SOLVING GALERKIN APPROXIMATIONS TO NONLINEAR TWO-POINT BOUNDARY VALUE PROBLEMS BY A GLOBALLY CONVERGENT 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, certain classes of zero finding and nonlinear programming problems, and two-point boundary value approximations based on shooting, finite differences, and spline collocation. The method is numerically stable and has been successfully applied to a wide range of practical engineering problems. Here the Chow-Yorke algorithm is proved globally convergent for a class of Galerkin approximations to nonlinear two-point boundary value problems. Several numerical implementations of the algorithm are briefly described, and computational results are presented for a fairly difficult magneto-hydrodynamics boundary value problem.

Key words. homotopy method, Chow-Yorke algorithm, globally convergent, two-point boundary value problem, Galerkin method, finite element method, nonlinear equations

1. Introduction. The Chow-Yorke algorithm (actually a family of algorithms) for nonlinear systems of equations was proposed in 1976, and since that time both the theory and the scope of its practical applicability have been greatly extended. This homotopy algorithm is accurately described as a globally convergent, probability-one algorithm. It is truly globally convergent in the sense that it will converge to a solution of the problem from an *arbitrary* starting point. The phrase "probability one" refers to the rigorous theoretical results which guarantee convergence for almost all choices of some parameter vector, i.e., with probability one.

Homotopy methods (both continuous [1] and simplicial [10, 24]) were originally very inefficient, and dismissed by some as inherently inferior to quasi-Newton algorithms. A common misconception is that homotopy algorithms are just continuation or an obvious extension of classical continuation. While this is superficially true, there are fundamental philosophical differences between these probability-one algorithms and standard continuation. These differences result in an elegant and rigorous theoretical foundation for globally convergent probability-one homotopy algorithms, and have subtle yet important implications for computer implementations [56]. Furthermore, there has been a series of practical engineering problems, successfully solved by homotopy methods, on which continuation and quasi-Newton methods either totally failed or experienced great difficulty [28-46]. Current implementations (as in HOMPACK [55]) of these globally convergent probability-one homotopy algorithms are reasonably efficient, and their robustness, stability, and accuracy have never been in doubt.

There are three distinct, but interrelated, aspects of homotopy methods: 1) construction of the right homotopy map, 2) theoretical proof of global convergence for this homotopy map, and 3) tracking the zero curve of this homotopy map. The first aspect is currently still an art, although this is much better understood now due to the accumulation of computational experience [28-46, 49]. Although much remains to be done, significant progress has been made on the second aspect. Global convergence has been proved for Brouwer fixed point problems [4, 48], certain classes of zero finding [48] and nonlinear programming (both unconstrained and constrained) problems [49], and two-point boundary value approximations based on shooting [51], finite differences [52], and spline collocation [54]. Recently Morgan [21-22] obtained some elegant results for polynomial systems, and the present work considers Galerkin approximations to nonlinear two-point boundary value problems. Various curve tracking algorithms have been around for a long time (e.g., [14-16]), but

there is an important distinction between general curve tracking algorithms and homotopy curve tracking algorithms. The object of the former is the zero curve *itself*, whereas the object of the latter is a point at $\lambda = 1$. This difference was emphasized in [47], [48], and [56], and the algorithms described here are more in the spirit of homotopy methods than a general tracker.

Section 2 outlines the theoretical foundation of globally convergent, probability-one homotopy methods, and proves some convergence theorems for Galerkin approximations to nonlinear two-point boundary value problems. Section 3 discusses several algorithms for tracking the homotopy curves, as well as some pertinent details of the software package HOMPACK used to obtain the numerical results. Section 4 considers a nontrivial two-point boundary value problem from fluid dynamics, presents numerical results, and illustrates the dependence of the solution on the problem parameters.

