SECOND ORDER BICYCLIC SPLITTING DIFFERENCE SCHEME FOR MULTIDIMENSIONAL ADVECTION-DIFFUSION PROBLEMS

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Abstract

A bicyclic splitting finite difference scheme for solving unsteady advection-diffusion problems, applicable for the multidimensional case, is presented. Different kind of discretizations for advection terms are considered. It is proved that the proposed new scheme has a discretization error of $O(\tau^2 + h_1^2 + \cdots + h_n^2)$ under some restrictions over the time step increment and it is stable. The new scheme is examined through numerical experiments for the two-dimensional advection-diffusion problem.

Key Words: Second order splitting method for non-commutative operators, Stability and convergence

1 Introduction

The numerical solution of advection-diffusion transport problems arises in many important applications in science and engineering. These problems occur in many applications such as in the transport of air and ground water pollutants, oil reservoir flow, in the modelling of semiconductors, etc. The great interest in the numerical solution of singularly perturbed problems has recently been demonstrated by many authors, see [2, 6, 7, 8] among many others.

The operator-splitting schemes are often used for solving initial value problems since they are economical as explicit schemes and can retain the unconditional stability inherent in some of the implicit schemes. This article is concerned with a bicyclic splitting method for numerical solution of the unsteady linear advection-diffusion problem with non-commutative operators. The main advantage of the bicyclic splitting method is that it is representative as well for multidimensional case. It is well known that there are a lot of difference schemes of the type of alternating direction scheme, which are unconditionally stable in the two-dimensional case with second order accuracy (most of them only for commutative operators). However, the construction of such schemes for multi-dimensional problems when the operators are not pair-wise commutative encounters considerable difficulties. In addition to this if the operators A_k defined in (3) depend on time, i.e. $A_k = A_k(t)$, the simple generalization of the splitting methods for $n \geq 3$ is impossible.

The article is organized in sections as follows: the problem is introduced in Section 2. Next, in Section 3, the bicyclic splitting method is presented. In Section 4 we show that the discretization error is of the second order in space and time. Some numerical results are presented and discussed in Section 5. Finally, some conclusions can be found in Section 6.

2 Advection-Diffusion Problem

Consider the unsteady linear advection-diffusion problem

$$\begin{aligned} &\frac{\partial \phi}{\partial t} + \sum_{k=1}^{n} v_k \frac{\partial \phi}{\partial x_k} = \nu \sum_{k=1}^{n} \frac{\partial^2 \phi}{\partial x_k^2}\ , \\ &\mathbf{x} = (x_1, \ldots, x_n) \in \Omega \subset \mathbb{R}^n, \\ &t \in \Omega_t = \{t_0 \leq t \leq T\}, \end{aligned} \quad (1)$$

Received on August 10, 2001.
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with initial condition

$$\phi(\mathbf{x}, t_0) = g(\mathbf{x}), \tag{2}$$

where the small scaling parameter $\nu > 0$ indicates advection dominated flow, $v_i = v_i(\mathbf{x}, t)$ are the velocity components. Proper boundary conditions of Dirichlet, Neumann or periodic type are imposed on the boundary $\Gamma = \partial\Omega$. We assume that

$$\Omega = \{a_1 \le x_1 \le b_1, a_2 \le x_2 \le b_2, \dots, a_n \le x_n \le b_n\}.$$

Let $A_k,\ k = 1, \dots, n$ denotes the advection-diffusion operator in direction x_k:

$$A_k = v_k \frac{\partial}{\partial x_k} - \nu \frac{\partial^2}{\partial x_k^2} \ . \tag{3}$$

Then the equation (1) can be written into the following evolution form

$$\frac{\partial \phi}{\partial t} + A\phi = 0, \quad \text{where} \quad A = \sum_{i=1}^{n} A_i. \tag{4}$$

3 Numerical method

3.1 Time splitting method

We use the bicyclic splitting scheme of additive type, which can be employed in the multi-dimensional case. The additive splitting was suggested by Samarskii in 1962 (see [10]) and the theory was developed in [5, 9, 11]. In these books the idea of bicyclic splitting is outlined as well.

