Higher-Order Accurate Schemes for a Variable Coefficient Singularly Perturbed Reaction-Diffusion Problem of Boundary Layer Type

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Abstract

This paper addresses the numerical approximation of linear, steady, one-dimensional, variable coefficient singular perturbation problems of reaction-diffusion type which exhibit boundary layers. Since the diffusion and reaction terms are of opposite sign, this is a special case of the linear source problem [1]. A generalization of the Miller scheme [10] is presented which is second-order accurate, uniformly in the small parameter. This new scheme is then combined with that of Hegarty [5] to yield another scheme which is formally fourth-order accurate. Finally, the Mehrstellenverfahren technique of L. Collatz [2] is applied to produce yet another scheme with formal fourth-order accuracy.

Mathematics Subject Classification: 65L10, 65L11, 65L12

Keywords: singular perturbation, reaction-diffusion, boundary layer

1 Introduction

A singular perturbation problem is said to be of reaction-diffusion type if the order of the problem is reduced by two when the small parameter is set

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to zero [14]. This is to be distinguished from a convection-diffusion problem [12] where the corresponding reduction in order is only one. Depending on the relative signs of the diffusion and reaction terms, the solution to such a reaction-diffusion equation may exhibit either boundary layer behavior [7] (the subject of the present paper) or become highly oscillatory [8, 9].

While the most general of such problems are nonlinear, transient and multidimensional, this paper focuses on the linear, steady-state, one-dimensional version with variable coefficients. This constitutes the extension of our treatment of the constant coefficient problem which was the subject of [7]. Within these confines, we present new methods of numerical approximation that are uniformly second-order accurate and formally fourth-order accurate. This will be achieved primarily by coupling the method of exponential fitting [3] with the Mehrstellenverfahren technique of L. Collatz [2].

In the development that follows, the focus will be on the boundary layer case. We begin by examining the local truncation error of central differencing which is uniformly zeroth-order accurate as applied to this problem, as well as that of Miller’s scheme [10] which is uniformly first-order accurate and Hegarty’s scheme which is uniformly second-order accurate. These considerations reveal that the respective local truncation errors predict the known asymptotic behaviors of these varied methods.

Motivated by this observation, it is then shown how to generalize the ideas developed in [7] to derive a variant of Miller’s scheme which is uniformly second-order accurate for variable coefficients. The approach taken herein amounts to the annihilation of all objectionable terms (i.e. terms that misbehave in the boundary layer) in the local truncation error. This new scheme is then combined with that of Hegarty to yield another scheme which is uniformly fourth-order accurate. The Mehrstellenverfahren technique (Hermitian method) of L. Collatz [2] is then applied to produce yet another scheme with formal fourth-order accuracy.

Finally, a comparison is made of central differencing, Miller’s scheme, Hegarty’s scheme as well as our new schemes on a variable coefficient boundary layer problem with known exact solution. These results are indeed very encouraging.

2 Reaction-Diffusion Equation

The subject of our investigation is the steady, one-dimensional, reaction-diffusion equation with variable coefficients. This self-adjoint equation may be cast in conservation form as

$$-\epsilon \cdot [a(x) \cdot v'(x)]' + b(x) \cdot v(x) = g(x); \ v(0) = v_L, \ v(1) = v_R,$$  \hspace{1cm} (1)
where we assume that \(0 < |\epsilon| \ll 1\), \(a(x) \geq \hat{a} > 0\), and \(b(x) \geq \hat{b} > 0\). Physically, \(\epsilon a(x)\) is the diffusion coefficient while \(b(x)\) is the reaction coefficient. Since \(\epsilon\) is a small parameter, we have here a singular perturbation problem. When (as herein) \(\epsilon > 0\), boundary layers may develop while, for \(\epsilon < 0\), the solution may be highly oscillatory [9].

