SOLUTION OF BOUNDARY-VALUE PROBLEMS BY ORTHOGONAL COLLOCATION

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Summary—New collocation methods are given for solving symmetrical boundary-value problems. Orthogonality conditions are used to select the collocation points. The accuracy obtained is comparable to that of least squares or variational methods and the calculations are simpler. Applications are given to one-dimensional eigenvalue problems and to parabolic and elliptic partial differential equations, encountered in problems of viscous flow, heat transfer and diffusion with chemical reaction.

Résumé—De nouvelles méthodes de classement sont données pour résoudre des problèmes symétriques de valeurs à la limite. Pour sélectionner ces points de classement on utilise des conditions d'oirthogonalité. La précision obtenue est comparable à celle des méthodes des carrés minima ou des variations et les calculs sont plus simples. Des applications sont données pour des problèmes de valeur caractéristic à une dimension et pour des équations partielles differentielles paraboliques et elliptiques rencontré dans les problèmes d'écoulement visqueux, de transfert de chaleur et de diffusion avec réaction chimique.

Zusammenfassung—Es werden neue Kollokationsmethoden zur Lösung symmetrischer Grenzwert-Probleme angegeben. Dabei werden Orthogonalitätsbedingungen zur Wahl der Kollokationspunkte verwendet Die erzielte Genauigkeit ist der Methode der kleinsten Quadrate bzw. der Variationals-Methode vergleichbar und die Berechnungen sind einfacher. Die Methoden werden auf eindimensionale Eigenwert-probleme und auf parabolische und elliptische Teil-Differentialgleichungen angewandt, wie man sie bei Problemen des viskosen Flusses, der Wärmeübertrangung und der Diffusion mit chemischer Reaktion antrifft.

INTRODUCTION

Trial-function expansions are widely used in solving boundary-value problems. The expansion coefficients are typically determined by variational principles or by weighted-residual methods [1–8], the latter being the more widely applicable. These methods are attractive because of the compactness of the results, as compared with conventional finite difference solutions. The finite-difference computations, on the other hand, are more easily automated. Here the conveniences of the two approaches are combined by using orthogonal polynomial expansions, fitted by collocation techniques.

Collocation methods have been used for more than 40 years to solve integral equations. They were apparently first applied to differential equations by Frazer *et al.* [9] and independently by Lanczos [10, 11]. The basic procedure for differential equations is as follows. Consider an unknown function $y(\mathbf{x})$ which satisfies the linear or non-linear differential equation

$$L^V(y) = 0 \quad \text{in } V \tag{1}$$

and the linear or non-linear boundary condition

$$L^S(y) = 0 \quad \text{on } S \tag{2}$$

where $\mathbf{x}$ is the position vector and S is a boundary adjoining the volume V. The dependent variable y is approximated by a series expansion $y^{(n)}$ containing n undetermined parameters; the parameters are then determined by applying eq. (1) or eq. (2) at each of n selected points.

Three classes of collocation methods are recognized. *Interior collocation* requires a function $y^{(n)}$ which satisfies the boundary conditions identically; the function is adjusted to satisfy eq. (1) at n points in V. *Boundary collocation* requires a function $y^{(n)}$ which satisfies the differential equation identically; the function is adjusted to satisfy eq. (2) at n points on S. *Mixed collocation* employs collocation points in both regions and is used when $y^{(n)}$ satisfies neither of the given equations. The present paper deals mainly with interior and boundary methods.

Comparatively little has been done on criteria for selecting the collocation points. An equidistant spacing is not generally appropriate, in view of the Runge divergence phenomenon [11] for equidistant polynomial interpolation. Lanczos [11] has pointed out that for one-dimensional problems in $-1 < x < 1$, the choice of the zeros of the Tschebysheff polynomial $T_n(x)$ as collocation points tends to minimize the maximum magnitude of the residual $L^V(y^{(n)})$. The Lanczos method as adapted by Clenshaw and Norton [12, 13] has recently found many applications. This method capitalizes on the good convergence properties of the expansion of $y^{(n)}$ in Tschebysheff polynomials; however, it does not take full advantage of the boundary conditions.

In this paper, new collocation methods are developed and applied to several simple geometries. The residual $L^V(y^{(n)})$ or $L^S(y^{(n)})$ is represented as an orthogonal polynomial over its region. By appropriate choices of the weight function in the orthogonality relation, we obtain collocation methods of accuracy comparable to the Galerkin interior and boundary methods. The collocation points thus selected are also

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optimal quadrature points for numerical integration of the solution over the same region.

Interior collocation principle

We begin by considering a symmetrical second-order boundary-value problem in one independent variable, x, in the region $x^2 < 1$. Here x may be the distance from the midplane in a slab, or the radial coordinate in a cylindrical or spherical system. The differential equation is

$$L^V(y) = 0 \quad \text{for } x^2 < 1 \tag{3}$$

and the boundary conditions are

$$y = y(1) \quad \text{at } x^2 = 1 \tag{4}$$

$$\frac{dy}{dx} = 0 \quad \text{at } x = 0 \tag{5}$$

For the slab, eq. (4) yields two conditions and eq. (5) is a corollary.

For interior collocation, the approximating function is chosen such that the boundary conditions are satisfied. A suitable function is

$$y^{(n)} = y(1) + (1 - x^2) \sum_{i=0}^{n-1} a_i^{(n)} P_i(x^2) \tag{6}$$

in which the $P_i(x^2)$ are polynomials of degree i in x^2, yet to be specified and the $a_i^{(n)}$ are undetermined constants.

A set of n equations is needed to determine the collocation points. We note that, once $y^{(n)}$ has been adjusted to satisfy eq. (3) at n collocation points, $x_1^2, \ldots, x_n^2$, the residual function $L^V(y^{(n)})$ either vanishes everywhere or contains a polynomial factor $G_n(x^2)$ of degree n in x^2, whose zeros are the collocation points. Then by analogy with Galerkin's method, which specifies that the residual be orthogonal to all the trial functions, we choose the collocation points by specifying that $G_n(x^2)$ be orthogonal to all the functions $(1 - x^2)P_i(x^2)$ of eq. (6) over the region V. Our specification is automatically satisfied by taking $G_n(x^2)$ and $P_i(x^2)$ from the orthogonal polynomial set defined by

$$\int_0^1 (1 - x^2) P_i(x^2) P_n(x^2) x^{a-1}\, dx = C_i \delta_{in} \tag{7}$$

for all positive integers i and n. Here the volume element dV has been replaced by the proportional quantity $x^{a-1}\,dx$; thus, for slabs $a = 1$, for cylinders $a = 2$ and for spheres $a = 3$.

The polynomials defined by eq. (7) are Jacobi polynomials [14, 15]. They are given explicitly by

$$\begin{aligned} P_i(x^2) &= F\left(-i, i + \frac{a}{2} + 1, \frac{a}{2}, x^2\right) \\ &= 1 + \frac{(-i)\left(i + \frac{a}{2} + 1\right)}{1!\left(\frac{a}{2}\right)} x^2 + \cdots \\ &\quad + \frac{(-i)(-i+1)\cdots(-1)\left(i + \frac{a}{2} + 1\right)\cdots\left(i + \frac{a}{2} + i\right)}{(i)!\left(\frac{a}{2}\right)\left(\frac{a}{2} + 1\right)\cdots\left(\frac{a}{2} + i - 1\right)} x^{2i} \end{aligned} \tag{8}$$

in which F is the hypergeometric function. The constant C_i of eq. (7) is correspondingly given by

$$C_i = \frac{[\Gamma(a/2)]^2 \Gamma(i+1)\Gamma(i+2)}{(4i + a + 2)\Gamma(i + a/2)\Gamma(i + a/2 + 1)} \tag{9}$$

The polynomials $P_i(x^2)$ and their constants C_i are given in Table 1 for several values of a and i. The collocation points $x_1, \ldots, x_n$, given by the zeros of $P_n(x^2)$, are shown in Tables 2–4. The orthogonality in eq. (7) ensures that the zeros of $P_n(x^2)$ are real, distinct and located within the open interval 0, 1. The completeness and other properties of these polynomials are summarized in [14, 15].

This completes the statement of the interior collocation principle. The key formula is eq. (7), which provides both the trial functions and the collocation points.

The collocation principle developed here is a discrete analog of Galerkin's method. The collocation principle is based on orthogonality, not of the residual function, but of a polynomial which vanishes at the same points. Numerical comparisons have thus far indicated that this collocation method gives about the same accuracy as the Galerkin method and is simpler to use. The two methods give identical results in problems with a residual of degree $d \leqslant 2n$ (e.g. for linear differential equations with constant coefficients). The relation between these and other approximate methods is discussed in Appendices A and B.

