

**ANALYTICAL UPSTREAM COLLOCATION SOLUTION
OF A QUADRATIC FORCED STEADY-STATE
CONVECTION-DIFFUSION EQUATION**

by

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The thesis presented by *Eric Paul Smith* entitled *Analytical Upstream Collocation Solution of a Quadratic Forced Steady-State Convection-Diffusion Equation* is hereby approved.

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ABSTRACT

In this thesis we present the exact solution to the Hermite collocation discretization of a quadratically forced steady-state convection-diffusion equation in one spatial dimension with constant coefficients, defined on a uniform mesh, with Dirichlet boundary conditions. To improve the accuracy of the method we use “upstream weighting” of the convective term in an optimal way. We also provide a method to determine where the forcing function should be optimally sampled. Computational examples are given, which support and illustrate the theory of the optimal sampling of the convective and forcing term.

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CHAPTER 1

INTRODUCTION

For many differential equations (DEs), often a numerical solution is sufficient or more practical to use than an exact (or continuous) solution. This is due to the difficulty or impossibility in finding an analytical solution for certain types of DEs. Unfortunately finding a numerical solution of a DE can be a difficult task. DEs where this is the case are models involving a combination of convection and diffusion processes. Some examples of such problems are modeling pollutant dispersal in a river estuary, atmospheric pollution, semi-conductor equations, viscous compressible flow past an aerofoil, financial value of share options and groundwater transport [5]. For these problems the convection-diffusion process makes up the whole problem, or is embedded in a larger problem [5]. The dimensionless parameter known as the Péclet number, which measure the relative dominance of convection to diffusion, can vary greatly in these problems. Finding an accurate numerical solution of convection-diffusion DEs at large Péclet is a difficult task. This is because many numerical techniques for this type of DE often give rise to oscillations that are not present in the exact solution. In order to ameliorate these undesirable oscillations, the technique

of upstream weighting is often used [1],[3],[4],[6],[7]. Unfortunately the technique also gives rise to “smearing” of the sharp solution profile of the exact solution of the DE.

In this thesis we will study the steady-state convection-diffusion equation

$$-D\frac{d^2u}{dx^2} + v\frac{du}{dx} = S(x) \quad (1.1)$$

with Dirichlet boundary condition, defined on the interval $[0, 1]$. Here D is the diffusion coefficient and v is the convection coefficient. Both are positive constants. Also, $S(x)$ is a forcing function. We choose this as our model because for a polynomial forcing term, we can compare the numerical solution of (1.1) with the exact solution. The difficulties in using a numerical method to solve (1.1) are also present in, and apply to, more complicated systems where we no longer have the advantage of knowing an exact solution. We will show how using the method of collocation with upstreaming, it is possible to select an upstream parameter such that oscillations can be eliminated and the smearing of the sharp solution profile of the continuous solution can be minimized. This will be done by first presenting previous work found in [1], [2], [3], [4], and [8] which reviews the method of collocation and the method of collocation with upstreaming. Then we will present Brill’s previous work in [3] and [4] which cover how to select an optimal parameter for the case when $S(x)$ is zero and linear. Finally we will present original work which gives the method of finding the optimal upstream parameter for when $S(x)$ is quadratic. This will be followed by numerical examples which illustrate the theory.

CHAPTER 2

NUMERICAL SOLUTION OF CONVECTION-DIFFUSION DIFFUSION DIFFERENTIAL EQUATION

2.1 Hermite Collocation

A discussion on the method of collocation can be found in [1], [2], [5], [6], [7] and [8]. It will be presented and summarized here for convenience. We begin the process of Hermite collocation by first taking our differential equation (1.1), with forcing term $S(x)$ on the interval $[0, 1]$. We then subdivide our interval into m subintervals and introduce Hermite basis functions defined for $\eta \in [-\frac{1}{2}, \frac{1}{2}]$:

$$f_j(x) = \begin{cases} \frac{1}{2}(1 + 2\eta)^2(1 - \eta) & x_{j-1} \leq x = x_j + (\eta - \frac{1}{2})h \leq x_j \\ \frac{1}{2}(1 - 2\eta)^2(1 + \eta) & x_j \leq x = x_j + (\eta + \frac{1}{2})h \leq x_{j+1} \\ 0 & \text{otherwise} \end{cases} \quad (2.1)$$

and

$$g_j(x) = \begin{cases} \frac{h}{8}(2\eta + 1)^2(2\eta - 1) & x_{j-1} \leq x = x_j + (\eta - \frac{1}{2})h \leq x_j \\ \frac{h}{8}(2\eta - 1)^2(2\eta + 1) & x_j \leq x = x_j + (\eta + \frac{1}{2})h \leq x_{j+1} \\ 0 & \text{otherwise} \end{cases} \quad (2.2)$$

where $h = \frac{1}{M}$. Note that $f_j(x_i)$ is defined such that it is equal to one for $i = j$, and zero otherwise. Similarly the derivative of $g_j(x_i)$ is equal to one for $i = j$, and zero otherwise as illustrated in Figure 2.1. Also $f'_i(x_j) = 0$ and $g_i(x_j) = 0$. Using these

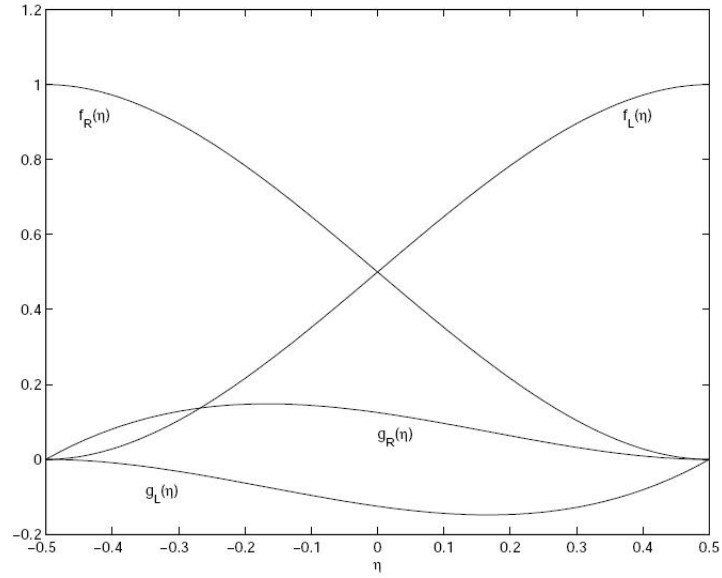


Figure 2.1: Basis functions f and g

basis functions we can form a piecewise cubic Hermite interpolating polynomial as follows:

$$\hat{u}(x) = \sum_{j=0}^m [u_j f_j(x) + u'_j g_j(x)]. \quad (2.3)$$

Putting this into (1.1) we obtain

$$-D \frac{d^2 \hat{u}}{dx^2} + v \frac{d \hat{u}}{dx} - S(x) = E(x) \quad (2.4)$$

where $E(x)$ is the residual.

Now to solve (2.4) we must first recognize that this equation has $2(m+1)$ coefficients, specifically u_j and u'_j for $j = 0, 1, \dots, m$. We can impose the condition that the residual $E(x)$ must be zero at two distinct collocation points in the interior of each of the m intervals. Given certain smoothness conditions, the location of the collocation points that will minimize local truncation error correspond to the points of Gaussian quadrature [8]. This corresponds to choosing the collocation points at $\eta = \pm \frac{1}{\sqrt{12}}$ in (2.1) and (2.2) for each subinterval $[-\frac{1}{2}, \frac{1}{2}]$. As shown in [8] and discussed in [4] this provides $O(h^4)$ local discretization error, and is often called ‘‘orthogonal’’ collocation.

Choosing the collocation points in this manner leads to a matrix equation with the repeated computational molecule

$$\begin{bmatrix} \frac{2\sqrt{3}D}{h^2} - \frac{v}{h} & \frac{(1+\sqrt{3})D}{h} + \frac{v}{2\sqrt{3}} & \frac{-2\sqrt{3}D}{h^2} + \frac{v}{h} & \frac{(-1+\sqrt{3})D}{h} - \frac{v}{2\sqrt{3}} \\ \frac{-2\sqrt{3}D}{h^2} - \frac{v}{h} & \frac{(1-\sqrt{3})D}{h} - \frac{v}{2\sqrt{3}} & \frac{2\sqrt{3}D}{h^2} + \frac{v}{h} & \frac{(-1-\sqrt{3})D}{h} + \frac{v}{2\sqrt{3}} \end{bmatrix} \begin{bmatrix} q_j \\ r_j \\ q_{j+1} \\ r_{j+1} \end{bmatrix} = \begin{bmatrix} S_{2j} \\ S_{2j+1} \end{bmatrix} \quad (2.5)$$

for $j = 0, 1, 2, \dots, m-1$. Here $q_j = u_j$ and $r_j = u'_j$, $j = 0, 1, 2, \dots, m$, and $S_k =$

$S(x_k)$. Note that this is a system of $2m$ equations in $2m + 2$ unknowns. If we have information about the boundary conditions, this will reduce the problem to a system of $2m$ equations in $2m$ unknowns. If we assume Dirichlet boundary conditions we have that the general solution of (2.5)[4] is:

$$q_j = c_1 + c_2\lambda^j + \frac{1}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k, \quad (2.6)$$

$$r_j = \rho c_2 \lambda^j + \frac{1}{2m} \sum_{k=0}^{2m-1} G'_{k,j} S_k, \quad (2.7)$$

where c_1 and c_2 are constants determined by the boundary conditions,

$$\lambda = \frac{\beta^2 + 6\beta + 12 + 6\beta\zeta(4 + \beta + \beta\zeta)}{\beta^2 - 6\beta + 12 + 6\beta\zeta(4 - \beta + \beta\zeta)}, \quad (2.8)$$

$$\rho = \frac{2\beta m(1 + \beta\zeta)}{\beta^2\zeta^2 + 4\beta\zeta + 2}, \quad (2.9)$$

where

$$\beta = \frac{hv}{D} = \frac{v}{mD} \quad (2.10)$$

is the Péclet number and S_k are the same as the right hand side of (2.5). The constants c_1 and c_2 are given by

$$c_2 = \frac{u(1) - u(0)}{\lambda^m - 1} \quad (2.11)$$

$$c_1 = u(0) - c_2.$$

The discrete Green's functions $G_{k,j}$ and $G'_{k,j}$ are

$$G_{k,j} = \begin{cases} A_k(\lambda^m - \lambda^j), & k = 0, 1, \dots, 2j - 1 \\ (C_k - A_k\lambda^m)(\lambda^j - 1), & k = 2j, 2j + 1, \dots, 2m - 1 \end{cases} \quad (2.12)$$

$$G'_{k,j} = \begin{cases} -\rho A_k \lambda^j, & k = 0, 1, \dots, 2j - 1 \\ \rho(C_k - A_k\lambda^m)\lambda^j, & k = 2j, 2j + 1, \dots, 2m - 1 \end{cases} \quad (2.13)$$

where

$$A_{2\ell} = \frac{(1 + \beta\zeta - \sqrt{3}\beta\zeta^2)\lambda_{\text{num}}\lambda^\ell + \rho_{\text{den}}(-6 - \sqrt{3}\beta - 6\beta\zeta + 6\sqrt{3}\beta\zeta^2)}{v(1 + \beta\zeta)\lambda_{\text{num}}\lambda^\ell(\lambda^m - 1)} \quad (2.14)$$

$$A_{2\ell+1} = \frac{(1 + \beta\zeta + \sqrt{3}\beta\zeta^2)\lambda_{\text{num}}\lambda^\ell + \rho_{\text{den}}(-6 + \sqrt{3}\beta - 6\beta\zeta - 6\sqrt{3}\beta\zeta^2)}{v(1 + \beta\zeta)\lambda_{\text{num}}\lambda^\ell(\lambda^m - 1)} \quad (2.15)$$

and

$$C_k = \begin{cases} \frac{1 + \beta\zeta - \sqrt{3}\beta\zeta^2}{v(1 + \beta\zeta)}, & k \text{ even} \\ \frac{1 + \beta\zeta + \sqrt{3}\beta\zeta^2}{v(1 + \beta\zeta)}, & k \text{ odd} \end{cases} \quad (2.16)$$

The symbols λ_{num} and ρ_{den} refer respectively to the numerator of (2.8) and denominator of (2.9).

2.2 Oscillations

By choosing to evaluate (2.4) at the collocation points $\eta = \pm \frac{1}{\sqrt{12}}$, we were motivated by [8] which gives that these points minimize the difference between the numerical and analytical solutions. However in [8], Prenter gives certain smoothness conditions that must be met in order for this particular choice to be optimal in the sense that we minimize the error between the numerical and continuous solution and have the upstreaming parameter within its interval of existence. If the Péclet number $\beta = \frac{hv}{D} > 2\sqrt{3}$, these smoothness conditions are violated. The result of this causes our numerical solution to be far less than optimal. If however we try and use a different method in hopes of obtaining a better numerical solution, such as finite central differences, we run into an even larger problem. For cases when $\beta > 2$ the method of central difference oscillates around the true solution [5]. This can be seen in Figure 2.2 which compares the exact solution to the central difference solution as in [3]. Here we use $\beta = 5$, $m = 10$, and $S(x) = 0$.