If we make the change of dependent variable

\[ u(x) := a(x)^{1/2} \cdot v(x), \quad (2) \]

then we obtain the following canonical form of the reaction-diffusion equation

\[ -\epsilon \cdot u''(x) + c(x) \cdot u(x) = f(x); \quad u(0) = u_L, \quad u(1) = u_R, \quad (3) \]

with

\[ c(x) := \frac{b(x)}{a(x)} + \epsilon \cdot \left[ \frac{a''(x)}{2a(x)} - \left( \frac{a'(x)}{2a(x)} \right)^2 \right] \quad f(x) := a^{-1/2}(x) \cdot g(x), \quad (4) \]

so that \(c(x) \geq \hat{c} > 0\) for sufficiently small \(\epsilon\).

In what follows, all functions appearing (especially, the coefficient \(c(x)\) and the source term \(f(x)\)) are assumed to possess sufficient smoothness to justify any operations to which we may subject them. Also, we define the parameter \(z := h\sqrt{c/\epsilon}\), which measures the strength of reaction relative to diffusion when scaled by the mesh width \(h := 1/N\) of Figure 1. For the problems of primary interest in this study, we have \(|z| \gg 1\). Lastly, in the ensuing derivations, we will restrict ourselves to \(\epsilon > 0\) (boundary layer case) where singular perturbation theory [11] reveals that the boundary layers may be as thin as \(O(\sqrt{\epsilon})\) and that in such a boundary layer \(u = O(1), \quad u' = O(1/\sqrt{\epsilon}), \quad u'' = O(1/\epsilon)\).

3 The Central Difference Scheme

If we discretize the two-point boundary value problem, Equation (3), using central differences, we obtain

\[ -\epsilon \cdot \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + c_i \cdot u_i = f_i. \quad (5) \]

The local truncation error of this scheme, which is easily established using Taylor series, is given by

\[ L.T.E. = \frac{h^2}{12} \cdot \left[ f_{i''} - c_i''u_i - 2c_i' u_i' - c_i u_i'' \right] + O(h^4). \quad (6) \]
In order to numerically resolve any boundary layers that arise, we require that \( h \sim \sqrt{\epsilon} \) (boundary layer width). Perusal of the above local truncation error then reveals that it is effectively \( O(1) \) due to the presence of the term containing \( u_i'' \). Thus, in spite of the fact that this scheme is formally second-order accurate, it is not uniformly accurate to any degree in the small parameter \( \epsilon \).

4 The Miller Scheme

Miller [10] has developed a scheme for Equation (3) which is uniformly first-order accurate for variable \( c(x) \) and uniformly second-order accurate for constant \( c \). This scheme is defined as follows:

\[
-\epsilon \cdot \frac{z_i^2}{2[\cosh z_i - 1]} \cdot \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + c_i \cdot u_i = f_i. \tag{7}
\]

The appearance of hyperbolic functions in this context is referred to as exponential fitting [11].

The local truncation error of this scheme is given by

\[
L.T.E. = \frac{h^2}{12} \cdot \left[ \frac{f_i''}{O(1)} - \frac{c_i'' u_i}{O(1)} - \frac{2c_i' u_i'}{O(1/\sqrt{\epsilon})} \right] + O(h^4). \tag{8}
\]

Notice that, in comparison to Equation (6), the undesirable term involving \( u_i'' \) has been eliminated. Thus, with \( h \sim \sqrt{\epsilon} \), the local truncation error is \( O(h) \) due to the presence of the term containing \( u_i' \). If \( c \) is constant, then this term vanishes and the local truncation error is \( O(h^2) \), independently of \( \epsilon \), so that,
in this special case only, the Miller scheme is thereby seen to be second-order accurate, uniformly in $\epsilon$.

