Numerical schemes for degenerate boundary value problems

1993 J. Phys. A: Math. Gen. 26 L413

(http://iopscience.iop.org/0305-4470/26/8/004)

J. Phys. A: Math. Gen. 26 (1993) L413–L421. Printed in the UK

LETTER TO THE EDITOR

Numerical schemes for degenerate boundary value problems

J W Mooney

Department of Mathematics, Glasgow Caledonian University, Glasgow G4 0BA, UK

Received 1 December 1992

Abstract. Methods for accurately determining solutions of degenerate boundary value problems are described. Nonlinear problems are first approximated by sequences of linear problems. A finite difference procedure which incorporates the effect of the degeneracy in the matrix of the linear discretized system of equations is developed. The simple tridiagonal structure of the matrix allows fast, accurate calculations to be performed with quite modest computer support. The results are readily improved using Richardson extrapolation.

Various physically important phenomena have been described using differential equations which degenerate at the boundary. These equations may be linear or nonlinear, and their solution causes numerical difficulties due to at least one of the derivatives of the solution becoming infinite at a boundary value [9]. In the case of nonlinear problems a quasilinearizaton technique [3] is often applicable, producing a sequence of degenerate linear differential equations converging to a solution of the nonlinear problem [15, 16]. However, approximation of a degenerate problem using a standard finite difference scheme is rarely satisfactory, particularly near the source of the degeneracy. Our aim is to illustrate how a new discretization technique can be used to provide accurate solutions simply and rather efficiently.

In many physical systems described by partial differential equations involving the Laplacian and the Dirichlet boundary conditions, the property of radial symmetry allows a reduction to a differential equation with one independent space variable (ordinary differential equation) or a partial differential equation in exactly two (one space, one time) variables. The dependency of the solution u on the 'radial' space variable r will then involve terms of the form $u''+(b/r)u'$. This is the case for nonlinear reaction-diffusion equations [10] where radially symmetric solutions play a useful role. The cubic Schrödinger equation in $(n+1)$-dimensional spacetime reduces to a form containing the space derivatives $u''+((n-1)/r)u'$. Particular cases arise in nonlinear optics, where $n=2$ and u is the envelope of an electromagnetic wave [12], and plasma physics, where $n=3$ and u is the envelope of a Langmuir wave [11]. There are physical applications for non-integral values of b also. In the theory of generalized axially symmetric heat potentials, values of b in the interval $[0, 2]$ arise when describing the conduction of heat in bodies of various shapes [1, 19]. Finally, even when a problem is not inherently symmetrical, radially symmetric solutions may be a launchpad for a perturbation analysis [18].

However, one major problem associated with the reduction process we have described arises when a boundary condition at $r=0$ is present. The differential form $u''+(b/r)u'$ will have an unwelcome singularity when $b\neq 0$, and degeneracy is said to occur at $r=0$.

0305-4470/93/080413+09$07.50

To analyse this situation further, we consider the ordinary differential equation $u''+(b/r)u'+f(r)g(u)=0$, where f and g are continuous functions. This is equivalent to the equation

$$(r^b u')' + r^b f(r)g(u) = 0. \tag{1}$$

When $f(r)=r^a$ and $g(u)=u^c$, with a, b, c real numbers and $c>0$, (1) is the Emden-Fowler equation. For $a=0$, $b=2$, $c=n$, typically 1.5 or 2.5, (1) is of importance in gas dynamics [5, 6]. There are more recent applications in fluid mechanics, relativistic mechanics, nuclear physics and chemically reacting systems and excellent bibliographies have been published [13, 21]. Equation (1) can be further reduced to the form $y''(x)+h(x, y(x))=0$ by a Liouville transformation. When f, g are power functions, then h is a product of powers of x and y. Consequently, there are many physical phenomena whose behaviour can be related to the solution y of the nonlinear equation $y''(x)=cx^p y^q(x)$, ($c=$ constant).

