An Efficient Algorithm Based on Quadratic Spline Collocation and Finite Difference Methods for Parabolic Partial Differential Equations

by

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Abstract

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An efficient algorithm which combines quadratic spline collocation methods (QSC) for the space discretization and classical finite difference methods (FDMs), such as *Crank-Nicolson*, for the time discretization to solve general *linear parabolic partial differential equations* has been studied. By combining QSC and finite differences, a form of the approximate solution of the problem at each time step can be obtained; thus the value of the approximate solution and its derivatives can be easily evaluated at any point of the space domain for each time step.

There are two typical ways for solving this problem: (a) using QSC in its standard formulation, which has low accuracy $\mathcal{O}(h^2)$ and low computational work. More precisely, it requires the solution of a tridiagonal linear system at each time step; (b) using optimal QSC, which has high accuracy $\mathcal{O}(h^4)$ and requires the solution of either two tridiagonal linear systems or an almost pentadiagonal linear system at each time step. A new technique is introduced here which has the advantages of the above two techniques; more precisely, it has high accuracy $\mathcal{O}(h^4)$ and almost the same low computational work as the standard QSC.

Dedication

To my families, especially to my lovely son, Bryan.

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Chapter 1

Introduction

In this chapter, we give the description of the problem which we are going to solve and some background and notation that we will use throughout this thesis.

We are interested in solving linear second-order parabolic *partial differential equations* (PDEs) in one space dimension. The typical example of such a problem is given by the heat equation, which is the non-stationary counterpart of the Laplace equation.

Let us define a spatial differential operator $\mathcal{L}$ by

$$\mathcal{L}u \equiv p(x,t)\frac{\partial^2 u}{\partial x^2} + q(x,t)\frac{\partial u}{\partial x} + f(x,t)u,$$

where p, q, and f are given functions.

The problem we want to solve is described by a parabolic PDE of the form

$$\frac{\partial u}{\partial t} = \mathcal{L}u + g(x,t),\ 0 < x < 1,\ 0 < t \le T, \tag{1.1}$$

subject to the initial condition

$$u(x,0) = \gamma(x), \quad 0 \le x \le 1, \tag{1.2}$$

and the boundary conditions

$$\mathcal{B}u \equiv \{u(0,t) = \beta_0(t),\ u(1,t) = \beta_1(t)\},\ 0 < t \le T, \tag{1.3}$$

where g, γ, β_0, and β_1 are given functions, and u is the unknown function to be determined (or approximated). We present the parabolic PDE problem with Dirichlet boundary conditions (1.3), but we will also consider periodic boundary conditions. Moreover, most methods presented in this thesis are easily extended to Neumann and general boundary conditions.

For the time discretization, we apply the *Crank-Nicolson* method. For the space discretization, we apply the *quadratic-spline* collocation method. The resulting method is referred to as the *Crank-Nicolson quadratic-spline* collocation method. First, we introduce the continuous-time collocation method. Then we talk about a discrete-time collocation method, the *Crank-Nicolson* collocation method. Finally, we focus on a particular collocation method, the *Crank-Nicolson quadratic-spline* collocation method and study several variants of it.

Following [8], we consider the interval $I = [0, 1]$ and a uniform partition

$$\Delta \equiv \{0 = x_0 < x_1 < \ldots < x_N = 1\}$$

of I with mesh size $h = \frac{1}{N}$. Let

$$I_i \equiv [x_{i-1}, x_i], \; i = 1, \ldots, N.$$

Let $\mathbf{P}^r(E)$ denote the set of polynomials of degree (at most) r on interval E. We define

$$\mathbf{P}^r_{\Delta,k} \equiv \{v \in \mathcal{C}^k(I) \mid v \in \mathbf{P}^r(I_i), i = 1, 2, \ldots, N\},$$

where $\mathcal{C}^k(I)$ is the set of functions with k continuous derivatives on I.

Thus, for example, the *Hermite piecewise-cubic* function space, the *cubic-spline* function space, and the *quadratic-spline* function space are given by $\mathbf{P}^3_{\Delta,1}$, $\mathbf{P}^3_{\Delta,2}$, and $\mathbf{P}^2_{\Delta,1}$, respectively.

After imposing the continuity conditions on the interior knots, it is easy to show that the dimension d of a function space $\mathbf{P}^r_{\Delta,k}$ is

$$d = (r + 1)N - (k + 1)(N - 1). \tag{1.4}$$

Therefore, the dimensions of $\mathbf{P}^3_{\Delta,1}$, $\mathbf{P}^3_{\Delta,2}$, $\mathbf{P}^2_{\Delta,1}$ are $2N+2,\ N+3,\ N+2$, respectively. Let

$$\{\phi_0, \phi_1, \ldots, \phi_{d-1}\}$$

be a set of piecewise polynomial basis functions of the function space $\mathbf{P}^r_{\Delta,k}$. Then any function $p(x) \in \mathbf{P}^r_{\Delta,k}$ can be written as

$$p(x) = \sum_{i=0}^{d-1} c_i \phi_i(x),$$

where c_i, $i = 0, \ldots, N$, are *degrees of freedom* (DOFs).

In [7], [8], the continuous-time collocation method is introduced for the function space $\mathbf{P}^3_{\Delta,1}$. Here, we present the continuous-time collocation method in a general way. In general, we seek a map $U(x,t) : [0,T] \to \mathbf{P}^r_{\Delta,k}$ such that U is an approximation to u of Problem (1.1)-(1.3). Recalling that $\dim(\mathbf{P}^r_{\Delta,k}) = d$, we need d relations for each time t to specify the approximate solution $U(x,t)$. Two of these conditions can obviously be obtained from the boundary conditions. The method of collocation requires that the remaining relations be obtained by having the differential equation satisfied at $d-2$ points in I. The $d-2$ points together with the two boundary points are called *collocation points* or *data points* and are denoted by

$$\{\tau_0 = 0 < \tau_1 < \ldots < \tau_{d-1} = 1\}.$$

More precisely, $U(x,t)$ is determined by satisfying

$$\begin{aligned} &(i) \quad \{\frac{\partial U}{\partial t} - \mathcal{L}U\}(\tau_i, t) = g(\tau_i, t),\ 1 \le i \le d-2, \\ &(ii) \quad U(0,t) = \beta_0(t),\ U(1,t) = \beta_1(t), \\ &(iii) \quad U(x,0) - \gamma(x) \text{ is small in a sense to be specified next.} \end{aligned} \tag{1.5}$$

Regarding condition (iii), a simple way to define $U(x,0)$ is to let $U(x,0)$ be the interpolant of γ in $\mathbf{P}^r_{\Delta,k}$.

So far, we have introduced the continuous-time collocation method. In order to actually compute an approximate solution to Problem (1.1)-(1.3) by the collocation method (1.5), we need to discretize the time variable. Let

$$\{0 = t_0 < t_1 < \ldots < t_M = T\}$$

be a partition of $[0, T]$. For simplicity, we use a uniform partition. More precisely, let Δt be the time stepsize, that is,

$$\Delta t = \frac{T}{M},\ t_j = j\Delta t,\ j = 0, \ldots, M,$$

where M is the number of timesteps. Define

$$t_{j+\frac{1}{2}} \equiv (j + \frac{1}{2})\Delta t,$$

and

$$\begin{aligned} U^j &\equiv U(x, t_j), \\ U^{j+\frac{1}{2}} &\equiv \frac{1}{2}(U^{j+1} + U^j), \\ \frac{\partial U^j}{\partial t} &\equiv \frac{U^{j+1} - U^j}{\Delta t}. \end{aligned} \tag{1.6}$$

With the above notation, the *Crank-Nicolson* collocation method corresponding to (1.5) is to find a map $U : \{t_0, \ldots, t_M\} \to \mathbf{P}^r_{\Delta,k}$ such that

$$\begin{aligned} &(i) \quad \{\frac{\partial U^j}{\partial t} - \mathcal{L}U^{j+\frac{1}{2}}\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}),\ 1 \le i \le d-2,\ 0 \le j \le M-1 \\ &(ii) \quad U^j(0) = \beta_0(t_j),\ U^j(1) = \beta_1(t_j),\ 0 < j \le M, \\ &(iii) \quad U^0 \text{ be the interpolant of } \gamma. \end{aligned} \tag{1.7}$$

If we let $\mathbf{P}^r_{\Delta,k} = \mathbf{P}^2_{\Delta,1}$ in (1.7), then we get the *Crank-Nicolson quadratic-spline* collocation method, referred to as the QSC-CN method.

In [14], [15], a cubic spline technique for the heat equation has been proposed. The main technique used in these two papers is based on some properties of cubic splines which are studied in [1]. These properties are described by equations relating the values of the cubic spline interpolant $S^j(x_i)$ of the values $u(x_i, t_j)$, its derivative values $S''^j(x_i)$, and the values $u(x_i, t_j)$ themselves. For simplicity, denote $u(x_i, t_j)$ by u_i^j. The following equation holds for $x \in I_i$, $i = 1, \ldots, N$:

$$\begin{aligned} S^j(x) &= S''^j(x_{i-1})\frac{(x_i - x)^3}{6h} + S''^j(x_i)\frac{(x - x_{i-1})^3}{6h} + (u_{i-1}^j - \frac{h^2}{6}S''^j(x_{i-1}))\frac{(x_i - x)}{h} \\ &\quad +(u_i^j - \frac{h^2}{6}S''^j(x_i))\frac{(x - x_{i-1})}{h}. \end{aligned} \tag{1.8}$$

By imposing the continuity of the first derivatives at the interior grid points, and using a certain implicit time discretization, the authors eliminate S'' and derive a general form of a finite difference formula which can be reduced to some frequently used finite difference formulae, for instance, *Crank-Nicolson* and *Douglas*. According to the method in [14], in order to get the cubic spline collocation approximation to the heat equation, first a finite difference method is used to obtain an approximation to u_i^j and a tridiagonal system is solved to obtain S''^0; then $S''^j(x_i)$ can be explicitly obtained for $j \geq 1$; finally, a cubic spline approximation is computed by (1.8). Since this method involves a finite difference method, we do not consider it as a pure cubic spline collocation method.

We say that a collocation approximation in $\mathbf{P}^r_{\Delta,k}$ is *optimal*, when it exhibits the same order of convergence as the interpolant in the same approximation space. From (1.4), we notice that the space of smooth splines, that is $\mathbf{P}^r_{\Delta,r-1}$, has the smallest dimension among all spaces $\mathbf{P}^r_{\Delta,k}$ of piecewise polynomials of the same degree r. Hence, spline collocation needs less data points and gives rise to smaller linear systems. However, standard spline collocation does not give rise to optimal order approximation. Certain modifications of the standard spline collocation methods can lead to optimal order approximations. In this thesis, we study a modified *quadratic-spline* collocation method for parabolic PDEs, which is of optimal order of convergence. Some previous work by other researchers is introduced in the following paragraphs.

In [7] and [8], Douglas and Dupont studied the continuous-time collocation method and the discrete-time collocation method based on $\mathbf{P}^r_{\Delta,1}$, with $r \geq 3$ for quasilinear parabolic equations in a single space variable. By collocation at the images of the Gauss-Legendre points in each I_i, uniform errors of order $\mathcal{O}(h^{r+1})$ and superconvergence results at the knots $\{x_i\}$ of order $\mathcal{O}(h^{2r-2})$ are obtained for the continuous-time collocation. For the discrete-time, *Crank-Nicolson*, collocation, $\mathcal{O}(h^{r+1} + (\Delta t)^2)$ convergence is obtained. In [9], the continuous-time and discrete-time collocation methods have been studied for semilinear parabolic initial-boundary value problems in two space variables based on the same function space as in [8]. Orders of convergence $\mathcal{O}(h^{r+1})$ for continuous-time and $\mathcal{O}(h^{r+1} + (\Delta t)^2)$ for discrete-time, *Crank-Nicolson*, approximation are obtained.

In [4], the continuous-time collocation method using smooth cubic splines is studied for two-point linear parabolic initial value problems of the form $u_t = u_{xx} - \sigma u + f(x,t),\ 0 < x < 1,\ t > 0$, subject to homogeneous Dirichlet boundary conditions. The authors introduce appropriate perturbation terms applied to the original collocation equations which result in $\mathcal{O}(h^4)$ convergence. However, since the analysis in [4] is based on the properties of certain matrices, it is not trivial to extend the analysis to more general boundary conditions or problems. In [3], Archer studied a modified version of the continuous-time cubic spline collocation method for more general problems (quasilinear parabolic problems) and found that a certain perturbation to the u_{xx} term of the operator leads to a fourth order approximation. This perturbation can be used for BVPs as well. Continuous time estimates of order $\mathcal{O}(h^4)$ are obtained.

The standard QSC-CN method defined by (1.7) with τ_i being the midpoints of I_i leads to second-order convergence with respect to both the space and time stepsizes. By adding an appropriate perturbation to $\mathcal{L}$ as described in [10] for BVPs, we obtain an optimal QSC-CN method which results in $\mathcal{O}(h^4 + \Delta t^2)$ error bounds at the collocation points $\{\tau_i\}$ and the knots $\{x_i\}$, and superconvergence for the first derivative at the Gauss points and for the second derivative at the collocation points.

The optimal QSC-CN method requires more computational work compared to the standard QSC-CN method. A new method introduced in this thesis attempts to reduce the computational work required by the optimal QSC-CN method without reducing the optimal order of convergence. Since this method is revised from the optimal QSC-CN method, we refer to it as the RQSC-CN method.

In Chapter 2, we present some results of the optimal *quadratic-spline* collocation method (QSC) on BVPs, which are needed for the development of the RQSC-CN method, and derive the linear systems arising from homogeneous Dirichlet and periodic boundary conditions. In Chapter 3, first, we introduce the optimal *one-step* and *two-step* QSC-CN methods; then we demonstrate how to derive the RQSC-CN method. In Chapter 4, we study the stability and convergence of the RQSC-CN method and make small changes to the RQSC-CN method giving rise to the RQSC-CN1 and RQSC-CN0 methods, which have better stability properties than the RQSC-CN method. In Chapter 5, we illustrate numerical results for a variety of problems. Finally, we conclude in Chapter 6 with a summary of the results presented in this thesis.

Chapter 2

Results of QSC for Two-point BVP

In this chapter, we review results on the optimal QSC methods for a second order two-point boundary value problem

$$\mathcal{L}u \equiv p(x)u'' + q(x)u' + f(x)u = g \text{ on } I = (0,1), \tag{2.1}$$

subject to Dirichlet boundary conditions

$$\mathcal{B}u \equiv \{u(0) = \beta_0,\ u(1) = \beta_1\}. \tag{2.2}$$

Most of the results presented in this chapter are from [10]. We employ the two boundary points and the midpoints of each I_i as the collocation points. More precisely, the set of collocation points is

$$\{\tau_0 = x_0, \tau_1 = \frac{x_0 + x_1}{2}, \ldots, \tau_N = \frac{x_{N-1} + x_N}{2}, \tau_{N+1} = x_N\}.$$

We use the notation introduced in Chapter 1 and uniform norms unless otherwise indicated.

First, we give some properties of a certain quadratic-spline interpolant and its derivatives. Then, we introduce the optimal QSC methods and results of convergence. Finally, we give the basis functions of $\mathbf{P}^2_{\Delta,1}$ and derive the matrices arising from the optimal QSC methods.

2.1 Approximate properties of the quadratic-spline interpolant

Let us adopt the notation $u^{(k)}(x)$ for the kth derivative of the single-variable function $u(x)$, for $k \geq 3$. Let $S(x)$ denote the quadratic-spline interpolant of $u(x)$ that satisfies

$$S(\tau_i) = \begin{cases} u(\tau_i) - \dfrac{h^4}{128} u^{(4)}(\tau_i), & i = 0, N+1 \\ u(\tau_i), & 1 \leq i \leq N. \end{cases} \tag{2.3}$$

Let S_i denote $S(\tau_i)$ and u_i denote $u(\tau_i)$. In general, the subscript for a function denotes the value of the function at the respective collocation point. The following theorems and relations are shown in [10].

Theorem 2.1.1 *If $u \in C^6(I)$, then at the midpoints τ_i of Δ, we have*

$$S_i' = u_i' + \frac{h^2}{24} u_i^{(3)} + \mathcal{O}(h^4)$$

and

$$S_i'' = u_i'' - \frac{h^2}{24} u_i^{(4)} + \mathcal{O}(h^4).$$

A subsequent theorem is shown in [10] by using Taylor's expansions.

Theorem 2.1.2 *If $u \in C^6(I)$, then at $\{\tau_i | i = 2, \ldots, N-1\}$, we have*

$$\begin{aligned} u_i^{(4)} &= (S_{i-1}'' - 2S_i'' + S_{i+1}'')/h^2 + \mathcal{O}(h^2) \\ u_i^{(3)} &= (S_{i+1}'' - S_{i-1}'')/(2h) + \mathcal{O}(h^2) \\ &= (S_{i-1}'' - 2S_i'' + S_{i+1}'')/h^2 + \mathcal{O}(h^2) \\ u_i'' &= (S_{i-1}'' + 22S_i'' + S_{i+1}'')/24 + \mathcal{O}(h^4) \\ u_i' &= -(S_{i-1}'' - 26S_i'' + S_{i+1}'')/24 + \mathcal{O}(h^4). \end{aligned} \tag{2.4}$$

For the points $\{\tau_0, \tau_1, \tau_N, \tau_{N+1}\}$, using extrapolation we get

$$\begin{aligned} u_0^{(k)} &= (3u_1^{(k)} - u_2^{(k)})/2 + \mathcal{O}(h^2) \\ u_1^{(k)} &= 2u_2^{(k)} - u_3^{(k)} + \mathcal{O}(h^2) \\ u_N^{(k)} &= 2u_{N-1}^{(k)} - u_{N-2}^{(k)} + \mathcal{O}(h^2) \\ u_{N+1}^{(k)} &= (3u_N^{(k)} - u_{N-1}^{(k)})/2 + \mathcal{O}(h^2) \end{aligned} \tag{2.5}$$

where $k = 3, 4$.

Define the discrete difference operator Λ by

$$\Lambda S_i \equiv (S_{i-1} - 2S_i + S_{i+1})/h^2. \tag{2.6}$$

Rewriting (2.4) and (2.5) using Λ, we have the following corollary:

Corollary 2.1.3 *Suppose the conditions of Theorem 2.1.1 and 2.1.2 are satisfied. Then the following relations hold*

$$u_i^{(k)} = \begin{cases} (5\Lambda S_2^{(k-2)} - 3\Lambda S_3^{(k-2)})/2 + \mathcal{O}(h^2), & i = 0 \\ 2\Lambda S_2^{(k-2)} - 3\Lambda S_3^{(k-2)} + \mathcal{O}(h^2), & i = 1 \\ \Lambda S_i^{(k-2)} + \mathcal{O}(h^2), & 2 \le i \le N-1 \\ 2\Lambda S_{n-1}^{(k-2)} - \Lambda S_{n-2}^{(k-2)} + \mathcal{O}(h^2), & i = N \\ (5\Lambda S_{n-1}^{(k-2)} - 3\Lambda S_{n-2}^{(k-2)})/2 + \mathcal{O}(h^2), & i = N+1 \end{cases}$$

where k=3,4.

The following theorem is shown in [13] and [11].

