Experimental studies on illposed singularly perturbed boundary value problems for parabolic differential equations

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Abstract. In this paper singularly perturbed parabolic initial-boundary value problems are considered which, in addition, are illposed. The latter means that at one end of the 1-d spatial domain two conditions (for the solution and its spatial derivative) are given while on the other end the corresponding quantities are to be determined. It is well-known that such problems are illposed in the mathematical sense. Here, in addition, boundary layers may occur which make the problems more difficult. For relatively simple examples numerical experiments have been carried out and numerical results are shown. The Conjugate Gradient Methods is used to find the desired quantities iteratively. It will be explained what has to be done in any iteration step. A regularisation is performed by means of discretization and by determining an optimal final iteration step via a stopping rule.

1. Introduction

Singularly perturbed differential equations have the essential feature that a small parameter multiplies the highest derivative. As a consequence, boundary layers may appear at parts of the boundary or even at inner locations. We restrict ourselves to a one-dimensional setting. Typical examples of singularly perturbed ordinary differential equations are displayed in the following Figures 1 and 2, (see the books [1], [2], [3] and the references therein). In parabolic equations, the boundary layers can move (in time). To make it as simple as possible, we do not consider moving boundary layers, and we assume that the solution of the parabolic equation exits and has the form $v_\varepsilon(x,t) = w(t)u_\varepsilon(x)$, where u_ε may be the solution of a singularly perturbed ordinary differential equation having boundary layers - or not.

In parabolic equations one type of inverse problems is the 'Inverse Heat Conduction Problem' or the 'noncharacteristic Cauchy problem' (see [4], [5], [6], [7] and many others). Here, the problem consists in determining the boundary data - i.e. temperature and heat flux - at inaccessible parts of the boundary from corresponding data at accessible parts. The latter are called the 'Cauchy data'. In a one-dimensional setting, the Cauchy data are given at one side of the spatial interval while the unknown quantities have to be determined at the other side. Such problems are known to be ill-posed in the mathematical sense (see, e.g. [8]).

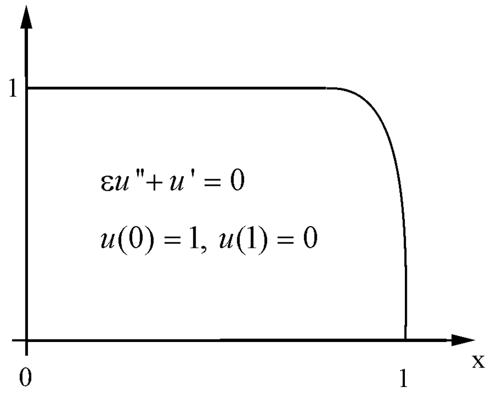

Figure 1. Example of singularly perturbed ode

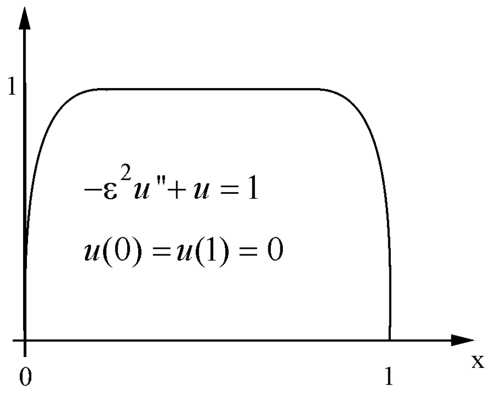

Figure 2. Example of singularly perturbed ode

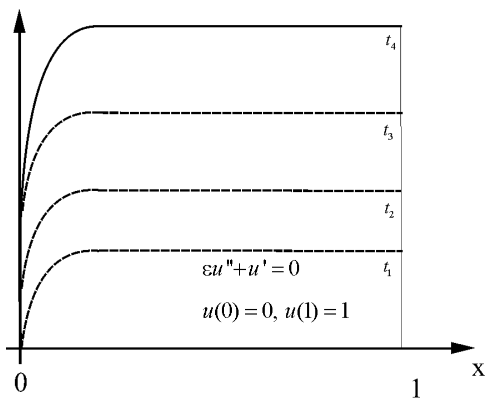

Figure 3. 2 Example of singularly perturbed parabolic equation, $v_\varepsilon(x,t) = w(t)u_\varepsilon(x)$

