and has simpler structure form, and uses only 3, 5 and 7

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nodes for 1-D, 2-D and 3-D problems, respectively. Compared with the FA and EDS scheme, the PENS scheme also has other obvious advantages: there is no "overflow" problem under the condition of high grid *Re* number and its approximate schemes remain its upwind property. In the contents followed, we will show how to constitute the PENS and PHD schemes of 1-D CD equation, and generalize it for 2-D incompressible N-S equation to constitute the second order PHD scheme of 2-D problem. Three 1-D CD problems and a 2-D cavity flow problem prove the good properties of the PENS and PHD schemes.

2. PERTURBATIONAL EXACT NUMERICAL SOLUTION (PENS) SCHEME FOR THE CONVECTION-DIFFUSION (CD) EQUATION

2.1 1-D CD equation

$$u\varphi_x = \mu\varphi_{xx} + S \tag{1}$$

Its first-order upwind difference scheme is

$$\frac{1}{\Delta x^2}\Big[\Big(1-\frac{1-\alpha}{2}u_i\Delta x\Big)\varphi_{i+1} - (2+\alpha u_i\Delta x)\varphi_i + \Big(1+\frac{1+\alpha}{2}u_i\Delta x\Big)\varphi_{i-1}\Big] + S_i = 0 \tag{2}$$

where $\alpha = \operatorname{sign} u_i$, $u_i = \frac{u_i}{\mu}$, $S_i = \frac{S_i}{\mu}$. Let the coefficients u_i of the first-order derivative and source term S_i be expanded into the power series of Δx:

$$u_p = u + u_1\Delta x + u_2\Delta x^2 + \cdots$$

$$S_p = S + S_1\Delta x + S_2\Delta x^2 + \cdots \tag{3}$$

Then we have the perturbational finite difference scheme and its modified differential equation

$$\frac{1}{\Delta x^2}\Big[\Big(1-\frac{1-\alpha}{2}u_p\Delta x\Big)\varphi_{i+1} - (2+\alpha u_p\Delta x)\varphi_i + \Big(1+\frac{1+\alpha}{2}u_p\Delta x\Big)\varphi_{i-1}\Big] + S_p = 0 \tag{4}$$

$$u_p\varphi_x = \varphi_{xx} + S_p + E_{p1}\Delta x + E_{p2}\Delta x^2 + \cdots \tag{5}$$

where

$$E_{p,2n-1} = \frac{\alpha u_p}{(2n)!}\frac{\partial^{2n}\varphi}{\partial x^{2n}}$$

$$E_{p,2n} = -\frac{u_p}{(2n+1)!}\frac{\partial^{2n+1}\varphi}{\partial x^{2n+1}} + \frac{2}{(2n+2)!}\frac{\partial^{2n+2}\varphi}{\partial x^{2n+2}}$$

$$(n = 1, 2, \cdots) \tag{6}$$

By using the relationship between the first- and second-order derivatives, which is provided by the CD Eq. (1), and supposing that u and S are constant in the grid interval (x_{i-1}, x_{i+1}), i.e. taking locally linearlized approximation, we get

$$\frac{\partial^{n+2}\varphi}{\partial x^{n+2}} = \frac{\partial^n}{\partial x^n}\Big(u\frac{\partial\varphi}{\partial x} - S_p - E_{p1}\Delta x - E_{p2}\Delta x - \cdots\Big) \tag{7}$$

$$u_p\Delta x = u_p\Delta x = \sum_{n=1}^{N}\frac{(u_i\Delta x)^{2n-1}}{(2n-1)!} + \alpha\sum_{n=1}^{N}\frac{(u_i\Delta x)^{2n}}{(2n)!}$$

$$\xrightarrow{N\to\infty} \sinh(u\Delta x) + \alpha[\cosh(u\Delta x) - 1] \tag{8a}$$

$$S_p = \frac{S}{u}u_p \tag{8b}$$

Substitute $u_p\Delta x$ and S_p with Eq. (8) in the scheme Eq. (4), after simple depuction, we get the PENS scheme

$$2\frac{1}{\Delta x^2}\{[(1-\alpha) + (1+\alpha)e^{-u\Delta x}]\varphi_{i+1} - [2 + (1+\alpha)e^{-u\Delta x} + (1-\alpha)e^{u\Delta x}]\varphi_i + [(1+\alpha) + (1-\alpha)e^{u\Delta x}]\varphi_{i-1}\} + \frac{S_i}{2u\Delta x}\cdot[2\alpha + (1-\alpha)e^{u\Delta x} - (1+\alpha)e^{-u\Delta x}] = 0 \tag{9}$$