Interior formulae based on ordinates

The interior method can be applied either by inserting eq. (6) into the differential equation at

Table 1. The polynomials $P_i(x^2)$ and constants C_i for $i \leqslant 3$

	$i=0$	$i=1$	$i=2$	$i=3$
$a=1$				
$P_i(x^2)$	1	$1-5x^2$	$1-14x^2+21x^4$	$1-27x^2+99x^4-\frac{429}{5}x^6$
C_i	$\frac{2}{3}$	$\frac{16}{21}$	$\frac{128}{165}$	$\frac{2048}{2625}$
$a=2$				
$P_i(x^2)$	1	$1-3x^2$	$1-8x^2+10x^4$	$1-15x^2+45x^4-35x^6$
C_i	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{12}$	$\frac{1}{16}$
$a=3$				
$P_i(x^2)$	1	$1-\frac{7}{3}x^2$	$1-6x^2+\frac{33}{5}x^4$	$1-11x^2+\frac{143}{5}x^4-\frac{143}{7}x^6$
C_i	$\frac{2}{15}$	$\frac{16}{405}$	$\frac{128}{6825}$	$\frac{2048}{187,425}$

$x = x_1, \ldots, x_n$ and solving for the coefficients $a_0^{(n)} \ldots a_{n-1}^{(n)}$, or by formulating an equivalent set of equations in terms of the unknown ordinates $y^{(n)}(x_1) \ldots y^{(n)}(x_n)$. Tables for the latter method are provided here. The derivation of the tables is described in Appendix C.

The gradient and Laplacian operators for the function $y^{(n)}(x)$ of eq. (6) are given by

$$\left(\frac{\mathrm{d}y^{(n)}}{\mathrm{d}x}\bigg|_{x=x_i}\right) = \sum_{j=1}^{n+1} A_{ij}^{(n)} y^{(n)}(x_j) \tag{10}$$

$$x^{1-a}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{a-1}\frac{\mathrm{d}y^{(n)}}{\mathrm{d}x}\right)\bigg|_{x=x_i} = \sum_{j=1}^{n+1} B_{ij}^{(n)} y^{(n)}(x_j) \tag{11}$$

for $i = 1, \ldots, n+1$. The coefficients $A_{ij}^{(n)}$ and $B_{ij}^{(n)}$ are given for slabs, cylinders and spheres in Tables 2, 3 and 4, respectively. Equations (10) and (11) are to be used to rewrite eq. (3) as a set of difference equations at the points $x_1, \ldots, x_n$. The operators for $i = n+1$ are not needed under the boundary condition of eq. (4), but are useful when derivatives occur in the boundary conditions; in the latter case the boundary is also a collocation position and the calculation becomes a mixed collocation method. These operators are exact for any even polynomial $y(x)$ of degree not exceeding $2n$.

Derivatives of higher order may be obtained by repeated application of eqs (10) and (11). One must arrange the calculations so that only even functions are differentiated at each stage; thus, if a derivative of odd order is desired, eq. (10) must be used last.

Integrals of the solution over the volume V can be calculated with high accuracy via the summation formula

$$\int_0^1 f(x)x^{a-1}\,\mathrm{d}x = \sum_{i=1}^{n+1} W_i^{(n)} f(x_i) \tag{12}$$

which requires knowledge of the solution only at the interior collocation points $x_1, \ldots, x_n$ and at the boundary, $x_{n+1} = 1$. The theory of formulae of this type is treated by Kopal [16]. Equation (12) is exact for any even polynomial function $f(x)$ of degree not exceeding $4n$; its high precision is due to the use of the zeros of the orthogonal polynomial $(1-x^2)P_n(x^2)$ as the quadrature points (see Appendix B). The weights $W_i^{(n)}$ are shown alongside the coordinates x_i in Tables 2–4. The values for $a = 1$ were first given by Radau [16, 17]; the other values are new.

For problems governed by an integral condition rather than a condition at the boundary, $y(1)$ will be unknown. An equation for $y(1)$ can then be obtained from the integral condition via eq. (12). This is another example of a mixed collocation method.

It is sometimes desirable to transform the calculated ordinates $y^{(n)}(x_1), \ldots, y^{(n)}(1)$ into an expansion of the form in eq. (6). To obtain the coefficient a_k we multiply eq. (6) by $P_k(x^2)x^{a-1}\,\mathrm{d}x$ and integrate from $x = 0$ to 1. With the aid of eq. (7) we get

$$a_k = \frac{1}{C_k}\int_0^1 [y^{(n)} - y(1)]P_k(x^2)x^{a-1}\,\mathrm{d}x$$

$$k = 0, \ldots, n-1. \tag{13}$$

Since the degree of $[y^{(n)} - y(1)]P_k(x^2)$ will not exceed $4n-2$, the integration can be done exactly by means of eq. (12); hence,

$$a_k = \frac{1}{C_k}\sum_{i=1}^{n} W_i[y^{(n)}(x_i) - y(1)]P_k(x_i^2)$$

$$k = 0, \ldots, n-1 \tag{14}$$

Thus, the expansion coefficients can be calculated by a weighted summation process. The necessary constants are given in Tables 1–4 for $n \leqslant 3$. The use of these tables is illustrated in Examples 1–3.

Table 2. Collocation constants for slab symmetry ($a = 1$)†

$n_t = n + 1$	i	x_i	W_i	A_{i1}	A_{i2}	A_{i3}	A_{i4}	B_{i1}	B_{i2}	B_{i3}	B_{i4}
2	1	$\sqrt{\frac{1}{5}}$	$\frac{5}{6}$	$-\frac{5}{2}x_1$	$\frac{5}{2}x_1$			$-\frac{5}{2}$	$\frac{5}{2}$		
2	1	0.44721	0.83333	−1.1180	1.1180			−2.5	2.5		
2	2	1	$\frac{1}{6}$	$-\frac{5}{2}$	$\frac{5}{2}$			$-\frac{5}{2}$	$\frac{5}{2}$		
2	2	1.00000	0.166667	−2.5000	2.5000			−2.5	2.5		
3	1	$\sqrt{\left(\frac{7-\sqrt{(28)}}{21}\right)}$	$\frac{14+\sqrt{7}}{30}$	$-\frac{7+2\sqrt{7}}{2}x_1$	$\frac{7+4\sqrt{7}}{2}x_1$	$-(\sqrt{7})x_1$		$-14+\frac{7\sqrt{7}}{2}$	$7-\frac{\sqrt{7}}{2}$	$7-3\sqrt{7}$	
3	1	0.285232	0.554858	−1.752962	2.507614	−0.754652		−4.739870	5.677124	−0.937254	
3	2	$\sqrt{\left(\frac{7+\sqrt{(28)}}{21}\right)}$	$\frac{14-\sqrt{7}}{30}$	$\frac{7-4\sqrt{7}}{2}x_2$	$-\frac{7-2\sqrt{7}}{2}x_2$	$(\sqrt{7})x_2$		$7+\frac{\sqrt{7}}{2}$	$-14-\frac{7\sqrt{7}}{2}$	$7+3\sqrt{7}$	
3	2	0.765055	0.378475	−1.370599	−0.653547	2.024146		8.322876	−23.260130	14.937254	
3	3	1	$\frac{1}{15}$	$-\frac{7-4\sqrt{7}}{2}$	$-\frac{7+4\sqrt{7}}{2}$	7		$-14+\frac{25\sqrt{7}}{2}$	$-14-\frac{25\sqrt{7}}{2}$	28	
3	3	1	0.066667	1.791503	−8.791503	7		19.071891	−47.071891	28	
4	1	0.20929922	0.41245880	−2.3889244	3.5135453	−1.7401020	0.61548115	−8.1079245	9.6033328	−2.0342937	0.53888539
4	2	0.59170018	0.34112269	−1.5027316	−0.84502256	3.3435154	−0.99576125	11.611597	−27.294644	19.309454	−3.6264063
4	3	0.87174015	0.21070423	0.81782916	−3.6741370	−0.57356542	3.4298732	−3.9821807	31.261322	−77.097432	49.818290
4	4	1	$\frac{1}{28}$	−1.4877192	5.6276304	−17.639911	$\frac{27}{2}$	−35.432632	122.93626	−200.00363	$\frac{225}{2}$

† For $n = 1$ and 2 all values are given twice: first exactly in terms of radicals and then in rounded decimal form. The same is done in Tables 3 and 4.