5 The Hegarty Scheme

Hegarty et al. [5] have developed another exponentially-fitted scheme for Equation (3) which is uniformly second-order accurate even for variable $c(x)$. Specifically,

$$\frac{\epsilon}{h^2} \cdot [r_i^- \cdot u_{i-1} + r_i^- \cdot u_i + r_i^+ \cdot u_{i+1}] = q_i^- \cdot f_{i-1} + q_i^+ \cdot f_{i+1}$$

where

$$c_i^\pm := c_i + \frac{(-1 \pm 1) + c_i(1 \pm 1)/2}{2}; \quad z_i^\pm := h\sqrt{c_i^\pm}/\epsilon,$$

$$r_i^\pm := \frac{z_i^\pm}{\sinh z_i^\pm}; \quad r_i^c := -z_i^- \cdot \coth z_i^- - z_i^+ \cdot \coth z_i^+,$$

$$q_i^\pm := \frac{\tanh (z_i^\pm/2)}{2z_i^\pm}; \quad q_i^c := q_i^- + q_i^+.$$

The local truncation error of this scheme is given by

$$L.T.E. = -\frac{h^2}{6} \cdot \left( f'' + c''_i u_i \right) + O(h^4).$$

Notice that, in comparison to Equation (8), the undesirable term involving $u_i'$ has been eliminated. Thus, the local truncation error is $O(h^2)$, independently of $\epsilon$, regardless of whether or not $c$ is constant. Note that this scheme does not reduce to Miller’s scheme when $c$ is constant. Versions of Hegarty’s scheme which work directly with Equation (1) rather than Equation (3) are presented in [13, 16].

6 The McCartin Scheme

Motivated by the above observed correlation between the behavior of the local truncation error in the boundary layer and the order of uniform accuracy of the corresponding scheme, we next present a variant of the Miller scheme, Equation (7), which is uniformly second-order accurate for the case of variable $c$. This provides an extension of the treatment of the constant coefficient case which was successfully examined in [7].
Conceptually, there are no further hurdles to be leaped. However, the complexity of the required calculations is considerably greater in this more general case. Fundamental to this development will be the identity

\[ u^{(m)} = -\frac{1}{\epsilon} f^{(m-2)} + \frac{1}{\epsilon} \left[ c^{(m-2)} \cdot u + (m - 2)c^{(m-3)} \cdot u' + \cdots + (m - 2)c' \cdot u^{(m-3)} + c \cdot u^{(m-2)} \right], \]  

for \( m = 3, \ldots \), obtained through recursive application of Equation (3).

We commence with

\[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 2 \cdot \sum_{n=1}^{\infty} \frac{h^{2n-2}}{(2n)!} \cdot u_i^{(2n)} \].

(15)

With \( h \sim \sqrt{\epsilon} \), substituting Equation (14) into Equation (15) and retaining only those terms which are either \( O(1) \) or \( O(h) \) yields

\[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \approx 2 \cdot \sum_{n=1}^{\infty} \frac{h^{2n-2}}{(2n)!} \cdot \left[ c_i' \cdot n \cdot (n - 1) \cdot \frac{c_i^{n-2}}{\epsilon^{n-1}} \cdot u_i' + \left( \frac{c_i}{\epsilon} \right)^{n-1} \cdot u_i'' \right]. \]

(16)

Factoring out terms not depending on \( n \) from Equation (16) and summing the resulting series produces

\[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \approx \frac{2(z_i^2 - 1)}{z_i^2} \cdot u'' + \frac{z_i \cosh z_i - \sinh z_i}{2z_i} \cdot \frac{c_i'}{c_i} \cdot u', \]

(17)

which, when solved for \( u'' \), provides the approximation

\[ u'' \approx \frac{z_i^2}{2(z_i^2 - 1)} \cdot \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i^2}{2(z_i^2 - 1)} \cdot \frac{z_i \cosh z_i - \sinh z_i}{2z_i} \cdot (\ln c_i') \cdot u'. \]

(18)

The appearance of \( u' \) in Equation (18) presents a new challenge which we meet as follows. Beginning this time with

\[ \frac{u_{i+1} - u_{i-1}}{2h} = \sum_{n=1}^{\infty} \frac{h^{2n-2}}{(2n-1)!} \cdot u_i^{(2n-1)}, \]

(19)

we again invoke Equation (14) and retain only terms of an order consistent with our previous approximations. Summation of the resulting series yields

\[ \frac{u_{i+1} - u_{i-1}}{2h} \approx \frac{\sinh z_i}{z_i} \cdot u'_i, \]