In this contribution we pose the question, whether in an inverse heat conduction problem the boundary data at the inaccessible part of the boundary can be determined if the underlying equation is singularly perturbed. More precisely, we consider two situations. At first, the Cauchy data are given at the side of the spatial interval where a boundary appears; at the other side no boundary layer exists. Secondly, at the side of the Cauchy data there is no boundary layer while at the other (inaccessible) part of the spatial interval a boundary layer appears. One may consider further situations - like boundary layers of both sides of the spatial interval or equations with inner layers - which will be the subjects of further studies.

The present study tries to answer the question of identifiability of boundary data in case of boundary layers by means of numerical methods. For the iterative solution of the illposed problem we use the Conjugate Gradient Method and solve the underlying parabolic problems by the Crank-Nicolson-Galerkin Method.

For the Conjugate Gradient Method solving Inverse Heat Conduction Problems we have a lot of experience (see [9], [10], [6], [11], [12], [13], [14]). Concerning the other aspect of solving singularly perturbed ordinary and partial differential equations we have used adaptive finite element methods to solve such problems effectively in [Rei81a], [Rei81b], [Rei82a], [Rei82b], [Rei85], [Rei91]. The adaptive and automatic construction of grids is no subject of this paper but can be exploited in further studies.

This paper is organized as follows. After this introduction, illposed singularly perturbed parabolic equations will be introduced. Then the variational approach for solving such problems is explained and the Conjugate Gradient Methods is presented in detail. Finally, experimental results for three examples are displayed and discussed. Conclusions and a list of references finalize this work.

2. Illposed Singularly Perturbed Parabolic Equations

We consider singularly perturbed parabolic partial differential equations of the form

$$v_t(x,t) = \varepsilon^2 v_{xx}(x,t) + c(x)v(x,t) + F(x,t),\ x \in [0,1],\ t \in (0,T]\,, \tag{1}$$

together with boundary conditions at $x = 0$ and $x = 1$ and an inital condition at $t = 0$,

$$v(x,0) = v_0(x) \tag{2}$$

Here, ε denotes a small positive parameter. We assume that $c = c(x)$ only depends on the spatial variable. The solution $v = v_\varepsilon(x,t)$ is assumed to be of the form $v_\varepsilon(x,t) = w(t)u_\varepsilon(x)$ where w can be of the form

$$w(t) = 1 - \exp(-t/\beta) \text{ or } w(t) = t\,. \tag{3}$$

The 'source term' $F = F_\varepsilon(x,t)$ in equation (1) is chosen appropriately.

With this framework we have in mind that $u_\varepsilon = u_\varepsilon(x)$ is some solution of a singularly perturbed ordinary differential equation having boundary layers at $x = 0$ or $x = 1$. We do not consider inner boundary layers. Also, we exclude moving boundary layers (in time).

In the associated *inverse problem*, for given c, F and

$$v_0 = v(x,0),\ \varphi(t) = v|_{x=0},\ g(t) = -\varepsilon^2 v_x|_{x=0} \tag{4}$$

one wants to find the heat flux

$$q(t) = \varepsilon^2 v_x|_{x=1}$$

where v is the solution of equation (1), (2) (see Fig. 4).