Table 3. Collocation constants for cylindrical symmetry ($a = 2$)

$n_t = n + 1$	i	x_i	W_i	A_{i1}	A_{i2}	A_{i3}	A_{i4}	B_{i1}	B_{i2}	B_{i3}	B_{i4}
2	1	$\sqrt{\frac{1}{3}}$	$\frac{3}{8}$	$-3x_1$	$3x_1$			-6	6		
2	1	0.577350	0.375	−1.73205	1.73205			−6	6		
2	2	1	$\frac{1}{8}$	−3	3			−6	6		
2	2	1	0.125	−3	3			−6	6		
3	1	$\sqrt{\left(\frac{4-\sqrt{6}}{10}\right)}$	$\frac{16-\sqrt{6}}{72}$	$(-4-\sqrt{6})x_1$	$\left(4+\frac{7}{3}\sqrt{6}\right)x_1$	$-\left(\frac{4}{3}\sqrt{6}\right)x_1$		$-\frac{64}{3}+\frac{14}{3}\sqrt{6}$	$\frac{32}{3}+\frac{2}{3}\sqrt{6}$	$\frac{32}{3}-\frac{16\sqrt{6}}{3}$	
3	1	0.393765	0.188202	−2.539584	3.825616	−1.286032		−9.902381	12.299660	−2.397279	
3	2	$\sqrt{\left(\frac{4+\sqrt{6}}{10}\right)}$	$\frac{16+\sqrt{6}}{72}$	$\left(4-\frac{7}{3}\sqrt{6}\right)x_2$	$-(4-\sqrt{6})x_2$	$\left(\frac{4}{3}\sqrt{6}\right)x_2$		$\frac{32}{3}-\frac{2}{3}\sqrt{6}$	$-\frac{64}{3}-\frac{14\sqrt{6}}{3}$	$\frac{32}{3}+\frac{16\sqrt{6}}{3}$	
3	2	0.803087	0.256243	−1.377677	−1.245195	2.622872		9.033674	−32.764286	23.730612	
3	3	1	$\frac{1}{18}$	$-4+\frac{7}{3}\sqrt{6}$	$-4-\frac{7}{3}\sqrt{6}$	8		$-\frac{64}{3}+\frac{54\sqrt{6}}{3}$	$-\frac{64}{3}-\frac{54\sqrt{6}}{3}$	$\frac{128}{3}$	
3	3	1	0.055556	1.715476	−9.715476	8		22.757482	−65.424149	42.666667	
4	1	0.29763730	0.11023111	−3.3597940	5.2924315	−3.1010284	1.1683909	−15.881426	19.636380	−5.2811862	1.5262327
4	2	0.63989598	0.19409673	−1.3980385	−1.5627540	4.3197367	−1.3589442	11.151861	−34.497415	29.235709	−5.8901550
4	3	0.88750181	0.16442216	0.69721650	−3.6766754	−1.1267583	4.1062172	−3.5405872	34.512110	−99.621159	68.649637
4	4	1	$\frac{1}{32}$	−1.2266754	5.4010626	−19.174387	15	−33.869987	136.24969	−252.37970	150

Table 4. Collocation constants for spherical symmetry ($a = 3$)

$n_t = n+1$	i	x_i	W_i	A_{i1}	A_{i2}	A_{i3}	A_{i4}	B_{i1}	B_{i2}	B_{i3}	B_{i4}
2	1	$\sqrt{\frac{3}{7}}$	$\frac{7}{30}$	$-\frac{7}{2}x_1$	$\frac{7}{2}x_1$			$-\frac{21}{2}$	$\frac{21}{2}$		
2	1	0.654654	0.233333	−2.29129	2.29129			−10.5	10.5		
2	2	1	$\frac{1}{10}$	$-\frac{7}{2}$	$\frac{7}{2}$			$-\frac{21}{2}$	$\frac{21}{2}$		
2	2	1	0.1	−3.5	3.5			−10.5	10.5		
3	1	$\sqrt{\left(\frac{15-\sqrt{60}}{33}\right)}$	$\frac{150-13\sqrt{15}}{1050}$	$-\left(\frac{9}{2}+\frac{3}{10}\sqrt{60}\right)x_1$	$\left(\frac{9}{2}+\frac{8}{10}\sqrt{60}\right)x_1$	$-\frac{1}{2}(\sqrt{60})x_1$		$-30+\frac{111}{60}\sqrt{60}$	$15+\frac{39}{60}\sqrt{60}$	$15-\frac{5}{2}\sqrt{60}$	
3	1	0.468849	0.0949059	−3.199326	5.015169	−1.815843		−15.669962	20.034878	−4.364917	
3	2	$\sqrt{\left(\frac{15+\sqrt{60}}{33}\right)}$	$\frac{150+13\sqrt{15}}{1050}$	$\left(\frac{9}{2}-\frac{8}{10}\sqrt{60}\right)x_2$	$\left(-\frac{9}{2}+\frac{3}{10}\sqrt{60}\right)x_2$	$\frac{1}{2}(\sqrt{60})x_2$		$15-\frac{39}{60}\sqrt{60}$	$-30-\frac{111}{60}\sqrt{60}$	$15+\frac{5}{2}\sqrt{60}$	
3	2	0.830224	0.1908084	−1.408702	−1.806741	3.215443		9.965122	−44.330038	34.364917	
3	3	1	$\frac{1}{21}$	$-\frac{9}{2}+\frac{8}{10}\sqrt{60}$	$-\frac{9}{2}-\frac{8}{10}\sqrt{60}$	9		$-30+\frac{147}{20}\sqrt{60}$	$-30-\frac{147}{20}\sqrt{60}$	60	
3	3	1	0.04761905	1.696773	−10.696773	9		26.932855	−86.932855	60	
4	1	0.36311746	0.04567809	−4.1308947	6.8819128	−4.5475386	1.7965205	−23.853064	30.593651	−9.7462944	3.0057072
4	2	0.67718628	0.12589831	−1.3388630	−2.2150478	5.2890548	−1.7351440	11.099906	−43.237662	40.818768	−8.6810122
4	3	0.89975799	0.13397916	0.62570332	−3.7406161	−1.6671150	4.7820278	−3.3228457	38.356814	−125.40927	90.375305
4	4	1	$\frac{1}{36}$	−1.0727282	5.3255695	−20.752841	$\frac{33}{2}$	−33.675598	152.37521	−311.19961	$\frac{385}{2}$

Boundary collocation principles

Boundary collocation is useful for linear partial differential equations, with linear or non-linear boundary conditions. The approximating function $y^{(n)}$ is formed by a linear combination of solutions of the differential equation. The boundary-condition residual $L^S(y^{(n)})$ is then set equal to zero at n selected points to determine the coefficients of combination.

A strict analogy with our interior collocation principle would dictate the use of orthogonalized solutions of the differential equation, $\Phi_0(x), \ldots, \Phi_{n-1}(x)$, to form the trial functions and to select the boundary collocation points. Such a procedure has definite merits if the same differential equation is to be solved many times; however, it has not been used here because of the success obtained with simpler methods.

For the present study we have used the zeros of various orthogonal polynomials, with appropriate symmetry on S, as boundary collocation points. This collocation procedure is analogous to the method of moments [1–3, 8], but is easier to apply. Each polynomial family is associated with a particular weight function $w(\mathbf{x})$, and gives rise to an optimal quadrature formula for integration of polynomials weighted by $w(\mathbf{x})$ over S. The choice $w(\mathbf{x}) = 1$ gives results similar to Galerkin's method. Example 3 shows that this choice is a good one, but that there are other interesting possibilities.

EXAMPLES

The collocation methods are demonstrated here for several linear problems. Non-linear problems will be treated in a later paper.

Example 1. *Transient diffusion with first-order reaction*

A catalyst slab with interior void fraction ε, initially filled with inert fluid, is exposed at time $t = 0$ to a reactant concentration c_{As} along the surfaces $z = \pm B$. The ensuing reaction is isothermal and first-order in the local reactant concentration c_A; the effective reactant diffusivity $\mathscr{D}_A$ is constant. Setting $y = c_A/c_{As}$, $x = z/B$, $T = \mathscr{D}t/B^2\varepsilon$ and $\Lambda^2 = B^2k_1/\mathscr{D}_A$, the problem can be stated in the dimensionless form:

D.E.:

$$\frac{\partial y}{\partial T} = \frac{\partial^2 y}{\partial x^2} - \Lambda^2 y \quad \text{in} \quad -1 < x < 1 \tag{15}$$

I.C.:

$$y = 0 \quad \text{for} \quad -1 < x < 1 \text{ at } T = 0 \tag{16}$$

B.C.1, 2:

$$y = 1 \quad \text{at } x = \pm 1 \text{ for } T = 0. \tag{17}$$

It is desired to compute the dimensionless mean reaction rate (effectiveness factor)

$$\eta = \frac{1}{2}\int_{-1}^{1} y\,dx \tag{18}$$

by interior collocation and to compare the results with the exact solution

$$\eta = \frac{\tanh\Lambda}{\Lambda} - 2\sum_{m=0}^{\infty} \frac{\exp\{-[\Lambda^2 + (m+\frac{1}{2})^2\pi^2]T\}}{\Lambda^2 + (m+\frac{1}{2})^2\pi^2} \tag{19}$$

obtained by Laplace transformation.