Let $x_i(i\Delta x)$ be fixed and Δx tends to zero, the solution of difference Eq. (9) tends to the exact solution of the linearlized CD Eq. (1). So that scheme Eq. (9) is a PENS scheme. This is a three-nodes scheme with diagonally predominant coefficient matrix and upwind effect. It remains the concise structure form of first-order upwind scheme. Especially, the exponential terms of the PENS scheme have the form of $\exp(-|u\Delta x|)$, so there is no "overflow" problem under the condition of high grid Reynolds number, which happens in normal exponential scheme very often. It deserves to point out that the central difference scheme of the CD Eq. (1) does not have the TVD property when $|u\Delta x|>2$, but the PENS scheme which got from perturbations of central difference scheme, has the TVD property for any value of $|u\Delta x|$ [1]. The result of 1-D problem has been generalized to 2- and 3-D problems, the PENS schemes of 2- and 3-D problems have the same advantages mentioned above, and uses 5 and 7 nodes respectively.

Expand the exponential term in PENS scheme Eq. (9) into the power-series of the grid Reynolds number, the approximate schemes of first-order, second-order, third-order … of PENS scheme can be obtained, and they are also called PHD scheme for convenience. The second-order PHD scheme is

$$\frac{1}{\Delta x^2}\{[1-\frac{1-\alpha}{2}u\Delta x(1+\frac{\alpha}{2}u\Delta x)]\varphi_{i+1}$$

$$[2+\alpha u\Delta x(1+\frac{\alpha}{2}u\Delta x)]\varphi_i+$$

$$[1+\frac{1+\alpha}{2}u\Delta x(1+\frac{\alpha}{2}u\Delta x)]\varphi_{i-1}\}+$$

$$S(1+\frac{\alpha}{2}u\Delta x)=0 \qquad (10)$$

The PHD scheme of higher order accurate can be obtained by keeping more terms of the power-series. For example, the third-order PHD scheme is

$$\frac{1}{\Delta x^2}\{[1-\frac{1-\alpha}{2}u\Delta x(1+\frac{\alpha}{2}u\Delta x+\frac{(u\Delta x)^2}{6})]\cdot$$

$$\varphi_{i+1}[2+\alpha u\Delta x(1+\frac{\alpha}{2}u\Delta x+\frac{(u\Delta x)^2}{6})]\varphi_i+$$

$$[1+\frac{1+\alpha}{2}u\Delta x(1+\frac{\alpha}{2}u\Delta x+\frac{(u\Delta x)^2}{6})]\varphi_{i-1}\}+$$

$$S(1+\frac{\alpha}{2}u\Delta x+\frac{(u\Delta x)^2}{6})=0 \qquad (11)$$

The other higher-order PHD schemes can be deduced as above. Various accurate PHD schemes all have upwind property. In fact, the first-order approximate scheme is the same as the normal first-order upwind scheme. Compared with the normal high-order accurate upwind schemes, second-, third-, … and higher-order PHD schemes have obvious advantages: they need less nodes inside, and near the boundary they do not reduce the order of accuracy and also do not need any special treatments. Other multi-node schemes[3] and compact schemes[2], which are multi-node scheme substantially, invokes additional physical contents and mathematical treatments which are not used in the deduction of the initial CD equation, and near the boundary they need to reduce its accuracy, or need some special treatments to keep the accuracy. Moreover, the second-order PHD scheme has an unusual advantage: not only the formula of u_p, S_p are the simplest, but they do not contain any derivative terms of u, S ever before linearlization, so the formulas of u_p and S_p in the locally linearlized CD equation are the same as those of nonlinear CD equation, that is, the second-order PHD scheme contains the effects of nonlinearity. Second order PHD scheme is used in this paper, and for linear and nonlinear problems, good results are obtained with it.