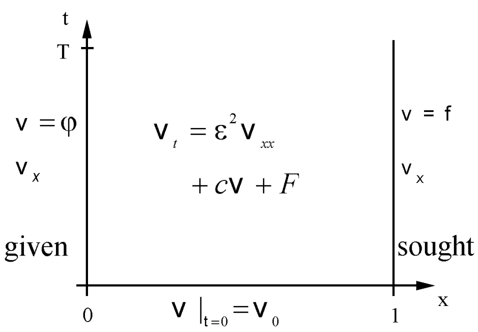

Figure 4. Inverse heat conduction problem

When q is available, also $f = v|_{x=1}$ can be determined. Alternatively, one can first try to find f and then determine q. Such a problem is also called *noncharacteristic Cauchy problem for a parabolic equation*; φ and g are called the *Cauchy data*.

In the following, we start with an initial guess for q and try to improve this iteratively until an appropriate stopping criterion is fulfilled. For this, we also use the notation

$$v = v_\varepsilon(x,t;q)\,.$$

We assume that the above inverse problem (1), (2), (4) has a unique solution.

3. Variational Approach and Conjugate Gradient Method

In the variational approach, instead of solving (1), (2), (4) one tries to minimize the functional

$$J(q) \;=\; \frac{1}{2}\big\|v(0,\cdot;q) - \varphi(\cdot)\big\|^2_{L^2(0,T)} \tag{5}$$

where v is the solution of the following *direct problem* (DP)

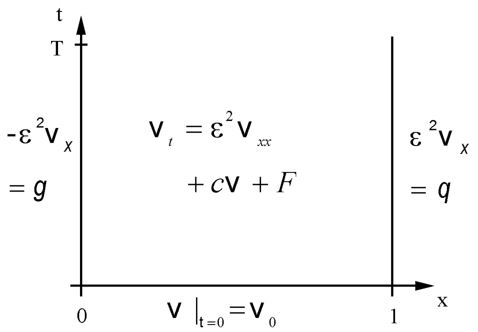

Figure 5. Direct problem

$$\textbf{(DP)} \begin{cases} v_t = \varepsilon^2 v_{xx} + cv + F \\ -\varepsilon^2 v_x|_{x=0} = g,\ \varepsilon^2 v_x|_{x=1} = q \\ v(\cdot,0) = v_0 \end{cases} \tag{6}$$

In (5) one can also add a penalty term, and minimize the functional.

$$J_\gamma(q) = \frac{1}{2}\big\|v(0,\cdot;q) - \varphi(\cdot)\big\|^2_{L^2(0,T)} + \gamma\|q\|^2_{L^2(0,T)}\,. \tag{7}$$

This is the well-known *Tikkonov regularization*, and $\gamma > 0$ is the *regularization parameter* which has to be chosen in an optimal way.

The Conjugate Gradient Method (abr.: CGM) is a suitable method for solving such minimisation problems. For this one needs the gradient of the functional (5) w.r.t. q. One can obtain the gradient by means of the solution of the associated *adjoint problem* (AP),

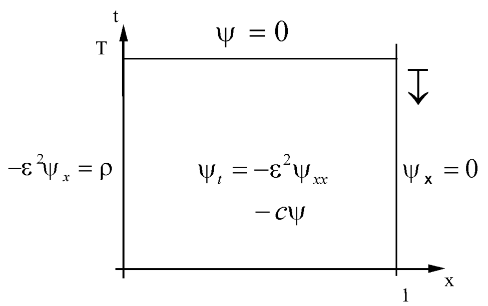

Figure 6. Adjoint problem

$$\textbf{(AP)} \begin{cases} \psi_t = -\varepsilon^2\psi_{xx} - c\psi,\ 0 \le x \le 1, \quad 0 \le t < T \\ \psi(x,T) = 0 \\ -\varepsilon^2\psi_x|_{x=0} = \underbrace{v(0,t;q) - \varphi(t)}_{=:\rho(t)=\text{ defect/residual}} \\ \psi_x|_{x=1} = 0 \end{cases} \tag{8}$$