These oscillations are potentially unmeaningful in the context of a physical solution of 1.1 since we might be modeling a quantity such as chemical concentration of a solute for which the values can only be between 0 and 1. Thus, we stay with the method of Hermite collocation and focus on the importance of optimizing it. In [3] Brill studies the topic in detail and shows that $\eta = \pm \frac{1}{\sqrt{12}}$ is optimal for only a small range of values for β . When β falls out of this range our numerical method may no longer capture sharp solution curves present in the analytical solution. Since

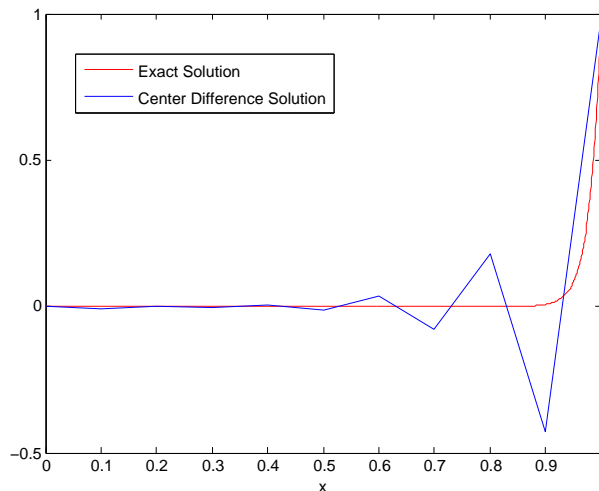


Figure 2.2: Oscillations present using central difference for $\beta > 2$

oscillations are unphysical, it is desirable to find a way to avoid oscillations, and yet still maintain a close correspondence to the continuous solution of the equation. This is discussed next.

2.3 Hermite Collocation with Upstreaming

Upstreaming was developed to alleviate the problem of oscillations in numerically approximating (1.1) [1]. The method of upstreaming is done by evaluating $\frac{d^2 \hat{u}}{dx^2}$ at the Gauss points, and evaluating $\frac{d \hat{u}}{dx}$ at the points $\eta = \pm \frac{1}{\sqrt{12}} - \zeta$. Here the ζ is considered the upstreaming parameter. The motivation for using upstreaming comes from the fact that information at the nodes depends more on information gathered upstream, than downstream, due to, for example, the velocity of the water in the model. Now because the support of each basis function f_j and g_j is in the interval $[-\frac{1}{2}, \frac{1}{2}]$, we

must, for upstreaming, have ζ lie in the interval $[0, \frac{1}{2} - \frac{1}{\sqrt{2}}]$. (Evaluating $\frac{d\hat{u}}{dx^2}$ in (2.4) at places where $\zeta < 0$ is considered downstreaming.) By using upstreaming we now have $O(h^2)$ local discretization error [1] rather than $O(h^4)$. Also if we do not choose the upstreaming parameter carefully we have the potential to cause another problem in our discrete solution in smearing. For example suppose we naively choose $\zeta = 0.2$ as our parameter. Although the discrete solution no longer exhibits oscillations, it can now appear smeared when compared to the continuous solution, see Figure 2.3. In this figure we use $\beta = 10$, $\zeta = 0.2$, and $S(x) = 0$. The problem of smearing is especially apparent for large β , see Figure 2.4. This figure presents the numerical solution using upstreaming with $\zeta = 0.2$ where $\beta = 10, 20, 30, 40, 50$.

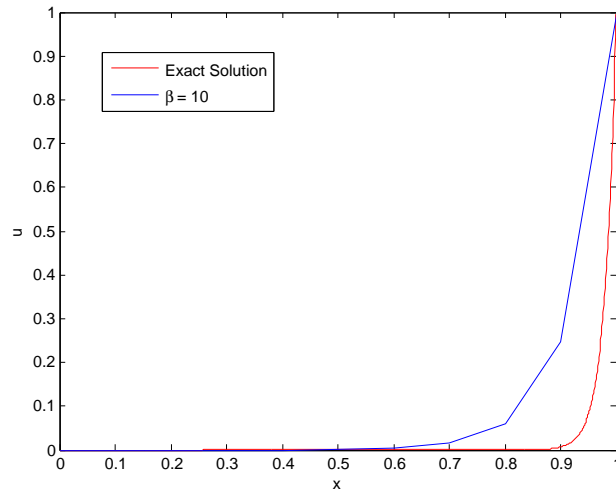


Figure 2.3: Smearing of solution using upstreaming with $\zeta = 0.2$, $\beta = 10$, and $S(x) = 0$

An important question to ask is, can an upstreaming parameter ζ be chosen that eliminates unwanted oscillations and gives a close correspondence with the continuous

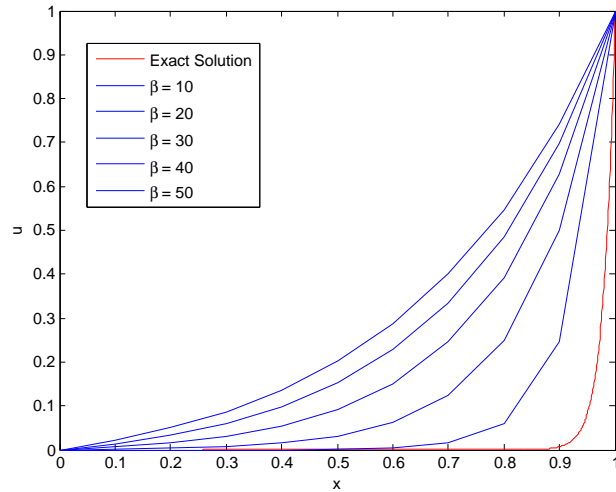


Figure 2.4: Smearing of solution using upstreaming with $\zeta = 0.2$, $\beta = 10, 20, 30, 40, 50$, and $S(x) = 0$

solution? In other words can we find the optimal ζ such that the difference between the discrete solutions, and continuous solution is minimized. Fortunately for some cases such a ζ does exist, as we will see in the next section.

CHAPTER 3

PREVIOUS WORK ON NUMERICAL SOLUTIONS

As shown in the previous chapter, Hermite collocation can be used to provide a numerical solution of (1.1). We have also shown how, without the method of upstreaming, unwanted oscillations can occur in our numerical solution. Care must be taken then in order to choose an upstreaming parameter that eliminates oscillations, but does not cause too much smearing of the numerical solution. In order to find out exactly how this parameter must be optimally chosen we will turn to previous work done for choosing the optimal upstreaming parameter for (1.1) when $S(x) = 0$ and when $S(x)$ is linear.

In [3], Brill focused on finding the optimal ζ for this homogeneous case. In his work it was found that ζ could be chosen optimally as a function of β via Table 3.1.

Similarly in [4], Brill focused on finding the optimal upstreaming parameter for when $S(x)$ was linear:

$$S(x) = \alpha_1 + \alpha_2 x \tag{3.1}$$

Table 3.1: Optimal ζ as a function of β

β interval	approx β interval	optimal ζ
$(0, 2\sqrt{3}]$	$(0, 3.46410]$	0
$[2\sqrt{3}, \sqrt{3} + 2^{-1/2} (3^{3/4} + 3^{5/4})]$	$[3.46410, 6.13572]$	$\frac{\sqrt{6\beta^2 - 36} - 6}{6\beta}$
$[\sqrt{3} + 2^{-1/2} (3^{3/4} + 3^{5/4}), 6 + 4\sqrt{3}]$	$[6.13572, 12.9282]$	$\frac{1}{2} - \frac{1}{\sqrt{12}}$
$[6 + 4\sqrt{3}, \infty]$	$[12.9282, \infty)$	$\frac{1}{2} - \frac{2}{\beta} - \frac{\sqrt{\beta^2 - 12\beta + 24}}{\sqrt{12}\beta} - \epsilon$

in (1.1). For this case it was assumed that ζ was already chosen optimally to evaluate $\frac{d\hat{u}}{dx}$. The method of upstreaming was also performed on the linear forcing term, using the upstreaming parameter ψ . In his work it was found that ψ was optimal when $\psi = -\zeta$. This gave way to easily finding the optimal ψ by again referencing Table 3.1 with ζ replaced by $-\psi$. From this we can see that an optimal upstreaming parameter may be possible for a more complicated forcing term. The next logical step is to explore the optimal parameter for when the forcing term is quadratic. This brings us to the main focus of this thesis.

CHAPTER 4

NUMERICAL SOLUTION, QUADRATIC FORCING

As discussed in the previous chapter Brill [3] [4] showed it is possible to optimally choose an upstreaming parameter when our forcing term is either zero or linear. This brings us to the question, “Can we optimally sample the forcing term in the quadratic case?” This is important because we want our forcing term to handle a variety of situations. One example which uses a quadratic forcing will be explained in detail in Chapter 5.2, and models the increase and decrease of a chemical solution in water. A situation such as this can not be modeled as accurately using only linear forcing terms. Fortunately, we can optimally sample a quadratic forcing term as the following original work will show. We begin in much the same way as the previous cases presented in [3] [4]. As we will see, however, the quadratic case gives rise not to a constant parameter, but a function for how to choose the optimal upstreaming parameter given certain conditions. As before we want to find the optimal locations

at which to evaluate the forcing function $S(x)$. To do this we will assume that

$$S(x) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 \quad (4.1)$$

We will also assume that the upstreaming parameter ζ for $\frac{d\hat{u}}{dx}$, and ψ for the $\alpha_1 + \alpha_2 x$ term, have already been chosen optimally. We will then evaluate the $\alpha_3 x^2$ term at the points

$$\left(\frac{2p+1}{2} + \kappa \pm \frac{1}{\sqrt{12}} \right) h, \quad (4.2)$$

where $p = 0, 1, \dots, m-1$. If $\kappa = 0$ then, as before, we are evaluating at the Gauss points. Since the support of the basis functions f_j or g_j is in the interval $[-\frac{1}{2}, \frac{1}{2}]$, we must have that κ must lie in $[\frac{1}{\sqrt{12}} - \frac{1}{2}, \frac{1}{2} - \frac{1}{\sqrt{12}}]$ or else we will end up sampling in a different interval. Given $S(x)$ as in (4.1), the exact solution of (1.1) with Dirichlet boundary conditions, evaluated at x_j for $j = 0, 1, 2, \dots, m$ is

$$u(x_j) = \gamma_0 + \gamma_1 \alpha_1 + \gamma_2 \alpha_2 + \gamma_3 \alpha_3 \quad (4.3)$$

where β is defined from (2.10), and

$$\begin{aligned}
\gamma_3 &= \frac{1}{3(\beta m)^2 v} \left[E(j) \frac{j}{m} - E(m) \frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right] \\
\gamma_2 &= \frac{1}{2\beta m v} \left[F(j) \frac{j}{m} - F(m) \frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right] \\
\gamma_1 &= \frac{1}{v} \left[\frac{j}{m} - \frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right] \\
\gamma_0 &= u(0) + [u(1) - u(0)] \frac{e^{\beta j} - 1}{e^{\beta m} - 1}
\end{aligned} \tag{4.4}$$

with (using dummy variable z)

$$\begin{aligned}
E(z) &= \beta^2 z^2 + 3\beta z + 6, \\
F(z) &= \beta z + 2.
\end{aligned} \tag{4.5}$$

Now the upstream collocation solution of the same problem is

$$q_j = \delta_0 + \delta_1 \alpha_1 + \delta_2 \alpha_2 + \delta_3 \alpha_3, \tag{4.6}$$

where

$$\begin{aligned}
\delta_3 &= \frac{1}{3(\beta m)^2 v} \left[\hat{E}(j) \frac{j}{m} - \hat{E}(m) \frac{\lambda^j - 1}{\lambda^m - 1} \right], \\
\delta_2 &= \frac{1}{2\beta m v} \left[\hat{F}(j) \frac{j}{m} - \hat{F}(m) \frac{\lambda^j - 1}{\lambda^m - 1} \right], \\
\delta_1 &= \frac{1}{v} \left[\frac{j}{m} - \frac{\lambda^j - 1}{\lambda^m - 1} \right], \\
\delta_0 &= u(0) + [u(1) - u(0)] \frac{\lambda^j - 1}{\lambda^m - 1},
\end{aligned} \tag{4.7}$$

with (again using dummy variable z)

$$\hat{E}(z) = \beta^2 (z^2 + 3\zeta^2 + 3z\zeta + 3z\kappa + 6\kappa\zeta + 3\kappa^2) + \beta (3z + 6\kappa + 12\zeta) + 6, \quad (4.8)$$

$$\hat{F}(z) = \beta z + 2(\beta\psi + \beta\zeta + 1).$$

The proof of arriving at (4.4) and (4.7) may be found in the Appendix. Now since ψ and ζ are both chosen optimally via Table 3.1 we need only focus on minimizing the difference between γ_3 and δ_3 . We ignore the difference between $\frac{e^{\beta j} - 1}{e^{\beta m} - 1}$ and $\frac{\lambda^j - 1}{\lambda^m - 1}$, and instead focus on $E(z)$ and $\hat{E}(z)$. Setting the difference of these two equal to zero we may obtain κ as a quadratic function in the variable z . The solutions of this equation are

$$K_1 = -\frac{2 + \beta z + 2\beta\zeta - \sqrt{4 + 4\beta z - 8\beta\zeta + (\beta z)^2}}{2\beta}, \quad (4.9)$$

$$K_2 = -\frac{2 + \beta z + 2\beta\zeta + \sqrt{4 + 4\beta z - 8\beta\zeta + (\beta z)^2}}{2\beta}. \quad (4.10)$$

This gives us two possible places that we might optimally choose κ . Exploring K_2 reveals that it is rarely inside the interval of existence for κ . The only time that K_2 is inside the interval of existence for κ is when $\zeta = 0$. This corresponds to having β in the interval $(0, 2\sqrt{3}]$ (see Table 3.1). For these values of ζ and β we have that K_1 is also equal to 0. Looking at other intervals for β shows that K_2 is not in the interval of existence, and in fact gets farther away from the interval of existence for larger values of z . (see Figure 4.1). In this figure we will look at the value of K_2

for $3 < \beta < 6$. The required interval of existence is represented by the area between the top two red lines. The other curves are the values of K_2 where $z = 1, 2, 3, 4, 5$. When $z = 1$ we can clearly see that the value of K_2 is not in the interval of existence. For greater values of z , we can see that the values of K_2 get farther away from the interval of existence. Since z will need to take on the values of j , which correspond to the intervals we are choosing our collocation points, it is necessary that our solution is able to stay within the interval of existence for large values of z . Since K_2 does not follow this criterion it will not be considered. Instead we will explore the behavior of K_1 . We do this by first noting that K_1 is a function of β , z , and ζ . If we vary the