2.2 *2-D CD equation*

By using result of 1-D CD equation, a PFD scheme for 2-D incompressible Navier-Stokes momentum equations can be deduced directly. The following is the deduction of the second-order PHD scheme of 2-D N-S equation. The nondimensional vorticity-stream function equations are

$$u\omega_x+v\omega_y=R_e^{-1}(\omega_{xx}+\omega_{yy})$$

$$\Psi_{xx}+\Psi_{yy}=-\omega \qquad (12)$$

Uing the time marching ADI method, the vorticity equation can be split into two equations:

$$\frac{\partial\omega}{2\partial t}+u\omega_x=R_e^{-1}\omega_{xx}+S_x$$

$$\frac{\partial\omega}{2\partial t}+v\omega_y=R_e^{-1}\omega_{yy}+S_y \qquad (13)$$

where $S_x=R_e^{-1}\omega_{yy}-v\omega_y$ and $S_y=R_e^{-1}\omega_{xx}-u\omega_x$. Perturbations are exerted on Eq. (13), deduction is the same as that of 1-D CD equation, the derivatives in S_x and S_y are discretized with the central difference, and finally the difference scheme of vorticity equation is given as

$$\frac{R_e}{2\Delta t}(\omega_{i,j}^{n+1/2}-\omega_{i,j}^{n})=\frac{1}{\Delta x^2}[(-\frac{1-\alpha}{2}u_p\Delta x)\cdot$$

$$\omega_{i+1,j}^{n+1/2}-(2+\alpha u_p\Delta x)\omega_{i,j}^{n+1/2}+$$

$$(1+\frac{1+\alpha}{2}u_p\Delta x)\,\omega^{n+1/2}_{i-1,j}] + S_{xp} \qquad (14)$$

$$\frac{R_e}{2\Delta t}(\omega^{n+1}_{i,j} - \omega^{n+1/2}_{i,j}) = \frac{1}{\Delta y^2}[(-\frac{1-\beta}{2}v_p\Delta y)\cdot$$

$$\omega^{n+1}_{i,j+1} - (2+\beta v_p\Delta y)\,\omega^{n+1}_{i,j} +$$

$$(1+\frac{1+\beta}{2}v_p\Delta y)\,\omega^{n+1}_{i,j-1}] + S_{yp} \qquad (15)$$

where

$\alpha = \mathrm{sign}(u),\ \beta = \mathrm{sign}(v),$

$u = u\cdot Re,\ v = v\cdot Re,$

$u_p\Delta x = u\Delta x + \frac{\alpha}{2}(u\Delta x)^2,$

$S_{xp} = ReS_x(1+\frac{\alpha}{2}u\Delta x),$

$v_p\Delta y = v\Delta y + \frac{\beta}{2}(v\Delta y)^2,$

$S_{yp} = ReS_y(1+\frac{\beta}{2}v\Delta y)$

In addition, the stream function equation is discretized with the central difference scheme and computed with the relaxation iteration method, and the relaxation coefficient is 0.5.

2.3 *Numerical Examples*

Example. 1 constant coefficient problem

$$\left.\begin{aligned} &\varepsilon z'' + z' - (1+\varepsilon)z = 0,\ -1 < x < 1\\ &z(-1) = 1+\exp(-2)\\ &z(1) = 1+\exp[\frac{-2(1+\varepsilon)}{\varepsilon}] \end{aligned}\right\} \qquad (16)$$

Its exact solution is $z_{ex} = \exp(x-1) + \exp[\frac{-(1+\varepsilon)}{\varepsilon(1+x)}]$. There is boundary-like steep change near $x = -1$ in this solution (see Fig. 1). Since it is a constant coefficient problem, the PENS scheme can be used. Computations show that the PENS scheme is practicable and gives highly accurate results. Fig. 1 gives a comparison of the solutions the first upwind scheme, central difference scheme, and PENS scheme with the exact solution as $\varepsilon = 0.01$ and $\Delta x = 0.02$. Results show that these three schemes can all simulate approximately boundary-layer-like steep change, but the PENS scheme can give more accurate results, the maximum error of the PENS scheme is less by two orders-of-multitude compared with those of the other two schemes.

