Optimal Quadratic Spline Collocation on Non-uniform Partitions

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Abstract

We extend the optimal quadratic spline collocation methods in [12] to non-uniform partitions. To develop optimal non-uniform partition methods, we use a mapping function from uniform to non-uniform partitions and develop expansions of the error at the non-uniform collocation points of some appropriately defined spline interpolants. The existence and uniqueness of the approximations are shown, under some conditions. Optimal global and local orders of convergence of the quadratic spline collocation approximations and derivatives are derived, similar to those of the respective methods for uniform partitions. The non-uniform partition methods are integrated with adaptive grid techniques. Numerical results on a variety of problems, including problems with layers, and a non-linear problem, verify the theoretically expected behaviour of the methods.

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1 Introduction

Consider a linear two-point Boundary Value Problem (BVP) described by the operator equation

$$\mathbf{L}u \equiv ru'' + pu' + qu = g \quad \text{in} \quad \Omega \equiv (0,1), \tag{1}$$

where r, p, q and g are given functions of x, and u is the unknown function of x, subject to boundary conditions on the boundary $\partial\Omega$ of Ω, described by

$$\mathbf{B}u \equiv \{\alpha_0 u(0) + \beta_0 u'(0) = \gamma_0, \alpha_1 u(1) + \beta_1 u'(1) = \gamma_1\}, \tag{2}$$

where α_i, β_i and γ_i, $i = 0, 1$ are given scalars. We focus the discussion to the above BVP, but some of the ideas and methods considered are useful for higher order and multi-dimensional BVPs.

Piecewise polynomial collocation is a commonly used method for the solution of (1)-(2). Let Δ be a partition for Ω. Based on Δ, a piecewise polynomial space $\mathcal{P}$ is defined. A set T of data points, called *collocation* points, is prescribed in $\overline{\Omega} \equiv \Omega \cup \partial\Omega$. The number of collocation points depends on the choice of the piecewise polynomial space. Let $T_{\mathbf{B}} \equiv T \cap \partial\Omega$ be the set of boundary collocation points. Let $T_{\mathbf{L}}$ the set of points at which (1) is collocated. Usually $T_{\mathbf{L}} \equiv T - T_{\mathbf{B}}$, but in some cases $T_{\mathbf{L}} \equiv T$, that is, the operator equation (1) is collocated on the boundary as well.

In its standard formulation, piecewise polynomial collocation seeks an approximation $u_\Delta \in \mathcal{P}$ to the solution u of (1)-(2), such that

$$\mathbf{L}u_\Delta = g \text{ in } T_\mathbf{L} \quad \text{and} \quad \mathbf{B}u_\Delta = \gamma \text{ on } T_\mathbf{B}. \tag{3}$$

The choice of collocation points is critical for the order of convergence of the arising method.

De Boor and Swartz [9] introduced and analyzed Gaussian collocation for one-dimensional mth order non-linear ODEs with m linear side conditions. For the second order BVP described by (1)-(2), Gaussian collocation determines a $\mathbf{C}^1$ piecewise $(k+1)$-degree polynomial approximation u_Δ by collocating at the k Gaussian points in each partition interval, and the 2 linear side conditions. Under some conditions, the global error in u_Δ is shown to be $O(H^{k+2})$, where H is the maximum partition length. Furthermore, at the nodes, the approximation and the first derivative have error $O(H^{2k})$, that is, they exhibit superconvergence for $k > 2$ and $k \geq 2$, respectively.

Splines are piecewise polynomials of degree k and continuity $\mathbf{C}^{k-1}$, that is, they exhibit the maximum possible smoothness. Spline collocation uses only one collocation point per subinterval and hence the linear system arising from (3) is the smallest possible among all types of piecewise polynomial collocation for the same number of partition points. Typical choices of spline collocation points are the nodes of the partition, if the degree of the splines is odd, and the midpoints, if the degree of the splines is even. It is worth noting that, when extending Gaussian collocation to two-dimensional domains through a tensor product approach, the number of collocation points per subrectangle is k^2, while for spline collocation it remains one. Thus the efficiency advantage of spline over Gaussian collocation becomes more apparent in two- and higher-dimensional problems.

However, the standard quadratic spline collocation methods applied to (1)-(2) produce $O(H^2)$ approximations even on uniform partitions. In contrast, quadratic spline interpolation at the midpoints gives an $O(H^3)$ global error bound, while, at the nodes of a uniform partition, it gives an $O(H^4)$ error bound.

Several researchers were concerned with developing optimal spline collocation methods, that is, methods that exhibit the same orders of convergence as interpolation in the same spline space. Optimal spline collocation methods on uniform partitions have been constructed based on acceleration techniques using appropriate perturbations $P_\mathbf{L}$ and $P_\mathbf{B}$ of the operators $\mathbf{L}$ and $\mathbf{B}$, respectively. The formulae that define these perturbation operators are derived by Taylor expansions at the collocation points of the errors between the exact solution u and an appropriately defined spline interpolant of u.

Two types of methods were formulated. The first type of method, called *one-step* or *extrapolated* method, involves determining a spline u_Δ such that

$$\mathbf{L}u_\Delta + P_\mathbf{L}u_\Delta = g \text{ in } T_\mathbf{L} \quad \text{and} \quad \mathbf{B}u_\Delta + P_\mathbf{B}u_\Delta = \gamma \text{ on } T_\mathbf{B}. \tag{4}$$

In this method, collocation is applied to a perturbed differential equation.

The second type of method, called *two-step* or *deferred-correction* method, involves determining first a spline $u_{\Delta[1]}$ that satisfies (3), and then a spline u_Δ, such that

$$\mathbf{L}u_\Delta = g - P_\mathbf{L}u_{\Delta[1]} \text{ in } T_\mathbf{L} \quad \text{and} \quad \mathbf{B}u_\Delta = \gamma - P_\mathbf{B}u_{\Delta[1]} \text{ on } T_\mathbf{B}. \tag{5}$$

Both methods are optimal. When the methods are extended to multi-dimensional BVPs, the deferred-correction method is more efficient in terms of time and memory requirements.

The first optimal spline collocation methods proposed to solve BVPs were based on cubic splines. For one-dimensional second-order BVPs and uniform partitions, Fyfe [11] proposed a deferred-correction cubic spline method, while [2] and [7] developed and analyzed an extrapolated cubic spline method. Extrapolated and deferred-correction quadratic spline methods, using the midpoints of the uniform partition intervals as collocation points, were proposed and analyzed in [12]. These optimal cubic and quadratic spline collocation methods were extended to two-dimensional second-order elliptic BVPs for rectangular domains in [14] and [5], respectively. Optimal quintic and quartic spline collocation methods [15], [18] were developed for one-dimensional fourth-order BVPs on uniform partitions. The orders of convergence of some optimal spline collocation methods and some Gaussian piecewise polynomial collocation methods are displayed in Tables 1 and 2.

d	2				3			
$m=2$	global	mid	nodal	Gauss	global	mid	nodal	Gauss
$u-u_\Delta$	3	4	4		4			
$u'-u'_\Delta$	2			3	3	4	4	
$u''-u''_\Delta$	1	2			2			3
$u^{(3)}-u^{(3)}_\Delta$	N/A	N/A	N/A	N/A	1	2		

d	4				5			
$m=4$	global	mid	nodal	Gauss	global	mid	nodal	Gauss
$u-u_\Delta$	5	6	6		6			
$u'-u'_\Delta$	4				5		6	
$u''-u''_\Delta$	3	4	4		4			
$u^{(3)}-u^{(3)}_\Delta$	2			3	3		4	
$u^{(4)}-u^{(4)}_\Delta$	1	2			2			

Table 1: Order of convergence of optimal spline collocation methods. Here, d is the degree of the spline ($d-1$ continuity), and m the order of the BVP. Blank entries denote that no local superconvergence result was found in the literature.

	$m=2, k=2, d=3$		$m=2, k=4, d=5$		$m=4, k=6, d=9$	
	global	nodal	global	nodal	global	nodal
$u-u_\Delta$	4		6	8	10	12
$u'-u'_\Delta$	3	4	5	8	9	12
$u''-u''_\Delta$	2		4		8	12
$u^{(3)}-u^{(3)}_\Delta$	1		3		7	12

Table 2: Order of convergence of degree $d = m + k - 1$ piecewise polynomial collocation ($m - 1$ continuity) for a mth order BVP at k Gaussian points in each subinterval. Blank entries denote that no local superconvergence result was found in the literature.

None of the above optimal spline collocation methods has been extended to non-uniform partitions.

The applicability of a discretization method to non-uniform partitions is essential for problems with rough solution behaviour, layers, etc, which are usually solved by adaptive techniques, and for multi-dimensional problems in non-rectangular domains. In the rest of the paper, we develop optimal non-uniform partition quadratic spline collocation (QSC) methods for linear one-dimensional second-order BVPs, while in [6] we do the same for cubic spline collocation (CSC) methods.

The outline of this paper is as follows. In Section 2, we present a technique of deriving optimal spline collocation methods for non-uniform partitions by mapping uniform to non-uniform partitions. We apply the technique to derive two QSC methods on non-uniform partitions, the two-step and the one-step methods. We emphasize that, at least numerically, this technique is *not* equivalent to applying a transformation of variables to the problem and obtaining a problem which can be solved effectively on a uniform grid. We prove the existence and uniqueness of the QSC approximation for a certain class of problems, and derive optimal global and local error bounds. We integrate our methods with adaptive grid techniques in Section 3. In the same section we explain how to compute an (approximation to the) mapping function from uniform to non-uniform partitions, for a given problem. In Section 4, we present numerical results that demonstrate the behaviour of the QSC methods on a variety of problems, including problems with boundary or interior layers, and a non-linear problem. In the last section, we make some concluding remarks and briefly mention possible extensions of this work.

2 Non-uniform Partition Quadratic Spline Collocation

Consider the two-point BVP (1)-(2). Let $\Delta \equiv \{x_0 = 0 < x_1 < \ldots < x_N = 1\}$ be a uniform partition of $\overline{\Omega}$ with stepsize $h = 1/N$ and $T \equiv \{\tau_0 = x_0, \tau_i = (x_i + x_{i-1})/2; i = 1, \ldots, N, \tau_{N+1} = x_N\}$ be a set of data points. Furthermore, define the Gaussian points $\delta_{ij} = x_i - \lambda_j h$; $j = 1, 2$, $i = 1, \ldots, N$, where $\lambda_1 = (3 - \sqrt{3})/6$ and $\lambda_2 = (3 + \sqrt{3})/6$.

Let $w(x) : \overline{\Omega} \to \overline{\Omega}$ be a bijective function in $\mathbf{C}^3$, with $w'(x) > 0$, $\forall x \in \overline{\Omega}$. Let $\Delta_w \equiv \{s_i = w(x_i), i = 0, \ldots, N\}$ be the partition of $\overline{\Omega}$ with respect to which the splines will be defined, and $T_w \equiv \{w_i = w(\tau_i), i = 0, \ldots, N+1\}$ be the set of collocation points. That is, for the initial development of the methods, we assume that the non-uniform grid points and collocation points are images of uniform grid points and collocation points, respectively. This assumption is relaxed in Section 3, where we allow any set of collocation points, and build an appropriate mapping from uniform to non-uniform collocation points. Let also $\sigma_{ij} \equiv w(\delta_{ij})$, $j = 1, 2$, $i = 1, \ldots, N$. Adopt the following notation: $h_i = w_{i+1} - w_i$, $i = 1, \ldots, N-1$, $h_i^a = s_i - w_i$, $i = 1, \ldots, N$, $h_i^b = w_{i+1} - s_i$ $i = 0, \ldots, N-1$, $H_i = s_{i+1} - s_i$, $i = 0, \ldots, N-1$, and $H = \max\{\max_{i=1,\ldots,N}\{h_i^a\}, \max_{i=0,\ldots,N-1}\{h_i^b\}\}$. Figure 1 shows the notation for the uniform grid and its non-uniform image for $N+1$ grid points. For any given $w(x)$, we denote by S_{Δ_w} the quadratic spline space with respect to the partition Δ_w.
We choose as basis functions for S_{Δ_w} the functions $\phi_i(x)$, $i = 0, \ldots, N+1$, where

$$\phi_i(x) \equiv \begin{cases} \frac{(x-s_{i-2})^2}{(s_i-s_{i-2})(s_{i-1}-s_{i-2})} & \text{for } s_{i-2} \le x \le s_{i-1} \\ \frac{(x-s_{i-2})(s_i-x)}{(s_i-s_{i-2})(s_i-s_{i-1})} + \frac{(s_{i+1}-x)(x-s_{i-1})}{(s_{i+1}-s_{i-1})(s_i-s_{i-1})} & \text{for } s_{i-1} \le x \le s_i \\ \frac{(s_{i+1}-x)^2}{(s_{i+1}-s_{i-1})(s_{i+1}-s_i)} & \text{for } s_i \le x \le s_{i+1} \\ 0 & \text{elsewhere.} \end{cases} \tag{6}$$

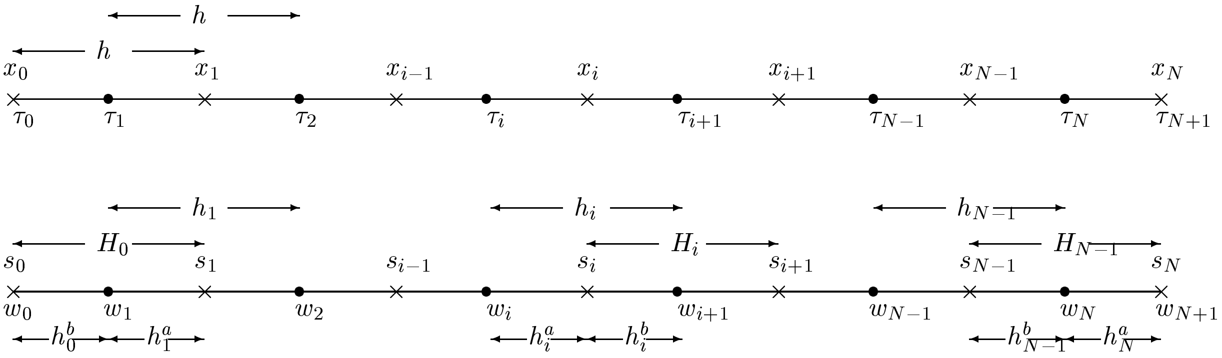

Figure 1: The uniform grid (above) and its non-uniform image (below, drawn as uniform for convenience).

