

SOLVING FINITE DIFFERENCE APPROXIMATIONS
TO NONLINEAR TWO-POINT BOUNDARY VALUE PROBLEMS
BY A HOMOTOPY METHOD

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ABSTRACT

The Chow-Yorke algorithm is a homotopy method that has been proved globally convergent for Brouwer fixed point problems, classes of zero finding, non-linear programming, and two-point boundary value problems. The method is numerically stable, and has been successfully applied to several practical nonlinear optimization and fluid dynamics problems. Previous application of the homotopy method to two-point boundary value problems has been based on shooting, which is inappropriate for fluid dynamics problems with sharp boundary layers. Here the Chow-Yorke algorithm is proved globally convergent for a class of finite difference approximations to nonlinear two-point boundary value problems. The numerical implementation of the algorithm is briefly sketched, and computational results are given for two fairly difficult fluid dynamics boundary value problems.

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I. INTRODUCTION

For the user of mathematical software, the ideal subroutine is a black box. The user specifies the problem and perhaps an error criterion, and the routine returns an answer and perhaps an indication of whether or not the error criterion was (likely) met. Such software exists for eigenvalues and eigenvectors, linear systems of equations, non-stiff initial value problems, and one-dimensional quadrature. For the first two areas, the sophistication and ease of use of EISPACK and LINPACK are well known. For the latter two areas, relieving the user of the burden of choosing step sizes or mesh points was a tremendous advance. The state of affairs with regard to nonlinear systems of equations is much more primitive, however. Although there is a huge amount of theory on nonlinear systems (for example, the book [14]), there is not software yet which approaches the black box ideal. Almost all the theory concerns locally convergent methods, which place the (sometimes extremely difficult) burden of choosing a good starting point on the user. Some of the recent quasi-Newton (or least change secant update) methods are robust and efficient, but the inescapable fact is that they still require good starting points (which is often not sufficiently emphasized). For example, with a Brouwer fixed point problem $x = f(x)$, where f maps some ball into itself, a fixed point exists, but the better quasi-Newton methods converge (as they are designed to [31, 32]) to a local minimum of $\|x - f(x)\|$. Typically economics and fluid dynamics problems have many such local minima nowhere near the fixed point, so a good starting point is essential.

A globally convergent algorithm (one that produces the correct answer regardless of its starting point) would seem to be the best foundation for nonlinear equations software. A globally convergent algorithm for nonlinear

equations sounds too good to be true. Actually, for Brouwer fixed points and a very large class of nonlinear systems of equations $F(x) = 0$, there are at least three distinct globally convergent algorithms. Because these algorithms are grounded in topology and differential geometry, were not discovered and advocated by numerical analysts, and were inefficient in their early implementations, they are not widely known or understood by numerical analysts. The excellent survey by Allgower and Georg [1] is an attempt to remedy that. The three algorithms are based on simplicial approximations (Eaves-Saigal [6,12,15]), retraction mappings (Kellogg-Li-Yorke [9]), and a parameterized Sard's theorem (Chow-Mallet-Paret-Yorke [4, 28]). Details can be found in the original references or [1]. This paper concentrates on the Chow-Yorke algorithm [27], the only one of the three that is both numerically stable and easy to understand.

The idea of the Chow-Yorke algorithm, various aspects of which have been around for a long time [1, 2, 5, 7, 8, 10, 11, 13, 14], is to track the zero curve of the homotopy map

$$\rho_a(\lambda, x) = \lambda f(x) + (1 - \lambda)(x - a)$$

emanating from $\lambda = 0$, $x = a$ until a zero of $f(x)$ is reached at $\lambda = 1$. Superficially this resembles standard imbedding [5], but there are two important differences. Here λ is not the imbedding parameter, but is a dependent variable just as x . Hence λ can increase and decrease along the zero curve, and need not increase monotonically from 0 to 1 (as in standard imbedding techniques). Furthermore, there are never any "singular points" along the zero curve, and turning points pose no special difficulty [28].

To be useful the Chow-Yorke algorithm must be globally convergent on the types of problems people actually solve. It has been proven globally convergent for Brouwer fixed points [4], the nonlinear complementarity problem [29], convex optimization problems with nonnegativity constraints

[26], and some two-point boundary value problems via shooting [30]. Actually the mathematical theory proves global convergence with probability one (i.e., it can fail only for starting points in a set of Lebesgue measure zero), but that has no practical significance since the exceptional set is nowhere dense. The intent of this paper is to prove the global convergence of the Chow-Yorke algorithm for the finite difference approximations to a class of nonlinear two-point boundary value problems, sketch the essence of the Chow-Yorke algorithm, and give some numerical results for two fluid dynamics problems. The intent here is not to prove very general theorems, but merely to justify the application of the Chow-Yorke algorithm to finite difference approximations of simple two-point boundary value problems. The computational results are on problems to which the theory is not obviously applicable.

Some theoretical results are presented in Section 2. The proofs rely heavily on theorems and descriptions published elsewhere, but at least the necessary facts are stated here. Section 3 sketches the numerical algorithm, which is described in detail in [28]. Computational results are given in Section 4. They are described in detail to make it clear exactly what equations were solved, and what the numerical experiments were.

Notation: E^n denotes n -dimensional Euclidean space; x_i denotes the i th component of a vector $x \in E^n$; the inner product $x^t y$ is simply written xy .