In the interval $t_{j-1} \le t \le t_{j+1}$ we solve the following one-dimensional problems

$$\frac{\phi^{j-1+\frac{k}{n}} - \phi^{j-1+\frac{k-1}{n}}}{\tau} + \Lambda_k^j \frac{\phi^{j-1+\frac{k}{n}} + \phi^{j-1+\frac{k-1}{n}}}{2} = 0, \quad k = 1, \dots, n, \tag{5}$$

$$\frac{\phi^{j+1-\frac{k-1}{n}} - \phi^{j+1-\frac{k}{n}}}{\tau} + \Lambda_k^j \frac{\phi^{j+1-\frac{k-1}{n}} + \phi^{j+1-\frac{k}{n}}}{2} = 0, \quad k = n, \dots, 1, \tag{6}$$

where τ is the time step increment, $\Lambda_k^j = \Lambda_k(t_j)$ are the difference approximations of the operators $A_k,\ k = 1, \dots, n$. The initial conditions for the one-dimensional problems (5), (6) are

$$\begin{aligned} \phi^{\frac{1}{n}}(\mathbf{x}, t_1) &= \phi(\mathbf{x}, t_0), \\ \phi^{j-1+\frac{1}{n}}(\mathbf{x}, t_j) &= \phi^{j-1}(\mathbf{x}, t_{j-1}), \\ \phi^{j-1+\frac{k}{n}}(\mathbf{x}, t_j) &= \phi^{j-1+\frac{k-1}{n}}(\mathbf{x}, t_j) \end{aligned} \tag{7}$$

for $k = 2, \dots, n$, and

$$\begin{aligned} \phi^{j+1-\frac{n-1}{n}}(\mathbf{x}, t_{j+1}) &= \phi^{j}(\mathbf{x}, t_j), \\ \phi^{j+1-\frac{k-1}{n}}(\mathbf{x}, t_{j+1}) &= \phi^{j+1-\frac{k}{n}}(\mathbf{x}, t_{j+1}) \end{aligned} \tag{8}$$

for $k = n-1, \dots, 1$.

After some manipulation the equations (5), (6) adopt the form

$$\left(E + \frac{\tau}{2}\Lambda_k^j\right)\phi^{j-1+\frac{k}{n}} = \left(E - \frac{\tau}{2}\Lambda_k^j\right)\phi^{j-1+\frac{k-1}{n}}, \quad k = 1, \dots, n, \tag{9}$$

$$\left(E + \frac{\tau}{2}\Lambda_k^j\right)\phi^{j+1-\frac{k-1}{n}} = \left(E - \frac{\tau}{2}\Lambda_k^j\right)\phi^{j+1-\frac{k}{n}}, \quad k = n, \dots, 1, \tag{10}$$

where E is the identity operator.

First we solve the equation for $\phi^{j-1+\frac{1}{n}}$ ($k = 1$ in (9)), with initial condition

$$\phi^{j-1+\frac{1}{n}}(\mathbf{x}, t_j) = \phi^{j-1}(\mathbf{x}, t_{j-1}),$$

and determine $\phi^{j-1+\frac{1}{n}}(\mathbf{x}, t_j)$, which is later used as an initial condition when determining $\phi^{j-1+\frac{2}{n}}(\mathbf{x}, t_j)$, and so on. On the next stage we solve the equations (10) in the same manner as equations (9) using $\phi^{j}(\mathbf{x}, t_j)$ as an initial condition for the first equation. We take $\phi^{j+1}(\mathbf{x}, t_{j+1})$ as an approximate solution of the problem (1), (2) at time t_{j+1}.

3.2 Spatial Discretization

We use a uniform grid in each direction x_k with size $h_k = (b_k - a_k)/(N_k - 1)$, where N_k is the total number of grid points in the direction x_k, $k = 1, 2, \dots, n$. We employ standard central difference approximation for the diffusion operator in (3). For comparison we consider different approximations for the advection operator in (3).