For illustration, we apply the numerical procedure to the degenerate two point boundary value problem [7]:

$$y''(x) = x^p y^q(x) \tag{2}$$

with $-2<p<0$, $q>1$, and $y(0)=1$, $y(a)=0$. The particular case $p=-\frac{1}{2}$, $q=\frac{3}{2}$ arises in the case of an ionized atom in Thomas–Fermi theory [8, 20].

We specify the nature of a degeneracy by means of the limit

$$\lim_{x\to p} \{y^R(x)(x-p)^P\} = k$$

where y^r is the rth derivative of any solution, p is a boundary point, k is a real constant, $R=\min\{r\colon y^r(a) \text{ is infinite}\}$, and P is the smallest positive rational number for which the limit is finite. The degeneracy is said to be of order (R, P) at $x=p$ or the differential equation to be (degenerate) of class D_P^R at $x=p$. The problem (2) will be approximated by sequences of linear two point boundary value problems each being discretized to form a tridiagonal matrix system. Accurate numerical solutions can be obtained when the equation is of class D_P^2, with $0<P<1$ at $x=0$. If $p<-1$, the problem is of class D_{-1-p}^1 and the solution of the discretized equations will not represent the solution of the nonlinear problem as accurately in this case.

The first step is to obtain algorithms for the sequence of linear boundary value problems which can be used to approximate the problem. The problem (2) is transformed to the form

$$\begin{aligned} &-\ddot{u}(t) + a^{2+p}qt^p u(t) = a^{2+p}t^p[(1-t)-u(t)]^q + a^{2+p}qt^p u(t) \\ &u(0)=u(1)=0 \end{aligned} \tag{3}$$

which is a generalization of the form (5.2) in [15], possessing homogeneous boundary conditions, and a solution $u(t)$ satisfying $u(t)=(1-t)-y(ta)=(1-x/a)-y(x)$, for x in $[0, a]$.

Generalizing on the method for developing the algorithm (3.3) in [15], we obtain

$$\begin{aligned} &-u''_{n+1}(t) + a^{2+p}qt^p u_{n+1}(t) = a^{2+p}t^p[(1-t)-u_n(t)]^q + a^{2+p}qt^p u_n(t) \\ &u_{n+1}(0)=u_{n+1}(1)=0 \end{aligned} \tag{4}$$

converging monotonically upwards from $u_0(t)=0$ and downwards from $u_0(t)=1-t$ to the solution of the transformed general Emden problem (3).

Putting $u_i(t)=(1-t)-w_i(t)$ in (4) above gives

$$\begin{aligned} &w''_{n+1}(t)-a^{2+p}qt^p w_{n+1}(t)=a^{2+p}t^p\{[w_n(t)]^q-qw_n(t)\} \\ &w_{n+1}(0)=1 \qquad w_{n+1}(1)=0 \end{aligned} \tag{5}$$

with $w(t)=y(ta)=y(x)$, and $w_n(t)$ converging to the solution of the problem

$$\begin{aligned} &w''(t)=a^{2+p}t^p w^q(t) \\ &w(0)=1 \qquad w(1)=0. \end{aligned} \tag{6}$$

This algorithmic scheme has linear or first-order convergence. A faster, one-sided scheme, may be obtained by quasilinearization. Thus, for a particular problem, this approach is capable of providing several numerical schemes whose results can be compared. Generalizing on the algorithm (3.4) in [15], we can obtain the second-order scheme

$$\begin{aligned} &-v''_{n+1}(t)=a^{2+p}t^p[(1-t)-v_n(t)]^q-a^{2+p}qt^p[(1-t)-v_n(t)]^{q-1}\{v_{n+1}(t)-v_n(t)\} \\ &v_{n+1}(0)=v_{n+1}(1)=0 \end{aligned} \tag{7}$$

which converges monotonically upwards from $v_0(t)=0$ to the solution of the transformed Emden problem (3) above, on the interval $[0,1)$.

