ANALYTICAL SOLUTION OF THE HERMITE COLLOCATION DISCRETIZATION OF THE STEADY-STATE CONVECTION-DIFFUSION EQUATION

Stephen H. Brill
Department of Mathematics
Boise State University
Boise, Idaho, U.S.A.
email: brill@math.boisestate.edu

Abstract

We give herein analytical formulas for the Hermite collocation solution of the steady-state convection-diffusion equation with constant coefficients defined on a uniform mesh in one spatial dimension. Both Dirichlet and Neumann boundary conditions are considered. Analysis is provided which compares the discrete collocation solution to the continuous solution. Unlike the solution obtained via the central difference discretization, the collocation solution is proven to be oscillation free, irrespective of the value of the Péclet number. For modest Péclet numbers, the collocation solution is shown to provide an excellent approximation to the solution of the continuous problem.

1 Introduction

In this paper, we study the numerical solution of the steady-state convection-diffusion equation

$$-D\frac{d^2u}{dx^2} + v\frac{du}{dx} = 0, \tag{1}$$

where the diffusion constant D and velocity constant v are both positive. In particular, we derive analytical formulas for the Hermite collocation solution of (1) on a uniform mesh.

It is well known (see, for example, [2]) that the solution of the standard central difference discretization of (1) exhibits oscillatory behavior that is not present in the continuous solution of (1). The formulas we derive show, in contrast, that the Hermite collocation solution of (1) does not suffer from these undesirable oscillations.

Although collocation has been widely studied, there has been very little work done on deriving analytical formulas for collocation discretizations of differential equations. In a previous paper ([1]) we give analytical formulas of the collocation solution of the ordinary differential equation (with appropriate boundary conditions)

$$\frac{d^2u}{dx^2} + \gamma u = 0,$$

where γ is a given constant. The present paper may be viewed as an extension of the previous one.

This paper is organized as follows. We first describe the collocation discretization of (1). We then derive analytic formulas for the solution of this discretization, from which we show that the collocation solution of (1) is oscillation free. We then compare the continuous solution and the collocation solution. After providing examples that illustrate the theory discussed herein, we conclude this paper with a short section summarizing our results.

2 Hermite Collocation Solution of Our Differential Equation

To begin, the differential equation (1) is defined on the interval $\mathcal{I} = [0, 1]$. Appropriate Dirichlet and/or Neumann boundary conditions are included. We partition the interval $\mathcal{I}$ into m uniform subintervals, each of length h, by $0 = x_0, x_1, x_2, \ldots, x_m = 1$. Note $x_j = jh$ and $mh = 1$.

The discretization proceeds by introducing a piecewise Hermite cubic interpolating polynomial

$$\widehat{u}(x) = \sum_{j=0}^{m} \left[u_j f_j(x) + u_j' g_j(x) \right]. \tag{2}$$

into the differential equation (1), obtaining

$$-D\frac{d^2\widehat{u}}{dx^2} + v\frac{d\widehat{u}}{dx} = E(x), \tag{3}$$

where $E(x)$ is an error function.

The Hermite basis functions, defined for $\eta \in \left[-\frac{1}{2}, \frac{1}{2}\right]$, are

$$f_j(x) = \begin{cases} f_L(\eta) = \frac{1}{2}(1+2\eta)^2(1-\eta), & x_{j-1} \le x = x_j + \left(\eta - \frac{1}{2}\right)h \le x_j \\ f_R(\eta) = \frac{1}{2}(1-2\eta)^2(1+\eta), & x_j \le x = x_j + \left(\eta + \frac{1}{2}\right)h \le x_{j+1} \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

and

$$g_j(x) = \begin{cases} g_L(\eta) = \frac{h}{8}(2\eta+1)^2(2\eta-1), & x_{j-1} \le x = x_j + \left(\eta - \frac{1}{2}\right)h \le x_j \\ g_R(\eta) = \frac{h}{8}(2\eta-1)^2(2\eta+1), & x_j \le x = x_j + \left(\eta + \frac{1}{2}\right)h \le x_{j+1} \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