2. Theory. Consider the two-point boundary value problem

$$y''(x) = f(x, y(x), y'(x)), \qquad 0 \le x \le 1, \tag{1}$$

$$y(0) = y(1) = 0, \tag{2}$$

where $y(x)$ is an $\hat{n}$-dimensional vector function and $f(x, u, v)$ is an $\hat{n}$-dimensional C^2 vector function. This is naturally posed in a weak form via a variational formulation using the space

$$V = \left\{ f \in H^1[0,1] \mid f(0) = f(1) = 0 \right\},$$

where $H^1[0,1]$ is the Hilbert space of all absolutely continuous functions on $[0,1]$ whose derivative lies in $L^2[0,1]$. Let $S_n \subset V$ be a finite-dimensional vector space with basis $\phi_1, \ldots, \phi_n$.

Using the finite-dimensional approximations

$$y_m(x) \approx A_m(x) = \sum_{i=1}^{n} \alpha_{mi} \phi_i(x), \qquad m = 1, \ldots, \hat{n}, \tag{3}$$

the standard Galerkin approximation to equations (1–2) is the nonlinear system of equations

$$\sum_{i=1}^{n} \alpha_{mi} \langle \phi_i', \phi_k' \rangle + \langle f_m(\cdot, A, A'), \phi_k \rangle = 0,$$

$$k = 1, \ldots, n, \quad m = 1, \ldots, \hat{n}. \tag{4}$$

Here

$$\langle u, v \rangle = \int_0^1 u(t) v(t) \, dt \tag{5}$$

is the inner product.

Example 1. Continuous piecewise linear functions.
Let $0 = x_0 < x_1 < \cdots < x_n < x_{n+1} = 1$ be a partition of $[0,1]$, and let S_n be the space of continuous, piecewise linear functions $f(x)$ with breakpoints $x_0, \ldots, x_{n+1}$ and $f(0) = f(1) = 0$. The

basis functions ϕ_i, $i = 1, \ldots, n$, are defined by $\phi_i(x_j) = \delta_{ij}$. Observe that in this case the equations (4) correspond to the difference equations

$$\frac{2}{h_k + h_{k+1}} \left[\frac{A_m(x_{k+1}) - A_m(x_k)}{h_{k+1}} - \frac{A_m(x_k) - A_m(x_{k-1})}{h_k} \right] =$$

$$\frac{2}{h_k + h_{k+1}} \langle f_m(\cdot, A, A'), \phi_k \rangle = f_m(x_k, A(x_k), A'(x_k)) + \mathcal{O}(h)$$

where $h_i = x_i - x_{i-1}$, $h = \max_j h_j$. This is a standard finite difference approximation to (1) (*cf.* [52] for the case of a uniform mesh).

Example 2. Chebyshev series (spectral methods).
Using the Chebyshev polynomials $\{T_n(x)\}_{n=0}^{\infty}$ for the interval $[-1, 1]$, take

$$\phi_{k-1}(x) = \begin{cases} T_k(2x - 1) - 1, & k \text{ even} \\ T_k(2x - 1) - (2x - 1), & k \text{ odd} \end{cases}$$

for $k = 2, 3, \ldots$. These $\phi_k(x)$ satisfy the zero boundary conditions, are dense in V, and are relatively well conditioned. The equations (4) in this case are not sparse. See Gottlieb and Orszag [12] for details.

A third example, generalizing Example 1, would be a space $S_n \subset C^{k-2}[0, 1]$ consisting of piecewise polynomials of order $k \geq 2$ with B-splines for the basis functions ϕ_i. This spline space is developed in Section 4.

