Optimal Hermite Collocation Solution of a Forced Convection-Diffusion Equation

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We give herein analytical formulas for the solution of the Hermite collocation discretization of a forced steady-state convection-diffusion equation in one spatial dimension and with constant coefficients, defined on a uniform mesh with Dirichlet boundary conditions. The accuracy of the method is enhanced by optimally employing “upstream weighting” of the convective term and optimally sampling the forcing function, avoiding both the “smearing” effect of numerical diffusion and unwanted oscillations, particularly for large Péclet numbers. Computational examples illustrate the efficacy of our approach.

1. INTRODUCTION

Convection-diffusion differential equations (DEs) arise in many areas of science and engineering, including transport of contaminants in groundwater. It is well known that the numerical solution of such equations is a difficult task when convection is the dominant process. Numerical techniques often give rise to spurious oscillations that are not present in the continuous (i.e., not numerical/discrete) solution of the DE. To ameliorate these physically unmeaningful (and therefore undesirable) oscillations, the technique of upstream weighting is often used ([1], [6]). While upstreaming can eliminate the oscillations, it is often at the expense of “smearing” the sharp solution profile of the continuous solution of the DE.

In this work, we study the convection-diffusion equation

$$-D\frac{d^2u}{dx^2} + v\frac{du}{dx} = S(x) \tag{1}$$

with Dirichlet boundary conditions, defined on the interval $[0,1]$. The convection coefficient v and diffusion coefficient D are both positive constants. For the purposes of numerical solution, we subdivide the domain $[0,1]$ into m equal subintervals and thus seek to solve (1) at the nodes $x_j = jh$, $j = 0, 1, 2, \ldots, m$, where $h = 1/m$.

In a previous work [3], we considered the case where the forcing function $S(x) \equiv 0$. Thus the present paper may be viewed as its logical extension.

This work is organized as follows. We begin with a brief discussion of Hermite collocation and how its standard implementation is changed for our purposes. We then provide the analytical solution of the matrix equation that arises from the Hermite collocation discretization of the DE (1), when upstream weighting is utilized. Subsequently, we give the result, derived in [3], that describes how to optimally select the upstream parameter

ζ. Next, we discuss optimal sampling of the forcing function $S(x)$. We then provide several computational examples which illustrate the theory. A short section summarizing our results concludes the paper.

2. PRELIMINARIES

Hermite collocation may be viewed as an example of the "Method of Weighted Residuals" (see [5]), where the basis functions are the standard cubic Hermite interpolating polynomials and the weighting functions are Dirac δ functions. Thus the method provides approximations q_j to $u(x_j)$ and r_j to $\frac{du}{dx}(x_j)$ at the $m+1$ nodes $x_j = jh$, $j = 0, 1, 2, \ldots, m$.

In the study of convection-diffusion DEs, the Péclet number β plays a fundamental role. It is defined as

$$\beta = \frac{vh}{D}.$$

In standard (also known in the literature as "orthogonal") collocation, all terms in (1) are evaluated at the points of Gaussian quadrature (the Gauss points) which, for a problem whose solution is sufficiently smooth, provides the greatest accuracy [4][7]. However, for our problems of interest which involve large Péclet numbers, the smoothness conditions of [4] and [7] are not met. We utilize the approach first given in [1] and then used successfully in [3], whereby only the second derivative term in (1) is evaluated at the Gauss points. The first derivative term in (1) is, in general, evaluated at some constant distance ζ to the left of the Gauss points. The value of ζ can vary from zero (in which case there is no upstreaming) to a maximum value of $\frac{1}{2} - \frac{1}{\sqrt{12}}$. The issue of how to optimally choose ζ as a function of β is discussed fully in [3].

The issue of where best to evaluate the forcing function $S(x)$ of (1) has, to our knowledge, not been studied in the literature. In this paper, we do give some preliminary results that pertain to this matter.

3. ANALYTICAL SOLUTION OF UPSTREAM COLLOCATION

We now give the main result of this paper. The proof of this result is completely straightforward, though computationally tedious.

