

NUMERICAL APPROXIMATION OF A TIME FRACTIONAL-DERIVATIVE INITIAL-BOUNDARY VALUE PROBLEM WITH BOUNDARY LAYERS

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Abstract. In this paper we consider a fractional differential equation where the time fractional derivative is of Caputo type. The diffusion parameter can take arbitrarily small values and then the solution exhibits in general a weak layer initially and boundary layers along both sides of the domain. This problem is approximated with a finite difference scheme which combines the L1 scheme and central differences; this scheme is defined on a graded mesh for the time variable and a Shishkin mesh for the space variable. Numerical results for a test problem are shown and they suggest that the proposed scheme gives accurate approximations to the solution.

Keywords: Fractional differential equation, Caputo fractional derivative, initial-boundary value problem, L1 scheme, weak singularity, boundary layers, Shishkin mesh, uniform convergence.

AMS classification: 34A08, 65L11, 65L12.

§1. Introduction

In this paper we consider the following class of initial-boundary value problems

$$D_t^\delta u - p \frac{\partial^2 u}{\partial x^2} + c(x, t)u = f(x, t), \quad (x, t) \in Q := (0, l) \times (0, T]; \quad (1a)$$

$$u(0, t) = \phi_L(t), \quad u(l, t) = \phi_R(t), \quad \text{for } t \in (0, T], \quad (1b)$$

$$u(x, 0) = \phi(x), \quad \text{for } x \in [0, l], \quad (1c)$$

where $0 < \delta < 1$, p is a positive constant, $c \geq 0$ for $(x, t) \in \bar{Q}$ and D_t^δ denotes the Caputo fractional derivative [1] in time, which is defined by

$$D_t^\delta g(x, t) := \frac{1}{\Gamma(1 - \delta)} \int_{s=0}^t (t - s)^{-\delta} \frac{\partial g(x, s)}{\partial s} ds \quad \text{for } (x, t) \in Q. \quad (2)$$

The behaviour of the solution of the problem (1) with $c \equiv c(x)$ was analysed in [5, 9] and it was shown that it has a layer at $t = 0$. To be more precise, assuming some regularity and compatibility conditions, the following estimates

$$\left| \frac{\partial^k u}{\partial x^k}(x, t) \right| \leq C, \quad \text{for } k = 0, 1, 2, 3, 4, \quad \left| \frac{\partial^\ell u}{\partial t^\ell}(x, t) \right| \leq C(1 + t^{\delta - \ell}) \quad \text{for } \ell = 1, 2, \quad (3)$$

for all $(x, t) \in [0, l] \times (0, 1]$ were proved rigorously in [9]. The estimates (3) were established assuming that the constant $p = O(1)$ and in this paper we explore how the solution behaves if the diffusion parameter p is close to zero. Observe that in the limit case $p = 0$, the highest order derivative in space has zero order and one would expect that, in general, the solution has large gradients (boundary layers) at both sides of the domain $x = 0$ and $x = l$, similarly to the case of a problem with a classical derivative in the time variable (see [3]). All these difficulties should be taken into consideration when approximating the solution to the problem (1).

In [9] the L1 approximation [7] and standard central differences were used to discretise the temporal and spatial variables, respectively. This discrete operator was defined both on a uniform and a graded mesh for the time discretisation and a uniform mesh for the space discretisation. However, this scheme cannot deal with all the difficulties in the solution u of the problem (1). We now propose in this paper to use a special mesh of Shishkin type [3] condensing in the boundary layer regions to approximate the solution u in the spatial direction, unlike the uniform mesh considered in [9] for the particular case of $p = O(1)$.

The paper is structured as follows: In Section 2 we describe our finite difference scheme in a general framework and it is used to approximate the discrete problem described in Section 3. In this section we also give the notation employed for the two-mesh differences and the orders of convergence of the scheme. This scheme is first applied to a test problem; the scheme uses a uniform mesh to discretise the time variable and both a uniform and a Shishkin mesh to discretise the space variable. In Section 4 a graded mesh is used to discretise the solution in the time direction and a Shishkin mesh in the space direction; an improvement in the computed orders of convergence associated with the scheme is observed when these special meshes are used in both directions.