The accuracy and convergence of the Galerkin approximation (3) to the exact solution $\phi(x)$ of (1-2) can be shown under various assumptions on the nonlinear right hand side $f(x, u, v)$ and generalizations of y'' to elliptic operators $L[w(x)] = \sum_{j=0}^{N}(-1)^{j-1} D^j(p_j(x)D^j w(x))$. To illustrate, some typical theorems from Ciarlet, Schultz, and Varga [5-9] will be quoted here. Following [5], assume that $\hat{n} = 1$, a classical solution $\phi(x)$ of (1-2) exists, the nonlinear right hand side has the form $f(x, y)$ (i.e., does not involve y'), and

$$\frac{\partial f(x, u)}{\partial u} \geq \gamma > -\Lambda \equiv -\inf_{\substack{w \in V \\ w \neq 0}} \frac{\displaystyle\int_0^1 (w'(t))^2 \, dt}{\displaystyle\int_0^1 (w(t))^2 \, dt} \tag{6}$$

for all $x \in [0, 1]$ and all real u. The appropriate norm (derived from an inner product based on a linearization of (4)) in this context is

$$\|w\|_\gamma = \left[\int_0^1 (w'(x))^2 + \gamma (w(x))^2 \, dx \right]^{1/2}, \quad w \in V,$$

where the constant γ is the same as that in (6). The accuracy of the Galerkin approximation $A(x)$ is given by

Theorem. Let $\phi(x)$ be the solution of (1-2) subject to the assumptions above, let S_n be any finite dimensional subspace of V of dimension n with basis $\phi_1, \ldots, \phi_n$, and let $\hat{A}_n(x) = \sum_{i=1}^{n} \hat{\alpha}_{ni} \phi_i(x)$,

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where $\hat{\alpha}_n$ is the (unique under the above assumptions) solution to (4). Then there exist constants C and K independent of n and S_n such that

$$\|\hat{A}_n - \phi\|_\infty \leq K\|\hat{A}_n - \phi\|_\gamma \leq C \inf_{w \in S_n} \|w - \phi\|_\gamma.$$

Theorem. Let $\phi(x)$ be the solution of (1-2) subject to the assumptions above, let $\left\{S_n\right\}_{n=1}^\infty$ be any sequence of finite dimensional subspaces of V such that $\bigcup_{n=1}^\infty S_n$ is dense in V in the norm $\|\cdot\|_\gamma$, and let $\left\{\hat{A}_n(x)\right\}_{n=1}^\infty$ be the sequence of functions obtained by solving (4) over the subspaces S_n respectively. Then $\left\{\hat{A}_n(x)\right\}_{n=1}^\infty$ converges *uniformly* to $\phi(x)$.

Generalizations of these theorems [5-9, 26] tend toward generalizing the differential operator on the left hand side in (1), weakening the smoothness assumptions on the right hand side in (1), and generalizing the boundary conditions (2), rather than the form of and growth conditions on $f(x, u, v)$. The homotopy theorems derived here require C^2 smoothness (piecewise C^2 is the absolute minimal requirement), and have rather mild growth restrictions on $f(x, u, v)$ compared to (6). Furthermore the f considered here can involve $y'(x)$ in a highly nonlinear way, whereas the $f = f(x, u)$ in (6) cannot involve $y'(x)$ at all. Roughly speaking, with the exception of smoothness, the limitations of the theoretical foundations for applying globally convergent homotopy methods to Galerkin approximations to nonlinear two-point boundary value problems derive more from the applicability of the Galerkin method itself than from the convergence conditions of the homotopy methods.

Let $Y = \left(\alpha_{11}, \alpha_{12}, \ldots, \alpha_{1n}, \alpha_{21}, \ldots, \alpha_{2n}, \ldots, \alpha_{\hat{n}1}, \ldots, \alpha_{\hat{n}n}\right)^t$. Then the system of equations (4) has the form

$$F(Y) = M\,Y + N(Y) = 0, \tag{7}$$

where

$$M = \begin{pmatrix} \bar{M} & 0 & \ldots & 0 \\ 0 & \bar{M} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \bar{M} \end{pmatrix}, \qquad \bar{M}_{ij} = \langle \phi_i', \phi_j' \rangle,$$