Theorem 2.1.4 *If $u \in C^4(I)$, then at the grid points $\{x_i | i = 0, \ldots, N\}$*

$$S(x_i) = u(x_i) + \mathcal{O}(h^4).$$

Now we consider Problem (2.1)-(2.2). Based on Theorem 2.1.1 and 2.1.2, we have

$$\mathcal{L}S_i = g_i - \frac{h^2}{24} p_i u_i^{(4)} + \frac{h^2}{24} q_i u_i^{(3)} + \mathcal{O}(h^4),\ 1 \le i \le N \tag{2.7}$$

and

$$S_0 = \beta_0 + \mathcal{O}(h^4),\ S_{N+1} = \beta_1 + \mathcal{O}(h^4).$$

Using Corollary 2.1.3, the right side of relations (2.7) is approximated without affecting the $\mathcal{O}(h^4)$ accuracy, to give rise to

$$\mathcal{L}S_i = \begin{cases} g_1 - \frac{h^2}{24} p_1 (2\Lambda S_2'' - \Lambda S_3'') + \frac{h^2}{24} q_1 (2\Lambda S_2' - \Lambda S_3') + \mathcal{O}(h^4), & i = 1 \\ g_i - \frac{h^2}{24} p_i \Lambda S_i'' + \frac{h^2}{24} q_i \Lambda S_i' + \mathcal{O}(h^4), & 2 \le i \le N-1 \\ g_n - \frac{h^2}{24} p_n (2\Lambda S_{n-1}'' - \Lambda S_{n-2}'') + \frac{h^2}{24} q_n (2\Lambda S_{n-1}' - \Lambda S_{n-2}') + \mathcal{O}(h^4), & i = N. \end{cases} \tag{2.8}$$

We define a perturbation operator $\mathcal{P}_{\mathcal{L}}$ by

$$\mathcal{P}_{\mathcal{L}} S_i \equiv \begin{cases} \frac{h^2}{24} p_1 (2\Lambda S_2'' - \Lambda S_3'') - \frac{h^2}{24} q_1 (2\Lambda S_2' - \Lambda S_3'), & i = 1 \\ \frac{h^2}{24} p_i \Lambda S_i'' - \frac{h^2}{24} q_i \Lambda S_i', & 2 \leq i \leq N-1 \\ \frac{h^2}{24} p_n (2\Lambda S_{n-1}'' - \Lambda S_{n-2}'') - \frac{h^2}{24} q_n (2\Lambda S_{n-1}' - \Lambda S_{n-2}'), & i = N. \end{cases} \quad (2.9)$$

and move the approximations of the derivatives of u in (2.8) to the left side. Then we have

$$(\mathcal{L} + \mathcal{P}_{\mathcal{L}}) S_i = g_i + \mathcal{O}(h^4), \text{ for } 1 \leq i \leq N. \quad (2.10)$$

2.2 Optimal quadratic-spline collocation methods for BVPs

Taking into account all the results presented in the previous section, we now define the two optimal QSC methods. The optimal QSC methods are based on the perturbation $\mathcal{P}_{\mathcal{L}}$ of the operator $\mathcal{L}$ of the problem.

2.2.1 Optimal one-step QSC method

The optimal one-step QSC method computes the approximation $w_\Delta \in \mathbf{P}^2_{\Delta,1}$ that satisfies

$$(\mathcal{L} + \mathcal{P}_{\mathcal{L}}) w_\Delta(\tau_i) = g(\tau_i), \quad \text{for } i = 1, \ldots, N, \quad (2.11)$$

and the boundary conditions

$$w_\Delta(\tau_0) = \beta_0, \text{ and } w_\Delta(\tau_{N+1}) = \beta_1.$$

We refer to this formulation as the optimal *one-step* QSC method, distinguished from the optimal *two-step* QSC method.

2.2.2 Optimal two-step QSC method

An alternative formulation of the method is to compute the approximate solution by two steps. In step one, we compute an intermediate approximation $v_\Delta \in \mathbf{P}^2_{\Delta,1}$ that satisfies

$$\mathcal{L}v_\Delta(\tau_i) = g(\tau_i), \text{ for } i = 1, \ldots, N,$$

and the boundary conditions

$$v_\Delta(\tau_0) = \beta_0, \text{ and } v_\Delta(\tau_{N+1}) = \beta_1.$$

In step two, using v_Δ to approximate the perturbation term in (2.11) and moving the perturbation term to the right side, we compute the final approximation $u_\Delta \in \mathbf{P}^2_{\Delta,1}$ that satisfies

$$\mathcal{L}u_\Delta(\tau_i) = g(\tau_i) - \mathcal{P}_\mathcal{L} v_\Delta(\tau_i), \text{ for } i = 1, \ldots, N,$$

and

$$u_\Delta(\tau_0) = \beta_0, \text{ and } u_\Delta(\tau_{N+1}) = \beta_1.$$

The existence and convergence of the approximation u_Δ are shown in [10] and are summarized as the following theorem.

Theorem 2.2.1 *If we assume that*

(a1) the functions p, q, f *and* g *are in* $C(I)$

(a2) the boundary value problem $\mathcal{L}u = g,\ \mathcal{B}u = 0$ *has a unique solution in* $C^4(I)$

(a3) the problem $u'' = 0,\ \mathcal{B}u = 0$ *has a unique solution,*

then the solution of two-step *QSC method* u_Δ *exists, and*

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

(ii) $|u(x) - u_\Delta(x)| = \mathcal{O}(h^4),$ *for* $x = x_i$ *and* $x = \tau_i$

(iii) $|u'(x_i + \lambda h) - u'_\Delta(x_i + \lambda h)| = \mathcal{O}(h^3)$

(iv) $|u''(x_i + h/2) - u''_\Delta(x_i + h/2)| = \mathcal{O}(h^2)$

where $\lambda = (3 \pm \sqrt{3})/6.$

Similar results hold for the solution w_Δ of the optimal *one-step* QSC method.

2.3 Basis functions and matrices

To implement the optimal QSC methods, we choose the set of quadratic B-splines as basis functions for $\mathbf{P}^2_{\Delta,1}$. More specifically,

let

$$\phi(x) = \frac{1}{2}\begin{cases} x^2, & \text{for } 0 \le x \le 1 \\ -2(x-1)^2 + 2(x-1) + 1, & \text{for } 1 \le x \le 2 \\ (3-x)^2, & \text{for } 2 \le x \le 3 \\ 0, & \text{elsewhere.} \end{cases} \tag{2.12}$$

Then, the basis functions for $\mathbf{P}^2_{\Delta,1}$ are given by

$$\phi_i(x) = \phi(\frac{x}{h} - i + 2),\ i = 0, \ldots, N+1. \tag{2.13}$$

Our analysis for the RQSC-CN method is based on functions satisfying some particular boundary conditions. More precisely, we assume that the function u satisfies homogeneous Dirichlet or periodic boundary conditions. It is worth mentioning that the RQSC-CN method can be used to solve the Problem (1.1)-(1.3) which has general Dirichlet boundary conditions, and can be extended to problems with Neumann and general boundary conditions.

2.3.1 Homogeneous Dirichlet boundary conditions

For homogeneous Dirichlet boundary conditions, we adjust the basis functions so that they satisfy the boundary conditions, and thus, decrease the dimension of $\mathbf{P}^2_{\Delta,1}$ from $N+2$ to N. Let $\mathbf{P}^2_{\Delta_{\partial d},1}$ denote the subspace of $\mathbf{P}^2_{\Delta,1}$ satisfying homogeneous Dirichlet boundary conditions. More precisely, the basis functions for $\mathbf{P}^2_{\Delta_{\partial d},1}$ are

$$\tilde{\phi}_1 = \phi_1 - \phi_0,\ \tilde{\phi}_i = \phi_i\ (i = 2, \ldots, N-1),\ \tilde{\phi}_N = \phi_N - \phi_{N+1}. \tag{2.14}$$

Thus, any quadratic spline $u_\Delta(x)$ in $\mathbf{P}^2_{\Delta_{\partial d},1}$ is written as

$$u_\Delta(x) = \sum_{i=1}^{N} c_i \tilde{\phi}_i(x), \tag{2.15}$$

where $\{c_1, \ldots, c_N\}$ are DOFs, and satisfies the boundary conditions by construction. Therefore, we do not need to have explicit equations for the boundary conditions.

In order to derive the linear system arising from the optimal QSC methods, we need the values of the quadratic spline basis functions and their derivatives at the collocation points. Based on the definition in (2.13), we can easily get the values shown in Table 2.1 in [5].

Table 2.1: Values of the quadratic spline basis functions and derivatives

	x_{i-2}	τ_{i-1}	x_{i-1}	τ_i	x_i	τ_{i+1}	x_{i+1}
ϕ_{i-2}	$1/2$	$1/8$	0	0	0	0	0
ϕ_{i-1}	$1/2$	$3/4$	$1/2$	$1/8$	0	0	0
ϕ_i	0	$1/8$	$1/2$	$3/4$	$1/2$	$1/8$	0
ϕ_{i+1}	0	0	0	$1/8$	$1/2$	$3/4$	$1/2$
ϕ_{i+2}	0	0	0	0	0	$1/8$	$1/2$
ϕ'_{i-2}	$-1/h$	$-1/(2h)$	0	0	0	0	0
ϕ'_{i-1}	$1/h$	0	$-1/h$	$-1/(2h)$	0	0	0
ϕ'_i	0	$1/(2h)$	$1/h$	0	$-1/h$	$-1/(2h)$	0
ϕ'_{i+1}	0	0	0	$1/(2h)$	$1/h$	0	$-1/h$
ϕ'_{i+2}	0	0	0	0	0	$1/(2h)$	$1/h$
ϕ''_{i-2}		$1/h^2$		0		0	
ϕ''_{i-1}		$-2/h^2$		$1/h^2$		0	
ϕ''_i		$1/h^2$		$-2/h^2$		$1/h^2$	
ϕ''_{i+1}		0		$1/h^2$		$-2/h^2$	
ϕ''_{i+2}		0		0		$1/h^2$	

Let $diag(d_1, d_2, \ldots, d_N)$ denote a diagonal matrix D with diagonal entries $D_{ii} = d_i, \ i = 1, \ldots, N$. Let

$$D_p = diag(p_1, p_2, \ldots, p_N), D_q = diag(q_1, q_2, \ldots, q_N), D_f = diag(f_1, f_2, \ldots, f_N),$$

and

$$\vec{g} = (g_1, g_2, \ldots, g_N)^T, \vec{c} = (c_1, c_2, \ldots, c_N)^T.$$

Taking into account (2.9) and Table 2.1, the equations in (2.11) representing the optimal *one-step* QSC method for homogeneous Dirichlet boundary conditions take the form of a linear system

$$\left(\frac{1}{h^2}D_p(Q_2+\frac{1}{24}Q_{xx})+\frac{1}{2h}D_q(Q_1-\frac{1}{24}Q_x)+D_fQ_0\right)\vec{c}=\vec{g}, \tag{2.16}$$

where

$$Q_0 = \frac{1}{8}\begin{bmatrix} 5 & 1 & 0 & \cdots & 0 \\ 1 & 6 & 1 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 1 & 6 & 1 \\ 0 & \cdots & 0 & 1 & 5 \end{bmatrix},$$

$$Q_1 = \begin{bmatrix} 1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & -1 & 0 & 1 \\ 0 & \cdots & 0 & -1 & -1 \end{bmatrix},$$

$$Q_2 = \begin{bmatrix} -3 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -3 \end{bmatrix},$$

and

$$Q_p = \begin{bmatrix} 2 & -5 & 4 & -1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 0 & 1 & -2 & 1 \\ 0 & \cdots & 0 & -1 & 4 & -5 & 2 \end{bmatrix},$$

$$\begin{aligned} Q_{xx} &= Q_p Q_2 \\ &= \begin{bmatrix} -11 & 16 & -14 & 6 & -1 & 0 & \cdots & 0 \\ -5 & 6 & -4 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -4 & 6 & -4 & 1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 1 & -4 & 6 & -4 & 1 \\ 0 & \cdots & 0 & 0 & 1 & -4 & 6 & -5 \\ 0 & \cdots & 0 & -1 & 6 & -14 & 16 & -11 \end{bmatrix}, \end{aligned}$$

$$\begin{aligned} Q_x &= Q_p Q_1 \\ &= \begin{bmatrix} 7 & -2 & -4 & 4 & -1 & 0 & \cdots & 0 \\ 3 & 0 & -2 & 1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & 0 & -2 & 1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & -1 & 2 & 0 & -2 & 1 \\ 0 & \cdots & 0 & 0 & -1 & 2 & 0 & -3 \\ 0 & \cdots & 0 & 1 & -4 & 4 & 2 & -7 \end{bmatrix}. \end{aligned}$$

Similarly, the linear systems arising from the optimal *two-step* QSC method for homogeneous Dirichlet boundary conditions are

$$(\frac{1}{h^2}D_pQ_2 + \frac{1}{2h}D_qQ_1 + D_fQ_0)\vec{c}_{one} = \vec{g} \tag{2.17}$$

for step one, and

$$(\frac{1}{h^2}D_pQ_2 + \frac{1}{2h}D_qQ_1 + D_fQ_0)\vec{c} = \vec{g} - (\frac{1}{h^2}D_p\frac{1}{24}Q_{xx} - \frac{1}{2h}D_q\frac{1}{24}Q_x)\vec{c}_{one} \tag{2.18}$$

for step two.

2.3.2 Periodic boundary conditions

For periodic boundary conditions, we also adjust the basis functions to incorporate the boundary conditions and decrease the dimension of $\mathbf{P}^2_{\Delta,1}$ from $N+2$ to N. We use $\mathbf{P}^2_{\Delta_{\partial p},1}$ to denote the subspace of $\mathbf{P}^2_{\Delta,1}$ satisfying periodic boundary conditions.

According to [16], we adjust the basis functions for the periodic boundary conditions as follows:

$$\hat{\phi}_1(x) \equiv \begin{cases} \phi_1(x) & x \in I_1 \cup I_2 \\ \phi_{N+1}(x) & x \in I_N \\ 0 & \text{otherwise,} \end{cases}$$

$$\hat{\phi}_j(x) \equiv \phi_j, \quad j = 2, \ldots, N-1,$$

$$\hat{\phi}_N(x) \equiv \begin{cases} \phi_0(x) & x \in I_1 \\ \phi_N(x) & x \in I_{N-1} \cup I_N \\ 0 & \text{otherwise.} \end{cases}$$

The linear system arising from the optimal *one-step* QSC method for periodic boundary conditions takes the form

$$(\frac{1}{h^2}D_p(Q_2' + \frac{1}{24}Q_2'^2) + \frac{1}{2h}D_q(Q_1' - \frac{1}{24}Q_2Q_1') + D_fQ_0')\vec{c} = \vec{g}, \tag{2.19}$$

where

$$Q'_0 = \frac{1}{8}\begin{bmatrix} 6 & 1 & 0 & 0 & \cdots & 1 \\ 1 & 6 & 1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 1 & 6 & 1 \\ 1 & \cdots & 0 & 0 & 1 & 6 \end{bmatrix},$$

$$Q'_1 = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & -1 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & -1 & 0 & 1 \\ 1 & \cdots & 0 & 0 & -1 & 0 \end{bmatrix},$$

$$Q'_2 = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & \cdots & 0 & 0 & 1 & -2 \end{bmatrix},$$

and, the linear systems arising from the optimal *two-step* QSC method for periodic boundary conditions are

$$(\frac{1}{h^2}D_pQ'_2 + \frac{1}{2h}D_qQ'_1 + D_fQ'_0)\vec{c}_{one} = \vec{g} \tag{2.20}$$

for step one, and

$$(\frac{1}{h^2}D_pQ'_2 + \frac{1}{2h}D_qQ'_1 + D_fQ'_0)\vec{c} = \vec{g} - (\frac{1}{h^2}D_p\frac{1}{24}Q'^2_2 - \frac{1}{2h}D_q\frac{1}{24}Q'_2Q'_1)\vec{c}_{one} \tag{2.21}$$

for step two.

In the next chapter, we introduce the optimal QSC-CN methods and the RQSC-CN method based on the results in this chapter.

Chapter 3

RQSC-CN Method

Consider Problem (1.1)-(1.2) subject to homogeneous Dirichlet boundary conditions

$$u(0,t) = 0,\ u(1,t) = 0,\ 0 < t \leq T. \tag{3.1}$$

In the following, the superscript j for a function denotes the value of the function at time step t_j. Similarly, the superscript for the DOFs denotes the DOFs at the respective time step. Recall that $\{\tilde{\phi}_1(x), \tilde{\phi}_2(x), \ldots, \tilde{\phi}_N(x)\}$ is the set of the basis functions for $\mathbf{P}^2_{\Delta_{\partial d},1}$. Then $\forall u^j_\Delta \in \mathbf{P}^2_{\Delta_{\partial d},1}$, we have

$$u^j_\Delta(x) = \sum_{i=1}^{N} c^j_i \tilde{\phi}_i(x), \tag{3.2}$$

where $\{c^j_1, \ldots, c^j_N\}$ are DOFs.

As we described in Chapter 1, the RQSC-CN method is revised from the optimal QSC-CN methods. We first illustrate the optimal QSC-CN methods. We use uniform partitions for both the space and time variables unless otherwise indicated.

3.1 Optimal one-step QSC-CN method

In order to obtain a higher order approximation than the standard QSC-CN method defined in (1.7), we need to add a perturbation $\mathcal{P}_\mathcal{L}$ to $\mathcal{L}$. The optimal *one-step* QSC-CN method is to find a map $w_\Delta : \{t_0, \ldots, t_M\} \to \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$\begin{aligned} (i) \quad & \{\frac{\partial w^j_\Delta}{\partial t} - (\mathcal{L} + \mathcal{P}_\mathcal{L}) w_\Delta^{j+\frac{1}{2}}\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}), \ 1 \le i \le N, \ 0 \le j \le M-1, \\ (ii) \quad & w^0_\Delta \text{ be the interpolant of } \gamma, \end{aligned} \tag{3.3}$$

where $\mathcal{P}_\mathcal{L}$ is defined in (2.9), and the notation of (1.6) is adopted for the terms $w^j_\Delta, w_\Delta^{j+1/2}$, and $\partial w^j_\Delta / \partial t$. Notice that in (3.3), there are no boundary conditions, since w_Δ belongs to the subspace $\mathbf{P}^2_{\Delta_{\partial d},1}$ and all functions in $\mathbf{P}^2_{\Delta_{\partial d},1}$ satisfy the boundary conditions by construction.

From (i) in (3.3) and (1.6), it follows that

$$\frac{w_\Delta^{j+1} - w_\Delta^j}{\Delta t} = \frac{1}{2}(\mathcal{L} + \mathcal{P}_\mathcal{L})(w_\Delta^{j+1} + w_\Delta^j) + g^{j+\frac{1}{2}}. \tag{3.4}$$

Therefore, we have

$$w_\Delta^{j+1} - \frac{\Delta t}{2}(\mathcal{L} + \mathcal{P}_\mathcal{L}) w_\Delta^{j+1} = w_\Delta^j + \frac{\Delta t}{2}(\mathcal{L} + \mathcal{P}_\mathcal{L}) w_\Delta^j + g^{j+\frac{1}{2}}. \tag{3.5}$$

Letting

$$\vec{c}^j = (c^j_1, \ldots, c^j_N)^T \text{ and } \vec{g}^{j+\frac{1}{2}} = (g_1^{j+\frac{1}{2}}, \ldots, g_N^{j+\frac{1}{2}})^T,$$

we obtain the matrix form of (3.5)

$$\begin{aligned} & (Q_0 - \frac{\Delta t}{2}(\frac{1}{h^2} D_p^{j+1}(Q_2 + \frac{1}{24} Q_{xx}) + \frac{1}{2h} D_q^{j+1}(Q_1 - \frac{1}{24} Q_x) + D_f^{j+1} Q_0))\vec{c}^{j+1} \\ = \ & (Q_0 + \frac{\Delta t}{2}(\frac{1}{h^2} D_p^j(Q_2 + \frac{1}{24} Q_{xx}) + \frac{1}{2h} D_q^j(Q_1 - \frac{1}{24} Q_x) + D_f^j Q_0))\vec{c}^j + \vec{g}^{j+\frac{1}{2}}. \end{aligned} \tag{3.6}$$

Thus, for each time step, we solve the system (3.6) once, and get the DOFs for the next time step. For the initial step, we compute the interpolant of u. More precisely, we solve

$$Q_0 \vec{c}^0 = (\gamma_1, \ldots, \gamma_N)^T.$$

Note that the matrix arising from (3.6) is not tridiagonal but almost pentadiagonal, due to the matrices Q_x and Q_{xx} arising from the perturbation term $\mathcal{P}_\mathcal{L}$. More specifically, the first and last rows of Q_x and Q_{xx} have some additional entries that make them deviate from the pure pentadiagonal structure. This makes the system (3.6) relatively complicated to solve. Since tridiagonal systems are easier to solve, we want to find some alternative method that requires the solution of tridiagonal systems only.