(20)

which, when solved for \( u'_i \), provides the approximation

\[ u'_i \approx \frac{z_i}{\sinh z_i} \cdot \frac{u_{i+1} - u_{i-1}}{2h}. \]

(21)
 Combining Equation (21) with Equation (18) results in the second derivative approximation
\[
u''_i \approx \frac{z_i^2}{2(cosh z_i - 1)} \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i cosh z_i - sinh z_i}{2 sinh z_i} \cdot (\ln c)'_i \cdot \frac{u_{i+1} - u_{i-1}}{2h} \right].
\] (22)

Utilizing Equation (22) in the approximation of Equation (3) results in the following primitive form of our new scheme
\[-\epsilon \frac{z_i^2}{2(cosh z_i - 1)} \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i cosh z_i - sinh z_i}{2 sinh z_i} \cdot (\ln c)'_i \cdot \frac{u_{i+1} - u_{i-1}}{2h} \right] + c_i u_i = f_i,
\] (23)
whose local truncation error is given by
\[L.T.E. = \frac{h^2}{12} \cdot \left[ \frac{f''_i}{O(1)} - \frac{c_i'' u_i}{O(1)} \right] + O(h^4).
\] (24)

Thus, we see that this has only half the magnitude of the corresponding expression, Equation (13), for Hegarty’s scheme. This new scheme also shares with Hegarty’s scheme the property of being uniformly second-order accurate.

Since \(\frac{z_i cosh z_i - sinh z_i}{2 sinh z_i} = \frac{z_i^2}{12} + O(z^4)\), making the further approximation \((\ln c)'_i = \ln (c_{i+1}/c_{i-1})/2h + O(h^2)\) contributes only an additional \(O(\epsilon z^2 h^2) = O(h^4)\) error which is independent of \(\epsilon\). Thus, this leads to a loss of neither formal nor uniform second-order accuracy and the principal term of the truncation error in Equation (24) is unaltered. The resulting McCartin scheme is thereby
\[-\epsilon \frac{z_i^2}{2(cosh z_i - 1)} \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i cosh z_i - sinh z_i}{2 sinh z_i} \ln \left( \frac{c_{i+1}}{c_{i-1}} \right) \cdot \frac{u_{i+1} - u_{i-1}}{4h^2} \right] + c_i u_i = f_i,
\] (25)

7 The McCartin-Hegarty Scheme

Comparison of the principal parts of the local truncation errors of the Hegarty scheme, Equation (13), and the McCartin scheme, Equation (24), leads to the surprising conclusion that an appropriate linear combination of these two schemes will yield a blended scheme which is formally fourth-order accurate. Specifically,
\[\frac{1}{3} \cdot L.T.E.\cdot Hegarty + \frac{2}{3} \cdot L.T.E.\cdot McCartin = O(h^4).
\] (26)

The resulting new scheme will be referred to as the McCartin-Hegarty scheme in what follows.
8 The McCartin-Hermite Scheme

Another route to achieving formal fourth-order accuracy employs the Mehrstel-lenverfahren technique (Hermitian method) of L. Collatz [2] wherein we approx-imate the \( O(h^2) \) terms of Equation (24) using

\[
f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2); \quad c_i'' = \frac{c_{i+1} - 2c_i + c_{i-1}}{h^2} + O(h^2)
\]

and incorporate these approximations into our scheme. The resulting Hermi-tian scheme is

\[
-\epsilon \cdot \frac{z_i^2}{2(\cosh z_i - 1)} \cdot \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i \cosh z_i - \sinh z_i}{2 \sinh z_i} \cdot \ln \left( \frac{c_{i+1}}{c_{i-1}} \right) \cdot \frac{u_{i+1} - u_{i-1}}{4h^2} \right] + \frac{c_{i+1} + 10c_i + c_{i-1}}{12} \cdot u_i = f_{i-1} + \frac{10f_i + f_{i+1}}{12}.
\]

(28)