Note that $\phi_i(x)$ and $\phi_i'(x)$ are well-defined at the nodes. Whenever we need $\phi_i''(s_j)$, we define it by right (without loss of generality) continuity for $s_i, i = 0, \ldots, N-1$, and by left continuity for s_N.
Let $S \in S_{\Delta_w}$ be the quadratic-spline interpolant of u such that

$$
\begin{aligned}
S''(w_1) &= u''(w_1) - \tfrac{1}{24}\{4(h_1^a - h_0^b)u^{(3)}(w_1) + (h_1^a + h_0^b)^2 u^{(4)}(w_1)\},\\
S(w_i) &= u(w_i), \quad i = 1, \ldots, N,\\
S''(w_N) &= u''(w_N) - \tfrac{1}{24}\{4(h_N^a - h_{N-1}^b)u^{(3)}(w_N) + (h_N^a + h_{N-1}^b)^2 u^{(4)}(w_N)\}.
\end{aligned} \tag{7}
$$

Note that the second set of relations in (7) is typical for a quadratic spline interpolant of u, while the first and third relations are a set of end-conditions that make the quadratic spline interpolant unique.

For simplicity, adopt the following notation: $S_i \equiv S(w_i)$, $S_i' \equiv S'(w_i)$ and $S_i'' \equiv S''(w_i)$. Notice that, when an integer subscript is attributed to the function w or its derivatives, it denotes values of the function or its derivatives, respectively, at collocation points of a uniform partition, i.e. $w_i = w(\tau_i)$, $w_i' = w'(\tau_i)$ and $w_i'' = w''(\tau_i)$, while, when it is attributed to other functions, it denotes values of the function at images through w of collocation points of a uniform partition, e.g. $u_i = u(w_i) = u(w(\tau_i))$, etc. Furthermore, let $e(x) \equiv u(x) - S(x)$, thus $e_i \equiv e(w_i)$. We will develop expansions of the errors of the derivatives of S at the collocation points.

2.1 Expansions of the errors of a quadratic spline interpolant

We begin by considering the second derivative error at the midpoints. In this section only, the symbols α, β, γ, α_1, β_1, γ_1, α_2, β_2 and γ_2 denote scalars defined within the section. By setting up the equations,

$$
\alpha_2 S_{i-1}'' + \beta_2 S_i'' + \gamma_2 S_{i+1}'' = \alpha S_{i-1} + \beta S_i + \gamma S_{i+1} \tag{8}
$$

for $i = 2, \ldots, N-1$, and solving for α, β, γ, α_2, β_2 and γ_2 with Maple we have

$$
\begin{aligned}
\alpha &= -2h_i, & \alpha_2 &= -h_i(h_{i-1}^a)^2,\\
\beta &= 2(h_i + h_{i-1}), & \beta_2 &= h_i(h_{i-1}^a)^2 + h_{i-1}(h_i^b)^2 - (h_i + h_{i-1})h_i h_{i-1},\\
\gamma &= -2h_{i-1}, & \gamma_2 &= -h_{i-1}(h_i^b)^2.
\end{aligned} \tag{9}
$$

It is worth noting that relations (8) hold for any quadratic spline $S \in S_{\Delta_w}$.
For later convenience, let $\wedge u_i \equiv \frac{1}{-(h_i+h_{i-1})h_i h_{i-1}}(\alpha_2 u_{i-1} + \beta_2 u_i + \gamma_2 u_{i+1})$, $i = 2, \ldots, N-1$.

LEMMA 1 *If $w(x) \in \mathbf{C}^3[\overline{\Omega}]$, then*

$$
\begin{array}{ll}
h_i = hw_i' + \frac{h^2}{2}w_i'' + O(h^3), & h_{i-1} = hw_i' - \frac{h^2}{2}w_i'' + O(h^3), \\
h_i^a = \frac{h}{2}w_i' + \frac{h^2}{8}w_i'' + O(h^3), & h_i^b = \frac{h}{2}w_i' + \frac{3h^2}{8}w_i'' + O(h^3), \\
h_{i-1}^b = \frac{h}{2}w_i' - \frac{h^2}{8}w_i'' + O(h^3), & h_{i-1}^a = \frac{h}{2}w_i' - \frac{3h^2}{8}w_i'' + O(h^3),
\end{array}
\tag{10}
$$

where the index i takes all possible values consistent with the definition of the stepsizes.

PROOF
Using the definitions of h_i, h_i^a and h_i^b, and Taylor expansions, the proof of this lemma is trivial. $\diamondsuit$

In the following, the symbol $\circ$ denotes composition of functions.

THEOREM 1 *If $u \in \mathbf{C}^6[\overline{\Omega}]$, $w(x) : \overline{\Omega} \to \overline{\Omega}$ is a bijective function in $\mathbf{C}^3$, with $w'(x) > 0$, $\forall x \in \overline{\Omega}$, $v = -\frac{1}{24}\{h^2(w'' \circ w^{-1})u^{(3)} + h^2(w' \circ w^{-1})^2 u^{(4)}\} \in \mathbf{C}^2[\overline{\Omega}]$, and S is defined by (7), then*

$$
S_i'' = u_i'' - \frac{1}{24}\{4(h_i^a - h_{i-1}^b)u_i^{(3)} + (h_i^a + h_{i-1}^b)^2 u_i^{(4)}\} + O(h^4), \tag{11}
$$

for $i = 1, \ldots, N$.

PROOF
Since $S_i = u_i$, $i = 1, \ldots, N$, and $u \in \mathbf{C}^6$, the right-hand side of (8) after applying Taylor expansion to $u_{i\pm1}$ is equivalent to

$$
\begin{aligned}
\alpha u_{i-1} + \beta u_i + \gamma u_{i+1} \;&=\; -h_{i-1}h_i(h_i + h_{i-1})[u_i'' + \frac{1}{3}(h_i - h_{i-1})u_i^{(3)} + \frac{1}{12}(h_i^2 - h_i h_{i-1} + h_{i-1}^2)u_i^{(4)}] \\
&+\; O(H^6), \quad i = 2, \ldots, N-1.
\end{aligned}
\tag{12}
$$

Moreover, using Taylor expansion of a function $f \in \mathbf{C}^4$ we can show

$$
\begin{aligned}
\alpha_2 f_{i-1} + \beta_2 f_i \;&+\; \gamma_2 f_{i+1} \\
&=\; -h_i h_{i-1}(h_i + h_{i-1})[f_i - \frac{(h_{i-1}^a + h_i^b)(h_{i-1}^a - h_i^b)}{h_i + h_{i-1}} f_i' + \frac{h_i(h_i^b)^2 + h_{i-1}(h_{i-1}^a)^2}{2(h_i + h_{i-1})} f_i''] \\
&+\; O(H^6), \quad i = 2, \ldots, N-1
\end{aligned}
\tag{13}
$$

By using Lemma 1 to expand h_i, h_i^a, h_i^b, relation (12) implies

$$
\wedge S_i'' = u_i'' + \frac{1}{3}h^2 w_i'' u_i^{(3)} + \frac{1}{12}h^2(w_i')^2 u_i^{(4)} + O(h^4), \quad i = 2, \ldots, N-1 \tag{14}
$$

and (13) implies

$$
\wedge f_i = f_i + \frac{3}{8}h^2 w_i'' f_i' + \frac{1}{8}h^2(w_i')^2 f_i'' + O(h^4), \quad i = 2, \ldots, N-1 \tag{15}
$$

Let $v = -\frac{1}{24}\{h^2(w'' \circ w^{-1})u^{(3)} + h^2(w' \circ w^{-1})^2 u^{(4)}\}$ and $f = u'' + v$. Then $f_i = u_i'' - \frac{1}{24}\{h^2 w_i'' u_i^{(3)} + h^2(w_i')^2 u_i^{(4)}\} = u_i'' - \frac{1}{24}\{4(h_i^a - h_{i-1}^b)u_i^{(3)} + (h_i^a + h_{i-1}^b)^2 u_i^{(4)}\} + O(h^4)$. As $u \in \mathbf{C}^6$, we have

$$
\wedge f_i = u_i'' + \frac{1}{3}h^2 w_i'' u_i^{(3)} + \frac{1}{12}h^2(w_i')^2 u_i^{(4)} + \frac{3}{8}h^4 w_i'' v_i' + \frac{1}{8}h^4(w_i')^2 v''(\xi_i) + O(h^4), \quad i = 2, \ldots, N-1, \tag{16}
$$

where $\xi_i \in (w_{i-1}, w_{i+1})$. As $v \in \mathbf{C}^2$ and $w \in \mathbf{C}^3$ we can regroup the h^4 terms as just $O(h^4)$. Hence,

$$\wedge(S_i'' - f_i) = O(h^4), \quad i = 2, \ldots, N-1. \tag{17}$$

Moreover, from the end-conditions in (7), we have

$$S_1'' - f_1 = O(h^4) \tag{18}$$

and

$$S_N'' - f_N = O(h^4). \tag{19}$$

Relations (18), (17) and (19) (in that order) form a system of equations that is strictly diagonally dominant. More specifically, using Lemma 1, and the fact that $w'(x) > 0$, $\forall x \in \overline{\Omega}$, we can show that $\frac{|\beta_2| - |\alpha_2| - |\gamma_2|}{|-(h_i + h_{i-1}) h_i h_{i-1}|} = \frac{1}{2} + O(h^2)$, which, for sufficiently small h, is greater than $\frac{1}{3}$. Therefore, the infinity norm of the inverse of the matrix of equations (18), (17) and (19) is bounded by 3.This implies that

$$S_i'' - f_i = O(h^4), \quad i = 1, \ldots, N.$$

$\diamondsuit$

REMARK 1 In the proof we assumed that $v \in \mathbf{C}^2[\overline{\Omega}]$ in order to bound the $O(h^4)$ terms in (16). We can substitute this assumption with the assumptions that $(w'' \circ w^{-1})v' \in \mathbf{C}[\overline{\Omega}]$ and $(w' \circ w^{-1})^2 v'' \in \mathbf{C}[\overline{\Omega}]$, which, sometimes, are less restrictive. (See also the numerical results on Problem 2.)

REMARK 2 The assumption that $w'(x) > 0, \forall x \in \overline{\Omega}$, together with Lemma 1 guarantee that the partition generated by w satisfies $H / \min\{\min_{i=1,\ldots,N}\{h_i^a\}, \min_{i=0,\ldots,N-1}\{h_i^b\}\} \leq C$, for some positive constant C, independent of h.

REMARK 3 Theorem 1 shows that, under the assumptions, $S_i'' - u_i''$ has a smooth expansion, since $S_i'' - u_i'' = -\frac{1}{24}\{h^2 w_i'' u_i^{(3)} + h^2 (w_i')^2 u_i^{(4)}\}$.