Notation: Throughout this paper we denote by $\|\cdot\|_D$ the maximum norm over the set D .

§2. Numerical scheme

This section describes the numerical scheme used to approximate the solution to problem (1). An arbitrary non-uniform mesh $\omega_{m,n}$ and the mesh steps h_m, τ_n are defined by

$$\omega_{m,n} := \{(x_m, t_n) : m = 0, 1, \dots, M, n = 0, 1, \dots, N\}, \quad h_m := x_m - x_{m-1}, \quad \tau_n := t_n - t_{n-1},$$

where M and N are two positive integers. In our finite difference scheme, the Caputo fractional derivative D_t^δ is approximated by the commonly used L1 approximation [7] (which we motivate below): The fractional derivative (2) is rewritten as

$$D_t^\delta u(x_m, t_n) = \frac{1}{\Gamma(1-\delta)} \sum_{k=0}^{n-1} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\delta} \frac{\partial u(x_m, s)}{\partial s} ds,$$

and the first-order partial derivative on each time interval $(t_k, t_{k+1}]$ is approximated by the forward finite difference operator

$$\frac{\partial u(x_m, s)}{\partial s} \approx \frac{u(x_m, t_{k+1}) - u(x_m, t_k)}{t_{k+1} - t_k} =: D_t^+ u(x_m, t_k), \quad s \in (t_k, t_{k+1}];$$

which has the associated truncation error

$$(D_t^+ u - u_t)(x_m, t_k) = \frac{1}{t_{k+1} - t_k} \int_{s=t_k}^{t_{k+1}} \int_{r=t_k}^s u_{rr}(x_m, r) dr ds.$$

The L1 approximation $D_N^\delta u_m^n$ is given by

$$\begin{aligned} D_N^\delta u_m^n &:= \frac{1}{\Gamma(1-\delta)} \sum_{k=0}^{n-1} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\delta} D_t^+ u_m^k ds \\ &= \frac{1}{\Gamma(2-\delta)} \sum_{k=0}^{n-1} \frac{u_m^{k+1} - u_m^k}{t_{k+1} - t_k} \left[(t_n - t_k)^{1-\delta} - (t_n - t_{k+1})^{1-\delta} \right], \end{aligned} \quad (4)$$

where u_m^n is the approximate solution computed at the mesh point (x_n, t_m) .

Let us now examine the truncation error associated with this approximation of the Caputo fractional derivative

$$\begin{aligned} (D_t^\delta - D_N^\delta)u(x_m, t_n) &= \frac{1}{\Gamma(1-\delta)} \sum_{k=0}^{n-1} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\delta} (u_s(x_m, s) - D_t^+ u(x_m, t_k)) ds \\ &= \frac{1}{\Gamma(1-\delta)} \sum_{k=0}^{n-1} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\delta} \frac{1}{t_{k+1} - t_k} \int_{p=t_k}^s u_{pp}(x_m, p) dp dr ds. \end{aligned}$$

In the case of a uniform mesh in time with $\tau := t_{n+1} - t_n$, $\forall n$, then the truncation error can be bounded as follows

$$|(D_t^\delta - D_N^\delta)u(x_m, t_n)| \leq \frac{\tau \|u_{tt}\|_{[0, \ell] \times [0, t_n]}}{\Gamma(1-\delta)} \int_{s=0}^{t_n} (t_n - s)^{-\delta} ds = \frac{\tau t_n^{1-\delta}}{\Gamma(2-\delta)} \|u_{tt}\|_{[0, \ell] \times [0, t_n]}.$$