The POLE scheme, constructed on the base of the Finite Variable Difference Method [7], is robust for large values of the mesh Reynolds number $Rm = (vh)/\nu$. This new scheme, called newly POLE, combines the QUICK scheme for $Rm \le 8/3$ and POLE scheme for $Rm > 8/3$. The accuracy of the POLE scheme is of the second order with respect to the mesh size Δx for Rm greater than 3 and of the third order at $Rm = 3$, while the QUICK scheme is only of the second order. From the view point of monotonicity, $Rm = 8/3$ is the critical value for the QUICK scheme, which is not monotone for $Rm > 8/3$.

It is possible to approximate all operators (including the advection term) using second order central differences. Such approximation (proposed by Arakawa [1]) has been employed in [4] for the nonlinear terms in the vectorial operator-splitting scheme for the Navier-Stokes equations. The efficiency of this central difference approximation for the convective terms in Navier-Stokes equations is clearly demonstrated in [4].

If the velocity components satisfy the condition

$$\sum_{k=1}^{n} \frac{\partial v_k}{\partial x_k} = 0 \tag{11}$$

then we can use the following representation

$$C_k = v_k \frac{\partial}{\partial x_k} + \frac{1}{2} \frac{\partial v_k}{\partial x_k} \tag{12}$$

of the advection operator in direction x_k in (3). The condition (11) ensures nonnegative definiteness of the operators A_k, i.e. the stability of the scheme. It is readily seen that the operator C_k satisfies the following condition $(C_k\phi, \phi) = 0$ if the functions v_k $(k = 1, \dots, n)$ and ϕ, satisfy appropriate conditions on the boundary (for example, if these functions are periodic, or satisfy homogeneous boundary conditions, etc.). Under the assumptions stated above we have

$$\begin{aligned} (C_k\phi, \phi) &= \int_\Omega \left(v_k \frac{\partial \frac{\phi^2}{2}}{\partial x_k} + \frac{\phi^2}{2} \frac{\partial v_k}{\partial x_k} \right) \mathrm{d}\mathbf{x} \\ &= \frac{1}{2} \int_\Omega \frac{\partial (v_k \phi^2)}{\partial x_k} \mathrm{d}\mathbf{x} = 0 \end{aligned} \tag{13}$$

The following difference approximation $\widetilde{C}_k$ of the operator C_k, see [1, 4, 5],

$$\begin{aligned} \widetilde{C}_k^j \phi_{i_k} &= \frac{1}{2h_k} \left[(v_k^j)_{i_k+\frac{1}{2}} \phi_{i_k+1} - (v_k^j)_{i_k-\frac{1}{2}} \phi_{i_k-1} \right], \\ v_k^j &= v_k(\mathbf{x}, t_j), \end{aligned} \tag{14}$$

where i_k denotes the number of grid points of the variable x_k, has the second order of spatial accuracy and satisfies

$$(\widetilde{C}_k^j \phi_{i_k}, \phi_{i_k}) = 0,$$

where the scalar product (α, β) is defined by

$$(\alpha, \beta) = \sum_{i_1 i_2 \dots i_n} \alpha_{i_1 i_2 \dots i_n} \beta_{i_1 i_2 \dots i_n} h_1 h_2 \dots h_n.$$

The multi-diagonal systems are solved by means of a specialized solver [3] which is a generalization of so called Thomas algorithm.