We now prove the counterpart of Theorem 1 for the first derivative error at the midpoints. Using Maple we can show the following relations for any $S \in S_{\Delta_w}$:

$$\begin{aligned}
\alpha_1 S_{i-1}' + \beta_1 S_i' + \gamma_1 S_{i+1}' &= \alpha S_{i-1} + \beta S_i + \gamma S_{i+1}, \quad i = 2, \ldots, N-1 && (20)\\
S_i' - S_{i-1}' &= h_{i-1}^b S_i'' + h_{i-1}^a S_{i-1}'', \qquad i = 2, \ldots, N && (21)\\
S_{i+1}' - S_i' &= h_i^b S_{i+1}'' + h_i^a S_i'', \qquad i = 1, \ldots, N-1, && (22)
\end{aligned}$$

where

$$\begin{array}{ll}
\alpha = -2 h_i h_i^a & \alpha_1 = h_i h_i^a h_{i-1}^a \\
\beta = 2(h_i h_i^a - h_{i-1} h_{i-1}^b) & \beta_1 = h_i h_{i-1}(h_i^a + h_{i-1}^2) + h_i^a h_{i-1}^b (h_i + h_{i-1}) \\
\gamma = 2 h_{i-1} h_{i-1}^b & \gamma_1 = h_{i-1} h_{i-1}^b h_i^b.
\end{array}$$

THEOREM 2 *Under the assumptions of Theorem 1,*

$$S_i' = u_i' + \frac{1}{24}(h_i^a + h_{i-1}^b)^2 u_i^{(3)} + O(h^4), \tag{23}$$

for $i = 1, \ldots, N$.

PROOF
Computing $\alpha_1 \times (21) - \gamma_1 \times (22) + (20)$ we have

$$\begin{aligned} & [\alpha S_{i-1} + \beta S_i + \gamma S_{i+1}] + [\alpha_1 (h^b_{i-1} S''_i + h^a_{i-1} S''_{i-1}) - \gamma_1 (h^b_i S''_{i+1} + h^a_i S''_i)] \\ = \; & (\alpha_1 + \beta_1 + \gamma_1) S'_i, \quad i = 2, \ldots, N-1. \end{aligned} \tag{24}$$

Now,

$$\begin{aligned} & \alpha S_{i-1} + \beta S_i + \gamma S_{i+1} = \alpha u_{i-1} + \beta u_i + \gamma u_{i+1} \\ = \; & h_i h_{i-1} [2(h^a_i + h^b_{i-1}) u'_i + (h_i h^b_{i-1} - h_{i-1} h^a_i) u''_i + \tfrac{1}{3}(h^2_i h^b_{i-1} + h^2_{i-1} h^a_i) u^{(3)}_i - \tfrac{1}{12}(h^3_i h^b_{i-1} + h^3_{i-1} h^a_i) u^{(4)}_i] \\ + \; & O(H^7), \quad i = 2, \ldots, N-1. \end{aligned} \tag{25}$$

Using Lemma 1 we have

$$\alpha_1 + \beta_1 + \gamma_1 = 2 h_i h_{i-1} (h^a_i + h^b_{i-1}) = 2 (w'_i)^3 h^3 + O(h^5). \tag{26}$$

By using (25), (26) and Lemma 1 we have

$$\frac{1}{\alpha_1 + \beta_1 + \gamma_1} (\alpha S_{i-1} + \beta S_i + \gamma S_{i+1}) = u'_i + \frac{1}{8} h^2 w''_i u''_i + \frac{1}{6} h^2 (w'_i)^2 u^{(3)}_i + O(h^4), \; i = 2, \ldots, N-1. \tag{27}$$

Moreover, by Theorem 1, Lemma 1 and the use of Maple we can show that

$$\begin{aligned} & \frac{1}{\alpha_1 + \beta_1 + \gamma_1} [\alpha_1 (h^b_{i-1} S''_i + h^a_{i-1} S''_{i-1}) - \gamma_1 (h^b_i S''_{i+1} + h^a_i S''_i)] \\ = \; & \frac{-\frac{1}{4} h^5 (w'_i)^3 w''_i u''_i - \frac{1}{4} h^5 (w'_i)^5 u^{(3)}_i + O(h^7)}{2 (w'_i)^3 h^3 + O(h^5)} \\ = \; & -\frac{1}{8} h^2 w''_i u''_i - \frac{1}{8} h^2 (w'_i)^2 u^{(3)}_i + O(h^4), \quad i = 2, \ldots, N-1. \end{aligned} \tag{28}$$

So combining (24), (27) and (28) we have

$$S'_i = u'_i + \frac{1}{24} h^2 (w'_i)^2 u^{(3)}_i + O(h^4), \quad i = 2, \ldots, N-1. \tag{29}$$

Furthermore, we can use (21), (22), (29), Lemma 1 and Theorem 1, and simplify with Maple to get

$$\begin{aligned} S'_1 &= S'_2 - h^b_1 S''_2 - h^a_1 S''_1 &&= u'_1 + \tfrac{1}{24} h^2 (w'_1)^2 u^{(3)}_1 + O(h^4) \\ S'_N &= S'_{N-1} + h^b_{N-1} S''_N + h^a_{N-1} S''_{N-1} &&= u'_N + \tfrac{1}{24} h^2 (w'_N)^2 u^{(3)}_N + O(h^4). \end{aligned}$$

But $h^2 (w'_i)^2 u^{(3)}_i = (h^a_i + h^b_{i-1})^2 u^{(3)}_i + O(h^4)$. ◊

Next, we develop expansions of the error of S at the nodes.

THEOREM 3 *Under the assumptions of Theorem 1,*

$$S(s_i) = u(s_i) - \frac{1}{16} (h^a_i - h^b_{i-1})(h^a_i + h^b_{i-1})^2 u^{(3)}(s_i) - \frac{1}{128} (h^a_i + h^b_{i-1})^4 u^{(4)}(s_i) + O(h^5), \tag{30}$$

for $i = 1, \ldots, N$, *and*

$$S(s_i) = u(s_i) - \frac{1}{16} (h^a_{i+1} - h^b_i)(h^a_{i+1} + h^b_i)^2 u^{(3)}(s_i) - \frac{1}{128} (h^a_{i+1} + h^b_i)^4 u^{(4)}(s_i) + O(h^5) \tag{31}$$

for $i = 0, \ldots, N-1$.

PROOF
By Taylor expansion

$$e(s_i) = e_i + h_i^a e_i' + \frac{1}{2}(h_i^a)^2 e_i'' + \frac{1}{6}(h_i^a)^3 u_i^{(3)} + \frac{1}{24}(h_i^a)^4 u_i^{(4)} + O((h_i^a)^5), \;\; i = 1, \ldots, N. \tag{32}$$

By noting that $e_i = 0$, and by using Theorems 2 and 1 for e_i' and e_i'', respectively, and Lemma 1, (32) becomes

$$\begin{aligned}
e(s_i) &= \{\frac{h}{2}w_i' + \frac{h^2}{8}w_i'' + O(h^3)\}\{-\frac{h^2}{24}(w_i')^2 u_i^{(3)} + O(h^4)\} \\
&+ \frac{1}{2}\{\frac{h^2}{4}(w_i')^2 + O(h^3)\}\{\frac{h^2}{24}w_i'' u_i^{(3)} + \frac{h^2}{24}(w_i')^2 u_i^{(4)} + O(h^4)\} \\
&+ \frac{1}{6}\{\frac{h^3}{8}(w_i')^3 + \frac{h^4}{32}(w_i')^2 w_i'' + \frac{h^4}{16}(w_i')^2 w_i'' + O(h^5)\}u_i^{(3)} + \frac{1}{24}\frac{h^4}{16}(w_i')^4 u_i^{(4)} + O(h^5) \\
&= \frac{h^4}{64}(w_i')^2 w_i'' u_i^{(3)} + \frac{h^4}{128}(w_i')^4 u_i^{(4)} + O(h^5) \\
&= \frac{h^4}{64}(w_i')^2 w_i'' u^{(3)}(s_i) + \frac{h^4}{128}(w_i')^4 u^{(4)}(s_i) + O(h^5) \\
&= \frac{1}{16}(h_i^a + h_{i-1}^b)(h_i^a - h_{i-1}^b)^2 u^{(3)}(s_i) + \frac{1}{128}(h_i^a + h_{i-1}^b)^4 u^{(4)}(s_i) + O(h^5).
\end{aligned}$$

Similarly,

$$e(s_i) = \frac{1}{16}(h_{i+1}^a - h_i^b)(h_{i+1}^a + h_i^b)^2 u^{(3)}(s_i) + \frac{1}{128}(h_{i+1}^a + h_i^b)^4 u^{(4)}(s_i) + O(h^5), \quad i = 0, \ldots, N-1.$$

$\diamondsuit$

Finally, we develop expansions of the error of the first derivative of S at the nodes.

THEOREM 4 *Under the assumptions of Theorem 1,*

$$S'(s_i) = u'(s_i) - \frac{1}{12}\{(h_i^a + h_{i-1}^b)^2 + 4(h_i^a - h_{i-1}^b)(h_i^a + h_{i-1}^b)\}u^{(3)}(s_i) + O(h^4) \tag{33}$$

for $i = 1, \ldots, N$, *and*

$$S'(s_i) = u'(s_i) - \frac{1}{12}\{(h_{i+1}^a + h_i^b)^2 - 4(h_{i+1}^a - h_i^b)(h_{i+1}^a + h_i^b)\}u^{(3)}(s_i) + O(h^4) \tag{34}$$

for $i = 0, \ldots, N-1$.

PROOF
By Taylor expansion

$$e'(s_i) = e_i' + h_i^a e_i'' + \frac{1}{2}(h_i^a)^2 u_i^{(3)} + \frac{1}{6}(h_i^a)^3 u_i^{(4)} + O((h_i^a)^4), \;\; i = 1, \ldots, N. \tag{35}$$

By using Theorems 2 and 1 for e_i' and e_i'', respectively, Lemma 1, and the Taylor relations $u_i^{(3)} = u^{(3)}(s_i) - h_i^a u^{(4)}(s_i) + O((h_i^a)^2)$ and $u_i^{(4)} = u^{(4)}(s_i) + O(h_i^a)$, (35) becomes

$$e'(s_i) = -\frac{h^2}{24}(w_i')^2 u_i^{(3)} + O(h^4)$$

$$\begin{aligned}
&+ \quad \{\frac{h}{2}w_i' + \frac{h^2}{8}w_i'' + O(h^3)\}\{\frac{h^2}{24}w_i''u_i^{(3)} + \frac{h^2}{24}(w_i')^2u_i^{(4)} + O(h^4)\} \\
&+ \quad \frac{1}{2}\{\frac{h}{2}w_i' + \frac{h^2}{8}w_i'' + O(h^3)\}^2u_i^{(3)} + \frac{1}{6}\{\frac{h}{2}w_i' + \frac{h^2}{8}w_i'' + O(h^3)\}^3u_i^{(4)} + O(h^4) \\
&= \quad \frac{1}{12}h^2(w_i')^2u_i^{(3)} + \frac{1}{12}h^3w_i'w_i''u_i^{(3)} + \frac{1}{24}h^3(w_i')^3u_i^{(4)} + O(h^4) \\
&= \quad \frac{1}{12}h^2(w_i')^2\{u^{(3)}(s_i) - h_i^a u^{(4)}(s_i) + O((h_i^a)^2)\} \\
&+ \quad \frac{1}{12}h^3w_i'w_i''\{u^{(3)}(s_i) - h_i^a u^{(4)}(s_i) + O((h_i^a)^2)\} + \frac{1}{24}h^3(w_i')^3\{u^{(4)}(s_i) + O(h_i^a)\} + O(h^4) \\
&= \quad \frac{1}{12}h^2(w_i')^2u^{(3)}(s_i) + \frac{1}{12}h^3w_i'w_i''u^{(3)}(s_i) + O(h^4) \\
&= \quad \frac{1}{12}(h_i^a + h_{i-1}^b)^2u^{(3)}(s_i) + \frac{1}{3}(h_i^a - h_{i-1}^b)(h_i^a + h_{i-1}^b)u^{(3)}(s_i) + O(h^4).
\end{aligned}$$

Similarly,

$$e'(s_i) = \frac{1}{12}(h_{i+1}^a + h_i^b)^2u^{(3)}(s_i) - \frac{1}{3}(h_{i+1}^a - h_i^b)(h_{i+1}^a + h_i^b)u^{(3)}(s_i) + O(h^4), \quad i = 0, \ldots, N-1.$$

$\diamondsuit$

THEOREM 5 *Under the assumptions of Theorem 1,*

$$|e(s_i)| = O(h^4), \tag{36}$$

$$|e'(\sigma_{ij})| = O(h^3), \tag{37}$$

$$|e''(w_i)| = O(h^2), \quad \textit{and} \tag{38}$$

$$\|e^{(k)}\|_\infty = O(h^{3-k}), \quad k = 0, 1, 2. \tag{39}$$

PROOF

Equations (36) and (38) are direct results of Theorems 3 and 1, respectively. To prove (37), we first consider some point $\sigma_i \equiv w(\tau_i + \mu h) = w_i + \mu h w_i' + O(h^2)$, for some constant μ. Then by Taylor expansion

$$e'(w_i + \mu h w_i' + O(h^2)) = e_i' + \mu h w_i' e_i'' + \frac{1}{2}\mu^2h^2(w_i')^2u_i^{(3)} + O(h^3). \tag{40}$$

By using Theorems 2 and 1 for e_i' and e_i'', respectively, (40) becomes

$$\begin{aligned}
e'(\sigma_i) &= -\frac{1}{24}h^2(w_i')^2u_i^{(3)} + \frac{1}{2}\mu^2h^2(w_i')^2u_i^{(3)} + O(h^3) \\
&= \{-\frac{1}{24} + \frac{1}{2}\mu^2\}h^2(w_i')^2u_i^{(3)} + O(h^3).
\end{aligned}$$

With $\mu = \pm\sqrt{3}/6$, the h^2 term vanishes. By noting that $\tau_i + \mu h = x_i - \lambda h$ when $\lambda = (3 \pm \sqrt{3})/6$, we are done.