3.2 Optimal two-step QSC-CN method

In this section, we let u_Δ^j denote the approximate solution computed by the optimal *two-step* QSC-CN method at time step t_j. Using the same technique introduced in Chapter Two for the optimal *two-step* QSC method for BVPs, we first compute an intermediate second order approximation ν_Δ^{j+1} by solving a linear system without the perturbation term; then, we use ν_Δ^{j+1} to approximate the perturbation term $\mathcal{P}_\mathcal{L} u_\Delta^{j+1}$ by $\mathcal{P}_\mathcal{L} \nu_\Delta^{j+1}$, and solve a system with the same matrix and a modified right side to obtain the DOFs for the next time step.

More precisely, we seek a map $u_\Delta : \{t_0, \ldots, t_M\} \to \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$\begin{array}{ll} (i) & \{\dfrac{\partial u_\Delta^j}{\partial t} - \mathcal{L} u_\Delta^{j+\frac{1}{2}}\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}) + \dfrac{\Delta t}{2}\mathcal{P}_\mathcal{L}(u_\Delta^j + \nu_\Delta^{j+1}),\ 1 \le i \le N,\ 0 \le j \le M-1, \\ & \text{where } \nu_\Delta^{j+1} \in \mathbf{P}^2_{\Delta_{\partial d},1} \text{ satisfies} \\ & \{\dfrac{\nu_\Delta^{j+1} - u_\Delta^j}{\Delta t} - \dfrac{1}{2}(\mathcal{L}\nu_\Delta^{j+1} + \mathcal{L} u_\Delta^j)\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}), \\ (ii) & u_\Delta^0 \text{ be the interpolant of } \gamma. \end{array} \tag{3.7}$$

The computation of u_Δ^j can be described as a two-step procedure. In step one, from (i) in (3.7), we compute ν_Δ^{j+1} satisfying

$$\nu_\Delta^{j+1} - \frac{\Delta t}{2}\mathcal{L}\nu_\Delta^{j+1} = u_\Delta^j + \frac{\Delta t}{2}\mathcal{L} u_\Delta^j + g^{j+\frac{1}{2}}. \tag{3.8}$$

That is, if $\nu_\Delta^{j+1} = \sum_{i=1}^N c_{\nu_i}^{j+1}\tilde{\phi}_i(x)$, we solve the linear system

$$\begin{aligned} & (Q_0 - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2 + \frac{1}{2h}D_q^{j+1}Q_1 + D_f^{j+1}Q_0))\vec{c}_\nu^{\,j+1} \\ = \ & (Q_0 + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j}Q_2 + \frac{1}{2h}D_q^{j}Q_1 + D_f^{j}Q_0))\vec{c}^{\,j} + \vec{g}^{\,j+\frac{1}{2}}. \end{aligned} \tag{3.9}$$

In step two, from (i) in (3.7) and (1.6), the equation we solve is given by

$$u_\Delta^{j+1} - \frac{\Delta t}{2}\mathcal{L}u_\Delta^{j+1} = u_\Delta^j + \frac{\Delta t}{2}\mathcal{L}u_\Delta^j + \frac{\Delta t}{2}\mathcal{P}_\mathcal{L}(u_\Delta^j + \nu_\Delta^{j+1}) + g^{j+\frac{1}{2}}. \tag{3.10}$$

That is, if $u_\Delta^{j+1} = \sum_{i=1}^N c_i^{j+1}\tilde{\phi}_i(x)$, we solve

$$\begin{aligned} &(Q_0 - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2 + \frac{1}{2h}D_q^{j+1}Q_1 + D_f^{j+1}Q_0))\vec{c}^{j+1} \\ = \ &(Q_0 + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^j(Q_2 + \frac{1}{24}Q_{xx}) + \frac{1}{2h}D_q^j(Q_1 - \frac{1}{24}Q_x) + D_f^jQ_0))\vec{c}^j \\ &+\frac{\Delta t}{2}(\frac{1}{24h^2}D_p^{j+1}Q_{xx} - \frac{1}{24h}D_q^{j+1}Q_x)\vec{c}_\nu^{j+1} + \vec{g}^{j+\frac{1}{2}}. \end{aligned} \tag{3.11}$$

Thus, we get the approximate solution u_Δ^{j+1} for time step t_{j+1}. For the initial step, we compute the interpolant of u. More precisely, we solve

$$Q_0\vec{c}^0 = (\gamma_1, \ldots, \gamma_N)^T.$$

The linear system arising from the optimal *two-step* QSC-CN method has nicer properties than the one arising from the optimal *one-step* QSC-CN method, for instance, the matrix is tridiagonal, therefore, easier to solve. However, we need to solve two systems at each time step. We can certainly save some computational work by saving some results from the first step and using them again in the second step. For instance, if we use LU decomposition to solve such a system for step one, we can save the LU decomposition and apply only back and forward substitutions in the second step.

3.3 RQSC-CN method

From the above discussion, we see that both the optimal *one-step* QSC-CN and *two-step* QSC-CN methods have some advantages and some disadvantages. The method presented in this section picks the advantages of the above two methods. More precisely, it requires the solution of the same simple system as the optimal two-step QSC-CN method, and only once for each time step.

For convenience, we adopt the notation $u^{(k)}(x,t)$ to denote the kth derivative of $u(x,t)$ with respect to x. Similar notation applies to other functions.

Lemma 3.3.1 *Consider the problem*

$$\begin{aligned} (i) \quad & u = u_1 + u_2 \\ (ii) \quad & \frac{\partial u_1}{\partial t} = \mathcal{L}_1 u + g(x,t) \\ (iii) \quad & \frac{\partial u_2}{\partial t} = h^2 \mathcal{L}_2 u \end{aligned} \tag{3.12}$$

where $\mathcal{L}_1, \mathcal{L}_2$ are second and fourth order linear spatial differential operators respectively. Assume $\{|g^{(k)}|, k = 0, \ldots, 4\}, \{|u^{(k)}|, k = 0, \ldots, 8\}$ are bounded. Then when applying the Forward Euler method to (iii) of (3.12) to discretize the time variable, the truncation error arising from time discretization is proportional to

$$h^2 \Delta t.$$

Proof:

By Taylor's expansions, when applying the Forward Euler method to (iii) of (3.12), we have

$$\frac{u_2^{j+1} - u_2^j}{\Delta t} - h^2 \mathcal{L}_2 u^j = \frac{\Delta t}{2} \frac{\partial^2 u_2}{\partial t^2}(\bar{t}), \tag{3.13}$$

where $\bar{t} \in [t_j, t_{j+1}]$. Notice that

$$\frac{\partial^2 u_2}{\partial t^2} = (\frac{\partial u_2}{\partial t})_t = h^2 (\mathcal{L}_2 u)_t = h^2 \mathcal{L}_2 (u_t) = h^2 \mathcal{L}_2 (\mathcal{L}_1 u + h^2 \mathcal{L}_2 u + g(x,t)) \tag{3.14}$$

Taking into account the assumptions of the lemma statement, and combining (3.13) and (3.14), we get the desired result. $\square$

Recall that the continuous-time one-step quadratic-spline collocation method corresponding to (3.3) is to find a map $u_C : [0,T] \to \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$\begin{aligned} (i) \quad & \{\frac{\partial u_C}{\partial t} - (\mathcal{L} + \mathcal{P}_{\mathcal{L}}) u_C\}(\tau_i, t) = g(\tau_i, t), \ 1 \le i \le N, \\ (ii) \quad & u_C(x, 0) \text{ be the interpolant of } \gamma. \end{aligned} \tag{3.15}$$

Suppose that we have two fictitious functions $u_1, u_2 \in \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$u_C(t) = u_1(t) + u_2(t). \tag{3.16}$$

More precisely, if $\vec{c}, \vec{c}_1, \vec{c}_2$ are the vectors of DOFs of u, u_1, u_2, respectively, we have

$$\vec{c} = \vec{c}_1 + \vec{c}_2.$$

We also require that u_1, u_2 satisfy the equations (3.17), (3.18), respectively

$$\{\frac{\partial u_1}{\partial t} - \mathcal{L}u_C\}(\tau_i, t) = g(\tau_i, t),\ 1 \le i \le N, \tag{3.17}$$

and

$$\{\frac{\partial u_2}{\partial t} - \mathcal{P}_{\mathcal{L}}u_C\}(\tau_i, t) = 0,\ 1 \le i \le N. \tag{3.18}$$

From (3.16), (3.17), and (3.18), it is easy to verify that u_C satisfies (3.15). Using the notation of (1.6), we discretize (3.17) as

$$\{\frac{\partial u_1^j}{\partial t} - \mathcal{L}u_C^{j+\frac{1}{2}}\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}),\ 1 \le i \le N,\ 0 \le j \le M-1. \tag{3.19}$$

This is a method similar to the Crank-Nicolson method, since we use central differences to discretize the time derivative and averaging for the $\mathcal{L}u_C$ term in (3.17). Notice that we cannot say that this is a pure Crank-Nicolson method, since u_1 is different from u_C. The forward Euler collocation method corresponding to (3.18) is to find a map $u_2 : \{t_0, \ldots, t_M\} \to \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$\{\frac{\partial u_2^j}{\partial t} - \mathcal{P}_{\mathcal{L}}u_C^j\}(\tau_i) = 0,\ 1 \le i \le N,\ 0 \le j \le M-1. \tag{3.20}$$

Notice that there is a common factor h^2 in $\mathcal{P}_{\mathcal{L}}$, defined in (2.9). By Lemma 3.3.1, if we let $\Delta t = \mathcal{O}(h^2)$, although we apply a first order time discretization (forward Euler) to (3.18), we still obtain a second order approximation since $h^2\mathcal{O}(\Delta t) = \mathcal{O}(\Delta t^2)$.

We can now give the first presentation of the RQSC-CN method. For the initial step $(t = 0)$, we solve

$$Q_0\vec{c}^0 = (\gamma_1, \ldots, \gamma_N)^T.$$

For each subsequent time step, we first use (3.20), which is an explicit method, to get the DOFs of u_2^{j+1}. Then substituting u_2^{j+1} in (3.19), taking into account (3.16), and solving (3.19), we obtain the DOFs of u_1^{j+1}. Finally, we obtain the DOFs of u_C^{j+1}, since $\vec{c}^{j+1} = \vec{c}_1^{j+1} + \vec{c}_2^{j+1}$.

We can give a simpler presentation of the RQSC-CN method that does not involve u_1 and u_2. Adding (3.19) to (3.20), leads to the RQSC-CN method. More precisely, the RQSC-CN method computes a map $u_C : \{t_0, \ldots, t_M\} \to \mathbf{P}^2_{\Delta_{\partial d},1}$ such that

$$\begin{array}{ll} (i) & \{\frac{\partial u_C^j}{\partial t} - (\mathcal{L}u_C^{j+\frac{1}{2}} + \mathcal{P}_{\mathcal{L}}u_C^j)\}(\tau_i) = g(\tau_i, t_{j+\frac{1}{2}}),\ 1 \le i \le N,\ 0 \le j \le M-1 \\ (ii) & u_C^0 \text{ be the interpolant of } \gamma. \end{array} \tag{3.21}$$

Since

$$u_C^j(x) = \sum_{i=1}^{N} c_i^j \tilde{\phi}_i(x),$$

it follows that, at each time step, the RQSC-CN method requires the solution of the linear system

$$\begin{aligned} & (Q_0 - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2 + \frac{1}{2h}D_q^{j+1}Q_1 + D_f^{j+1}Q_0))\vec{c}^{j+1} \\ = \ & (Q_0 + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^j(Q_2 + \frac{1}{12}Q_{xx}) + \frac{1}{2h}D_q^j(Q_1 - \frac{1}{12}Q_x) + D_f^jQ_0))\vec{c}^j + \vec{g}^{j+\frac{1}{2}} \end{aligned} \tag{3.22}$$

By solving (3.22), we get the DOFs for next time step. Notice that, in (3.21), the term $\mathcal{L}u_C$ is treated implicitly by Crank-Nicolson, while the term $\mathcal{P}_{\mathcal{L}}u_C$ is treated explicitly by Forward Euler. Since (3.21) involves discretizing (3.15) partly by an implicit method and partly by an explicit method, we consider the RQSC-CN method as a semi-implicit method.

We can motivate (3.21) in a different way, once we have noticed that there is a common factor h^2 in $\mathcal{P}_{\mathcal{L}}$. We explain the derivation of (3.21) as follows:

Recall that in the optimal *two-step* QSC-CN method, we compute an intermediate solution ν_Δ^{j+1} to approximate u_Δ^{j+1} in the term $\mathcal{P}_{\mathcal{L}}u_\Delta^{j+1}$. It turns out that ν_Δ^{j+1} is a $\mathcal{O}(h^2)$ approximation to $\mathcal{P}_{\mathcal{L}}u_\Delta^{j+1}$, but, since $\mathcal{P}_{\mathcal{L}}$ includes an h^2 factor, substituting ν_Δ^{j+1} for u_Δ^{j+1}

in the term $\mathcal{P}_{\mathcal{L}} u_{\Delta}^{j+1}$ introduces an $\mathcal{O}(h^4)$ error. Now, notice that u_{Δ}^{j} is an $\mathcal{O}(\Delta t)$ approximation to u_{Δ}^{j+1}, as well as to ν_{Δ}^{j+1}. Just as we argued before, since $\mathcal{P}_{\mathcal{L}}$ includes an h^2 factor, in (i) of (3.7), if we substitute u_{Δ}^{j} for ν_{Δ}^{j+1} in $\mathcal{P}_{\mathcal{L}} \nu_{\Delta}^{j+1}$, we introduce an $h^2\mathcal{O}(\Delta t)$ error. If we assume that $\mathcal{O}(\Delta t) = \mathcal{O}(h^2)$, then the error introduced by substituting u_{Δ}^{j} for ν_{Δ}^{j+1} in $\mathcal{P}_{\mathcal{L}} \nu_{\Delta}^{j+1}$, is $\mathcal{O}(h^4)$. Substituting $\mathcal{P}_{\mathcal{L}} u_{\Delta}^{j}$ for $\mathcal{P}_{\mathcal{L}} \nu_{\Delta}^{j+1}$ in (i) of (3.7), results in (3.21).

Comparing (3.11) and (3.22), we notice that the matrices of the left sides are the same. Therefore, for the RQSC-CN method, we only need to solve one tridiagonal system with the same matrix as that of the optimal *two-step* QSC-CN method to get the DOFs for each time step. However, as will be seen in Chapter 4, the RQSC-CN method is not unconditionally stable whereas the optimal *one-step* and *two-step* QSC-CN methods are.

3.4 Periodic boundary conditions

In this section, we indicate the linear systems arising from the optimal *one-step*, *two-step* QSC-CN and the RQSC-CN methods with periodic boundary conditions. The reason we present the periodic case is that the stability analysis can be carried out easily for periodic boundary conditions.

For periodic boundary conditions, we have the same equations as (3.3), (3.7), and (3.21) corresponding to the respective methods. The matrix forms are slightly different from those for homogeneous boundary conditions.

The linear system arising from the optimal *one-step* QSC method and periodic boundary conditions is

$$\begin{aligned} &(Q_0' - \frac{\Delta t}{2}(\frac{1}{h^2} D_p^{j+1}(Q_2' + \frac{1}{24} Q_2'^2) + \frac{1}{2h} D_q^{j+1}(Q_1' - \frac{1}{24} Q_2' Q_1') + D_f^{j+1} Q_0'))\vec{c}^{j+1} \\ = \; &(Q_0' + \frac{\Delta t}{2}(\frac{1}{h^2} D_p^{j}(Q_2' + \frac{1}{24} Q_2'^2) + \frac{1}{2h} D_q^{j}(Q_1' - \frac{1}{24} Q_2' Q_1') + D_f^{j} Q_0'))\vec{c}^{j} + \vec{g}^{j+\frac{1}{2}} \quad (3.23) \end{aligned}$$

For the optimal *two-step* QSC-CN method and periodic boundary conditions, the linear systems are

$$\begin{aligned}&(Q_0' - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2' + \frac{1}{2h}D_q^{j+1}Q_1' + D_f^{j+1}Q_0'))\vec{c}_\nu^{j+1}\\ = \; &(Q_0' + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j}Q_2' + \frac{1}{2h}D_q^{j}Q_1' + D_f^{j}Q_0'))\vec{c}^{j} + \vec{g}^{j+\frac{1}{2}}\end{aligned} \tag{3.24}$$

for step one, and

$$\begin{aligned}&(Q_0' - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2' + \frac{1}{2h}D_q^{j+1}Q_1' + D_f^{j+1}Q_0'))\vec{c}^{j+1}\\ = \; &(Q_0' + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j}(Q_2' + \frac{1}{24}Q_2'^2) + \frac{1}{2h}D_q^{j}(Q_1' - \frac{1}{24}Q_2'Q_1') + D_f^{j}Q_0'))\vec{c}^{j}\\ &+\frac{\Delta t}{2}(\frac{1}{24h^2}D_p^{j+1}Q_2'^2 - \frac{1}{24h}D_q^{j+1}Q_2'Q_1')\vec{c}_\nu^{j+1} + \vec{g}^{j+\frac{1}{2}}\end{aligned} \tag{3.25}$$

for step two.

For the RQSC-CN method and periodic boundary conditions, the linear system is

$$\begin{aligned}&(Q_0' - \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j+1}Q_2' + \frac{1}{2h}D_q^{j+1}Q_1' + D_f^{j+1}Q_0'))\vec{c}^{j+1}\\ = \; &(Q_0' + \frac{\Delta t}{2}(\frac{1}{h^2}D_p^{j}(Q_2' + \frac{1}{12}Q_2'^2) + \frac{1}{2h}D_q^{j}(Q_1' - \frac{1}{12}Q_2'Q_1') + D_f^{j}Q_0'))\vec{c}^{j} + \vec{g}^{j+\frac{1}{2}}\end{aligned} \tag{3.26}$$

Chapter 4

Stability and Convergence Analysis

In this chapter, we study the stability and convergence of the RQSC-CN method introduced in the previous chapter for a simple *linear parabolic PDE*

$$\frac{\partial u}{\partial t} = p\frac{\partial^2 u}{\partial x^2} \quad \text{in} \;\; 0 < x < 1,\; 0 < t \leq T, \tag{4.1}$$

where p is a positive constant, subject to homogeneous Dirichlet boundary conditions

$$u(0,t) = 0,\; u(1,t) = 0,\; \text{for } 0 \leq t \leq T, \tag{4.2}$$

or periodic boundary conditions

$$u(0,t) = u(1,t),\; \text{and } \frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(1,t),\; \text{for } 0 \leq t \leq T, \tag{4.3}$$

and initial condition

$$u(x,0) = \gamma(x),\; \text{for } 0 \leq x \leq 1. \tag{4.4}$$

All the matrices in this chapter have been defined in Chapter 2.

4.1 Stability

4.1.1 Periodic boundary conditions

For Problem (4.1)-(4.4) with periodic boundary conditions, the RQSC-CN method requires the solution of a linear system

$$(Q_0' - \frac{1}{2}\sigma Q_2')\vec{c}^{j+1} = (Q_0' + \frac{1}{2}\sigma Q_2' + \frac{1}{24}\sigma Q_2'^2)\vec{c}^j, \tag{4.5}$$

which is a special case of (3.26) with $\sigma = p\frac{\Delta t}{h^2}$. Letting

$$Q = (Q_0' - \frac{1}{2}\sigma Q_2')^{-1}(Q_0' + \frac{1}{2}\sigma Q_2' + \frac{1}{24}\sigma Q_2'^2),$$

we have

$$\vec{c}^{j+1} = Q\vec{c}^j.$$

We refer to Q as the iteration matrix for (4.5).

