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A Bicyclic Splitting Difference Scheme for Unsteady Advection-Diffusion Problem

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ABSTRACT

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

Keywords: Stability and convergence of numerical methods, Finite numerical methods (IVP of PDE)

1. Introduction

The numerical solution of advection-diffusion transport problems arise 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 modeling 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.

This article is concerned with the numerical solution of the unsteady linear advection-diffusion problem

$$\frac{\partial \phi}{\partial t} + \sum_{k=1}^n v_k \frac{\partial \phi}{\partial x_k} = \nu \sum_{k=1}^n \frac{\partial^2 \phi}{\partial x_k^2}, \quad \mathbf{x} = (x_1, \dots, x_n) \in \Omega \subset \mathbb{R}^n, t \in \Omega_t = \{t_0 \leq t \leq T\}, \quad (1.1)$$

with initial condition

$$\phi(\mathbf{x}, t_0) = g(\mathbf{x}), \quad (1.2)$$

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

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

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

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$$A_k = v_k \frac{\partial}{\partial x_k} - v \frac{\partial^2}{\partial x_k^2}. \quad (1.3)$$

Then the equation (1.1) can be written into the following evolution form

$$\frac{\partial \phi}{\partial t} + A\phi = 0, \quad \text{where } A = \sum_{i=1}^n A_i. \quad (1.4)$$

The advantage of the operator-splitting schemes for solving the initial value problem (1.4), (1.2) is that they are economical as explicit schemes and can retain the unconditional stability inherent in some of the implicit schemes. 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 pairwise commutative (namely $A_k A_l \neq A_l A_k$) encounters considerable difficulties. In addition to this if the operators A_k depend on time, i.e. $A_k = A_k(t)$, like the advection operator in the above problem, the simply generalization of the splitting methods for $n > 2$ is impossible.

2. Numerical method

2.1. Time splitting method

We use the bicyclic splitting scheme of additive type, which can be employed in the multidimensional 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 also.

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

$$\frac{\phi^{j-1+\frac{k}{n}} - \phi^{j-1+\frac{k-1}{n}}}{\tau} + \Lambda_k^j \frac{\phi^{j-1+\frac{k}{n}} + \phi^{j-1+\frac{k-1}{n}}}{2} = 0, \quad k = 1, \dots, n, \quad (2.1)$$

$$\frac{\phi^{j+1-\frac{k-1}{n}} - \phi^{j+1-\frac{k}{n}}}{\tau} + \Lambda_k^j \frac{\phi^{j+1-\frac{k-1}{n}} + \phi^{j+1-\frac{k}{n}}}{2} = 0, \quad k = n, \dots, 1, \quad (2.2)$$

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 (2.1), (2.2) are

$$\phi^{\frac{1}{n}}(x, t_1) = \phi(x, t_0),$$

$$\phi^{j-1+\frac{1}{n}}(x, t_j) = \phi^{j-1}(x, t_{j-1}), \quad \phi^{j-1+\frac{k}{n}}(x, t_j) = \phi^{j-1+\frac{k-1}{n}}(x, t_j) \quad (2.3)$$

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

$$\phi^{j+1-\frac{n-1}{n}}(x, t_{j+1}) = \phi^j(x, t_j), \quad \phi^{j+1-\frac{k-1}{n}}(x, t_{j+1}) = \phi^{j+1-\frac{k}{n}}(x, t_{j+1}) \quad (2.4)$$

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

After some manipulation the equations (2.1), (2.2) adopt the form

$$\left(E + \frac{\tau}{2} \Lambda_k^j\right) \phi^{j-1+\frac{k}{n}} = \left(E - \frac{\tau}{2} \Lambda_k^j\right) \phi^{j-1+\frac{k-1}{n}}, \quad k = 1, \dots, n, \quad (2.5)$$

$$\left(E + \frac{\tau}{2}\Lambda_k^j\right)\phi^{j+1-\frac{k-1}{n}} = \left(E - \frac{\tau}{2}\Lambda_k^j\right)\phi^{j+1-\frac{k}{n}}, \quad k = n, \dots, 1. \quad (2.6)$$

First we solve the equation for $\phi^{j-1+\frac{1}{n}}$ ($k=1$ in (2.5)), 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 (2.6) in the same manner as equations (2.5) 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 (1.1), (1.2) at time t_{j+1} .