Finally, we may recover the McCartin scheme of [7] in the case of constant \( c \), together with its attendant uniform fourth-order accuracy, via the following modification of Equation (28)

\[
-\epsilon \cdot \frac{z_i^2}{2(\cosh z_i - 1)} \cdot \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{z_i \cosh z_i - \sinh z_i}{2 \sinh z_i} \cdot \ln \left( \frac{c_{i+1}}{c_{i-1}} \right) \cdot \frac{u_{i+1} - u_{i-1}}{4h^2} \right] + \frac{c_{i+1} + 10c_i + c_{i-1}}{12} \cdot u_i = f_i + \frac{1}{z_i^2} \cdot \left[ 1 - \frac{z_i^2}{2(\cosh z_i - 1)} \right] \cdot (f_{i+1} - 2f_i + f_{i-1}).
\]

(29)

In the remainder of this paper, Equation (29) will be referred to as the McCartin-Hermite scheme.

A side benefit of the present approach is that it clearly indicates what is required to achieve a given level of uniform accuracy. For example, uniform third-order accuracy would involve \( c_i'' \), which is approximable on a three point stencil, whereas uniform fourth-order accuracy would entail \( c_i''' \), which is not so approximable.

9 Boundary Layer Test Problem

We now present the results of some numerical experiments aimed at demonstrating the efficacy of the new schemes developed above. First, we present a model problem for which we know the exact solution. Then, this test problem is used as the basis for comparison of our schemes with those commonly used in the literature for the boundary layer case. These new schemes provide greatly improved results in all instances examined.

The variable coefficient two-point boundary value problem

\[
-\epsilon \cdot u'' + \frac{1}{(x+1)^2} \cdot u = 0; \quad u(0) = 1, \quad u(1) = \sqrt{2}
\]

(30)
possesses the analytical solution [17, p. 94] [6, p. 435]

\[ u(x) = \frac{\sqrt{x + 1}}{1 + 2^{-r}} \cdot \left\{ \left( \frac{x + 1}{2} \right)^r + \left( \frac{1}{x + 1} \right)^r \right\}; \quad r := \sqrt{\frac{1}{4} + \frac{1}{\epsilon}}. \] 

(31)

Figure 2 displays the development of the boundary layers as \( \epsilon \to 0^+ \) for the case of \( u_L = 1 \) and \( u_R = \sqrt{2} \). The successive frames correspond to the solution of the boundary value problem, Equation (31), for \( \epsilon = 2^{-m} (m = 8, \ldots, 13) \).

In the maximum norm, we have [4, p. 157]

\[ ||u(x; \epsilon) - u_h(x; \epsilon)||_\infty \leq Ch^p, \] 

(32)

where \( h := 1/N \) is the mesh parameter, \( C \) is the asymptotic error constant and \( p \) is the asymptotic rate of convergence which is estimated as [4, p. 159]

\[ p \approx p_N := \log_2 \left( \frac{||u_{N/2} - u||_\infty}{||u_N - u||_\infty} \right). \] 

(33)

Figures 3 through 8 display, for each method, the exact (solid line) and numerical (circles) solutions on the left with the corresponding error (dots)
on the right for $\epsilon = 2^{-13}$ and $N = 32$ where $h = 1/N$. Tables 1 through
6 contain the corresponding maximum error and convergence rate estimated
from Equation (33) for $\epsilon = 2^{-m}$ ($m = 8, \ldots, 13$) and $N = 2^n$ ($n = 5, \ldots, 9$).

Table 1 clearly shows the formal second-order accuracy of the Central Dif-
ference scheme as $h \to 0$ for fixed $\epsilon$. However, the nonuniform nature of this
convergence is evidenced by the growth of the errors as $\epsilon \to 0$ for fixed $h$. Ta-
ble 2 shows a similar nonuniform convergence for the Miller scheme. However,
accuracy has now been considerably enhanced by the elimination of the $O(1/\epsilon)$
term in the local truncation error.

This contrasts sharply with Table 3 where the uniform second-order accu-
ry of the Hegarty scheme for $h \to 0$ with fixed $\epsilon$ as well as $\epsilon \to 0$ with fixed
$h$ is prominently displayed. Likewise, Table 4 clearly indicates the uniform
second-order accuracy of the McCartin scheme, but the error for small $h$ has
now been halved as predicted by the respective local truncation errors.

