THE HERMITE SCHEME FOR SEMILINEAR SINGULAR PERTURBATION PROBLEMS*1)

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Abstract

A numerical method for singularly perturbed semilinear boundary value problems is given. The method uses the fourth order Hermite scheme on a special discretization mesh. Its stability and convergence are investigated in the discrete L^1 norm.

§1. Introduction

We shall consider the following singularly perturbed boundary value problem:

$$T_u := -\varepsilon^2 u'' + c(x, u) = 0, \ x \in I = [0, 1],$$

 $u(0) = u(1) = 0,$ (1)

where $\varepsilon \in (0, \varepsilon^*]$ (usually $\varepsilon^* << 1$). Throughout the paper we shall assume:

$$c \in C^6(I \times I\!\! R),$$
 (2.a)

$$c_{u}(x,u) > \gamma^{2}, (x,u) \in I \times IR, \gamma > 0.$$
 (2.b)

These conditions guarantee that the problem (1) has a unique solution u_{ϵ} , $u_{\epsilon} \in C^{B}(I \times IR)$, which exhibits two boundary layers at the endpoints of I. In particular, the following estimates hold, see [22]:

$$|u_{\varepsilon}^{(k)}(x)| \leq M[1 + \varepsilon^{-k}(\exp(-\gamma x/\varepsilon) + \exp(\gamma(x-1)/\varepsilon))], \ x \in I, \ k = 0(1)6,$$
 where M does not depend on ε .

Because of such a behaviour of u_{ϵ} it is necessary to use special methods to solve the problem numerically. We shall use a finite-difference scheme on a special non-equidistant discretization mesh which is dense in the layers. The mesh will guarantee that the local truncation errors of the scheme will be uniform (by "uniform" we shall always mean "uniform in ϵ "); hence the discretization will be uniformly consistent

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with the continuous problem. Then the uniform convergence (the convergence of the numerical solution towards the restriction of u_{ϵ} on the mesh) will follow if we show that our discretization is uniformly stable. Usually, as in Doolan, Miller, Schilders [7], Herceg, Vulanović [13], Herceg [8, 9, 10], Herceg, Petrović [12], Herceg, Vualnović, Petrović [14], Vulanović, Herceg, Petrović [26], Vulanović [21, 22, 23], the stability is shown in the maximum norm; hence the pointwise uniform convergence follows. The order of the convergence depends on the scheme used. Higher order convergence was proved in Vulanović, Herceg, Petrović [26], Herceg, Vulanović, Petrović [14] and Herceg [9], while Herceg [10], and Herceg, Petrović [12] used higher order schemes in the layers only. These papers, as well as Vulanović [23], Herceg, Vulanović [13] and Vulanović [23], use the approach of special discretization meshes. The concept of exponential fitting was used in Doolan, Miller, Schilders [7], Herceg [8], Vulanović [21], and Vulanović [23]. The method from [3] is based on piecewise linear interpolation, and for the use of spline-difference schemes see Surla [16, 17, 18, 19]. For other papers which deal with the numerical solution of the problem (1), see Herceg [9].

In this paper we shall use a discretization of the same type as in Herceg [9], Herceg, Vulanović, Petrović [14]. Basically, the Hermite scheme is used, but at some mesh points it is replaced by the standard central scheme. Such a switch is used in order to prove the uniform stability. For the same reason Herceg [9] and Herceg, Vulanović, Petrović [14] have a restriction on the nonlinearity of c(x, u). Essentially, the following is required:

$$c_u(x,u) \le \Gamma, x \in I, u \in IR; \quad 5\gamma^2 - 2\Gamma > 0.$$
 (4)

Obviously, such an assumption is unpleasant, and our aim here will be to avoid it. We shall prove the uniform stability in the discrete L^1 norm (cf. Vulanovi \acute{c} [24], [25] where this norm was used for discretizations of quasilinear singular perturbation problems) and for this (4) is not needed. Such a result was announced in Herceg [9] and Herceg, Vulanovi \acute{c} , Petrovi \acute{c} [14].

Thus we shall obtain the uniform convergence in the discrete L^1 norm. The L^1 -error will be estimated by

$$M[\varepsilon n^{-4} + n^{-1}\exp(-pn)]$$

where n is the number of mesh steps, p is a positive constant independent of n and ε , and throughout the paper M denotes a positive generic constant independent of n and ε . From this we shall get that

$$M[n^{-3}+\varepsilon^{-1}\exp(-pn)]$$

is the upper bound for the maximal pointwise error. This is worse than Mn^{-4} from Herceg [9]. However, we point out that the numerical method which will be given here is essentially the same as the method from Herceg [9] (the deferent pointwise error estimates result from the different norms used); hence we might expect the uniform fourth order pointwise convergence to be still present. Our numerical experiments confirm that.