Note that $\hat{u}$ in (2) interpolates the values $u_j = u(x_j)$ and $u'_j = \frac{du}{dx}(x_j)$, $j = 0, 1, \ldots, m$, because $f_j(x_k) = \delta_{jk}$, $\frac{df_j}{dx}(x_k) = 0$, $g_j(x_k) = 0$, and $\frac{dg_j}{dx}(x_k) = \delta_{jk}$. Here δ_{jk} is the Kronecker symbol.

It is clear that (3) has $2(m+1)$ coefficients, namely u_j and u'_j, $j = 0, 1, 2, \ldots m$. However, the imposition of boundary conditions reduces this number to $2m$. To generate the $2m$ equations necessary to find these undetermined coefficients, we enforce that the error function $E(x)$ in (3) is identically zero at two distinct "collocation points" in the interior of each of the m subintervals.

Given certain smoothness conditions, the optimal (in terms of minimizing discretization error) location of the collocation points within each subinterval corresponds to the points of Gaussian quadrature [3]. In this work, we will use these optimal collocation points, which correspond to choosing the collocation points as $\eta = \pm \frac{1}{\sqrt{12}}$ (see (4) and (5)) in each subinterval $\left[-\frac{1}{2}, \frac{1}{2}\right]$ (given in local η coordinates).

It is straightforward to see that choosing the collocation points in this manner leads to a matrix equation with the repeated computational molecule

$$\begin{bmatrix} \frac{2\sqrt{3}D}{h^2} - \frac{v}{h} & \frac{(1+\sqrt{3})D}{h} + \frac{v}{2\sqrt{3}} & \frac{-2\sqrt{3}D}{h^2} + \frac{v}{h} & \frac{(-1+\sqrt{3})D}{h} - \frac{v}{2\sqrt{3}} \\ \frac{-2\sqrt{3}D}{h^2} - \frac{v}{h} & \frac{(1-\sqrt{3})D}{h} - \frac{v}{2\sqrt{3}} & \frac{2\sqrt{3}D}{h^2} + \frac{v}{h} & \frac{(-1-\sqrt{3})D}{h} + \frac{v}{2\sqrt{3}} \end{bmatrix} \begin{bmatrix} q_j \\ r_j \\ q_{j+1} \\ r_{j+1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{6}$$

for $j = 0, 1, 2, \ldots, m-1$. Here $q_j = u_j$ and $r_j = u'_j$, $j = 0, 1, 2, \ldots, m$. Note that the matrix equation represented by (6) is a system of $2m$ equations in $2(m+1)$ unknowns.

3 Analytical Solution of Collocation Discretization

We begin by separately adding the two equations in (6) together and then subtracting the first from the second. We then multiply each term in the first of these equations (i.e., the one obtained via addition) by $\frac{6h}{D}$ and multiply each term in the second of these equations (i.e., the one obtained via subtraction) by $\frac{-\sqrt{3}h^2 v}{D^2}$, producing the molecule

$$\begin{bmatrix} -\frac{12\beta}{h} & 12 & \frac{12\beta}{h} & -12 \\ \frac{12\beta}{h} & 6\beta + \beta^2 & -\frac{12\beta}{h} & 6\beta - \beta^2 \end{bmatrix} \begin{bmatrix} q_j \\ r_j \\ q_{j+1} \\ r_{j+1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{7}$$

$j = 0, 1, 2, \ldots, m-1$. The dimensionless parameter $\beta = \frac{hv}{D}$ is known as the Péclet number.