4 Stability and Convergence of Bicyclic Difference Scheme

In this paragraph the consistency and stability of the bicyclic scheme will be shown. Hereafter, $\|\cdot\|$ denotes the usual maximum norm, i.e., $\|u\| = \sup_{x\in\Omega} |u(x)|$. The bicyclic scheme has a second order of discretization error with respect to the time and space, i.e., the following theorem is valid

Theorem *Consider the problem (4), (2) with the assumptions*

$$\frac{\tau}{2} \|\Lambda_k^j\| < 1, \quad A_k \geq 0, \tag{15}$$

and the discretization as described in 3.1 and 3.2, using a uniform mesh. If $u \in C^4(\overline{\Omega})$, *then the discretization error satisfies*

$$\|\phi^{j+1}(\mathbf{x}, t_{j+1}) - \phi(\mathbf{x}, t_{j+1})\| = O(\tau^2 + h^2).$$

Proof: In order to show the consistency of the difference scheme consider first the truncation error with respect to the time step. Upon the denotation $T_k = (E + \frac{\tau}{2}\Lambda_k^j)^{-1}(E - \frac{\tau}{2}\Lambda_k^j)$ from equation (9) it follows that

$$\phi^j = T_n^j T_{n-1}^j \dots T_1^j \phi^{j-1}$$

and in a similar way from (10)

$$\phi^{j+1} = T_1^j T_2^j \dots T_n^j \phi^j.$$

In the full cycle one obtains

$$\phi^{j+1} = T^j \phi^{j-1}, \text{ where } T^j = \prod_{k=1}^{n} T_k^j \prod_{k=n}^{1} T_k^j.$$

If the inequality (15) is satisfied, then for the operator T^j the following expansion is valid, independently of the fact that the operators A_k are pairwise commutative or not,

$$T^j = E - 2\tau\Lambda^j + 2\tau^2(\Lambda^j)^2 + O(\tau^3),$$

where

$$\Lambda^j = \sum_{k=1}^{n} \Lambda_k^j.$$

It is easy to show that the bicyclic difference scheme approximates the Crank-Nicolson difference scheme in the interval $t_{j-1} \leq t \leq t_{j+1}$

$$\frac{\phi^{j+1} - \phi^{j-1}}{2\tau} + \Lambda^j \frac{\phi^{j+1} + \phi^{j-1}}{2} = 0$$

of the order $O(\tau^2)$, i.e., the truncation error of the bicyclic scheme (9), (10) with respect to τ is of the second order.

It should be noticed that the *conventional splitting scheme approximates the Crank-Nicolson scheme with second order only if the operators A_k are pairwise commutative, and of the order $O(\tau)$ if they are not pairwise commutative.* The bicyclic splitting overcomes under the condition (11) the restriction of pairwise commutativity to obtain the second order accuracy.

By using Kellog's lemma, see [5] for the details, it can be proved that

$$\|T^j\| \leq 1 \quad \text{if} \quad A_k \geq 0,\, k = 1, \dots, n,$$

i.e., the bicyclic scheme is stable if $A_k \geq 0$. For the skew-symmetric scheme for the operator A_k we have $A_k \geq 0$, i.e. $(A_k\phi, \phi) \geq 0$. While for the standard central difference scheme, if $\frac{|v_k|h_k}{2\nu} \leq 1$, then $A_k \geq 0$. It follows (under the assumptions) that we have the estimate

$$\|\phi^{j+1}(\mathbf{x}, t_{j+1}) - \phi(\mathbf{x}, t_{j+1})\| = O(\tau^2 + h^2)$$

for the POLE and skew-symmetric scheme. For the upwind scheme the discretization error is of the order $O(\tau^2 + h)$. ■

It should be mentioned that the first condition in (15) that ensures the second order consistency with respect to τ is rather restrictive. It means that both the stability and convergence of the difference scheme can be proved under quite a strong condition such as $\tau = O(h^2)$, where $h^2 = \sum_{k=1}^{n} h_k^2$. For weaker norms the estimate $O(\tau^2 + h^2)$ can be obtained under less restrictive conditions on the scheme parameters. The estimate $O(\tau + h^2)$ for the non-cyclic additive scheme for the heat conduction operator is proved in [10].

5 Numerical Results

The accuracy of the developed bicyclic splitting difference scheme and algorithm are examined by tests involving several values of the parameters ν, τ, and h. We conducted a number of calculations in order to verify the practical convergence and the $O(\tau^2 + h^2)$-approximation of the difference scheme.