Theorem 1 *The collocation solution of (1), combined with Dirichlet boundary conditions, is*

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

$$r_j = \rho\, c_2\,\lambda^j + \frac{1}{2m}\sum_{k=0}^{2m-1} G'_{k,j} S_k, \tag{3}$$

where c_1 and c_2 are constants determined by boundary conditions,

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

and

$$\lambda = \frac{\beta^2 + 6\beta + 12 + 6\beta\zeta(4 + \beta + \beta\zeta)}{\beta^2 - 6\beta + 12 + 6\beta\zeta(4 - \beta + \beta\zeta)}. \tag{5}$$

Additionally, $S_k = S(c_k)$ is the value of the forcing function at the kth point c_k at which $S(x)$ is evaluated. Finally, the discrete Green's functions $G_{k,j}$ and $G'_{k,j}$ for $j = 0, 1, 2, \ldots, m$ and $k = 0, 1, 2, \ldots, 2m-1$ are given by

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

and

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

Here

$$C_k = \begin{cases} \dfrac{1 + \beta\zeta - \sqrt{3}\beta\zeta^2}{(1+\beta\zeta)v} & \text{if } k \text{ is even} \\[2ex] \dfrac{1 + \beta\zeta + \sqrt{3}\beta\zeta^2}{(1+\beta\zeta)v} & \text{if } k \text{ is odd,} \end{cases}$$

$$A_{2j} = \frac{(1 + \beta\zeta - \sqrt{3}\beta\zeta^2)\lambda_{num}\lambda^j + \rho_{den}(-6 - \sqrt{3}\beta - 6\beta\zeta + 6\sqrt{3}\beta\zeta^2)}{v\lambda^j Q(\lambda^m - 1)},$$

$$A_{2j+1} = \frac{(1 + \beta\zeta + \sqrt{3}\beta\zeta^2)\lambda_{num}\lambda^j + \rho_{den}(-6 + \sqrt{3}\beta - 6\beta\zeta - 6\sqrt{3}\beta\zeta^2)}{v\lambda^j Q(\lambda^m - 1)},$$

$$Q = 12 + 6\beta + \beta^2 + 36\beta\zeta + 12\beta^2\zeta + \beta^3\zeta + 30\beta^2\zeta^2 + 6\beta^3\zeta^2 + 6\beta^3\zeta^3 m$$

and ρ_{den} and λ_{num} are, respectively, the denominator of (4) and numerator of (5).

The points c_k, $k = 0, 1, 2, \ldots, 2m-1$, must satisfy the linear constraints

$$x_0 \le c_0 \le c_1 \le x_1 \le c_2 \le c_3 \le x_2 \le \cdots \le x_{m-1} \le c_{2m-2} \le c_{2m-1} \le x_m \tag{6}$$

with respect to the nodes.

Since we are given the Dirichlet boundary conditions $u(0) = q_0 = b_0$ and $u(1) = q_m = b_1$ we conclude from (2) with $j = 0, m$, that $c_2 = \frac{b_1 - b_0}{\lambda^m - 1}$ and $c_1 = b_0 - \frac{b_1 - b_0}{\lambda^m - 1}$.

4. OPTIMAL UPSTREAM WEIGHTING

In [3], we considered the only the homogeneous problem (i.e., when the forcing function $S(x) \equiv 0$ in (1)). In that work, we determined how to choose the upstream parameter ζ as a function of the Péclet number β in an optimal fashion and in such a way as to avoid any spurious oscillations in the collocation solution. The algorithm is given in Table 1 and depicted in Figure 1.

It should be noted that the number ϵ in the final entry of Table 1 is a small positive number large enough to ensure that the computed value of $\frac{1}{2} - \frac{2}{\beta} - \frac{\sqrt{\beta^2 - 12\beta + 24}}{\sqrt{12\beta}} - \epsilon$ is indeed smaller than that of $\frac{1}{2} - \frac{2}{\beta} - \frac{\sqrt{\beta^2 - 12\beta + 24}}{\sqrt{12\beta}}$. For the results given in [3], we used $\epsilon = 10^{-6}$.

Table 1
Optimal ζ as a function of β.

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

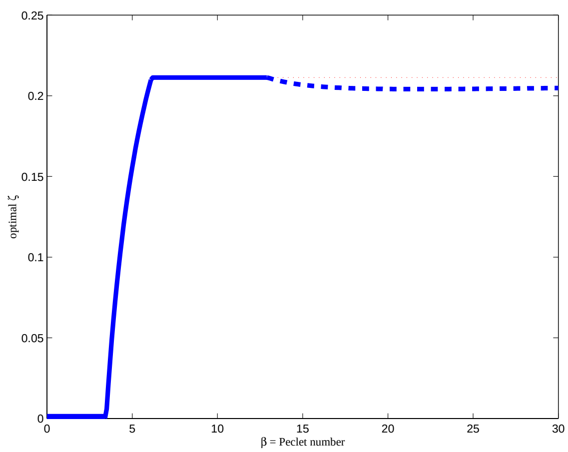

Figure 1. Optimal ζ as a function of β.