Now putting $v_1(t)=(1-t)-w_i(t)$ in (7) gives

$$\begin{aligned} &w''_{n+1}(t)-a^{2+p}qt^p[w_n(t)]^{q-1}w_{n+1}(t)=a^{2+p}t^p\{[w_n(t)]^q-q[w_n(t)]^q\} \\ &w_{n+1}(0)=1 \qquad w_{n+1}(1)=0 \end{aligned} \tag{8}$$

converging monotonically downwards from $u_0(t)=1-t$ to the solution of problem (6). Taking $a=1$, and therefore $t=x$, $w(t)=y(x)$ in the problem (6) and the approximating sequences (5) and (8), gives the respective sequences

$$\begin{aligned} &y''_{n+1}(x)-qx^p y_{n+1}(x)=x^p\{[y_n(x)]^q-qy_n(x)\} \\ &y_{n+1}(0)=1 \qquad y_{n+1}(1)=0 \end{aligned} \tag{9}$$

and

$$\begin{aligned} &y''_{n+1}(x)-qx^p[y_n(x)]^{q-1}y_{n+1}(x)=(1-q)x^p[y_n(x)]^q \\ &y_{n+1}(0)=1 \qquad y_{n+1}(1)=0 \end{aligned} \tag{10}$$

converging to the solution of the generalized Emden problem

$$\begin{aligned} &y''(x)=x^p y^q(x) \qquad 0<x<1 \\ &y(0)=1 \qquad y(1)=0. \end{aligned} \tag{11}$$

The next step is to discretize these sequences effectively. Choosing a uniform grid:

$$0=x_0<x_1<\ldots<x_{N-1}<X_N=1$$

with $h=1/N$, $x_r=rh$, $r=1(1)N$ then, for $x=x_r$, $1\leqslant r\leqslant N-1$, we have for any iterative solution y:

$$\begin{aligned} &y(x+h)-2y(x)+y(x-h) \\ &\qquad =h^2y^{(2)}(x)+2h^4y^{(4)}(x)/4!+2h^6y^{(6)}(x)/6!+\cdots. \end{aligned}$$

Using (9) with $y^{(2)}(x)$ in place of $y''_{n+1}(x)$, then $y^{(2)}$ is expressible in terms of $y(x)$ and the previous iterate $y_n(x)$. For instance, for the first iterate in (9) with $y_0(x)=0$, we have

$$y_{r+1}-(2+qh^{2+p}r^p)y_r+y_{r-1}=2h^4y_r^{(4)}/4!+2h^6y_r^{(6)}/6!+\cdots$$

where $y_r=y(x_r)=y(rh)$, for $1\leqslant r\leqslant N-1$. However, since the derivatives contain negative powers of x that are large for values of $x=rh$ close to zero, the accuracy can be seen to be at best $O(h^{2+p})$. At least $O(h^2)$ accuracy is required for the effective use of the 'deferred approach to the limit' technique on the resulting discretization schemes. To accomplish this, all h^{2+p} terms are collected on the left-hand side giving, after a little algebra for series, the first lower iterate in (9):

$$y_{r+1}-(2+qh^{2+p}r^p\sum\alpha_{r,m})y_r+y_{r-1}=O(h^{3+p}) \qquad (1\leqslant r\leqslant N-1) \quad (12)$$

where $\Sigma\,\alpha_{r,m}=r^2[(1+1/r)^{p+2}+(1-1/r)^{p+2}-2]/(p+1)(p+2)$ $(p>-1)$. The sum is the addition of all coefficients of terms in h^{2+p}. For subsequent (all) iterates, the general expression is

$$y_{r+1}-(2+qv_r(h))y_r+y_{r-1}=v_r(h)f_r+O(h^{3+p}) \qquad (1\leqslant r\leqslant N-1) \qquad (13)$$

where $v_r(h)=h^{2+p}r^p\,\Sigma\,\alpha_{r,m}$, $f_r=\{[Y_r]^q-qY_r\}$, with Y_r being value of previous iterate Y at $x_r=rh$, $\Sigma\,\alpha_{r,m}$ as in [12], and $p>-1$.