Example 1. First it will be shown that the solution of our scheme has $O(h^2)$-approximation if the velocity components are

$$\begin{aligned} v_1 &= t \cos x_1 (\cos x_1 + \sin x_2), \\ v_2 &= t \sin x_1 (\cos x_1 + \sin x_2). \end{aligned} \tag{16}$$

The analytical solution is

$$\phi = (\cos x_1 + \sin x_2) \exp(-\nu t) \tag{17}$$

in the domain $\Omega = \{0 \leq x_1 \leq 2\pi, 0 \leq x_2 \leq 2\pi\}$ and $\Omega_t = \{0 \leq t \leq T\}$. The accuracy of the scheme with respect to the grid sizes h_k is examined by tests with different values of h_k, namely $h_k = \pi/8, \pi/16, \pi/32, \pi/64$ for fixed $\nu = 10^{-5}$ and $\tau = 0.002$. For this value of τ, the spatial discretization errors are substantial in comparison with the temporal discretization error. In this way we are able to see the decrease of the error due to the spatial discretization. The value of T is chosen to be $T = 1$. In this test we check the accuracy of the both schemes–skew-symmetric central difference scheme (SCD) and POLE scheme. The differences between the numerical and analytical solution along the horizontal cross section $y = \pi/4$ for the POLE scheme is presented in Fig.1(a). These results confirm the $O(h^2)$ accuracy of the solutions, obtained with both schemes. In this case the convergence of the POLE scheme is faster than those of the central difference scheme. There are no oscillations in the solutions with the both schemes.

To test the accuracy of the solution due to the temporal discretization we perform calculations with central difference scheme for time steps $\tau = 0.2, 0.1, 0.05, 0.025$ and fixed values of $\nu = 10^{-2}$, $h_k = \pi/32$, $T = 1.2$. Fig.1(b) clearly shows the $O(\tau^2)$ differences between the numerical and analytical solution. Note that the solution of this example and velocity components depend on t, x_1, x_2.

The computational results of the above test show that the bicyclic splitting scheme is robust for very small values of the parameter ν. We are able to obtain an accurate solution even for $\nu = 0$.

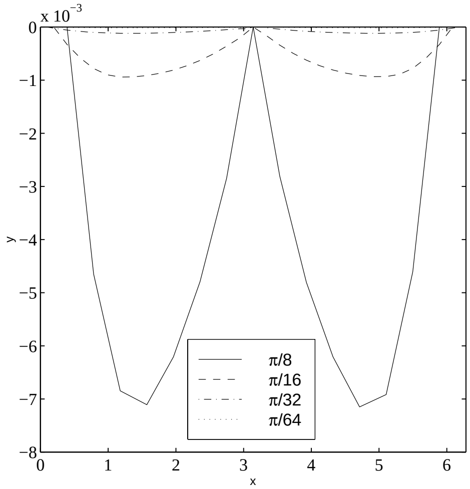
Example 2. We consider the advection-diffusion problem with the following initial condition

$$\phi(x_1, x_2, 0) = \exp\{-[(10x_1 - 3)^2 + (10x_2 - 3)^2)]\} \tag{18}$$

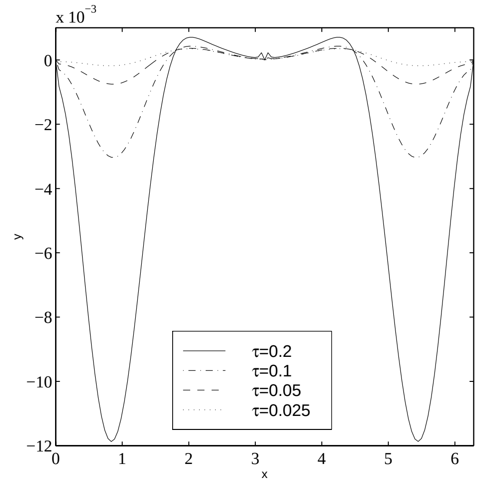
and $v_1 = v_2 = 0.1$, $h_1 = h_2 = 0.0125$, $\tau = 0.01$. The initial condition is shown in Fig.3. The numerical solution at $T = 4$ for $\nu = 10^{-2}$ is presented in Fig.2(b), while those for $\nu = 10^{-3}$ in Fig.2(c). In these cases the diffusion term is dominant and we observe smearing of the wave due to the viscosity ν. The numerical solution for $\nu = 0$ is shown in Fig.2(d). In this case in the equation (1) only the advection term is presented and the initial wave propagates with no reduction in the amplitude if the velocity components are constant. The analytical solution of this problem is