On the other hand, the second order spatial derivative u_{xx} is approximated by the standard formula

$$u_{xx}(x_m, t_n) \approx \delta_x^2 u_m^n := \frac{2}{h_{m+1} + h_m} \left(\frac{u_{m+1}^n}{h_{m+1}} - \frac{u_m^n - u_{m-1}^n}{h_m} \right),$$

with $h_m := x_m - x_{m-1}$ for $m = 1, 2, \dots, M$. Note also that the truncation error associated with the second-order derivative in space (on a nonuniform mesh) satisfies

$$\begin{aligned} \left| (\delta_x^2 u - u_{xx})(x_m, t_n) \right| &= \frac{2}{h_{m+1} + h_m} \left| \frac{1}{h_{m+1}} \int_{r=x_m}^{x_{m+1}} \int_{s=x_m}^r u_{ss}(s, t_n) - u_{xx}(x_m, t_n) ds dr \right. \\ &\quad \left. - \frac{1}{h_m} \int_{r=x_{m-1}}^{x_m} \int_{s=x_m}^r u_{ss}(s, t_n) - u_{xx}(x_m, t_n) ds dr \right| \\ &\leq C \left(|h_{m+1} - h_m| \left| \frac{\partial^3 u}{\partial x^3}(x_m, t_n) \right| + \frac{h_{m+1}^3 + h_m^3}{h_{m+1} + h_m} \left| \frac{\partial^4 u}{\partial x^4}(\xi, t_n) \right| \right), \end{aligned}$$

for $0 < m < M$, $0 < n \leq N$ and $\xi \in (x_m, x_{m+1})$. In the case of a uniform mesh in space with $h := x_{m+1} - x_m$, $\forall m$, then this spatial truncation error can be bounded as follows

$$\left| (\delta_x^2 u - u_{xx})(x_m, t_n) \right| \leq Ch^2 \|u_{xxx}\|_{[0, \ell] \times [0, t_n]}.$$

Our discretization of problem (1) is given by

$$L_N^\delta u_n^m := D_N^\delta u_n^m - p \delta_x^2 u_n^m + c(x_m, t_n) u_n^m = f(x_m, t_n) \text{ for } 1 \leq m \leq M-1, 1 \leq n \leq N, \quad (5a)$$

$$u_0^n = \phi_L(t_n), \quad u_M^n = \phi_R(t_n) \text{ for } 0 < n \leq N, \quad (5b)$$

$$u_m^0 = \phi(x_m) \text{ for } 0 \leq m \leq M. \quad (5c)$$

For a uniform mesh in both space and time this scheme has the associated truncation error bound

$$\left| L_N^\delta (u_n^m - u(x_m, t_n)) \right| \leq Ch^2 \|u_{xxx}\|_{[0,l] \times [0,t_n]} + C\tau t_n^{1-\delta} \|u_{tt}\|_{[0,l] \times [0,t_n]}.$$

A suitable stability argument is required to deduce an error bound from this truncation error bound. Observe that

$$D_N^\delta z_m^n \equiv \frac{(t_n - t_{n-1})^{1-\delta}}{\Gamma(2-\delta)} D^+ z_m^n + \frac{1}{\Gamma(1-\delta)} \sum_{k=0}^{n-2} D^+ z_m^k \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\delta} ds, \quad n \geq 2.$$

Based on this observation and using the recurrence relation linking each time level, for a uniform mesh in both space and time, one can deduce (see [4]) the stability bound

$$\begin{aligned} |u_n^m - u(x_m, t_n)| &\leq C \frac{\tau^\delta}{n^{1-\delta} - (n-1)^{1-\delta}} \left\| L_N^\delta (u_n^m - u(x_m, t_n)) \right\|_{[0,l] \times [0,t_n]} \\ &\leq C(n\tau)^\delta \left\| L_N^\delta (u_n^m - u(x_m, t_n)) \right\|_{[0,l] \times [0,t_n]} \\ &\leq Ch^2 t_n^\delta \|u_{xxx}\|_{[0,l] \times [0,t_n]} + Ct_n \tau \|u_{tt}\|_{[0,l] \times [0,t_n]}. \end{aligned}$$

