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SPLINE DIFFERENCE SCHEME AND MINIMUM PRINCIPLE FOR A REACTION-DIFFUSION PROBLEM[1]

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Abstract. The linear singularly perturbed reaction-diffusion problem is considered. The spline difference scheme on the Shishkin mesh is used to solve the problem numerically. With the special position of collocation points, the obtained scheme satisfies the discrete minimum principle. Numerical experiments which confirm theoretical results are presented.

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1. Introduction

We consider the singularly perturbed reaction-diffusion boundary value problem

$$\begin{aligned} Ly := \varepsilon^2 y''(x) - b(x)y(x) &= f(x), \qquad x \in (0,1), \\ y(0) = \gamma_0, \ y(1) &= \gamma_1, \end{aligned} \tag{1}$$

where $0 < \varepsilon \ll 1$. The functions b and f are assumed to be sufficiently smooth and $b(x) \geq \beta^2 > 0$, $x \in [0,1] = I$. Under these assumptions the problem (1) has a unique solution which exhibits two exponential boundary layers of width $\mathcal{O}\left(\varepsilon \ln 1/\varepsilon\right)$ at two subintervals of the domain. Boundary layers are the regions, where the solution and its derivatives change rapidly. Most of the traditional numerical methods fail to catch the rapid change of the solution, and its failure in turn pollutes the numerical approximation on the whole domain. Therefore special measures are required to obtain good numerical approximations. Properly layer-adapted meshes have been used often to overcome these difficulties and to yield methods that converge uniformly no matter how small is the perturbation parameter, see [1, 2] for surveys. We use a piecewise uniform Shishkin mesh which can be chosen a priori when one has some knowledge of the structure of these layers. For the construction of the mesh, we use the solution decompositions from [6] and related estimates for the components and their derivatives.

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Lemma 1.1. *[6] Let $b, f \in C^2(I)$. Then the problem (1) has unique solution $y(x) \in C^4(I)$ and this can be decomposed as*

$$y(x) = v(x) + w(x) + g(x)$$

where for $i = 0, 1, 2, 3, 4$

$$|v^{(i)}(x)| \le C, \quad |w^{(i)}(x)| \le C\varepsilon^{-i}e^{-x\beta/\varepsilon}, \quad |g^{(i)}(x)| \le C\varepsilon^{-i}e^{-(1-x)\beta/\varepsilon}$$

and C is constant independent of ε.

Throughout the paper C denotes any positive constant that may take different values in different formulas, but always independent of ε and the number of mesh nodes.

Problem of this type is numerically treated by spline collocation method in [3, 4], for example. In [3] a semilinear reaction-diffusion problem is considered. The spline collocation method on slightly modified Shishkin mesh is applied. The uniform convergency of order $\mathcal{O}(N^{-2}\ln^2 N)$ is achieved.

In [5] the spline difference scheme for the singularly perturbed problem with two small parameters is derived. The collocation points are moved from the standard position in order to obtain inverse monotone matrix for the discrete analogue. This fact enabled application of barrier function method in the proof of the uniform convergency of order $\mathcal{O}(N^{-2}\ln^2 N)$ in the layer points and $\mathcal{O}(N^{-2})$ elsewhere. We emphasize that the problem of the form (1) is not involved in [5].

Here we used technique form [5] for the problem (1) and obtain the more precisely error estimate then one obtained in [3] on the standard Shishkin mesh. That is the consequence of special choice of collocation points.

2. The mesh construction and the derivation of the spline difference scheme

We approximate the solution y of the problem (1) with the quadratic spline $u(x), x \in I$ on a piecewise uniform Shishkin mesh $\triangle_N$ defined by

$$\triangle_N : x_0 = 0,\ x_1,\ x_2,\ \dots,\ x_N = 1,$$

where

$$x_i = \begin{cases} \frac{4\sigma i}{N}, & 0 \le i \le \frac{N}{4}, \\ \sigma + \frac{2}{N}(i - \frac{N}{4})(1 - 2\sigma), & \frac{N}{4} \le i \le \frac{3N}{4}, \\ 1 - \sigma + (i - \frac{3N}{4})\frac{4\sigma}{N}, & \frac{3N}{4} \le i \le N. \end{cases} \tag{2}$$