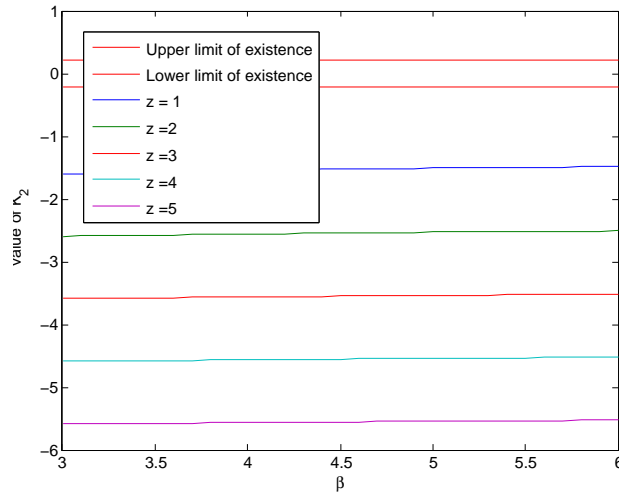


Figure 4.1: Value of K_2 for β in $[3.46410, 6.13572]$

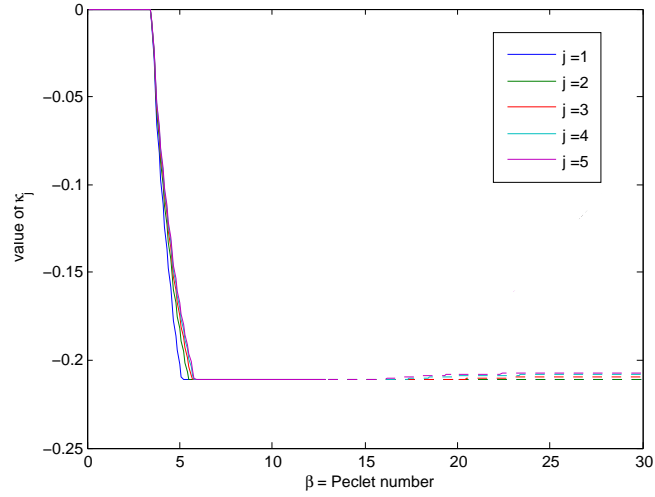
value of K_1 for several values of β , z and ζ , we can see that K_1 takes on very similar behavior to $-\zeta$. Exploring this further we take the limit and see that as (βz) goes to

infinity we have that K_1 goes to $-\zeta$:

$$\lim_{\beta z \rightarrow \infty} K_1 = -\zeta = \psi \quad (4.11)$$

Since we can calculate β in our differential and discrete equation we can calculate β , we can find the value of ζ . K_1 would then only have the unknown variable of z . Since z is just a “dummy” variable, and actually is j or m from (4.4) and (4.7), it will vary depending on what subinterval we are in. Recall that m represent the number of intervals we would like to subdivide our discrete solution into and j represents which subinterval we are considering. When calculating the value of K_1 , m is fixed but j will vary depending on what subinterval is being considered. The optimal place to sample our quadratic term will then be different for every interval. For this reason we can say that the optimal κ depends on j . Hence we will use κ_j to represent the optimal sampling parameter for the quadratic term. In other, words given β and a subinterval j we can choose $\kappa_j = K_1(j)$; (see Figure 4.2 for an illustration) Table 4.1 gives a summary of these results.

From this table we can choose an optimal κ depending on our interval. From (4.11) we can also say that if we have a large β or we are in a subinterval with large index j , then we can sample the terms of our forcing function $S(x)$ at approximately $-\zeta$.

Figure 4.2: Value of κ_j for $j = 1, 2, \dots, 5$ Table 4.1: Optimal κ_j as a function of β and ζ

approx β interval	optimal κ_j
$(0, 3.46410]$	0
$[3.46410, 6.13572]$	$-\frac{2+\beta j+2\beta\zeta-\sqrt{4+4\beta j-8\beta\zeta+(\beta j)^2}}{2\beta}$
$[6.13572, 12.9282]$	$-\frac{1}{2} + \frac{1}{\sqrt{12}}$
$[12.9282, \infty)$	$-\frac{2+\beta j+2\beta\zeta-\sqrt{4+4\beta j-8\beta\zeta+(\beta j)^2}}{2\beta}$

CHAPTER 5

NUMERICAL EXPERIMENTS

In this section we give results of numerical experiments that illustrate the theory presented above. We do this by first choosing two problems from which we can see the advantages and limitations of the method. The rest of the data presented from these problems will be found in the appendix. Later in this chapter we present a more physical problem using the groundwater transport model and show how the method can be used to find an approximate solution. This is an excellent model to use Hermite collocation on since on a large scale one of the dominant transport mechanisms is convection [11].

5.1 Example Problems

For our first two problems we will solve (1.1) where

$$S(x) = 3 - 2x + 3x^2 \tag{5.1}$$

and

$$S(x) = -10 + 200x - 400x^2 \quad (5.2)$$

The boundary conditions will be

$$u(0) = 1 \quad (5.3)$$

$$u(1) = 0$$

We will call these problems A and B respectively and will fix the number of subintervals to $m = 10$, as well as the convection coefficient $v = 10$. We will vary the value of the diffusion coefficient $D = 1.0, 0.25, 0.1, 0.05, 0.02$, which will in turn produce $\beta = 1, 4, 10, 20, 50$. For a given value of β , we will use the optimal value of ζ as determined from Table 3.1. We will also evaluate the linear term of $S(x)$ at optimal ψ . To illustrate the optimal choice of κ , we will sample the quadratic term of $S(x)$ at $\kappa + a$. Here we will choose κ via Table 4.1 and let $a = [-0.20, -0.18, \dots, 0.18, 0.20]$. We will only look at values of a , where $\kappa + a \in [-\frac{1}{2} + \frac{1}{\sqrt{12}}, \frac{1}{2} - \frac{1}{\sqrt{12}}]$.

In this first Figure 5.1 we see that optimal choice of all the upstreaming parameters, shown by the blue boxes, provides a very close correspondence to the exact solution in red. As demonstrated by the green crosses and plus signs, other choices for sampling the quadratic term seem to do equally as well. Although some smearing seems to be present at the later points, any choice for the quadratic upstreaming parameter seems to do sufficiently well.

The next Figure 5.3 uses the same parameters as before, with the exception of

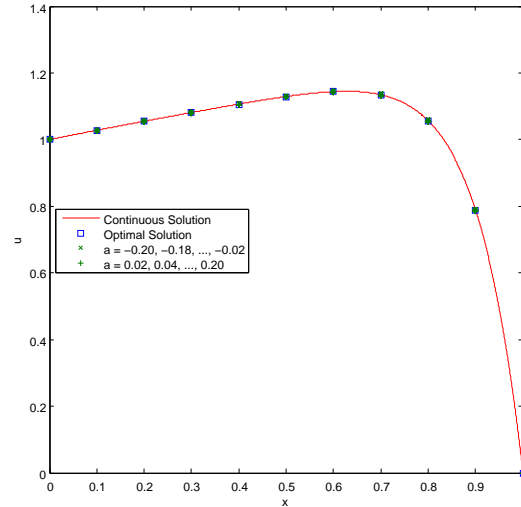


Figure 5.1: $\beta = 1$, Problem A

D which is now 0.25 to produce $\beta = 4$. Although the value of β has increased we still see little difference between optimal sampling of the quadratic term and other possible sampling. The second to last point, however, shows that no matter what is used to sample the quadratic term, that it can not quite capture the profile of the exact solution. It might seem reasonable then that we simply increase the step size in order to gain more accuracy. We must remember however that β is also affected by the interval size so that by increasing the number of intervals, we lower the value of β . If β is lowered enough, then the method of upstreaming is not even useful. Figure 5.2 shows how when we increase the number of points m we reduce the error.

Figure 5.4 begins to show a hint of a smearing problem as the value of x increases. The green crosses and plus signs no longer follow as closely to the exact solution. Optimal sampling of the quadratic term, however, remains its close correspondence to

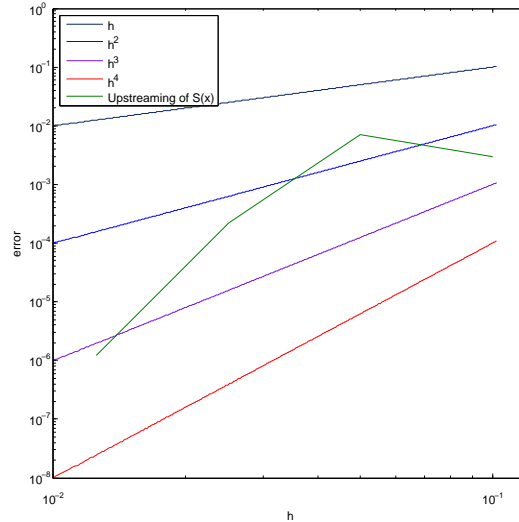


Figure 5.2: Error When Upstreaming $S(x)$

the exact solution. Despite some smearing occurring, it is still unclear the magnitude this problem can present. To get a better idea of this we turn to problem B.

In Figure 5.5 we can see lots of smearing when we do not choose optimal sampling of the quadratic term, even though $\beta = 1$. This comes partly from the larger coefficients of problem B, which exaggerate the smearing present. As expected optimal sampling of the quadratic term maintains a close correspondence with the exact solution.

As we again increase β to 4, Figure 5.6 shows lots of smearing when we do not sample optimally. An interesting feature here occurs at the second to last point. Here we can see that optimal sampling did not fall on the exact solution. In this case it seems that our choice of where to sample the quadratic term was not optimal. If we were to choose $\kappa + 0.06$ however, which corresponds to the green plus sign that did

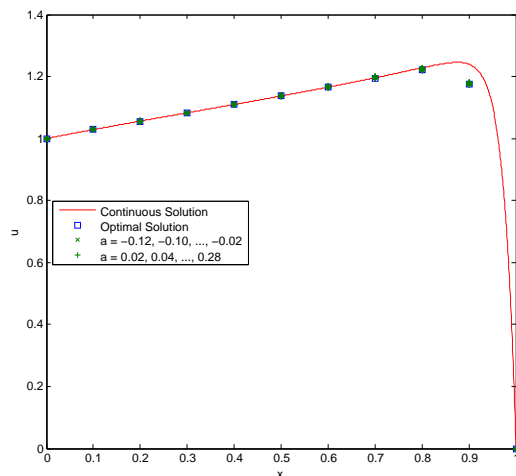
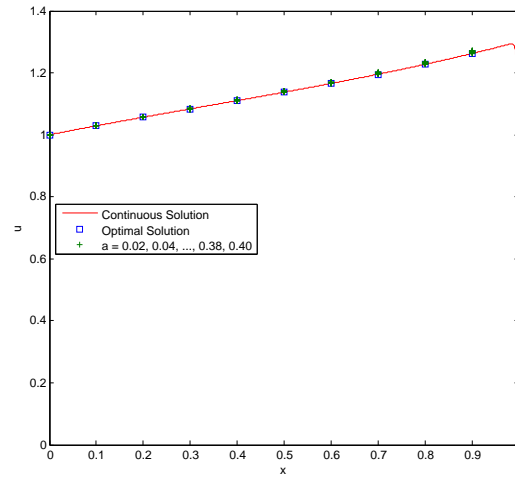
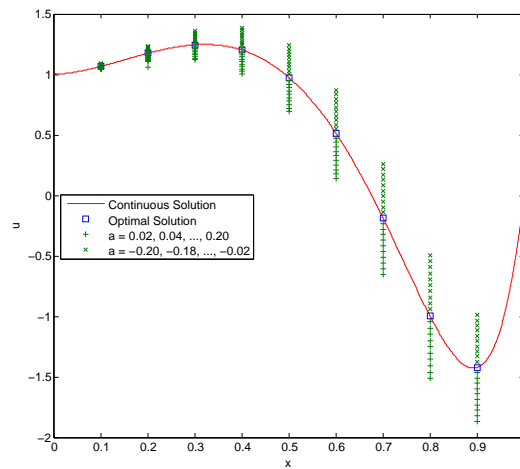
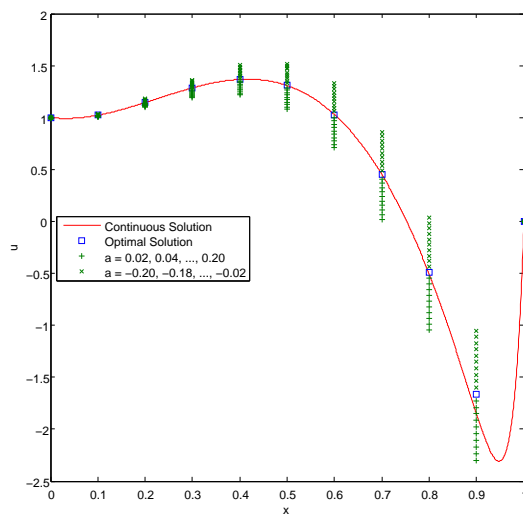
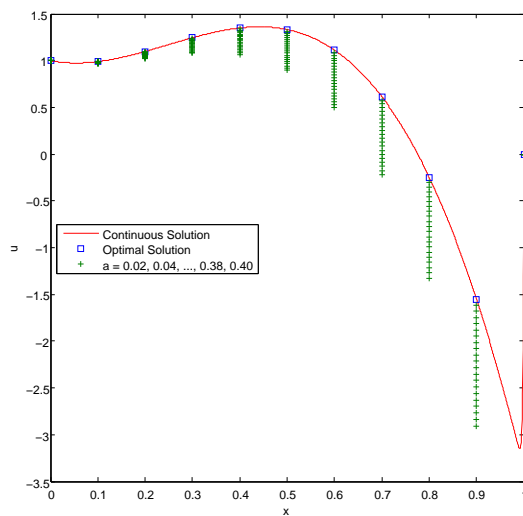


Figure 5.3: $\beta = 4$, Problem A

match the closest to the exact solution at $x = 0.9$, we would have not had such a close correspondence between our numerical and exact solution for $x = 0.2, 0.3, \dots, 0.8$. This shows that choosing κ according to Table 4.1 remains the best choice.