Now, $e(x) = e_i + cH_{i-1}e_i' + \frac{1}{2}(cH_{i-1})^2e_i'' + O(H_{i-1}^3)$ for $x \in [s_{i-1}, s_i]$ with $-1 < c < 1$. Thus, by using Lemma 1 and the bounds for the local errors we have

$$\begin{aligned}
\|e(x)\|_\infty &= O(h^4) + O(h)O(h^2) + O(h^2)O(h) + O(h^3) \\
&= O(h^3).
\end{aligned}$$

The other global errors follow similarly. $\diamondsuit$

2.2 Approximations to the high derivatives

We now develop approximations to the high derivatives of u at the collocation points using values of S, S' and S'' at the collocation points.

THEOREM 6 *Under the assumptions of Theorem 1,*

$$u_i^{(k)} = \frac{2h_i S_{i-1}^{(k-2)} - 2(h_{i-1}+h_i)S_i^{(k-2)} + 2h_{i-1}S_{i+1}^{(k-2)}}{h_{i-1}(h_{i-1}+h_i)h_i} + O(h^2), \tag{41}$$

for $k = 3, 4$ *and* $i = 2, \ldots, N-1$.

PROOF
Equation (41) for $k = 3$ follows from the relation $u_i^{(3)} = \frac{2h_i u'_{i-1} - 2(h_{i-1}+h_i)u'_i + 2h_{i-1}u'_{i+1}}{h_{i-1}(h_{i-1}+h_i)h_i} + O(h_i - h_{i-1})$, (23), and the use of Lemma 1 for $h_i - h_{i-1}$ and $h_i^a + h_{i-1}^b$. Similarly, equation (41) for $k = 4$ follows from the relation $u_i^{(4)} = \frac{2h_i u''_{i-1} - 2(h_{i-1}+h_i)u''_i + 2h_{i-1}u''_{i+1}}{h_{i-1}(h_{i-1}+h_i)h_i} + O(h_i - h_{i-1})$, (11), and the use of Lemma 1 for $h_i - h_{i-1}$, $h_i^a - h_{i-1}^b$ and $h_i^a + h_{i-1}^b$. ◇

For convenience, we adopt the notation $\sqcap u_i \equiv \frac{2h_i u_{i-1} - 2(h_{i-1}+h_i)u_i + 2h_{i-1}u_{i+1}}{h_{i-1}(h_{i-1}+h_i)h_i}$. From Theorem 6 we have $u_i^{(4)} = \sqcap S''_i + O(h^2)$ and $u_i^{(3)} = \sqcap S'_i + O(h^2)$ for $i = 2, \ldots, N-1$.

COROLLARY 1 *Under the assumptions of Theorem 1, for* $k = 3, 4$,

$$\begin{aligned}
(42)\quad u_0^{(k)} &= \frac{(h_0^b + h_1)(h_1 + h_2) - h_0^b h_2}{h_1 h_2} \sqcap S_2^{(k-2)} - \frac{(h_0^b + h_1)}{h_2} \sqcap S_3^{(k-2)} + O(h^2),\\
(43)\quad u_1^{(k)} &= \frac{(h_1 + h_2) \sqcap S_2^{(k-2)} - h_1 \sqcap S_3^{(k-2)}}{h_2} + O(h^2),\\
(44)\quad u_N^{(k)} &= \frac{(h_{N-1} + h_{N-2}) \sqcap S_{N-1}^{(k-2)} - h_{N-1} \sqcap S_{N-2}^{(k-2)}}{h_{N-2}} + O(h^2),\\
(45)\, u_{N+1}^{(k)} &= \frac{(h_N^a + h_{N-1})(h_{N-1} + h_{N-2}) - h_N^a h_{N-2}}{h_{N-1}h_{N-2}} \sqcap S_{N-1}^{(k-2)} - \frac{(h_N^a + h_{N-1})}{h_{N-2}} \sqcap S_{N-2}^{(k-2)} + O(h^2).
\end{aligned}$$

PROOF
Equations (42) and (43) come from the relations $u_0^{(k)} = \frac{(h_0^b + h_1)u_1^{(k)} - h_0^b u_2^{(k)}}{h_1} + O(h^2)$, $u_1^{(k)} = \frac{(h_1+h_2)u_2^{(k)} - h_1 u_3^{(k)}}{h_2} + O(h^2)$ and Theorem 6. Equations (45) and (44) follow similarly. ◇

2.3 The Method of Optimal QSC

Consider solving the BVP (1)-(2). Based on the relations from Theorems 1-4 we observe that the interpolant S of u satisfies the relations

$$\mathbf{L}S_i = g_i - \frac{r_i}{24}\{4(h_i^a - h_{i-1}^b)u_i^{(3)} + (h_i^a + h_{i-1}^b)^2 u_i^{(4)}\} + \frac{p_i}{24}(h_i^a + h_{i-1}^b)^2 u_i^{(3)} + O(h^4), \;\; i = 1, \ldots, N \tag{46}$$

and

$$\begin{aligned}
\mathbf{B}S_0 &= \gamma_0 - \frac{\beta_0}{12}\{(h_1^a + h_0^b)^2 - 4(h_1^a - h_0^b)(h_1^a + h_0^b)\}u_0^{(3)} + O(h^4),\\
(47)\quad \mathbf{B}S_{N+1} &= \gamma_{N+1} - \frac{\beta_{N+1}}{12}\{(h_N^a + h_{N-1}^b)^2 + 4(h_N^a - h_{N-1}^b)(h_N^a + h_{N-1}^b)\}u_{N+1}^{(3)} + O(h^4).
\end{aligned}$$

Notice that due to Lemma 1, Theorem 6 and Corollary 1, relations (46) and (47) can be written as

$$\mathbf{L}S_i = g_i - P_{\mathbf{L}}S_i + O(h^4), \ \ i = 1, \dots, N \tag{48}$$

and

$$\mathbf{B}S_i = \gamma_i - P_{\mathbf{B}}S_i + O(h^4), \ \ i = 0, N+1, \tag{49}$$

where

$$\begin{aligned} P_{\mathbf{L}}S_1 &= \frac{r_1}{24}\{4(h_1^a - h_0^b)\frac{(h_1+h_2)\sqcap S_2' - h_1 \sqcap S_3'}{h_2} + H_0^2\frac{(h_1+h_2)\sqcap S_2'' - h_1\sqcap S_3''}{h_2}\} \\ &- \frac{p_1}{24}H_0^2\frac{(h_1+h_2)\sqcap S_2' - h_1\sqcap S_3'}{h_2}, \end{aligned} \tag{50}$$

$$P_{\mathbf{L}}S_i = \frac{r_i}{24}\{(h_i - h_{i-1})\sqcap S_i' + H_{i-1}^2 \sqcap S_i''\} - \frac{p_i}{24}H_{i-1}^2\sqcap S_i', \quad i = 2, \dots, N-1 \tag{51}$$

$$\begin{aligned} P_{\mathbf{L}}S_N &= \frac{r_N}{24}\{4(h_N^a - h_{N-1}^b)\frac{(h_{N-1}+h_{N-2})\sqcap S_{N-1}' - h_{N-1}\sqcap S_{N-2}'}{h_{N-2}} \\ &\quad + H_{N-1}^2\frac{(h_{N-1}+h_{N-2})\sqcap S_{N-1}'' - h_{N-1}\sqcap S_{N-2}''}{h_{N-2}}\} \\ &- \frac{p_N}{24}H_{N-1}^2\frac{(h_{N-1}+h_{N-2})\sqcap S_{N-1}' - h_{N-1}\sqcap S_{N-2}'}{h_{N-2}}, \end{aligned} \tag{52}$$

$$P_{\mathbf{B}}S_0 = \frac{\beta_0}{12}\{H_0^2 - 4(h_1^a - h_0^b)H_0\}\{\frac{(h_0^b+h_1)(h_1+h_2) - h_0^b h_2}{h_1 h_2}\sqcap S_2' - \frac{(h_0^b + h_1)}{h_2}\sqcap S_3'\}, \tag{53}$$

$$\begin{aligned} P_{\mathbf{B}}S_{N+1} &= \frac{\beta_{N+1}}{12}\{H_{N-1}^2 + 4(h_N^a - h_{N-1}^b)H_{N-1}\} \\ &\quad \{\frac{(h_N^a + h_{N-1})(h_{N-1}+h_{N-2}) - h_N^a h_{N-2}}{h_{N-1}h_{N-2}}\sqcap S_{N-1}' - \frac{(h_N^a + h_{N-1})}{h_{N-2}}\sqcap S_{N-2}'\}. \end{aligned} \tag{54}$$

Let $T_{w\mathbf{L}} \equiv \{w_i, i = 1, \dots, N\}$ and $T_{w\mathbf{B}} \equiv \{s_0, s_N\}$. We now present an optimal *two-step QSC method* to determine an approximation $u_\Delta \in S_{\Delta_w}$ of the solution of the BVP (1)-(2).
Step 1: Determine $u_{\Delta[1]} \in S_{\Delta_w}$ by forcing it to satisfy

$$\mathbf{L}u_{\Delta[1]} = g \ \text{ in } \ T_{w\mathbf{L}}, \tag{55}$$

$$\mathbf{B}u_{\Delta[1]} = \gamma \ \text{ on } \ T_{w\mathbf{B}}. \tag{56}$$

Step 2: Determine $u_\Delta \in S_{\Delta_w}$ by forcing it to satisfy

$$\mathbf{L}u_\Delta = g - P_{\mathbf{L}}u_{\Delta[1]} \ \text{ in } \ T_{w\mathbf{L}}, \tag{57}$$

$$\mathbf{B}u_\Delta = \gamma - P_{\mathbf{B}}u_{\Delta[1]} \ \text{ on } \ T_{w\mathbf{B}}. \tag{58}$$

We also present an *optimal one-step QSC method* which determines an approximation $\widehat{u_\Delta} \in S_{\Delta_w}$ of the solution of the BVP (1)-(2) by the equations

$$\tilde{\mathbf{L}}\widehat{u_\Delta} \equiv \mathbf{L}\widehat{u_\Delta} + P_{\mathbf{L}}\widehat{u_\Delta} = g \ \text{ in } \ T_{w\mathbf{L}}, \tag{59}$$

$$\tilde{\mathbf{B}}\widehat{u_\Delta} \equiv \mathbf{B}\widehat{u_\Delta} + P_{\mathbf{B}}\widehat{u_\Delta} = \gamma \ \text{ on } \ T_{w\mathbf{B}}. \tag{60}$$

From relations (48)-(49), we get an intuition why u_Δ and $\widehat{u_\Delta}$ are optimal approximations to u. A formal proof, though it is very similar to the one in [12], is given in the next section for completeness.