2.2. Spatial Discretization

We use a uniform grid in each direction x_k with a steps size $h_k = (b_k - a_k) / (N_k - 1)$, where N_k is the total number of grid points in direction x_k , $k = 1, 2, \dots, n$. We employ standard central difference approximation for the diffusion operator in (1.3). For comparison we consider different approximations for the advection operator in (1.3).

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 $Rm \leq 8/3$ and POLE scheme for $Rm > 8/3$. The accuracy of the POLE scheme is of second order with respect to the mesh size Δx for Rm greater than 3 and of third order at $Rm = 3$, while the QUICK scheme is of second order. From the view point of the 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 advective term) with central differences with second order of approximation. 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

$$\sum_{k=1}^n \frac{\partial v_k}{\partial x_k} = 0 \quad (2.7)$$

then we can use the following representation

$$C_k = v_k \frac{\partial}{\partial x_k} + \frac{1}{2} \frac{\partial v_k}{\partial x_k} \quad (2.8)$$

of the advection operator in direction x_k in (1.3). It is readily 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 above assumptions we have

$$(C_k \phi, \phi) = \int_{\Omega} \left(v_k \frac{\partial \phi^2}{\partial x_k} + \frac{\phi^2}{2} \frac{\partial v_k}{\partial x_k} \right) d\mathbf{x} = \frac{1}{2} \int_{\Omega} \frac{\partial (v_k \phi^2)}{\partial x_k} d\mathbf{x} = 0 \quad (2.9)$$

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

$$\widetilde{C}_k^j \phi_{i_k} = \frac{1}{2h_k} \left[(v_k^j)_{i_k + \frac{1}{2}} \phi_{i_k + 1} - (v_k^j)_{i_k - \frac{1}{2}} \phi_{i_k - 1} \right], \quad v_k^j = v_k(x, t_j), \quad (2.10)$$

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

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

where the scalar product is

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

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

3. Convergence Analysis of Bicyclic Difference Scheme

Upon denotation $T_k = (E + \frac{\tau}{2} \Lambda_k^j)^{-1} (E - \frac{\tau}{2} \Lambda_k^j)$ from equation (2.5) 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 (2.6)

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

In full cycle one obtains

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

If the inequality

$$\frac{\tau}{2} \|\Lambda_k^j\| < 1 \quad (3.1)$$

is satisfied then for the operator T^j the following expansion is valid

$$T^j = E - 2\tau \Lambda^j + 2\tau^2 (\Lambda^j)^2 + O(\tau^3), \quad \text{where } \Lambda^j = \sum_{k=1}^n \Lambda_k^j$$

independently of that the operators A_k are pairwise commutative or not. It is easy to be shown 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 order $O(\tau^2)$. While the onecyclic splitting scheme approximates the respective Crank-Nicolson scheme of second order only if the operators A_k are pairwise commutative, and of order $O(\tau)$ if they are not pairwise commutative. Hence, in the interval $t_{j-1} \leq t \leq t_{j+1}$ the truncation error of the bicyclic scheme (2.5), (2.6) with respect to τ is of second order.

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

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

i.e., the bicyclic scheme is absolutely 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 should be mentioned that the condition (3.1) which ensures the consistency of second order with respect to τ is rather restrictive. It means that both the stability and convergence of the difference scheme can be proven under severe conditions for the time step $\tau = O(h^2)$, 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 proven in [10].

It follows (under some additional restriction of smoothness) that we have the estimate

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

for the POLE and skewsymmetric scheme, while for the upwind scheme the discretization error is of order $O(\tau + h)$. The accuracy of the scheme with respect to the time is of second order, independently of that the operators Λ_k are pairwise commutative or not.

4. Numerical Results

The accuracy of the developed here bicyclic splitting difference scheme and algorithm are checked by tests involving different values of the parameters of the scheme: ν , the time step increment τ and grid spacing 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

$$v_1 = t \cos x_1 (\cos x_1 + \sin x_2), \quad v_2 = t \sin x_1 (\cos x_1 + \sin x_2). \quad (4.1)$$

The analytical solution is

$$\phi = (\cos x_1 + \sin x_2) \exp(-\nu t) \quad (4.2)$$

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 time 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 Figure 4.1—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 of the solutions with the both schemes.