$$\phi(x_1, x_2, t) = \exp\{-[(t - 10x_1 + 3)^2 + (t - 10x_2 + 3)^2)]\}.$$

Fig.2(d) shows the numerical solution obtained by the central difference scheme at the moment $T = 4$.



(a) POLE scheme for different h_k, $\tau = 0.002$, $T = 1$, $\nu = 10^{-5}$



(b) SCD scheme for different τ, $h = \pi/128$, $T = 1.2$, $\nu = 10^{-2}$

Fig.1: Difference between $\phi_{\text{num.}} - \phi_{\text{anal.}}$, Example 1.

Table 1: Maximal value (location) of the solutions for different value of τ and h_k. Exact values—1.0000(0.7000).

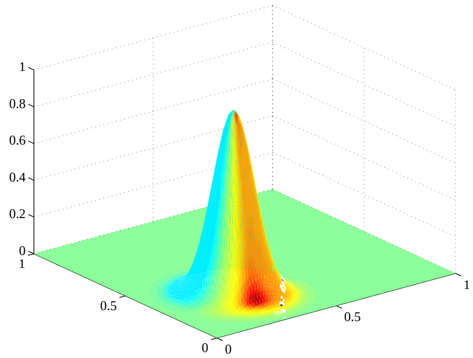
Sch.	τ / h_k	1/40	1/80	1/160	1/320
SCD	0.1	0.9430(0.6780)	0.9923(0.6922)	0.9985(0.6965)	0.9993(0.6977)
POLE		0.7791(0.7246)	0.9537(0.7085)	0.9941(0.7000)	0.9991(0.6988)
SCD	0.02	0.9473(0.6791)	0.9948(0.6938)	0.9996(0.6984)	1.0000(0.6995)
POLE		0.7737(0.7257)	0.9493(0.7102)	0.9915(0.7000)	0.9991(0.7000)
SCD	0.01	0.9474(0.6791)	0.9949(0.6939)	0.9997(0.6984)	1.0000(0.6996)
POLE		0.7735(0.7257)	0.9492(0.7103)	0.9914(0.7000)	0.9991(0.7000)
SCD	0.005	0.9474(0.6791)	0.9949(0.6939)	0.9997(0.6984)	1.0000(0.6996)
POLE		0.7735(0.7258)	0.9491(0.7103)	0.9914(0.7000)	0.9991(0.7000)

Fig.3 presents the exact solution and the numerical solutions on the diagonal cross section for central difference, POLE (second order upwind scheme for $\nu = 0$), and the first order upwind scheme. There is a very small reduction of the amplitude of the initial wave in SCD solution due to discretization. For the POLE solution this reduction is a little more, while for the upwind scheme—large. Table 1 presents the maximal value and location of the wave for different values of h_k and τ at the moment $T = 4$ for CD scheme and POLE scheme for $\nu = 0$.