Lastly we will look at Figure 5.7 to emphasize how much smearing can occur. Although smearing of the exact solution when we do not optimally sample is obvious, it is interesting to note that the difference between optimal sampling of the quadratic term and any other possible choice is very small. The last row of green plus signs represents a difference of only 0.4 from the optimal choice of κ , yet it results in the numerical solution to be off from the exact solution by as much as 1.5, as seen at $x = 0.9$.

Figure 5.4: $\beta = 50$, Problem AFigure 5.5: $\beta = 1$, Problem B

Figure 5.6: $\beta = 4$, Problem BFigure 5.7: $\beta = 50$, Problem B

5.2 Groundwater Transport Model

With so much attention paid to the method of Hermite collocation we must keep in mind that (1.1) is a model of a physical system. One such example we can look at is for modeling the spread of pollution in an underground aquifer in one spatial dimension. For this problem D will represent how well the pollutant is able to diffuse through

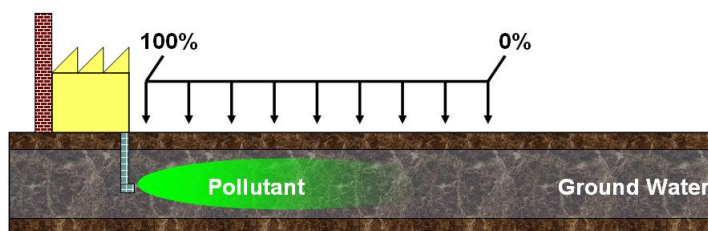


Figure 5.8: Pollution concentration in underground water model

out the ground water and v will represent the velocity of the ground water. $S(x)$ in this case will represent many processes which might include adding or subtracting pollution through interaction with the water and with the soil. In this example we will use $D = 10m^2$ per day and $v = 2m$ per day as suggested by [5]. u in (1.1) will represent the concentration of the pollutant in the groundwater. We will want to know the concentration of the pollutant over $100m$ intervals over a total of $1000m$. Interaction from an adjacent aquifer is causing pure water to be added in the intervals of $0m$ to $333m$ and from $666m$ to $1000m$. A broken waste pipe is causing more pollution to enter the aquifer in the interval of $333m$ to $666m$. The aquifer is completely contaminated at $0m$ and has pure water at $1000m$. After scaling the

coefficients so that $x = 1$ unit is equivalent to $1000m$ we get values of $v = .002$, $D = 10^{-5}$, and $h = 0.1$. Putting these into (1.1) and multiplying by 10^6 to eliminate decimals we get the equation

$$-10 \frac{d^2 u}{dx^2} + 2000 \frac{du}{dx} = -4000 + 18000x - 18000x^2 \quad (5.4)$$

with boundary conditions

$$u(0) = 1 \quad u(1) = 0 \quad (5.5)$$

This produces the Péclet number $\beta = 20$. Applying Hermite collocation with upstreaming we get the numerical solution. From Figure 5.9 we can see the effects

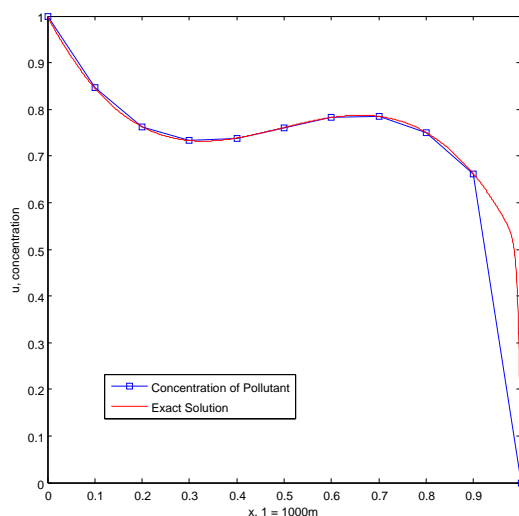


Figure 5.9: Numerical solution for groundwater transport model

that the broken pipe and pure water from the other aquifer has on the concentration of the pollutant. This is highlighted by the short drop off in concentration early on,

which is followed by a short up turn, and eventual decline. Here optimal sampling is critical in order to capture the effects of the quadratic forcing term.

CHAPTER 6

CONCLUSIONS

6.1 Sampling

From the calculations presented, we can clearly see that when the forcing term $S(x)$ is quadratic, that it can be sampled in an optimal way. Unfortunately when $S(x)$ is quadratic the method for choosing the optimal sampling term is more complicated than either the homogeneous or linear case. The important part however, is that it can be done, and that a method is provided. This allows it to be extended into more complicated convection-diffusion DEs where an exact solution may not be available.

Also calculating an optimal κ_j might not be necessary for certain values of β and j . This is because for large values of βj we have that $\kappa_j \approx -\zeta$. This comes from the proof of (4.11) where $z = j$, which can be found in Appendix C. Specifically, we can be sure that κ_j is within ϵ of $-\zeta$ as long as $\beta j > M$ where $M = \frac{1}{\epsilon}$. This means that given a sufficiently large value of βj we can simply sample all the terms of a quadratic $S(x)$ at $-\zeta$ instead of having to compute κ_j .

6.2 Future Directions

From previous work we have seen how to sample (1.1) optimally for a few forcing terms. Specifically when $S(x)$ is homogeneous, linear, and quadratic. The next logical step is, of course, to start working with $S(x)$ as a third degree polynomial. From this more information could be gathered which might eventually extend to a forcing term that is an n^{th} degree polynomial. This is important in that we might model even more complicated forcing terms via Taylor polynomials.

Already it appears that the value of ζ will play a role in determining where to sample more complicated forcing terms. It is hypothesized that for large values of β that the optimal sampling of the forcing term should be done at approximately $-\zeta$. As seen in Figure 6.1, this hypothesis seem very promising. This figure shows the effect of sampling all the terms of $S(x)$ at $-\zeta$ for when $S(x) = -60 + 380x - 760x^2 + 480x^3$. Here $D = 0.02$, $v = 10$, $m = 10$, producing $\beta = 50$, with boundary conditions $u(0) = 1$, $u(1) = 0$. As we can see the numerical solution does an excellent job at capturing the behavior of the exact solution. If we were to not use upstreaming we end up with a poor approximation to the exact solution.

One alarming aspect is how complicated the equation for choosing the optimal sampling term becomes as the forcing terms grows in degree. Although for the homogeneous and linear forcing term case, it seems quite manageable, the quadratic case reveals that more information is needed to find the optimal sampling term. For the quadratic case this involves knowing the value of β , as well as the interval that the

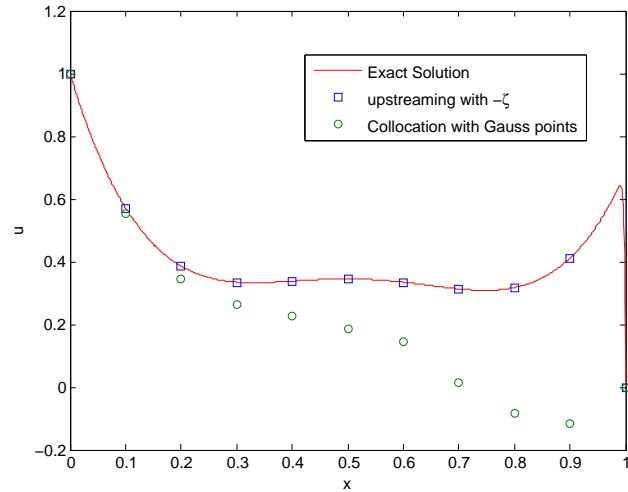


Figure 6.1: $\beta = 4$, Problem B

sampling is to be done. For more complicated forcing terms, more information might be needed as well, causing another level of complexity to be added on.

Also not discussed in this thesis are cases where $S(x)$ is a trigonometric or a step function. In both these cases it is not known if the forcing term can be sampled optimally. This limits our ability to handle potentially useful scenarios when considering our DE.

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APPENDIX A

PROOF OF (4.6)

To prove (4.6) we must show that it is equivalent to (2.6).

Therefore we begin by starting with (2.6)

$$q_j = c_1 + c_2 \lambda^j + \frac{1}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k \quad (\text{A.1})$$

Here the forcing term S_k represents the forcing term evaluated at k .

$$S(x) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 \quad (\text{A.2})$$

The case for when $S(x) = \alpha_1 + \alpha_2 x$ has already been studied by Brill in [4]. Doing so gives us $\delta_0 + \delta_1 \alpha_1 + \delta_2 \alpha_2$ in (4.6). Therefore we will only focus on the $\alpha_3 x^2$ term.

Because of this we will use

$$\begin{aligned}
S_{2\ell} &= \left(\ell + \frac{1}{2} + \kappa - \frac{1}{\sqrt{12}} \right)^2 \left(\frac{1}{m^2} \right) \\
&= \left(\ell^2 + 2 \left(\frac{1}{2} + \kappa - \frac{1}{\sqrt{12}} \right) \ell + \left(\frac{1}{2} + \kappa - \frac{1}{\sqrt{12}} \right)^2 \right) \left(\frac{1}{m^2} \right) \\
S_{2\ell+1} &= \left(\ell + \frac{1}{2} + \kappa + \frac{1}{\sqrt{12}} \right)^2 \left(\frac{1}{m^2} \right) \\
&= \left(\ell^2 + 2 \left(\frac{1}{2} + \kappa + \frac{1}{\sqrt{12}} \right) \ell + \left(\frac{1}{2} + \kappa + \frac{1}{\sqrt{12}} \right)^2 \right) \left(\frac{1}{m^2} \right)
\end{aligned} \tag{A.3}$$

where the α_3 has already been factored out. To evaluate the sum we first recognize that $G_{k,j}$ is piecewise defined as in (2.12). From this we have that

$$\frac{\alpha_3}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k = \frac{\alpha_3}{2m} \left[\sum_{k=0}^{2j-1} A_k (\lambda^m - \lambda^j) S_k + \sum_{k=2j}^{2m-1} (C_k - A_k \lambda^m) (\lambda^j - 1) S_k \right] \tag{A.4}$$

To evaluate the first of these sums in (A.4) we recognize that A_k and S_k are also piecewise defined as in (2.14), (2.15), and (A.3). To evaluate the second sum in (A.4) we recognize that C_k is piecewise defined as in (2.16). Substituting in this information gives us that (A.4) is

$$\begin{aligned}
\frac{\alpha_3}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k &= \frac{\alpha_3}{2m} (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [A_{2\ell} S_{2\ell} + A_{2\ell+1} S_{2\ell+1}] \\
&\quad + \frac{\alpha_3}{2m} (\lambda^j - 1) \sum_{\ell=j}^{m-1} [C_{2\ell} S_{2\ell} + C_{2\ell+1} S_{2\ell+1} - \lambda^m (A_{2\ell} S_{2\ell} + A_{2\ell+1} S_{2\ell+1})]
\end{aligned} \tag{A.5}$$

Putting (A.3) into (A.5), gathering like terms, and factoring out $\frac{1}{m^2}$ gives us

$$\frac{\alpha_3}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k = \frac{\alpha_3}{2m^3} (E_1 + E_2 + E_3 + E_4 + E_5 + E_5) \quad (\text{A.6})$$

where

$$E_1 = (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [\ell^2 (A_{2\ell} + A_{2\ell+1})] + (\lambda^j - 1) \sum_{\ell=j}^{m-1} [\ell^2 (C_{2\ell} + C_{2\ell+1} - \lambda^m (A_{2\ell} + A_{2\ell+1}))] \quad (\text{A.7})$$

$$E_2 = (1 + 2\kappa)(\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [\ell (A_{2\ell} + A_{2\ell+1})] + (1 + 2\kappa)(\lambda^j - 1) \sum_{\ell=j}^{m-1} [\ell (C_{2\ell} + C_{2\ell+1} - \lambda^m (A_{2\ell} + A_{2\ell+1}))] \quad (\text{A.8})$$

$$E_3 = - \left(\frac{1}{\sqrt{12}} \right) (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [\ell (A_{2\ell} - A_{2\ell+1})] - \left(\frac{1}{\sqrt{12}} \right) (\lambda^j - 1) \sum_{\ell=j}^{m-1} [\ell (C_{2\ell} - C_{2\ell+1} - \lambda^m (A_{2\ell} - A_{2\ell+1}))] \quad (\text{A.9})$$

$$E_4 = \left(\frac{1}{2} + \kappa \right)^2 (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [A_{2\ell} + A_{2\ell+1}] + \left(\frac{1}{2} + \kappa \right)^2 (\lambda^j - 1) \sum_{\ell=j}^{m-1} [C_{2\ell} + C_{2\ell+1} - \lambda^m (A_{2\ell} + A_{2\ell+1})] \quad (\text{A.10})$$

$$\begin{aligned}
E_5 = & -(1 + 2\kappa) \left(\frac{1}{\sqrt{12}} \right) (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [A_{2\ell} - A_{2\ell+1}] \\
& - (1 + 2\kappa) \left(\frac{1}{\sqrt{12}} \right) (\lambda^j - 1) \sum_{\ell=j}^{m-1} [C_{2\ell} - C_{2\ell+1} - \lambda^m (A_{2\ell} - A_{2\ell+1})]
\end{aligned} \tag{A.11}$$

$$\begin{aligned}
E_6 = & \left(\frac{1}{12} \right) (\lambda^m - \lambda^j) \sum_{\ell=0}^{j-1} [A_{2\ell} + A_{2\ell+1}] \\
& + \left(\frac{1}{12} \right) (\lambda^j - 1) \sum_{\ell=j}^{m-1} [C_{2\ell} + C_{2\ell+1} - \lambda^m (A_{2\ell} + A_{2\ell+1})]
\end{aligned} \tag{A.12}$$