2.4 Convergence Analysis and Error Bounds

The convergence analysis of the QSC methods for non-uniform partitions is similar to that for uniform partitions [12], but we present it here mainly for completeness. For this section we will assume that $r(x) = 1$ in (1) and that, without loss of generality, we have homogeneous boundary conditions, that is $\mathbf{B}u = 0$ in (2). In order to analyze the QSC methods, we adopt the approach used by many [17], [16], [7], [12], [15] for proving existence, uniqueness and error bounds for piecewise polynomial collocation. According to this approach, we introduce an integral representation of equations (55), (57), (59) and of the differential equation (1). For this purpose, we assume that the BVP $u'' = 0, \mathbf{B}u = 0$ has a unique solution. This implies that there is a Green's function $G(x,t)$ for this problem. If we assume that $u, u_{\Delta[1]}$, u_Δ and $\widehat{u_\Delta}$ satisfy homogeneous boundary conditions, then u, $u_{\Delta[1]}$ and u_Δ can be obtained via the Green's function $G(x,t)$ and the respective second derivatives. That is, we have

$$
\begin{aligned}
u(x) &= \int_0^1 G(x,t)u''(t)dt, & u'(x) &= \int_0^1 G_x(x,t)u''(t)dt,\\
u_{\Delta[1]}(x) &= \int_0^1 G(x,t)u''_{\Delta[1]}(t)dt, & u'_{\Delta[1]}(x) &= \int_0^1 G_x(x,t)u''_{\Delta[1]}(t)dt,\\
u_\Delta(x) &= \int_0^1 G(x,t)u''_\Delta(t)dt, & u'_\Delta(x) &= \int_0^1 G_x(x,t)u''_\Delta(t)dt,\\
\widehat{u_\Delta}(x) &= \int_0^1 G(x,t)\widehat{u_\Delta}''(t)dt, & \widehat{u_\Delta}'(x) &= \int_0^1 G_x(x,t)\widehat{u_\Delta}''(t)dt.
\end{aligned}
$$

Let L be the set of bounded functions in $\overline{\Omega}$, that are continuous except possibly at the nodes $\{s_i\}_0^N$ of any partition, where their values are determined by right (without loss of generality) continuity for $s_i, i = 0, \dots, N-1$, and by left continuity for s_N, and where we impose the additional condition that, for each $f \in L$, the limits $\lim_{x \to s_i -} f(x)$ exist for all $i = 1, \dots, N-1$. Note that although $\lim_{x\to s_i -} f(x)$ exists, it may be different than $f(s_i)$. Note also that L includes all continuous functions in $\overline{\Omega}$, and all piecewise constant functions with respect to any partition. We assume that the coefficient functions $p(x)$ and $q(x)$ in (1) are continuous, and introduce the compact operator K that maps L to $\mathbf{C}[\overline{\Omega}]$ by

$$Kf(x) = p(x)\int_0^1 G_x(x,t)f(t)dt + q(x)\int_0^1 G(x,t)f(t)dt. \tag{61}$$

Equation (1) can now be written as

$$u'' + Ku'' = g \tag{62}$$

and equations (55) and (57) as

$$(u''_{\Delta[1]} + Ku''_{\Delta[1]})_i = g_i, \tag{63}$$

$$(u''_\Delta + Ku''_\Delta)_i = \tilde{g}_i, \tag{64}$$

respectively, where $\tilde{g} \equiv g - P_{\mathbf{L}} u_{\Delta[1]}$.

Furthermore, we introduce the operator P_Δ which maps functions in L to step functions via piecewise constant interpolation at the midpoints $\{w_i\}_1^N$. That is, for $f \in L$, $P_\Delta f = f(w_i)$ for $x \in [s_{i-1}, s_i)$, $i = 1, \dots, N$ and $P_\Delta f(s_N) = f(w_N)$. Based on the notation introduced, and taking into account the uniqueness of the piecewise constant interpolant for a given set of midpoint values, we can rewrite equations (63) and (64) in the form

$$u''_{\Delta[1]} + P_\Delta K u''_{\Delta[1]} = P_\Delta g, \tag{65}$$

$$u''_{\Delta} + P_\Delta K u''_{\Delta} = P_\Delta \tilde{g}, \tag{66}$$

respectively, since $P_\Delta u''_{\Delta[1]} = u''_{\Delta[1]}$ and $P_\Delta u''_\Delta = u''_\Delta$.

By the definition of P_Δ, $\|f - P_\Delta f\|_\infty \to 0$ as $h \to 0$ for all $f \in L$, that is, the sequence of operators P_Δ converges strongly to the identity operator $I : L \to L$. Moreover, $\|P_\Delta f\|_\infty \le \|f\|_\infty$. The compactness of K, and the strong convergence and uniform boundedness of P_Δ imply that $\|K - P_\Delta K\|_\infty \to 0$ as $h \to 0$.

THEOREM 7 *If*
(A1) the coefficients p and q, and the right-hand side g are in $\mathbf{C}[\Omega]$,
(A2) the BVP $\mathbf{L}u = g, \mathbf{B}u = 0$ has a unique solution,
(A3) the BVP $u'' = 0, \mathbf{B}u = 0$ has a unique solution,
(A4) the assumptions of Theorem 1 hold,
then $u_{\Delta[1]} \in S_{\Delta_w}$ defined by (55)-(56) exists, is unique, and satisfies the global error estimates

$$\|u - u_{\Delta[1]}\|_\infty = O(h^2), \ \|u' - u'_{\Delta[1]}\|_\infty = O(h^2), \ \textit{and} \ \|u'' - u''_{\Delta[1]}\|_\infty = O(h), \tag{67}$$

and the local error estimates

$$|(u - u_{\Delta[1]})^{(k)}(w_i)| = O(h^2), \ k = 0, 1, 2, \ \textit{and} \ i = 1, \ldots, N. \tag{68}$$

PROOF
Assumption (A2) and the equivalence of (1) and (62) imply that $(I + K)^{-1}$ exists and is bounded. Since $\|K - P_\Delta K\|_\infty \to 0$ as $h \to 0$, Neumann's theorem [16] implies that $(I + P_\Delta K)^{-1}$ exists and is uniformly bounded for sufficiently small h. The unique solvability of (65) follows from the existence and uniform boundedness of $(I + P_\Delta K)^{-1}$. The existence and uniqueness of $u''_{\Delta[1]}$ and the use of the Green's function $G(x,t)$ in association with (56) lead to the existence and uniqueness of $u_{\Delta[1]}$.

To establish the error bounds (67) and (68), simplify relations (48) and (49) to

$$\mathbf{L}S_i = g_i + O(h^2), \ \ i = 1, \ldots, N \text{ and} \tag{69}$$

$$\mathbf{B}S_i = O(h^2), \ \ i = 0, N+1. \tag{70}$$

From (55), (56), (69) and (70), we obtain

$$\mathbf{L}(S - u_{\Delta[1]})_i = O(h^2), \ \ i = 1, \ldots, N \text{ and} \tag{71}$$

$$\mathbf{B}(S - u_{\Delta[1]})_i = O(h^2), \ \ i = 0, N+1. \tag{72}$$

Notice that, because of assumption (A3), there is a linear function l such that $\mathbf{B}(S - u_{\Delta[1]})_j = \mathbf{B}l_j = O(h^2)$, $j = 0, N+1$, with $\|l\|_\infty = O(h^2)$, $\|l'\|_\infty = O(h^2)$, and thus $\mathbf{L}l_i = O(h^2)$, $i = 1, \ldots, N$. From $\mathbf{L}(S - u_{\Delta[1]} - l)_i = O(h^2)$ and $\mathbf{B}(S - u_{\Delta[1]} - l)_j = 0$, we conclude that

$$(I + P_\Delta K)(S'' - u''_{\Delta[1]} - l'') = O(h^2).$$

The uniform boundedness of $(I + P_\Delta K)^{-1}$ yields

$$\|S'' - u''_{\Delta[1]} - l''\|_\infty = O(h^2). \tag{73}$$

Since $\mathbf{B}(S - u_{\Delta[1]} - l)_j = 0$, $j = 0, N+1$, we have

$$(S - u_{\Delta[1]} - l)^{(k)}(x) = \int_0^1 G_x^{(k)}(x,t)(S'' - u''_{\Delta[1]} - l'')(t)dt.$$

This implies that

$$\|S - u_{\Delta[1]} - l\|_\infty = O(h^2),\ \|S' - u'_{\Delta[1]} - l'\|_\infty = O(h^2). \tag{74}$$

The error bounds (67) and (68) now follow from Theorem 5, the definition of l, the triangle inequality and relations (73) and (74). $\diamondsuit$

REMARK 4 Assumption (A4) implies that $u \in \mathbf{C}^6[\overline{\Omega}]$. However, we can relax this condition and assume that $u \in \mathbf{C}^4[\overline{\Omega}]$, and still obtain the results of Theorem 7, since the simplified relations $\mathbf{L}S_i = g_i + O(h^2)$ and $\mathbf{B}S_j = O(h^2)$ arising from (46) and (47), respectively, can be proved under the relaxed assumption.

The next theorem gives the optimal error bounds that u_Δ satisfies. To proceed with the proof, we make the assumption that
(A5) $S'_i - (u'_{\Delta[1]})_i$ and $S''_i - (u''_{\Delta[1]})_i$, $i = 0, \ldots, N+1$, have smooth expansions.
We do not provide a mathematical proof of this statement, however, extensive numerical experiments have shown that the statement holds. Of course, we can equivalently assume that $u'_i - (u'_{\Delta[1]})_i$ and $u''_i - (u''_{\Delta[1]})_i$, have smooth expansions, since, by Theorems 1, 2, and 4, we know that $S'_i - u'_i$ and $S''_i - u''_i$ have smooth expansions.

THEOREM 8 *Under the assumptions of Theorem 7, and assumption (A5), $u_\Delta \in S_{\Delta_w}$ defined by (57)-(58) exists, is unique, and satisfies the global error estimates*

$$\|(u - u_\Delta)^{(k)}\|_\infty = O(h^{3-k}),\ k = 0, 1, 2, \tag{75}$$

and the local error estimates

$$|(u - u_\Delta)(x)| = O(h^4) \text{ for } x = s_i \text{ and } w_i,\ |(u - u_\Delta)'(\sigma_{ij})| = O(h^3),\ |(u - u_\Delta)''(w_i)| = O(h^2). \tag{76}$$

PROOF
As in the proof of Theorem 7, the existence and uniform boundedness of $(I + P_\Delta K)^{-1}$ imply existence and uniqueness of u''_Δ in (66), which in turn implies existence and uniqueness of u_Δ.

We now establish the optimal error bounds (75) and (76). By (A5), we conclude that $\sqcap S_i^{(k)} = \sqcap(u_{\Delta[1]}^{(k)})_i + O(h^2)$, $k = 1, 2$. Therefore relations (48) and (49) imply

$$\begin{aligned} \mathbf{L}S_i &= \tilde{g}_i + O(h^4),\ \ i = 1, \ldots, N \text{ and} && (77)\\ \mathbf{B}S_i &= \tilde{\gamma}_i + O(h^4),\ \ i = 0, N+1, && (78) \end{aligned}$$

where $\tilde{\gamma} \equiv \gamma - P_{\mathbf{B}} u_{\Delta[1]}$. From (57), (58), (77) and (78), we obtain

$$\mathbf{L}(S - u_\Delta)_i = O(h^4), \quad i = 1, \ldots, N \text{ and} \tag{79}$$

$$\mathbf{B}(S - u_\Delta)_i = O(h^4), \quad i = 0, N+1. \tag{80}$$

Notice that there is a linear function l such that $\mathbf{B}(S - u_\Delta)_j = \mathbf{B} l_j = O(h^4)$, $j = 0, N+1$, with $\|l\|_\infty = O(h^4)$, $\|l'\|_\infty = O(h^4)$, and thus $\mathbf{L} l_i = O(h^4)$, $i = 1, \ldots, N$. From $\mathbf{L}(S - u_\Delta - l)_i = O(h^4)$ and $\mathbf{B}(S - u_\Delta - l)_j = 0$, we conclude that

$$(I + P_\Delta K)(S'' - u''_\Delta - l'') = O(h^4).$$

Applying the arguments used in the proof of Theorem 7 and with $\sigma_{ij} = w(x_i - \lambda_j h)$, we obtain the optimal results (75) and (76). $\diamondsuit$

We now turn to the analysis of the one-step QSC method. In order to write (59) in integral form, we introduce some more notations. Let $D_\Delta : L \to \mathbf{R}^N$ be defined by $(D_\Delta f)_i = f(\tau_i)$ for $i = 1, \ldots, N$, $E_p = \text{diag}(p(\tau_i)), E_q = \text{diag}(q(\tau_i))$ be $N \times N$ diagonal matrices and M_Δ be the operator which maps $\mathbf{R}^N$ to step functions via piecewise constant interpolation at the midpoints $\{w_i\}_1^N$.