To test the accuracy of the solution due to the time discretization we perform calculations with central difference scheme for time steps $\tau = 0.2, 0.1, 0.05, 0.025$ and fixed values of $\nu = 10^{-2}, h_k = \pi/32, T = 1.2$. Figure 4.1—b) clearly shows the $O(\tau^2)$ differences between the numerical and

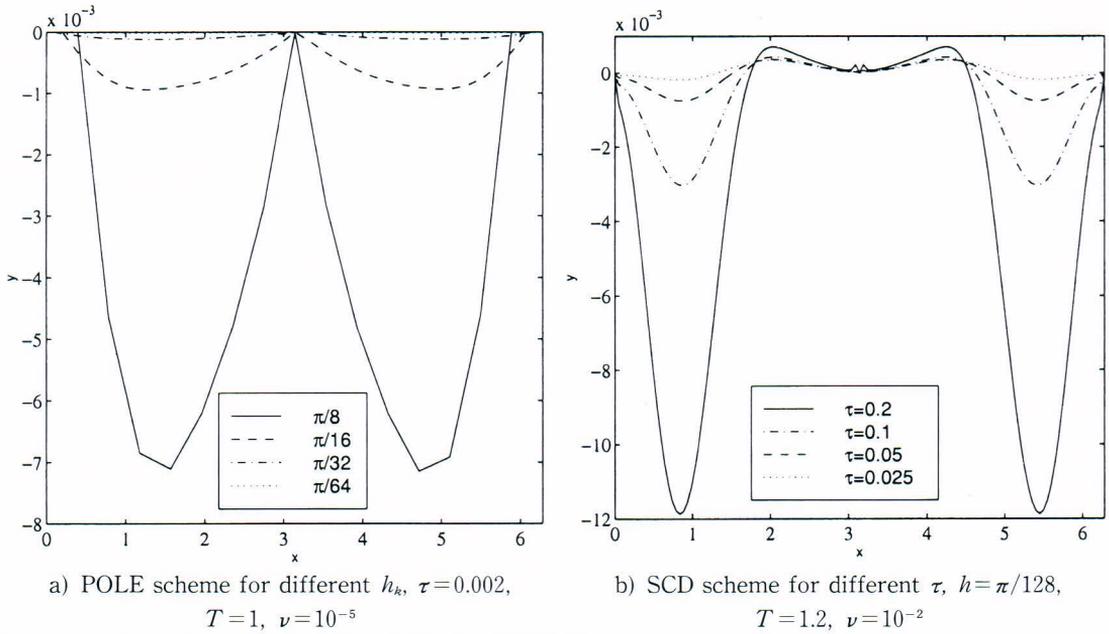


Figure 4.1: Example 1—difference between $\phi_{\text{num.}} - \phi_{\text{anal.}}$.

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

$$\phi(x_1, x_2, 0) = \exp\{-[(10x_1 - 3)^2 + (10x_2 - 3)^2]\} \quad (4.3)$$

and $v_1 = v_2 = 0.1$, $h_1 = h_2 = 0.0125$, $\tau = 0.01$. The initial condition is shown in Figure 4.2–a).

The numerical solution for $\nu = 10^{-2}$ is presented in Figure 4.2–b), while those for $\nu = 10^{-3}$ in Figure 4.2–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 Figure 4.2–d). In this case in the equation (1.1) 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

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

Figure 4.2–d) shows the numerical solution obtained by the central difference scheme at the moment $t=4$. The Figure 4 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 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 numeri-