Evaluating the sums in each of these using the formulas for arithmetic-geometric series found in [9] and [10] we obtain

$$\begin{aligned}
E_1 = & \left(\frac{1}{3v} + \frac{24\rho_{den}\lambda}{\lambda_{num}v(\lambda-1)^2} \right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1} \right] \\
& + \left(-\frac{1}{v} + \frac{12\rho_{den}\lambda}{\lambda_{num}v(\lambda-1)} \right) \left[j^2 - \frac{m^2(\lambda^j - 1)}{\lambda^m - 1} \right] \\
& + \left(\frac{2}{3v} \right) \left[j^3 - \frac{m^3(\lambda^j - 1)}{\lambda^m - 1} \right]
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
E_2 = & (1 + 2\kappa) \left(-\frac{1}{v} + \frac{12\rho_{den}\lambda}{\lambda_{num}v(\lambda-1)} \right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1} \right] \\
& + (1 + 2\kappa) \left(\frac{1}{v} \right) \left[j^2 - \frac{m^2(\lambda^j - 1)}{\lambda^m - 1} \right]
\end{aligned} \tag{A.14}$$

$$\begin{aligned}
E_3 = & \left(-\frac{2}{\sqrt{12}}\right) \left(\frac{\sqrt{12}\beta\zeta^2}{2v(1+\beta\zeta)} + \frac{\sqrt{12}\beta\lambda(\rho_{den} - 6\rho_{den}\zeta^2)}{\lambda_{num}v(\lambda-1)(1+\beta\zeta)}\right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1}\right] \\
& + \left(-\frac{2}{\sqrt{12}}\right) \left(\frac{-\sqrt{12}\beta\zeta^2}{2v(1+\beta\zeta)}\right) \left[j^2 - \frac{m^2(\lambda^j - 1)}{\lambda^m - 1}\right]
\end{aligned} \tag{A.15}$$

$$E_4 = \left(\frac{1}{2} + \kappa\right)^2 \left(\frac{2}{v}\right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1}\right] \tag{A.16}$$

$$E_5 = -(1 + 2\kappa) \left(\frac{1}{\sqrt{12}}\right) \left(\frac{-\sqrt{12}\beta\zeta^2}{v(1+\beta\zeta)}\right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1}\right] \tag{A.17}$$

$$E_6 = \left(\frac{1}{12}\right) \left(\frac{2}{v}\right) \left[j - \frac{m(\lambda^j - 1)}{\lambda^m - 1}\right] \tag{A.18}$$

Finally we combine and simplify to arrive at

$$\frac{\alpha_2}{2m} \sum_{k=0}^{2m-1} G_{k,j} S_k = \left(\frac{\alpha_2}{2m^3}\right) \left(\frac{2}{3\beta^2 v}\right) \left[j\hat{E}(j) - \hat{E}(m)\frac{m(\lambda^j - 1)}{\lambda^m - 1}\right] \tag{A.19}$$

where

$$\hat{E}(z) = \beta^2 (z^2 + 3\zeta^2 + 3z\zeta + 3z\kappa + 6\kappa\zeta + 3\kappa^2) + \beta (3z + 6\kappa + 12\zeta) + 6 \quad (\text{A.20})$$

Doing one last simplification gives us $\delta_3\alpha_3$ from (4.6). Using this as well as the $\delta_0 + \delta_1\alpha_1 + \delta_2\alpha_2$ we can say that

$$q_j = \delta_0 + \delta_1\alpha_1 + \delta_2\alpha_2 + \delta_3\alpha_3 \quad (\text{A.21})$$

where

$$\begin{aligned} \delta_3 &= \frac{1}{3(\beta m)^2 v} \left[\hat{E}(j) \frac{j}{m} - \hat{E}(m) \frac{\lambda^j - 1}{\lambda^m - 1} \right] \\ \delta_2 &= \frac{1}{2\beta m v} \left[\hat{F}(j) \frac{j}{m} - \hat{F}(m) \frac{\lambda^j - 1}{\lambda^m - 1} \right] \\ \delta_1 &= \frac{1}{v} \left[\frac{j}{m} - \frac{\lambda^j - 1}{\lambda^m - 1} \right] \\ \delta_0 &= u(0) + [u(1) - u(0)] \frac{\lambda^j - 1}{\lambda^m - 1} \end{aligned} \quad (\text{A.22})$$

with

$$\hat{E}(z) = \beta^2 (z^2 + 3\zeta^2 + 3z\zeta + 3z\kappa + 6\kappa\zeta + 3\kappa^2) + \beta (3z + 6\kappa + 12\zeta) + 6 \quad (\text{A.23})$$

$$\hat{F}(z) = \beta z + 2(\beta\psi + \beta\zeta + 1)$$

Therefore (4.6) is equivalent to (2.6) as desired.

APPENDIX B

PROOF OF (4.3)

To find the continuous solution for the case where the forcing term is quadratic we start with (1.1) where $S(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2$ as in (4.1).

$$-D \frac{d^2 u}{dx^2} + v \frac{du}{dx} = \alpha_0 + \alpha_1 x + \alpha_2 x^2 \quad (\text{B.1})$$

We will also use the following Dirichlet boundary conditions

$$u(0) = u_0 \quad u(1) = u_1 \quad (\text{B.2})$$

For simplifying later we will also define the Péclet number β .

$$\beta = \frac{hv}{D} = \frac{v}{mD} \quad (\text{B.3})$$

In much the same way as the proof of (4.6), the general solution to this problem

is

$$u(x) = u(0) - \frac{u(1) - u(0)}{e^{\beta m} - 1} + \left(\frac{u(1) - u(0)}{e^{\beta m} - 1} \right) e^{\beta m x} + \int_0^1 G(\xi, x_j) S(\xi) d\xi \quad (\text{B.4})$$

where G is the continuous Green's function as discussed in [4].

$$G(\xi, x_j) = \begin{cases} A(\xi) [e^{\beta m} - e^{\beta j}], & 0 \leq \xi \leq x_j \\ \left[\frac{1}{v} - A(\xi) e^{\beta m} \right] (e^{\beta j} - 1), & x_j \leq \xi \leq 1 \end{cases} \quad (\text{B.5})$$

and

$$A(\xi) = \frac{1 - e^{-\beta m \xi}}{v(e^{\beta m} - 1)} \quad (\text{B.6})$$

Evaluating this and using $e^{\beta m} = e^{\frac{v}{D}}$ we arrive at

$$\begin{aligned} u(x) &= \frac{\alpha_2 x^2}{2v} + \frac{x^2 D \alpha_3}{v^2} + \frac{\alpha_3 x^3}{3v} \\ &\quad - \frac{(-6u_1 v^3 + 3a_2 v^2 + 6\alpha_3 v D + 2\alpha_3 v^2 + 6v^3 u_0 + 6\alpha_1 v^2 + 6D v \alpha_2 + 12D^2 \alpha_3) e^{\frac{vx}{D}}}{6v^3 \left(e^{\left(\frac{v}{D}\right)} - 1 \right)} \\ &\quad + \frac{x\alpha_1}{v} + \frac{x D \alpha_2}{v^2} + \frac{2x D^2 \alpha_3}{v^3} \\ &\quad + \frac{6v^3 u_0 e^{\left(\frac{v}{D}\right)} - 6u_1 v^3 + 3\alpha_2 v^2 + 6\alpha_3 v D + 2\alpha_3 v^2 + 6\alpha_1 v^2 + 6D v \alpha_2 + 12D^2 \alpha_3}{6v^3 \left(e^{\left(\frac{v}{D}\right)} - 1 \right)} \end{aligned} \quad (\text{B.7})$$

Now we will evaluate the solution at the x_j 's by substituting $x = \frac{j}{m}$

$$\begin{aligned}
u(x_j) &= \frac{\alpha_2 j^2}{2vm^2} + \frac{j^2 D\alpha_3}{v^2 m^2} + \frac{\alpha_3 j^3}{3vm^3} \\
&\quad - \frac{(-6u_1 v^3 + 3\alpha_2 v^2 + 6\alpha_3 vD + 2\alpha_3 v^2 + 6v^3\alpha_0 + 6\alpha_1 v^2 + 6Dv\alpha_2 + 12D^2\alpha_3)e^{\frac{vj}{Dm}}}{6v^3 \left(e^{\left(\frac{v}{D}\right)} - 1 \right)} \\
&\quad + \frac{j\alpha_1}{vm} + \frac{jD\alpha_2}{v^2 m} + \frac{2jD^2\alpha_3}{v^3 m} \\
&\quad + \frac{6v^3 u_0 e^{\left(\frac{v}{D}\right)} - 6u_1 v^3 + 3\alpha_2 v^2 + 6\alpha_3 vD + 2\alpha_3 v^2 + 6\alpha_1 v^2 + 6Dv\alpha_2 + 12D^2\alpha_3}{6v^3 \left(e^{\left(\frac{v}{D}\right)} - 1 \right)}
\end{aligned} \tag{B.8}$$

To help us simplify this, and get a better understanding of the solution we can gather the coefficients of the α 's. We'll start with the the terms that do not contain any α .

$$\begin{aligned}
&\frac{u_1 e^{\frac{vj}{Dm}}}{e^{\frac{v}{D}} - 1} - \frac{u_0 e^{\frac{vj}{Dm}}}{e^{\frac{v}{D}} - 1} + \frac{u_0 e^{\frac{v}{D}}}{e^{\frac{v}{D}} - 1} - \frac{u_1}{e^{\frac{v}{D}} - 1} \\
&= \frac{1}{e^{\beta m} - 1} (u_1 e^{\beta j} - u_0 e^{\beta j} + u_0 e^{\beta m} - u_1) \\
&= \frac{1}{e^{\beta m} - 1} (u_1 (e^{\beta j} - 1) + u_0 (e^{\beta m} - e^{\beta j})) \\
&= u_0 + (u_1 - u_0) \left(\frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right)
\end{aligned} \tag{B.9}$$

We will call this term γ_0 :

$$\gamma_0 = u_0 + (u_1 - u_0) \left(\frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right) \tag{B.10}$$

Next we will gather the coefficients of α_1

$$\begin{aligned}
& -\frac{e^{\left(\frac{vj}{Dm}\right)}\alpha_1}{v\left(e^{\frac{v}{D}}-1\right)}+\frac{j\alpha_1}{mv}+\frac{\alpha_1}{v\left(e^{\left(\frac{v}{D}\right)}-1\right)} \\
& =\frac{\alpha_1\left(-e^{\left(\frac{vj}{Dm}\right)}m+je^{\left(\frac{v}{D}\right)}-j+m\right)}{vm\left(e^{\left(\frac{v}{D}\right)}-1\right)} \\
& =\alpha_1\left[\frac{-e^{\beta j}m+je^{\beta m}-j+m}{vm\left(e^{\beta m}-1\right)}\right] \\
& =\alpha_1\frac{1}{v}\left[\frac{j}{m}-\frac{e^{\beta j}-1}{e^{\beta m}-1}\right]
\end{aligned} \tag{B.11}$$

From this we can clearly see the coefficient of α_1 , which we will call γ_1 :

$$\gamma_1=\frac{1}{v}\left[\frac{j}{m}-\frac{e^{\beta j}-1}{e^{\beta m}-1}\right] \tag{B.12}$$

In much the same way we can gather the coefficients of α_2

$$\begin{aligned}
& \frac{\alpha_2j^2}{2vm^2}-\frac{e^{\beta j}\alpha_2}{2v\left(e^{\frac{v}{D}}-1\right)}-\frac{e^{\beta j}D\alpha_2}{v^2\left(e^{\frac{v}{D}}-1\right)}+\frac{jD\alpha_2}{mv^2}+\frac{\alpha_2}{2v\left(e^{\frac{v}{D}}-1\right)}+\frac{D\alpha_2}{v^2\left(e^{\frac{v}{D}}-1\right)} \\
& =\frac{\alpha_2j^2}{2vm^2}-\frac{e^{\beta j}\alpha_2}{2v\left(e^{\beta m}-1\right)}-\frac{e^{\beta j}D\alpha_2}{v^2\left(e^{\beta m}-1\right)}+\frac{jD\alpha_2}{mv^2}+\frac{\alpha_2}{2v\left(e^{\beta m}-1\right)}+\frac{D\alpha_2}{v^2\left(e^{\beta m}-1\right)} \\
& =\frac{\alpha_2}{2\beta mv}\left[(\beta j+2)\left(\frac{j}{m}\right)-(\beta m+2)\left(\frac{e^{\beta j}-1}{e^{\beta m}-1}\right)\right]
\end{aligned} \tag{B.13}$$

From this we obtain the coefficient of α_2 which we will call γ_2 :

$$\gamma_2=\frac{1}{2\beta mv}\left[(\beta j+2)\left(\frac{j}{m}\right)-(\beta m+2)\left(\frac{e^{\beta j}-1}{e^{\beta m}-1}\right)\right] \tag{B.14}$$

Lastly we will gather to coefficients of α_3 .

$$\begin{aligned} & \frac{j^2 D \alpha_3}{v^2 m^2} + \frac{\alpha_3 j^3}{3 v m^3} - \frac{e^{\beta j} \alpha_3 D}{v^2 (e^{\beta m} - 1)} - \frac{e^{\beta j} \alpha_3}{3 v (e^{\beta m} - 1)} - \frac{2 e^{\beta j} D^2 \alpha_3}{v^3 (e^{\beta m} - 1)} \\ & + \frac{\alpha_3}{e^{\beta m} - 1} \left[-\frac{e^{\beta j} D 3 v}{3 v^3} - \frac{e^{\beta j} v^2}{3 v^3} - \frac{2 e^{\beta j} D^2 3}{3 v^3} + \frac{D 3 v}{3 v^3} + \frac{v^2}{3 v^3} + \frac{2 D^2 3}{3 v^3} \right] \end{aligned} \quad (\text{B.15})$$

$$\begin{aligned} & = \alpha_3 \left[\frac{j^3}{3 v m^3} + \frac{j^2 D}{v^2 m^2} + \frac{2 j D^2}{m v^3} \right] \\ & + \frac{\alpha_3}{e^{\beta m} - 1} \left[\frac{e^{\beta j} (-D 3 v - v^2 - D^2 6)}{3 v^3} + \frac{D 3 v + v^2 + D^2 6}{3 v^3} \right] \\ & = \alpha_3 \left[\frac{j^3}{3 v m^3} + \frac{j^2 D}{v^2 m^2} + \frac{2 j D^2}{m v^3} \right] + \frac{\alpha_3}{e^{\beta m} - 1} \left[\frac{(D 3 v + v^2 + D^2 6) (-e^{\beta j} + 1)}{3 v^3} \right] \quad (\text{B.16}) \\ & = \left(\frac{\alpha_3 D^2}{3 v^3} \right) \left[(\beta^2 j^2 + 3 \beta j + 6) \left(\frac{j}{m} \right) - \left(\frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right) (\beta^2 m^2 + 3 \beta m + 6) \right] \\ & = \left(\frac{\alpha_3}{3 \beta^2 m^2 v} \right) \left[(\beta^2 j^2 + 3 \beta j + 6) \left(\frac{j}{m} \right) - (\beta^2 m^2 + 3 \beta m + 6) \left(\frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right) \right] \end{aligned}$$

From this we obtain the coefficient of α_3 , which we will call γ_3 :

$$\gamma_3 = \frac{1}{3 (\beta m)^2 v} \left[(\beta^2 j^2 + 3 \beta j + 6) \left(\frac{j}{m} \right) - (\beta^2 m^2 + 3 \beta m + 6) \left(\frac{e^{\beta j} - 1}{e^{\beta m} - 1} \right) \right] \quad (\text{B.17})$$

This give us that

$$u(x_j) = \gamma_0 + \gamma_1 \alpha_1 + \gamma_2 \alpha_2 + \gamma_3 \alpha_3 \quad (\text{B.18})$$

which corresponds with equation (4.3) as desired.