The realistic a priori bounds (3) make the analysis of the convergence more delicate than the classical argument given above. For example, if $n = 1$, the truncation error associated with the Caputo time fractional derivative satisfies the crude estimate

$$|(D_t^\delta - D_N^\delta)u(x_m, t_1)| \leq C, \text{ for } 0 < m < M.$$

Therefore, one needs a more sophisticated approach to derive appropriate error estimates from the stability of the discrete operator. The convergence of the scheme (5) is investigated in [9]. In particular, if $p = O(1)$, $c \equiv c(x)$ and the scheme is defined on a uniform mesh, then under suitable hypotheses on the data of the problem, the error satisfies

$$\|u - u_m^n\|_\omega \leq C \left(h^2 + \tau^\delta \right), \quad (6)$$

where C is a constant independent of N and M , but it depends on the data problem, as for example on δ and p . It is shown in [9] that this estimate is sharp when $p = O(1)$, by means of some numerical results. In the next section we approximate a test problem with the numerical scheme (5) but, unlike in [9], we allow the parameter p to be arbitrarily small. Therefore, the dependence of the partial derivatives on the parameter p will be crucial when the truncation error of the scheme (5) is analysed.

§3. Numerical experiments

Consider the following test problem

$$D_t^\delta u - p \frac{\partial^2 u}{\partial x^2} = \frac{1}{\pi^2} x^2 (\pi - x)^2 \quad (7a)$$

for $(x, t) \in Q := (0, \pi) \times (0, 1]$, with

$$u(0, t) = t^2, \quad u(\pi, t) = t^2, \quad \text{for } t \in (0, 1], \quad (7b)$$

$$u(x, 0) = \sin^3(x), \quad \text{for } x \in [0, \pi]. \quad (7c)$$

We shall consider in our numerical experiments several values of δ and p .

The solution of this problem is unknown and we shall estimate the errors using the two-mesh principle [2]: Let u_m^n be the computed solution with the scheme (5) on the mesh $\{(x_m, t_n)\}$ for $m = 0, 1, \dots, M$ and $n = 0, 1, \dots, N$. To estimate the errors we compute a new approximation $z_{m/2}^n$ using the same scheme but it is defined on the mesh $\{(x_{m/2}, t_{n/2})\}$ for $m = 0, 1, \dots, 2M$ and $n = 0, 1, \dots, 2N$ where $x_{m+1/2} := (x_{m+1} + x_m)/2$ and $t_{n+1/2} := (t_{n+1} + t_n)/2$. Thus, the finer mesh includes the mesh points of the coarser mesh and their midpoints.

We then compute the two-mesh differences

$$d_{M,N}^\delta := \max_{\substack{0 \leq m \leq M, \\ 0 \leq n \leq N}} |u_m^n - z_m^n|; \quad (8)$$

and from these values one computes the estimated orders of convergence by

$$q_{M,N}^\delta = \log_2 \left(\frac{d_{M,N}^\delta}{d_{2M,2N}^\delta} \right). \quad (9)$$

In Figure 1 we display the computed solution for $N = M = 64$ and the values of $\delta = 0.7, 0.3$ (the order of the Caputo fractional derivative) and $p = 1, 10^{-6}$ (the diffusion parameter). The solution has been computed using a fine mesh in the vicinity of $t = 0$ and $x = 0, \pi$ (which are described in Sections 3.1 and 4) and we observe that the solution exhibits initial and boundary layers.

In this section we consider a uniform mesh for the discretisation of the time and space variables. We first consider the values of $p = 1$ and $\delta = 0.3, 0.5, 0.7$. The numerical results are given in Table 1, where the maximum two-mesh differences appears in the first row of each block and their corresponding orders of convergence in the second row. We use this format in all the tables of this paper. The numerical results of this table are in agreement with the error estimate (6); they indicate that the method converges at the rate of $O(\tau^\delta)$ and therefore the error estimates proved in [9] are sharp.