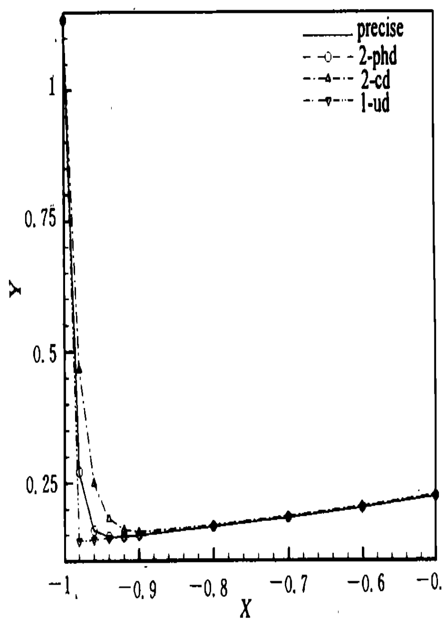

Fig. 1 Constant coefficient problem

Example. 2 Air-pocket problem

$$\left.\begin{aligned} &\varepsilon z'' - [(1-2x)z]' = 0,\\ &0 < x < 1,\ z(0) = z(1) = 1 \end{aligned}\right\} \qquad (17)$$

Its exact solution is $z_{ex}(x) = \exp[\frac{x}{\varepsilon(1-x)}]$. From the exact solution we know that its maximum value can be very large in the interval (0, 1) if ε is small enough, then its numerical simulation is very difficult. Fig. 2 gives a comparison of the solutions of the first upwind-, central difference-, and second-order PHD schemes with the exact solution as $\varepsilon = 0.1$ and $\Delta x = 0.01$. From Table 1, we can conclude that the central difference scheme gives only intolerable results though it is of second-order while highly accurate results are obtained with the second-order PHD scheme.

Example. 3 steady burgers problem

$$\left.\begin{aligned} &zz' = \frac{z''}{R_e},\ -1 < x < 1,\\ &z(-1) = \mathrm{th}(\frac{R_e}{2}),\ z(1) = -\mathrm{th}(\frac{R_e}{2}) \end{aligned}\right\} \qquad (18)$$

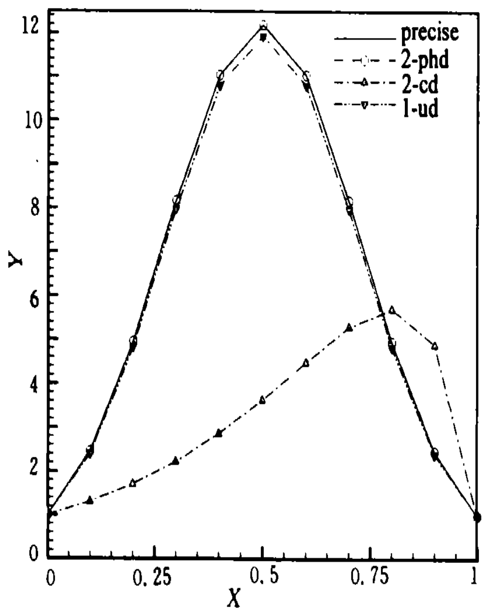

Fig. 2 Air-pocket problem

This is one of the classical problems in simulating shock wave, and its exact solution is $z_{ex}(x) = -\operatorname{th}(\frac{xR_e}{2})$. Fig. 3 gives a comparison of the solutions of the first upwind-, central difference-, and second order PHD shcemes with the exact solution as $\varepsilon = 0.1$ and $\Delta x = 0.1$. Table. 1 shows the maximum errors of the three schemes, from which we can see that the errors of the PHD scheme is very small. As the Reynolds number increases, the second-order PHD scheme can still capture exactly "shock wave"-like steep change and numerical solutions are very precise even the Reynolds number is 10^5, but resolutions of the first order upwind scheme and central difference scheme are very low.