2. THEORY

Consider first the simple two-point boundary value problem

$$(1) \quad y''(x) = f(x, y(x), y'(x)), \quad 0 \leq x \leq 1,$$

$$(2) \quad y(0) = y(1) = 0,$$

where $y(x)$ is a scalar function, and $f(x, u, v)$ is C^2 . General boundary conditions and $y(x)$ a vector will be considered later. Partition the interval $[0,1]$ into $n+1$ equal subintervals of length $h = \frac{1}{(n+1)}$, let $x_i = ih$, $i = 0, \dots, n+1$, y_i be an approximation to an exact solution $y(x)$ at x_i . The following standard finite difference approximations will be used:

$$(3) \quad y''(x_i) = \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1}))}{h^2} + O(h^2)$$

$$(4) \quad y'(x_i) = \frac{y(x_{i+1}) - y(x_{i-1}))}{2h} + O(h^2)$$

$$(5) \quad y'(x_0) = \frac{-3y(x_0) + 4y(x_1) - y(x_2)}{2h} + O(h^2)$$

$$(6) \quad y'(x_{n+1}) = \frac{y(x_n) - 4y(x_{n+1}) + 3y(x_{n+2}))}{2h} + O(h^2).$$

Substituting (3), (4) into (1-2), neglecting terms of order h^2 , and replacing $y(x_i)$ by y_i , results in

$$(7) \quad G(Y) = AY + h^2 F(Y) = 0$$

where

$$Y = \begin{bmatrix} Y_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ Y_n \end{bmatrix} \quad A = \begin{bmatrix} 2 & -1 & 0 & & \\ -1 & 2 & -1 & \bigcirc & \\ 0 & -1 & 2 & & \\ & & & \ddots & \\ \bigcirc & & & & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}$$

and $F_i^h(Y) = f(x_i, Y_i, (Y_{i+1} - Y_{i-1}) / 2h)$, $i = 1, \dots, n$.

Thus the two-point boundary value problem (1-2) is approximated by the nonlinear system of equations (7). A homotopy method is used to solve (7). The following lemma from [29] will be useful.

Lemma 1. Let $F : E^n \rightarrow E^n$ be a C^2 map such that for some $r > 0$, $xF(x) \geq 0$ whenever $\|x\| = r$. Then F has a zero in $\{x \in E^n \mid \|x\| \leq r\}$, and for almost all $a \in E^n$, $\|a\| < r$, there is a zero curve γ of $\rho_a(\lambda, x) = \lambda F(x) + (1 - \lambda)(x - a)$,

along which the Jacobian matrix $D\rho_a(\lambda, x)$ has full rank, emanating from $(0, a)$ and reaching a zero \bar{x} of F at $\lambda = 1$. Furthermore, γ has finite arc length if $DF(\bar{x})$ is nonsingular.

The function $\rho_a : [0, 1] \times E^n \rightarrow E^n$ in Lemma 1 is the homotopy map. It is important to note that: 1) λ need not increase monotonically along the zero curve γ , 2) the Jacobian matrix of the homotopy map has full rank at every point along γ (this feature is convenient but not crucial to the success of a numerical method, see [35]); 3) γ is guaranteed to reach a zero of F with probability one.

Theorem 1. Let $F^h(Y)$ in (7) be a C^2 mapping, and suppose that

$$(8) \quad \lim_{\|Y\| \rightarrow \infty} \frac{\|F^h(Y)\|}{\|Y\|} \leq 9.$$

For $W \in E^n$, define $\rho_W : [0,1) \times E^n \rightarrow E^n$ by

$$\rho_W(\lambda, Y) = \lambda G(Y) + (1 - \lambda)(Y - W).$$

Then for almost all $W \in E^n$ there exists a zero curve γ of ρ_W , along which the Jacobian matrix $D\rho_W(\lambda, Y)$ has full rank, emanating from $(0, W)$ and reaching a zero \tilde{Y} of G (at $\lambda = 1$). Furthermore, if $DG(\tilde{Y})$ is nonsingular then γ has finite length.

Proof. By Lemma 1, it is sufficient to prove that $YG(Y) \geq 0$ for all Y sufficiently large. The matrix A in (7) is symmetric and positive definite with smallest eigenvalue $2(1 - \cos \frac{\pi}{n+1}) \geq \frac{9.5}{(n+1)^2} = 9.5h^2$ (for $n \geq 4$) [5]. By hypothesis, there exists $r > 0$ such that $\|F^h(Y)\| \leq 9.4\|Y\|$ for $\|Y\| \geq r$. Now for $\|Y\| \geq r$,

$$(9) \quad YG(Y) = YAY + h^2 YF^h(Y) \geq (9.5h^2)\|Y\|^2 - h^2\|Y\|(9.4\|Y\|) = .1h^2\|Y\|^2 > 0$$

using the symmetry of A and the Cauchy-Schwartz inequality. Q.E.D.

Corollary 1. If the condition (8) in Theorem 1 is replaced by $\lim_{\|Y\| \rightarrow \infty} \frac{\|F^h(Y)\|}{\|Y\|} \leq C < \pi^2$ for $0 < h < h_0$, then there exists $h_1 > 0$ such that Theorem 1 holds for $0 < h < h_1$.