From [6], we know that the eigenvalues of Q_2' are

$$\lambda_i = -4\sin^2(\frac{(i-1)\pi}{N}),\ i = 1, \dots, N. \tag{4.6}$$

Since $Q_0' = \frac{1}{8}(8I + Q_2')$, Q_0' and Q_2' have the same eigenvectors. Thus, the eigenvalues of Q_0' are

$$1 + \frac{1}{8}\lambda_i.$$

Therefore, $(Q_0' - \frac{1}{2}\sigma Q_2')^{-1}$ exists and the eigenvalues of $Q$are

$$\lambda_{Qi} = \frac{1 + \frac{\lambda_i}{8} + \sigma\frac{\lambda_i}{2} + \sigma\frac{\lambda_i^2}{24}}{1 + \frac{\lambda_i}{8} - \sigma\frac{\lambda_i}{2}}. \tag{4.7}$$

From (4.6), we have

$$-4 \le \lambda_i \le 0.$$

Then, it is easy to show that

$$|\lambda_{Qi}| \le 1.$$

In the particular case that $\lambda_i = 0$, we have $|\lambda_{Qi}| = 1$. Since Q is symmetric and real, we have shown that

$$\|Q\|_2 = \max\{|\lambda_{Qi}|\} \leq 1.$$

Therefore, this method is unconditionally stable. We have, therefore, shown the following theorem.

Theorem 4.1.1 *The RQSC-CN method applied to Problem (4.1), (4.3), (4.4) is unconditionally stable.*

4.1.2 Homogeneous Dirichlet boundary conditions

As we mentioned in Chapter 3, in the case of Dirichlet boundary conditions, the RQSC-CN method is not unconditionally stable; there is some condition that has to be satisfied for stability. Unfortunately, we cannot prove a rigorous result at this time. Shown by numerical results, we have the following conjecture:

Conjecture 4.1.2 *The RQSC-CN method applied to Problem (4.1), (4.2), (4.4) is conditionally stable. The condition that needs to be satisfied for stability is*

$$\sigma \leq 5.06,$$

where $\sigma = p\frac{\Delta t}{h^2}$.

For the case of homogeneous Dirichlet boundary conditions, the RQSC-CN method applied to Problem (4.1), (4.2), (4.4) requires the solution of a linear system

$$(Q_0 - \frac{1}{2}\sigma Q_2)\vec{c}^{j+1} = (Q_0 + \frac{1}{2}\sigma Q_2 + \frac{1}{24}\sigma Q_{xx})\vec{c}^{j}, \text{ where } Q_{xx} = Q_p Q_2, \tag{4.8}$$

which is a special case of (3.22) with $\sigma = p\frac{\Delta t}{h^2}$. Then, the iteration matrix for each time step is

$$Q = (Q_0 - \frac{1}{2}\sigma Q_2)^{-1}(Q_0 + \frac{1}{2}\sigma Q_2 + \frac{1}{24}\sigma Q_{xx}). \tag{4.9}$$

We are unable to find explicit formulae for the eigenvalues of Q, so we compute them numerically. The spectral radii of the matrix Q computed by *Matlab* for certain choices of σ and N are shown in Table 4.1.

Table 4.1: The spectral radii of the iteration matrix for the RQSC-CN method

σ	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
0.01	0.9985	0.9996	0.9999	1.0000	1.0000	1.0000
0.1	0.9847	0.9962	0.9990	0.9998	0.9999	1.0000
0.25	0.9622	0.9904	0.9976	0.9994	0.9998	1.0000
0.5	0.9258	0.9809	0.9952	0.9988	0.9997	0.9999
1.0	0.8569	0.9622	0.9904	0.9976	0.9994	0.9998
1.5	0.8088	0.9438	0.9856	0.9964	0.9991	0.9998
2.0	0.8755	0.9258	0.9809	0.9952	0.9988	0.9997
2.5	0.9168	0.9165	0.9762	0.9940	0.9985	0.9996
3.0	0.9446	0.9443	0.9715	0.9928	0.9982	0.9995
3.5	0.9643	0.9641	0.9668	0.9916	0.9979	0.9995
4.0	0.9789	0.9788	0.9788	0.9904	0.9976	0.9994
4.5	0.9901	0.9901	0.9901	0.9901	0.9973	0.9993
4.75	0.9948	0.9947	0.9947	0.9947	0.9971	0.9993
4.85	0.9965	0.9964	0.9964	0.9964	0.9971	0.9993
4.95	0.9982	0.9981	0.9981	0.9981	0.9981	0.9993
5.0	0.9990	0.9989	0.9989	0.9989	0.9989	0.9992
5.03	0.9995	0.9993	0.9993	0.9993	0.9993	0.9993
5.06	0.9999	0.9998	0.9998	0.9998	0.9998	0.9998
5.07	1.0001	0.9999	0.9999	0.9999	0.9999	0.9999
5.1	1.0005	1.0004	1.0004	1.0004	1.0004	1.0004
5.5	1.0061	1.0059	1.0059	1.0059	1.0059	1.0059
6.0	1.0119	1.0116	1.0116	1.0116	1.0116	1.0116

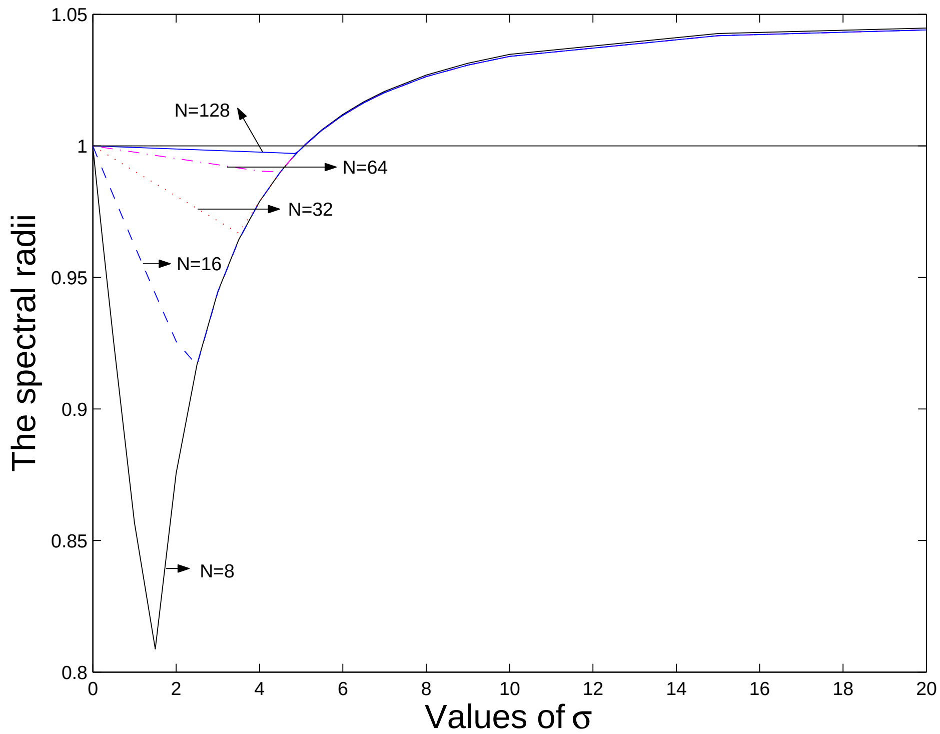


Figure 4.1: The spectral radii of the iteration matrix for the RQSC-CN method

In Figure 4.1, we plot the spectral radii versus σ for different values of N. From Table 4.1 and Figure 4.1, we notice that the spectral radii of the iteration matrix are less than or equal to one when $\sigma \leq 5.06$. For a fixed N, there is an optimal σ, which minimizes the spectral radii, for instance, the optimal σ for $N = 8$ is about 1.5. In addition, this optimal σ seems to be proportional to $\ln N$ for the range $N = 8$ up to $N = 128$. For a fixed σ, the spectral radii become larger as N increases. But as σ tends to, or goes beyond the critical point, 5.06, the spectral radii behave almost in the same way no matter what N is. Furthermore, the larger N is, the less sensitive the spectral radii are to the values of σ. We may expect that the spectral radii tend to one as N tends to infinity for all $\sigma \leq 5.06$. It is worth mentioning that the spectral radii seem to be below 1.05 for all σ.

4.1.3 Some improvements

Certainly, having a condition for stability is a disadvantage of the RQSC-CN method. We are seeking some modifications applied to this method which may make it much more stable. If we compare $Q_2'^2$ in (4.5) and Q_{xx} in (4.8), we find that $Q_2'^2$ is symmetric while Q_{xx} is not. Since the RQSC-CN method is stable for periodic boundary conditions, this motivates us to seek some improvements which can make Q_{xx} in (4.8) simpler and closer to being symmetric. As we know, the additional entries in the first and last rows in Q_{xx} arise from the approximation of $u_C^{(4)}$ at τ_1, τ_N. We try to use some different ways to approximate $u_C^{(4)}$ which will reduce the additional entries in Q_{xx}.

First, we use $u_C^{(4)}(\tau_2)$ to approximate $u_C^{(4)}(\tau_1)$, and $u_C^{(4)}(\tau_{N-1})$ to approximate $u_C^{(4)}(\tau_N)$. Although this is just a first order approximation, it makes Q_{xx} have fewer entries in the first and last rows than the matrix arising from the original approximation. More precisely, our perturbation term $\mathcal{P}_\mathcal{L}$ becomes

$$\mathcal{P}_\mathcal{L} u_i \equiv \begin{cases} \frac{h^2}{24}\Lambda u_2'', & i = 1 \\ \frac{h^2}{24}\Lambda u_i'', & 2 \le i \le N-1 \\ \frac{h^2}{24}\Lambda u_{n-1}'', & i = N \end{cases} \tag{4.10}$$

and the matrix Q_p in (4.8) is changed to

$$Q_{p_1} = \begin{bmatrix} 1 & -2 & 1 & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & 1 & -2 & 1 \end{bmatrix}. \tag{4.11}$$

Shown by numeric results, the method arising by using Q_{p_1} instead of Q_p in (4.8) is not only unconditionally stable but also convergent. To our delight, we can still get $\mathcal{O}(h^4)$ convergence even though we sacrifice some accuracy at τ_1, τ_N. We refer to this method as the RQSC-CN1 method. The spectral radii of the iteration matrix Q computed by *Matlab* for certain choices of σ are shown in Table 4.2.

Table 4.2: The spectral radii of the iteration matrix for the RQSC-CN1 method

σ	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
0.01	0.9985	0.9996	0.9999	1.0000	1.0000	1.0000
0.1	0.9847	0.9962	0.9990	0.9998	0.9999	1.0000
0.25	0.9622	0.9904	0.9976	0.9994	0.9998	1.0000
0.5	0.9258	0.9809	0.9952	0.9988	0.9997	0.9999
1	0.8569	0.9622	0.9904	0.9976	0.9994	0.9998
1.5	0.7929	0.9438	0.9856	0.9964	0.9991	0.9998
2	0.7699	0.9258	0.9809	0.9952	0.9988	0.9997
2.5	0.8159	0.9081	0.9762	0.9940	0.9985	0.9996
3	0.8481	0.8907	0.9715	0.9928	0.9982	0.9995
3.5	0.8719	0.8736	0.9668	0.9916	0.9979	0.9995
4	0.8901	0.8901	0.9622	0.9904	0.9976	0.9994
4.5	0.9046	0.9046	0.9575	0.9892	0.9973	0.9993
5	0.9163	0.9163	0.9529	0.9880	0.9970	0.9992
5.5	0.9260	0.9260	0.9484	0.9868	0.9967	0.9992
6	0.9341	0.9341	0.9438	0.9856	0.9964	0.9991
6.5	0.9410	0.9410	0.9410	0.9845	0.9961	0.9990
7	0.9469	0.9469	0.9469	0.9833	0.9958	0.9989
8	0.9566	0.9566	0.9566	0.9809	0.9952	0.9988
9	0.9642	0.9642	0.9642	0.9785	0.9946	0.9986
10	0.9702	0.9702	0.9702	0.9762	0.9940	0.9985
15	0.9880	0.9880	0.9880	0.9880	0.9910	0.9977
20	0.9966	0.9966	0.9966	0.9966	0.9966	0.9970

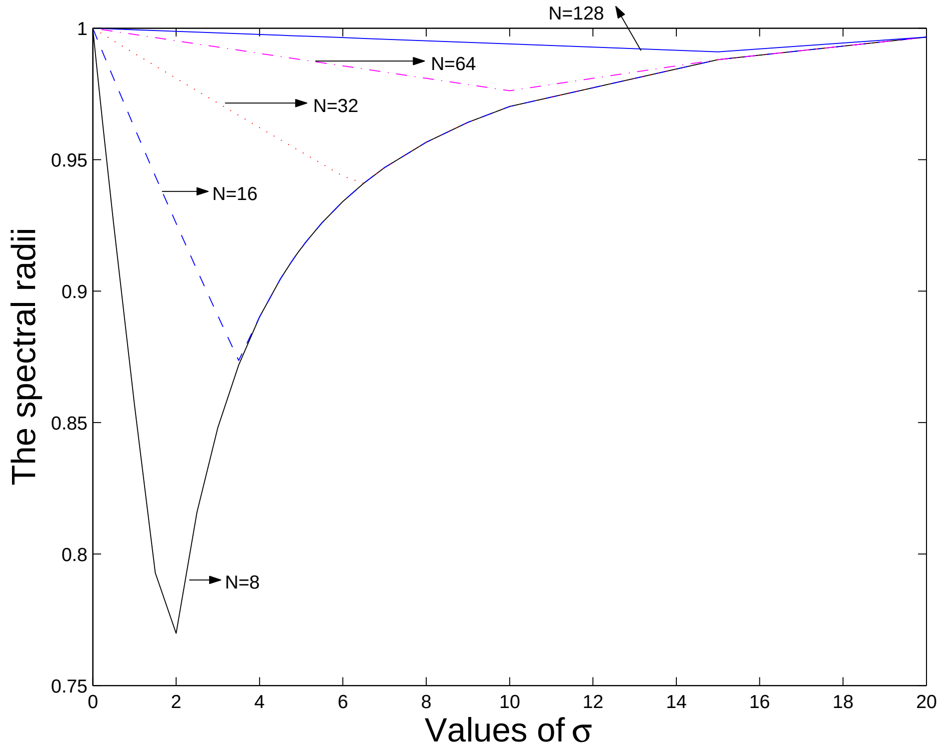


Figure 4.2: The spectral radii of the iteration matrix for the RQSC-CN1 method

In Figure 4.2, we plot the spectral radii versus σ for different values of N. From Table 4.2 and Figure 4.2, we notice that the spectral radii of the iteration matrix behave similarly to those in Figure 4.1, except that the spectral radii for the RQSC-CN1 method are always less than or equal to one for all σ. It also seems that the spectral radii tend to one as N tends to infinity for all σ.

In [3], Archer proposes a modified version of the standard cubic spline collocation method for certain parabolic problems which also involves introducing some perturbation term to $\mathcal{L}$. There are quite a few choices for the perturbation at the boundary points [12]. Archer chooses not to add any perturbation at the boundary points. This choice is simple and easy to apply. Archer has proved that the modified method without perturbation at the boundary points leads to $\mathcal{O}(h^4)$ convergence at grid points. Motivated by this idea, we let $\mathcal{P}_{\mathcal{L}}$ to be zero at $\{\tau_1, \tau_N\}$. This makes the matrix Q_{xx} even nicer than that for the

RQSC-CN1 method. More precisely, the perturbation term $\mathcal{P}_{\mathcal{L}}$ becomes

$$\mathcal{P}_{\mathcal{L}} u_i \equiv \begin{cases} 0, & i = 1 \\ \frac{h^2}{24}\Lambda u_i'', & 2 \le i \le N-1 \\ 0, & i = N \end{cases} \tag{4.12}$$

and the matrix Q_p in (4.8) is changed to

$$Q_{p_0} = \begin{bmatrix} 0 & 0 & 0 & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & 0 & 0 & 0 \end{bmatrix}.$$

Shown by numeric results, the method arising by using Q_{p_0} instead of Q_p in (4.8) appears to be not only unconditionally stable but also convergent. To our delight, we can still get $\mathcal{O}(h^4)$ convergence even though we do not add any perturbation at τ_1, τ_N. We refer to this method as the RQSC-CN0 method. The spectral radii of the iteration matrix Q computed by *Matlab* for certain choices of σ are shown in Table 4.3.

Table 4.3: The spectral radii of the iteration matrix for the RQSC-CN0 method

σ	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
0.01	0.9985	0.9996	0.9999	1.0000	1.0000	1.0000
0.1	0.9847	0.9962	0.9990	0.9998	0.9999	1.0000
0.25	0.9622	0.9904	0.9976	0.9994	0.9998	1.0000
0.5	0.9258	0.9809	0.9952	0.9988	0.9997	0.9999
1	0.8569	0.9622	0.9904	0.9976	0.9994	0.9998
1.5	0.7928	0.9438	0.9856	0.9964	0.9991	0.9998
2	0.7330	0.9258	0.9809	0.9952	0.9988	0.9997
2.5	0.7181	0.9081	0.9762	0.9940	0.9985	0.9996
3	0.7524	0.8907	0.9715	0.9928	0.9982	0.9995
3.5	0.7784	0.8736	0.9668	0.9916	0.9979	0.9995
4	0.7989	0.8568	0.9622	0.9904	0.9976	0.9994
4.5	0.8154	0.8404	0.9575	0.9892	0.9973	0.9993
5	0.8291	0.8290	0.9529	0.9880	0.9970	0.9992
5.5	0.8406	0.8406	0.9484	0.9868	0.9967	0.9992
6	0.8505	0.8505	0.9438	0.9856	0.9964	0.9991
6.5	0.8591	0.8591	0.9393	0.9845	0.9961	0.9990
7	0.8667	0.8666	0.9347	0.9833	0.9958	0.9989
8	0.8794	0.8792	0.9258	0.9809	0.9952	0.9988
9	0.8896	0.8893	0.9169	0.9785	0.9946	0.9986
10	0.8980	0.8977	0.9081	0.9762	0.9940	0.9985
15	0.9247	0.9245	0.9245	0.9645	0.9910	0.9977
20	0.9392	0.9392	0.9392	0.9529	0.9880	0.9970

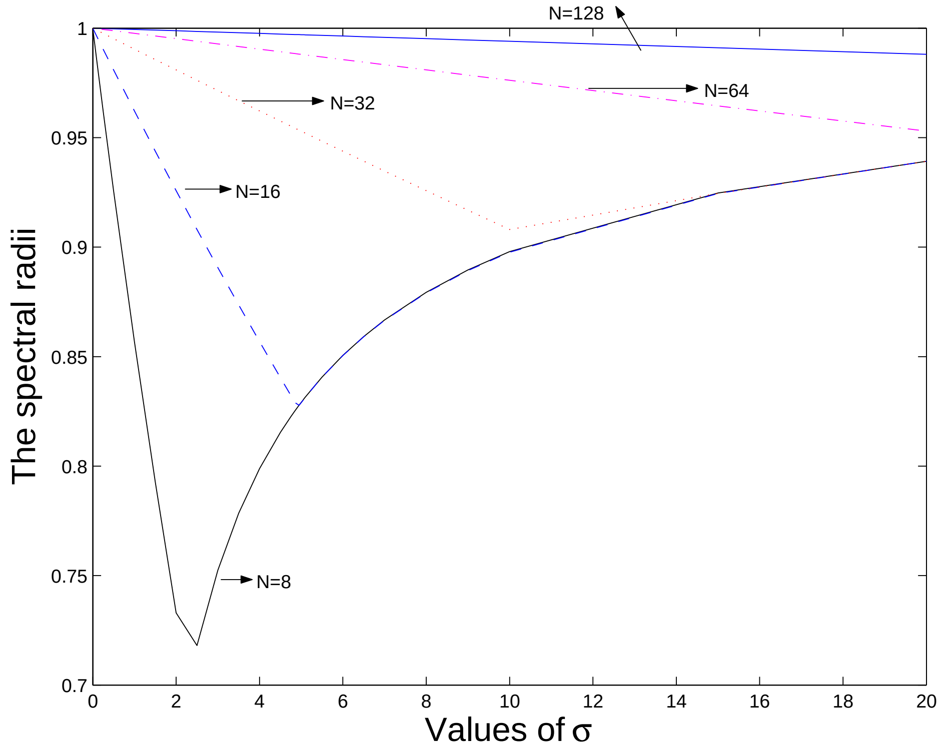


Figure 4.3: The spectral radii of the iteration matrix for the RQSC-CN0 method

In Figure 4.3, we plot the spectral radii versus σ for different values of N. From Table 4.3 and Figure 4.3, we notice that the spectral radii of the iteration matrix behave quite similarly to those in Figure 4.2. Moreover, the spectral radii for the RQSC-CN0 method are smaller than the respective ones for the RQSC-CN1 method and grow more slowly than those for the RQSC-CN1 method as σ increases. Furthermore, for a fixed N, the optimal σ that minimizes the spectral radius of the iteration matrix of the RQSC-CN0 method is larger than that of the RQSC-CN1 method. We may say that the RQSC-CN0 method appears to be better than the RQSC-CN1 method as far as stability is concerned.