If we now add the two equations in (7) together, we eliminate q_j and q_{j+1}, obtaining

$$r_{j+1} = \rho\, r_j, \tag{8}$$

where

$$\rho = \frac{\beta^2 + 6\beta + 12}{\beta^2 - 6\beta + 12}. \tag{9}$$

Additionally, manipulation of the first equation in (7) yields the relation

$$q_{j+1} - q_j = \frac{h}{\beta}(r_{j+1} - r_j). \tag{10}$$

We now use (8) and (10), combined with appropriate boundary conditions, to determine formulas for q_j and r_j, in terms of only the boundary conditions, the parameter ρ, the Péclet number β, and the number of subintervals m. We note that the use of a Neumann-type boundary condition at both endpoints of the domain of the differential equation (1) results in an ill-posed problem and thus this case will not be considered further.

Below we consider separately the three remaining combinations of Dirichlet and Neumann boundary conditions. The formula for the sum of a finite geometric series

$$\sum_{k=0}^{\ell-1} \rho^k = \frac{\rho^\ell - 1}{\rho - 1} \tag{11}$$

will be used in each case.

3.1 Case I: $u(0) = q_0 = b_0$ and $u(1) = q_m = b_1$.

Repeated application of (8) gives

$$r_j = \rho^j r_0; \tag{12}$$

thus

$$r_{j+1} - r_j = (\rho - 1)\rho^j r_0.$$

Therefore, letting

$$\alpha = \frac{h}{\beta}(\rho - 1) r_0, \tag{13}$$

we obtain from (10)

$$q_{j+1} = q_j + \alpha \rho^j. \tag{14}$$

Using (11) and (14), we now write, for $j = 1, 2, 3, \ldots, m$,

$$q_j = q_0 + \alpha \, \frac{\rho^j - 1}{\rho - 1}; \tag{15}$$

thus, from (13) we arrive at (for $j = m$)

$$r_0 = \frac{\beta(b_1 - b_0)}{h(\rho^m - 1)}. \tag{16}$$

Therefore, using (12), we have

$$r_j = \frac{\beta m(b_1 - b_0)}{\rho^m - 1} \, \rho^j. \tag{17}$$

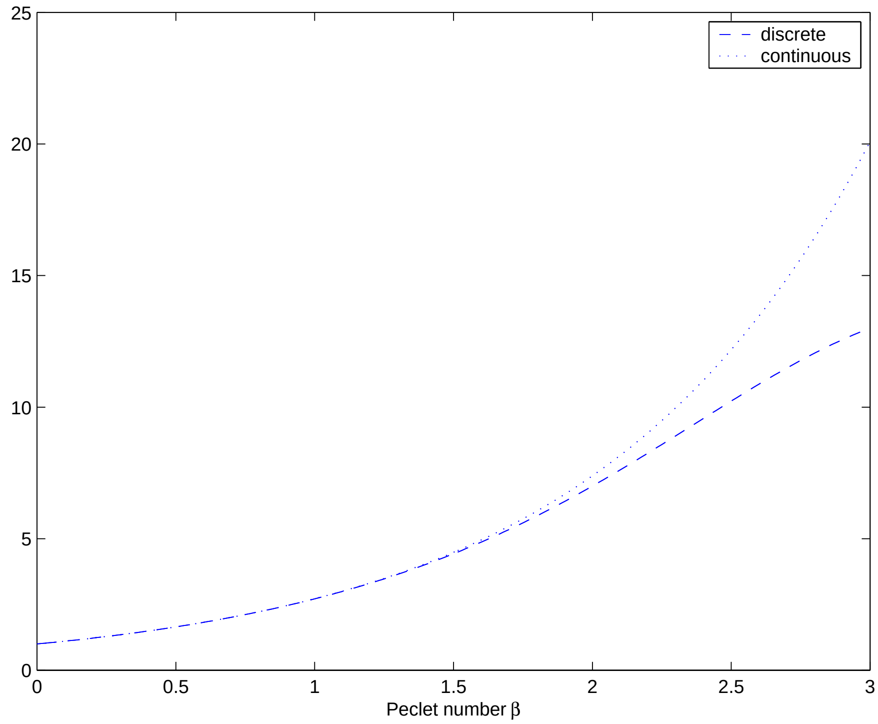

Figure 1: e^{β} (continuous) and $\rho = \dfrac{\beta^2 + 6\beta + 12}{\beta^2 - 6\beta + 12}$ (discrete)