We choose

$$\sigma = \min\left\{\frac{1}{4}, \frac{2\varepsilon}{\beta}\ln N\right\}.$$

The mesh step size is defined by

$$h_i = x_i - x_{i-1}, \quad \text{for } i = 1, ..., N.$$

The mesh is equidistant on the sets

$$\Omega_0 := [0, \sigma] \cup [1 - \sigma, 1], \qquad \Omega_v := [\sigma, 1 - \sigma].$$

We suppose that $\sigma = \frac{2\varepsilon}{\beta} \ln N$ since in the opposite case we can use the standard uniform mesh. Shishkin mesh $\triangle_N$ is fine on Ω_0 and coarse on Ω_v with mesh step sizes

$$h = 8\beta^{-1}\varepsilon N^{-1} \ln N \quad \text{and} \quad H = 2(1 - 2\sigma)N^{-1},$$

respectively. We also introduce notation $i_0 = N/4$.

We choose collocation points in a nonstandard way:

$$\begin{aligned} \xi_i &= \alpha_{1i}x_{i-1} + (1 - \alpha_{1i})x_i, \text{ on } [x_{i-1}, x_i], \; i = 1, ..., N - 1, \\ \eta_i &= \alpha_{2i}x_i + (1 - \alpha_{2i})x_{i+1}, \text{ on } [x_i, x_{i+1}] \; i = 1, ..., N - 1, \end{aligned} \tag{3}$$

where $0 < \alpha_{1i}, \alpha_{2i} < 1$.

As an approximation function we use the quadratic spline

$$u(x) = u_i + (x - x_i)u'_i + \tfrac{1}{2}(x - x_i)^2 u''_i, \;\; x \in [x_i, x_{i+1}], \tag{4}$$

$$u(x) \in C^1[0, 1] \tag{5}$$

Thus, we define the collocation equations as follows:

$$\varepsilon^2 u''(\xi_i) - b(\xi_i)u(\xi_i) = f(\xi_i), \qquad \xi_i \in [x_{i-1}, x_i], \tag{6}$$

$$\varepsilon^2 u''(\eta_i) - b(\eta_i)u(\eta_i) = f(\eta_i), \qquad \eta_i \in [x_i, x_{i+1}], \tag{7}$$

where $u''(\xi_i) = u''_{i-1}, \quad u''(\eta_i) = u''_i, \quad \xi_i$ and η_i are defined by (3) and (4).

From (3), (4), (5) and (7) we obtain

$$u'_i = \frac{(u_{i+1} - u_i)Q_i + h^2_{i+1}u_i b^+_i + f^+_i h^2_{i+1}}{h_{i+1}P_i}, \tag{8}$$

$$u'_{i+1} = \frac{2(u_{i+1} - u_i)}{h_{i+1}} - \frac{(u_{i+1} - u_i)Q_i + h^2_{i+1}u_i b^+_i + f^+_i h^2_{i+1}}{h_{i+1}P_i},$$

where $b^+_i = b(\eta_i), f^+_i = f(\eta_i)$ and

$$Q_i = -2\varepsilon^2 + b^+_i(1 - \alpha_{2i})^2 h^2_{i+1},$$

$$P_i = -2\varepsilon^2 - b^+_i \alpha_{2i}(1 - \alpha_{2i})h^2_{i+1}.$$

On the interval $[x_{i-1}, x_i]$ using (3), (4), (5) and (6) we obtain

$$u'_i = \frac{2(u_i - u_{i-1})}{h_i} - \frac{(u_i - u_{i-1})\Omega_i + h^2_i u_{i-1}b^-_i + f^-_i h^2_i}{h_i D_i}, \tag{9}$$

where $b_i^- = b(\xi_i), f_i^- = f(\xi_i)$ and

$$\Omega_i = -2\varepsilon^2 + b_i^-(1-\alpha_{1i})^2 h_i^2.$$

$$D_i = -2\varepsilon^2 - b_i^- \alpha_{1i}(1-\alpha_{1i})h_i^2,$$

From (8) and (9) we obtain the difference scheme

(10)

$$L_N u_i := r_i^- u_{i-1} + r_i^c u_i + r_i^+ u_{i+1} \;=\; q_i^- f_i^- + q_i^+ f_i^+,\ i = 1, \dots, N-1,$$