APPENDIX C

PROOF OF (4.11)

To prove that

$$\lim_{\beta z \rightarrow \infty} K_1 = -\zeta \tag{C.1}$$

We begin by letting $\epsilon > 0$ be given. We also let $M = \frac{1}{\epsilon}$ and assume that $\beta z > M$.

We want to show that

$$\left| -\frac{2 + \beta z + 2\beta\zeta - \sqrt{4 + 4\beta z + (\beta z)^2 - 8\beta\zeta}}{2\beta} + \zeta \right| < \epsilon \tag{C.2}$$

Starting with the left side of the inequality we have

$$\begin{aligned} & \left| -\frac{2 + \beta z + 2\beta\zeta - \sqrt{4 + 4\beta z + (\beta z)^2 - 8\beta\zeta}}{2\beta} + \zeta \right| \\ &= \left| \frac{-2 - \beta z - 2\beta\zeta + \sqrt{4 + 4\beta z + (\beta z)^2 - 8\beta\zeta}}{2\beta} + \frac{2\beta\zeta}{2\beta} \right| \\ &= \left| \frac{-2 - \beta z + \sqrt{4 + 4\beta z + (\beta z)^2 - 8\beta\zeta}}{2\beta} \right| \end{aligned} \tag{C.3}$$

Multiplying the top and bottom by $(-2 - \beta z) - \sqrt{4 + 4\beta z + (\beta z)^2 - \beta\zeta}$ and simplifying we obtain

$$\left| \frac{-4\zeta}{(2 + \beta z) + \sqrt{(2 + \beta z)^2 - 8\beta\zeta}} \right| \quad (\text{C.4})$$

By reverse triangle inequality we have that

$$\sqrt{(2 + \beta z)^2 - 8\beta\zeta} \geq \sqrt{(2 + \beta z)^2} - \sqrt{8\beta\zeta} \quad (\text{C.5})$$

Therefore (C.4) is less than

$$\left| \frac{-4\zeta}{(2 + \beta z) + \sqrt{(2 + \beta z)^2 - \sqrt{8\beta\zeta}}} \right| \quad (\text{C.6})$$

Simplifying this we obtain

$$\left| \frac{-4\zeta}{2(2 + \beta z) - \sqrt{8\beta\zeta}} \right| \quad (\text{C.7})$$

Now the max that ζ can be is $\frac{1}{2} - \frac{1}{\sqrt{12}} \approx 0.211324$. Therefore we can replace ζ with $\frac{1}{4}$ to obtain the greater expression

$$\left| \frac{-1}{2(2 + \beta z) - \sqrt{8\beta\zeta}} \right| \quad (\text{C.8})$$

Now z is an integer, so for $z > 1$ we have that $z > \zeta$. This allows us to replace the ζ under the root and obtain the greater expression

$$\left| \frac{-1}{2(2 + \beta z) - \sqrt{8\beta z}} \right| \quad (\text{C.9})$$

Finally we have that for $\beta z > 8$ the following is true

$$\sqrt{8\beta z} < \sqrt{(\beta z)^2} = \beta z < 4 + \beta z \quad (\text{C.10})$$

Therefore we can replace the root in (C.9) with $4 + \beta z$ and obtain the greater expression

$$\left| \frac{-1}{4 + 2\beta z - (4 + \beta z)} \right| \quad (\text{C.11})$$

Simplifying this we obtain

$$\left| \frac{-1}{\beta z} \right| = \frac{1}{\beta z} < \frac{1}{M} = \epsilon \quad (\text{C.12})$$

as desired.

APPENDIX D

MAPLE CODE

The Maple Code used by the author implements the upstream collocation method on a convection-diffusion differential equation which is forced. In order to run, the following parameters must be entered in.

- D the diffusion constant
- v the convection constant
- $F [1], F [2], F [3]$ the forcing term
- PTS a list of points where the solution will be approximated at
- a boundary condition at the first point
- b boundary condition at the last point

Before the CollocationAuto procedure may be run, the ListCount procedure must be run. This procedure takes PTS and returns p the number of points that will be used. This will be used by the CollocationAuto procedure.

Once ListCount is run then the CollocationAuto procedure may be run. In the procedure we use the previously defined parameters p , D, v , a and b . An additional “wander” parameter w is also entered. When $w = 0$ the procedure will use the optimal κ_j as defined in Table 4.1. If $w \neq 0$ the procedure will use $\kappa_j + w$ to find an approximate solution.

CollocationAuto displays β , ζ , ψ , and w as well as the approximate values for each point listed in *PTS*. If desired CollocationAuto can also display a plot of these points by using the PLOT command near the end of the procedure.

APPENDIX E

ADDITIONAL DATA

The remaining data from the numerical experiments which were not presented in Chapter 4 are presented here for the reader. In all the tables the first and last column come from the imposed boundary conditions and so always remain 1 and 0 respectively. Each term in the table as been rounded to three decimal places.

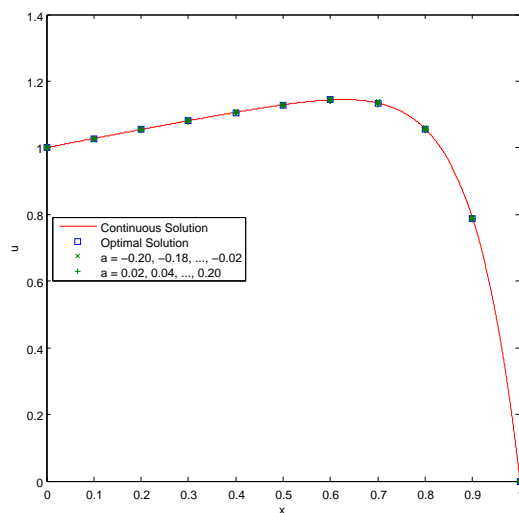
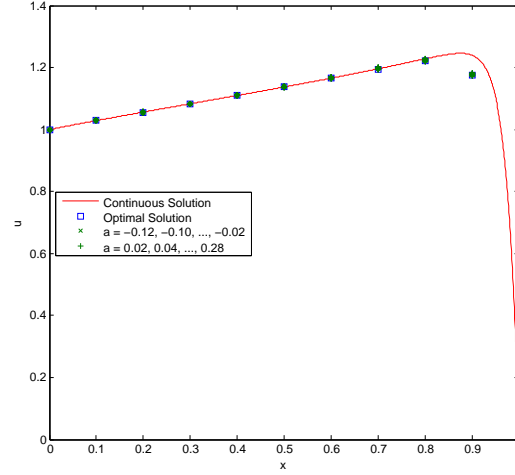


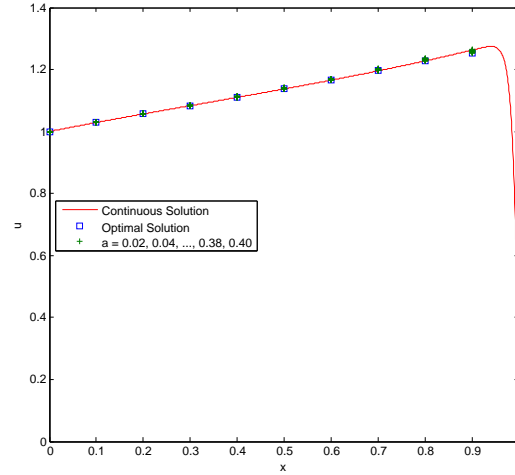
Figure E.1: $\beta = 1$, Problem A

Table E.1: Data for $\beta = 1$, Problem A

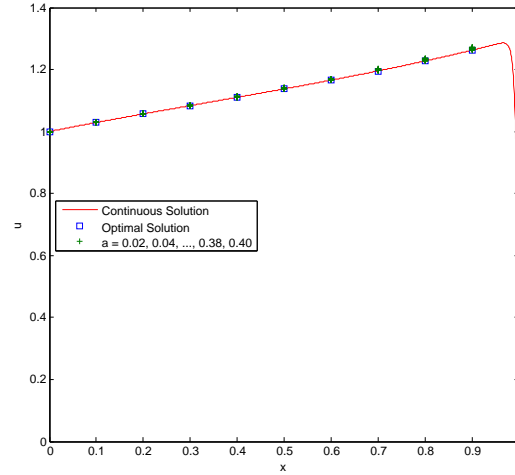
	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.028	1.055	1.081	1.106	1.129	1.144	1.135	1.057	0.790	0.000
Opt.	1.000	1.028	1.055	1.081	1.106	1.129	1.144	1.134	1.057	0.789	0.000
+ 0.02	1.000	1.028	1.055	1.081	1.107	1.129	1.144	1.135	1.057	0.789	0.000
+ 0.04	1.000	1.028	1.055	1.081	1.107	1.130	1.144	1.135	1.057	0.789	0.000
+ 0.06	1.000	1.028	1.055	1.081	1.107	1.130	1.145	1.135	1.058	0.790	0.000
+ 0.08	1.000	1.028	1.055	1.081	1.107	1.130	1.145	1.136	1.058	0.790	0.000
+ 0.10	1.000	1.028	1.055	1.082	1.107	1.130	1.145	1.136	1.059	0.790	0.000
+ 0.12	1.000	1.028	1.055	1.082	1.107	1.130	1.145	1.137	1.059	0.791	0.000
+ 0.14	1.000	1.028	1.055	1.082	1.107	1.131	1.146	1.137	1.059	0.791	0.000
+ 0.16	1.000	1.028	1.055	1.082	1.108	1.131	1.146	1.137	1.060	0.791	0.000
+ 0.18	1.000	1.028	1.055	1.082	1.108	1.131	1.146	1.138	1.060	0.791	0.000
+ 0.20	1.000	1.028	1.055	1.082	1.108	1.131	1.147	1.138	1.061	0.792	0.000
- 0.02	1.000	1.028	1.055	1.081	1.106	1.129	1.144	1.134	1.056	0.788	0.000
- 0.04	1.000	1.028	1.055	1.081	1.106	1.129	1.143	1.134	1.056	0.788	0.000
- 0.06	1.000	1.028	1.055	1.081	1.106	1.129	1.143	1.133	1.055	0.788	0.000
- 0.08	1.000	1.028	1.055	1.081	1.106	1.128	1.143	1.133	1.055	0.787	0.000
- 0.10	1.000	1.028	1.055	1.081	1.106	1.128	1.142	1.133	1.055	0.787	0.000
- 0.12	1.000	1.028	1.055	1.081	1.106	1.128	1.142	1.132	1.054	0.787	0.000
- 0.14	1.000	1.028	1.054	1.080	1.105	1.128	1.142	1.132	1.054	0.787	0.000
- 0.16	1.000	1.028	1.054	1.080	1.105	1.128	1.142	1.132	1.054	0.786	0.000
- 0.18	1.000	1.028	1.054	1.080	1.105	1.127	1.141	1.131	1.053	0.786	0.000
- 0.20	1.000	1.028	1.054	1.080	1.105	1.127	1.141	1.131	1.054	0.787	0.000