We note that from Theorem 6 and Lemma 1 we have

$$u_i^{(k)} = \frac{S_{i-1}^{(k-2)} - 2S_i^{(k-2)} + S_{i+1}^{(k-2)}}{h^2 (w'_i)^2} + \frac{O(h) S_{i-1}^{(k-2)} + O(h^2) S_i^{(k-2)} + O(h) S_{i+1}^{(k-2)}}{h^2 (w'_i)^2} + O(h^2),$$

for $k = 3, 4$ and $i = 2, \ldots, N-1$. Close to the boundary we have

$$\begin{aligned}
u_1^{(k)} &= \frac{2S_1^{(k-2)} - 5S_2^{(k-2)} + 4S_3^{(k-2)} - S_4^{(k-2)}}{h^2 (w'_1)^2} \\
&+ \frac{O(h) S_1^{(k-2)} + O(h) S_2^{(k-2)} + O(h) S_3^{(k-2)} + O(h) S_4^{(k-2)}}{h^2 (w'_1)^2} + O(h^2), \\
u_N^{(k)} &= \frac{2S_N^{(k-2)} - 5S_{N-1}^{(k-2)} + 4S_{N-2}^{(k-2)} - S_{N-3}^{(k-2)}}{h^2 (w'_N)^2} \\
&+ \frac{O(h) S_N^{(k-2)} + O(h) S_{N-1}^{(k-2)} + O(h) S_{N-2}^{(k-2)} + O(h) S_{N-3}^{(k-2)}}{h^2 (w'_N)^2} + O(h^2),
\end{aligned}$$

where each $O(h)$ term involves the value of at least one of the first three derivatives of w. Hence, from Theorems 1 and 2, we have

$$u''_i = \frac{1}{24}(S''_{i-1} + 22S''_i + S''_{i+1}) + O(h) S''_{i-1} + O(h^2) S''_i + O(h) S''_{i+1} \tag{81}$$

$$+ \frac{w''_i}{24 (w'_i)^2}(S'_{i-1} - 2S'_i + S'_{i+1}) + O(h) S'_{i-1} + O(h^2) S'_i + O(h) S'_{i+1} + O(h^4) \tag{82}$$

$$u'_i = \frac{1}{24}(-S'_{i-1} + 26S'_i - S'_{i+1}) + O(h) S'_{i-1} + O(h^2) S'_i + O(h) S'_{i+1} + O(h^4), \tag{83}$$

for $i = 2, \ldots, N-1$. It is important to note that there is at most a constant number (actually two) of $O(h)$ terms in each of (81), (82) and (83).

We have similar results for u_i'' and u_i' for $i = 1, N$. Let Ψ and Φ be the almost tridiagonal $N \times N$ matrices defined in [12], that is,
$\Psi_{i,i} = 22/24$, $\Psi_{i-1,i} = \Psi_{i+1,i} = 1/24$, $i = 2, \dots, N-1$,
$\Psi_{1,1} = \Psi_{N,N} = 26/24$, $\Psi_{1,2} = \Psi_{N,N-1} = -5/24$, $\Psi_{1,3} = \Psi_{N,N-2} = 4/24$, $\Psi_{1,4} = \Psi_{N,N-3} = -1/24$,
$\Phi_{i,i} = 26/24$, $\Phi_{i-1,i} = \Phi_{i+1,i} = -1/24$, $i = 2, \dots, N-1$,
$\Phi_{1,1} = \Phi_{N,N} = 22/24$, $\Phi_{1,2} = \Phi_{N,N-1} = 5/24$, $\Phi_{1,3} = \Phi_{N,N-2} = -4/24$, $\Phi_{1,4} = \Phi_{N,N-3} = 1/24$, with the rest of the entries of Ψ and Φ equal to 0. Let also Γ be a matrix which differs from Ψ only on the diagonal, more specifically, $\Gamma_{i,i} = -2/24$, $i = 2, \dots, N-1$, and $\Gamma_{1,1} = \Gamma_{N,N} = 2/24$. Relations (81) for $i = 2, \dots, N-1$, and the respective boundary relations give rise to the matrix $\tilde{\Psi} = \Psi + h\Sigma$, where $h\Sigma$ is an $N \times N$ matrix that represents the $O(h)$ and $O(h^2)$ terms. Similarly, relations (82) for $i = 2, \dots, N-1$, and the respective boundary relations give rise to the matrix $\tilde{\Gamma} = \Theta\Gamma + h\mathrm{Z}$, where $\Theta = \mathrm{diag}(\frac{w_i''}{24(w_i')^2})$, and $h\mathrm{Z}$ is an $N \times N$ matrix representing the $O(h)$ and $O(h^2)$ terms. Finally, relations (83) for $i = 2, \dots, N-1$, and the respective boundary relations give rise to the matrix $\tilde{\Phi} = \Phi + h\Upsilon$, where $h\Upsilon$ is an $N \times N$ matrix representing the $O(h)$ and $O(h^2)$ terms. Note that the matrices Σ, Z and Υ have at most 4 non-zero entries per row, and their entries involve values of the first 3 derivatives of w. Thus, assuming $w \in \mathbf{C}^3$, $||\Sigma||_\infty$, $||\mathrm{Z}||_\infty$ and $||\Upsilon||_\infty$ are bounded. Since $w'(x) > 0$, $\forall x \in \overline{\Omega}$, $||\Theta||_\infty$ is bounded as well. Also, from the boundedness of $||\Psi^{-1}||_\infty$ and the fact that $\tilde{\Psi} = \Psi(\mathbf{I} + h\Psi^{-1}\Sigma)$, we have the boundedness of $||\tilde{\Psi}^{-1}||_\infty$, for sufficiently small h.

We now rewrite (59) equivalently as

$$\widehat{u_\Delta}'' + R_\Delta \widehat{u_\Delta}'' = M_\Delta \tilde{\Psi}^{-1} D_\Delta g, \tag{84}$$

where R_Δ is the integral operator defined by

$$\begin{aligned} R_\Delta f \;\; &\equiv \;\; M_\Delta \tilde{\Psi}^{-1} \tilde{\Gamma} D_\Delta \int_0^1 G_x(x,t) f(t) dt + M_\Delta \tilde{\Psi}^{-1} E_p \tilde{\Phi} D_\Delta \int_0^1 G_x(x,t) f(t) dt \\ &+ \;\; M_\Delta \tilde{\Psi}^{-1} E_q D_\Delta \int_0^1 G(x,t) f(t) dt. \end{aligned}$$

LEMMA 2 *The sequence of operators R_Δ converges strongly to the integral operator K in L.*

PROOF
Consider the convergence of $\|R_\Delta f - M_\Delta D_\Delta K f\|_\infty$ for $f \in L$. According to the definition of R_Δ and the use of the triangular inequality we obtain

$$\begin{aligned} \|R_\Delta f - M_\Delta D_\Delta K f\|_\infty \;\; &\le \;\; \|M_\Delta \tilde{\Psi}^{-1} \tilde{\Gamma} D_\Delta \textstyle\int_0^1 G_x f dt\|_\infty \\ &+ \;\; \|M_\Delta \tilde{\Psi}^{-1} E_p \tilde{\Phi} D_\Delta \textstyle\int_0^1 G_x f dt - M_\Delta \tilde{\Psi}^{-1} \tilde{\Psi} E_p D_\Delta \int_0^1 G_x f dt\|_\infty \\ &+ \;\; \|M_\Delta \tilde{\Psi}^{-1} E_q D_\Delta \textstyle\int_0^1 G f dt - M_\Delta \tilde{\Psi}^{-1} \tilde{\Psi} E_q D_\Delta \int_0^1 G f dt\|_\infty. \end{aligned}$$

From the boundedness of $||M_\Delta||_\infty$, $||\tilde{\Psi}^{-1}||_\infty$, $||\mathrm{Z}||_\infty$, $||\Sigma||_\infty$ and $||\Upsilon||_\infty$, and the definitions of $\tilde{\Gamma}$, $\tilde{\Psi}$ and $\tilde{\Phi}$, we have

$$\begin{aligned} \|R_\Delta f - M_\Delta D_\Delta K f\|_\infty \le C \;\; &\{\|\Theta\Gamma D_\Delta \textstyle\int_0^1 G_x f dt\|_\infty \\ &+\|E_p \Phi D_\Delta \textstyle\int_0^1 G_x f dt - \Psi E_p D_\Delta \int_0^1 G_x f dt\|_\infty \\ &+\|E_q D_\Delta \textstyle\int_0^1 G f dt - \Psi E_q D_\Delta \int_0^1 G f dt\|_\infty\} + O(h), \end{aligned} \tag{85}$$

for some constant $C > 0$. Notice that $\Gamma D_\Delta \int_0^1 G_x f dt$ is bounded by the modulus of continuity over a $3h$ interval. Hence, the first term of (85) is $O(h)$. The treatment of the other two terms and the rest of the proof of the lemma is identical to that in [12]. $\diamondsuit$

With techniques identical to those in [12], we can now show that, under the assumptions of Theorem 7, $\widehat{u_\Delta}$ exists, is unique, and satisfies the same error bounds as u_Δ.

3 Construction of Mapping Function using Adaptive Techniques

In previous sections we have shown that for a smooth enough mapping function w, we can develop an optimal QSC method for the set of collocation points T_w corresponding to the non-uniform grid Δ_w. However, we have not discussed the selection of an appropriate mapping function, given a certain BVP. In this section we discuss the use of adaptive techniques to generate mapping functions appropriate for the problem considered.

The primary idea is to first construct a non-uniform grid s_i, $i = 0, \ldots, N$, using adaptive techniques, then construct a monotone Hermite piecewise cubic interpolant w such that $w(s_0) = s_0, w(s_N) = s_N$ and $w(\tau_i) = (s_{i-1} + s_i)/2$, $i = 1, \ldots, N$, where τ_i are the midpoints defined in Section 2.

We use the adaptive techniques and the idea of grading functions presented in [3] to construct the non-uniform grid. According to these techniques, the partition points are distributed so that the error in some chosen norm (or semi-norm) is equidistributed among the subintervals of the partition. Depending on the norm chosen, a different grading function arises, based on which the partition points are constructed. All grading functions involve high derivatives of u, which, under realistic situations, is not known. Therefore, u_Δ is substituted in place of u, to obtain the respective approximate grading functions.

According to [3], with u_Δ being a piecewise polynomial of degree 2, and the chosen norm being the H^1 semi-norm, the grading function is $\xi_{q5}(x) = \int_0^x (u^{(3)})^{2/5} dx / \int_0^1 (u^{(3)})^{2/5} dx$, while, if the chosen norm is the H^0 norm, the grading function is $\xi_{q7}(x) = \int_0^x (u^{(3)})^{2/7} dx / \int_0^1 (u^{(3)})^{2/7} dx$. De Boor [8] suggests that, for a method with error proportional to $h^p u^{(q)}$, a good grading function is $\int_0^x |u^{(q)}|^{1/p} dx / \int_0^1 |u^{(q)}|^{1/p} dx$. For QSC we take $q = 3$ (as the error formula for the interpolant suggests) and $p = 3$ (the global order), resulting in the grading function $\xi_{q6}(x) = \int_0^x (u^{(3)})^{2/6} dx / \int_0^1 (u^{(3)})^{2/6} dx$. An alternative is to equidistribute the arc length, as [1] suggests, resulting in the grading function $\xi_{q2}(x) = \int_0^x \sqrt{1 + (u')^2} dx / \int_0^1 \sqrt{1 + (u')^2} dx$.

The following algorithm is taken from [3] and adapted for the QSC method. Given a grading function $\xi(x)$ and a number of subintervals N, the algorithm computes points s_i, $i = 0, \ldots, N$, with $\xi(s_0) = \xi(0) = 0$ and $\xi(s_N) = \xi(1) = 1$, such that $\xi(s_i) - \xi(s_{i-1}) \approx 1/N$, $i = 1, \ldots, N$, or equivalently $\xi(s_i) \approx i/N$.

The algorithm works iteratively, with a stopping criterion suggested in [3]. That is, if $\xi(x) = \int_0^x \hat{u} dx / \int_0^1 \hat{u} dx$, for some appropriate *monitor* function $\hat{u}$, at each iteration, we calculate the "drift" $\max_i \{\int_{s_i}^{s_{i+1}} \hat{u} dx\} - \int_0^1 \hat{u} dx / N$ from the target placement of the points. The stopping criterion is then $drift < tol$, where tol is a user chosen tolerance. During the experiments, we noticed that sometimes the drift oscillates, resulting in the partition points vibrating with small amplitude. However, we noticed that the partition points were already distributed reasonably well. This phenomenon was also noticed in [3]. It may result in the adaptive algorithm ending without reaching the stopping criterion and leaving us with the last set of points, even if those were not the points of the smallest drift. To get the "most" from the adaptive method, at each iteration we save the set of partition points that gives the smallest drift, and use these to compute the interpolant.

Once we have the non-uniform grid, we use the algorithm for monotone piecewise cubic interpolation from [10] to generate the mapping function w. In this way, the mapping function is in $\mathbf{C}^1$, that is, it does not satisfy the assumptions of the theorems. However, it has worked well in all experiments, as will be shown in the next section. It is worth noting that a piecewise linear $\mathbf{C}^0$ interpolant did not give satisfactory results.