Similarly, in the case of the iterates (10), collecting all h^{2+p} terms on the left-hand side gives

$$y_{r+1}-\{2+qv_r(h)[Y_r]^{q-1}\}y_r+y_{r-1}=v_r(h)g_r+O(h^{3+p}) \qquad (1\leqslant r\leqslant N-1) \qquad (14)$$

where $g_r=(1-q)[Y_r]^q$, with Y_r being value of previous iterate Y at $x_r=rh$, and $v_r(h)$, $\Sigma\,\alpha_{r,m}$ as defined in (13) and (12). For $p>-1$ we have $O(h^2)$ convergence for schemes (13) and (14).

All the discretization schemes have the form

$$A_{n+1}Y_{n+1}=B_n \qquad n=0,1,2,\ldots$$

where Y_{n+1}, an $N-1$ column vector, is the approximation to the $(n+1)$th iterate, A_{n+1} is a tridiagonal matrix of order $N-1$, and B_n is an $N-1$ column vector containing the boundary conditions and data relating to the nth iterate. Specifically, each matrix A has a constant value 1 in both the sub- and the super-diagonal and the diagonal element a_r of A_{n+1} for $1\leqslant r\leqslant N-1$ is given by

$$a_r=-(2+qh^{2+p}r^p\sum\alpha_{r,m}) \qquad (15)$$

for iterations (9) with $p>-1$, $q>1$.

$$a_r=-\{2+q(h^{2+p}r^p\sum\alpha_{r,m})[Y_r]^{q-1}\} \qquad (16)$$

for iterations (10) with $p>-1$, $q>1$, where Y is the previous iterate. The elements b_r $(1\leqslant r\leqslant N-1)$ in the column vector B_n are given by $[\{b_r\}]^T=[-1,0,0,\ldots,0,0]^T+[\{\beta_r\}]^T$, with:

$$\beta_r=(h^{2+p}r^p\sum\alpha_{r,m})f_r \qquad (17)$$

for iterations (9) with $p>-1$ and $q>1$, where $f_r=\{[Y_r]^q-qY_r\}$, with Y being the previous iterate {initially $Y_r\equiv0$ for increasing or $Y_r=(1-x_r)=(1-rh)$ for a decreasing sequence}.

$$\beta_r=(h^{2+p}r^p\sum\alpha_{r,m})g_r \qquad (18)$$

for iterations (10) with $p>-1$ and $q>1$, where $g_r=(1-q)[Y_r]^q$, with Y being the previous iterate {initially $Y_r=(1-x_r)=(1-rh)$ giving a decreasing sequence}.

A tridiagonal routine is used to solve $A_{n+1}Y_{n+1}=B_n$, $n=0, 1, \ldots$. Computations for a number of problems are presented in [17], and comparisons are made with previous methods. The results show high accuracy with a small amount of computer effort. In conclusion, the procedure is demonstrated fully for the ionized atom Thomas-Fermi boundary value problem (problem (11) with $p=-\frac{1}{2}$ and $q=\frac{3}{2}$).

We discuss the ionized atom Thomas-Fermi problem in detail:

$$\begin{aligned} &y''(x)=x^{-1/2}y^{3/2}(x) \qquad 0<x<1 \\ &y(0)=1 \qquad y(1)=0. \end{aligned} \tag{19}$$

The approximating sequences for this problem consist of the linear boundary value problems

$$\begin{aligned} &y''_{n+1}(x)-\tfrac{3}{2}x^{-1/2}y_{n+1}(x)=x^{-1/2}\{[y_n(x)]^{3/2}-\tfrac{3}{2}y_n(x)\} \\ &y_{n+1}(0)=1 \qquad y_{n+1}(1)=0 \end{aligned} \tag{20a}$$