The gradient is then obtained by

$$J'(q) = \psi(x,t;q)|_{x=1}\,. \tag{9}$$

Note, that the parabolic equation (8) is backward in time but wellposed. Indeed the transformation

$$\tau = T - t,\ \hat\psi = \hat\psi(x,\tau) = \psi(x, T-\tau)$$

yields the following equations equivalent to (8),

$$(\mathrm{AP}) \iff \begin{cases} \hat{\psi}_\tau = \varepsilon^2 \hat{\psi}_{xx} + c\hat{\psi},\ 0 \le x \le 1,\ 0 < \tau \le T \\ \hat{\psi}(x,0) = 0(\text{ initial cond.}) \\ -\varepsilon^2 \hat{\psi}_x|_{x=0} = \rho(T-\tau),\ \hat{\psi}_x|_{x=1} = 0 \end{cases} \tag{10}$$

The CGM for solving the minimisation problem (5), (6) proceeds as follows:

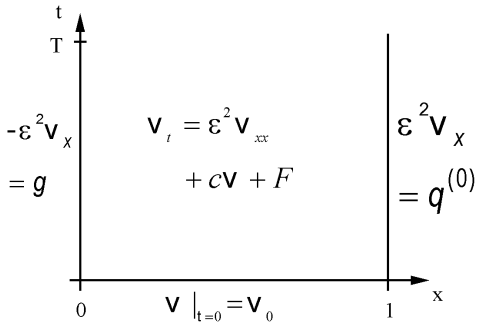

Figure 7. Step 0 of CGM

Step 0: Guess $q = q(t) = q^{(0)}(t)$ (e.g. $q^{(0)} = 0$) and solve

$$(\mathrm{DP}) \begin{cases} v_t = \varepsilon^2 v_{xx} + cv + F,\ 0 \le x \le 1,\ 0 < t \le T \\ -\varepsilon^2 v_x|_{x=0} = g,\ \varepsilon^2 v_x|_{x=1} = q^{(0)}, \\ v|_{t=0} = v_0\,; \end{cases}$$

with solution $v^{(0)} = v(x,t;q^{(0)})$; determine *defect* $\rho^{(0)} = v^{(0)}(0,\cdot) - \varphi(\cdot)$ and set $k = 0$.

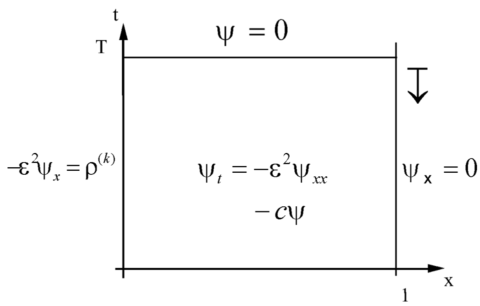

Figure 8. Step 1 of CGM

Step 1: Solve (AP) with $q^{(k)}$ ($\rightarrow$ solution $\psi^{(k)}$) i.e.

$$\begin{aligned} &\psi_t^{(k)} = -\varepsilon^2 \psi_{xx}^{(k)} - c\psi^{(k)}, \quad 0 \le x \le 1, \quad 0 \le t < T\,, \\ &\psi^{(k)}(x,T) = 0\,, \quad 0 \le x \le 1, \\ &-\varepsilon^2 \psi_x^{(k)}|_{x=0} = \underbrace{v^{(k)}(0,\cdot) - \varphi(\cdot)}_{\rho^{(k)}}, \quad \psi_x^{(k)}|_{x=1} = 0, \\ &\qquad\qquad 0 \le t < T\,; \end{aligned}$$

set $d^{(0)} = -r^{(0)} (k=0)$, $d^{(k)} = -r^{(k)} + \beta_k d^{(k-1)}$ $(k \ge 1)$ where $\beta_k = \|r^{(k)}\|_{L^2}^2 / \|r^{(k-1)}\|_{L^2}^2 (k \ge 1)$, $r^{(k)} = \psi^{(k)}|_{x=1}$.