Figure E.2: $\beta = 4$, Problem ATable E.2: Data for $\beta = 4$, Problem A

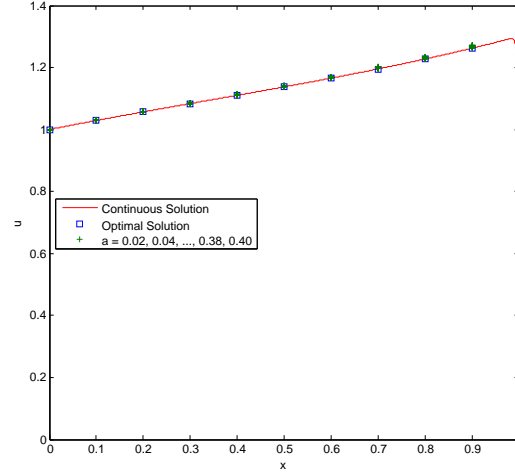
	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.029	1.056	1.083	1.110	1.137	1.166	1.196	1.228	1.240	0.000
Opt.	1.000	1.029	1.056	1.083	1.110	1.137	1.166	1.195	1.222	1.175	0.000
+ 0.02	1.000	1.029	1.056	1.083	1.110	1.137	1.166	1.196	1.223	1.176	0.000
+ 0.04	1.000	1.029	1.056	1.083	1.110	1.137	1.166	1.196	1.223	1.176	0.000
+ 0.06	1.000	1.029	1.056	1.083	1.110	1.138	1.166	1.196	1.224	1.177	0.000
+ 0.08	1.000	1.029	1.056	1.083	1.110	1.138	1.166	1.197	1.224	1.177	0.000
+ 0.10	1.000	1.029	1.056	1.083	1.110	1.138	1.167	1.197	1.224	1.178	0.000
+ 0.12	1.000	1.029	1.056	1.083	1.110	1.138	1.167	1.197	1.225	1.178	0.000
+ 0.14	1.000	1.029	1.056	1.083	1.111	1.138	1.167	1.198	1.225	1.179	0.000
+ 0.16	1.000	1.029	1.056	1.084	1.111	1.138	1.167	1.198	1.226	1.179	0.000
+ 0.18	1.000	1.029	1.056	1.084	1.111	1.139	1.168	1.198	1.226	1.180	0.000
+ 0.20	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.226	1.180	0.000
+ 0.22	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.227	1.181	0.000
+ 0.24	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.227	1.181	0.000
+ 0.26	1.000	1.029	1.057	1.084	1.111	1.139	1.169	1.200	1.228	1.182	0.000
+ 0.28	1.000	1.029	1.057	1.084	1.111	1.139	1.169	1.200	1.228	1.182	0.000
- 0.02	1.000	1.029	1.056	1.083	1.110	1.137	1.165	1.195	1.222	1.175	0.000
- 0.04	1.000	1.029	1.056	1.083	1.110	1.137	1.165	1.195	1.222	1.175	0.000
- 0.06	1.000	1.029	1.056	1.083	1.109	1.137	1.165	1.194	1.221	1.174	0.000
- 0.08	1.000	1.029	1.056	1.083	1.109	1.136	1.165	1.194	1.221	1.174	0.000
- 0.10	1.000	1.029	1.056	1.083	1.109	1.136	1.164	1.194	1.220	1.173	0.000
- 0.12	1.000	1.029	1.056	1.083	1.109	1.136	1.164	1.194	1.220	1.173	0.000

Figure E.3: $\beta = 10$, Problem ATable E.3: Data for $\beta = 10$, Problem A

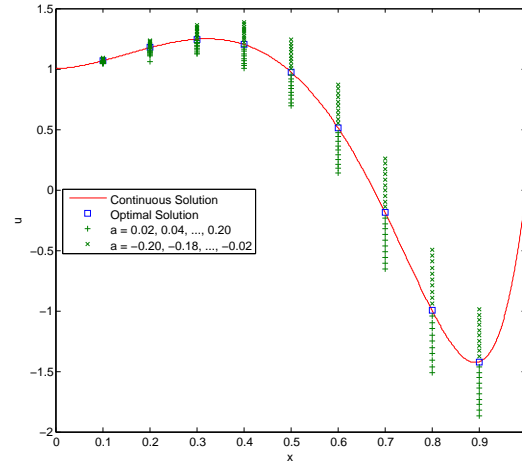
	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.029	1.057	1.083	1.110	1.137	1.166	1.195	1.228	1.262	0.000
Opt.	1.000	1.029	1.057	1.083	1.110	1.137	1.166	1.196	1.228	1.253	0.000
+ 0.02	1.000	1.029	1.057	1.083	1.110	1.137	1.166	1.196	1.228	1.254	0.000
+ 0.04	1.000	1.029	1.057	1.084	1.110	1.138	1.166	1.196	1.228	1.254	0.000
+ 0.06	1.000	1.029	1.057	1.084	1.110	1.138	1.166	1.196	1.229	1.255	0.000
+ 0.08	1.000	1.029	1.057	1.084	1.110	1.138	1.166	1.196	1.229	1.255	0.000
+ 0.10	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.230	1.256	0.000
+ 0.12	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.230	1.256	0.000
+ 0.14	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.198	1.230	1.257	0.000
+ 0.16	1.000	1.029	1.057	1.084	1.111	1.139	1.167	1.198	1.231	1.257	0.000
+ 0.18	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.198	1.231	1.258	0.000
+ 0.20	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.258	0.000
+ 0.22	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.259	0.000
+ 0.24	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.259	0.000
+ 0.26	1.000	1.029	1.057	1.084	1.112	1.139	1.169	1.200	1.233	1.260	0.000
+ 0.28	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.200	1.233	1.260	0.000
+ 0.30	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.200	1.234	1.261	0.000
+ 0.32	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.201	1.234	1.261	0.000
+ 0.34	1.000	1.029	1.057	1.085	1.112	1.140	1.170	1.201	1.235	1.262	0.000
+ 0.36	1.000	1.029	1.057	1.085	1.112	1.140	1.170	1.201	1.235	1.263	0.000
+ 0.38	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.202	1.235	1.263	0.000
+ 0.40	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.202	1.236	1.264	0.000

Figure E.4: $\beta = 20$, Problem ATable E.4: Data for $\beta = 20$, Problem A

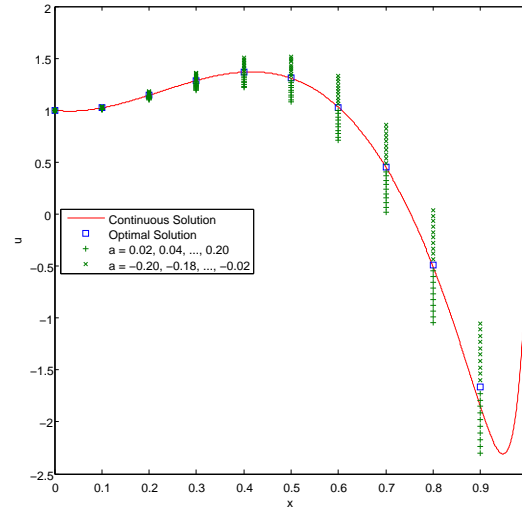
	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.029	1.057	1.084	1.110	1.137	1.166	1.195	1.227	1.262	0.000
Opt.	1.000	1.029	1.057	1.084	1.110	1.137	1.166	1.195	1.227	1.262	0.000
+ 0.02	1.000	1.029	1.057	1.083	1.110	1.138	1.166	1.196	1.228	1.263	0.000
+ 0.04	1.000	1.029	1.057	1.084	1.110	1.138	1.166	1.196	1.228	1.263	0.000
+ 0.06	1.000	1.029	1.057	1.084	1.111	1.138	1.166	1.196	1.229	1.264	0.000
+ 0.08	1.000	1.029	1.057	1.084	1.111	1.138	1.166	1.197	1.229	1.264	0.000
+ 0.10	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.229	1.265	0.000
+ 0.12	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.230	1.265	0.000
+ 0.14	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.230	1.266	0.000
+ 0.16	1.000	1.029	1.057	1.084	1.111	1.139	1.167	1.198	1.231	1.266	0.000
+ 0.18	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.198	1.231	1.267	0.000
+ 0.20	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.198	1.231	1.267	0.000
+ 0.22	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.268	0.000
+ 0.24	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.268	0.000
+ 0.26	1.000	1.029	1.057	1.084	1.112	1.139	1.169	1.199	1.233	1.269	0.000
+ 0.28	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.200	1.233	1.269	0.000
+ 0.30	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.200	1.233	1.270	0.000
+ 0.32	1.000	1.029	1.057	1.085	1.112	1.140	1.169	1.200	1.234	1.270	0.000
+ 0.34	1.000	1.029	1.057	1.085	1.112	1.140	1.169	1.201	1.234	1.271	0.000
+ 0.36	1.000	1.029	1.057	1.085	1.112	1.140	1.170	1.201	1.235	1.271	0.000
+ 0.38	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.201	1.235	1.272	0.000
+ 0.40	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.202	1.236	1.272	0.000

Figure E.5: $\beta = 50$, Problem ATable E.5: Data for $\beta = 50$, Problem A

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.029	1.057	1.084	1.110	1.137	1.166	1.195	1.227	1.262	0.000
Opt.	1.000	1.029	1.057	1.084	1.110	1.137	1.166	1.195	1.227	1.262	0.000
+ 0.02	1.000	1.029	1.057	1.084	1.110	1.138	1.166	1.196	1.228	1.263	0.000
+ 0.04	1.000	1.029	1.057	1.084	1.111	1.138	1.166	1.196	1.228	1.263	0.000
+ 0.06	1.000	1.029	1.057	1.084	1.111	1.138	1.166	1.196	1.228	1.264	0.000
+ 0.08	1.000	1.029	1.057	1.084	1.111	1.138	1.166	1.197	1.229	1.264	0.000
+ 0.10	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.229	1.264	0.000
+ 0.12	1.000	1.029	1.057	1.084	1.111	1.138	1.167	1.197	1.230	1.265	0.000
+ 0.14	1.000	1.029	1.057	1.084	1.111	1.139	1.167	1.197	1.230	1.266	0.000
+ 0.16	1.000	1.029	1.057	1.084	1.111	1.139	1.167	1.198	1.230	1.266	0.000
+ 0.18	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.198	1.231	1.267	0.000
+ 0.20	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.198	1.231	1.267	0.000
+ 0.22	1.000	1.029	1.057	1.084	1.111	1.139	1.168	1.199	1.232	1.268	0.000
+ 0.24	1.000	1.029	1.057	1.084	1.112	1.139	1.168	1.199	1.232	1.268	0.000
+ 0.26	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.199	1.232	1.269	0.000
+ 0.28	1.000	1.029	1.057	1.084	1.112	1.140	1.169	1.200	1.233	1.269	0.000
+ 0.30	1.000	1.029	1.057	1.085	1.112	1.140	1.169	1.200	1.233	1.270	0.000
+ 0.32	1.000	1.029	1.057	1.085	1.112	1.140	1.169	1.200	1.234	1.270	0.000
+ 0.34	1.000	1.029	1.057	1.085	1.112	1.140	1.169	1.201	1.234	1.271	0.000
+ 0.36	1.000	1.029	1.057	1.085	1.112	1.140	1.170	1.201	1.235	1.271	0.000
+ 0.38	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.201	1.235	1.272	0.000
+ 0.40	1.000	1.029	1.057	1.085	1.112	1.141	1.170	1.202	1.235	1.272	0.000

Figure E.6: $\beta = 1$, Problem BTable E.6: Data for $\beta = 1$, Problem B

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.067	1.175	1.245	1.202	0.974	0.512	-0.188	-0.997	-1.424	0.000
Opt.	1.000	1.067	1.175	1.245	1.202	0.975	0.513	-0.187	-0.994	-1.421	0.000
+ 0.02	1.000	1.065	1.169	1.233	1.183	0.947	0.476	-0.233	-1.045	-1.464	0.000
+ 0.04	1.000	1.062	1.062	1.221	1.164	0.920	0.439	-0.279	-1.097	-1.509	0.000
+ 0.06	1.000	1.060	1.156	1.209	1.144	0.892	0.402	-0.325	-1.148	-1.553	0.000
+ 0.08	1.000	1.057	1.149	1.197	1.125	0.864	0.365	-0.371	-1.200	-1.597	0.000
+ 0.10	1.000	1.055	1.142	1.185	1.105	0.836	0.327	-0.418	-1.252	-1.642	0.000
+ 0.12	1.000	1.052	1.136	1.172	1.086	0.808	0.290	-0.464	-1.304	-1.687	0.000
+ 0.14	1.000	1.050	1.129	1.160	1.066	0.779	0.252	-0.511	-1.356	-1.732	0.000
+ 0.16	1.000	1.047	1.122	1.147	1.046	0.751	0.214	-0.558	-1.409	-1.777	0.000
+ 0.18	1.000	1.044	1.115	1.134	1.026	0.722	0.175	-0.606	-1.462	-1.822	0.000
+ 0.20	1.000	1.042	1.108	1.121	1.006	0.693	0.137	-0.653	-1.515	-1.867	0.000
- 0.02	1.000	1.070	1.181	1.257	1.221	1.002	0.549	-0.141	-0.944	-1.377	0.000
- 0.04	1.000	1.072	1.188	1.269	1.239	1.029	0.586	-0.096	-0.893	-1.333	0.000
- 0.06	1.000	1.074	1.194	1.281	1.258	1.056	0.622	-0.051	-0.842	-1.290	0.000
- 0.08	1.000	1.076	1.200	1.292	1.277	1.083	0.658	-0.006	-0.792	-1.247	0.000
- 0.10	1.000	1.079	1.206	1.304	1.295	1.109	0.694	0.039	-0.742	-1.203	0.000
- 0.12	1.000	1.081	1.212	1.315	1.313	1.136	0.729	0.083	-0.692	-1.161	0.000
- 0.14	1.000	1.083	1.218	1.326	1.331	1.162	0.765	0.127	-0.643	-1.118	0.000
- 0.16	1.000	1.085	1.224	1.338	1.349	1.188	0.800	0.171	-0.593	-1.075	0.000
- 0.18	1.000	1.087	1.230	1.349	1.367	1.214	0.835	0.215	-0.544	-1.033	0.000
- 0.20	1.000	1.089	1.236	1.360	1.385	1.240	0.870	0.259	-0.495	-0.991	0.000