4.2 Convergence

In this section, we study the convergence of the RQSC-CN method for Problem (4.1), (4.2), (4.4).

At each time step, let u^m denote the exact solution at time t_m, i.e.

$$u^m(x) = u(x, t_m) = u(x, m\Delta t), \tag{4.13}$$

u_C^m be the approximation to u^m computed by the RQSC-CN method and u_I^m be the quadratic-spline interpolant of u^m satisfying (2.3). Notice that u_I^m does not satisfy homogeneous Dirichlet boundary conditions if $(u^m)^{(4)} \neq 0$ at the boundaries. For simplicity, we give the convergence proof by assuming

$$(u^m)^{(4)}(x) = 0, \quad \text{at } x = x_0,\ x_N. \tag{4.14}$$

Then we can use the same adjusted basis functions as (2.14) for u_I^m. The proof for general functions with $(u^m)^{(4)} \neq 0$ at the two boundary points uses a similar approach, but is more complicated to describe. Initially, $u^0 = \gamma$ and $u_C^0 = u_I^0$, taking into account assumption (4.14). We assume that the initial solution function $\gamma(x) \in C^6(I)$. That is, $\gamma(x)$ has bounded derivatives up to sixth order, i.e.

$$|\gamma^{(k)}(x)| \leq C,\ 0 \leq x \leq 1,\ k = 0, 1, \ldots, 6, \tag{4.15}$$

where C is a constant. The maximum principle [2] then guarantees that $u(x, t)$ also has bounded derivatives up to sixth order with respect to x for all t, i.e.

$$|u^{(k)}(x, t)| \leq C,\ 0 \leq x \leq 1,\ 0 < t \leq 1,\ k = 0, 1, \ldots, 6, \tag{4.16}$$

where C is the same constant as in (4.15). Since $u(x, t)$ satisfies (4.1), we have

$$u_{ttt} = (u_t)_{tt} = (pu_{xx})_{tt} = p^3 u_{xxxxxx}. \tag{4.17}$$

Therefore, u_{ttt} and u_{xxtt} are also bounded for all x and t.

In (4.1), discretizing the time variable with the Crank-Nicolson Method, and using Taylor's expansions, we get

$$u^{m+1} - \frac{1}{2}\Delta t \mathcal{L} u^{m+1} = u^m + \frac{1}{2}\Delta t \mathcal{L} u^m + \Delta t R^{m+1}, \tag{4.18}$$

where

$$R^{m+1} \equiv \frac{\Delta t^2}{24} u_{ttt}^{m_1} - \frac{\Delta t^2}{16}(u_{xxtt}^{m_2} + u_{xxtt}^{m_3}),\ m_1 \in [m, m+1],\ m_2 \in [m, m+\frac{1}{2}],\ m_3 \in [m+\frac{1}{2}, m+1]. \tag{4.19}$$

Clearly,

$$R^m = \mathcal{O}(\Delta t^2),\ \text{for all } x,\ t \text{ and } m. \tag{4.20}$$

Recall the definitions of the discrete operators Λ in (2.6) and $\mathcal{P}_{\mathcal{L}}$ in (2.9). We next summarize, in a form of *Theorem 4.2.1*, some results shown in [10].

Theorem 4.2.1 *According to [10], under the assumption $u^0 \in C^6(I)$, we have, for all $0 \le m \le M$*

$$\begin{aligned}
\|(u_I^m)^{(k)} - (u^m)^{(k)}\|_\infty &= \mathcal{O}(h^{3-k}),\ k = 0, 1, 2 \\
|u_I^m(x) - u^m(x)| &= \mathcal{O}(h^4),\ \textit{for } x = x_i \\
|(u_I^m)'(x) - (u^m)'(x)| &= \mathcal{O}(h^3),\ \textit{for } x = x_i + \lambda h,\ \lambda = (3 \pm \sqrt{3})/6 \\
|(u_I^m)''(x) - (u^m)''(x)| &= \mathcal{O}(h^2),\ \textit{for } x = \tau_i
\end{aligned}$$

and

$$|u_I^m(x) - u^m(x)| = 0,\ \textit{for } x = \tau_i, \tag{4.21}$$

$$|(\mathcal{L} + \mathcal{P}_{\mathcal{L}})u_I^m(x) - \mathcal{L}u^m(x)| = \mathcal{O}(h^4),\ \textit{for } x = \tau_i. \tag{4.22}$$

For later convenience, let

$$R_1^m \equiv \mathcal{L}u^m - (\mathcal{L} + \mathcal{P}_{\mathcal{L}})u_I^m, \tag{4.23}$$

and notice that

$$R_1^m = \mathcal{O}(h^4),\ \text{for } x = \tau_i \text{ and for all } m. \tag{4.24}$$

We will make use of the following lemma:

Lemma 4.2.2 *Let $u_\Delta, v_\Delta \in \mathbf{P}^2_{\Delta_{\partial d},1}$ satisfy (4.25), (4.26), respectively,*

$$u_\Delta - \frac{1}{2}\Delta t \mathcal{L} u_\Delta = g_u, \ 0 < x < 1, \tag{4.25}$$

$$v_\Delta - \frac{1}{2}\Delta t \mathcal{L} v_\Delta = g_v, \ 0 < x < 1, \tag{4.26}$$

at the collocation points, where $g_v = g_u + \mathcal{O}(h^r)$. Then we have

$$\|u_\Delta^{(k)} - v_\Delta^{(k)}\|_\infty = \mathcal{O}(h^{r-k}), \ k = 0, 1, 2. \tag{4.27}$$

Proof: Letting $\vec{c}_u, \vec{c}_v$ be the DOFs for u_Δ, v_Δ respectively, from (4.25) and (4.26), we have

$$A\vec{c}_u = \vec{g}_u, \tag{4.28}$$

$$A\vec{c}_v = \vec{g}_v = \vec{g}_u + \mathcal{O}(h^r), \tag{4.29}$$

where

$$A \equiv Q_0 - \frac{1}{2}\sigma Q_2.$$

Subtracting (4.29) from (4.28), we have

$$A(\vec{c}_u - \vec{c}_v) = \mathcal{O}(h^r).$$

Writing down the matrix A explicitly, by simple mathematical manipulation, we have, for $i = 1, \ldots, N$,

$$|A_{ii}| \geq \sum_{j=1, j\neq i}^{N} |A_{ij}| + \frac{1}{2}.$$

Therefore, A^{-1} exists and $\|A^{-1}\|_\infty$ is bounded independently of h. Consequently, we have

$$\|\vec{c}_u - \vec{c}_v\|_\infty \leq \|A^{-1}\|_\infty \mathcal{O}(h^r) = \mathcal{O}(h^r). \tag{4.30}$$

Noticing that the quadratic spline basis functions are bounded, from (4.30), we have

$$\|u_\Delta^{(k)} - v_\Delta^{(k)}\|_\infty = \mathcal{O}(h^{r-k}), \ k = 0, 1, 2. \qquad \square$$

Lemma 4.2.3 *If $u^0 \in C^6(I)$, then*

$$\mathcal{P}_{\mathcal{L}}(u_I^{m+1} - u_I^m) = \mathcal{O}(h^4 + h^2\Delta t), \text{ for } x = \tau_i \text{ and for all } m. \tag{4.31}$$

Proof: Since $u^0 \in C^6(I)$, we have (4.16). From [10], we know that

$$\Lambda(u_I^{m+1})'' = (u^{m+1})^{(4)} + \mathcal{O}(h^2)$$

and

$$\Lambda(u_I^m)'' = (u^m)^{(4)} + \mathcal{O}(h^2),$$

and by Taylor's expansions we get

$$(u^{m+1})^{(4)} = (u^m)^{(4)} + \mathcal{O}(\Delta t).$$

Therefore

$$\Lambda(u_I^{m+1})'' = \Lambda(u_I^m)'' + \mathcal{O}(h^2 + \Delta t). \tag{4.32}$$

Based on the definition of $\mathcal{P}_{\mathcal{L}}$, and (4.32), we have the desired result. □

For later convenience, define

$$R_2^m \equiv \frac{1}{2}\mathcal{P}_{\mathcal{L}}(u_I^{m+1} - u_I^m), \tag{4.33}$$

and notice that, from Lemma 4.2.3, we have

$$R_2^m = \mathcal{O}(h^4 + h^2\Delta t), \text{ for } x = \tau_i \text{ and for all } m. \tag{4.34}$$

We now come to the main convergence theorem.

Theorem 4.2.4 *If $u^0 \in C^6(I)$, $\sigma \le 5.06$, and $\Delta t = \mathcal{O}(h^2)$, we have for $m = 0, \ldots, M$,*

$$\begin{aligned}
\|(u_C^m)^{(k)} - (u^m)^{(k)}\|_\infty &= \mathcal{O}(h^{3-k}), \; k = 0, 1, 2 \\
|u_C^m(x) - u^m(x)| &= \mathcal{O}(h^4), \; \textit{for } x = x_i \textit{ and } x = \tau_i \\
|(u_C^m)'(x) - (u^m)'(x)| &= \mathcal{O}(h^3), \; \textit{for } x = x_i + \lambda h, \; \lambda = (3 \pm \sqrt{3})/6 \\
|(u_C^m)''(x) - (u^m)''(x)| &= \mathcal{O}(h^2), \; \textit{for } x = \tau_i.
\end{aligned}$$

Proof: We first prove that at each time step t_{m+1}

$$\|(u_C^{m+1})^{(k)} - (u_I^{m+1})^{(k)}\|_\infty = t_{m+1}\mathcal{O}(h^{4-k}),\ k = 0, 1, 2. \tag{4.35}$$

All the following equations are satisfied at the collocation points τ_i, $i = 1, \ldots, N$, unless otherwise indicated. We ignore errors with order higher than $\mathcal{O}(h^4)$.

By (4.21) and (4.22) in *Theorem 4.2.1*, and by the definition (4.23), we have

$$u_I^{m+1} - \frac{1}{2}\Delta t(\mathcal{L} + \mathcal{P}_\mathcal{L})u_I^{m+1} = u^{m+1} - \frac{1}{2}\Delta t\mathcal{L}u^{m+1} + \frac{1}{2}\Delta t R_1^{m+1}. \tag{4.36}$$

Using (4.18), relation (4.36) is rewritten as

$$u_I^{m+1} - \frac{1}{2}\Delta t(\mathcal{L} + \mathcal{P}_\mathcal{L})u_I^{m+1} = u^m + \frac{1}{2}\Delta t\mathcal{L}u^m + \Delta t(R^{m+1} + \frac{1}{2}R_1^{m+1}). \tag{4.37}$$

Using (4.21), (4.22) and (4.23) again, relation (4.37) becomes

$$u_I^{m+1} - \frac{1}{2}\Delta t(\mathcal{L} + \mathcal{P}_\mathcal{L})u_I^{m+1} = u_I^m + \frac{1}{2}\Delta t(\mathcal{L} + \mathcal{P}_\mathcal{L})u_I^m + \Delta t(R^{m+1} + \frac{1}{2}R_1^{m+1} + \frac{1}{2}R_1^m). \tag{4.38}$$

Moving $\frac{1}{2}\Delta t\mathcal{P}_\mathcal{L}u_I^{m+1}$ to the right side, we have

$$u_I^{m+1} - \frac{1}{2}\Delta t\mathcal{L}u_I^{m+1} = u_I^m + \frac{1}{2}\Delta t(\mathcal{L} + \mathcal{P}_\mathcal{L})u_I^m + \frac{1}{2}\Delta t\mathcal{P}_\mathcal{L}u_I^{m+1} + \Delta t(R^{m+1} + \frac{1}{2}R_1^{m+1} + \frac{1}{2}R_1^m). \tag{4.39}$$

Using the definition of R_2^m, relation (4.39) is written as

$$u_I^{m+1} - \frac{1}{2}\Delta t\mathcal{L}u_I^{m+1} = u_I^m + \frac{1}{2}\Delta t(\mathcal{L} + 2\mathcal{P}_\mathcal{L})u_I^m + \Delta t(R^{m+1} + \frac{1}{2}R_1^{m+1} + \frac{1}{2}R_1^m + R_2^m). \tag{4.40}$$

Define

$$g_I^m \equiv u_I^m + \frac{1}{2}\Delta t(\mathcal{L} + 2\mathcal{P}_\mathcal{L})u_I^m \tag{4.41}$$

and

$$\epsilon^m \equiv R^{m+1} + \frac{1}{2}R_1^{m+1} + \frac{1}{2}R_1^m + R_2^m. \tag{4.42}$$

Then relation (4.40) is written as

$$u_I^{m+1} - \frac{1}{2}\Delta t\mathcal{L}u_I^{m+1} = g_I^m + \Delta t\epsilon^m. \tag{4.43}$$

From (4.20), (4.24), and (4.34), we have

$$\epsilon^m = \mathcal{O}(\Delta t^2 + \Delta t h^2 + h^4), \tag{4.44}$$

which, by letting $\Delta t = \mathcal{O}(h^2)$, gives

$$\epsilon^m = \mathcal{O}(h^4). \tag{4.45}$$

Recall that

$$A \equiv Q_0 - \frac{1}{2}\sigma Q_2,$$

and define

$$B \equiv Q_0 + \frac{1}{2}\sigma Q_2 + \frac{1}{24}\sigma Q_{xx}. \tag{4.46}$$

We rewrite (4.43), for the collocation points τ_i, $i = 1, \ldots, N$, in the format of linear system as

$$A\vec{c}_I^{m+1} = B\vec{c}_I^m + \Delta t \vec{\epsilon}^m, \tag{4.47}$$

where $\vec{c}_I^m$ is the $N \times 1$ vector of DOFs of u_I^m, and $\vec{\epsilon}^m$ is the $N \times 1$ vector of values of ϵ^m at τ_i, $i = 1, \ldots, N$.

That is

$$\vec{c}_I^{m+1} = A^{-1}B\vec{c}_I^m + A^{-1}\Delta t \vec{\epsilon}^m. \tag{4.48}$$

We define

$$\vec{\varepsilon}^m \equiv A^{-1}\vec{\epsilon}^m. \tag{4.49}$$

Since, by *Lemma 4.2.2*, $\|A^{-1}\|$ is bounded independently of h, and by (4.45) $\|\vec{\epsilon}^m\|_\infty = \mathcal{O}(h^4)$, we have

$$\|\vec{\varepsilon}^m\|_\infty = \mathcal{O}(h^4). \tag{4.50}$$

Rewrite (4.48) as

$$\vec{c}_I^{m+1} = A^{-1}B\vec{c}_I^m + \Delta t \vec{\varepsilon}^m. \tag{4.51}$$

According to the RQSC-CN method, the collocation equations are given by

$$\vec{c}^{m+1} = A^{-1}B\vec{c}^m, \tag{4.52}$$

where $\vec{c}^m$ is the $N \times 1$ vector of DOFs of u_C^m.

Subtracting (4.52) from (4.51), we have

$$\vec{c}_I^{m+1} - \vec{c}^{m+1} = Q(\vec{c}_I^m - \vec{c}^m) + \Delta t \vec{\varepsilon}^m, \tag{4.53}$$

where we recall that $Q = A^{-1}B$ is the iteration matrix of the RQSC-CN method.

It can be easily shown by induction that

$$\vec{c}_I^{m+1} - \vec{c}^{m+1} = Q^{m+1}(\vec{c}_I^0 - \vec{c}^0) + \Delta t(Q^m \vec{\varepsilon}^0 + Q^{m-1}\vec{\varepsilon}^1 + \ldots + Q\vec{\varepsilon}^{m-1} + \vec{\varepsilon}^m). \tag{4.54}$$

Since $c^0 = c_I^0$, the term $Q^{m+1}(\vec{c}_I^0 - \vec{c}^0)$ in (4.54) cancels. According to *Conjecture 4.1.2*, under the stability condition $\sigma \leq 5.06$, we have $|\lambda_i| \leq 1$, for all eigenvalues λ_i of Q. This is equivalent to $\|Q^m\|_\infty \to 0$, as $m \to \infty$. In addition, it is easy to show that $\|Q\|_\infty \leq \kappa$, where κ is a positive constant independent of h. Therefore, we have for $j = 0, \ldots, m$

$$\|Q^j \vec{\varepsilon}^{m-j}\|_\infty = \mathcal{O}(h^4).$$

Then, from (4.54), we get

$$\|\vec{c}_I^{m+1} - \vec{c}^{m+1}\|_\infty = t_{m+1}\mathcal{O}(h^4). \tag{4.55}$$

Then, with similar arguments as in *Lemma 4.2.2*, we obtain (4.35). Finally, by *Theorem 4.2.1* and the use of the triangle inequality, the desired results are easily obtained. $\square$

As we have mentioned, the above proof holds for functions with $u^{(4)} = 0$ at the boundaries. Next, we will show that *Theorem* 4.2.4 holds for general functions. To complete the proof, we will need to adjust the RQSC-CN method, as described in the rest of the section.

When $u^{(4)} \neq 0$ at the boundaries, the relations (4.35) to (4.43) still hold for u_I. However, since $u_I \neq 0$ at the boundaries, we cannot use the adjusted basis functions anymore to represent it. We will use the original basis functions (2.13) instead. Let

$$u_I^m = \sum_{i=0}^{N+1} c_{I_i}^{m'} \phi_i(x). \tag{4.56}$$

Then, we have

$$\frac{1}{8}\begin{bmatrix} 4 & 4 & 0 & \cdots & 0 \\ 1 & 6 & 1 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 1 & 6 & 1 \\ 0 & \cdots & 0 & 4 & 4 \end{bmatrix}_{(N+2)\times(N+2)} \begin{bmatrix} c_{I_0}^{m'} \\ c_{I_1}^{m'} \\ \vdots \\ c_{I_N}^{m'} \\ c_{I_{N+1}}^{m'} \end{bmatrix} = \begin{bmatrix} -\frac{h^4}{128}(u_0^m)^{(4)} \\ u_1^m \\ \vdots \\ u_N^m \\ -\frac{h^4}{128}(u_{N+1}^m)^{(4)} \end{bmatrix}. \tag{4.57}$$

Define

$$\vec{c}_I^{m'} = (c_{I_0}^{m'}, \ldots, c_{I_{N+1}}^{m'})^T. \tag{4.58}$$

It is worth mentioning that $\vec{c}_I^{m'}$ is different from $\vec{c}_I^{m}$, and we use a prime to distinguish it from $\vec{c}_I^{m}$. Notice that $\vec{c}_I^{m'}$ is a $(N+2)\times 1$ vector, while $\vec{c}_I^{m}$ is a $N\times 1$ vector.