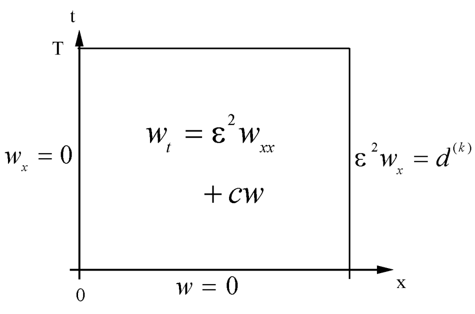

Figure 9. Step 2 of CGM

Step 2: Solve (DP) with $g = 0$, $F = 0$ with initial-boundary conditions

$$\begin{aligned} &w_x|_{x=0} = 0,\ \varepsilon^2 w_x\,|_{x=1} = d^{(k)},\ 0 < t \le T \\ &w|_{t=0} = 0 \end{aligned}$$

$\big(\longrightarrow$ solution $w = w^{(k)} = w^{(k)}(x,t;d^{(k)})\big)$ and set $\alpha_k = \|r^{(k)}\|_{L^2}^2 \,/\, \|w^{(k)}\big(0,\cdot;d^{(k)}\big)\big)\|_{L^2}^2$, $q^{(k+1)} = q^{(k)} + \alpha_k d^{(k)}$

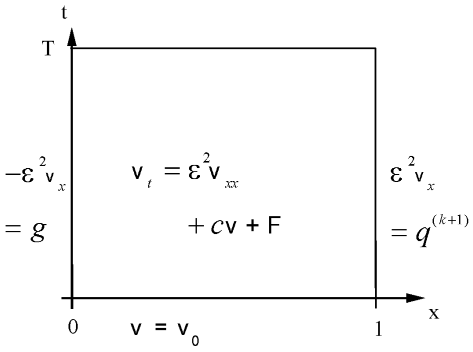

Figure 10. Step 3 of CGM

Step 3: Solve (DP) with
$-\varepsilon^2 v_x|_{x=0} = g, \quad \varepsilon^2 v_x|_{x=1} = q^{(k+1)}$
($\longrightarrow$ solution $v^{(k+1)}$) and determine *defect*
$\rho^{(k+1)} = v^{(k+1)}(0,\cdot) - \varphi(\cdot)$.
Go to Step 1 with $k+1 \longrightarrow k$.
Remark: Only 2 direct solutions are needed in every iteration step!

Note that perturbations of the Cauchy data are allowed. Here, we consider only perturbations of φ,

$$\|\varphi - \varphi_\delta\|_{L^2(0,T)} \leq \delta\,. \tag{11}$$

The stopping rule due to Morozov [21] stops at the first index $k = k(\delta)$ where the defect is of the magnitude of the data perturbation; more precisely, when

$$\|v^{(k)}(0,\cdot;q^{(k)}) - \varphi_\delta(\cdot)\|_{L^2(0,T)} \leq \gamma_1\delta\,. \tag{12}$$

Here, γ_1 is a constant close to one, $\gamma_1 \approx 1$. If we use discretization or projection methods of accuracy $O(h)$ to solve the underlying parabolic equations numerically, the stopping rule has to be extended to

$$\|v^{(k)}(0,\cdot;q^{(k)}) - \varphi_\delta(\cdot)\|_{L^2(0,T)} \leq \gamma_1(\delta + h\|q^{(k)}\|_{L^2})\,. \tag{13}$$

(s. Nemirowski [22]).

The following results are well-known for the CGM:

- The CGM is a 'regularization method', i.e. the stopping rule gives final $k's$; $k = k\,(\delta, h)\; s.t.$, $q = q^{\left(k(\delta,h)\right)} \longrightarrow q(\delta \longrightarrow 0,\, h \longrightarrow 0)$
- There may be orders of convergence under strong assumptions.
- Big errors can occur near the final time T (explanation known; improvements possible).
- In (7), γ can be also determined in an optimal way by a stopping rule.

Note that everything depends on the small parameter $\varepsilon > 0$ which is assumed to be fixed.