In addition, it follows directly from (13), (15), and (16) that

$$q_j = b_0 + \frac{b_1 - b_0}{\rho^m - 1}(\rho^j - 1). \tag{18}$$

With the boundary conditions under consideration, the continuous solution of (1) and its derivative with respect to x, both evaluated at $x_j = jh = \frac{j}{m}$, are

$$u(x_j) = b_0 + \frac{b_1 - b_0}{e^{\beta m} - 1}\left(e^{\beta j} - 1\right) \tag{19}$$

(compare to (18)) and

$$u'(x_j) = \frac{\beta m (b_1 - b_0)}{e^{\beta m} - 1}\, e^{\beta j} \tag{20}$$

(compare to (17)).

3.2 Case II: $u(0) = q_0 = b_0$ and $u'(1) = r_m = b'_1$.

Repeated application of (8) gives

$$r_j = b'_1\, \rho^{j-m}. \tag{21}$$

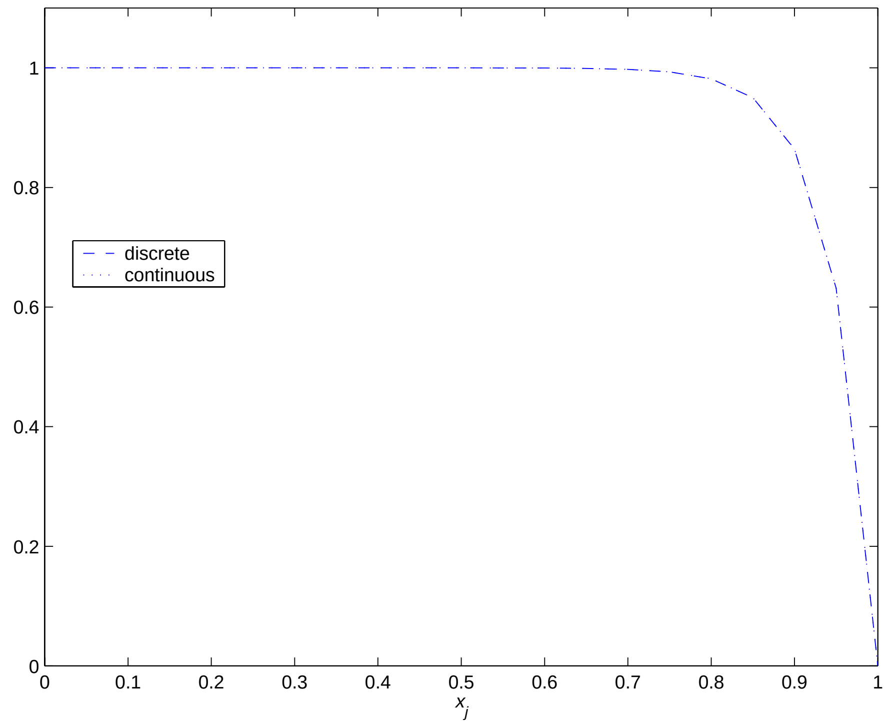

Figure 2: Comparison of discrete and continuous solutions: $\beta = 1$

Also, using (8), we obtain

$$r_{j+1} - r_j = (\rho - 1)\, r_j.$$

Thus, using (10) and (21), we have

$$q_{j+1} = q_j + \frac{h}{\beta}(\rho - 1)\, b'_1\, \rho^{j-m}. \tag{22}$$

Using (11) and (22), we conclude, for $j = 1, 2, 3, \ldots, m$,

$$q_j = b_0 + \frac{b'_1}{\beta m \rho^m}(\rho^j - 1). \tag{23}$$

With the boundary conditions under consideration, the continuous solution of (1) and its derivative with respect to x, both evaluated at $x_j = jh = \frac{j}{m}$, are

$$u(x_j) = b_0 + \frac{b'_1}{\beta m e^{\beta m}}(e^{\beta j} - 1) \tag{24}$$

(compare to (23)) and

$$u'(x_j) = b'_1 e^{\beta(j-m)} \tag{25}$$

(compare to (21)).