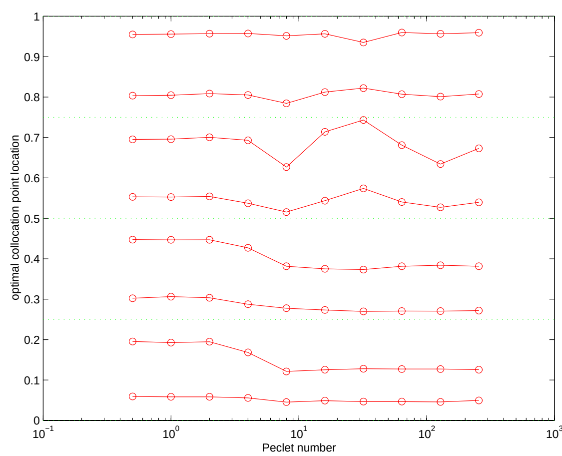

Figure 2. Optimal locations for forcing function evaluation as a function of Péclet number.

5. NUMERICAL EXPERIMENTS

Numerical experiments in [3] deal with only the homogeneous version of (1). In discussing these results, we will confine ourselves only with the nonhomogeneous term $S(x)$. In some sense we are "cheating" in compiling these results, as we will use knowledge of the continuous solution of the boundary value problem (BVP) as a guide. However, the results are sufficiently promising to motivate future work in which we will not "cheat".

Specifically, we study the collocation solution of the BVP

$$\begin{cases} -D\dfrac{d^2u}{dx^2} + 10\dfrac{du}{dx} = 10 - 20x \\ u(0) = 1 \\ u(1) = 0 \end{cases} \tag{7}$$

with $m = 4$ and where D is chosen to obtain Péclet numbers of the form 2^k, for $k = -1, 0, 1, \ldots, 8$. When appropriate, we used $\epsilon = 10^{-5}$. (Using $\epsilon = 10^{-6}$, as was done in [3], led to catastrophic roundoff error.) For each value of D, we compute q_j, $j = 1, 2, 3, \ldots, m-1$ from (2). Note that these q_j's each depend on $c_0, c_1, c_2, \ldots, c_{2m-1}$. Now, because of the nature of the differential equation in (7), we can compute its continuous analytical solution $u(x)$ at each of the nodes x_j. Since each q_j should approximate the corresponding $u(x_j)$, we seek to find the values of $c_0, c_1, c_2, \ldots, c_{2m-1}$ that minimize the maximum value of $|u(x_j) - q_j|$, subject to the linear constraints (6). Actually, since we consider that the homogeneous part of this problem has been solved in [3], we consider only the nonhomogeneous portions of $u(x_j)$ and q_j in the "minimax" problem described above.

We solve this minimax problem using the function `fminimax` as found in the "Optimization Toolbox" in the MATLAB software package. The solution of the minimax problem, i.e., the locations at which we should sample the forcing function, are depicted in Figure 2. We note that optimal sampling points are very close to the Gauss points for small values of the Péclet number. As β increases, the optimal points move away from their Gaussian locations.

Now using these optimal locations, we then compute q_j, $j = 1, 2, 3, \ldots, m-1$, from (2). We then show these values of q_j, along with the continuous solution of the corresponding BVP in Figures 3 to 12. In examining these figures, we see that for almost all examples, the discrete collocation solution (depicted by the circles) and the continuous solution (depicted by the solid curve) are visually indistinguishable. In the case where $\beta = 4$ (i.e., in Figure 6), where the error is visually detected, the source of this error is to be found in the homogeneous part of the problem, not in the nonhomogeneous part which is addressed by our optimization routine.

6. SUMMARY AND CONCLUSIONS

Herein we give analytical formulas for the Hermite collocation solution of the one-dimensional nonhomogeneous convection-diffusion equation defined on a uniform mesh with Dirichlet boundary conditions. We collocate the diffusion term at the Gauss points, the convective term at optimal locations determined in [3], and the forcing function at optimal locations determined by optimization software. Especially for large Péclet numbers, the discrete collocation solution is visually indistinguishable from the continuous solution.

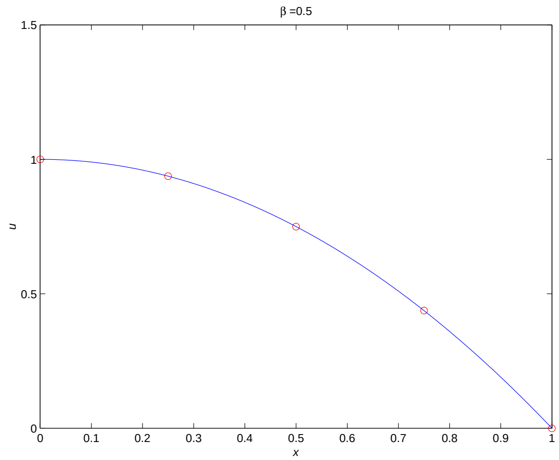

Figure 3. Continuous and discrete collocation solutions: $\beta = 0.5$.