The problem is symmetrical about $x = 0$, so that y may be approximated by eq. (6) with time-dependent coefficients $a_i^{(n)}(T)$. The spatial derivatives of $y^{(n)}$ are obtained via Table 2; thus eq. (15) is approximated at the collocation points by

$$\frac{dy^{(n)}(x_i)}{dT} = \sum_{j=1}^{n+1} B_{ij}^{(n)} y^{(n)}(x_j) - \Lambda^2 y^{(n)}(x_i)$$

$$i = 1, \ldots, n. \tag{20}$$

Setting $y_{n+1} = 1$ according to eq. (17) and converting to matrix notation, we get

$$\frac{d}{dT}[y^{(n)}] = [B^{(n)} - \Lambda^2 I][y^{(n)}] + [K^{(n)}] \tag{21}$$

with the initial condition

$$[y^{(n)}] = [0] \quad \text{at } T = 0. \tag{22}$$

Here $[y^{(n)}]$ is the column vector of dimensionless concentrations $y^{(n)}(x_1, T), \ldots, y^{(n)}(x_n, T)$; $[B^{(n)}]$ is the $n \times n$ matrix of coefficients $B_{ij}^{(n)}$ for i and $j < n$, and $[K^{(n)}]$ is the column vector of coefficients $B_{ij}^{(n)}$ for $i = 1, \ldots, n$, $j = n + 1$.

Equations (21) and (22) are solvable by standard methods [18]. The result may be written via Sylvester's theorem as

$$[y^{(n)}] = \sum_{r=1}^{n} \frac{(1 - e^{-\lambda_r T})}{\lambda_r} \prod_{\substack{k=1 \\ k \neq r}}^{k=n} \frac{[(\Lambda^2 - \lambda_k)I - B^{(n)}]}{(\lambda_r - \lambda_k)} [K^{(n)}] \tag{23}$$

in which $\lambda_1, \ldots, \lambda_n$ are the eigenvalues (assumed distinct) of the matrix $[\Lambda^2 I - B^{(n)}]$. The n-point collocation approximation for the mean reaction rate is found by inserting the elements of $[y^{(n)}]$ into eq. (12):

$$\eta^{(n)} = \sum_{j=1}^{n} W_j^{(n)} y^{(n)}(x_j) + W_{n+1}^{(n)}. \tag{24}$$

Here eq. (17) has again been used to evaluate $y^{(n)}(x_{n+1})$.

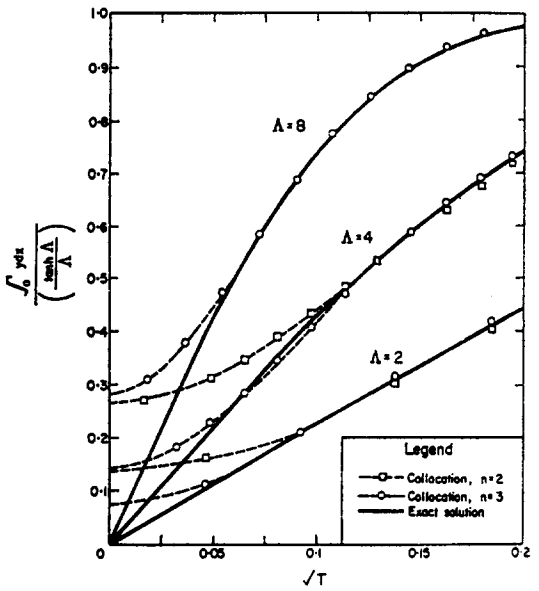

Fig. 1. Approximate and exact solutions for unsteady-state effectiveness factors, Example 1.

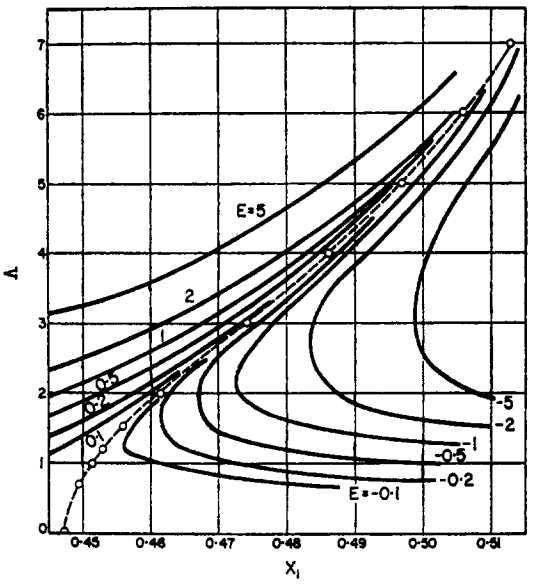

Fig. 2. Effect of interior collocation position, x_1, on accuracy of steady-state effectiveness factor calculation with $n = 1$. Curves are contours of constant percentage error, $E = 100\,(\eta^{(1)} - \eta)/\eta$; the dotted curve is for $E = 0$.

Figure 1 shows the exact solution for η, along with the collocation approximations for $n = 2$ and $n = 3$. At small values of T the collocation approximations are high, since eq. (24) gives $\eta^{(n)} = W_{n+1}^{(n)}$ when the interior concentrations are zero; this error is inherent in the polynomial approximations but diminishes rapidly with increasing n. At larger values of T the collocation approximations are remarkably good; the approximation $\eta^{(3)}$ is accurate within 0.8% for $T \geqslant 0.01$ and $\Lambda \leqslant 8$.

In the limit as $T \to \infty$, eq. (23) approaches the steady-state solution of eq. (21):

$$[y^{(n)}] = [\Lambda^2 I - B^{(n)}]^{-1}[K^{(n)}]. \qquad (25)$$

The effectiveness factors computed from this solution are shown in Table 6. The first approximation, given by

$$\eta^{(1)} = \frac{5}{6}\frac{2.5}{2.5 + \Lambda^2} + \frac{1}{6} \qquad (26)$$

is accurate within 0.005% for $\Lambda \leqslant 2$; the higher approximations $\eta^{(2)}$ and $\eta^{(3)}$ are still better.

Other choices of collocation points have been tested for the steady-state problem, to see how the accuracy is affected. The results for $n = 1$ are shown in Fig. 2; the contours give the percentage error $E = 100(\eta^{(1)} - \eta)/\eta$ for each combination of x_1 and Λ, and the dotted contour is for $E = 0$. The value $x_1 = 0.44721$, given in Table 2, is clearly optimal for $\Lambda \ll 1$, and give less than 1% error up to $\Lambda = 2$.

The optimum x_1 for this problem is nearly constant for $\Lambda < 0.5$, but increases thereafter with increasing Λ. This trend arises because the parabolic concentration profile $y^{(1)}$ becomes a less satisfactory approximation when Λ is large.

Table 5. Steady-state effectiveness factors for example 1

Thiele modulus	Collocation solutions eqs (27) and (28)			Exact solution eq. (22)
(Λ)	$\eta^{(1)}$	$\eta^{(2)}$	$\eta^{(3)}$	η
0.0	1.00000	1.00000	1.00000	1.00000
0.5	0.92424	0.92424	0.92424	0.92424
1.0	0.76190	0.76159	0.76159	0.76159
2.0	0.48718	0.48202	0.48201	0.48201
4.0	0.27928	0.25041	0.24984	0.24983
8.0	0.19799	0.13175	0.12534	0.12500
∞	0.16667	0.06667	0.03571	0.00000

Table 6. Eigenvalues of eqs (30)–(32), case 1

	λ_1	λ_2	λ_3
Collocation, $n = 1$	2.5	—	—
Collocation, $n = 2$	2.467437	25.53	—
Collocation, $n = 3$	2.46740111	22.29	87.7
Exact values	2.46740110...	22.21...	61.7

The steady-state problem has also been solved for $n = 2$, with various choices of x_1 and x_2. The collocation points of Table 2 with $n = 2$ proved to be optimal near $\Lambda = 0$, and satisfactory for a larger range of Λ as illustrated in Table 5.

On the basis of Fig. 2, one might choose a compromise value of x_1, such as $x_1 = 0.498$, which gives less than 5% error up to $\Lambda = 6$. Such an approach however, is based on hindsight; the error contours could not be plotted unless the solution were already known. We therefore recommend the x_i of Tables 2–4

as the best points that can be chosen *a priori* for collocation of the polynomial in eq. (6).

Example 2. *Eigenvalue problems*

The interior collocation method has been applied to several eigenvalue problems of the form

$$\text{D.E.:} \quad \nabla^2 y + \lambda f(x) y = 0 \quad \text{in } 0 < x < 1 \tag{27}$$

B.C.1.:

$$y = 0 \quad \text{at } x = 1 \tag{28}$$

B.C.2.:

$$\frac{dy}{dx} = 0 \quad \text{at } x = 0 \tag{29}$$

with various even functions $f(x)$, where $f(x) > 0$ for $0 < x < 1$. Non-trivial solutions $y(x)$ occur only for certain values of the parameter λ; approximations to the first n of these eigenvalues are desired.