on using (9), and

$$\begin{aligned} &y''_{n+1}(x)-\tfrac{3}{2}x^{-1/2}[y_n(x)]^{1/2}y_{n+1}(x)=-\tfrac{1}{2}x^{-1/2}[y_n(x)]^{3/2} \\ &y_{n+1}(0)=1 \qquad y_{n+1}(1)=0 \end{aligned} \tag{20b}$$

on using (10). The sequence $\{y_{n+1}\}$, $n\geqslant 0$, in (20a) converges monotonically from $y_0=0$, or from $y_0=1-x$, to the solution $y(x)$ of the Thomas-Fermi problem (19). The sequence $\{y_{n+1}\}$ in (20b) converges downwards from $y_0=1-x$ to the solution $y(x)$ of problem (19). The next step is to obtain finite difference approximations for the equations (20a) and (20b).

Discretizing the scheme (20a) gives, as in (13):

$$y_{r+1}+a_r y_r+y_{r-1}=v_r f_r+O(h^{5/2}) \tag{21}$$

for $1\leqslant r\leqslant N-1$, with $y_0=1$, $y_N=0$ where

$$a_r=-2\{1+h^{3/2}[(r+1)^{3/2}+(r-1)^{3/2}-2r^{3/2}]\} \tag{21a}$$

from (12), (15),

$$v_r=\tfrac{4}{3}h^{3/2}[(r+1)^{3/2}+(r-1)^{3/2}-2r^{3/2}] \tag{21b}$$

and

$$f_r=[Y_r]^{3/2}-\tfrac{3}{2}Y_r\} \tag{21c}$$

with Y being the previous iterate. Hence we first solve the tridiagonal scheme $AY_1=B_0$, where A is a fixed tridiagonal matrix with sub and super diagonal elements equal to 1 and rth ($1\leqslant r\leqslant N-1$) diagonal element a_r given by (21a). In the scheme $AY_1=B_0$ the column

$$B_0=[v_1f_1-1, v_2f_2, \ldots, v_{N-1}f_{N-1}]^T \tag{22}$$

with v_r given by (21b) and f_r by (21c). If Y in (21c) is taken to be $Y=[0, 0, 0, \ldots, 0, 0]^T$, then the solution Y_1 of (22) is the first (discretized) *lower* Picard iterate for problem (19). This iterate is given in table 1a for several discretizations $h=1/N$. However, if Y in (21c) is taken to be

$$Y=[(1-h), (1-2h), \ldots, (1-rh), \ldots, (1-(N-1)h)]^T \tag{23}$$

Table 1a. First Picard lower bounds $y_1(x)$ for solution of (19). Lower bound $y_1(x)$ is the extrapolated limit of $y_h(x)$, using (27) $y_h(x)$ is solution of discretized first lower Picard iterate (22) $h=1/N=1/1600$, $x=x_r=rh$ for $0\leqslant r\leqslant N$. $D_h=y_{2h}-y_h$, $D_{2h}=y_{4h}-y_{2h}$ actual numerical values = table entries $\times 10^{-9}$.

$y_1(x)$	$y_h(x)$ $N=1600$	D_h (1)	$y_{2h}(x)$ $N=800$	D_{2h} (2)	$y_{4h}(x)$ $N=400$	$y_{8h}(x)$ $N=200$	x
816 341 088	816 341 161	219	816 341 380	862	816 342 242	816 345 597	0.1
676 635 195	676 635 271	227	676 635 498	895	676 636 393	676 639 899	0.2
560 264 866	560 264 937	211	560 265 148	834	560 265 982	560 269 256	0.3
459 468 617	459 468 680	187	459 468 867	739	459 469 606	459 472 510	0.4
369 682 481	369 682 534	159	369 682 693	628	369 683 321	369 685 793	0.5
287 802 887	287 802 930	129	287 803 059	510	287 803 569	287 805 576	0.6
211 536 747	211 536 780	98	211 536 878	387	211 537 265	211 538 790	0.7
139 089 613	139 089 635	66	139 089 701	261	139 089 962	139 090 992	0.8
068 993 124	068 993 135	34	068 993 169	132	068 993 301	068 993 823	0.9

then the solution Y_1 of (22) is the first (discretized) *upper* Picard iterate for problem (19). This iterate is given in table 1*b* for several discretizations $h=1/N$.