Define

$$\tilde{u}_0^m = -\frac{h^4}{128}(u_0^m)_{xxxx} \quad \text{and} \quad \tilde{u}_{N+1}^m = -\frac{h^4}{128}(u_{N+1}^m)_{xxxx}. \tag{4.59}$$

From the first and last equations in (4.57), we have

$$c_{I_0}^{m'} = 2\tilde{u}_0^m - c_{I_1}^{m'} \quad \text{and} \quad c_{I_{N+1}}^{m'} = 2\tilde{u}_{N+1}^m - c_{I_N}^{m'}. \tag{4.60}$$

At the midpoints $\tau_i, i = 1, \ldots, N$, we have

$$u_I^m = \frac{1}{8}\begin{bmatrix} 1 & 6 & 1 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 1 & 6 & 1 \end{bmatrix}_{N\times(N+2)} \begin{bmatrix} c_{I_0}^{m'} \\ \vdots \\ c_{I_{N+1}}^{m'} \end{bmatrix}. \tag{4.61}$$

Substituting (4.60) for $c_{I_0}^{m'}$ and $c_{I_{N+1}}^{m'}$ in (4.61), we have

$$u_I^m = Q_0 \vec{c}_{I_R}^{m'} + \tilde{r}_{Q_0}^m, \tag{4.62}$$

where $\vec{c}_{I_R}^{m'} = (c_{I_1}^{m'}, \ldots, c_{I_N}^{m'})^T$ is a $N \times 1$ restriction of $\vec{c}_I^{m'}$, obtained by omitting the first and last components, and

$$\tilde{r}_{Q_0}^m = (2(Q_0)_{2,1}\tilde{u}_0^m, 0, \ldots, 0, 2(Q_0)_{N-1,N}\tilde{u}_{N+1}^m)^T. \tag{4.63}$$

Similarly, we have

$$(u_I^m)_{xx} = Q_2 \vec{c}_{I_R}^{m'} + \tilde{r}_{Q_2}^m, \tag{4.64}$$

where

$$\tilde{r}_{Q_2}^m = (2(Q_2)_{2,1}\tilde{u}_0^m, 0, \ldots, 0, 2(Q_2)_{N-1,N}\tilde{u}_{N+1}^m)^T. \tag{4.65}$$

Now, the relation (4.47) for general functions with $u^{(4)} \neq 0$ at boundaries becomes

$$A\vec{c}_{I_R}^{m+1'} + \tilde{r}_A^{m+1} = B\vec{c}_{I_R}^{m'} + \tilde{r}_B^m + \Delta t \vec{\epsilon}^m, \tag{4.66}$$

where

$$\tilde{r}_A^{m+1} = (2A_{2,1}\tilde{u}_0^{m+1}, 0, \ldots, 0, 2A_{N-1,N}u_{N+1}^{m+1})^T$$

and

$$\tilde{r}_B^m = (2B_{2,1}\tilde{u}_0^m, 0, \ldots, 0, 2B_{N-1,N}u_{N+1}^m)^T.$$

That is

$$A\vec{c}_{I_R}^{m+1'} = B\vec{c}_{I_R}^{m'} - \tilde{r}_A^{m+1} + \tilde{r}_B^m + \Delta t \vec{\epsilon}^m. \tag{4.67}$$

Let

$$u_C^m = \sum_{i=0}^{N+1} c_i^{m'} \phi_i(x), \tag{4.68}$$

and define

$$\vec{c}^{m'} = (c_0^{m'}, \ldots, c_{N+1}^{m'})^T \text{ and } \vec{c}_R^{m'} = (c_1^{m'}, \ldots, c_N^{m'})^T. \tag{4.69}$$

Let $c_0^{m'}, c_1^{m'}, c_N^{m'}$, and $c_{N+1}^{m'}$ satisfy relations similar to those in (4.60), more precisely,

$$c_0^{m'} = 2\tilde{u}_0^m - c_1^{m'} \text{ and } c_{N+1}^{m'} = 2\tilde{u}_{N+1}^m - c_N^{m'}. \tag{4.70}$$

Recall that the RQSC-CN method for functions with $u^{(4)} = 0$ at the boundaries computes the DOFs of u_C^{m+1} by solving

$$A\vec{c}^{m+1} = B\vec{c}^m.$$

For $u^{(4)} \neq 0$ at the boundaries, we adjust the RQSC-CN method to compute the DOFs of u_C^{m+1} by solving

$$A\vec{c}_R^{m+1'} = B\vec{c}_R^{m'} - \tilde{r}_A^{m+1} + \tilde{r}_B^m. \tag{4.71}$$

This means that, instead of satisfying the Dirichlet boundary conditions exactly, the collocation approximation u_C^{m+1} satisfies perturbed boundary conditions that are the same as those that u_I^{m+1} satisfies.

Initially, let $\vec{c}_R^{0'} = \vec{c}_{I_R}^{0'}$. Subtracting (4.71) from (4.67), we have

$$A(\vec{c}_{I_R}^{m+1'} - \vec{c}_R^{m+1'}) = B(\vec{c}_{I_R}^{m'} - \vec{c}_R^{m'}) + \Delta t \vec{\epsilon}^m, \tag{4.72}$$

which leads to

$$\vec{c}_{I_R}^{m+1'} - \vec{c}_R^{m+1'} = Q(\vec{c}_{I_R}^{m'} - \vec{c}_R^{m'}) + \Delta t \vec{\varepsilon}^m. \tag{4.73}$$

This is a relation similar to (4.53). Then by similar arguments as before, we obtain

$$\|\vec{c}_{I_R}^{m+1'} - \vec{c}_R^{m+1'}\|_\infty = t_{m+1}\mathcal{O}(h^4).$$

Finally, by (4.60) and (4.70), we have

$$\|\vec{c}_I^{m+1'} - \vec{c}^{m+1'}\|_\infty = t_{m+1}\mathcal{O}(h^4).$$

□

We need to add a few notes regarding the adjustment we applied to the RQSC-CN method to obtain the proof of convergence of the method for functions with $u^{(4)} \neq 0$ at the boundaries. First, this adjustment may seem unrealistic, since it involves the values of $u^{(4)}$ at the boundaries. However, we can use an $\mathcal{O}(h^2)$ approximation to $u^{(4)}$ instead of $u^{(4)}$ itself, without affecting the steps of the proof, since such an approximation will introduce an $\mathcal{O}(h^6)$ error which will have no impact on the orders of convergence. (Recall that the adjustment involves an $\mathcal{O}(h^4)$ perturbation at the boundaries.) An $\mathcal{O}(h^2)$ approximation to $(u^{m+1})^{(4)}(x_0)$ can be obtained by first approximating $(u^{m+1})^{(4)}(x_0)$ by $(u^m)^{(4)}(x_0)$, then approximating the latter by an appropriate finite difference formula involving the values of $(u_C^m)^{(4)}$ at the six leftmost midpoints. Similar approximation can be obtained for $(u^{m+1})^{(4)}(x_N)$. Thus, the adjustment is easily computable and involves little extra computational effort. Second, it is important to note that the adjustment to the RQSC-CN method is only needed for the proof of convergence. Extensive numerical experiments on functions with $u^{(4)} \neq 0$ at the boundaries using the RQSC-CN method without adjustment indicate that the optimal orders of convergence hold. However, we were unable to complete the proof of convergence without the adjustment for functions with $u^{(4)} \neq 0$ at the boundaries.

Chapter 5

Numerical Results

In this chapter, we present a variety of numerical results to demonstrate the performance of the methods discussed in previous chapters. First, we test the convergence of the RQSC-CN method for Problems (1.1)-(1.3) and (4.1)-(4.4). Next, we demonstrate the convergence of the RQSC-CN1 and RQSC-CN0 methods. Finally, we compare the numerical results of the RQSC-CN, RQSC-CN1 and RQSC-CN0 methods to those of the optimal *two-step* QSC-CN method.

From the analysis of the convergence in Chapter 4, we expect that the resulting errors in the infinity norm would be $\mathcal{O}(h^3)$ globally and $\mathcal{O}(h^4)$ at the grid points $\{x_i\}$ and midpoints $\{\tau_i\}$. We are also expecting some superconvergence behaviour for derivatives, i.e. we are expecting $\mathcal{O}(h^3)$ for u_x at the points $\{\lambda_i\}$ where $\lambda_i = x_i + (3 \pm \sqrt{3})h$, and $\mathcal{O}(h^2)$ for u_{xx} at the midpoints.

In all our experiments, we first choose the problem, i.e. pick the coefficients p, q and f of u_{xx}, u_x, and u, respectively; then we adjust $\gamma(x), \beta_0(t), \beta_1(t)$, and $g(x,t)$ so that a predetermined function satisfies the problem. Therefore, we can use this true solution to compute the errors and the respective orders of convergence. For all problems considered, the domain is $[0,1] \times [0,1]$. The errors and the respective orders of convergence are computed at $t = 0.1k,\ k = 0, 1, \ldots, 10$, and the maximum is picked. The errors are presented in the format $x.y \pm k$, which means $x.y \times 10^{\pm k}$. We use the subscripts, x_i, τ_i and λ_i, to denote the discrete infinity (maximum) norms of the errors at the points $\{x_i\}, \{\tau_i\}$, and $\{\lambda_i\}$, respectively, and the subscript ∞, to denote the continuous infinity (maximum) norm of the error (global error). The global error is approximated by computing the maximum error at 1000 points in the space domain for each $t = 0.1k,\ k = 0, 1, \ldots, 10$, and picking the maximum over all $k = 0, 1, \ldots, 10$. The methods are programmed in *Matlab*, which, by default, uses double precision. In the discussion that follows, when we refer to zero errors from numerical experiments, we mean errors close to the machine epsilon.

5.1 RQSC-CN Method

5.1.1 Dirichlet Boundary Conditions

In this section, we consider the Problem (1.1)-(1.3).

Problem 1

We perform a test to indicate the maximum degree of polynomials with respect to x, which leads to zero errors at the grid points and midpoints.

In (1.1), letting $p(x,t) = 1, q(x,t) = 0$, and $f(x,t) = -1$, the problem becomes

$$u_t = u_{xx} - u + g(x,t),\ 0 < x < 1, 0 < t < 1.$$

We choose $u(x,t) = x^3(t^2 - 1)$ and $\sigma = \Delta t/h^2 = 1$. For such a function, the third and higher derivatives with respect to t are zero, therefore, the time discretization does not introduce any error. The boundary functions β_0 and β_1 are determined such that $u(x,t)$ satisfies the boundary conditions.

The infinity norms of the observed errors for $N = 8$ to 128 points in the partition Δ and the respective orders of convergence are shown in Table 5.1. It can be observed that we obtain zero errors within the machine precision for u at the points $\{x_i, \tau_i\}$. We also get zero errors for derivatives at superconvergence points. More precisely, we get zero errors for u_x and u_{xx} at the points $\{\lambda_i\}$ and $\{\tau_i\}$, respectively. If we increase the degree of x to four, we cannot get zero errors for u at $\{x_i, \tau_i\}$ and for derivatives at $\{\lambda_i, \tau_i\}$ anymore. It seems that the maximum degree of x which leads to zero errors at the respective points is three.

Table 5.1: Errors and respective orders of convergence of the RQSC-CN method for Problem 1.

N	$\|u-u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x}-\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2}-\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	2.8-17	2.8-17	2.3-05	3.3-16	9.8-04	1.9-03	9.4-02	5.3-15	9.4-02
16	2.8-17	2.8-17	2.9-06	1.3-15	2.4-04	4.9-04	4.7-02	1.4-14	4.7-02
32	2.8-17	2.8-17	3.7-07	2.3-15	6.1-05	1.2-04	2.3-02	1.1-13	2.3-02
64	6.7-16	6.7-16	4.6-08	1.1-14	1.5-05	3.0-05	1.2-02	3.4-13	1.2-02
128	6.2-15	6.2-15	5.7-09	4.7-14	3.8-06	7.6-06	5.9-03	1.8-12	5.8-03

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	-	-	3.00	-	2.00	2.00	1.00	-	1.00
32	-	-	3.00	-	2.00	2.00	1.00	-	1.00
64	-	-	3.00	-	2.00	2.00	1.00	-	1.00
128	-	-	3.00	-	2.00	2.00	1.00	-	1.00

Problem 2

With this problem, we want to demonstrate the convergence of the RQSC-CN method for a smooth function $u \in \mathcal{C}^\infty$, and a problem with variable coefficients. In (1.1), letting

$$p(x,t) = 2 + \sin t,\ \ q(x,t) = \frac{16x}{1+4x^2}\frac{1}{1+t},\ \ f(x,t) = \frac{8}{1+4x^2}e^{-t},$$

the problem becomes

$$u_t = (2+\sin t)u_{xx} + \frac{16x}{1+4x^2}\frac{1}{1+t}u_x + \frac{8}{1+4x^2}e^{-t}u + g(x,t),\ \ 0 < x < 1, 0 < t < 1.$$

The functions γ, g, β_0, and β_1 are chosen such that $u(x,t) = e^{x+t}$ is the true solution. For the time step, we choose $\Delta t = h^2$.

The infinity norms of the observed errors for $N = 8$ to 128 points in the partition Δ are shown in Table 5.2. From these we derive estimates of the orders of convergence. It can be observed that the optimal orders of convergence and superconvergence are obtained for a function in $\mathcal{C}^\infty$. Although the convergence analysis in Chapter 4 is carried out for some special problem, the optimal orders of convergence and superconvergence by the RQSC-CN method are also observed for a general problem and general Dirichlet boundary conditions. These results indicate that the conditions of Theorem 4.2.4 under which the optimal convergence of the RQSC-CN method is obtained are only sufficient and not necessary.

Table 5.2: Errors and respective orders of convergence of the RQSC-CN method for Problem 2.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	6.2-06	1.5-05	1.2-04	2.4-04	4.5-03	9.2-03	4.5-01	4.5-03	4.4-01
16	3.9-07	9.4-07	1.5-05	2.9-05	1.2-03	2.2-03	2.3-01	1.2-03	2.2-01
32	2.4-08	5.9-08	1.8-06	3.6-06	3.0-04	5.5-04	1.1-01	3.0-04	1.1-01
64	1.5-09	3.7-09	2.3-07	4.5-07	7.5-05	1.4-04	5.8-02	7.5-05	5.4-02
128	9.5-11	2.3-10	2.8-08	5.7-08	1.9-05	3.4-05	2.9-02	1.9-05	2.7-02

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.00	3.98	3.02	3.01	1.95	2.07	0.98	1.96	1.01
32	4.00	4.00	3.01	3.01	1.98	1.98	0.99	1.98	1.00
64	4.00	4.00	3.01	3.00	1.99	1.99	1.00	1.99	1.02
128	4.00	4.00	3.02	3.00	1.99	2.04	1.00	1.99	1.00

Problem 3

With this problem, we study the convergence of the RQSC-CN method for various smoothness assumptions on u. The problem arises from an one-dimensional BVP in [10]. By adding some terms involving the time variable, we get a parabolic PDE. In (1.1), letting

$$p(x,t)=1, q(x,t)=\frac{16x}{1+4x^2}, f(x,t)=\frac{8}{1+4x^2},$$

the problem becomes

$$u_t=u_{xx}+\frac{16x}{1+4x^2}u_x+\frac{8}{1+4x^2}u+g(x,t),\ 0<x<1, 0<t<1.$$

First, we test the convergence for various smoothness assumptions on u with respect to x. Let $u(x,t)=x^{\alpha/2}e^t$, where $\alpha=11,9,7$, which puts u in $\mathcal{C}^{5.5},\mathcal{C}^{4.5},\mathcal{C}^{3.5}$ with respect to x, respectively. Again, the functions γ, g, β_0, and β_1 are chosen such that u is the true solution to this problem. We refer to this problem as Problem 3(i). Next, we test the convergence for various smoothness assumptions on u with respect to t. Let $u(x,t)=e^x t^{\alpha/2}$, where $\alpha=7,5,3$, which puts u in $\mathcal{C}^{3.5},\mathcal{C}^{2.5},\mathcal{C}^{1.5}$ with respect to t, respectively. We refer to this problem as Problem 3(ii).

For the time step size, we choose $\sigma=1$, thus $\Delta t=h^2$. The infinity norms of the observed errors and the respective orders of convergence are shown in Tables 5.3 - 5.5 for Problem 3(i) and Tables 5.6 - 5.8 for Problem 3(ii).

From the results, we see that for Problem 3(i), when u is in $\mathcal{C}^4$ with respect to x, the orders of convergence of u and its derivatives are optimal, while for a function in $\mathcal{C}^{3.5}$, the orders of convergence and superconvergence are 0.5 less than the optimal orders. This indicates that $\mathcal{C}^4$ is the minimum continuity required to obtain the optimal orders of convergence. The minimum continuity with respect to t is $\mathcal{C}^2$. When u is in $\mathcal{C}^{1.5}$ with respect to t, the orders of convergence are one less than the optimal orders only at the grid points and midpoints. An interesting observation is that the orders of superconvergence for the derivatives are preserved.

Table 5.3: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(i) with $\alpha = 11$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	4.1-04	1.1-03	4.0-03	1.8-02	1.3-01	2.9-01	1.4+01	3.6-01	1.4+01
16	2.8-05	6.8-05	4.8-04	2.2-03	3.5-02	7.0-02	7.2+00	9.3-02	6.9+00
32	1.8-06	4.3-06	5.9-05	2.8-04	9.2-03	1.7-02	3.6+00	2.3-02	3.4+00
64	1.2-07	2.7-07	7.2-06	3.6-05	2.3-03	4.1-03	1.8+00	5.9-03	1.7+00
128	7.3-09	1.7-08	8.8-07	4.5-06	5.9-04	1.0-03	9.2-01	1.5-03	8.6-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	3.87	4.01	3.05	3.02	1.87	2.07	0.96	1.98	0.99
32	3.94	3.99	3.03	2.99	1.94	2.06	0.98	1.98	1.03
64	3.97	3.99	3.02	2.98	1.97	2.02	0.99	1.99	1.02
128	3.99	3.99	3.04	2.99	1.99	2.02	1.00	1.99	0.97

Table 5.4: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(i) with $\alpha = 9$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.2-04	3.2-04	1.8-03	5.3-03	6.3-02	1.3-01	6.5+00	1.0-01	6.4+00
16	8.0-06	1.9-05	2.1-04	6.4-04	1.7-02	3.2-02	3.3+00	2.6-02	3.2+00
32	5.1-07	1.2-06	2.6-05	7.9-05	4.3-03	7.9-03	1.7+00	6.5-03	1.6+00
64	3.2-08	7.5-08	3.3-06	9.8-06	1.1-03	2.0-03	8.3-01	1.6-03	7.8-01
128	2.0-09	4.7-09	4.0-07	1.2-06	2.7-04	4.8-04	4.2-01	4.1-04	3.9-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	3.95	4.05	3.04	3.05	1.92	2.08	0.98	2.01	1.00
32	3.98	4.01	3.02	3.01	1.96	2.01	0.99	2.00	1.01
64	3.99	4.00	3.02	3.00	1.98	2.00	0.99	2.00	1.02
128	4.00	4.00	3.03	3.00	1.99	2.04	1.00	2.00	0.98

Table 5.5: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(i) with $\alpha = 7$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.0-04	1.7-04	5.7-04	2.2-03	2.2-02	4.4-02	2.2+00	3.5-02	2.2+00
16	8.1-06	1.2-05	7.0-05	3.5-04	5.7-03	1.1-02	1.1+00	1.2-02	1.1+00
32	6.3-07	9.4-07	8.7-06	5.8-05	1.4-03	2.7-03	5.6-01	4.3-03	5.4-01
64	5.2-08	8.2-08	1.1-06	1.0-05	3.6-04	6.9-04	2.8-01	1.5-03	2.7-01
128	4.5-09	7.2-09	1.4-07	1.8-06	9.1-05	1.7-04	1.4-01	5.4-04	1.3-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	3.69	3.75	3.02	2.65	1.97	2.04	0.99	1.52	1.02
32	3.68	3.72	3.01	2.57	1.99	2.00	1.00	1.50	0.99
64	3.61	3.53	3.01	2.53	1.99	1.98	1.00	1.50	1.01
128	3.54	3.51	3.01	2.51	2.00	2.01	1.00	1.50	1.01

Table 5.6: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(ii) with $\alpha = 7$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	7.6-05	7.8-05	9.9-05	4.0-04	1.5-03	3.6-03	1.7-01	2.1-03	1.6-01
16	4.7-06	4.9-06	7.7-06	2.7-05	4.2-04	8.1-04	8.4-02	4.4-04	8.1-02
32	2.9-07	3.1-07	6.9-07	2.1-06	1.1-04	2.0-04	4.2-02	1.1-04	4.1-02
64	1.8-08	1.9-08	8.3-08	2.1-07	2.7-05	5.1-05	2.1-02	2.7-05	2.0-02
128	1.2-09	1.2-09	1.0-08	2.4-08	6.9-06	1.2-05	1.1-02	6.9-06	1.0-02

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.01	3.99	3.68	3.89	1.83	2.13	0.99	2.23	1.01
32	4.00	4.00	3.49	3.73	1.95	2.00	0.99	2.01	1.00
64	4.00	4.00	3.06	3.28	1.98	1.99	1.00	2.00	1.02
128	4.00	4.00	3.02	3.16	1.99	2.04	1.00	2.00	1.00

Table 5.7: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(ii) with $\alpha = 5$.