$$u_0 = \gamma_0, \qquad u_N = \gamma_1,$$

where

$$r_i^- = \frac{S_i}{2D_i}, \quad r_i^+ = \frac{Q_i h_i}{2h_{i+1}P_i}, \quad r_i^c = -1 + \frac{h_i h_{i+1} b_i^+}{2P_i} - \frac{Q_i h_i}{2h_{i+1}P_i} + \frac{\Omega_i}{2D_i},$$

$$q_i^- = -\frac{h_i^2}{2D_i}, \qquad q_i^+ = -\frac{h_i h_{i+1}}{2P_i}, \text{ and } S_i = -2\varepsilon^2 + b_i^- h_i^2 \alpha_{1i}^2.$$

The coefficients of the scheme depend on x_{i-1}, x_i and x_{i+1}. For a fixed i we have two intervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$ which are involved in the construction of the scheme. Further on, when it is clear from the context, we will drop the index i from $\alpha_{1i}, \alpha_{2i}, a_i^-, a_i^+$ and so on.

The parameters α_1 and α_2 provide two degrees of freedom which we use to ensure that the corresponding matrix of the system (10) is an $M-$ matrix, i. e.:

$$r_i^- \;\geq\; 0, \qquad r_i^+ \;\geq\; 0, \qquad r_i^c \;<\; 0.$$

Since $D_i < 0$, the first condition $r^- \;\geq\; 0$ is fulfilled if α_1 is determined in such a way that the following condition is satisfied:

$$S_i \;\leq\; 0.$$

Since $P_i < 0$, the second condition $r_i^+ \;\geq\; 0$ is fulfilled if α_2 is determined in such a way that the following condition is satisfied:

$$Q_i \;\leq\; 0.$$

If α_1 and α_2 are determined to provide conditions $r_i^- \geq 0$ and $r_i^+ \geq 0$ then $q_i^- > 0$, $q_i^+ > 0$ and

$$r_i^c = -r_i^- - r_i^+ - b_i^- q_i^- - b_i^+ q_i^+ < 0,$$

so the corresponding matrix has $L-$form and strictly diagonal dominant matrix. Thus we have the following theorem holds.

Theorem 2.1. *(Discrete Minimum Principle) Let α_1 and α_2 be determined so that $S_i \leq 0$ and $Q_i \leq 0$. If W is any mesh function with properties $L_N W \leq 0$, $W_0 \geq 0$, $W_N \geq 0$ then $W \geq 0$.*

Remark 1. We put $\alpha_1 = \alpha_2 = 1/2$ whenever the mesh steps provide $r^- \geq 0$ and $r^+ \geq 0$ which is the case in boundary layer regions.

3. Convergence results

The discrete minimum principle allow us to apply the barrier function technique for the error estimation. To that aim we first determine α_{1i} and α_{2i}.

Lemma 3.1. *Let the parameters α_1 and α_2 be determined as follows*

$$\alpha_{1i} = \alpha_{2i} = \frac{1}{2}, \qquad 0 \le i \le i_0 - 1, \quad N - i_0 + 1 \le i \le N,$$

$$(1-\alpha_{2i_0})^2 = \frac{2\varepsilon^2}{b_{i_0}^+ H^2}, \qquad \alpha_{1i_0} = \frac{1}{2},$$

$$\alpha_{2j} = \frac{1}{2}, \qquad \alpha_{1j}^2 = \frac{2\varepsilon^2}{b_j^- H^2}, \qquad \textit{for} \quad j = N - i_0$$

for $i_0 + 1 \le i \le N - i_0 + 1$ we put $\alpha_{2i} = 1 - \alpha_{1i}$ while α_{1i} is determened so that $S_i \le 0$ and $Q_i \le 0$.

Then discrete analogue (10) satisfies discrete minimum principle.