Proof. For n large enough, the smallest eigenvalue $\lambda_1 = 2(1 - \cos \frac{\pi}{n+1})$ of A can be made arbitrarily close to $\frac{\pi^2}{(n+1)^2} = \pi^2 h^2$ from below. Also for $\|Y\|$ sufficiently large, $\|F^h(Y)\| \leq (C + \delta)\|Y\| < \pi^2\|Y\|$. Therefore

for n and $\|Y\|$ large enough, $\pi^2 h^2 > \lambda_1 > (C + \delta)h^2$, which when used in (9) gives the desired result. n large enough translates to h small enough, so the theorem holds for $0 < h < h_1$. Q.E.D.

Corollary 2. The conclusion of Theorem 1 holds if $f(x, u, v)$ in (1) is a C^2 mapping and bounded.

Consider now the differential equation (1) with the general boundary conditions

$$(10) \quad C \begin{bmatrix} y(0) \\ y'(0) \\ y(1) \\ y'(1) \end{bmatrix} = \begin{bmatrix} \alpha_{11}y(0) + \alpha_{12}y'(0) + \alpha_{13}y(1) + \alpha_{14}y'(1) \\ \alpha_{21}y(0) + \alpha_{22}y'(0) + \alpha_{23}y(1) + \alpha_{24}y'(1) \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = b,$$

with rank $C = 2$. Making the finite difference substitutions (3-6) in (1) and (10) leads to a system of equations of the form

$$(11) \quad \underline{G}(Y) = \underline{A}^h Y + h^2 \underline{F}^h(Y) = 0$$

where $\underline{Y} = (Y_0, \dots, Y_{n+1})^t$, \underline{A}^h is a matrix of order $n+2$ representing the linear differential operator and boundary conditions, and \underline{F}^h is a nonlinear operator arising from the nonlinear term of (1).

The following two Lemmas are from [30].

Lemma 2. Let $g : E^m \rightarrow E^m$ be a C^2 map and define $\rho_a : [0,1) \times E^m \rightarrow E^m$ by

$$\rho_a(\lambda, y) = \lambda g(y) + (1 - \lambda)(y - a).$$

Then for almost all $a \in E^m$ there is a zero curve γ of ρ_a emanating from $(0, a)$ along which $D\rho_a(\lambda, y)$ has full rank.

Lemma 3. If the zero curve γ in Lemma 2 is bounded, it has an accumulation point $(1, \bar{y})$, where $g(\bar{y}) = 0$. Furthermore if $Dg(\bar{y})$ is nonsingular, then γ has finite arc length.

Theorem 2. Let $\underline{F}^h(\underline{y})$ in (11) be a C^2 mapping, and suppose that \underline{G} satisfies one of the following:

- 1) there exists $r > 0$ such that $\underline{y} - \underline{w}$ and $\underline{G}(\underline{y})$ do not point in opposite directions for $\|\underline{y}\| = r$, $\|\underline{w}\| < r$;
- 2) there exists $r > 0$ such that $\underline{y} \underline{G}(\underline{y}) \geq 0$ for $\|\underline{y}\| = r$;
- 3) \underline{A}^h is positive semidefinite ($\underline{y} \underline{A}^h \underline{y} \geq 0$ for all \underline{y}); and there exists $r > 0$ such that

$$\underline{y} \underline{F}^h(\underline{y}) \geq 0 \text{ for } \|\underline{y}\| = r.$$

For $\underline{W} \in E^{n+2}$, define $\rho_{\underline{W}} : [0,1) \times E^{n+2} \rightarrow E^{n+2}$ by

$$\rho_{\underline{W}}(\lambda, \underline{Y}) = \lambda \underline{G}(\underline{Y}) + (1 - \lambda)(\underline{Y} - \underline{W}).$$

Then for almost all $\underline{W} \in E^{n+2}$, $\|\underline{W}\| < r$, there exists a zero curve γ of $\rho_{\underline{W}}$, along which the Jacobian matrix $D\rho_{\underline{W}}(\lambda, \underline{Y})$ has full rank, emanating from $(0, \underline{W})$ and reaching a zero $\underline{\tilde{Y}}$ of \underline{G} (at $\lambda = 1$). Furthermore, if $D\underline{G}(\underline{\tilde{Y}})$ is nonsingular, then γ has finite arc length.

Proof. It is sufficient to prove the theorem under condition 1), since 3) implies 2), which in turn implies 1). Condition 1) says that $\rho_{\underline{W}} \neq 0$ for $0 \leq \lambda < 1$ on the surface of the ball $\|\underline{Y}\| \leq r$. Therefore γ , if it exists, must lie entirely within the ball $\|\underline{Y}\| \leq r$. The existence of γ for almost all \underline{W} and γ reaching $\lambda = 1$ follow directly from Lemmas 2 and 3 above. The finite arc length of γ for $D\underline{G}(\underline{\tilde{Y}})$ nonsingular also follows from Lemma 3. Q.E.D.

Corollary 1. Suppose the matrix \underline{A}^h in (11) is positive definite and $f(x, u, v)$ in (1) is a bounded C^2 mapping. Then the conclusion of Theorem 2 holds.