Let us finally note that problems of type (1) arise in practice as models for chemical catalysis reactions and the Michaelis-Menten process in biology, Bohl [1]. For other applications see [2] and [3].

§2. The Numerical Method

Let us introduce the discretization mesh I_h with the mesh points

$$x_i = \lambda(t_i), \ t_i = ih, \ i = 0, 1, \dots, n; \quad h = \frac{1}{n}, \ n = 2m, m \in \mathbb{N} \setminus \{1\},$$

where λ is a mesh generating function:

$$\lambda(t) = \left\{ egin{array}{l} \mu(t) = rac{lpha arepsilon t}{q-t}, & t \in [0,lpha], \ \mu'(lpha)(t-lpha) + \mu(lpha), & t \in [lpha,0.5], \ 1-\lambda(1-t), & t \in [0.5,1]. \end{array}
ight.$$

Here q is an arbitrary number from (0, 0.5) and $a \in (0, q/\epsilon^*]$. The point α is determined from

$$\mu'(\alpha)(0.5-\alpha)+\mu(\alpha)=0.5,$$

 $\mu'(\alpha)(0.5-\alpha)+\mu(\alpha)=0.5,$ which reduces to a quadratic equation and α is easy to find:

$$\alpha = \frac{q - \sqrt{aq\varepsilon(1 - 2q + 2a\varepsilon)}}{1 + 2a\varepsilon}.$$

We have $\lambda \in C^1(I)$ and

$$0 < \lambda'(t) \le M, \ t \in I. \tag{5}$$

Such a mesh generating function was introduced in Vulanović [22] and used in our other papers, and in Herceg [9] in particular.

Let

$$h_i = x_i - x_{i-1}, i = 1(1)n, \bar{h}_i = (h_i + h_{i+1})/2, i = 1(1)n - 1.$$

It is obvious that

$$h_i \leq h_{i+1}, i = 1(1)m - 1, h_i = h_{n-i+1}, i = 1(1)m.$$
 (6)

By w^h, v^h etc. we shall denote mesh functions defined on $I_h/\{0,1\}$. They will be identified with \mathbb{R}^{n-1} - column vectors:

$$w^h = [w_1, w_2, \cdots, w_{n-1}]^T, \quad w_i := w_i^h.$$

In particular, we shall take

$$u_{\epsilon}^{h} = [u_{\epsilon}(x_{1}), u_{\epsilon}(x_{2}), \cdots, u_{\epsilon}(x_{n-1})]^{T}.$$

Let $||\cdot||_{\infty}$ and $||\cdot||_1$ be the usual norms in \mathbb{R}^{n-1} . The discrete L^1 norm is given by

$$||w^h||_1^h = ||Hw^h||_1 = \sum_{i=1}^{n-1} \bar{h}_i |w_i|, \quad H = \operatorname{diag}(\bar{h}_1, \bar{h}_2, \cdots, \bar{h}_{n-1});$$

see [24, 25]. The corresponding matrix norms will be denoted in the same way. In particular, we have

$$||A||_1^h = ||HAH^{-1}||_1, A \in \mathbb{R}^{n-1,n-1}.$$

We shall use two approximations of the differentiations operator T: the Hermitian approximation (see [9], [14]):

$$T_H w_i = -\varepsilon^2 D w_i + b_1(i) c_{i-1} + b_0(i) c_i + b_2(i) c_{i+1}, \ i = 1(1)n - 1$$

and the central approximation:

$$T_c w_i = -\varepsilon^2 D w_i + c_i, \ i = 1(1)n - 1.$$

Here

$$Dw_{i} = [(w_{i+1} - w_{i})/h_{i+1} + (w_{i_{1}} - w_{i})/h_{i}]/\bar{h}_{i},$$

$$b_{1}(i) = (h_{i}^{2} - h_{i+1}^{2} + h_{i}h_{i+1})/12h_{i}\bar{h}_{i},$$

$$b_{2}(i) = (h_{i+1}^{2} - h_{i}^{2} + h_{i}h_{i+1})/12h_{i+1}\bar{h}_{i},$$

$$b_{0}(i) = 1 - b_{1}(i) - b_{2}(i),$$

$$c_{j} = c(x_{j}, w_{j}).$$

These two approximations will be combined to make a discrete problem on the mesh I_h , corresponding to (1).