4. Experimental Results

In our experimental studies, we have considered three examples with the following solutions of (1):

Example 1: $v(x,t) = \left(1 - \exp(-\frac{t}{0.4})\right) \frac{1-\exp\left(-(1-x)/\varepsilon\right)}{1-\exp(-1/\varepsilon)}$

Example 2: $v(x,t) = t\left\{x + \frac{\exp\left(-(1+x)/\varepsilon\right) - \exp\left(-(1-x)/\varepsilon\right)}{1-\exp(-2/\varepsilon)}\right\}$

Example 3: $v(x,t) = \left(1 - \exp(-\frac{t}{0.4})\right) \frac{1-\exp(-x/\varepsilon)}{1-\exp(-1/\varepsilon)}$

The functions F are chosen accordingly; c is set to be -1. In Example 1 a boundary layer appears at $x = 1$ (see Fig. 12) while in the remaining part of the spatial interval the solution is nearly constant. Because of the exponential factor $w(t) = 1 - \exp(-t/0.4)$, for $t \approx 1$ and larger the solution is nearly a stationary one.

In Example 2, again a boundary layer appears at $x = 1$ while in the remaining x-interval the solution is nearly linear. The factor w is here chosen to be $w(t) = t$. Example 3 is obtained from Example 1 by using the transformation $x \longrightarrow 1 - x$. Hence, the boundary layer appears at $x = 0$.

As we have said in the beginning, in Example 1 and 2 we try to identify the boundary data at the side of the x-interval where the boundary layer appears; the Cauchy data are given at $x = 0$ where no boundary layer exists. In Example 3 the situation is just the converse: The boundary layer appears at the side where Cauchy data are given while at the inaccessible part of the boundary no boundary layer shows up.

All examples are computed with the Crank–Nicolson–Galerkin Method (abr. CNG) with continuous, piecewise linear basis functions for the spatial approximation. If nothing else is said we have used

$$\triangle x = 0.125,\ \triangle t = 0.05,\ T = 1.0,\ \delta = 10^{-8}\,.$$

For the ε's we have taken $\varepsilon^2 = 0.1$ and $\varepsilon^2 = 0.005$. In the first case, because of the relatively large ε, no boundary layer appears.

In Figure 11 very good numerical results can be seen for Example 1 at two different times. Here, $\varepsilon^2 = 0.1$ which is the case of no boundary layers. Figure 12 shows the exact solution for three different times for the same example but with boundary layer at $x = 1$ - due to $\varepsilon^2 = 0.005$. In the following Figure 13 the numerical solutions (together with the exact solution) are displayed for two different times. Near the boundary layer (at $x = 1$) the numerical results become worse. However, the results are not completely bad. Here, the CGM has stopped after two iterations while in Figure 11 twenty iterations have been performed. In Figure 14 the desired heat flux and its numerical approximation at $x = 1$ is seen for Example 1 and $\varepsilon^2 = 0.005$. The exact heat flux in this example is given by $\varepsilon^2 v_x(1,t) = -\varepsilon \frac{1-\exp(-t/0.4)}{1-\exp(-1/\varepsilon)}$. Due to the factor ε, the heat flux at $x = 1$ is nearly zero. The absolute error for the numerical heat flux is moderate.

Numerical results for Example 2 are shown in Figure 15 to Figure 17. In Figure 15 the results for a relatively large ε, $\varepsilon^2 = 0.1$, are again very good. Also, the results for $\varepsilon^2 = 0.005$ in Figures 16 and 17 are good. The exact heat flux at $x = 1$ (s. Figure 17) is again nearly zero,

$$\varepsilon^2 v_x(1,t) = \varepsilon t \left\{ \varepsilon - \frac{1 + \exp(-2/\varepsilon)}{1 - \exp(-2/\varepsilon)} \right\} ;$$

the numerical heat flux is nearly zero, as well.