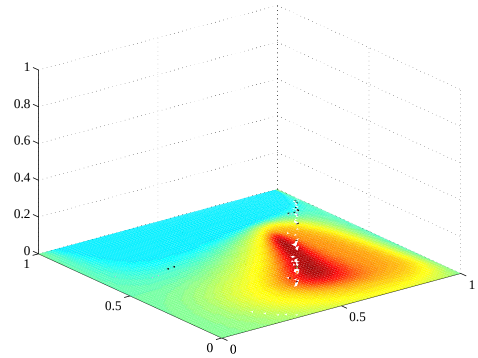
The exact values of these characteristics of the solution are 1. and $(0.7, 0.7)$. The numerical values are interpolated in the following way: 9-point stencil is formed with the extrema in its central point and the function is approximated with 2D second-order polynomials on the stencil with third order of approximation. Upon setting the partial derivatives equal to zero the location of the wave is identified. After that the amplitude of the wave is calculated from the polynomial in the location. It is seen from the table that the results for the maximal value of the SCD scheme are more accurate then those of the POLE scheme, while for the location of the maximal value the POLE scheme gives better results for $h_k \leq 1/160$.

6 Conclusions

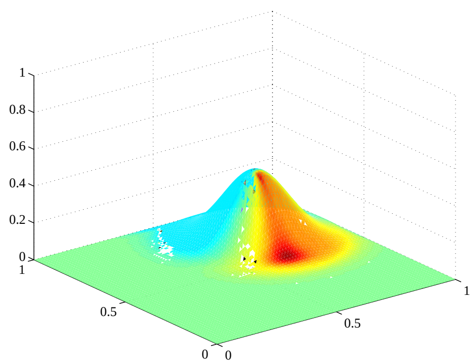
In brief, the conclusions are summarized as follows. A finite difference method for the unsteady advection-diffusion problem has been developed, based on bi-



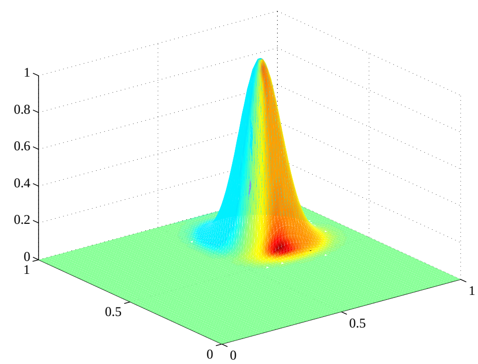
(a) Initial condition (18)



(b) SCD solution for $\nu = 10^{-2}$ at $T = 4$



(c) SCD solution for $\nu = 10^{-3}$ at $T = 4$



(d) SCD solution for $\nu = 0$ at $T = 4$

Fig.2: Example 2, $h_1 = h_2 = 0.0125$, $\tau = 0.01$.

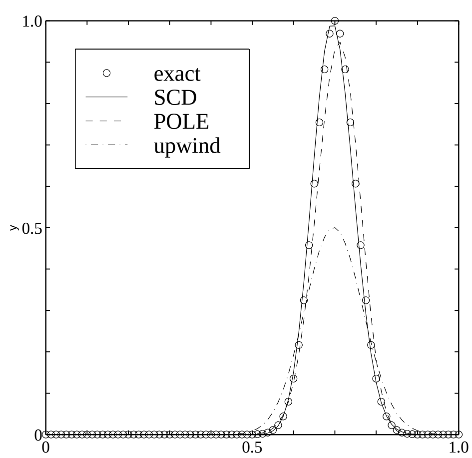


Fig.3: Diagonal cross section, $\nu = 0$, $T = 4$.

cyclic splitting with different spatial approximations for advective term—POLE and central difference scheme. This method was chosen in order to obtain a stable numerical solution of high order accuracy with a low computational cost. A convergence analysis shows the second order of the discretization error. The numerical experiments demonstrates the advantages of our method. The consistency and convergence of the scheme are verified numerically via mandatory tests with different resolutions and time increments.

Acknowledgements. The authors are indebted to the referees for helpful suggestions. The support for R.M. from Japan Science and Technology Agency under STA Fellowship ID No. 200131 and for T.M. from Japan Society for the Promotion of Science under Grant No. P99745 is gratefully acknowledged. The work of C.C. is supported in part by Grant LEQSF (1999-2002)-RD-A-49 from the Louisiana Board of Regents.

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