Proof. f bounded implies \underline{F}^h in (11) is bounded, and therefore $h^2 \underline{Y} \underline{F}^h(\underline{Y}) = O(\|\underline{Y}\|)$. Let $n = \min_{\|\underline{Y}\|=1} \underline{Y} \underline{A}^h \underline{Y} > 0$. Then $\underline{Y} \underline{G}(\underline{Y}) = \underline{Y} \underline{A}^h \underline{Y} + h^2 \underline{Y} \underline{F}^h(\underline{Y}) \geq n \|\underline{Y}\|^2 + O(\|\underline{Y}\|) > 0$ for $\|\underline{Y}\|$ large enough, which is condition 2) in Theorem 2. Q.E.D.

Corollary 2. If $f(x, u, v)$ in (1) is a bounded C^2 mapping and the boundary conditions (10) are of the form

$$y(0) = b_1, \quad y(1) = b_2,$$

then the conclusion of Theorem 2 holds.

Proof. By Corollary 1, it is sufficient to show that the matrix \underline{A}^h in (11) is positive definite. With these boundary conditions,

$$\underline{A}^h = \begin{pmatrix} 1 & 0 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 & 0 \\ & & & & -1 & 2 & -1 \\ & & & & 0 & 0 & 1 \end{pmatrix}$$

$$\text{and } \underline{y}^T \underline{A}^h \underline{y} = y_0^2 - y_0 y_1 + y_1^2 + \sum_{i=1}^{n-1} (y_{i+1} - y_i)^2 + y_n^2 - y_n y_{n+1} + y_{n+1}^2 > 0 \text{ for } \underline{y} \neq \underline{0}, \text{ Q.E.D.}$$

Condition 1) in Theorem 2 is the most general situation in which the homotopy method is guaranteed globally convergent. However, it is virtually impossible to verify in practice, with a few notable exceptions [29].

Condition 3) is easier to verify, but is frequently not satisfied for practical problems. For most practical problems the homotopy method works very well, even though the above theory is not directly or demonstrably applicable.

Finally, consider the case where $y(x) = (y_1(x), \dots, y_m(x))$ in (1) is a m -dimensional vector function. Let $y_i^{(k)}$ be an approximation to the exact solution $y_k(x_i)$ and $Y = (Y^{(1)}, \dots, Y^{(m)}) \in E^{mn}$. Then the matrix in (7) becomes a block diagonal matrix with each diagonal block the same as A in (7), and $F^h(Y)$ is defined accordingly. The proofs of Theorem 1 and its corollaries are valid for the vector case also, so

Theorem 3. Theorem 1 and its corollaries are valid for the two-point boundary value problem (1-2), where $y(x) = (y_1(x), \dots, y_m(x))$ is a m -dimensional vector function, and Y , A , $F^h(Y)$ in (7) are defined as described.

The vector case with general boundary conditions (10) is not so easy, because there are many ways of forming the matrix \underline{A}^h in (11). The most advantageous way to merge the boundary conditions with the finite difference matrix to form \underline{A}^h depends on the problem. Without being more specific, assume \underline{A}^h in (11) is formed in some reasonable way, and that $\underline{F}^h(\underline{Y})$ is defined accordingly. Here $\underline{Y} \in E^{m(n+2)}$. The proof of Theorem 2 carries over to the vector case, but not necessarily the corollaries' proofs, since they depended on a specific structure in \underline{A}^h . Hence

Theorem 4. Theorem 2 is valid for the two-point boundary value problem (1), (10), where $y(x) = (y_1(x), \dots, y_m(x))$ is a m -dimensional vector function, C is a $2m \times 4m$ matrix of rank $2m$, and $\underline{Y}, \underline{A}^h, \underline{F}^h(\underline{Y})$ in (11) are defined such that (11) is a consistent approximation to (1), (10).

The boundary condition approximations based on (5), (6) are just one of many possibilities, and there was no particular reason for that choice. For example, adding an extra point to the left of zero or staggering the mesh points around zero and then using a central difference approximation for $y'(0)$ could have been done.

3. Algorithm

The general idea of the algorithm is apparent from Theorems 1 and 2: Just follow the zero curve γ emanating from $(0, W)$ until a zero \tilde{Y} of $G(Y)$ is reached (at $\lambda = 1$). Of course it is nontrivial to develop a viable numerical algorithm based on that idea, but at least conceptually, the algorithm is clear and simple. The numerical algorithm was described in detail in [28], and various aspects and applications of it are in [29-30]. [27] contains computer code for the algorithm. Since the algorithm has been thoroughly described elsewhere, only a brief outline of it and how it differs from standard continuation will be given here. The homotopy map is

$$\rho_W(\lambda, Y) = \lambda G(Y) + (1 - \lambda)(Y - W),$$

which has the same form as a standard continuation or embedding mapping. However, there are two crucial differences. In standard continuation, the embedding parameter λ increases monotonically from 0 to 1 as the trivial problem $Y - W = 0$ is continuously deformed to the problem $G(Y) = 0$. The present homotopy method permits λ to both increase and decrease along γ with no adverse effect, that is, turning points present no special difficulty. The second important difference is that there are never any "singular points" which plague standard continuation methods. The way in which the zero curve γ of ρ_W is followed and the full rank of $D\rho_W$ along γ guarantee this. Observe that Lemma 2 guarantees that γ cannot just "stop" at an interior point of $[0, 1] \times E^n$.