Tables 5 and 6 testify to the formal fourth-order accuracy of the McCartin-
Hegarty and McCartin-Hermite schemes where both schemes are seen to yield
errors of the same order of magnitude. For $\epsilon = 2^{-13}$ with $N = 22$, both formally
fourth-order accurate schemes provide accuracy ($\approx 1.7 \times 10^{-5}$) comparable to
that of the uniformly second-order accurate McCartin scheme with $N = 64$.

## 10 Conclusion

In the preceding sections, new higher-order accurate schemes for the steady,
one-dimensional, variable coefficient reaction-diffusion equation of boundary
layer type have been presented. These included a scheme of uniform second-
order accuracy as well as a pair formally fourth-order accurate schemes. De-
tailed derivations as well as extensive comparisons to existing schemes have
been provided. The computational efficacy of the uniformly second-order ac-
curate McCartin scheme is underscored by the fact that the maximum error
for $\epsilon = 2^{-13}$ with $N = 22$ is $3 \times 10^{-5}$ which is comparable to that of the
corresponding error of the uniformly first-order accurate Miller scheme with
$N = 512$ thereby indicating that only $\sqrt{N}$ grid points need be used for com-
parable accuracy.

These boundary layer test case results provide compelling numerical evi-
dence for the validity of the following:

**Conjecture 1 (Equivalence of Uniform Consistency and Convergence)**

For $c(x)$ and $f(x)$ sufficiently smooth and $u(x)$ defined by

$$\mathcal{L}[u] := -\epsilon \cdot u''(x) + c(x) \cdot u(x) - f(x) = 0; \quad u(0) = u_L, \ u(1) = u_R,$$

$k^{th}$-order uniform consistency is equivalent to $k^{th}$-order uniform convergence.
That is to say,
\[ \mathcal{L}_h[u_h] = 0 \Rightarrow ||u - u_h||_\infty < C h^k \ (C \text{ independent of } \epsilon) \]
if and only if
\[ \mathcal{L}_h[u] = \mathcal{L}[u] + \sum_{l=k}^{\infty} C_l h^l, \]
where
\[ \lim_{h \to 0, \epsilon = h^2} C_l = O(h^{k-l}). \]

There are a number of directions in which this work could be extended. For example, the derivation for a non-uniform mesh would be straightforward but tedious. It is anticipated that this would result in the loss of one order of formal accuracy. Also, the fitted operators presented herein could be combined with corresponding fitted uniform meshes [15]. Finally, treatment of multiple spatial dimensions, transients, and nonlinearities would each be of substantial interest. The extension to the treatment of the highly oscillatory case [8] with variable coefficients, where the diffusion and reaction terms are of the same sign, will appear in [9].

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References


Figure 3: Central Difference Scheme ($\epsilon = 2^{-13}, N = 32$)

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Table 1: Central Difference Scheme: Error and Convergence Rate
Variable coefficient reaction-diffusion problem of boundary layer type

Figure 4: Miller Scheme ($\epsilon = 2^{-13}, N = 32$)

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Table 2: Miller Scheme: Error and Convergence Rate
Figure 5: Hegarty Scheme ($\epsilon = 2^{-13}, N = 32$)

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Table 3: Hegarty Scheme: Error and Convergence Rate
Figure 6: McCartin Scheme ($\epsilon = 2^{-13}, N = 32$)

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Table 4: McCartin Scheme: Error and Convergence Rate
Figure 7: McCartin-Hegarty Scheme ($\epsilon = 2^{-13}, N = 32$)

Table 5: McCartin-Hegarty Scheme: Error and Convergence Rate

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Variable coefficient reaction-diffusion problem of boundary layer type

Figure 8: McCartin–Hermite Scheme ($\epsilon = 2^{-13}, N = 32$)

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Table 6: McCartin–Hermite Scheme: Error and Convergence Rate

Received: January 3, 2016; Published: March 31, 2016