One possible explanation for the relatively good results in the above mentioned figures may be that the CGM is started with initial guess $q^{(0)} = 0$. This is already a good approximation for the desired heat flux at $x = 1$ as explained above. In Figure 18 for Example 1 one can see the initial approximation $v^{(0)}(x,t)$, for $t = 1$ and with $\Delta x = 1/16$, calculated with a 'bad' initial guess $q^{(0)} = 0.5$ for the heat flux at $x = 1$; here again $\varepsilon^2 = 0.005$. It can be observed that the defect at $x = 0$, $\rho^{(0)}(1) = v^{(0)}(0,1;q^{(0)}) - \varphi(1)$, nearly vanishes. Hence, in Step 1 of the CGM the gradient obtained by the solution of the Adjoint Problem nearly vanishes, and further iterations of the CNG yield no improvements. It can be even observed that further iterations produce useless results with large errors. One may conjecture that the boundary layer at $x = 1$ is responsible for the fact that boundary data at the boundary layer location have no influence on the solution outside the boundary layer.

In Example 3 the situation is just the converse, namely the Cauchy data are at the boundary layer location and no boundary layer is at $x = 1$. Again, the initial guess for the heat flux at $x = 1$ is $q^{(0)} = 0.5$. In Figure 19 it can be seen that, similarly to the last figure, the boundary values at $x = 1$ have nearly no influence on the boundary values at $x = 0$ of the numerical solution and, hence, the defect and the gradient nearly vanishes. Here, again $\Delta x = 1/16$. One may say that a 'numerical boundary layer' appears at $x = 1$ while the (analytical) boundary layer is at $x = 0$. Here, as in the previous figure, further iterations will not improve the numerical approximations of the heat flux at $x = 1$ – they even produce larger and larger errors.

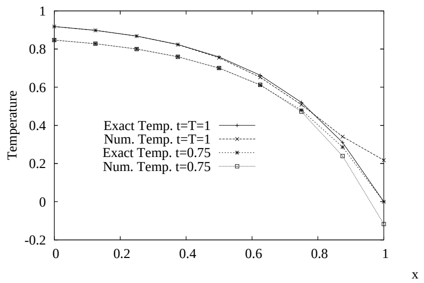

Figure 11. Ex. 1: Temp. (in x) for 2 times, $\varepsilon^2 = 0.1$.

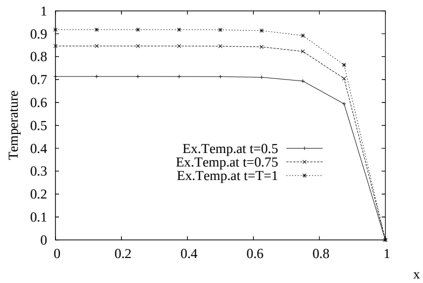

Figure 12. Ex. 1: Solution (in x) at 3 times, $\varepsilon^2 = 0.005$.

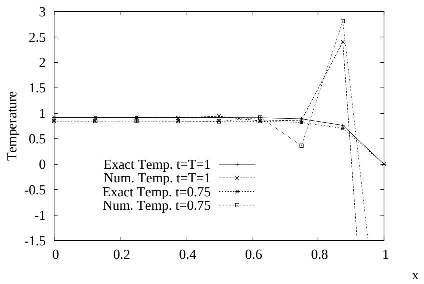

Figure 13. Ex. 1: Temp. (in x) for 2 times, $\varepsilon^2 = 0.005$.

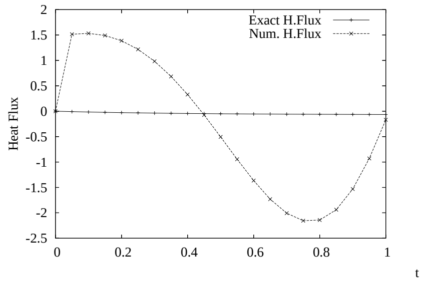

Figure 14. Ex. 1: Heat Flux at $x = 1$ for $\varepsilon^2 = 0.005$.