We now approximate the problem (7) but we consider a smaller value of p ; we choose $p = 10^{-6}$. The values for the parameters N, M and δ are the same as in Table 1. The numerical results for these parameter settings are given in Table 2 and they indicate that our numerical scheme (5) does not converge when the diffusion parameter is very small and M is reasonable large (i.e., independent of p). In Figure 2 we display the two mesh differences for $p = 10^{-6}$

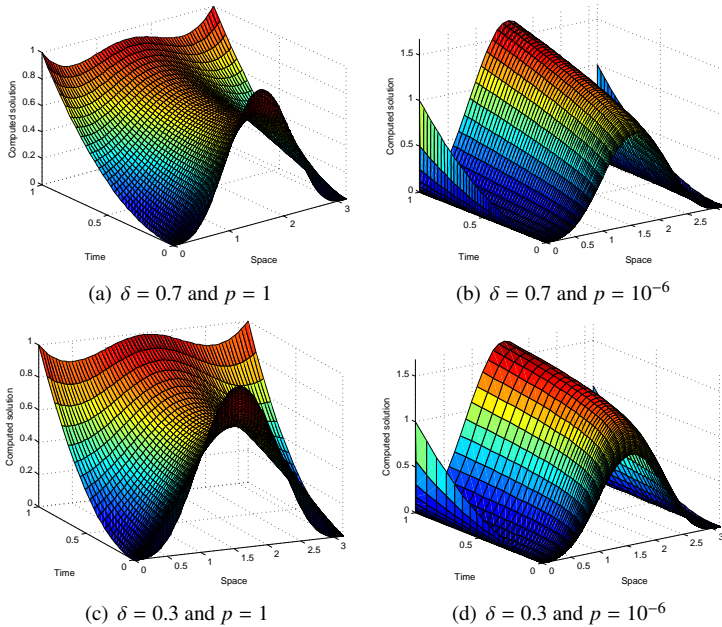


Figure 1: Test problem (7): Computed solution on $[0, \pi] \times [0, 1]$, using the special meshes described in Sections 3.1 and 4 for $\delta = 0.3, 0.7$ and $p = 1, 10^{-6}$.

and several values of δ , N and M . These plots show how the two-mesh differences behave depending on the values of the parameters. The large values for the two-mesh differences in the vicinity of $x = 0$ and $x = \pi$ motivate the use of a special mesh in space so that the resulting method gives accurate approximations to the solution. This special mesh is described in the next section.

3.1. Numerical results using a Shishkin mesh in space

This section uses a special mesh of Shishkin type [3] for the space discretisation. This type of meshes has been extensively used to approximate a wide set of singularly perturbed problems (see [6, 8] and the references therein) and they are also proposed to approximate the problem (1) when p is very small. We consider the standard mesh which is used to approximate the singularly perturbed 1D linear problem of reaction-diffusion problem: $-\varepsilon u'' + b(x)u = g(x)$ whose solution exhibits two boundary layers at both endpoints of the domain and the layers have a width of order $O(\sqrt{\varepsilon})$.

We recall that this mesh is defined by means of a transition parameter

$$\sigma = \min \{ \pi/4, 2\sqrt{p} \ln M \},$$

which is used to split the interval $[0, \pi]$ into three subintervals $[0, \sigma]$, $[\sigma, \pi - \sigma]$ and $[\pi - \sigma, \pi]$ and within each of them the mesh distributes $M/4$, $M/2$ and $M/4$ points equidistantly,

Table 1: Test problem (7) with $p = 1$ and several values of δ : Maximum two-mesh differences using a uniform mesh in time and space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	1.442E-002 0.037	1.405E-002 0.028	1.379E-002 0.038	1.343E-002 0.055	1.292E-002 0.076	1.226E-002
$\delta = 0.5$	1.843E-002 0.188	1.618E-002 0.238	1.372E-002 0.296	1.118E-002 0.348	8.781E-003 0.390	6.700E-003
$\delta = 0.7$	1.433E-002 0.550	9.789E-003 0.624	6.352E-003 0.659	4.023E-003 0.647	2.568E-003 0.678	1.606E-003

Table 2: Test problem (7) with $p = 10^{-6}$ and several values of δ : Maximum two-mesh differences using a uniform mesh in time and space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	2.323E-002 0.300	1.887E-002 0.300	1.533E-002 0.300	1.245E-002 -0.214	1.444E-002 -0.969	2.826E-002
$\delta = 0.5$	1.172E-002 0.500	8.290E-003 0.500	5.862E-003 0.500	4.145E-003 -1.588	1.247E-002 -1.130	2.728E-002
$\delta = 0.7$	4.740E-003 0.700	2.918E-003 0.700	1.796E-003 -0.757	3.035E-003 -1.797	1.055E-002 -1.293	2.585E-002

respectively. Thus, if $\sigma = \pi/4$ the mesh is uniform and otherwise is a piecewise uniform mesh condensing in the layer regions.