The solutions contain only even powers of x; accordingly y may be approximated by eq. (6) and eq. (29) is thereby satisfied. Evaluation of $\nabla^2 y^{(n)}$ via eq. (11) and elimination of $y^{(n)}(x_{n+1})$ via eq. (28), gives the collocation equations

$$\sum_{j=1}^{n} B_{ij}^{(n)} y^{(n)}(x_j) + \lambda f(x_i) y^{(n)}(x_i) = 0, \quad i = 1, \ldots, n \tag{30}$$

or in matrix notation

$$[M^{(n)}][y^{(n)}] = [y^{(n)}]\lambda, \tag{31}$$

where $[M^{(n)}]$ is the $n \times n$ matrix with elements given by

$$M_{ij}^{(n)} = -B_{ij}^{(n)}/f(x_i), \quad i = 1, \ldots, n \qquad j = 1, \ldots, n \tag{32}$$

and $[y^{(n)}]$ is the column vector with elements $y^{(n)}(x_1), \ldots, y^{(n)}(x_n)$.

Equation (31) yields non-trivial solutions $[y^{(n)}]$ only when λ is an eigenvalue of the matrix $[M^{(n)}]$. Thus, the eigenvalues and right eigenvectors of $[M^{(n)}]$ are approximations to the first n eigenvalues and eigenfunctions of eqs (27)–(29). The approximations converge rapidly with increasing n, as the following results illustrate.

Case 1: $f(x) = 1, a = 1$. This is a standard example. The kth eigenfunction is $c_k \cos(k - \frac{1}{2})\pi x$, where c_k is an arbitrary constant; the kth eigenvalue is $(k - \frac{1}{2})^2\pi^2$. The collocation approximations $\lambda_1^{(n)}, \ldots, \lambda_n^{(n)}$ are found as the eigenvalues of the $n \times n$ matrix of elements $M_{ij}^{(n)} = -B_{ij}^{(n)}$ obtained from Table 2. The results are given in Table 6 and show good convergence with increasing n; they approach the exact values from above in each case. The lowest eigenvalues are approximated most accurately and the same situation can be expected for the eigenfunctions.

Since $L^V(y^{(n)})$ is a polynomial of the same degree as $y^{(n)}$ in this problem, the results are identical to those of the Rayleigh–Ritz and Galerkin methods for the same trial functions. For further discussion of this point, see Appendix A.

Table 7. Eigenvalues of eqs (30)–(32), case 2 (Graetz problem)

	λ_1	λ_2	λ_3
Collocation, $n = 1$	4.5	—	—
Galerkin, $n = 1$	4.0	—	—
Collocation, $n = 2$	3.679	48.32	
Galerkin, $n = 2$	3.665	36.33	—
Collocation, $n = 3$	3.65714	24.70	244
Exact values	3.656793	22.30473	56.9605

Case 2: $f(x) = 2(1 - x^2), a = 2$. This case arises in the Graetz–Nusselt problem [19] of heat transfer to a Newtonian fluid in laminar flow through a tube. The smallest eigenvalue, λ_1, is the asymptotic value of the local Nusselt number for large distances into the heat-transfer region.

Calculation of the matrix $[M^{(n)}]$ according to eq. (32), and determination of the eigenvalues, gives the results shown in Table 7. For comparison, exact values computed from the results of Abramowitz [20] are included. The initial approximation by collocation is less accurate here than in case 1, because of the higher degree of $f(x)$; however, the approximations for larger n converge satisfactorily. Galerkin's method is somewhat more accurate than orthogonal collocation in this case.

Case 3:

$$f(x) = \frac{2(1 - x^2) + (4/(\alpha + 1))(\tau_R/\tau_{\frac{1}{2}})^{\alpha - 1}(1 - x^{\alpha + 1})}{1 + (4/(\alpha + 3))(\tau_R/\tau_{\frac{1}{2}})^{\alpha - 1}},$$

$$a = 2.$$

This case arises in the extension of the Graetz–Nusselt problem to an Ellis fluid, presented by Matsuhisa and Bird [21]. The smallest eigenvalue is the ultimate value of the local Nusselt number; it depends on the dimensionless parameters $\tau_R/\tau_{1/2}$ and α. The notations α, τ_R and $\tau_{1/2}$ are the same as in reference [21].

Matsuhisa and Bird computed values of λ_1 by a single iteration of the method of Stodola and Vianello [22], which is a form of the Schwarz method [2, 16]. This method gives good precision but the integrations are tedious in the present problem and higher approximations have not been carried out.

The solution by collocation is straightforward. The complicated form of $f(x)$ raises no special difficulty, since only the numerical values $f(x_1), \ldots, f(x_n)$ are required. The matrix $[M^{(n)}]$ is computed via eq. (32) and its eigenvalues are computed by standard methods.

Table 8 shows the collocation approximations to λ_1 as functions of $\tau_R/\tau_{1/2}$ and α. The first approximations are high, as in Table 7, and are not included. The second and third approximations coincide within

Table 8. Collocation solutions for ultimate Nusselt number in laminar flow of an Ellis fluid through an isothermal tube

n	$\tau_R/\tau_{1/2}$	$a = 1.5$	2	2.5	3	3.5	5
2	0.1	3.706	3.697	3.687	3.681	3.680	3.679
3		3.690	3.677	3.666	3.660	3.658	3.657
2	0.2	3.714	3.712	3.700	3.690	3.685	3.680
3		3.699	3.695	3.680	3.669	3.663	3.658
2	0.5	3.727	3.748	3.749	3.741	3.729	3.700
3		3.715	3.736	3.735	3.724	3.710	3.678
2	1	3.737	3.787	3.826	3.857	3.881	3.921
3		3.727	3.781	3.821	3.850	3.872	3.905
2	2	3.748	3.830	3.920	4.016	4.115	4.397
3		3.741	3.831	3.925	4.022	4.119	4.391
2	5	3.762	3.877	4.004	4.128	4.240	4.503
3		3.757	3.885	4.019	4.143	4.251	4.497
2	10	3.771	3.900	4.031	4.150	4.255	4.506
3		3.768	3.912	4.049	4.167	4.267	4.500
2	100	3.792	3.926	4.047	4.158	4.259	4.506
3		3.793	3.942	4.067	4.175	4.270	4.500
2	∞	3.805	3.930	4.048	4.158	4.259	4.506
3		3.809	3.946	4.068	4.175	4.270	4.500

0.6%, as in Table 7, and the third approximations are thus judged to be accurate to four digits.

Example 3. *An elliptic partial differential equation*

As a final example, consider the differential equation

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = -1 \tag{33}$$

in the square region $x^2 < 1$, $y^2 < 1$, with the boundary conditions

$$v = 0 \quad \text{at } x = \pm 1 \text{ and at } y = \pm 1. \tag{34}$$

These dimensionless equations describe the axial velocity $v(x, y)$ of a Newtonian fluid of constant density and viscosity, in developed laminar flow through a square duct.

The exact solution for v has been obtained in series form by Boussinesq, and the results are summarized in Dryden *et al.* [23]. The main quantities of interest are the dimensionless volumetric flow rate $q = \int\int v\,dx\,dy$ and the dimensionless centreline velocity v_{max}. Stewart [24] has used this problem to demonstrate the variational methods of Hill and Power [25] and Johnson [26], which provide upper and lower bounds on q. Here the same problem is used to demonstrate the interior and boundary collocation methods.

1. *Interior collocation.* A suitable polynomial expression for v, subject to the boundary conditions and the symmetry conditions $v(x, y) = v(y, x)$; $v(-x, y) = v(x, y)$, is

$$v^{(n)} = (1 - x^2)(1 - y^2) \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} a_{ij}^{(n)} P_i(x^2) P_j(y^2),$$

$$a_{ij}^{(n)} = a_{ji}^{(n)}. \tag{35}$$

Here $P_i(x^2)$ and $P_j(y^2)$ are defined by eq. (8) with $a = 1$. This expansion is a direct extension of eq. (6) and can be fitted analogously.

Because of the symmetry, the problem is solvable by considering one octant of the duct, as shown in Fig. 3. The collocation points are selected by assigning each coordinate the set of values listed for x_i in Table 2. The derivatives $\partial^2 v/\partial x^2$ and $\partial^2 v/\partial y^2$ are obtained by applying Table 2 in each coordinate direction. These derivatives are inserted into eq. (33) to obtain the collocation equations, which are then solved for the local values of $v^{(n)}$ at the collocation points.