For the approximation of all integrals arising in the algorithm we use the midpoint rule, since for QSC the midpoints are points of high accuracy and no discontinuities. Note that the approximation to u' is given directly by the derivative of the standard (first step) QSC approximation, while the approximation to $u^{(3)}$ is computed as shown in Section 2.2.
The outline of the algorithm, which we refer to as **PlaceMap**, is as follows:

Pick N (usually $N = 32$) and initial mesh s_i, $i = 0, \dots, N$ (usually uniform)
Pick grading function $\xi(x)$
For $itadpt = 1, \dots, maxstep$ do
    Use the first step of QSC on mesh s_i, $i = 0, \dots, N$, with $\tau_i = (s_{i-1} + s_i)/2$, $i = 1, \dots, N$,
        to approximate u
    Approximate the appropriate derivatives of u at τ_i, $i = 1, \dots, N$
    Compute new points s_i, $i = 0, \dots, N$, redistributed according to ξ
    Calculate drift
    If drift smaller than all previous iterations, save s_i, $i = 0, \dots, N$
    If $drift < tol$ then exit loop
End
Use s_i, $i = 0, \dots, N$, to construct monotone Hermite interpolant w
Output N, s_i, $i = 0, \dots, N$, w, and approximation to u

In the case that the data of the problem are given only on certain points, and we do not have a way to evaluate the source terms and the coefficient functions of the problem at the points chosen by the adaptive technique, the QSC method is still applicable. Given a set of points $T_w \equiv \{w_0 = 0 < w_1 < \dots < w_{N+1} = 1\}$, we can construct a monotone Hermite piecewise cubic interpolant w such that $w(\tau_i) = w_i$, $i = 0, \dots, N+1$, where τ_i are the collocation points (midpoints and boundary nodes) defined in Section 2. Once we have the mapping function w, we can define the nodes $s_i = w(x_i)$, $i = 0, \dots, N$, of the partition, then setup the equations (55)-(58), since all stepsizes and basis functions we need are now defined.

It is important to note that the algorithm **PlaceMap** is usually applied to a relatively small grid size N, usually $N = 32$. Once w has been constructed, this same w is used to generate the nodes and the collocation points for other grid sizes, by mapping points of a uniform partition of any grid size to the respective points of a non-uniform partition. There are some alternatives to this procedure, which we briefly discuss. (a) We can apply the adaptive algorithm for any chosen N, and construct a mapping function based on the computed grid points. Thus the mapping function may be different for each N. This procedure is more costly, since both the adaptive and the interpolation algorithms are applied for larger N's. We tested this procedure numerically for some problems, but since the error results were compatible with those using the same mapping computed with a small N, we present only the latter in the next section. It is worth pointing out that, if the mapping function is to be constructed only once, the size of the grid on which it is constructed is crucial for the success of the method. In general, the appropriate grid size is not known apriori, thus, in most realistic situations, the mapping needs to be constructed for any N, or for a large enough N, determined based on the problem. (b) We can get rid of the mapping completely, by applying the adaptive algorithm for any chosen N, then computing the position of the non-uniform midpoints by Taylor expansions based at the grid points. More specifically, once the grid points are computed, we have H_i, $i = 0, \ldots, N-1$, and from these the stepsizes h_i^a, $i = 1, \ldots, N$, and h_i^b, $i = 0, \ldots, N-1$, can be computed using the expansions of Lemma 1 and similar expansions for H_i, $i = 0, \ldots, N-1$. We developed $O(h^3)$ and $O(h^4)$ approximations of h_i^a and h_i^b and tested them numerically on some problems. The order of convergence obtained was about 3 or a bit above 3, but below the optimal 4. Therefore, we do not present these results. From the above discussion, it becomes clear that it is difficult to get rid of the mapping function in non-uniform QSC, since the method requires both the non-uniform "midpoints" w_i, and the grid points s_i. In [6], a non-uniform mapping-free CSC method is presented.

For practical purposes, a user needs to solve a problem within a certain error tolerance. The above procedure of adaptive placement of grid points and mapping function computation can be useful in this context, if it is combined with grid size and error estimators. Extrapolation through two runs, one of double size as the other can be used to estimate the error and the grid size needed to reach a given tolerance. However, for the grid size estimator to be reliable, a procedure is needed to gradually advance the grid size, until enough points are taken so that the solution behaviour is properly captured. In [6], we present such a procedure, which can be used for QSC as well as for CSC.

4 Numerical Results

In this section, we present numerical results to demonstrate the convergence of the QSC method for BVPs with non-uniform grids. All computations in this section were carried out in double precision. The QSC methods and algorithm **PlaceMap** were programmed in MATLAB by us. The linear systems arising from the QSC method were solved by Gauss elimination using the backslash operator or the lu function in MATLAB. We used the MATLAB functions $pchip$ and $ppval$ to construct and evaluate a monotone Hermite piecewise cubic interpolant.

In all tables, the notation $x.y \pm z$ means $x.y \times 10^{\pm z}$. The observed error is denoted by ϵ. The uniform norm $\|\cdot\|_\infty$ is approximated by the maximum absolute value on a constant grid of 1001 evaluation points, independently of the discretization grid.

We run some experiments with predefined mapping functions w, and some with the mapping functions constructed by the adaptive technique of Section 3. In the adaptive methods, we used $tol = 10^{-2}$, $maxstep = 20$ and a grid size of $N = 32$ to construct w, for each problem, independently of the size of the discretization grid used to solve the problem. Thus the overhead from constructing the adaptive grid is constant. For notational convenience, let w_{q2}, w_{q5}, w_{q6}, and w_{q7} be the Hermite interpolant mappings resulting from applying the adaptive algorithm in Section 3 to the grading functions ξ_{q2}, ξ_{q5}, ξ_{q6}, and ξ_{q7}, respectively.

The first problem is used to test the convergence of the QSC method with a predefined w. The operator has variable coefficients and the boundary conditions are mixed.

PROBLEM 1
$$\exp(x)u'' + \sin(x)u' - \tfrac{1}{2+x}u = g \quad \text{in} \quad (0,1),$$
$$u(0) - u'(0) = \gamma(0), \;\; u(1) + u'(1) = \gamma(1).$$

The function g is chosen so that $u(x) = \sin(x)$ is the solution. The mapping function is $w(x) = \frac{\exp(x)-1}{\exp(1)-1}$, and it is intentionally chosen so that it does not have any particular properties that fit this problem. Table 3 shows that our method has optimal convergence both globally and locally, for general differential equations with general mixed boundary conditions, and an "arbitrary" w.

QSC	$\|\epsilon(x)\|_\infty$		$\|\epsilon(s_i)\|$		$\|\epsilon'(\sigma_{ij})\|$		$\|\epsilon''(w_i)\|$	
N	error	order	error	order	error	order	error	order
32	6.80-7		1.65-7		5.67-7		4.63-5	
64	7.48-8	3.2	9.91-9	4.1	7.41-8	2.9	1.21-5	1.9
128	8.72-9	3.1	6.04-10	4.0	9.60-9	2.9	3.11-6	2.0
256	1.06-9	3.0	3.73-11	4.0	1.22-9	3.0	7.86-7	2.0

Table 3: Observed errors and respective orders of convergence corresponding to Problem 1 solved by QSC with the mapping function $w(x) = \frac{\exp(x)-1}{\exp(1)-1}$.

The next problem is designed to analyze the effect of the smoothness of w on the convergence of QSC.

PROBLEM 2
$$u'' + u' - u = g \quad \text{in} \quad (0,1), \quad u(0) = 0, \;\; u(1) = 1.$$

The function g is chosen so that $u(x) = x^q$, $q > 0$, is the solution to the problem. We note that for $q \in \mathbf{I}^+$, q should be greater than 2, otherwise the approximate and the exact solution would be the same. The mapping function is chosen to be of the form $w(x) = x^p$, $p > 0$. In order to satisfy the condition $v \in \mathbf{C}^2$ of Theorem 1 we need $q \geq 4 + 2/p$, while to satisfy the (looser) conditions of Remark 1, we need $q \geq 2 + 4/p$, thus if $q \geq 3$ then $p \geq 4$. Table 4 shows that when $q = 3$, we have optimal convergence even for $p = 1.5$. Moreover, it shows that, even for a non-smooth function $u(x) = x^{1.5}$, there are mapping functions, such as $w(x) = x^3$, that map the uniform grid to non-uniform grids that produce optimal results. One advantage of QSC over some other spline collocation methods is that it evaluates the second derivatives at midpoints instead of grid points and thus avoids potential singularities at the end points. Table 5 shows that a non-smooth mapping function $w(x) = x^{0.5}$ ($w'(0)$ is unbounded) can still give rise to a non-uniform grid with optimal convergence provided that the exact solution u has a sufficiently high degree q. Also notice that the fact that, for $p > 1$, $w'(0) = 0$, did not affect the optimal convergence. These results indicate that the conditions of the theorems are only sufficient and not necessary.

Problem 3 was taken from [4]. Its solution has a boundary layer at the left endpoint. The parameter η controls the sharpness of the boundary layer.

PROBLEM 3
$$\{(1 + \eta x)u'\}' = 0 \quad \text{in} \quad (0,1), \quad u(0) = 0, \;\; u(1) = 1.$$

QSC	$q=3, p=1.5$		$q=3, p=4$		$q=1.5, p=1$		$q=1.5, p=2$		$q=1.5, p=3$	
N	error	order	error	order	error	order	error	order	error	order
32	1.49-7		1.55-5		1.28-4		4.71-6		1.42-6	
64	9.37-9	4.0	1.02-6	4.0	4.60-5	1.4	6.32-7	2.9	9.07-8	4.0
128	5.87-10	4.0	6.53-8	4.0	1.63-5	1.5	8.27-8	2.9	5.75-9	4.0

Table 4: Observed midpoint errors and respective orders of convergence corresponding to Problem 2 solved by QSC.

QSC	$q=5$		$q=6$		$q=7$	
N	error	order	error	order	error	order
32	1.31-4		9.97-5		1.03-5	
64	2.40-5	2.4	1.26-5	3.0	6.41-7	4.0
128	4.48-6	2.4	1.58-6	3.0	3.74-8	4.0

Table 5: Observed midpoint errors and respective orders of convergence corresponding to Problem 2 solved by QSC with $p=0.5$.

The analytical solution to this problem is $u(x) = \frac{\log(1+\eta x)}{\log(1+\eta)}$. The approximate solutions for this BVP with different parameters η and mapping functions $w_I(x) = x$ and $w_{x3}(x) = x^3$ are analyzed. Figure 2 plots u for various values of η. The function u with large η increases very sharply near $x = 0$. In order to accurately capture this property in the approximate solution, many grid points near $x = 0$ and fewer near $x = 1$ should be used. The function w_{x3} is an example of a function that maps the uniform grid to such a non-uniform grid, whereas the function w_I maps the uniform grid to itself. Table 6 shows that for $\eta = 1$, both grids Δ_{w_I} and $\Delta_{w_{x3}}$ resulting from w_I and w_{x3}, respectively, produce optimal results. However, the numerical results worsen for the grid Δ_{w_I} as η increases, but remain optimal for the grid $\Delta_{w_{x3}}$. Asymptotically, we expect both the uniform and non-uniform grids to give optimal convergence, but, for this problem, the uniform grid will require a very large N to reach the optimal asymptotic behaviour. Figure 3 shows that the approximate solution arising from w_{x3} is visibly more accurate than that arising from w_I, even for a moderate η. Table 7 shows that the QSC solution arising from w_{x3} has optimal local convergence.

We next test the performance of QSC on Problem 3 with mapping functions w_{q6} and w_{q7}, respectively, and compare it with the performance when the mapping function is $w_e(x) = ((1+\eta)^x - 1)/\eta$, which is the inverse of the exact solution u, and which, for this problem, is expected to produce good results. The adaptive method for w_{q6} and w_{q7} reached the tolerance in 7 and 6 iterations, respectively. Table 8 shows that the approximate solutions arising from w_{q6}, w_{q7} and w_e have optimal global and local convergence for the points indicated. It should be noted that w_e produces errors very close to those of w_{q6}. Certainly, under realistic situations, it is not always possible to construct an analytic formula for a mapping function such as w_e.

The solution of the fourth problem has layers at both boundaries.

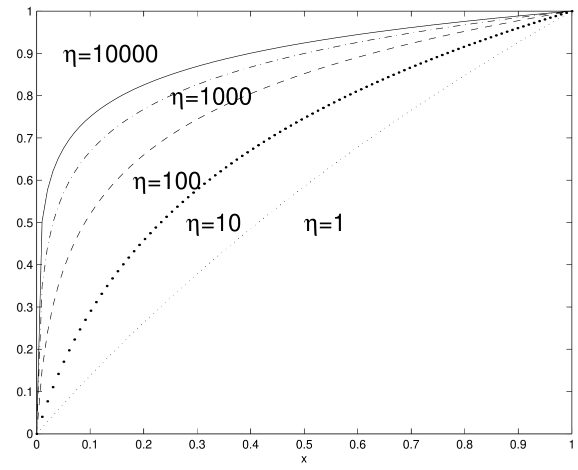

Figure 2: Exact solution u of Problem 3 with different η constants.