The numerical results for our scheme (5) using a uniform mesh in time and a Shishkin mesh in space are displayed in Table 3 for the value of $p = 10^{-6}$. Similar results have been obtained for smaller values of the parameter p . We have considered the same values for the parameters N, M and δ as in the previous tables. These numerical results suggest that our scheme converges even for $p \ll 1$. The observed order of convergence is δ and then the temporal errors again dominates the spatial errors.

Table 3: Test problem (7) with $p = 10^{-6}$ and several values of δ : Maximum two-mesh differences using a uniform mesh in time and a Shishkin mesh in space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	2.323E-002 0.300	1.887E-002 0.300	1.533E-002 0.300	1.245E-002 0.300	1.011E-002 0.300	8.215E-003
$\delta = 0.5$	1.213E-002 0.549	8.290E-003 0.500	5.862E-003 0.500	4.145E-003 0.500	2.931E-003 0.500	2.073E-003
$\delta = 0.7$	1.449E-002 1.397	5.503E-003 1.465	1.993E-003 0.850	1.106E-003 0.700	6.806E-004 0.700	4.189E-004

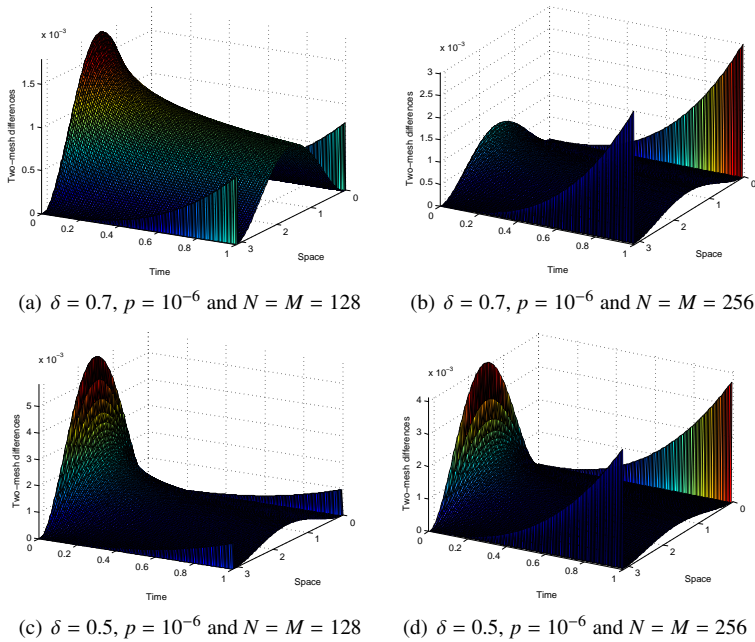


Figure 2: Test problem (7): Two-mesh differences for the scheme (5) using a uniform mesh.

§4. Numerical results using a graded mesh in time and a Shishkin mesh in space

In [9] the Caputo fractional derivative is approximated on a graded mesh

$$t_j = \left(\frac{j}{N}\right)^r, \quad j = 0, 1, \dots, N, \quad (10)$$

where $r \geq 1$ is the grading exponent. If $r = 1$, then the mesh is uniform. In that paper it was established that the error associated to the discretization of the Caputo fractional derivative (2) converges at the rate $O(M^{-(2-\delta)})$ if $r \geq (2 - \delta)/\delta$.