Parameterize γ by arc length s so $\lambda = \lambda(s)$, $Y = Y(s)$ along γ . Then

$$\rho_W(\lambda(s), Y(s)) = 0$$

and

$$(12) \quad \frac{d}{ds} p_w(\lambda(s), Y(s)) = 0,$$

$$(13) \quad \left\| \left(\frac{d\lambda}{ds}, \frac{dY}{ds} \right) \right\|_2 = 1.$$

Taking

$$(14) \quad \lambda(0) = 0, Y(0) = W,$$

the zero curve γ is the trajectory of the initial value problem (12-14). When $\lambda(\bar{s}) = 1$, the corresponding $Y(\bar{s})$ is a zero of $G(Y)$. Thus all the sophisticated ODE techniques currently available can be brought to bear on the problem of tracking γ [17,18].

ODE software requires $\left(\frac{d\lambda}{ds}, \frac{dY}{ds} \right)$ explicitly, and (12), (13) only implicitly define the derivative $\left(\frac{d\lambda}{ds}, \frac{dY}{ds} \right)$. This can be calculated by finding the kernel of the $n \times (n+1)$ matrix

$$Dp_w(\lambda(s), Y(s)),$$

which has full rank by Lemma 2. It is here that a substantial amount of computation is incurred, and it is imperative that the number of derivative evaluations be kept small. The recommended techniques for these calculations are given in [3,28].

Remember that tracking γ was merely a means to an end, namely a zero \tilde{Y} of $G(Y)$. Since γ itself is of no interest, one should not waste computational effort following it too closely. On the other hand, since γ is the only sure way to \tilde{Y} , losing γ can be fatal. The tradeoff between computational efficiency and reliability, and some practical advice based on computational experience, is also in [28].

4. NUMERICAL RESULTS.

All the results reported here were obtained on an IBM 370/158 using a double precision version of the code FIXPT in [27]. FIXPT was compiled with the FORTRAN H Extended compiler, and the answers were obtained accurate to 8 places unless otherwise mentioned. The execution times are in seconds. The examples here are intended to show the performance of the algorithm on realistic problems, and that the homotopy method works even though the theory in Section 2 is not obviously applicable.

The first example concerns the motion of a fluid squeezed between two parallel plates with prescribed normal velocity. The equations are [19], [30]

$$\begin{aligned} S(\eta f'''' + 3f'' + mf'f'' - ff''') &= f^{(4)} \\ f(0) = f''(0) = 0, \quad f(1) = 1, \quad f'(1) = 0, \\ m &= 0 \text{ (axisymmetric case).} \end{aligned}$$

With $x_1 = f$, $x_2 = f''$, the second order formulation is

$$\begin{aligned} x_1'' &= x_2 \\ x_2'' &= S(\eta x_2' + 3x_2 - x_1 x_2') \\ x_1(0) &= 0, \quad x_1(1) = 1 \\ x_2(0) &= 0, \quad x_1'(1) = 0. \end{aligned}$$

Note that the boundary conditions are unbalanced. This was handled by relating x_1 , x_1' , x_1'' , and x_2 at $\eta = 1$. The nonlinear system $G(Z) = 0$ corresponding to (7) is given in Table 1.

The dimension of the nonlinear system is $NEQ = 2n + 1$. Take $S = -4.226$. Starting from $W = 0$ with $n = 4$, the algorithm required 2.25 seconds of CPU time and 118 Jacobian evaluations, with an arc length of 20.0547. Starting from zero for larger n is expensive because most of the components of the solution are large resulting in a very long zero curve γ , and demonstrates nothing other than the global convergence. The results are shown in Table 2, with starting points

$$W = (0, 0, 1, 1, -1, -1, -1, -1, 2) \quad (n = 4)$$

$$W = (3*0, 3*.5, 3*1, 3*-.5, 6*-1, 2) \quad (n = 9)$$

$$W = (3*0, 4*.5, 7*1, 3*-1, 3*-2, 4*-4, -2, -1, 0, 1, 2) \quad (n = 14)$$

$$W = (3*0, 6*.5, 10*1, 4*-1, 5*-3, 5*-4, -3, -2, -1, 0, 1, 2) \quad (n = 19)$$

n	4	9	14	19
NEQ	9	19	29	39
CPU time	2.00	11.37	27.11	63.39
Jacobian evaluations	108	139	118	127
arc length	8.1771	11.8233	6.0622	4.4201
$x_2(1)$	2.7033820	2.1986139	2.1178779	2.0902818
extrapolated values		2.0303579	2.0532891	2.0548011
			2.0561555	2.0553051
				2.0552484

Table 2. Squeezing of a fluid between parallel plates.

The extrapolation was based on an asymptotic expansion in powers of h^2 , which should hold since all the finite difference approximations were $O(h^2)$ accurate [5]. The last extrapolated value compares well to the exact solution $x_2(1) = f''(1) = 2.05514$. (It is known that centered difference methods may have difficulties on such problems [33, 34].)