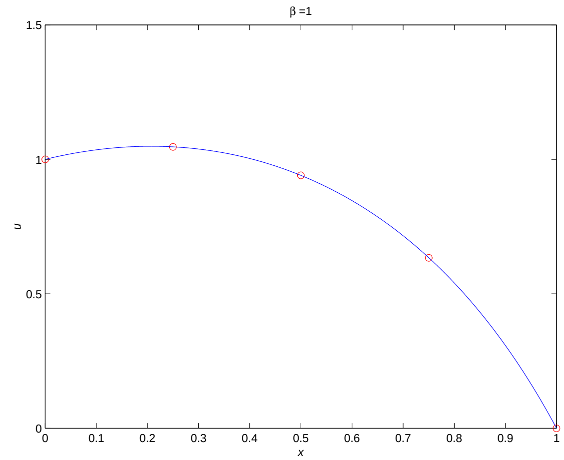

Figure 4. Continuous and discrete collocation solutions: $\beta = 1$.

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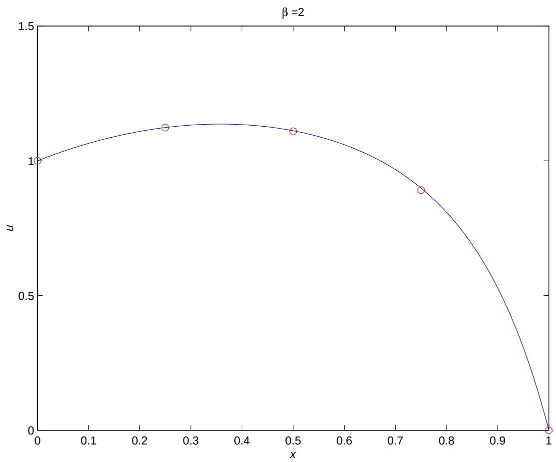

Figure 5. Continuous and discrete collocation solutions: $\beta = 2$.

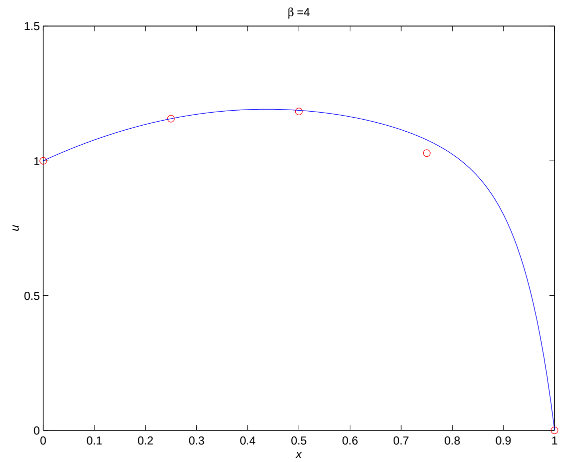

Figure 6. Continuous and discrete collocation solutions: $\beta = 4$.

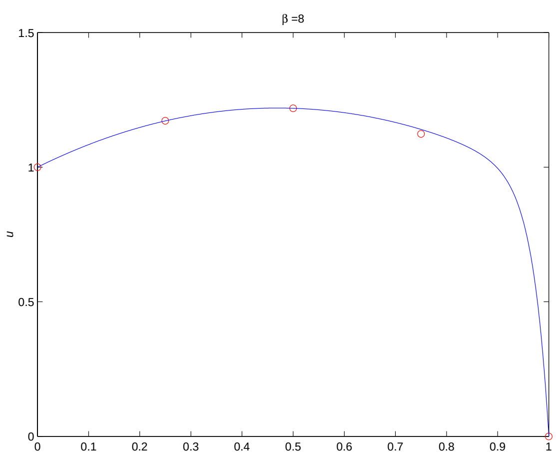

Figure 7. Continuous and discrete collocation solutions: $\beta = 8$.