The simplest case, $n = 1$, involves a single collocation point $(x_1, y_1) = (\sqrt{\frac{1}{5}}, \sqrt{\frac{1}{5}})$. The approximations to the partial derivatives are

$$\left.\frac{\partial^2 v^{(1)}}{\partial x^2}\right|_{x_1, y_1} = -2.5 v^{(1)}(x_1, y_1) + 2.5(0) \tag{36}$$

$$\left.\frac{\partial^2 v^{(1)}}{\partial y^2}\right|_{x_1, y_1} = -2.5 v^{(1)}(x_1, y_1) + 2.5(0) \tag{37}$$

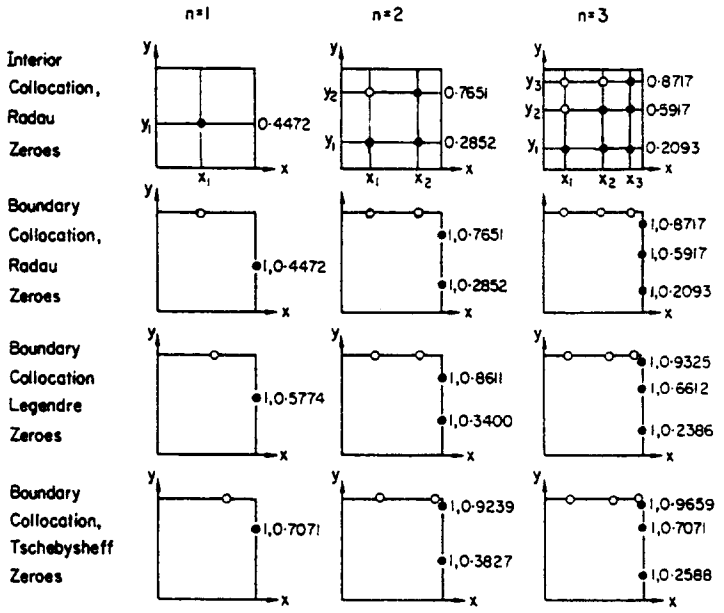

Fig. 3. Collocation points for the square-duct problem, first quadrant. The residual is equated to zero at the solid points; it correspondingly vanishes, by symmetry, at the circled points

Table 9. Volumetric flow rate and maximum velocity for Example 3

	Approximate solutions				Exact
	Boundary collocation (Radau zeroes)	Interior collocation (Radau zeroes)	Boundary collocation (Legendre zeroes)	Boundary collocation (Tschebysheff zeroes)	Boussinesq series solution
$q^{(1)}$	$\frac{8}{15} = 0.53333$	$\frac{5}{9} = 0.55556$	$\frac{2}{3} = 0.66667$	$\frac{5}{6} = 0.83333$	
$q^{(2)}$	$\frac{59}{105} = 0.56190$	$\frac{253}{450} = 0.56222$	$\frac{76}{135} = 0.56296$	$\frac{337}{600} = 0.56167$	$q = 0.562305$
$q^{(3)}$	0.562279	0.562302	0.562336	—	
$q^{(4)}$	0.562304	—	0.562311	—	
$v_{\max}^{(1)}$	$\frac{3}{10} = 0.30000$	$\frac{5}{16} = 0.31250$	$\frac{1}{3} = 0.33333$	$\frac{3}{8} = 0.37500$	
$v_{\max}^{(2)}$	$\frac{33}{112} = 0.29464$	$\frac{151}{512} = 0.29492$	$\frac{53}{180} = 0.29444$	$\frac{47}{160} = 0.29375$	$v_{\max} = 0.294685$
$v_{\max}^{(3)}$	0.294686	—	0.294694	—	
$v_{\max}^{(4)}$	0.294686	—	0.294685	—	

and the resulting collocation equation is

$$-5v^{(1)}(x_1, y_1) = -1 \tag{38}$$

which yields $v^{(1)}(x_1, y_1) = \frac{1}{5}$. Application of eq. (12) gives

$$\begin{aligned} q^{(1)} &= \int_{-1}^{1}\int_{-1}^{1} v^{(1)}\,dx\,dy \\ &= 4\sum_{k=1}^{2}\sum_{m=1}^{2} W_k^{(1)} W_m^{(1)} v^{(1)}(x_k, y_m) \\ &= 4[(\tfrac{5}{6})(\tfrac{5}{6})(\tfrac{1}{5}) + 0 + 0 + 0] \\ &= \tfrac{5}{9}. \end{aligned} \tag{39}$$

Insertion of $v^{(1)}(x_1, y_1)$ in eq. (35) gives the velocity profile

$$v^{(1)} = \tfrac{5}{16}(1 - x^2)(1 - y^2) \tag{40}$$

and the centreline velocity $v_{\max}^{(1)} = \frac{5}{16}$. Table 9 shows that these results are quite accurate.

The next approximation, $n = 2$, yields three collocation points: $(x_1, y_1) = (0.285232, 0.285232)$, $(x_2, y_1) = (0.765055, 0.285232)$ and $(x_2, y_2) = (0.765055, 0.765055)$. The point $(x_1, y_2) = (0.285232, 0.765055)$ lies in the second octant and is omitted because of symmetry (see Fig. 3). The three collocation equations, obtained via Table 2, may be written in matrix

form as

$$\begin{bmatrix} -28+7\sqrt{7} & 14-\sqrt{7} & 0 \\ 7+\frac{1}{2}\sqrt{7} & -28 & 7-\frac{1}{2}\sqrt{7} \\ 0 & 14+\sqrt{7} & -28-7\sqrt{7} \end{bmatrix} \begin{bmatrix} v^{(2)}(x_1,y_1) \\ v^{(2)}(x_2,y_1) \\ v^{(2)}(x_2,y_2) \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} \tag{41}$$

and solved by elimination to obtain

$$v^{(2)}(x_1,y_1) = \frac{9+2\sqrt{7}}{56}$$

$$v^{(2)}(x_2,y_1) = \tfrac{1}{8}$$

$$v^{(2)}(x_2,y_2) = \frac{9-2\sqrt{7}}{56}. \tag{42}$$

Insertion of these results in eq. (35) gives

$$v^{(2)} = (1-x^2)(1-y^2) \times \begin{bmatrix} \frac{253}{800} - \frac{21}{1600}(1-5x^2+1-5y^2) \\ + \frac{63}{12800}(1-5x^2)(1-5y^2) \end{bmatrix} \tag{43}$$

as the second approximation to the velocity profile.

Higher approximations are found analogously by collocating at $n(n+1)/2$ points arranged as shown in Fig. 3 and solving for $n(n+1)/2$ values of v. The results for q and v_{max} converge rapidly, as shown in Table 9, and for most purposes the results with $n = 2$ would be sufficient. Here again, the interior collocation method is identical with the Rayleigh–Ritz and Galerkin methods (see Appendix A). From the theory of the Rayleigh–Ritz method it follows that the successive approximations $q^{(1)}, q^{(2)}, \ldots$ should converge toward the true q from below; the numerical results confirm this.

2. *Boundary collocation.* For this procedure we require an approximating function which satisfies eq. (33) identically. A suitable one is

$$v^{(n)} = v_P(x,y) + \sum_{i=0}^{n-1} c_i^{(n)} \varphi_i(x,y) \tag{44}$$

in which

$$v_P = -\tfrac{1}{4}(x^2+y^2)$$

$$\varphi_0 = 1$$

$$\varphi_1 = x^4 - 6x^2y^2 + y^4$$

$$\varphi_2 = x^8 - 28x^6y^2 + 70x^4y^4 - 28x^2y^6 + y^8$$

$$\varphi_3 = x^{12} - 66x^{10}y^2 + 495x^8y^4 - 924x^6y^6 + 495x^4y^8 - 66x^2y^{10} + x^{12}. \tag{45}$$

Here v_P satisfies the complete eq. (33) and the φ_i satisfy the homogeneous equation

$$\partial^2\varphi_i/\partial x^2 + \partial^2\varphi_i/\partial y^2 = 0.$$

The approximate solution is determined by choosing the constants $c_i^{(n)}$ to satisfy the boundary conditions of eq. (34) at a selected set of points. In view of the symmetry, we consider only the boundary residual for the first octant,

$$L^S(v^{(n)})|_{x=1} = -\tfrac{1}{4}(1+y^2) + \sum_{i=0}^{n-1} c_i^{(n)} \varphi_i(1,y)$$

$$0 \leqslant y \leqslant 1 \tag{46}$$

and set this function equal to zero at n values of y. The boundary residual will automatically vanish at the corresponding points in the other seven octants.

When the constants $c_i^{(n)}$ are chosen to make the residual of eq. (46) vanish at n points $y_1, \ldots, y_n$, then the right-hand side of this equation becomes divisible by a polynomial $G_n(y^2) = (y^2 - y_1^2)\ldots(y^2 - y_n^2)$. By analogy with the method of moments, which would require the residual to be orthogonal to a set of n chosen functions on the interval $0 \leqslant y \leqslant 1$, we choose $G_n(y^2)$ to be member of a set of polynomials $\psi_0(y^2), \psi_1(y^2), \ldots$ that are orthogonal on the same interval. The collocation points must then be the zeros of the polynomial $\psi_n(y^2)$ in the chosen set.

Three choices of orthogonal polynomials are tested here: Legendre polynomials, Tschebysheff polynomials, and Radau polynomials. The zeros of these polynomials have been widely tabulated, since they are the quadrature points in the numerical integration formulae of Gauss, Tschebysheff, and Radau [16] for the integration limits $-1, 1$. Each of these choices of collocation points minimizes the boundary residual in a weighted least-squares sense, but with a different weight function $w(y)$ as discussed below.