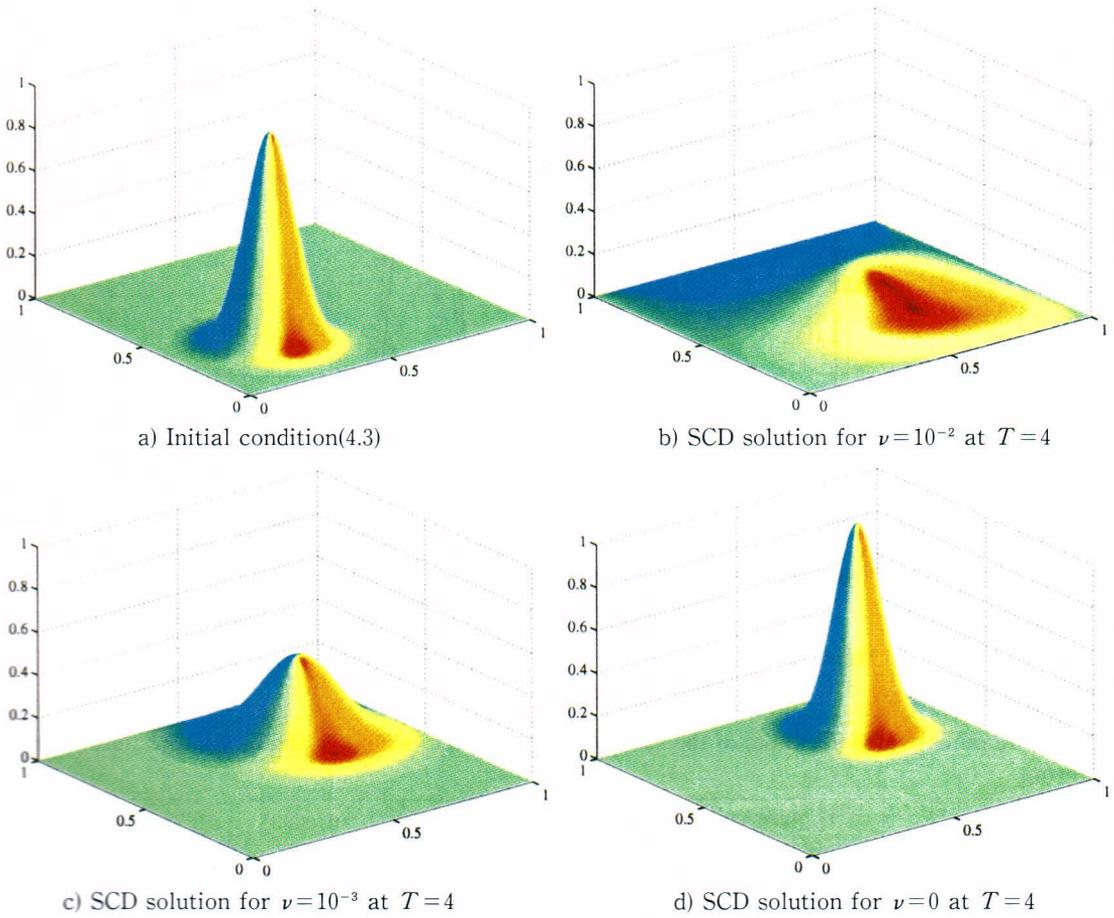


Figure4.2: Example 2, $h_1 = h_2 = 0.0125$, $\tau = 0.01$.

cal 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 vortex is identified. After that the amplitude of the vortex is calculated from the polynomial in the location. It is seen from the table that the results for the maximal value of SCD scheme is more accurate than those of POLE scheme, while for the location of the maximal value the POLE scheme gives better results for $h_k \leq 1/160$.

5. Conclusions

A finite difference method for the unsteady advection-diffusion problem has been presented, based on bicyclic 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 at a higher order of accuracy with a low computational cost. The numerical experiments show the advantages of the method. The consistency and convergence of the scheme are verified numerically via mandatory tests with different resolutions and time increments.

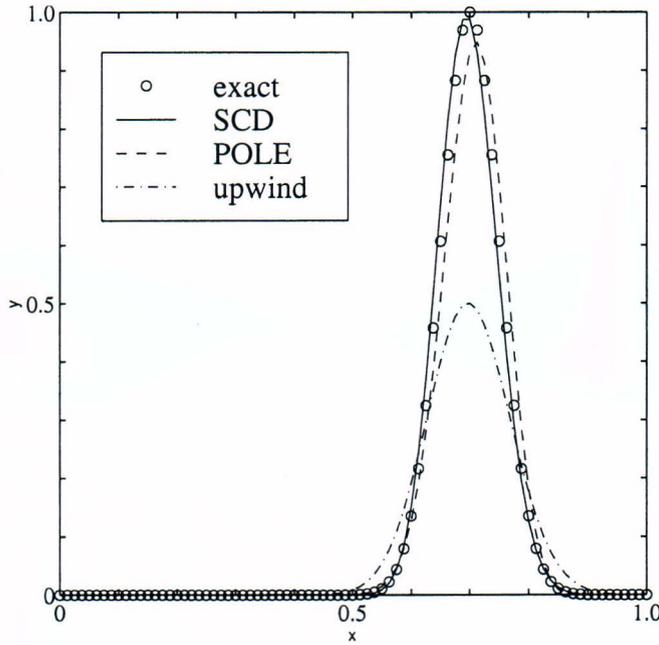


Figure 4.3: Diagonal cross section. Example 2, $\nu=0$, $T=4$.

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=0.025	1/80=0.0125	1/160=0.00625	1/320=0.003125
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)

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