The next step is to solve $AY_2=B_1$, where B_1 is defined as for B_0 but with f_r now given in terms of the iterate Y_1 (i.e. $Y=Y_1$). This enables a sequence of iterates Y_1, $Y_2, \ldots$ to be constructed which converges to the solution of the discretized problem (19) at the grid points $x_r=rh$, $1\leqslant r\leqslant N-1$. The convergence rate is linear.

Finally, we describe the discretization of the quadratic scheme (20*b*). This gives, from (14),

$$y_{r+1}+a_r y_r+y_{r-1}=v_r g_r+O(h^{5/2}) \tag{24a}$$

for $1\leqslant r\leqslant N-1$, with $y_0=1$ and $y_N=0$, where

$$a_r=-2\{1+h^{3/2}[(r+1)^{3/2}+(r-1)^{3/2}-2r^{3/2}][Y_r]^{1/2}\} \tag{24b}$$

v_r is given in (21*b*), and

$$g_r=-\tfrac{1}{2}[Y_r]^{3/2} \tag{24c}$$

with Y being the previous iterate.

Table 1b. First Picard upper bounds $y^1(x)$ for solution of (19). Upper bound $y^1(x)$ is the extrapolated limit of $y_h(x)$, using (27) $y_h(x)$ is solution of discretized first upper Picard iterate (22) $h=1/N=1/1600$, $x=x_r=rh$ for $0\leqslant r\leqslant N$. $D_h=y_{2h}-y_h$, $D_{2h}=y_{4h}-y_{2h}$ actual numerical values = table entries $\times 10^{-9}$.

$y^1(x)$	$y_h(x)$ $N=1600$	D_h (1)	$y_{2h}(x)$ $N=800$	D_{2h} (2)	$y_{4h}(x)$ $N=400$	$y_{8h}(x)$ $N=200$	x
850 718 983	850 719 042	175	850 719 217	690	850 719 907	850 722 597	0.1
729 624 593	729 624 655	184	729 624 839	725	729 625 564	729 628 409	0.2
626 610 569	622 610 627	173	622 610 800	684	622 611 484	622 614 172	0.3
524 332 582	524 332 634	155	524 332 789	613	524 333 402	524 335 814	0.4
431 691 062	431 691 106	133	431 691 239	528	431 691 767	431 693 846	0.5
342 650 317	342 650 354	110	342 650 464	435	342 650 899	342 652 612	0.6
255 798 924	255 798 952	84	255 799 036	336	255 799 372	255 800 697	0.7
170 144 790	170 144 809	58	170 144 867	232	170 145 099	170 146 012	0.8
085 012 173	085 012 183	30	085 012 213	121	085 012 334	085 012 811	0.9

Hence we first solve the tridiagonal scheme

$$A_1 Y_1 = B_0 \tag{25}$$

where A_1 has the same form as the matrix A in (22) but with the diagonal elements a_r, as given by (24a), iterate dependent (on Y). The column $B_0 = [v_1 g_1 - 1, v_2 g_2, \ldots, v_{N-1} g_{N-1}]^T$, with v_r given by (21b) and g_r by (24c), where Y is as in (23a). The solution Y_1 is the first (discretized) *upper* Newton iterate for the problem (19). This iterate is given in table 1c for several discretizations $h = 1/N$. We next solve $A_2 Y_2 = B_1$, where A_2 has diagonal elements given by (24a) with $Y = Y_1$, the previously found iterate, and the column B_1 is the same as B_0 but with g_r now in terms of the previous iterate $Y = Y_1$. Then the quadratically convergent sequence (20b) discretizes as $A_{n+1} Y_{n+1} = B_n$, $n = 0, 1, \ldots$, producing a sequence $\{Y_{n+1}\}$ converging to the solution of the discretized problem (19) at the grid points $x_r = rh$ $(1 \leqslant r \leqslant N-1)$.