In [30] this squeezing problem was solved by the same code FIXPT, using instead a nonlinear system, equivalent to the original problem, defined by shooting. The shooting approach produces more accurate solutions than the finite difference method here, and it also yields the first and third derivatives throughout the interval, which the method here does not. The only difficulties with shooting (on this problem) are instability and the magnitude of the solution (which involves higher derivatives), both due to the pronounced boundary layers [19]. The shooting approach took 53 seconds on an Amdahl 470 V6. Allowing for the different machines, the CPU times for the shooting method in [30] and the finite difference method here are comparable. Since the shooting technique in [30] is more accurate, yields more information, is easier to program, and has approximately the same execution time as the finite difference method here, it is clearly preferable (for this squeezing problem).

In many fluid dynamics problems, the boundary layers become more pronounced as certain parameters increase [20, 21, 22]. As these parameters increase, shooting becomes more and more unstable. In extreme cases shooting completely fails, because unless it is started right at the correct initial conditions the solution to the differential equation becomes so large that the ODE solver never reaches the other end of the interval. An example of such a problem is in [20].

Frequently a stretching transformation alleviates the problem, but this doesn't help if there are multiple boundary layers whose locations change as the parameters change (as in [21], for example). Other possibilities are collocation and multiple shooting [5], but these were not tried. Shooting completely fails on the following problem, for the aforementioned reasons.

A model of the polar ice cap is given by the equations [22].

$$R(f'f'' - ff''') = f^{(4)} + \gamma k' ,$$

$$R(f'k - fk') = k'' - \gamma f' ,$$

$$R(gf' - fg') = g'' + \gamma h + B ,$$

$$R(gk - fh') = h'' - \gamma g ,$$

$$f(0) = -1 , f(1) = -\beta , f'(0) = f'(1) = 0 ,$$

$$k(0) = k(1) = g(0) = g(1) = h(0) = h(1) = 0 .$$

With $x_1 = f$, $x_2 = f''$, $x_3 = g$, $x_4 = h$, $x_5 = k$, the second order formulation is

$$x_1'' = x_2$$

$$x_2'' = R(x_1'x_2 - x_1x_2') - \gamma x_5'$$

$$x_3'' = R(x_3x_1' - x_1x_3') - \gamma x_4 - B$$

$$x_4'' = R(x_3x_5 - x_1x_4') + \gamma x_3$$

$$x_5'' = R(x_1'x_5 - x_1x_5') + \gamma x_1'$$

$$x_1(0) = -1 , x_1(1) = -\beta , x_1'(0) = x_1'(1) = 0 ,$$

$$x_3(0) = x_3(1) = x_4(0) = x_4(1) = x_5(0) = x_5(1) = 0 .$$

The unbalanced boundary conditions are handled as in the previous problem. Let

$z = (x_1(h) , \dots , x_1(nh) , x_2(0) , \dots , x_2(1) , x_3(h) , \dots , x_3(nh) , x_4(h) , \dots , x_4(nh) , x_5(h) , \dots , x_5(nh))$. The finite difference equations are

listed in Tables 3 and 4. The dimension of the nonlinear system is

$$NEQ = 5n + 2 .$$

Table 5 lists the results corresponding to starting points

$W = 0$ ($n = 4$)

$W = (-1, -.5, 0, .5, .5, 3*1, 2, 30, 20, 10, 5, 0, -2, -4, -6, -8, -10, -11, 18*0, 0, 6*-.5, 2*0)$ ($n = 9$)

$W = (-1, 3*-.5, 0, 3*.5, 3*1, 2*1.5, 2, 20, 17, 12, 7, 2, 0, -1, -2, -4, -6, -8, -9, 4*-11, 28*0, 2*0, -.2,$

$8*-.5, -.1, 2*0)$ ($n = 14$)

$W = (-1, 4*-.5, 3*0, 3*.5, 3*1, 3*1.5, 2*2, 23, 3*20, 10, 5, 0, -1, -2, -3, -4, -5, -6, -7, -8, -9, 5*-11,$

$38*0, 3*0, 3*-.5, 3*-1, 3*-.6, 3*-.3, 3*-.1, 0)$ ($n = 19$)

For $\gamma = R = 20$ shooting is successful, although with difficulty. For $\gamma = R > 25$ (and $\beta = -2$) shooting completely fails. An interesting note is that shooting succeeds for $\gamma > 25$, $R > 25$, $\beta \geq 0$, but becomes progressively worse as β decreases. As might be expected, the finite difference approach is impervious to the values of γ , R , and β .

Table 6 lists the results for a different set of parameters with starting points

$W = 0$ ($n = 4$)

$W = (-1, -.5, 0, 2*.5, 3*1, 2, 25, 20, 10, 5, 0, -2, -4, -6, -8, 2*-10, 27*0)$ ($n = 9$)

$W = (-1, 3*-.5, 0, 3*.5, 3*1, 2*1.5, 2, 23, 20, 14, 7, 2, 0, -1, -2, -4, -6, -8, -9, 4*-11, 42*0)$ ($n = 14$)

$W = (-1, 4*-.5, 3*0, 3*.5, 3*1, 3*1.5, 2*2, 23, 3*20, 10, 5, 0, -1, -2, -3, -4, -5, -6, -7, -8, -9,$

$5*-11, 57*0)$ ($n = 19$)

For $\gamma = 1$, $\beta = -2$ shooting begins to fail around $R = 20$, but the finite difference approach handles $R = 50$ with no difficulty, requiring only slightly more time than for $R = 30$.