N	$\Vert u - u_C \Vert_{x_i,\tau_i,\infty}$			$\Vert \frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x} \Vert_{\lambda_i,\tau_i,\infty}$			$\Vert \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2} \Vert_{x_i,\tau_i,\infty}$		
8	3.2-05	3.2-05	4.5-05	1.5-04	1.6-03	3.4-03	1.7-01	1.7-03	1.6-01
16	2.0-06	2.0-06	5.4-06	1.3-05	4.3-04	8.0-04	8.4-02	4.3-04	8.1-02
32	1.3-07	1.3-07	6.7-07	1.5-06	1.1-04	2.0-04	4.2-02	1.1-04	4.1-02
64	8.1-09	8.1-09	8.3-08	1.8-07	2.7-05	5.1-05	2.1-02	2.7-05	2.0-02
128	5.1-10	5.1-10	1.0-08	2.1-08	6.9-06	1.2-05	1.1-02	6.9-06	1.0-02

N	$u_C\vert_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\vert_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\vert_{x_i,\tau_i,\infty}$		
16	3.97	3.95	3.06	3.55	1.93	2.09	0.99	2.00	1.01
32	3.98	3.98	3.02	3.15	1.97	1.99	0.99	1.99	1.00
64	3.99	3.99	3.01	3.08	1.99	1.99	1.00	1.99	1.02
128	3.99	3.99	3.02	3.04	1.99	2.04	1.00	2.00	1.00

Table 5.8: Errors and respective orders of convergence of the RQSC-CN method for Problem 3(ii) with $\alpha = 3$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	6.4-04	6.3-04	6.4-04	3.3-03	3.0-03	3.5-03	1.7-01	1.2-02	1.6-01
16	8.3-05	8.3-05	8.3-05	4.2-04	8.0-04	8.0-04	8.4-02	1.6-03	8.1-02
32	1.0-05	1.0-05	1.0-05	5.3-05	2.0-04	2.0-04	4.2-02	2.0-04	4.1-02
64	1.3-06	1.3-06	1.3-06	6.6-06	5.1-05	5.1-05	2.1-02	2.7-05	2.0-02
128	1.6-07	1.6-07	1.6-07	8.3-07	1.2-05	1.2-05	1.1-02	6.9-06	1.0-02

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	2.94	2.93	2.94	2.98	2.79	2.14	0.99	2.90	1.00
32	2.98	2.99	2.99	2.98	1.98	1.98	0.99	2.98	1.00
64	2.99	2.99	2.99	2.99	1.99	1.99	1.00	2.86	1.02
128	3.00	3.00	3.00	3.00	1.99	2.04	1.00	1.99	1.00

5.1.2 Periodic Boundary Conditions

In this section, we present the numerical results of the RQSC-CN method for Problem (4.1)-(4.4), subject to periodic boundary conditions.

Problem 4

Consider the parabolic problem

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2},\ 0 < x < 1,\ 0 < t < 1, \tag{5.1}$$

subject to periodic boundary conditions and initial condition (4.4).

Let $\gamma(x) = \sin 2\pi x$. The unique solution to this problem is given explicitly by $u(x,t) = e^{-4\pi^2 t} \sin 2\pi x$. We choose a relatively large $\sigma = 20$ to show that the RQSC-CN method is unconditionally stable when the problem has periodic boundary conditions.

The infinity norms of the observed errors and the respective orders of convergence are shown in Table 5.9. It can be observed that the optimal orders of convergence and superconvergence are obtained. This agrees with the analysis, in which it was shown that the RQSC-CN method for Problem (4.1)-(4.4) with periodic boundary conditions is unconditionally stable and convergent.

Table 5.9: Errors and respective orders of convergence of the RQSC-CN method for Problem 4.

N	$\|u-u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x}-\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2}-\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	6.8-01	6.3-01	6.8-01	4.2-00	3.9-00	4.5-00	2.6+01	2.6-00	2.6+01
16	4.1-02	4.1-02	4.1-02	2.6-01	2.5-01	2.6-01	7.8-00	1.6-00	7.6-00
32	2.2-03	2.1-03	2.2-03	1.4-02	1.4-02	1.9-02	3.9-00	8.4-02	3.8-00
64	2.2-04	2.2-04	2.2-04	1.4-03	2.5-03	4.8-03	1.9-00	1.6-02	1.9-00
128	1.5-05	1.5-05	1.5-05	9.1-05	6.3-04	1.2-03	9.7-01	4.0-03	9.5-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.04	3.96	4.04	4.03	3.93	4.10	1.72	3.99	1.75
32	4.26	4.24	4.26	4.26	4.22	3.80	1.00	4.26	1.02
64	3.32	3.31	3.32	3.32	2.43	2.00	1.00	2.41	0.99
128	3.89	3.89	3.89	3.89	2.00	1.97	1.00	2.00	1.00

5.1.3 Homogeneous Dirichlet Boundary Conditions

In this section, we consider Problem (4.1)-(4.4) with homogeneous Dirichlet boundary conditions. We verify by numerical experiments that the RQSC-CN method is stable under the condition in *Conjecture* 4.1.2.

Problem 5

For this problem, we will test the condition for stability in *Conjecture* 4.1.2. Consider the parabolic problem

$$\frac{\partial u(x,t)}{\partial t} = p\frac{\partial^2 u(x,t)}{\partial x^2} + g(x,t),\ 0 < x < 1,\ 0 < t < 1, \tag{5.2}$$

where p is constant, subject to homogeneous Dirichlet boundary conditions and initial condition (4.4).

The functions $g(x,t)$ and $\gamma(x)$ are chosen such that the unique solution is given explicitly by

$$u(x,t) = e^{-t/10}\sin \pi x.$$

First, we show that the RQSC-CN method is stable and convergent for $\sigma = p\frac{\Delta t}{\Delta x^2} \leq 5.06$. We choose two values of p to show that the stability depends on p and $r = \frac{\Delta t}{\Delta x^2}$. Letting $\sigma = 5.06$, the infinity norms of the observed errors and the respective orders of convergence are shown in Table 5.10 an Table 5.11. It can be observed that the optimal orders of convergence and superconvergence are obtained under the condition in *Conjecture* 4.1.2 for this problem.

Next, we show that RQSC-CN method is not stable when $\sigma > 5.06$. We choose $\sigma = 5.1, 5.2$. The reason that we choose a relatively large σ instead of choosing $\sigma = 5.07, 5.08$, is that for a small σ which is just above the critical point, 5.06, we need more time steps for the errors to be amplified enough to demonstrate the instability. As a result, it is hard to show the instability of the RQSC-CN method by numerical results for marginal values of σ. In this case, we only present the errors and the respective orders of convergence of the function u. The corresponding results are shown in Table 5.12 and Table 5.13. From the results, we can see that RQSC-CN method is not stable for $\sigma = 5.1, 5.2$. Moreover, the larger the σ is, the more unstable the method is. We also notice that for stability, if we double p, we should reduce r in half, which is consistent to the relation $\sigma = pr$.

Table 5.10: Errors and respective orders of convergence of the RQSC-CN method for Problem 5 ($\sigma = 5.06, p = 1, r = 5.06$).

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.9-04	7.3-05	5.1-04	3.1-03	2.0-02	3.9-02	1.9+00	6.2-02	1.9+00
16	1.2-05	2.8-06	6.1-05	3.8-04	5.1-03	9.5-03	9.7-01	1.6-02	9.4-01
32	7.3-07	1.6-07	7.6-06	4.8-05	1.3-03	2.4-03	4.8-01	4.0-03	4.7-01
64	4.5-08	9.8-09	9.5-07	6.0-06	3.2-04	6.1-04	2.4-01	9.9-04	2.4-01
128	2.8-09	6.1-10	1.2-07	7.4-07	7.9-05	1.5-04	1.2-01	2.5-04	1.2-01
256	1.8-10	3.8-11	1.5-08	9.3-08	2.0-05	3.8-05	6.1-02	6.2-05	6.0-02
512	1.1-11	1.8-12	1.8-09	1.2-08	4.9-06	9.4-06	3.0-02	1.5-05	3.0-02

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.01	4.72	3.05	3.01	2.01	2.03	1.00	1.97	1.02
32	4.00	4.13	3.01	3.00	2.00	2.00	1.00	1.99	0.99
64	3.97	4.02	3.00	3.00	2.00	1.97	1.00	2.00	1.00
128	4.00	4.00	3.00	3.00	2.00	2.02	1.00	2.00	1.01
256	4.00	4.01	3.00	3.00	2.00	1.96	1.00	2.00	0.98
512	4.00	4.39	3.00	3.00	2.00	2.03	1.00	2.00	1.01

Table 5.11: Errors and respective orders of convergence of the RQSC-CN method for Problem 5 ($\sigma = 5.06, p = 2, r = 2.53$).

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.9-04	6.2-05	5.1-04	3.1-03	2.0-02	3.9-02	1.9+00	6.2-02	1.9+00
16	1.2-05	2.1-06	6.1-05	3.8-04	5.1-03	9.5-03	9.7-01	1.6-02	9.4-01
32	7.3-07	1.1-07	7.6-06	4.8-05	1.3-03	2.4-03	4.8-01	4.0-03	4.7-01
64	4.5-08	7.0-09	9.5-07	6.0-06	3.2-04	6.1-04	2.4-01	9.9-04	2.4-01
128	2.8-09	4.3-10	1.2-07	7.4-07	7.9-05	1.5-04	1.2-01	2.5-04	1.2-01
256	1.8-10	2.7-11	1.5-08	9.3-08	2.0-05	3.8-05	6.1-02	6.2-05	6.0-02
512	1.1-11	1.1-12	1.8-09	1.2-08	4.9-06	9.4-06	3.0-02	1.5-05	3.0-02

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.01	4.92	3.05	3.01	2.01	2.04	1.00	1.97	1.02
32	4.00	4.18	3.01	3.00	2.00	2.00	1.00	1.99	0.99
64	4.00	4.02	3.00	3.00	2.00	1.97	1.00	2.00	1.00
128	4.00	4.00	3.00	3.00	2.00	2.02	1.00	2.00	1.01
256	4.00	4.01	3.00	3.00	2.00	1.96	1.00	2.00	0.98
512	4.00	4.61	3.00	3.00	2.00	2.03	1.00	2.00	1.01

Table 5.12: Errors and respective orders of convergence of the RQSC-CN method for Problem 5 with $p = 1, \sigma = 5.2, 5.1, r = 5.2, 5.1$, respectively. A '-' indicates that no results are produced.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	$\sigma = 5.2, r = 5.2$			$\sigma = 5.1, r = 5.1$		
8	1.88-04	7.28-05	5.06-04	1.88-04	7.32-05	5.06-04
16	1.16-05	2.80-06	6.13-05	1.16-05	2.77-06	6.13-05
32	7.26-07	1.61-07	7.59-06	7.26-07	1.59-07	7.59-06
64	4.54-08	9.93-09	9.47-07	4.54-08	9.81-09	9.47-07
128	2.84-09	6.19-10	1.19-07	2.84-09	6.12-10	1.19-07
256	7.91-06	8.07-06	9.02-06	1.77-10	3.85-11	1.48-08
512	-	-	-	2.00-07	2.05-07	2.07-07

N	$u_C\|_{x_i,\tau_i,\infty}$					
	$\sigma = 5.2, r = 5.2$			$\sigma = 5.1, r = 5.1$		
16	4.01	4.70	3.05	4.01	4.72	3.05
32	4.00	4.12	3.01	4.00	4.13	3.01
64	4.00	4.02	3.00	4.00	4.02	3.00
128	4.00	4.00	3.00	4.00	4.00	3.00
256	-11	-14	-6.5	4.00	3.99	3.00
512	-	-	-	-10	-12	-3.0

Table 5.13: Errors and respective orders of convergence of the RQSC-CN method for Problem 5 with $p = 2, \sigma = 5.2, 5.1, r = 2.6, 2.55$, respectively. A '-' indicates that no results are produced.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	$\sigma = 5.2, r = 2.6$			$\sigma = 5.1, r = 2.55$		
8	1.88-04	6.24-05	5.07-04	1.88-04	6.24-05	5.07-04
16	1.16-05	2.07-06	6.13-05	1.16-05	2.06-06	6.13-05
32	7.26-07	1.15-07	7.59-06	7.26-07	1.14-07	7.59-06
64	4.54-08	7.04-09	9.47-07	4.54-08	6.98-09	9.47-07
128	8.26-09	8.38-09	1.19-07	2.84-09	4.35-10	1.19-07
256	9.04+04	9.23+04	1.03+05	1.77-10	2.75-11	1.48-08
512	-	-	-	7.34+01	7.53+01	7.61+01

N	$u_C\|_{x_i,\tau_i,\infty}$					
	$\sigma = 5.2, r = 2.6$			$\sigma = 5.1, r = 2.55$		
16	4.01	4.91	3.05	4.01	4.92	3.05
32	4.00	4.18	3.01	4.00	4.18	3.01
64	4.00	4.02	3.00	4.00	4.02	3.00
128	2.46	-0.3	3.00	4.00	4.00	3.00
256	-43	-43	-40	4.00	3.99	3.00
512	-	-	-	-39	-41	-32

5.2 RQSC-CN1 and RQSC-CN0 Methods

In this section, we study the convergence and stability of the RQSC-CN1 and RQSC-CN0 methods for Problem (4.1)-(4.4) subject to homogeneous Dirichlet boundary conditions. Recall that, for the RQSC-CN1 method, we use $u^{(4)}(\tau_2)$ and $u^{(4)}(\tau_{n-1})$ to approximate $u^{(4)}(\tau_1)$ and $u^{(4)}(\tau_n)$, respectively. More precisely, $\mathcal{P}_{\mathcal{L}}$ is changed as shown in (4.10). For the RQSC-CN0 method, we do not add any perturbation at $\{\tau_1, \tau_n\}$, that is, in this case, $\mathcal{P}_{\mathcal{L}}$ becomes as shown in (4.12).

Problem 6

Consider the following equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + g(x,t), \quad 0 < t \leq 1$$

subject to (4.4) and (4.2).

The functions γ and g are chosen such that the true solution is $u(x,t) = \sin(2\pi x)e^{-t}$. We choose a relatively large $\sigma = 20$ to give evidence that the RQSC-CN1 and RQSC-CN0 methods are unconditionally stable.

The infinity norms of the observed errors and respective orders of convergence of the RQSC-CN1 and RQSC-CN0 methods are shown in Table 5.14 and Table 5.15, respectively. It can be observed that the optimal orders of convergence and superconvergence are obtained.

Table 5.14: Errors and respective orders of convergence of the RQSC-CN1 method for Problem 6.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	8.2-03	9.9-03	1.1-02	1.2-01	1.7-01	3.7-01	1.5+01	1.4-00	1.5+01
16	2.7-04	3.2-04	6.4-04	8.3-03	4.1-02	7.7-02	7.8-00	2.5-01	7.6-00
32	1.2-05	1.7-05	6.1-05	7.6-04	1.0-02	1.9-02	3.9-00	6.3-02	3.8-00
64	7.3-07	9.8-07	7.6-06	9.5-05	2.5-03	4.8-03	1.9-00	1.6-02	1.9-00
128	4.5-08	5.9-08	9.5-07	1.2-05	6.3-04	1.2-03	9.7-01	4.0-03	9.5-01
256	2.8-09	3.6-09	1.2-07	1.5-06	1.6-04	3.0-04	4.8-01	9.9-04	4.7-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.93	4.95	4.09	3.85	2.03	2.28	1.00	2.51	1.01
32	4.52	4.26	3.38	3.44	2.01	2.02	1.00	1.97	1.02
64	4.00	4.10	3.01	3.00	2.00	2.00	1.00	1.99	0.99
128	4.00	4.05	3.00	3.00	2.00	1.97	1.00	2.00	1.00
256	4.00	4.03	3.00	3.00	2.00	2.02	1.00	2.00	1.01

Table 5.15: Errors and respective orders of convergence of the RQSC-CN0 method for Problem 6.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	3.1-03	3.6-03	4.6-03	6.1-02	1.7-01	3.2-01	1.5+01	9.0-01	1.5+01
16	1.9-04	1.8-04	5.1-04	6.2-03	4.1-02	7.7-02	7.8-00	2.5-01	7.6-00
32	1.2-05	1.3-05	6.1-05	7.6-04	1.0-02	1.9-02	3.9-00	6.3-02	3.8-00
64	7.3-07	8.7-07	7.6-06	9.5-05	2.5-03	4.8-03	1.9-00	1.6-02	1.9-00
128	4.5-08	5.5-08	9.5-07	1.2-05	6.3-04	1.2-03	9.7-01	4.0-03	9.5-01
256	2.8-09	3.5-09	1.2-07	1.5-06	1.6-04	3.0-04	4.8-01	9.9-04	4.7-01

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	4.05	4.35	3.17	3.32	2.03	2.04	1.00	1.87	1.01
32	4.01	3.74	3.05	3.01	2.01	2.02	1.00	1.97	1.02
64	4.00	3.93	3.01	3.00	2.00	2.00	1.00	1.99	0.99
128	4.00	3.97	3.00	3.00	2.00	1.97	1.00	2.00	1.00
256	4.00	3.98	3.00	3.00	2.00	2.02	1.00	2.00	1.01

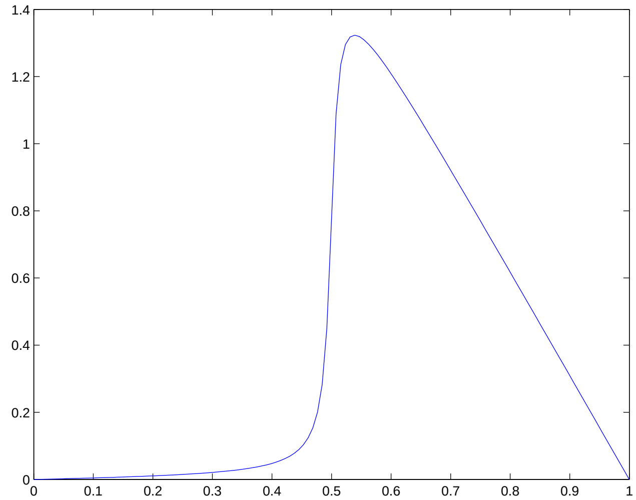
Problem 7

We consider a problem with the same PDE as *Problem 6* but with the exact solution

$$u(x,t) = (1-x)(\arctan(\nu(x-\mu)) + \arctan(\nu\mu))e^{-t},$$

where $\mu = 0.5,\ \nu = 10$.

The solution exhibits an interior layer, therefore, this problem is harder to solve. At the initial step, the function is shown in the following figure.



We choose a relatively large $\sigma = 20$ to give evidence that the RQSC-CN1 and RQSC-CN0 methods are unconditionally stable.

The infinity norms of the observed errors and the respective orders of convergence of the RQSC-CN1 and RQSC-CN0 methods are shown in Table 5.16 and Table 5.17, respectively. Since this function has a very steep interior layer, small step sizes are needed to obtain the optimal orders of convergence.