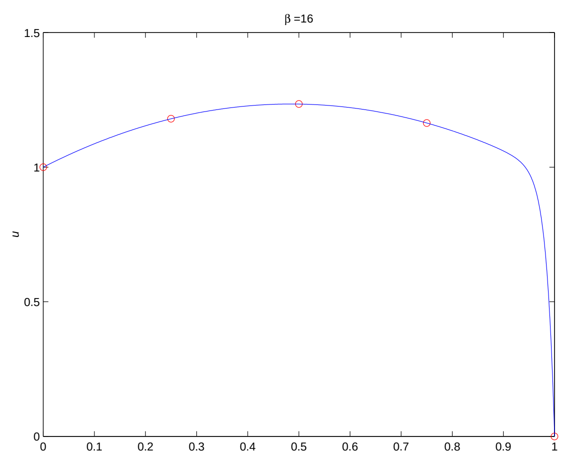

Figure 8. Continuous and discrete collocation solutions: $\beta = 16$.

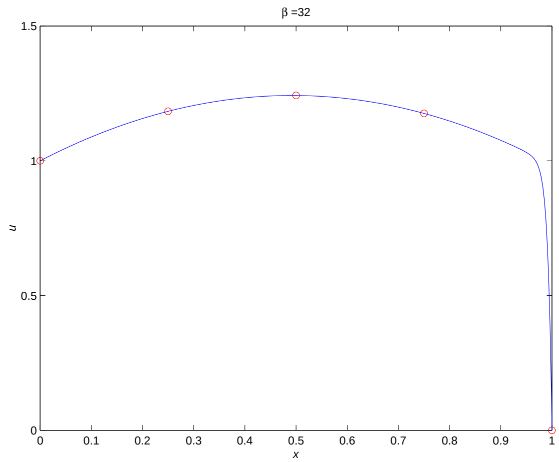

Figure 9. Continuous and discrete collocation solutions: $\beta = 32$.

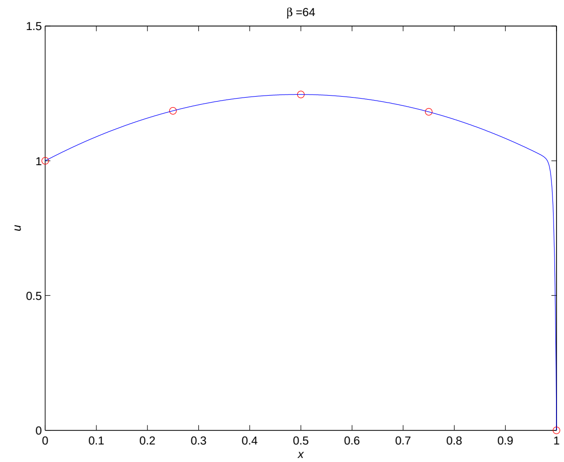

Figure 10. Continuous and discrete collocation solutions: $\beta = 64$.

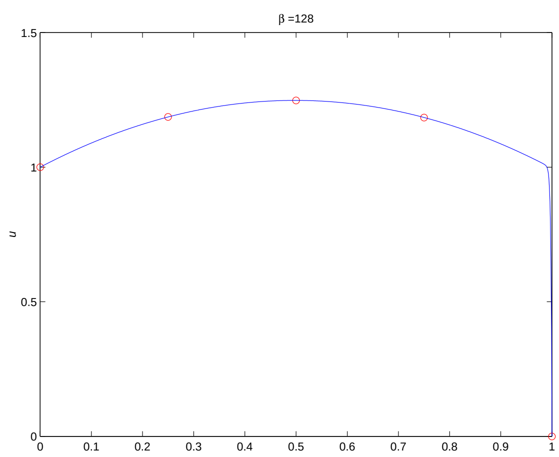

Figure 11. Continuous and discrete collocation solutions: $\beta = 128$.

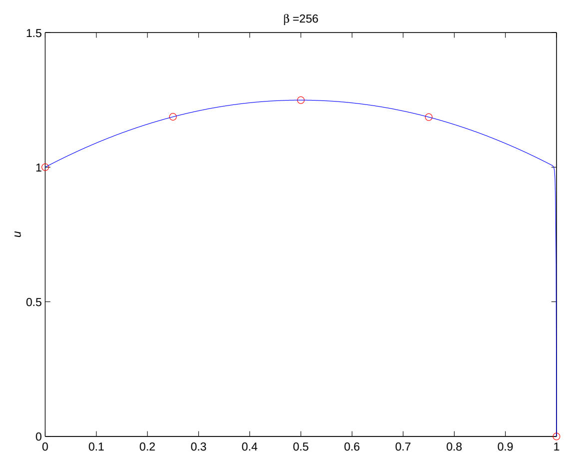

Figure 12. Continuous and discrete collocation solutions: $\beta = 256$.