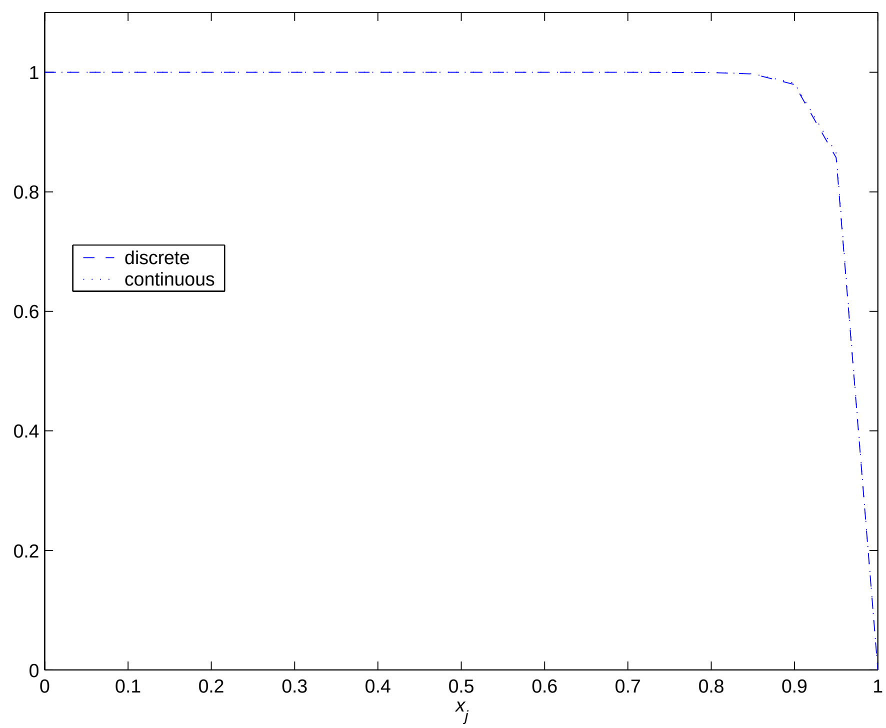

Figure 3: Comparison of discrete and continuous solutions: $\beta = 2$

3.3 Case III: $u'(0) = r_0 = b'_0$ and $u(1) = q_m = b_1$.

Repeated application of (8) gives

$$r_j = b'_0\, \rho^j. \tag{26}$$

Using (10) and (26) provides

$$q_j = q_{j+1} - \frac{(\rho - 1)b'_0}{\beta m} \rho^j$$

which, in combination with (11), gives

$$q_j = b_1 + \frac{b'_0}{\beta m}(\rho^j - \rho^m). \tag{27}$$

With the boundary conditions under consideration, the continuous solution of (1) and its derivative with respect to x, both evaluated at $x_j = jh = \frac{j}{m}$, are

$$u(x_j) = b_1 + \frac{b'_0}{\beta m}(e^{\beta j} - e^{\beta m}) \tag{28}$$

(compare to (27)) and

$$u'(x_j) = b'_0 e^{\beta j} \tag{29}$$

(compare to (26)).

4 Analysis

In this section we provide two analyses. We prove that the collocation discretization of (1) is oscillation free, which is in contrast to central differencing. We then compare the accuracy of the discrete collocation solution with respect to the continuous solution.