Now we analyze $L_N C$ and truncation error. Thus,

$$L_N C = C(r_i^- + r_i^c + r_i^+) = -C(b_i^- q_i^- + b_i^+ q_i^+)$$

and according to Lemma 3.1 we have

$$L_N C \ge \begin{cases} CN^{-2}\ln^2 N, & 0 \le i \le i_0 - 1, \ N - i_0 + 1 \le i \le N, \\ CN^{-1}\ln N, & i = i_0, \ i = N - i_0, \\ C, & i_0 < i < N - i_0. \end{cases} \tag{11}$$

The truncation error $\tau_i(y) = L_N(y_i - u_i)$ will be estimated separately for the functions v, w and g. Let

$$u_i = V_i + W_i + G_i$$

where V_i, W_i and G_i are approximation for v_i, w_i and g_i respectively. Using the Taylor expansion up to the third derivative, we obtain

$$\tau_i(y) = \sum_{j=1}^{6} \pi_j(y), \tag{12}$$

where

$$\pi_1(y) = \frac{r_i^+}{3!} h_{i+1}^3 y'''(s_1), \qquad \pi_2(y) = -\frac{r_i^-}{3!} h_i^3 y'''(\bar{s}_1),$$

$$\pi_3(y) = \varepsilon^2 q_i^- \alpha_1 h_i y'''(\bar{s}_2), \qquad \pi_4(y) = -\varepsilon^2 q_i^+ (1-\alpha_2) h_{i+1} y'''(s_2),$$

$$\pi_5(y) = -\frac{b_i^- q_i^-}{3!} \alpha_1^3 h_i^3 y'''(\bar{s}_3), \qquad \pi_6(y) = \frac{b_i^+ q_i^+}{3!} (1-\alpha_2)^3 h_{i+1}^3 y'''(s_3),$$

$$x_i \le s_j \le x_{i+1}, \quad x_{i-1} \le \bar{s}_j \le x_i, \quad j = 1, 2, 3.$$

Since

$$|r_i^-| \le C,\ |r_i^+| \le C,$$

for $\varepsilon \le CN^{-1}$ from (12) we obtain

$$\tau_i(v) = \begin{cases} C\varepsilon^3 N^{-3}\ln^3 N, & 0 \le i \le i_0,\ N - i_0 \le i \le N \\ CN^{-3}, & i_0 + 1 \le i \le N - i_0 - 1. \end{cases} \tag{13}$$

Thus we can use barrier function of the form CN^{-2} for sufficiently large C. From (11) and (13) we obtain

$$|v_i - V_i| \le CN^{-2}, \qquad i = 0, \dots, N. \tag{14}$$

For the error estimation of the functions w and g, we use Taylor expansion up to the fourth derivative. Then we have

$$\tau_i(y) = T_{3i}(y) + \sum_{j=1}^{6} \bar{\pi}_j(y) \tag{15}$$

where

$$\begin{aligned} T_{3i}(y) &= \Big(\alpha_1 h_i q_i^- \varepsilon^2 - (1-\alpha_2) h_{i+1} q_i^+ \varepsilon^2 - \frac{1}{6} q_i^- b_i^- h_i^3 \alpha_1^3 \\ &\quad + \frac{1}{6} q_i^+ b_i^+ h_{i+1}^3 (1-\alpha_2)^3 + \frac{1}{6} r_i^+ h_{i+1}^3 - \frac{1}{6} r_i^- h_i^3 \Big) y_i^{'''} \end{aligned}$$

$$\begin{aligned} \bar{\pi}_1(y) &= \frac{1}{4!} r_i^+ h_{i+1}^4 y^{IV}(\nu_1), & \bar{\pi}_2(y) &= \frac{1}{4!} r_i^- h_i^4 y^{IV}(t_1), \\ \bar{\pi}_3(y) &= -\frac{1}{2} q^- \varepsilon^2 \alpha_1^2 h_i^2 y^{IV}(t_2), & \bar{\pi}_4(y) &= -\frac{1}{2} q_i^+ \varepsilon^2 (1-\alpha_2)^2 h_{i+1}^2 y^{IV}(\nu_2), \\ \bar{\pi}_5(y) &= \frac{1}{4!} q_i^- b_i^- \alpha_1^4 h_i^4 y^{IV}(t_3), & \bar{\pi}_6(y) &= \frac{1}{4!} q_i^+ b_i^+ (1-\alpha_2)^4 h_{i+1}^4 y^{IV}(\nu_3). \end{aligned}$$

where $x_i \le \nu_j \le x_{i+1}$ and $x_{i-1} \le t_j \le x_i$ for $j = 1, 2, 3$.