Table 1c. First Newton upper bounds $\underline{y}^1(x)$ for solution of (19). Upper bound $\underline{y}^1(x)$ is the extrapolated limit of $y_h(x)$, using (27) $y_h(x)$ is solution of discretized first upper Newton iterate (25) $h = 1/N = 1/1600$, $x = x_r = rh$ for $0 \leqslant r \leqslant N$. $D_h = y_{2h} - y_h$, $D_{2h} = y_{4h} - y_{2h}$ actual numerical values = table entries $\times 10^{-9}$.

$\underline{y}^1(x)$	$y_h(x)$ $N = 1600$	D_h (1)	$y_{2h}(x)$ $N = 800$	D_{2h} (2)	$y_{4h}(x)$ $N = 400$	$y_{8h}(x)$ $N = 200$	x
849 621 180	849 621 239	177	849 621 416	694	849 622 110	849 624 817	0.1
727 501 050	727 501 112	186	727 501 298	733	727 502 031	727 504 903	0.2
619 644 832	619 644 890	175	619 645 065	694	619 645 759	619 648 484	0.3
520 800 241	520 800 294	158	520 800 452	625	520 801 077	520 803 534	0.4
427 928 975	427 929 021	137	427 929 158	540	427 929 698	427 931 825	0.5
339 023 757	339 023 795	113	339 023 908	446	339 024 354	339 026 113	0.6
252 669 004	252 669 033	87	252 669 120	346	252 669 466	252 670 828	0.7
167 836 520	167 836 540	60	167 836 600	238	167 836 838	167 837 777	0.8
083 782 101	083 782 111	31	083 782 142	124	083 782 266	083 782 753	0.9

The discretized problems (21) and (24) were solved for several mesh widths h between $h = 0.5 \times 10^{-2}$ and $h = 0.625 \times 10^{-3}$ and the difference columns (1) and (2) obtained as indicated in the tables. These difference columns were used with either of the 'deferred approach to the limit' formulae:

$$s = \frac{d}{3} + p \tag{26}$$

$$s = \frac{19d}{45} - \frac{e}{45} + p \tag{27}$$

where h is the uniform mesh width, s is the solution using the 'deferred correction' formula, p is the approximate solution y_h with mesh size h, and d, e are the differences $y_h - y_{2h}$, $y_{2h} - y_{4h}$, respectively. This produces the columns for $s = y_1$, y^1, $\underline{y}^1$, and $\underline{y}$ shown in tables 1 and 2. For an $O(h^2)$ accurate discretization process, formula (27) is the more accurate. The $O(h^2)$ accuracy is demonstrated by the difference columns (1), (2) in the tables being in the ratio 1:4. In the tables, $y_1(x)$ and $y^1(x)$ are the first lower and upper bounds for the solution of the Thomas-Fermi problem (19), obtained by using (20a) with $y_0(x) = 0$ and $y_0(x) = 1 - x$, respectively. Also, $\underline{y}^1(x)$ is the first

Table 2. Accurate numerical solution of (19) by iteration. Solution $\underline{y}(x)$ is the extrapolated limit of $y_h(x)$, using (27) $y_h(x)$ is iterated solution of either scheme (21) or scheme (24) $h=1/N=1/1600$, $x=x_r=rh$ for $0\leqslant r\leqslant N$. $D_h=y_{2h}-y_h$, $D_{2h}=y_{4h}-y_{2h}$ actual numerical values = table entries $\times 10^{-9}$.