4.1 No Oscillations in Collocation

For Péclet numbers greater than 2, the standard central difference discretization of (1) produces spurious oscillations. For example, let the boundary conditions be $u(0) = 0$ and $u(1) = 1$. If we let q_j^{CD} be the central difference approximation to $u(x_j)$, then the solution obtained is (for $\beta \neq 2$) [2]

$$q_j^{CD} = \frac{\lambda^j - 1}{\lambda^m - 1},$$

where

$$\lambda = \frac{2 + \beta}{2 - \beta}.$$

If $\beta > 2$, then $\lambda < -1$. Thus q_j^{CD} and q_{j+1}^{CD} have opposite signs; i.e., the central difference solution oscillates. On the other hand, the continuous solution of the boundary value problem is (take (19) with $b_0 = 0$ and $b_1 = 1$)

$$u(x_j) = \frac{e^{\beta j} - 1}{e^{\beta m} - 1},$$

which, since $\beta > 0$, is monotonic.

With respect to (18), (23), and (27), it is clear that the issue of whether the collocation solution oscillates rests on the behavior of ρ^j. However, since the Péclet number β is always positive, it is easy to show that ρ, defined in (9), is always greater than unity. Thus the collocation solution cannot oscillate.

4.2 Comparison of Collocation and Continuous Solutions

When we compared the discrete collocation solution to the continuous solution in the previous subsection, in all instances the relevant difference between the two was that the role of e^β in the continuous solution was played by ρ in the collocation solution. To see how good an approximation ρ is to e^β, we expand each in a Taylor series about $\beta = 0$:

$$\rho = 1 + \beta + \frac{1}{2}\beta^2 + \frac{1}{6}\beta^3 + \frac{1}{24}\beta^4 + \frac{1}{144}\beta^5 + \mathcal{O}(\beta^6)$$

$$e^\beta = 1 + \beta + \frac{1}{2}\beta^2 + \frac{1}{6}\beta^3 + \frac{1}{24}\beta^4 + \frac{1}{120}\beta^5 + \mathcal{O}(\beta^6)$$

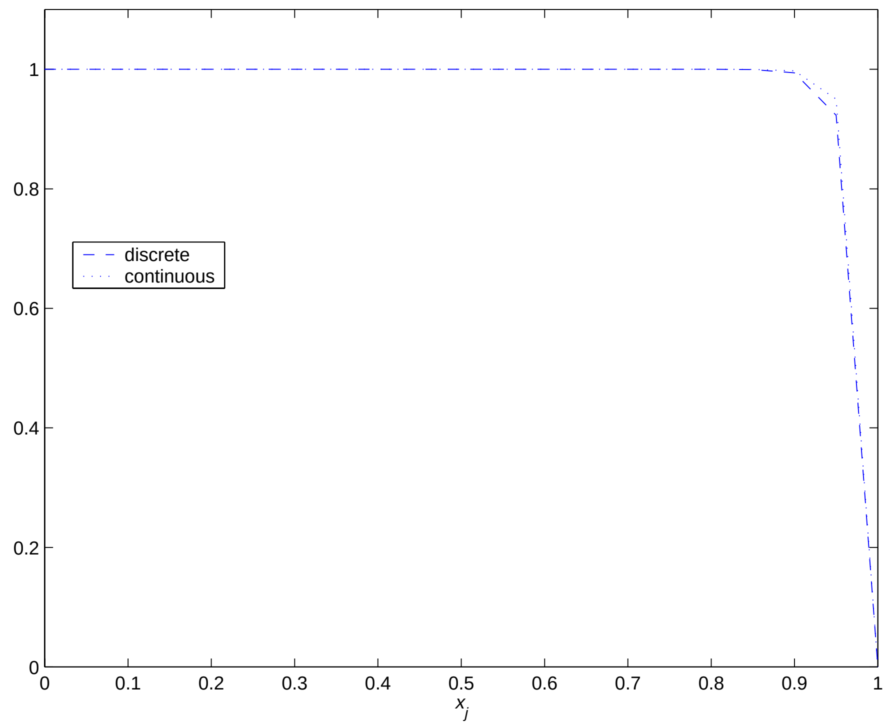

Figure 4: Comparison of discrete and continuous solutions: $\beta = 3$

The graphs of these two functions are given in Figure 1.