Now we use (15) and analyze $\tau_i(v)$ and $\tau_i(g)$. It is easy to verify that

$$|\tau_i(w)| \le CN^{-4} \ln^4 N, \qquad 0 \le i \le i_0 - 1. \tag{16}$$

Also we have

$$|\tau_i(g)| \le CN^{-4} \ln^4 N, \qquad N - i_0 + 1 \le i \le N. \tag{17}$$

For $i = i_0$ we analyze the following parts of $T_{3i}(w)$:

$$\begin{aligned} a &= -(1-\alpha_2) h_{i+1} q_i^+ \varepsilon^2 w_i^{'''} \\ b &= (q_i^+ b_i^+ (1-\alpha_2)^3 h_{i+1}^3 / 3!) w_i^{'''} \\ d &= (r_i^+ h_{i+1}^3 / 3!) w_i^{'''}. \end{aligned}$$

Since $(1-\alpha_{2i_0})^2 = \dfrac{2\varepsilon^2}{b_{i_0}^{+}H^2}$, we obtain that $Q_i = 0$, $|P_i| \geq C\varepsilon h_{i+1}$ and $d = 0$.

Since $(1-\alpha_2) \leq C\varepsilon N^{-1}$ and $e^{-\frac{x_{i_0}\beta}{\varepsilon}} = N^{-2}$ we have

$$|a|, |b| \leq CN^{-3}\ln N.$$

The other terms in $T_{3i}(w)$ are easy for estimation and finally we obtain

$$|T_{3i}(w)| \leq CN^{-3}\ln N, \qquad i = i_0.$$

Similarly, we obtain

$$\sum_{j=1}^{6} |\bar{\pi}_j(w)| \leq CN^{-3}\ln N, \qquad i = i_0.$$

At the point x_{N-i_0} we use analogous arguments. Thus, we have

$$|\tau_i(w)| \leq CN^{-3}\ln N, \qquad i = i_0 \quad \text{and} \tag{18}$$

$$|\tau_i(g)| \leq CN^{-3}\ln N, \qquad i = N - i_0. \tag{19}$$

For $i_0 + 1 \leq i \leq N - i_0 - 1$ we have coarse mesh. Since $\alpha_{1i} = 1 - \alpha_{2i}$ and

$$|w_i^{'''}| \leq C\frac{1}{\varepsilon^3}e^{-x_{i_0+1}\beta/\varepsilon} = Ce^{-x_{i_0}\beta/\varepsilon}\frac{e^{-H\beta/\varepsilon}}{\varepsilon^3} \leq CN^{-2}H^{-3} \leq CN,$$

$$|w_i^{IV}| \leq CN^2,$$

we obtain

$$|\tau_i(w)| \leq CN^{-2}, \qquad i_0 + 1 \leq i \leq N - i_0. \tag{20}$$

For the function g we use similar arguments and conclude

$$|\tau_i(g)| \leq CN^{-2}, \qquad i_0 \leq i \leq N - i_0 - 1. \tag{21}$$

Now we use the barrier function ψ_i to estimate the error due to w:

$$\psi_i = \begin{cases} CN^{-2}\ln^2 N, & 0 \leq i \leq i_0 - 1 \\ CN^{-2}, & i_0 \leq i \leq N. \end{cases}$$

From (11), (16), (18) and (20) we obtain

$$L_N(\psi_i \pm (w_i - W_i)) \geq 0$$

and consequently

$$|w_i - W_i| = \begin{cases} CN^{-2}\ln^2 N, & 0 \leq i \leq i_0 - 1 \\ CN^{-2}, & i_0 \leq i \leq N. \end{cases} \tag{22}$$

According to (11), (17), (19) and (21), the similar estimate is valid for the function g:

$$
(23) \qquad |g_i - G_i| = \begin{cases} CN^{-2}\ln^2 N, & N-i_0+1 \le i \le N \\ CN^{-2}, & i_0 \le i \le N-i_0. \end{cases}
$$

From (14), (22) and (23), we obtain the following theorem.