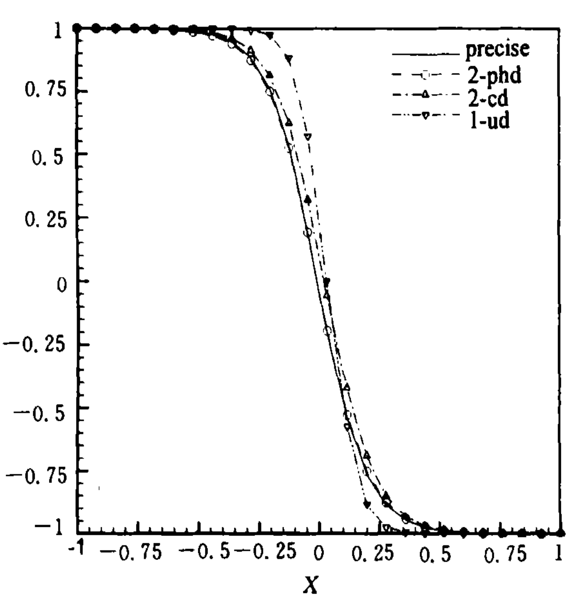

Fig. 3 Steady burgers equation

[HJ]Example. 4 2-D flow in a square cavity

Here the second-order accurate PHD scheme was given in Section 2. 2 and used to compute a square cavity flow with one boundary moving, and computations were based on the vorticity-stream function equations of incompressible fluid. The vorticity equation is discretized with the second-order PHD scheme relevant with time, and the stream function equation is discretized with the central difference scheme. The implicit ADI method for the vorticity equation and the relaxation iteration method for stream function equation are combined to compute the stream function in a square cavity with $Re = 100$ and $Re = 1000$. In this numerical simulation, the maximum iteration errors are less than 10^{-5} when convergent results are obtained. For $Re = 100$, the ceneter of primary vortex is located at $x = 0.6172$, $y = 0.7344$, the maximum value of stream funetion is -0.10325. For $Re = 1000$, the center of primary vortex is located at $x = 0.5313$, $y = 0.5703$, and the maximum value of stream function is -0.1109. All these results are in good agreement with those of Ghia et al.[6] and Charls-Henri et al.[7], they both use second-order accurate discretization, Fig. 4 and Fig. 5 are the streamline figures and vorticity contours for $Re = 100$ and $Re = 1000$, respectively.

3. CONCLUSION

The PFD method[1] is a kind of high-order accurate compact difference method, but its idea is different from multi-nodes method[3] and the normal compact method[2]. In the PFD method the concept of difference approximation of differential equations is expanded, and non-derivative terms (including coefficients) are also discretized besides derivative terms in the differential equation studied. On the premises that the derivatives are approximated by direct differences (i. e. second order center difference, upwind and backward differences) and 1-, 2-, 3-D problem use 3, 5, 7 nodes respectively, derivative coefficients and source terms are expanded into the power series of grid-size. By removing the truncated error terms in the modified differential equation of the CD-difference equation, a PENS seheme of locally linearlized CD equation is obtained. The approximate schemes of PENS scheme, including the first-, second-, third- …order accuracy are also called PHD scheme. They can be obtained by expanding the exponential terms in the PENS scheme into the power series of grid Reynold number. Compared with other high-order accurate difference schemes (such as multi-node[3] high-order-accurate schemes and compact difference schemes[2]), the most notable characteristic of the PENS scheme is that the physical considerations and mathematical treatments adopted in deducing them do not go beyond those in the deduction of the CD equations.

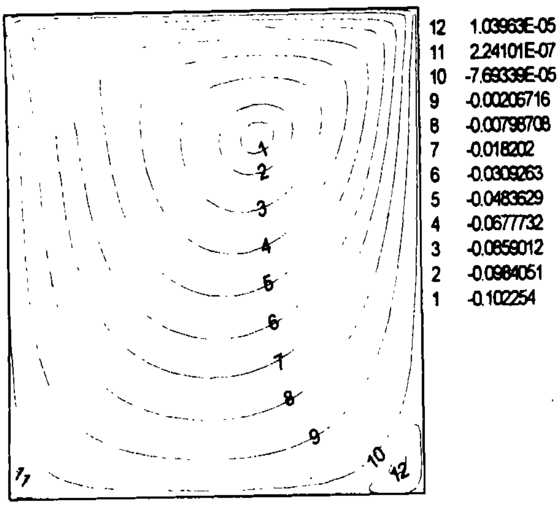

Fig. 4(a) Streamlines (Re = 100, 128 × 128)

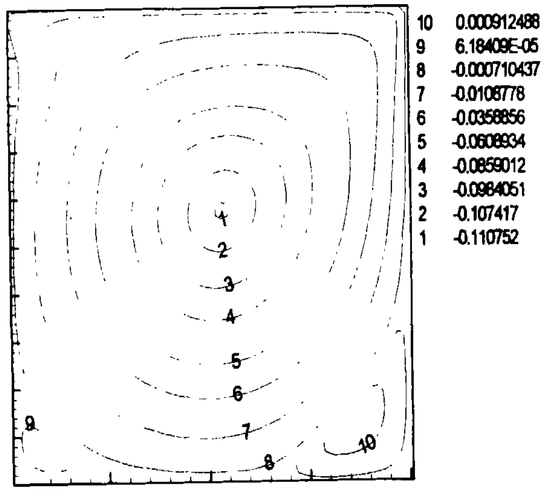

Fig. 5(a) Streamlines (Re = 1000, 128 × 128)