The results of these three choices are shown in Table 9. Collocation at the Radau zeros gives the closest approximations both for q and for v_{max}; collocation at the Tschebysheff zeros is the least accurate for both quantities. These differences can be understood qualitatively in terms of the weight functions for the three polynomial families: unity for the Legendre polynomials, $(1-y^2)$ for the Radau polynomials, and $(1-y^2)^{-1/2}$ for the Tschebysheff polynomials. The Radau weighting tends to give highest accuracy near the centres of the walls, whereas the Tschebysheff weighting emphasizes the corners.

In this problem, Legendre boundary collocation converges toward the correct q from above, whereas

Radau boundary collocation converges from below. The Legendre collocation results for $n \leqslant 2$ are identical with the upper bounds on q obtained by a variational method with equivalent trial functions [24]. These results merit further study, to see if comparable upper and lower bounds can be obtained in other problems.

CONCLUSION

The collocation methods developed here permit rapid solution of many types of second-order boundary-value problems. The finite-difference formulation is attractive because of its simplicity and is more efficient computationally than existing finite-difference methods.

These collocation methods differ from other weighted residual methods in that the residual here is not directly orthogonalized, but is matched to an orthogonal function at its zeros. The necessity of integrating the residual is thereby avoided, and the calculations are correspondingly simplified. The accuracy is comparable to that of Galerkin's method.

Of the two orthogonal collocation methods described here, the interior method is the more versatile since it can be used for non-linear differential equations. Furthermore, by treating $y(1)$ in eq. (6) as an unknown function, one can handle various types of boundary or integral conditions; in such cases the interior method becomes a mixed method as discussed under eqs (11) and (12). Applications of the interior method to non-linear problems are underway, and will be reported in a later paper.

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NOTATION

a	geometric constant: 1 for slabs, 2 for cylinders, 3 for spheres
$a_i^{(n)}$	coefficients in eq. (6)
$A_{ij}^{(n)}$	coefficients in eq. (10)
$B_{ij}^{(n)}$	coefficients in eq. (11)
$c_i^{(n)}$	coefficients in eq. (44)
C_i	constant in eq. (9)
$E(u)$	interpolation error in eq. (B2)
$[I]$	unit matrix
K	derivative bound in eq. (B2)
L^S	boundary-condition operator in eq. (2)
$L^S(y^{(n)})$	boundary-condition residual for approximate function $y^{(n)}$
L^V	differential-equation operator in eq. (1) or eq. (3)
$L^V(y^{(n)})$	differential-equation residual for approximate function $y^{(n)}$
$M_{ij}^{(n)}$	elements of matrix $[M^{(n)}]$, defined in eq. (32)
n	number of collocation points in one space dimension
$p_n(u)$	$[=(u-u_1)\ldots(u-u_n)]$
$p_n'(u_j)$	$[=\mathrm{d}p_n(u)/\mathrm{d}u]$ at $u=u_j$
$P_n(u)$	polynomial given by eq. (8), with $i=n$ and $x^2=u$
$P_n'(u_j)$	$[=\mathrm{d}P_n(u)/\mathrm{d}u]$ at $u=u_j$
q	$(=4v_{av})$ dimensionless volume flow rate through square duct. In notation of [22], $q=Q\mu L(\mathscr{P}_0-\mathscr{P}_L)^{-1}B^{-4}$
S	boundary region of eq. (2)
T	dimensionless time defined above eq. (15)
u	x^2
v	dimensionless velocity in square duct. In notation of [24], $v=v_z\mu L(\mathscr{P}_0-\mathscr{P}_L)^{-1}B^{-2}$.
V	volume over which eq. (1) or eq. (3) is applied.
$W_i^{(n)}$	coefficients in eq. (12)
x	position coordinate defined above eq. (3)
y	dependent variable in eqs (1)–(5); position coordinate in Example 3
$y^{(n)}$	approximating function in eq. (6)

Greek letters

$\Gamma(z)$	the gamma function of z
δ_{in}	Kronecker symbol: unity if $i=n$, zero otherwise
η	effectiveness factor, defined in eq. (18)
λ_i	ith eigenvalue
Λ	Thiele modulus, defined above eq. (15)

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APPENDIX A: COMPARISON OF INTERIOR APPROXIMATION METHODS

Our interior method is briefly compared here with several other methods, for the general problem in eqs (3)–(6).

The Galerkin interior method determines the approximate solution by setting the differential-equation residual $L^V(y^{(n)})$ orthogonal to all the trial functions. For the $y^{(n)}$ function of eq. (6), the orthogonality relations over V become

$$\int_0^1 (1-x^2)P_i(x^2)[L^V(y^{(n)})]x^{a-1}\,dx = 0$$

$$i = 0, \ldots, n-1. \tag{A1}$$

Our collocation method, on the other hand, uses the orthogonality relation

$$\int_0^1 (1-x^2)P_i(x^2)[(x^2-x_1^2)\ldots(x^2-x_n^2)]$$

$$x^{a-1}\,dx = 0, \quad i = 0, \ldots, n-1 \tag{A2}$$

to define the collocation points $x_1, \ldots, x_n$ where $L^V(y^{(n)})$ is to vanish. The two methods agree if $L^V(y^{(n)})$ is a polynomial of degree $d \leqslant n$ in x^2.

The Ritz and Rayleigh–Ritz variational principles, when applicable, give the same solution for $y^{(n)}$ as Galerkin's method [8]. Hence, the variational solutions for $y^{(n)}$ are equivalent to the collocation method given here, as long as $L^V(y^{(n)})$ is a polynomial of degree $d \leqslant n$ in x^2. The upper or lower bounds given by the Rayleigh–Ritz method can be obtained directly from the results of the collocation solutions (see Examples 2 and 3). Many other variational principles have been proved equivalent to Galerkin's interior method [27] and are correspondingly related to the interior collocation method given here.

A weighted least-squares method may be written for this symmetrical problem as

$$\frac{\partial}{\partial a_i^{(n)}} \int_0^1 w(x^2)[L^V(y^{(n)})]^2 x^{a-1}\,dx = 0$$

$$i = 0, \ldots, n-1 \tag{A3}$$

where $w(x^2)$ is a weight function, positive for $x^2 < 1$. For comparison, eqs (A2) can be combined to give

$$\frac{\partial}{\partial(x_i^2)} \int_0^1 (1-x^2)[(x^2-x_1^2)\ldots(x^2-x_n^2)]^2$$

$$x^{a-1}\,dx = 0, \quad i = 1, \ldots, n \tag{A4}$$

which shows that our interior collocation points also satisfy a least-squares criterion. Thus, if one chooses $w(x^2) = 1 - x^2$ and if $L^V(y^{(n)})$ is a polynomial of degree $d \leqslant n$ in x^2, then eqs (A3) lead to the same results as our interior method.

The Lanczos selected-points method [10, 11] may be applied here by setting $L^V(y^{(n)}) = 0$ at the zeros of a different form of Jacobi polynomial, namely, the Tschebysheff polynomial $T_{2n}(x)$. These collocation points satisfy the orthogonality conditions

$$\int_0^1 \frac{x^{2i}}{\sqrt{(1-x^2)}}[(x^2-x_1^2)\ldots(x^2-x_n^2)]\,dx = 0$$

$$i = 0, \ldots, n-1 \tag{A5}$$

and the function in the brackets is $T_{2n}(x)$. In comparison with the x_i of eq. (A2), the Tschebysheff zeros are distributed closer to $x^2 = 1$, because the weight function $(1-x^2)^{-1/2}$ goes to infinity at that point.

The Tschebysheff polynomials are optimal for ordinary interpolation in a finite interval, with the terminal values unspecified. However, for interior collocation these polynomials have several disadvantages: (i) the resulting collocation points are concentrated near $x^2 = 1$, where the uncertainty in the solution is the least; (ii) the function $y^{(n)}$ is prescribed at $x^2 = 1$ and is therefore not optimally interpolated by Tschebysheff polynomials; (iii) the weight function in eq. (A5) prevents any equivalence with the Rayleigh–Ritz or Galerkin methods; (iv) the zeros of $T_{2n}(x^2)$ are poorly situated for numerical integration of the solution over V. A brief demonstration of the method may be obtained by extrapolating Fig. 2 to $x_1 = 0.70711$, the positive zero of $T_2(x)$; the results are definitely inferior to those obtained via Table 2.

In boundary collocation, the Tschebysheff polynomials work somewhat better, since objections (i) and (ii) do not apply. Some numerical results are given in Table 9; the values for $n = 2$ are good.

APPENDIX B: ALTERNATE DERIVATION OF INTERIOR METHOD

The interior collocation method owes its accuracy to a property of eq. (12): the minimization of the integration remainder term. To prove this property, we use a method similar to Kopal's analysis [16] of the Gauss integration formula.