Figure E.7: $\beta = 4$, Problem BTable E.7: Data for $\beta = 4$, Problem B

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.022	1.143	1.285	1.367	1.308	1.030	0.452	-0.505	-1.854	0.000
Opt.	1.000	1.021	1.142	1.284	1.365	1.307	1.028	0.451	-0.491	-1.664	0.000
+ 0.02	1.000	1.020	1.138	1.275	1.351	1.285	0.997	0.409	-0.545	-1.726	0.000
+ 0.04	1.000	1.019	1.134	1.267	1.336	1.262	0.966	0.367	-0.599	-1.789	0.000
+ 0.06	1.000	1.017	1.130	1.258	1.322	1.240	0.934	0.324	-0.654	-1.853	0.000
+ 0.08	1.000	1.016	1.126	1.249	1.307	1.218	0.902	0.282	-0.709	-1.916	0.000
+ 0.10	1.000	1.015	1.122	1.241	1.292	1.195	0.870	0.239	-0.764	-1.980	0.000
+ 0.12	1.000	1.013	1.117	1.232	1.277	1.172	0.838	0.195	-0.819	-2.044	0.000
+ 0.14	1.000	1.012	1.113	1.223	1.262	1.149	0.806	0.152	-0.875	-2.109	0.000
+ 0.16	1.000	1.011	1.109	1.214	1.246	1.126	0.773	0.109	-0.931	-2.173	0.000
+ 0.18	1.000	1.009	1.104	1.205	1.231	1.103	0.740	0.065	-0.987	-2.238	0.000
+ 0.20	1.000	1.008	1.099	1.195	1.215	1.079	0.707	0.021	-1.043	-2.303	0.000
- 0.02	1.000	1.022	1.146	1.292	1.379	1.329	1.059	0.493	-0.437	-1.601	0.000
- 0.04	1.000	1.023	1.150	1.300	1.394	1.350	1.090	0.534	-0.383	-1.539	0.000
- 0.06	1.000	1.024	1.154	1.308	1.408	1.372	1.121	0.576	-0.330	-1.477	0.000
- 0.08	1.000	1.025	1.158	1.316	1.422	1.393	1.151	0.617	-0.277	-1.415	0.000
- 0.10	1.000	1.026	1.161	1.324	1.435	1.414	1.182	0.658	-0.224	-1.354	0.000
- 0.12	1.000	1.027	1.165	1.332	1.449	1.435	1.212	0.698	-0.172	-1.293	0.000
- 0.14	1.000	1.028	1.168	1.340	1.462	1.465	1.242	0.739	-0.119	-1.232	0.000
- 0.16	1.000	1.029	1.172	1.347	1.476	1.477	1.271	0.779	-0.067	-1.171	0.000
- 0.18	1.000	1.030	1.175	1.355	1.489	1.498	1.301	0.819	-0.016	-1.111	0.000
- 0.20	1.000	1.031	1.179	1.362	1.502	1.518	1.330	0.859	0.036	-1.051	0.000

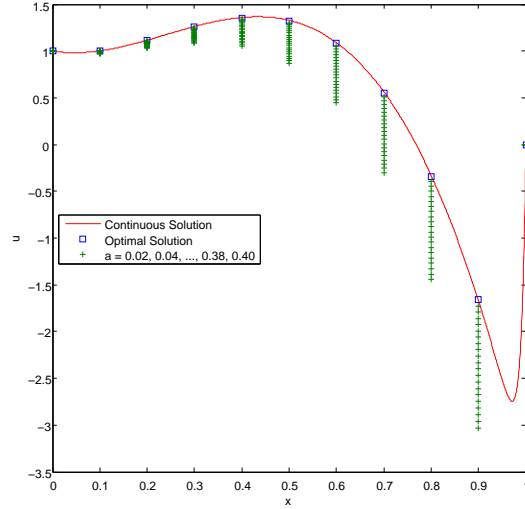
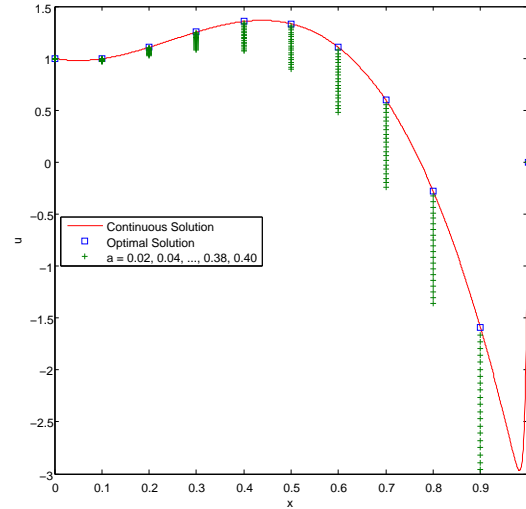


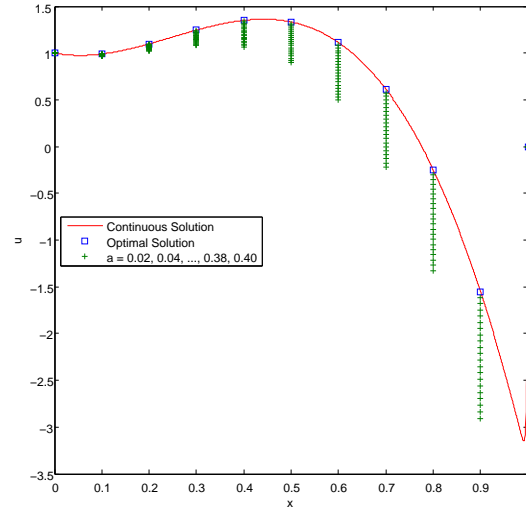
Figure E.8: $\beta = 10$, Problem B

Table E.8: Data for $\beta = 10$, Problem B

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	1.002	1.116	1.262	1.360	1.329	1.091	0.565	-0.329	-1.671	0.000
Opt.	1.000	1.000	1.112	1.257	1.353	1.321	1.081	0.553	-0.342	-1.661	0.000
+ 0.02	1.000	0.999	1.109	1.249	1.339	1.300	1.051	0.513	-0.395	-1.727	0.000
+ 0.04	1.000	0.998	1.105	1.241	1.326	1.279	1.021	0.472	-0.448	-1.793	0.000
+ 0.06	1.000	0.997	1.102	1.233	1.312	1.258	0.991	0.431	-0.501	-1.859	0.000
+ 0.08	1.000	0.996	1.098	1.225	1.298	1.236	0.960	0.390	-0.554	-1.926	0.000
+ 0.10	1.000	0.995	1.094	1.217	1.284	1.215	0.930	0.349	-0.608	-1.993	0.000
+ 0.12	1.000	0.994	1.090	1.209	1.270	1.193	0.899	0.307	-0.662	-2.060	0.000
+ 0.14	1.000	0.993	1.086	1.200	1.255	1.171	0.868	0.266	-0.716	-2.127	0.000
+ 0.16	1.000	0.991	1.082	1.192	1.241	1.149	0.837	0.224	-0.770	-2.195	0.000
+ 0.18	1.000	0.990	1.078	1.184	1.227	1.127	0.805	0.181	-0.825	-2.263	0.000
+ 0.20	1.000	0.989	1.074	1.175	1.212	1.105	0.774	0.139	-0.880	-2.332	0.000
+ 0.22	1.000	0.988	1.070	1.166	1.197	1.082	0.742	0.096	-0.935	-2.400	0.000
+ 0.24	1.000	0.986	1.066	1.157	1.182	1.060	0.710	0.053	-0.991	-2.469	0.000
+ 0.26	1.000	0.985	1.061	1.149	1.167	1.037	0.678	0.010	-1.046	-2.538	0.000
+ 0.28	1.000	0.984	1.057	1.140	1.152	1.014	0.646	-0.033	-1.102	-2.608	0.000
+ 0.30	1.000	0.982	1.052	1.131	1.137	0.991	0.613	-0.077	-1.158	-2.678	0.000
+ 0.32	1.000	0.981	1.048	1.121	1.121	0.968	0.580	-0.121	-1.215	-2.748	0.000
+ 0.34	1.000	0.979	1.043	1.112	1.106	0.944	0.547	-0.165	-1.271	-2.818	0.000
+ 0.36	1.000	0.978	1.039	1.103	1.090	0.921	0.514	-0.209	-1.328	-2.889	0.000
+ 0.38	1.000	0.976	1.034	1.093	1.074	0.897	0.481	-0.253	-1.386	-2.960	0.000
+ 0.40	1.000	0.975	1.029	1.084	1.058	0.873	0.447	-0.298	-1.443	-3.031	0.000

Figure E.9: $\beta = 20$, Problem BTable E.9: Data for $\beta = 20$, Problem B

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	0.994	1.105	1.251	1.354	1.332	1.107	0.597	-0.276	-1.596	0.000
Opt.	1.000	0.994	1.104	1.251	1.353	1.331	1.106	0.596	-0.277	-1.595	0.000
+ 0.02	1.000	0.993	1.101	1.243	1.340	1.311	1.076	0.556	-0.329	-1.661	0.000
+ 0.04	1.000	0.992	1.097	1.236	1.327	1.290	1.047	0.516	-0.381	-1.726	0.000
+ 0.06	1.000	0.991	1.094	1.228	1.313	1.270	1.017	0.476	-0.434	-1.793	0.000
+ 0.08	1.000	0.990	1.090	1.220	1.300	1.249	0.987	0.436	-0.487	-1.859	0.000
+ 0.10	1.000	0.989	1.087	1.212	1.286	1.228	0.957	0.395	-0.540	-1.926	0.000
+ 0.12	1.000	0.988	1.083	1.204	1.272	1.206	0.927	0.354	-0.593	-1.993	0.000
+ 0.14	1.000	0.987	1.079	1.196	1.258	1.185	0.896	0.313	-0.646	-2.060	0.000
+ 0.16	1.000	0.986	1.076	1.188	1.244	1.163	0.866	0.271	-0.700	-2.128	0.000
+ 0.18	1.000	0.985	1.072	1.180	1.230	1.142	0.835	0.230	-0.754	-2.196	0.000
+ 0.20	1.000	0.984	1.068	1.172	1.216	1.120	0.804	0.188	-0.808	-2.264	0.000
+ 0.22	1.000	0.983	1.064	1.163	1.201	1.098	0.773	0.146	-0.863	-2.333	0.000
+ 0.24	1.000	0.981	1.060	1.155	1.187	1.076	0.741	0.103	-0.917	-2.401	0.000
+ 0.26	1.000	0.980	1.056	1.146	1.172	1.053	0.709	0.061	-0.972	-2.470	0.000
+ 0.28	1.000	0.979	1.051	1.137	1.157	1.031	0.678	0.018	-1.028	-2.540	0.000
+ 0.30	1.000	0.977	1.047	1.129	1.142	1.008	0.646	-0.025	-1.083	-2.609	0.000
+ 0.32	1.000	0.976	1.043	1.120	1.127	0.985	0.613	-0.068	-1.139	-2.679	0.000
+ 0.34	1.000	0.975	1.038	1.111	1.112	0.962	0.581	-0.111	-1.195	-2.750	0.000
+ 0.36	1.000	0.973	1.034	1.102	1.097	0.939	0.548	-0.155	-1.251	-2.820	0.000
+ 0.38	1.000	0.972	1.029	1.093	1.081	0.916	0.516	-0.199	-1.308	-2.891	0.000
+ 0.40	1.000	0.970	1.025	1.083	1.066	0.892	0.483	-0.243	-1.364	-2.962	0.000

Figure E.10: $\beta = 50$, Problem BTable E.10: Data for $\beta = 50$, Problem B

	0.000	0.100	0.200	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
Con.	1.000	0.990	1.098	1.245	1.350	1.333	1.115	0.615	-0.246	-1.550	0.000
Opt.	1.000	0.990	1.098	1.244	1.349	1.333	1.115	0.615	-0.247	-1.550	0.000
+ 0.02	1.000	0.989	1.095	1.237	1.336	1.313	1.086	0.575	-0.298	-1.615	0.000
+ 0.04	1.000	0.988	1.091	1.230	1.323	1.292	1.056	0.536	-0.350	-1.680	0.000
+ 0.06	1.000	0.987	1.088	1.222	1.310	1.272	1.027	0.496	-0.402	-1.746	0.000
+ 0.08	1.000	0.986	1.084	1.214	1.297	1.251	0.997	0.455	-0.454	-1.812	0.000
+ 0.10	1.000	0.985	1.081	1.207	1.283	1.230	0.967	0.415	-0.507	-1.878	0.000
+ 0.12	1.000	0.984	1.077	1.199	1.270	1.209	0.937	0.374	-0.560	-1.945	0.000
+ 0.14	1.000	0.983	1.073	1.191	1.256	1.188	0.907	0.333	-0.613	-2.012	0.000
+ 0.16	1.000	0.982	1.070	1.183	1.242	1.167	0.877	0.292	-0.666	-2.079	0.000
+ 0.18	1.000	0.981	1.066	1.175	1.228	1.145	0.846	0.251	-0.720	-2.147	0.000
+ 0.20	1.000	0.980	1.062	1.167	1.214	1.123	0.815	0.210	-0.774	-2.215	0.000
+ 0.22	1.000	0.979	1.058	1.158	1.200	1.102	0.784	0.168	-0.828	-2.283	0.000
+ 0.24	1.000	0.977	1.054	1.150	1.185	1.080	0.753	0.126	-0.882	-2.351	0.000
+ 0.26	1.000	0.976	1.050	1.142	1.171	1.057	0.722	0.084	-0.937	-2.420	0.000
+ 0.28	1.000	0.975	1.046	1.133	1.156	1.035	0.690	0.041	-0.992	-2.489	0.000
+ 0.30	1.000	0.974	1.042	1.124	1.141	1.013	0.658	-0.001	-1.047	-2.558	0.000
+ 0.32	1.000	0.972	1.038	1.116	1.126	0.990	0.626	-0.044	-1.102	-2.628	0.000
+ 0.34	1.000	0.971	1.033	1.107	1.111	0.967	0.594	-0.087	-1.158	-2.697	0.000
+ 0.36	1.000	0.970	1.029	1.098	1.096	0.944	0.562	-0.131	-1.214	-2.767	0.000
+ 0.38	1.000	0.968	1.024	1.089	1.081	0.921	0.529	-0.174	-1.270	-2.838	0.000
+ 0.40	1.000	0.967	1.020	1.080	1.066	0.898	0.497	-0.218	-1.327	-2.909	0.000