Let

$$Q = \frac{3}{5}(7 + \sqrt{14}) = 6.4449944\cdots$$

and

$$I'_h = \{x_i \in I_h: q - Qh < t_{i-1}, \alpha \text{ or } 1 - \alpha < t_{i+1} < 1 - Qh\}$$

(note that I'_h may be empty). Note that [9] uses a different (smaller) value of Q. This is the only difference between the two methods, caused by technical reasons.

The discrete problem is given by

$$Fw^h=0, (7)$$

where

First we shall investigate the stability of the operator F.

Theorem 1. Let $c \in C^1(I \times IR)$ and let (2b) hold. Then the discrete problem has a unique solition w_{ϵ}^h which is a point of attraction of SOR-Nowton and Newton-SOR methods with the relaxation parameter $\omega \in (0,1]$. Moreover, the following stability inequality holds for any $w_{\epsilon}^h, v_{\epsilon}^h$:

$$||w^h - v^h||_1^h \le \frac{12}{\gamma^2} ||Fw^h - Fv^h||_1^h.$$
 (8)

Proof. The Trechet derivative $F'(w^h)$ of F at arbitrary w^h is a tridiagonal matrix:

with

$$A_{i} = -\varepsilon^{2}/h_{i}\bar{h}_{i} + a_{1}(i)c_{u}(x_{i-1,w_{i-1}}),$$

$$B_{i} = 2\varepsilon^{2}/h_{i}h_{i+1} + a_{0}(i)c_{u}(x_{i},w_{i}),$$

$$C_{i} = -\varepsilon^{2}/h_{i+1}\bar{h}_{i} + a_{2}(i)c_{u}(x_{i+1},w_{i+1}),$$

where

$$a_j(i) = \begin{cases} b_j(i), & x_i \in I_h \setminus I'_h, \\ 0, & x_i \in I'_h, & j = 1, 2, \end{cases}$$
 $a_0(i) = 1 - a_1(i) - a_2(i).$

Let us write formally

$$C_0=A_n=0.$$

We shall show that

$$||F'(w^h)^{-1}||_1^h \le 12/\gamma^2 \tag{9}$$

and (8) will be immediate (note that $\|\cdot\|_{\infty}$ was used in Herceg [9] and because of that a condition of type (4) was needed). At the same time, (9) will imply the rest of the assertion; see Ortega, Rheinboldt [15].

In order to prove (9) we shall show

$$\sigma_i := |B_i| - |C_{i-1}|\bar{h}_i - |A_{i+1}|\bar{h}_{i+1}/\bar{h}_i \ge \gamma^2/12, \ i = 1(1)n - 1. \tag{10}$$

This means that $HF'(w^h)H^{-1}$ is strictly diagonally dominant by columns and it follows that

$$||(HF'(w^h)H^{-1})^{-1}||_1 \le 12/\gamma^2;$$

see Varah [20]. This is in fact inequality (9) since

$$||(HF'(w^h)H^{-1})^{-1}||_1 = ||HF'(w^h)^{-1}H^{-1}||_1 = ||F'(w^h)^{-1}||_1^h;$$

cf. Vulanović [24, 25].

Let us prove (10) for i = 1(1)m (for other indices the proof is analogous by the symmetry (6)). This proof is similar to the proof from Herceg [9]. It always holds that

$$B_i > 0$$
.

If x_{i-1} , x_i , $x_{i+1} \in I'_h$ we have

$$C_{i-1} \leq 0, \ A_{i+1} \leq 0$$

and it easily follows that

$$\sigma_i \geq \gamma^2$$
.

Now suppose x_{i-1} , $x_i, x_{i+1} \in I_h \setminus I'_h$ and let us consider the hardest possible situation when

$$C_{i-1} \geq 0, \ A_{i+1} \geq 0;$$

cf. Herceg [9]. Using estimates from Herceg [9] and Herceg, Vulanović, Petrović [14]:

$$b_0(i) \geq \frac{5}{6}, \ \frac{1}{6} \geq b_2(i) \geq \frac{1}{12}, \ b_2(i) \geq b_1(i) \geq -\frac{1}{6},$$

we get

$$\begin{split} \sigma &\geq \frac{\gamma^2}{\bar{h}_i} [b_0(i)\bar{h}_i - |b_1(i+1)|\bar{h}_{i+1} - b_2(i-1)\bar{h}_{i-1}] \\ &\geq \frac{\gamma^2}{\bar{h}_i} [\frac{5}{6}\bar{h}_i \frac{1}{6}\bar{h}_{i+1} - \frac{1}{6}\bar{h}_{i-1}] \geq [\frac{2}{3} - \frac{1}{6}\frac{\bar{h}_{i+1}}{\bar{h}_i}]\gamma^2 \geq \frac{\gamma^2}{12}. \end{split}$$