Consider the interpolation of an even function $f(x)$ in $-1 \leqslant x \leqslant 1$, using the fixed interpolation points $x = \pm 1$ and the disposable interior points $\pm x_1, \ldots, \pm x_n$. By fitting $f(x)$ at all of these points, and df/dx at the interior points, we obtain the interpolation formula

$$f(x) = \left\{\frac{p_n(u)}{p_n(1)}\right\}^2 f(1) + \sum_{j=1}^{n} \left\{1 - \frac{p_n''(u_j)}{p_n'(u_j)}(u - u_j)\right\}\left\{\frac{u-1}{u_j - 1}\right\} \times \left\{\frac{p_n(u)}{(u-u_j)p_n'(u_j)}\right\}^2 f(u_j) + \sum_{j=1}^{n} (u - u_j)\left\{\frac{u-1}{u_j-1}\right\}\left\{\frac{p_n(u)}{(u-u_j)p_n'(u_j)}\right\}^2 f'(u_j) \tag{B1}$$

in which u is x^2, $p_n(u)$ is $(u - u_1) \ldots (u - u_n)$ and primes denote derivatives with respect to u. This formula is exact for $f(u)$ of degree not exceeding $2n$ (and hence for $f(x)$ of degree not exceeding $4n$); for $f(u)$ of higher degree the error $E(u)$ is bounded by

$$|E(u)| \leqslant \frac{K}{(2n+1)!}(1-u)\{p_n(u)\}^2 \tag{B2}$$

at each point in the region $-1 \leqslant x \leqslant 1$. Here K is the maximum absolute value of $(d^{2n+1}f/du^{2n+1})$ in the same region. Equation (B1) is similar to the Hermite $(n+1)$-point formula [16], except that here the derivative is left unspecified at the last point.

Equation (B1) can be integrated over V to obtain a quadrature formula for $f(x)$, exact for $f(x)$ of degree not exceeding $4n$. Equation (B2) can be integrated in the same manner to obtain an error bound for the quadrature when applied to functions of higher degree. The error bound is

$$\left|\int_0^1 E(x)x^{a-1}\,dx\right| \leqslant \frac{K}{(2n+1)!} \int_0^1 (1-u)\{p_n(u)\}^2 \tfrac{1}{2}u^{(a/2)-1}\,du \tag{B3}$$

and depends accordingly on the choice of interpolation points. Making this error bound stationary with respect to each of the u_i, we obtain

$$\int_0^1 (1-u)\{p_n(u)\}\left\{\frac{p_n(u)}{u-u_i}\right\}u^{(a/2)-1}\,du = 0 \qquad i = 1, \ldots, n \tag{B4}$$

which can be arranged to give

$$\int_0^1 (1-x^2)p_n(x^2)x^{2i}x^{a-1}\,dx = 0 \qquad i = 0, \ldots, n-1 \tag{B5}$$

The polynomial $p_n(x^2)$ thus defined is equivalent to $P_n(x^2)$ expect for a numerical factor. Thus, the error bound in eq. (B3) is made stationary by taking $x_1^2, \ldots, x_n^2$ as the positive zeros of $P_n(x^2)$. The stationary value is a minimum, since the integral on the right of (B3) has positive second derivatives with respect to all the u_i.

Integration of eq. (B1) over the volume V gives

$$\int_0^1 f(x)x^{a-1}\,dx = f(1)\int_0^1 \frac{1}{2}\left\{\frac{p_n(u)}{p_n(1)}\right\}^2 u^{(a/2)-1}\,du + \sum_{j=1}^{n} f(u_j) \times \int_0^1 \frac{1}{2}\left\{\frac{u-1}{u_j-1}\right\}\left\{\frac{p_n(u)}{(u-u_j)p_n'(u_j)}\right\}^2 u^{(a/2)-1}\,du + \sum_{j=1}^{n}\left\{f'(u_j) - \frac{p_n''(u_j)}{p_n'(u_j)}f(u_j)\right\} \times \int_0^1 \frac{1}{2}(u-u_j)\left\{\frac{u-1}{u_j-1}\right\} \times \left\{\frac{p_n(u)}{(u-u_j)p_n'(u_j)}\right\}^2 u^{(a/2)-1}\,du \tag{B6}$$

Now if the error bound on this formula is minimized, by choosing $u_1, \ldots, u_n$ to satisfy eq. (B4), then the integral in the last term vanishes identically for $j = 1, \ldots, n$. Hence the optimal form of eq. (B6) is that given in eq. (12), in which the derivatives of $f(x)$ do not appear. The integration coefficients of eq. (12) are given in terms of the Jacobi polynomials by

$$W_i^{(n)} = \int_0^1 \frac{1}{2}\left\{\frac{u-1}{u_i-1}\right\}\left\{\frac{P_n(u)}{(u-u_i)P_n'(u_i)}\right\}^2 u^{(a/2)-1}\,du \qquad i = 1, \ldots, n \tag{B7}$$

$$W_{n+1}^{(n)} = \int_0^1 \frac{1}{2}\left\{\frac{P_n(u)}{P_n(1)}\right\}^2 u^{(a/2)-1}\,du \tag{B8}$$

and are accordingly positive. The error bound for eq. (12) can be correspondingly evaluated as

$$\left|\int_0^1 E(x)x^{a-1}\,dx\right| \leqslant K\frac{n!(n+1)!\Gamma(n+a/2)\Gamma(n+a/2+1)}{(2n+1)!(4n+a+2)[\Gamma(2n+a/2+1)]^2} \tag{B9}$$

with the aid of eqs (8) and (9); this bound is the minimum of eq. (B3) with respect to $u_1, \ldots, u_n$.

Equation (12) can be used to relate the interior method to more familiar principles. For example, application of eq. (12) to eq. (A1) gives

$$\sum_{j=1}^{n} W_j^{(n)}(1-x_j^2)P_i(x_j^2)[L_V(y^{(m)})|_{x=x_j}] = 0 \qquad i = 0, \ldots, \infty \tag{B10}$$

which requires that the residual vanish at each interior quadrature point; this is the interior collocation principle.

The summation on the left of eq. (B10) is the optimal n-point estimator of the corresponding integral

for *all* values of i. Thus, the collocation method gives the minimum n-point error bound on the integral of eq. (A1) for $i = 0, \ldots, \infty$, the minimization being done in the choice of $x_1, \ldots, x_n$. This minimum property enables the collocation method to give good results even when the integrand in the eq. (A1) is of too high a degree to be integrated exactly by eq. (12).

Application of eq. (12) to the least-squares principle, [eq. (A3)] again gives eq. (B10) provided one chooses $w(x) = 1 - x^2$. Other weight functions lead to other quadrature formulae and other collocation principles; thus, the weight $(1 - x^2)^{-1/2}$ leads, for $a = 1$, to the Lanczos method discussed under eq. (A5).

APPENDIX C: CALCULATION OF DIFFERENTIATION AND INTEGRATION COEFFICIENTS

The coefficients in Tables 3, 4 and 5 were computed by writing eqs (10), (11) and (12) for the functions $y = x^0$, $y = x^2$, $\ldots$, $y = x^{2n}$ and solving the resulting systems of equations for the arrays $A_{ij}^{(n)}$, $B_{ij}^{(n)}$ and $W_i^{(n)}$. The calculations may be summarized compactly in matrix form:

$$[A_{ij}^{(n)}] = \begin{bmatrix} (dx^0/dx)|_{x_1} & \cdots & (dx^{2n}/dx)|_{x_1} \\ \vdots & \cdots & \vdots \\ (dx^0/dx)|_{x_{n+1}} & \cdots & (dx^{2n}/dx)|_{x_{n+1}} \end{bmatrix} \begin{bmatrix} Q \end{bmatrix}^{-1} \tag{C1}$$

$$[B_{ij}^{(n)}] = \begin{bmatrix} \nabla^2(x^0)|_{x_1} & \cdots & \nabla^2(x^{2n})|_{x_1} \\ \vdots & \cdots & \vdots \\ \nabla^2(x^0)|_{x_{n+1}} & \cdots & \nabla^2(x^{2n})|_{x_{n+1}} \end{bmatrix} \begin{bmatrix} Q \end{bmatrix}^{-1} \tag{C2}$$

$$[W_{ij}^{(n)}] = \left[\int_0^1 x^{0+a-1}\,dx \quad \cdots \quad \int_0^1 x^{2n+a-1}\,dx \right] \begin{bmatrix} Q \end{bmatrix}^{-1} \tag{C3}$$

in which

$$[Q] = \begin{bmatrix} 1 & x_1^2 & \cdots & x_1^{2n} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & x_{n+1}^2 & \cdots & x_{n+1}^{2n} \end{bmatrix} \tag{C4}$$

The collocation points $x_1, \ldots, x_n$ that appear here are the roots of $P_n(x^2) = 0$ and x^{n+1} is unity. The roots were located approximately by Graeffe's method and refined to 10-digit accuracy by Newton's method. The calculations in eqs (C1)–(C3) were then done with standard matrix subroutines.