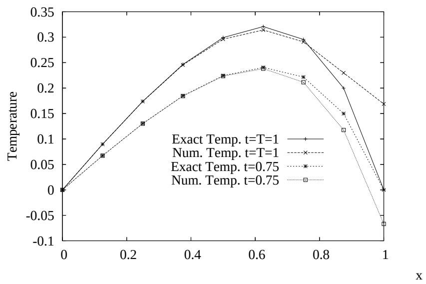

Figure 15. Ex. 2: Temp. (in x) for 2 times, $\varepsilon^2 = 0.1$.

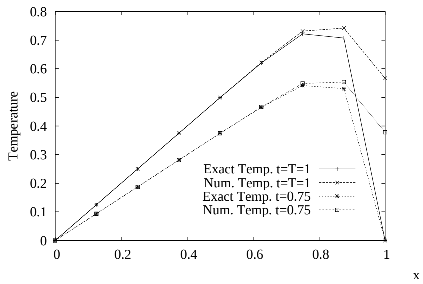

Figure 16. Ex. 2: Temp. (in x) for 2 times, $\varepsilon^2 = 0.005$.

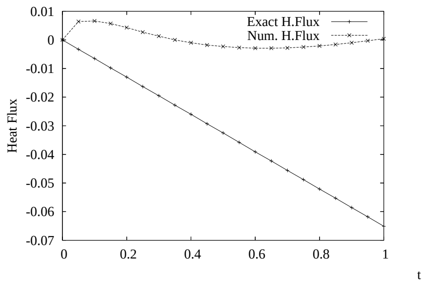

Figure 17. Ex. 2: Heat Flux at $x = 1$ for $\varepsilon^2 = 0.005$.

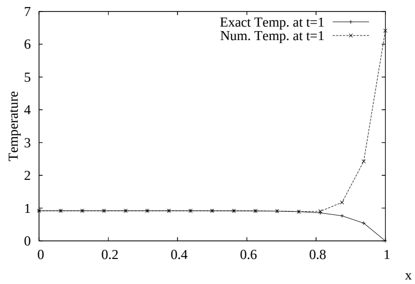

Figure 18. Ex. 1: Temp. (in x), $\varepsilon^2 = 0.005$, for $q^{(k)} = 0.5, k = 0$.

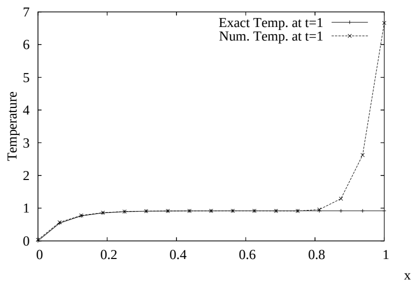

Figure 19. Ex. 3: Temp. (in x), $\varepsilon^2 = 0.005$, for $q^{(k)} = 0.5, k = 0$.

5. Questions and Conclusions

Our numerical experiments have left a series of problems open. First of all, for small ε it is not clear whether the boundary values (heat flux and temperature) can be identified at the inaccessible part of the boundary. This is an open question in cases when the Cauchy data are at the boundary layer location or when the boundary layer appears at the inaccessible part of the boundary.

The above examples are given in dimensionless form – in space and time. It is well-known that boundary data cannot be identified if the inaccessible parts are to far away from the accessible parts where the Cauchy data are given. Here, the influence of small ε's should be analysed with regard to 'far' and 'close'.

There are numerical methods for noncharacteristic Cauchy problems for parabolic equations, like the Beck method (see [4], [11], [12]) which may be more stable in cases of small ε's.

Singularly perturbed equations should be numerically solved with adapted grids. The choice of the grid points could be done a-priorily – like the Shishkin mesh (see [3], [23]) – or a-posteriorily with automatically chosen grids (see e.g. [15], [16], [18], [19], [20]). Finally, the influence of the small ε on iterative methods for solving the illposed problems is completely open.

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