The last inequality follows because we have

$$2\bar{h}_{i+1} \le 7\bar{h}_i. \tag{11}$$

Indeed, if $t_{i-1} \geq \alpha$, it holds that $\bar{h}_{i+1} = \bar{h}_i$, and if, on the other hand, $t_{i-1} < \alpha$, we use

$$t_{i-1} \le q - Qh \tag{12}$$

(which holds because $x_i \in I_h \setminus I'_h$) to get

$$\frac{\bar{h}_{i+1}}{\bar{h}_i} \leq \frac{\mu'(t_{i+1})}{\mu'(t_{i-1})} \leq \left(\frac{q-t_{i-1}}{q-t_{i+2}}\right)^2$$

(note that $t_{i+2} < q$). Finally, (11) follows since (12) is equivalent to

$$\left(\frac{q-t_{i-1}}{q-t_{i+2}}\right)^2 \leq \frac{7}{2}.$$

Note that for i=1 we have $C_0=0$ and that situation is better than the one considered. This is also true for the case when $x_{i-1} \in I_h \setminus I'_h(x_{i-1}, x_i \in I_h \setminus I'_h)$ and $x_i, x_{i+1} \in I'_h(x_{i+1} \in I'_h)$. Thus (10) is proved and so is the theorem.

Let us mention that besides SOR-Newton methods, AOR-Newton methods (see Cvetković, Herceg [4,5,6], Herceg, Cvetković [11]) may be used to solve the discrete problem (7).

Now let us consider the consistency error

$$r^h = Fu_\varepsilon^h$$
.

Let

$$d = \varepsilon h^4 + h \cdot \exp(-pn),$$

where

$$p = \operatorname{aq} \gamma/Q$$
.

Theorem 2. Let (2) hold. Then it follows that

$$||r^h||_1^h \le Md. \tag{13}$$

Proof. We shall estimate $\bar{h}_i|r_i|$, i=1(1)m-1, where r_i are components of r^h . For i=m(1)n the estimates can be obtained analogously. We shall use (3) which reduces to

$$|u_{\varepsilon}^{(k)}(x)| \le M[1 + \varepsilon^{-k} \exp(-\gamma x/\varepsilon)], \ x \in [0, 0.5], \ k = 0(1)6.$$
 (14)

As in Herceg [9], Vulanović [22], Herceg, Vulanović, Pereović [14] and our other papers, we distinguish the following three cases:

$$1^{\circ} t_{i-1} \geq \alpha,$$

$$2^{\circ}$$
 $t_{i-1} < \alpha$ and $t_{i-1} \leq q - Qh$,

$$3^{\circ} q - Qh < t_{i-1} < \alpha$$
.

In cases 1^0 and 2^0 it holds that $x_i \in I_h \setminus I_h'$. By expanding r_i in the same way as in Herceg [9], and using the same technique we can prove

$$|\bar{h}_i|r_i| \le M\varepsilon h^5. \tag{15}$$

When case 3^0 holds we have $x_i \in I_h'$ and the central scheme is used:

$$r_i = \varepsilon^2 [u^n_{\epsilon}(x_i) - Du_{\epsilon}(x_i)].$$

Now we have to use a technique different from Herceg [9]. We use the following integral representation of r_i :

$$\bar{h}_i r_i = -\frac{1}{2h_{i+1}} \int_{x_i}^{x_{i+1}} (s - x_{x+1})^2 u_{\epsilon}^{n'}(s) ds - \frac{1}{2h_i} \int_{x_i}^{x_{i-1}} (s - x_{i-1})^2 u_{\epsilon}^{n'}(s) ds.$$