We define our scheme (5) on the graded mesh (10) which discretizes the time variable and the Shishkin mesh to discretize the space variable. This scheme is used to discretize the domain associated with the test problem (7) when p is small. In Tables 4, 5 and 6 we show the numerical results obtained with this scheme for $p = 10^{-5}$, $p = 10^{-6}$ and $p = 10^{-7}$ and the computed orders of convergence in these tables are greater than in Table 3. Hence, we see that the use of a non-uniform mesh in both space and time, with each mesh suitably adapted to any difficulty present in the solution, can improve the convergence of the numerical solutions. When the order of p is smaller than N^{-2} and the spatial mesh is nonuniform, we have observed that the maximum two-mesh differences occurs at the transition points $x = \sigma, 1 - \sigma$ —where the spatial mesh is not uniform—instead of inside the boundary layer regions (see Figure 3). This causes a reduction in the spatial orders of convergence as can be observed in Tables 4, 5 and 6. The convergence of this method will be analysed in a future paper.

Table 4: Test problem (7) with $p = 10^{-5}$ and several values of δ : Maximum two-mesh differences using a graded mesh in time and a Shishkin mesh in space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	1.121E-002 1.399	4.250E-003 1.505	1.497E-003 1.417	5.606E-004 0.372	4.331E-004 0.918	2.293E-004
$\delta = 0.5$	1.296E-002 1.397	4.919E-003 1.481	1.763E-003 1.583	5.885E-004 0.419	4.402E-004 0.913	2.337E-004
$\delta = 0.7$	1.514E-002 1.385	5.797E-003 1.450	2.122E-003 1.550	7.248E-004 0.761	4.276E-004 0.890	2.308E-004

 Table 5: Test problem (7) with $p = 10^{-6}$ and several values of δ : Maximum two-mesh differences using a graded mesh in time and a Shishkin mesh in space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	1.121E-002 1.399	4.250E-003 1.505	1.497E-003 1.601	4.934E-004 1.652	1.571E-004 0.743	9.381E-005
$\delta = 0.5$	1.296E-002 1.397	4.919E-003 1.481	1.763E-003 1.583	5.885E-004 1.634	1.896E-004 0.996	9.504E-005
$\delta = 0.7$	1.515E-002 1.385	5.797E-003 1.450	2.122E-003 1.550	7.248E-004 1.591	2.406E-004 1.389	9.185E-005

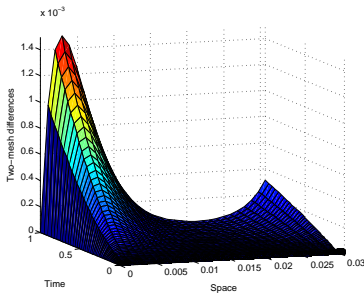
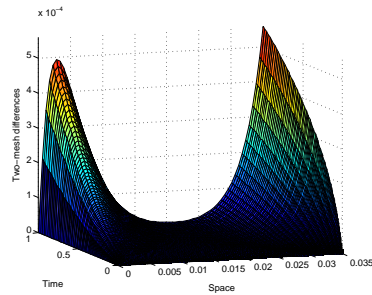

 (a) $\delta = 0.3$, $p = 10^{-5}$ and $N = M = 128$

 (b) $\delta = 0.3$, $p = 10^{-5}$ and $N = M = 256$

 Figure 3: Test problem (7): Two-mesh differences near $x=0$ for the scheme (5) using a graded mesh in time and a Shishkin mesh in space.

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Table 6: Test problem (7) with $p = 10^{-7}$ and several values of δ : Maximum two-mesh differences using a graded mesh in time and a Shishkin mesh in space.

	N=M=32	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\delta = 0.3$	1.121E-002 1.399	4.250E-003 1.505	1.497E-003 1.601	4.934E-004 1.652	1.571E-004 1.689	4.871E-005
$\delta = 0.5$	1.296E-002 1.397	4.919E-003 1.481	1.763E-003 1.583	5.885E-004 1.634	1.896E-004 1.667	5.971E-005
$\delta = 0.7$	1.515E-002 1.385	5.797E-003 1.450	2.122E-003 1.550	7.248E-004 1.591	2.406E-004 1.607	7.900E-005

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