Theorem 3.1. *Let $b, f \in C^2(I)$. Let y be the exact solution of (1) and u its approximation obtained by (10) on the Shishkin mesh defined by (2). If collocation points are given by Lemma 3.1 and $\varepsilon \le CN^{-1}$, then*

$$
|y(x_i) - u_i| \le \begin{cases} CN^{-2}\ln^2 N, & 0 \le i \le i_0 - 1,\ N-i_0+1 \le i \le N \\ CN^{-2}, & i_0 \le i \le N-i_0. \end{cases}
$$

4. Numerical results

We test the following problem

$$
\varepsilon^2 y'' - y = \cos^2(\pi x) + 2\varepsilon^2\pi^2\cos(2\pi x),
$$

$$
y(0) = y(1) = 0.
$$

Its exact solution is

$$
y(x) = \frac{e^{-\frac{x}{\varepsilon}} + e^{\frac{x-1}{\varepsilon}}}{1 + e^{-\frac{1}{\varepsilon}}} - \cos^2(\pi x).
$$

Let $u^N = (u_0, \dots, u_N)^T$ be the numerical solution. For each $N = 2^{-k}$, $k = 5, 6, \dots, 10$ and $\varepsilon^2 = 2^{-l}$, $l = 10, 11, \dots, 20$ we shall report

$$
E_N = \max_{0 \le j \le N} |y(x_j) - u_j|.
$$

Assuming convergence of order CN^{-p}, for some p, for fixed ε we compute E_N for two consecutive values of k. Because of

$$
\frac{E_N}{E_{2N}} \approx \frac{(N^{-k})^p}{(N^{-2k})^p} = 2^{-p},
$$

we estimate the convergence order p for each fixed ε from

$$
P_N = \frac{\ln E_N - \ln E_{2N}}{\ln 2}, \text{ for } N = 2^k \text{ and } k = 4, 5, \dots 10.
$$

In Table 1 we present E_N and P_N in the case of $\varepsilon^2 = 2^{-10}, 2^{-11}, \dots, 2^{-20}$ and in Table 2 are given values of α_1. The positions of the points α_{1i} are determined so that $S_i \le 0$ and $Q_i \le 0$ without the strong criterium for transition points.

ε^2/N	32	64	128	256	512	1024
2^{-10}	6.224e-3	1.970e-3	4.815e-4	1.197e-4	2.988e-5	7.467e-6
	1.660	2.032	2.008	2.002	2.000	
2^{-11}	6.235e-3	2.136e-3	7.092e-4	2.306e-4	5.987e-5	1.496e-5
	1.545	1.591	1.620	1.946	2.001	
2^{-12}	6.238e-3	2.137e-3	7.095e-4	2.308e-4	7.287e-4	2.247e-5
	1.545	1.591	1.620	1.663	1.697	
2^{-13}	6.239e-3	2.138e-3	7.096e-4	2.308e-4	7.287e-4	2.247e-5
	1.545	1.591	1.620	1.663	1.697	
2^{-14}	6.239e-3	2.138e-3	7.096e-4	2.308e-4	7.288e-4	2.247e-5
	1.545	1.591	1.620	1.663	1.697	
...	...	...	...	...	...	...
2^{-20}	6.239e-3	2.138e-3	7.096e-4	2.308e-4	7.288e-4	2.247e-5
	1.545	1.591	1.620	1.663	1.697	

Table 1: E_N and P_N for our test problem

ε^2/N	32	64	128	256	512	1024
2^{-10}	0.5	0.5	0.5	0.5	0.5	0.5
2^{-11}	0.5	0.5	0.5	0.5	0.5	0.5
2^{-12}	0.25	0.5	0.5	0.5	0.5	0.5
2^{-13}	0.25	0.5	0.5	0.5	0.5	0.5
2^{-14}	0.125	0.25	0.5	0.5	0.5	0.5
2^{-15}	0.125	0.25	0.5	0.5	0.5	0.5
2^{-16}	0.625	0.125	0.25	0.5	0.5	0.5
2^{-17}	0.625	0.125	0.25	0.5	0.5	0.5
2^{-18}	0.3125	0.625	0.125	0.25	0.5	0.5
2^{-19}	0.3125	0.625	0.125	0.25	0.5	0.5
2^{-20}	0.15625	0.3125	0.625	0.25	0.25	0.5

Table 2: α_1 for our test problem

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