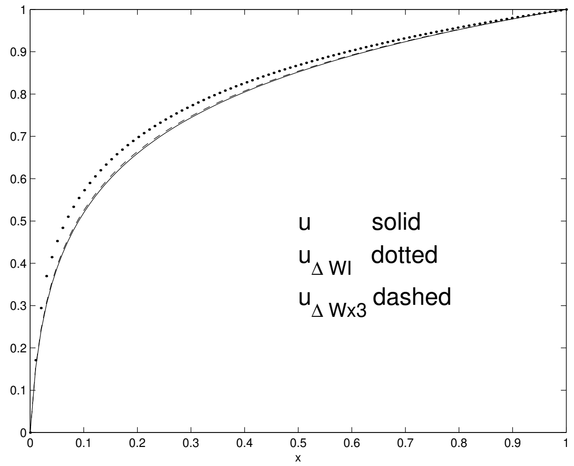

Figure 3: Exact solution u of Problem 3 with $\eta = 100$ and approximate solutions computed by QSC based on mapping functions w_I and w_{x3} for $N = 32$ grid.

QSC	w_I				w_{x3}			
	$\|\epsilon(x)\|_\infty$		$|\epsilon(w_i)|$		$\|\epsilon(x)\|_\infty$		$|\epsilon(w_i)|$	
N	error	order	error	order	error	order	error	order
	$\eta = 1$							
16	5.42-6		9.38-7		1.95-5		2.26-6	
32	6.48-7	3.1	6.42-8	3.8	2.36-6	3.0	6.01-8	5.2
64	8.30-8	3.0	4.14-9	3.9	2.95-7	3.0	2.84-9	4.4
128	1.05-8	3.0	2.61-10	4.0	3.49-8	3.1	1.64-10	4.1
	$\eta = 100$							
16	6.99-2		6.57-2		4.38-3		4.19-3	
32	2.40-2	1.5	2.26-2	1.5	2.47-4	4.1	2.36-4	4.1
64	5.29-3	2.0	5.29-3	2.0	1.73-5	3.8	1.43-5	4.0
128	9.85-4	2.4	9.82-4	2.4	1.08-6	4.0	8.91-7	4.0
	$\eta = 10,000$							
16	5.64-1		5.57-1		1.52+1		1.37+1	
32	6.89-1	-0.2	6.51-1	-0.2	3.49-1	5.4	3.39-1	5.4
64	7.79-1	-0.1	7.46-1	-0.1	7.93-3	5.4	7.87-3	5.4
128	7.82-1	-0.0	7.58-1	-0.0	3.94-4	4.2	4.02-4	4.3
256	6.51-1	0.2	6.40-1	0.2	2.42-5	4.0	2.40-5	4.0

Table 6: Observed errors and respective orders of convergence corresponding to Problem 3 solved by QSC with different η constants and mapping functions w_I and w_{x3}.

QSC	$\lvert\epsilon(s_i)\rvert$		$\lvert\epsilon'(\sigma_{ij})\rvert$		$\lvert\epsilon''(w_i)\rvert$	
N	error	order	error	order	error	order
32	3.53-1		2.38+3		2.20+7	
64	7.76-3	5.5	5.17+1	5.5	4.45+5	5.6
128	3.97-4	4.2	2.65+0	4.2	3.36+4	3.7
256	2.36-5	4.0	1.71-1	3.9	8.05+3	2.0

Table 7: Observed errors and respective orders of convergence corresponding to Problem 3 solved by QSC with $\eta = 10,000$ and mapping function w_{x3}.

QSC	w_e				w_{q6}				w_{q7}			
	$\lVert\epsilon(x)\rVert_\infty$		$\lvert\epsilon(w_i)\rvert$		$\lVert\epsilon(x)\rVert_\infty$		$\lvert\epsilon(w_i)\rvert$		$\lVert\epsilon(x)\rVert_\infty$		$\lvert\epsilon(w_i)\rvert$	
N	error	order	error	order	error	order	error	order	error	order	error	order
32	1.62-3		1.64-3		1.70-3		1.69-3		6.32-3		6.32-3	
64	1.14-4	3.8	1.10-4	3.9	1.27-4	3.7	1.24-4	3.8	4.87-4	3.7	4.76-4	3.7
128	7.43-6	3.9	6.93-5	4.0	8.32-6	3.9	7.82-6	4.0	3.86-5	3.7	3.91-5	3.6
256	5.12-7	3.8	4.34-7	4.0	5.45-7	3.9	4.92-7	4.0	3.18-6	3.6	3.01-6	3.7

Table 8: Observed errors and respective orders of convergence corresponding to Problem 3 solved by QSC with $\eta = 10,000$ and mapping functions w_e, w_{q6}, and w_{q7}.

PROBLEM 4 $$u'' + u' - u = g \quad \text{in} \quad (0,1), \quad u(0) = 0, \;\; u(1) = 0.$$

The function g is chosen so that $u(x) = \frac{\log(1+x\eta)\log(1+(1-x)\eta)}{\log(1+\eta)^2}$ is the solution to the problem. The solution has a narrow layer at each of the boundaries. The adaptive method applied to w_{q5} or w_{q6} required 9 iterations to reach the tolerance. Table 9 shows that the approximate solution arising from w_{q5} has less derivative error than the one arising from w_{q6} while the opposite is true if we look at the function error.

QSC	w_{q5}				w_{q6}			
	$\lvert\epsilon(w_i)\rvert$		$\lvert\epsilon'(\sigma_{ij})\rvert$		$\lvert\epsilon(w_i)\rvert$		$\lvert\epsilon'(\sigma_{ij})\rvert$	
N	error	order	error	order	error	order	error	order
32	6.13-2		1.50-0		4.28-3		1.22+1	
64	4.38-3	3.8	3.50-1	2.1	4.61-4	3.2	4.90+0	1.3
128	2.74-4	4.0	4.39-2	3.0	3.71-5	3.6	9.80-1	2.3
256	1.79-5	3.9	5.97-3	2.9	2.88-6	3.7	1.82-1	2.4

Table 9: Observed errors and respective orders of convergence corresponding to Problem 4 solved by QSC with $\eta = 10,000$ and mapping functions w_{q5} and w_{q6}.

The fifth problem was taken from [3] and its solution has an interior layer.

PROBLEM 5 $$-(1/\nu + \nu(x-\mu)^2)u'' - (2\nu(x-\mu))u' = g \quad \text{in} \quad (0,1), \quad u(0) = 0, \;\; u(1) = 0.$$

The function g is chosen so that the exact solution to this problem is $u(x) = (1-x)(\arctan(\nu(x-\mu)) + \arctan(\nu\mu))$, which for large ν has an interior layer near μ. The adaptive method applied to w_{q5} and w_{q6} did not reach the tolerance in 20 iterations, but the minimum drift was obtained in 5 and 11 iterations, respectively. The adaptive method applied to w_{q7} and w_{q2} required 5 and 11 iterations, respectively to reach the tolerance. Table 10 shows that the approximate solution arising from QSC with the mapping functions approximated by the respective Hermite interpolants have optimal local convergence.

QSC	w_{q5}		w_{q6}		w_{q7}		w_{q2}	
N	error	order	error	order	error	order	error	order
32	2.43-3		7.14-4		1.19-3		1.27-1	
64	2.84-4	3.1	4.82-5	3.9	1.12-4	3.4	5.78-3	4.5
128	1.77-5	4.0	3.03-6	4.0	7.09-6	4.0	4.63-4	3.6
256	1.12-6	4.0	1.91-7	4.0	4.43-7	4.0	3.08-5	3.9

Table 10: Observed grid point errors and respective orders of convergence corresponding to Problem 5 solved by QSC with $\mu = .5$ and $\nu = 100$, and mapping functions w_{q5}, w_{q6}, w_{q7} and w_{q2}.

Finally, we present results from the application of QSC to a non-linear problem, taken from [17].

PROBLEM 6 $$u'' - \exp(u) = 0 \quad \text{in} \quad (0,1), \quad u(0) = u(1) = 0.$$

The unique solution to this problem is $u = 2\log(\zeta \sec(\zeta(x-0.5)/2)) - \log 2$, where $\zeta = 1.3360556949061$. (The value of ζ was calculated as the unique root of $z - \sqrt{2}\cos(z/4) = 0$ [9]). We solve this problem using the two-step QSC method and each of the following two iteration schemes: the simple scheme [17] $u^{[k+1]''} - u^{[k+1]} = \exp(u^{[k]}) - u^{[k]}$ and the scheme arising from Newton's method [9], $u^{[k+1]''} - \exp(u^{[k]})u^{[k+1]} = \exp(u^{[k]}) - \exp(u^{[k]})u^{[k]}$. We apply the non-linear iteration first to the first step of QSC until convergence and then to the second step of QSC until convergence. The non-linear iteration of the first step uses the zero vector as initial guess, while that of the second step uses the last solution of the first step. The stopping criterion is the infinity norm of the difference of the degrees of freedom vectors between two consecutive iterations, and the non-linear iteration tolerance (grid dependent) is $10^{-2}h^2$ for the first step and $10^{-2}h^4$ for the second. (Note that, when the degrees of freedom of two quadratic splines differ at most by a certain tolerance, the two quadratic splines also differ at most by the tolerance, since the infinity norm of the quadratic spline interpolation matrix is equal to 1.) Due to the simple shape of the solution, the application of the adaptive technique of Section 3 to Problem 6 resulted in a uniform partition, that is, the "drift" corresponding to the initial uniform partition was below the adaptive technique tolerance $tol = 10^{-2}$. Table 11 shows that the QSC method applied to Problem 6 exhibits optimal convergence. It is worth noting that the second step of QSC requires fewer non-linear iterations than the first step, a fact which can be attributed to the choice of initial guess for the second step, as discussed above. It is also worth noting that, in several cases, Newton's method requires fewer iterations, but also requires the QSC matrix to be formed at each iteration. Moreover, Newton's method is applicable to other non-linear problems, while the particular simple iteration scheme is designed for this problem.

	simple iteration						Newton's					
QSC	Step 1			Step 2			Step 1			Step 2		
N	$itnl$	error	order	$itnl$	error	order	$itnl$	error	order	$itnl$	error	order
16	3	1.59-05		2	2.53-08		3	1.60-05		2	2.63-08	
32	3	3.95-06	2.01	2	1.88-09	3.75	3	3.99-06	2.00	2	1.85-09	3.83
64	4	9.98-07	1.99	3	1.18-10	3.99	3	9.98-07	2.00	2	1.19-10	3.96
128	4	2.49-07	2.00	3	7.35-12	4.00	3	2.50-07	2.00	2	7.49-12	3.99

Table 11: Observed number of non-linear iterations $itnl$, grid point errors and respective orders of convergence for both steps of QSC on Problem 6.

5 Final remarks

One may consider that the technique of mapping uniform to non-uniform points and solving the problem on the non-uniform partition is mathematically equivalent to applying a transformation of variables to the problem and obtaining a problem which can be solved effectively on a uniform grid. We emphasize that, at least numerically, this is not true. Our technique computes an approximation to $w(x)$ and to the location of the non-uniform grid points and collocation points, then applies collocation on the non-uniform partition. To implement the transformation of variables technique, we need to compute, an approximation to $w(x)$, $w'(x)$ and $w''(x)$, then apply collocation to the transformed problem (which involves w, w' and w'') on the uniform partition. When we attempted to do that, we found that our numerical results were significantly affected. More specifically, the order of convergence was hardly above 2, and the actual errors significantly larger. Therefore, we did not choose (and do not recommend) this approach.

The technique used in this paper to extend the optimal quadratic spline collocation methods from uniform to non-uniform partitions can be used for other (smooth) spline collocation methods (e.g. cubic) and higher order BVPs (e.g. quartic or quintic splines and fourth-order BVPs). However, the development of appropriate spline interpolants (i.e. the derivation of the boundary relations the spline interpolant has to satisfy) and the derivation of the expansions of the derivative errors of the interpolant at the non-uniform collocation points is quite cumbersome and not straightforward. The generalization of the spline interpolant definition and derivative error expansions to higher degree splines is a challenging piece of research. In [6], we develop, analyze and test non-uniform CSC methods. However, due to the fact that the CSC methods are based on grid points only, they are essentially mapping-free.

The QSC methods described in this paper can be relatively easily extended to two-dimensional (and higher-dimensional) rectangular domains, if the domain discretization is also rectangular. However, a rectangular discretization is usually not the most effective one. Moreover, the analysis of the methods for multi-dimensional domains is not straightforward. More work is also needed to extend the methods to non-rectangular domains, for example, following the approach of [13], and to general quadrilateral discretizations. The development of efficient linear solvers for the resulting system of equations is another interesting extension of this work.

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