$\underline{y}(x)$	$y_h(x)$ $N=1600$	D_h (1)	$y_{2h}(x)$ $N=800$	D_{2h} (2)	$y_{4h}(x)$ $N=400$	$y_{8h}(x)$ $N=200$	x
849 474 382	849 474 441	177	849 474 618	695	849 475 313	849 478 024	0.1
727 231 852	727 231 915	187	727 232 102	735	727 232 837	727 235 717	0.2
619 294 515	619 294 575	176	619 294 751	697	619 295 448	619 298 186	0.3
520 414 506	520 414 560	158	520 414 718	629	520 415 347	520 417 819	0.4
427 550 017	427 550 063	138	427 550 201	544	427 550 745	427 552 888	0.5
338 686 150	338 686 188	114	338 686 302	450	338 686 752	338 688 526	0.6
252 398 194	252 398 223	88	252 398 311	349	252 398 660	252 400 035	0.7
167 649 022	167 649 042	61	167 649 103	240	167 649 343	167 650 291	0.8
083 686 767	083 686 778	32	083 686 810	125	083 686 935	083 687 427	0.9

upper bound obtained using (20*b*) with $y_0(x)=1-x$. Applying (20*a*) and (20*b*) iteratively, the iterates $y_8(x)$, $y^7(x)$ and $\underline{y}^3(x)$ were found to be identical to nine decimal places for each discretization $h=1/N$ used, and are given as discretized solutions $y_h(x)$ for problem (19) in table 2. Applying the formula (26) or (27) gives the column for $s=\underline{y}(x)$, the approximate solution of (19) to nine decimal places given in table 2.

The tabulated results agree with those in [4]. These are given without the decimal point for clarity, the actual values being multiplied by 10^{-9}.

In conclusion, when the interval length a in (6) is larger than 20, at least 100 iterations are required for the scheme (9) but only 6 for the scheme (10). In these cases, Chan's method [4] is expensive. The discretization schemes were realized using double precision on an IBM PC (640K) with maths co-processor. The method can be used with other boundary conditions and on problems where there is a degeneracy of class D_p^2, $0<P<1$, on the boundary. Finally, other more general physical problems may often reduce to a problem of the form (11).

References

[1] Alexiades V 1982 *Arch. Rat. Mech. Anal.* **79** 325

[2] Ascher U M, Mattheij R M M and Russell R D 1988 *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations* (Englewood Cliffs, NJ: Printice-Hall)

[3] Bellman R E and Kalaba R 1965 *Quasilinearisation and Nonlinear Boundary Value Problems* (New York: Elsevier)

[4] Chan C Y and Hon Y C 1987 *Quart. Appl. Math.* **45** 591

[5] Chandrasekhar S 1942 *Principles of Stellar Dynamics* ch 5 (Chicago: University of Chicago Press)

[6] Chandrasekhar S 1957 *Introduction to the Study of Stellar Structure* ch 4 (New York: Dover)

[7] Emden R 1907 *Anwendungen der mechanischen Warmetheorie auf Kosmologie und meteorologischen Probleme* (Leipzig: Teubner)

[8] Fermi E 1927 *R. C. Accad. Naz. Lincei* (6) **6** 602

[9] Fox L 1980 *Computational Techniques for Ordinary Differential Equations* ed I Gladwell and D K Sayers (London: Academic Press)

[10] Gidas B, Ni W M and Nirenberg L 1979 *Commun. Math. Phys.* **68** 209

[11] Goldman M V 1984 *Rev. Mod. Phys.* **56** 709

[12] Kelley P L 1965 *Phys. Rev. Lett.* **15** 1005

[13] Kwong M K 1990 *ZAMP* **41** 79

[14] Mooney J W and Roach G F 1976 *Proc. R. Soc. Edinburgh* (A) **76** 81
[15] Mooney J W 1978 *Quart. Appl. Math.* **36** 305
[16] Mooney J W 1979 *Math. Meth. Appl. Sci.* **1** 554
[17] Mooney J W 1992 *Monotone Computational Procedures for Generalised Emden Equations* Glasgow Polytechnic Math. Tech. Report
[18] Oliker V I 1987 *Inverse Problems* **3** 743
[19] Solomon A D 1979 *Solar Energy* **22** 251
[20] Thomas L H 1927 *Proc. Camb. Phil. Soc.* **23** 542
[21] Wong J S W 1975 *SIAM Review* **17** 339