Then from (14) and (5) we get

$$|\bar{h}_i|r_i| \leq M \left[\varepsilon^2 h^2 + \frac{1}{\varepsilon h_{i+1}} \int_{x_i}^{x_{i+1}} (s - x_{i+1})^2 \exp(-\gamma s/\varepsilon) ds\right]$$

$$+\frac{1}{2h_i}\int_{x_{i-1}}^{x_i}(s-x_{i-1})^2\exp\left(-\gamma s/\varepsilon\right)ds$$

and after two partial integrations there follows

$$|\bar{h}_i|r_i| \le M[\varepsilon^2 h^2 + \bar{h}_i \cdot \exp(-\gamma x_{i-1}/\varepsilon)] \le M[\varepsilon^2 h^2 + h \cdot \exp(-aq\gamma/(q - t_{i-1}))]$$

 $\le M[\varepsilon^2 h^2 + h \cdot \exp(-aq\gamma/Qh)] = M[\varepsilon^2 h^2 + h \cdot \exp(-pn)].$

Because of

$$q - Qh < t_{i-1} < \alpha \le q - M\sqrt{\varepsilon} < q$$

case 3° can be true only if

$$\sqrt{\varepsilon} \leq Mh$$
,

and it follows that

$$|\bar{h}_i|r_i| \leq M[\varepsilon^2 h^4 + h \cdot \exp(-pn)].$$

Also note that case 30 can happen at 7 points at most. Thus we have

$$||r^h||_1^h \leq \sum_{i \neq i} \bar{h}_i |r_i| + Md, \quad x_i \in I_h \setminus I_h'$$

and from (15) we get (13).

By combining Theorems 1 and 2 we have the convergence theorem:

Theorem 3. Let (2) hold. Then it follows that

$$||w_{\epsilon}^h - u_{\epsilon}^h||_1^h \leq Md.$$

Since

$$||w^h||_1^h \geq \bar{h}_1 ||w^h||_{\infty} \geq M\varepsilon h ||w^h||_{\infty},$$

we have the following

Corollary. Let (2) hold. Then it follows that

$$||w_{\varepsilon}^{h}-u_{\varepsilon}^{h}||_{\infty}\leq M[h^{3}+\varepsilon^{-1}\cdot\exp\left(-pn\right)].$$

The last result is almost the third order uniform pointwise convergence, but as we have said, we expect numerical results to show

$$||w_{\varepsilon}^h - u_{\varepsilon}^h||_{\infty} \leq Mh^4$$
.

Note that from Vulanović [24] it follows that

$$||w_{\epsilon}^h - u_{\epsilon}^h||_1^h \leq Mh$$

holds for the central scheme on an arbitrary locally almost equidistant mesh. The result of Theorem 3 is much better because of the use of the special scheme on the special mesh.

§3. Numerical Results

We shall concider the following test example, Bohl [1]:

$$-\varepsilon^2 u' + \frac{u-4}{5-u} = 0, \ u(0) = u(1) = 0.$$

It is known, Bohl [1], that $0 \le u_{\varepsilon} \le 4$. So we have

$$\Gamma=1\geq c_u(x,u)\geq \frac{1}{25}=\gamma^2.$$

Note that (4) does not hold. This problem was considered in [2], [3], [4], [5], [6], [7] as well.

In the following Table we present the numerical order of convergence. Here we determine numerically the order of uniform convergence of our scheme as usual when the exact solution is not known:

Ord =
$$\frac{\log E_n - \log E_{2n}}{\log 2},$$

where

$$E_n := ||u_{\epsilon}^* - u||_{\infty}$$

and for each fixed $\varepsilon, u_{\varepsilon}^*$ is the numerical solution to our problem with n=1024 mesh points. This solution we compare with the other numerical solutions obtained by our method for n=4, 8, 16, 32, 64, 128, 256, 512. The corresponding nonlinear systems are solved by one-step Newton-Gauss-Seidel methods. For numerical solutions u we consider the iterate u^k for which

$$||Fu^k||_{\infty} < 10^{-7} \text{ and } ||u^k - u^{k-1}||_{\infty} < 10^{-11}.$$

In each case the start approximation is $u^0 = [0, 4, 4, \dots, 4, 0]^T$.

All computations have been carried out on the ATARI 1040 ST with 48 bits accuracy

in floating point.

Table

$n \setminus \varepsilon$	2-4	2-8	2^{-16}	2^{-24}
4	-	•	:-	: ·
8	3.8985	6.6896	14.528	20.0523
16	4.1643	2.5064	1.5343	1.5318
32	3.7656	1.9034	2.6312	2.6157
64	3.8134	4.0804	4.5252	4.5490
128	3.9943	4.0018	4.0025	4.0026
25 6	4.0767	4.0170	4.0211	4.0210
512	4.0847	4.1704	4.0981	4.0980

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