By examining Figure 1, we see that ρ and e^{β} are visually indistinguishable for $0 < \beta < 1.5$. As β increases from 1.5, the approximation of e^{β} that ρ provides worsens. Thus we expect the collocation solution of (1) to do an excellent job approximating the continuous solution for Péclet numbers less than 1.5. As we let the Péclet number increase from 1.5, we expect that the collocation approximation to the continuous solution becomes commensurately of poorer quality.

5 Examples

Here we provide numerical evidence to support the theoretical conclusions we made in the previous paragraph. We solve the differential equation (1) with boundary conditions $u(0) = 1$ and $u(1) = 0$. For all examples, we use $m = 20$ and $D = 0.025$. We select v to produce Péclet numbers $\beta = 1, 2, 3, 6, 12$. The graphs in Figures 2 through 6 are obtained by plotting the values q_j and $u(x_j)$. In all cases, the data for the discrete collocation solution (the q_j's) are interpolated linearly using a dashed line while the data for the continuous solution (the $u(x_j)$'s) are interpolated linearly using a dotted line.

In examining Figures 2 through 6, we see that for Péclet numbers $\beta = 1$ and $\beta = 2$, the discrete and continuous solutions are visually indistinguishable. When

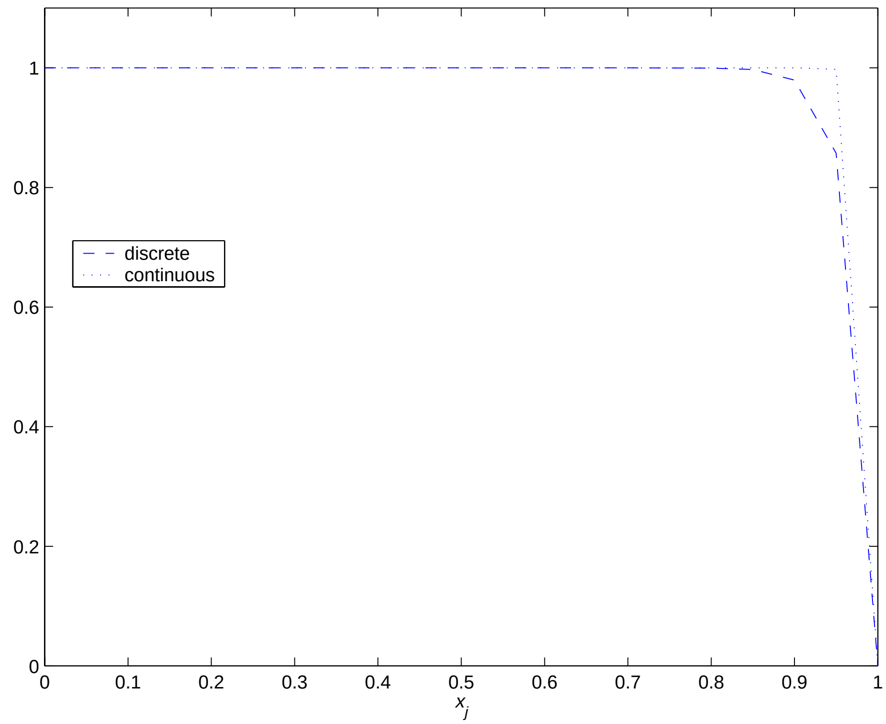

Figure 5: Comparison of discrete and continuous solutions: $\beta = 6$

$\beta = 3$, we see a small difference between the two solutions at $x_j = 0.95$. When the Péclet number increases to 6 and then to 12, the differences between the discrete and continuous solutions become more pronounced. This is consistent with the behavior observed in Figure 1, where the approximation of e^β produced by the collocation method (i.e., ρ) becomes progressively worse as β increases from the value 2.