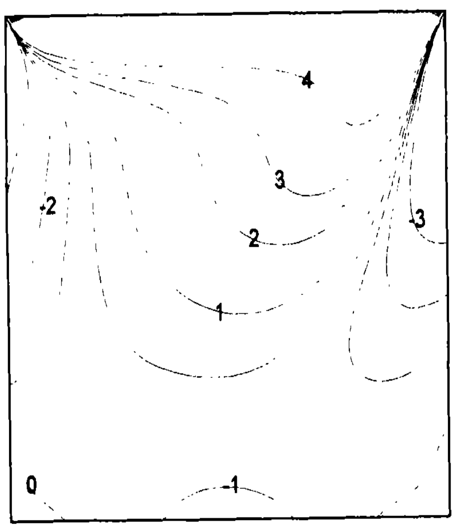

Fig. 4(b) Vorticity contours (Re = 100, 128 × 128)

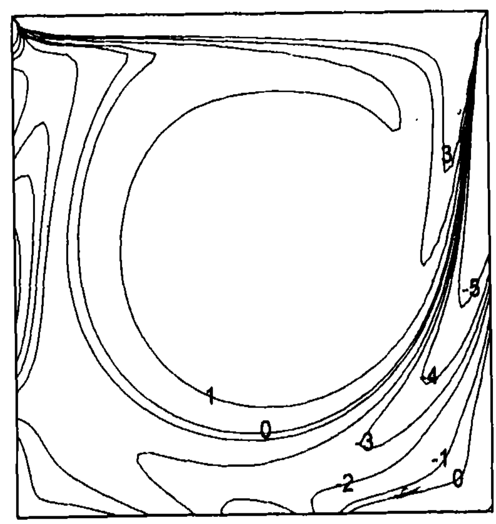

Fig. 5(b) Vorticity contours (Re = 1000, 128 × 128)

The PENS scheme is similar to the FA scheme[4,5] and EDS[5] scheme, which are all exponential schemes and have some advantages in common: they all can reflect convective upwind effect; they have not problems of negative density and pseudo numerical convection; they are unanimous convergent and steady for any large Re number. But the PENS scheme has more advantages that can not be seen in FA and EDS scheme: it does not have "overflow" problem in the case of high grid Reynolds number, and it is much simpler than the FA scheme and uses much less time and memories in computations.

In the PHD schemes, the upwind effect and simple structure form of the PENS scheme are remained. The PHD schemes use only 3, 5, and 7 nodes for 1-, 2-, and 3-D problems respectively, and for nodes near the boundary, they do not need any special treatments to get the same accuracy as the nodes inside. Three 1-D CD problems and a 2-D cavity flow problem proved the good properties of PENS and PHD schemes, and satisfactory numerical results are obtained.

Table 1. Maximum absolute errors (m. a. e.) and maximum relative errors (m. r. e.) of first-order upwind difference (1-UD) scheme, the second-order central difference (2-CD) scheme and the perturbational finite difference (PFD) scheme for 1-D C-D equations (examples 1-3). Here the PFD scheme is substituted with the PENS scheme in Example 1 and with second-order PHD scheme in Examples 2 and 3).

Example	ε	Δx	1-UD scheme		2-CD) scheme		PFD scheme	
			m. a. e.	m. r. e.	m. a. e.	m. r. e.	m. a. e.	m. r. e.
1	0.1	0.1	0.14	0.30	0.029	0.080	0.0030	0.0082
	0.01	0.02	0.20	0.72	0.13	0.49	0.0011	0.0031
	0.001	0.02	0.049	0.36	0.80	5.8	0.0033	0.0089
2	1	0.1	0.0067	0.0052	0.49	0.38	0.0016	0.0012
	0.1	0.01	0.26	0.021	8.7	0.72	0.047	0.0038
	0.05	0.001	17.0	0.12	145	0.98	0.16	0.0011
3	0.1	0.08	0.38	1.9	0.14	0.72	0.00151	0.012
	10^{-3}	0.08	2.0	2.0	3.28	3.28	6.10×10^{-4}	6.10×10^{-4}
	10^{-5}	0.08	2.0	2.0	2.0	2.0	6.25×10^{-8}	6.25×10^{-8}

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