5. CONCLUSION

Three conclusions can be drawn from Sections 2 and 4. First, the Chow-Yorke algorithm is theoretically applicable to the finite difference approximations to simple nonlinear two-point boundary value problems, and practically applicable to a much wider class than the present theory indicates. Second, the homotopy method is indeed globally convergent, and the code in [27] requires no jiggling of parameters and starting points to make it work. Third, and this observation has been made before [26,28], the homotopy method levels the difficulty of problems. Trivial problems take almost as much time as extremely difficult problems. Whenever a quasi-Newton method does converge to the correct answer, the quasi-Newton method is usually at least an order of magnitude more efficient than the homotopy method. The question, of course, is how to know when a quasi-Newton method will work. For non-oscillatory well conditioned problems Saigal and Todd's accelerated simplicial algorithm [16] is much more efficient than the Chow-Yorke algorithm, but the final verdict is not in yet. One final note: The differential geometry foundation of the Chow-Yorke algorithm is very powerful, and has been used to generate globally convergent nonlinear homotopies for problems on which the simplicial algorithms fail [25].

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$$\begin{bmatrix}
 \alpha_{11}h - \frac{3}{2}\alpha_{12} & 2\alpha_{12} & \frac{1}{2}\alpha_{12} & 0 & \dots & 0 & \frac{1}{2}\alpha_{14} & -2\alpha_{14} & \alpha_{13}h + \frac{3}{2}\alpha_{14} \\
 -1 & 2 & -1 & 0 & \dots & 0 & 0 & 0 & 0 \\
 0 & -1 & 2 & -1 & \dots & 0 & 0 & 0 & 0 \\
 0 & 0 & -1 & 2 & \dots & 0 & 0 & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & 0 & 0 & 0 & \dots & 2 & -1 & 0 & 0 \\
 0 & 0 & 0 & 0 & \dots & -1 & 2 & -1 & 0 \\
 0 & 0 & 0 & 0 & \dots & 0 & -1 & 2 & -1 \\
 \alpha_{21}h - \frac{3}{2}\alpha_{22} & 2\alpha_{22} & \frac{1}{2}\alpha_{22} & 0 & \dots & 0 & \frac{1}{2}\alpha_{24} & -2\alpha_{24} & \alpha_{23}h + \frac{3}{2}\alpha_{24}
 \end{bmatrix}
 \begin{bmatrix}
 Y_0 \\
 Y_1 \\
 Y_2 \\
 Y_3 \\
 \vdots \\
 Y_{n-2} \\
 Y_{n-1} \\
 Y_n \\
 Y_{n+1}
 \end{bmatrix}
 +
 \begin{bmatrix}
 -hb_1 \\
 h^2 f\left(x_1, Y_1, \frac{Y_2 - Y_0}{2h}\right) \\
 \vdots \\
 h^2 f\left(x_n, Y_n, \frac{Y_{n+1} - Y_{n-1}}{2h}\right) \\
 -hb_2
 \end{bmatrix}
 = 0$$

Figure 1. Detail for Equation (11).

$$\begin{array}{l}
 h^2 z_{n+1} \\
 h^2 z_{n+2} \\
 h^2 z_{n+3} \\
 \vdots \\
 h^2 z_{2n-1} \\
 h^2 z_{2n} \\
 h^2 S \left(\frac{z_n + 2}{2} + 3z_{n+1} - z_1 \frac{z_n + 2}{2h} \right) \\
 h^2 S \left(2 \frac{z_n + 3 - z_{n+1}}{2} + 3z_{n+2} - z_2 \frac{z_n + 3 - z_{n+1}}{2h} \right) \\
 h^2 S \left(3 \frac{z_n + 4 - z_{n+2}}{2} + 3z_{n+3} - z_3 \frac{z_n + 4 - z_{n+2}}{2h} \right) \\
 \vdots \\
 h^2 S \left(n \frac{z_{2n} + 1 - z_{2n-1}}{2} + 3z_{2n} - z_n \frac{z_{2n} + 1 - z_{2n-1}}{2h} \right)
 \end{array}$$

= 0

Table 1. Finite difference equations for squeezing problem. (Cont.)