We observe also that when the discrete and continuous solutions diverge from each other, it is near the right-hand boundary condition. This is due to the fact that both continuous and discrete solutions are exponential in nature: as the exponent j increases, the difference between ρ^j and $e^{\beta j}$ increases commensurately (see (18) and (19)). Furthermore, as β increases, the rapid change that the continuous solution exhibits near $x = 1$ becomes more pronounced. However, the discrete collocation solution is not capable of capturing this sharp front for larger values of β. Qualitatively, we may say that the collocation solution "smears" the sharp solution profile of the continuous solution (for larger values of the Péclet number).

6 Summary and conclusions

In this work we derived analytical solutions of the Hermite collocation discretization of the one-dimensional steady-state convection-diffusion equation with constant coefficients defined on a uniform mesh. All possible combinations of Dirichlet and

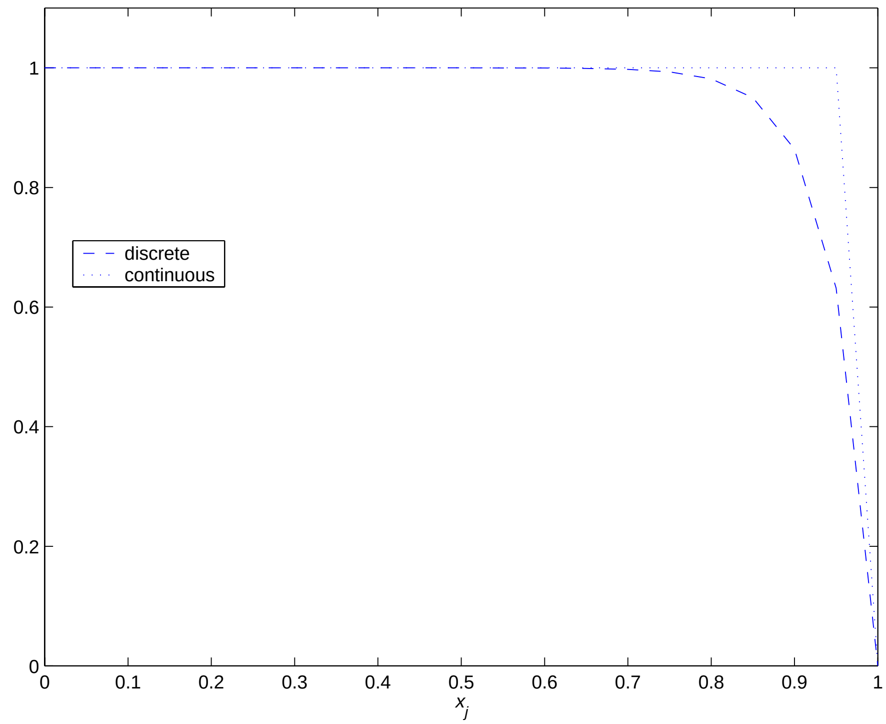

Figure 6: Comparison of discrete and continuous solutions: $\beta = 12$

Neumann boundary conditions were considered. The collocation solution was proven to be oscillation free, unlike the standard central difference discretization. Excellent agreement between continuous and discrete collocation solutions may be expected when the Péclet number is no greater than 2. However, for Péclet numbers beyond this value, agreement between continuous and discrete solutions deteriorates, particularly at values near the right end of the domain.

References

[1] S. H. Brill, Analytical Solution of Hermite Collocation Discretization of Self-Adjoint Ordinary Differential Equations, submitted to *Mathematics of Computation*.

[2] K. W. Morton, *Numerical Solution of Convection-Diffusion Problems*, Chapman, London (1996).

[3] P. M. Prenter, *Splines and Variational Methods*, John Wiley & Sons, New York (1975).