Table 5.16: Errors and respective orders of convergence of the RQSC-CN1 method for Problem 7.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.0-01	1.1-01	1.2-01	1.0-00	7.3-01	1.5-00	2.6+01	1.0+01	4.1+01
16	2.4-03	2.6-03	3.6-03	9.5-02	1.7-01	3.0-01	2.3+01	3.1-00	2.9+01
32	2.2-04	3.7-05	3.3-04	1.4-02	4.7-02	7.3-02	1.5+01	8.0-01	1.6+01
64	1.3-05	1.9-06	3.4-05	1.6-03	1.1-02	1.9-02	7.9-00	2.6-01	7.7-00
128	7.7-07	1.1-07	4.0-06	2.0-04	2.6-03	4.4-03	4.0-00	6.7-02	3.7-00
256	4.8-08	7.1-09	4.7-07	2.5-05	6.5-04	1.1-03	2.0-00	1.7-02	1.8-00

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	5.41	5.46	5.00	3.44	2.09	2.32	0.14	1.73	0.51
32	3.45	6.13	3.48	2.74	1.86	2.02	0.67	1.96	0.88
64	4.13	4.24	3.26	3.12	2.11	1.95	0.90	1.63	1.01
128	4.03	4.08	3.09	3.02	2.06	2.08	0.97	1.94	1.05
256	3.99	4.01	3.07	2.99	2.01	2.02	1.00	2.00	1.06

Table 5.17: Errors and respective orders of convergence of the RQSC-CN0 method for Problem 7.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$			$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
8	1.0-01	1.2-01	1.2-01	1.0-00	7.4-01	1.5-00	2.6+01	1.0+01	4.1+01
16	2.4-03	2.6-03	3.6-03	9.5-02	1.7-01	3.0-01	2.3+01	3.1-00	2.9+01
32	2.2-04	3.7-05	3.3-04	1.4-02	4.7-02	7.3-02	1.5+01	8.0-01	1.6+01
64	1.3-05	2.0-06	3.4-05	1.6-03	1.1-02	1.9-02	7.9-00	2.6-01	7.7-00
128	7.7-07	1.2-07	4.0-06	2.0-04	2.6-03	4.4-03	4.0-00	6.7-02	3.7-00
256	4.8-08	7.1-09	4.7-07	2.5-05	6.5-04	1.1-03	2.0-00	1.7-02	1.8-00

N	$u_C\|_{x_i,\tau_i,\infty}$			$\frac{\partial u_C}{\partial x}\|_{\lambda_i,\tau_i,\infty}$			$\frac{\partial^2 u_C}{\partial x^2}\|_{x_i,\tau_i,\infty}$		
16	5.43	5.47	5.00	3.45	2.10	2.33	0.14	1.73	0.51
32	3.45	6.13	3.48	2.74	1.86	2.02	0.67	1.96	0.88
64	4.13	4.25	3.26	3.12	2.11	1.95	0.90	1.63	1.01
128	4.03	4.08	3.09	3.02	2.06	2.08	0.97	1.94	1.05
256	3.99	4.02	3.07	2.99	2.01	2.02	1.00	2.00	1.06

5.3 Comparison

As we have discussed, the optimal *one-step QSC-CN* and *two-step QSC-CN* methods have their advantages and disadvantages. The RQSC-CN method has the advantages of these two methods, that is, the RQSC-CN method solves only one system at each time step like the *one-step* method and the system is as sparse (tridiagonal) as the linear systems of the *two-step* method. The orders of convergence of the RQSC-CN method are the same as the above two methods, but the computational work of the RQSC-CN method is much less. More specifically, it is about half of the computational work of the two-step QSC-CN method, and less than half of the work of the one-step QSC-CN method.

In this section, we want to present how the errors of the RQSC-CN, RQSC-CN1, and RQSC-CN0 methods behave compared to those of the *two-step QSC-CN* method.

Problem 8

In this test, we compare the RQSC-CN method with the optimal *two-step QSC-CN* method. We consider Problem 3(i) with $\alpha = 9, 7$. We solve it by the optimal two-step QSC-CN method. For convenience, we copy the results from Problem 3 and put the results from the RQSC-CN and optimal two-step QSC-CN methods into one table. The infinity norms of the errors and the respective orders of convergence for u, u_x, and u_{xx} are shown in Tables 5.18 - 5.21.

From the results, the orders of convergence of these two methods are almost the same and the RQSC-CN method is as accurate as the optimal *two-step* QSC-CN method. For the few cases where the results of the RQSC-CN method are slightly different from those of the optimal *two-step* QSC-CN method, we notice that the RQSC-CN method is slightly more accurate when the grid size increases. Furthermore, these two methods have similar sensitivity to discontinuity as far as orders of convergence are concerned.

Table 5.18: Errors and respective orders of convergence of the RQSC-CN and optimal two-step QSC-CN methods for Problem 8 for u with $\alpha = 9$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN			Two-step		
8	1.25-04	3.21-04	1.76-03	1.25-04	3.04-04	1.75-03
16	8.03-06	1.93-05	2.14-04	8.03-06	1.80-05	2.13-04
32	5.09-07	1.20-06	2.64-05	5.09-07	1.10-06	2.64-05
64	3.20-08	7.48-08	3.27-06	3.20-08	6.80-08	3.26-06
128	2.00-09	4.67-09	4.00-07	2.01-09	4.23-09	4.01-07

N	$u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN			Two-step		
16	3.96	4.05	3.04	3.96	4.08	3.04
32	3.98	4.01	3.02	3.98	4.03	3.02
64	3.99	4.00	3.02	3.99	4.01	3.02
128	4.00	4.00	3.03	4.00	4.01	3.03

Table 5.19: Errors and respective orders of convergence of the RQSC-CN and optimal two-step QSC-CN methods for Problem 8 for u_x and u_{xx} with $\alpha = 9$.

N	RQSC-CN			Two-step		
	$\Vert\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\Vert_{\lambda_i,\infty}$		$\Vert\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\Vert_{\tau_i}$	$\Vert\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\Vert_{\lambda_i,\infty}$		$\Vert\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\Vert_{\tau_i}$
8	5.28-03	1.33-01	1.04-01	5.00-03	1.33-01	1.03-01
16	6.35-04	3.16-02	2.59-02	6.42-04	3.16-02	2.56-02
32	7.87-05	7.86-03	6.49-03	8.18-05	7.85-03	6.37-03
64	9.82-06	1.97-03	1.63-03	1.03-05	1.97-03	1.60-03
128	1.23-06	4.77-04	4.08-04	1.30-06	4.77-04	4.03-04

N	RQSC-CN			Two-step		
	$\Vert\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\Vert_{\lambda_i,\infty}$		$\Vert\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\Vert_{\tau_i}$	$\Vert\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\Vert_{\lambda_i,\infty}$		$\Vert\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\Vert_{\tau_i}$
16	3.05	2.08	2.01	2.96	2.07	2.02
32	3.01	2.01	2.00	2.97	2.01	2.00
64	3.00	2.00	2.00	2.99	2.00	2.00
128	3.00	2.04	2.00	2.99	2.04	1.99

Table 5.20: Errors and respective orders of convergence of the RQSC-CN and optimal two-step QSC-CN methods for Problem 8 for u with $\alpha = 7$.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN			Two-step		
8	1.05-04	1.66-04	5.70-04	7.13-05	1.41-04	5.65-04
16	8.13-06	1.24-05	7.05-05	5.98-06	1.14-05	7.01-05
32	6.34-07	9.40-07	8.75-06	5.48-07	9.90-07	8.72-06
64	5.18-08	8.16-08	1.09-06	5.24-08	8.71-08	1.08-06
128	4.45-09	7.16-09	1.37-07	5.02-09	7.69-09	1.36-07

N	$u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN			Two-step		
16	3.69	3.75	3.02	3.57	3.63	3.01
32	3.68	3.72	3.01	3.45	3.53	3.01
64	3.61	3.53	3.01	3.39	3.51	3.01
128	3.54	3.51	3.01	3.38	3.50	3.00

Table 5.21: Errors and respective orders of convergence of the RQSC-CN and optimal two-step QSC-CN methods for Problem 8 for u_x and u_{xx} with $\alpha = 7$.

N	RQSC-CN			Two-step		
	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$
8	2.20-03	4.44-02	3.49-02	2.13-03	4.42-02	3.57-02
16	3.48-04	1.08-02	1.22-02	3.56-04	1.08-02	1.25-02
32	5.85-05	2.71-03	4.31-03	6.18-05	2.70-03	4.41-03
64	1.01-05	6.88-04	1.53-03	1.09-05	6.88-04	1.56-03
128	1.78-06	1.70-04	5.40-04	1.92-06	1.70-04	5.51-04

N	RQSC-CN			Two-step		
	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$
16	2.65	2.04	1.52	2.58	2.04	1.52
32	2.57	2.00	1.50	2.53	2.00	1.50
64	2.53	1.98	1.50	2.51	1.98	1.50
128	2.51	2.01	1.50	2.50	2.01	1.50

Problem 9

From the results of Problem 6, we notice that the errors and orders of convergence of the RQSC-CN1 method are quite similar to those of the RQSC-CN0 method. Therefore, in this test, we only compare the RQSC-CN1 method with the optimal *two-step QSC-CN* method.

We solve Problem 6 again with the same $\sigma = 20$ by the optimal *two-step QSC-CN* method. The infinity norms of the errors and the respective orders of convergence of u, u_x, and u_{xx} for the *two-step* method together with those for the RQSC-CN1 method are shown in Tables 5.22 - 5.23.

From the results, the orders of convergence of these two methods are almost the same and the RQSC-CN1 method is as accurate as the optimal *two-step* QSC-CN method except for the values of u at the midpoints for this problem. Furthermore, the RQSC-CN1 method is as stable as the optimal *two-step QSC-CN* method for this problem.

Table 5.22: Errors and respective orders of convergence of the RQSC-CN1 and optimal two-step QSC-CN methods for Problem 9 for u.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN1			Two-step		
8	8.2-03	9.9-03	1.1-02	3.1-03	3.9-03	5.3-03
16	2.7-04	3.2-04	6.4-04	1.9-04	3.7-05	5.1-04
32	1.2-05	1.7-05	6.1-05	1.2-05	2.8-07	6.1-05
64	7.3-07	9.8-07	7.6-06	7.3-07	2.3-09	7.6-06
128	4.5-08	5.9-08	9.5-07	4.5-08	6.0-10	9.5-07
256	2.8-09	3.6-09	1.2-07	2.8-09	4.7-11	1.2-07

N	$u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN1			Two-step		
16	4.93	4.95	4.09	4.05	6.73	3.38
32	4.52	4.26	3.38	4.01	7.03	3.05
64	4.00	4.10	3.01	4.00	6.91	3.01
128	4.00	4.05	3.00	4.00	1.96	3.00
256	4.00	4.03	3.00	4.00	3.68	3.00

Table 5.23: Errors and respective orders of convergence of the RQSC-CN and optimal two-step QSC-CN methods for Problem 9 for u_x and u_{xx}.

N	RQSC-CN1			Two-step		
	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$
8	1.2-01	3.7-01	1.4-00	6.7-02	3.2-01	1.1-00
16	8.3-03	7.7-02	2.5-01	6.2-03	7.7-02	2.5-01
32	7.6-04	1.9-02	6.3-02	7.6-04	1.9-02	6.3-02
64	9.5-05	4.8-03	1.6-02	9.5-05	4.8-03	1.6-02
128	1.2-05	1.2-03	4.0-03	1.2-05	1.2-03	4.0-03
256	1.5-06	3.0-04	9.9-04	1.5-06	3.0-04	9.9-04

N	RQSC-CN1			Two-step		
	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$
16	3.85	2.28	2.51	3.45	2.04	2.21
32	3.44	2.02	1.97	3.01	2.02	1.97
64	3.00	2.00	1.99	3.00	2.00	1.99
128	3.00	1.97	2.00	3.00	1.97	2.00
256	3.00	2.02	2.00	3.00	2.02	2.00

Problem 10

We consider Problem (1.1)-(1.3), and compare the stability properties of the RQSC-CN0 and the optimal *two-step* QSC-CN methods when the coefficient of u_x is considerably larger than that of u_{xx}. We set $f(x,t) = 0$ and consider several constant values of $p(x,t)$ and $q(x,t)$.

In (1.1), letting

$$p(x,t) = 0.1,\ q(x,t) = 100,\ f(x,t) = 0,\ T = 1,$$

the problem becomes

$$u_t = 0.1u_{xx} + 100u_x + g(x,t),\ 0 < x < 1, 0 < t < 1.$$

The functions γ, g, β_0, and β_1 are chosen such that $u(x,t) = e^{x+t}$ is the true solution. For the time step, we first choose $\sigma = 0.1$. Recalling that $\sigma = p\frac{\Delta t}{h^2}$, we have $\Delta t = h^2$.

The infinity norms of the observed errors for $N = 8$ to 64 points in the partition Δ are shown in Table 5.24. We notice that the optimal *two-step* QSC-CN method gives reasonable results for all N and the respective Δt, while the RQSC-CN0 method gives huge errors for small N ($N < 64$), and, therefore, large Δt. These numerical experiments, indicate that the optimal *two-step* QSC-CN method is stable and convergent even for large Δt, while the RQSC-CN0 method is stable and convergent when Δt is small enough. Furthermore, when Δt is small enough so that the RQSC-CN0 method is stable and convergent, the RQSC-CN0 method is more accurate than the optimal *two-step* QSC-CN method.

Table 5.24: Errors and respective orders of convergence of the RQSC-CN0 and optimal two-step QSC-CN methods for Problem 10.

N	$\|u - u_C\|_{x_i,\tau_i,\infty}$					
	RQSC-CN0			Two-step		
8	9.4+21	4.7+22	4.7+22	7.2-02	6.6-02	7.7-02
16	1.3+44	2.5+44	2.6+44	1.1-04	8.6-04	8.6-04
32	4.7+76	6.8+76	7.1+76	2.3-06	1.6-05	1.6-05
64	4.6-09	1.0-08	2.2-07	8.3-08	2.9-07	3.1-07

N	RQSC-CN0			Two-step		
	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$	$\|\frac{\partial u}{\partial x} - \frac{\partial u_C}{\partial x}\|_{\lambda_i,\infty}$		$\|\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u_C}{\partial x^2}\|_{\tau_i}$
8	8.6+23	1.4+24	2.2+25	1.1-00	1.7-00	2.7+01
16	8.9+45	1.3+46	3.7+47	3.2-02	5.2-02	1.6-00
32	4.8+78	6.9+78	3.7+80	1.1-03	2.0-03	1.2-01
64	1.4-06	1.4-04	2.4-04	4.2-05	1.4-04	8.4-03

We investigated this issue further, and attempted to find numerically the problem parameters and the relations they need to satisfy, in order for the RQSC-CN0 method to be stable and convergent. The parameters we considered are Δt, N, p, q, as well as the length L of the spatial domain, since, though all methods considered are developed for the $[0,1]$ spatial interval, they can be extended to any spatial domain in a straightforward way. Through several experiments, we found that Δt must satisfy the relation

$$\Delta t \leq c\frac{p}{q^2}, \tag{5.3}$$

where c is a constant, with $c \approx 25$. The relation (5.3) seems to be a sufficient condition for the RQSC-CN0 method to be stable and convergent.

To support our argument, we solve Problem 10 for various values of the parameters Δt, N, p, q and L, and present selected results. To find the relation Δt should satisfy, we pick certain values for N, p, q and L, and compute the solution of Problem 10 by the RQSC-CN0 method with several values of Δt, and try to determine the maximum Δt for which the method is stable and convergent. Clearly, we could not test all possible values of Δt, but, for each set of values for N, p, q and L, we started the tests with some value of Δt that gave reasonable results, then increased Δt, up to the point the errors started becoming huge and, therefore, unacceptable. For example, when $\Delta t = 10^{-d}$ gave reasonable results, we increased Δt by increments of $5 \times 10^{-d-1}$, until the results were unacceptable. In Table 5.25, we present the maximum Δt, calculated as described above, and the associated errors.

The first four rows of Table 5.25 have N, q, L fixed and p varying. The next three rows have N, p, L fixed and q varying. The next four rows have p, q, L fixed and N varying. The last three rows have N, p, q fixed and L varying. These experiments indicate that the maximum Δt for which the RQSC-CN0 method is stable and convergent depends approximately linearly to p, inversely to q^2, and does not depend on N and L. Clearly, relation (5.3) seems to hold with remarkable accuracy. We included the value of $25\frac{p}{q^2}$ in the table, to emphasize how well the numerically calculated maximum Δt agrees with

$25\frac{p}{q^2}$. There are a few cases (rows 1, 3 and 7 in Table 5.25) in which we found a Δt slightly larger than $25\frac{p}{q^2}$, that results in a stable and convergent method. In all other cases, we have full agreement between the maximum Δt and $25\frac{p}{q^2}$.

Table 5.25: The maximum Δt which makes the RQSC-CN0 method stable and convergent for Problem 10, for the indicated values of N, p, q and L. The respective errors are also shown.

L	N	p	q	$25\frac{p}{q^2}$	Δt	$\|u - u_C\|_{x_i,\tau_i,\infty}$		
1	16	0.1	100	0.00025	0.0003	3.6-07	1.8-06	1.5-05
1	16	1	100	0.0025	0.0025	3.6-07	6.1-07	1.5-05
1	16	2	100	0.005	0.0055	9.4-07	1.3-06	1.4-05
1	16	4	100	0.01	0.01	9.4-06	8.4-06	1.5-05
1	16	1	50	0.01	0.01	3.1-06	3.3-06	1.4-05
1	16	1	100	0.0025	0.0025	3.6-07	6.1-07	1.5-05
1	16	1	200	0.000625	0.000675	3.6-07	7.9-07	1.5-05
1	4	1	100	0.0025	0.0025	2.6-02	3.0-02	3.0-02
1	8	1	100	0.0025	0.0025	5.5-06	1.5-05	1.2-04
1	16	1	100	0.0025	0.0025	3.6-07	6.1-07	1.5-05
1	32	1	100	0.0025	0.0025	1.7-07	1.9-07	1.8-06
1	16	1	50	0.01	0.01	3.1-06	3.3-06	1.4-05
2	16	1	50	0.01	0.01	3.3-05	4.4-05	3.2-04
4	16	1	50	0.01	0.01	2.2-03	5.6-03	2.0-02

Chapter 6

Conclusions

An efficient algorithm based on the quadratic-spline collocation and Crank-Nicolson methods for linear parabolic PDEs is introduced and studied in this thesis. The RQSC-CN method is derived from the optimal *one-step* and *two-step* QSC-CN methods. Both the optimal *one-step* and *two-step* methods have advantages and disadvantages. More precisely, the *two-step* method solves a simple system (tridiagonal) at each time step, but solves it twice; the *one-step* method solves a system once at each time step, but the matrix has more non-zero entries than that in the *two-step* method. This motivates us to develop the RQSC-CN method which solves the same simple system as in the *two-step* method only once for each time step.

Stability and convergence are studied for Problem (4.1)-(4.4). To our delight, numerical results indicate that the RQSC-CN method works well not only for Problem (4.1)-(4.4), but also for some instances of the more general Problem (1.1)-(1.3) (the RQSC-CN method is unstable for some particular instances even when σ is small). We can also obtain the same orders of convergence and superconvergence for derivatives at certain points as those obtained by the optimal *two-step* method. As far as sensitivity to discontinuity of the solution is concerned, the RQSC-CN method behaves in a similar way as the optimal *two-step* QSC-CN method. Furthermore, the RQSC-CN method is as accurate as the optimal *two-step* QSC-CN method.

The RQSC-CN method requires less computational work than either the optimal *one-step* or *two-step* QSC-CN methods while it preserves the accuracy and optimal orders of convergence. But it is not unconditionally stable even for a simple problem like Problem (4.1)-(4.4). Some modifications are applied to the RQSC-CN method to make it stable. As a result, we develop the RQSC-CN1 and RQSC-CN0 methods which, as shown by numerical results, we conjecture to be unconditionally stable while maintaining the orders of convergence for Problem (4.1)-(4.4).

For a problem as general as Problem (1.1)-(1.3), stability is much more complicated to analyze. It seems that in this case the stability depends not only on the matrices but also on the coefficients of u, u_x, u_{xx}. For further research, the properties of the stability and convergence of the RQSC-CN, RQSC-CN1, and RQSC-CN0 methods for the general Problem (1.1)-(1.3) may be studied.

Although we have not derived any method based on higher degree splines, the techniques (semi-implicit method) introduced in Section 3.3 may be applied to the *cubic spline collocation* method since, when using the cubic spline collocation method, we also have a perturbation term $\mathcal{P}_{\mathcal{L}}$ which may be discretized by a first order explicit method with respect to t.

The parabolic PDE considered in this thesis is one-dimensional in space. The methods developed though can be extended to parabolic PDEs in two or more space dimensions in a natural way, using tensor products. We believe that the benefits in efficiency from the RQSC-CN method will be more substantial when the method is extended to multiple space dimensions.

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