$2z_1 - z_2$	$h^2 z_n + 2 + 1$
$- z_1 + 2z_2 - z_3$	$h^2 z_n + 3$
\vdots	\vdots
$- z_n - 2 + 2z_n - 1 - z_n$	$h^2 z_{2n}$
$- z_n - 1 + 2z_n$	$h^2 z_{2n} + 1 + \beta$
$- 8z_1 + z_2 + 2h^2 z_n + 1$	-7
$- z_n + 1 + 2z_n + 2 - z_n + 3$	$\frac{hR}{2}((z_2 + 1)z_n + 2 - z_1(z_n + 3 - z_n + 1)) - \frac{\gamma h}{2} z_{4n} + 4$
$- z_n + 2 + 2z_n + 3 - z_n + 4$	$\frac{hR}{2}((z_3 - z_1)z_n + 3 - z_2(z_n + 4 - z_n + 2)) - \frac{\gamma h}{2}(z_{4n} + 5 - z_{4n} + 3)$
\vdots	\vdots
$- z_{2n} - 1 + 2z_{2n} - z_{2n} + 1$	$\frac{hR}{2}((z_n - z_n - 2)z_{2n} - z_n - 1(z_{2n} + 1 - z_{2n} - 1)) - \frac{\gamma h}{2}(z_{5n} + 2 - z_{5n})$
$- z_{2n} + 2z_{2n} + 1 - z_{2n} + 2$	$\frac{hR}{2}((- \beta - z_n - 1)z_{2n} + 1 - z_n(z_{2n} + 2 - z_{2n})) + \frac{\gamma h}{2} z_{5n} + 1$
$z_n - 1 - 8z_n + 2h^2 z_{2n} + 2$	-7\beta
$2z_{2n} + 3 - z_{2n} + 4$	$\frac{hR}{2}(z_{2n} + 3(z_2 + 1) - z_1 z_{2n} + 4) - \gamma h^2 z_{3n} + 3 - Bh^2$
$- z_{2n} + 3 + 2z_{2n} + 4 - z_{2n} + 5$	$\frac{hR}{2}(z_{2n} + 4(z_3 - z_1) - z_2(z_{2n} + 5 - z_{2n} + 3)) - \gamma h^2 z_{3n} + 4 - 8h^2$
\vdots	\vdots
$- z_{3n} + 2z_{3n} + 1 - z_{3n} + 2$	$\frac{hR}{2}(z_{3n} + 1(z_n - z_n - 2) - z_n - 1(z_{3n} + 2 - z_{3n})) - \gamma h^2 z_{4n} + 1 - Bh^2$
$- z_{3n} + 1 + 2z_{3n} + 2$	$\frac{hR}{2}(z_{3n} + 2(- \beta - z_n - 1) + z_n z_{3n} + 1) - \gamma h^2 z_{4n} + 2 - 8h^2$

= 0

Table 3. Finite difference equations for polar ice cap problem (part 1).

$$\begin{aligned}
& \left[\begin{aligned} & 2z_{3n} + 3 - z_{3n} + 4 \\ & - z_{3n} + 3 + 2z_{3n} + 4 - z_{3n} + 5 \\ & \vdots \\ & - z_{4n} + 2z_{4n} + 1 - z_{4n} + 2 \\ & - z_{4n} + 1 + 2z_{4n} + 2 \\ & \\ & 2z_{4n} + 3 - z_{4n} + 4 \\ & - z_{4n} + 3 + 2z_{4n} + 4 - z_{4n} + 5 \\ & \vdots \\ & - z_{5n} + 2z_{5n} + 1 - z_{5n} + 2 \\ & - z_{5n} + 1 + 2z_{5n} + 2 \end{aligned} \right] \\
& + \\
& \left[\begin{aligned} & Rh^2(z_{2n} + 3z_{4n} + 3 - z_1 \frac{z_{3n} + 4}{2h}) + \gamma h^2 z_{2n} + 3 \\ & Rh^2(z_{2n} + 4z_{4n} + 4 - z_2 \frac{z_{3n} + 5 - z_{3n} + 3}{2h}) + \gamma h^2 z_{2n} + 4 \\ & \vdots \\ & Rh^2(z_{3n} + 1z_{5n} + 1 - z_n - 1 \frac{z_{4n} + 2 - z_{4n}}{2h}) + \gamma h^2 z_{3n} + 1 \\ & Rh^2(z_{3n} + 2z_{5n} + 2 + z_n \frac{z_{4n} + 1}{2h}) + \gamma h^2 z_{3n} + 2 \\ & \\ & \frac{hR}{2} ((z_2 + 1)z_{4n} + 3 - z_1 z_{4n} + 4) + \frac{\gamma h}{2} (z_2 + 1) \\ & \frac{hR}{2} ((z_3 - z_1)z_{4n} + 4 - z_2 (z_{4n} + 5 - z_{4n} + 3)) + \frac{\gamma h}{2} (z_3 - z_1) \\ & \vdots \\ & \frac{hR}{2} ((z_n - z_n - 2)z_{5n} + 1 - z_n - 1(z_{5n} + 2 - z_{5n})) + \frac{\gamma h}{2} (z_n - z_n - 2) \\ & \frac{hR}{2} ((-\beta - z_n - 1)z_{5n} + 2 + z_n z_{5n} + 1) + \frac{\gamma h}{2} (-\beta - z_n - 1) \end{aligned} \right] \\
& = 0
\end{aligned}$$

Table 4. Finite difference equations for polar ice cap problem (part 2).

n	4	9	14	19
NEQ	22	47	72	97
CPU time	18.4	114.8	483.7	1153.9
Jacobian evaluations	155	138	176	179
arc length	38.80661	18.47349	17.41116	20.33562
f'' (0)	26.924488	23.570686	23.185378	23.068960
extrapolated values		22.452752	22.877132	22.919280
			22.930180	22.933329
				22.933539

Table 5. $\gamma = R = 30$, $\beta = -2$, $B = .5$.

n	4	9	14	19
NEQ	22	47	72	97
CPU time	17.4	141.3	546.8	1225.3
Jacobian evaluations	141	165	194	186
arc length	39.40252	13.53256	19.01427	22.85432
$f''(1)$	-10.525653	-11.197161	-11.299751	-11.337634
extrapolated values		-11.420997	-11.381823	-11.386341
			-11.376926	-11.387847
				-11.388575

Table 6. $\gamma = 1$, $R = 50$, $\beta = -2$, $B = .5$.