$$N(Y) = \Big(\langle f_1(x, A(x), A'(x)),\, \phi_1(x) \rangle, \ldots, \langle f_1(x, A(x), A'(x)),\, \phi_n(x) \rangle,$$

$$\langle f_2(x, A(x), A'(x)),\, \phi_1(x) \rangle, \ldots, \langle f_2(x, A(x), A'(x)),\, \phi_n(x) \rangle,$$

$$\vdots$$

$$\langle f_{\hat{n}}(x, A(x), A'(x)),\, \phi_1(x) \rangle, \ldots, \langle f_{\hat{n}}(x, A(x), A'(x)),\, \phi_n(x) \rangle \Big).$$

Thus the two-point boundary value problem (1-2) is approximated by the nonlinear system of equations (7), which has dimension

$$p = \hat{n}\, n.$$

A homotopy method is used to solve (7).

Since $(u, v) \to \langle u', v' \rangle$ is an inner product on V and $\phi_1, \ldots, \phi_n$ are linearly independent, the Gram matrix $\bar{M}$ is symmetric and positive definite. Therefore M is also symmetric, positive definite.

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Let E^p denote p-dimensional real Euclidean space. The following four lemmas from [51], [51], [50], [52] respectively will be useful.

Lemma 1. Let $F : E^p \to E^p$ be a C^2 map, $a \in E^p$, and define $\rho_a : [0,1) \times E^p \to E^p$ by

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

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

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

Lemma 3. Let $F : E^p \to E^p$ be a C^2 map such that for some $r > 0$, $xF(x) \geq 0$ whenever $\|x\| = r$. Then F has a zero in $\{x \in E^p \mid \|x\| \leq r\}$, and for almost all $a \in E^p$, $\|a\| < r$, 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.

Lemma 3 is a special case of the following more general lemma.

Lemma 4. Let $F : E^p \to E^p$ be a C^2 map such that for some $r > 0$ and $\tilde{r} > 0$, $F(x)$ and $x - a$ do not point in opposite directions $(\mu F(x) + (x - a) \neq 0 \ \forall \mu > 0)$ for $\|x\| = r$, $\|a\| < \tilde{r}$. Then F has a zero in $\{x \in E^p \mid \|x\| \leq r\}$, and for almost all $a \in E^p$, $\|a\| < \tilde{r}$, 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.

Theorem 1. Let $N(Y)$ in (7) be a C^2 mapping, and suppose there exist constants C and ν such that

$$\limsup_{\|Y\|_2 \to \infty} \frac{\|N(Y)\|_2}{\|Y\|_2^\nu} = C, \qquad 0 \leq \nu < 1. \tag{8}$$

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

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

Then for almost all $W \in E^p$ 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 F (at $\lambda = 1$). Furthermore, if $DF(\tilde{Y})$ is nonsingular, then γ has finite arc length.

Proof. As observed above, the matrix M in (7) is symmetric and positive definite. Therefore all its eigenvalues are real and positive. Let $\Gamma > 0$ be the smallest eigenvalue of M. Then a simple argument shows that for $Y \neq 0$,

$$Y^t M Y \geq \Gamma \|Y\|_2^2 > 0. \tag{9}$$

Choose $\epsilon > 0$. Using (8) and (9) yields

$$Y^t F(Y) = Y^t M Y + Y^t N(Y) \geq \Gamma \|Y\|_2^2 - \|Y\|_2 (C + \epsilon) \|Y\|_2^\nu > 0$$

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for $\|Y\|_2$ sufficiently large. Therefore there exists $r > 0$ such that $Y^t F(Y) \geq 0$ for $\|Y\|_2 = r$. The result now follows directly from Lemma 3. $\qquad Q.E.D$

Theorem 2. Let $N(Y)$ in (7) be a C^2 mapping and $\Gamma > 0$ defined by (9). If

$$\limsup_{\|Y\|_2 \to \infty} \frac{\|N(Y)\|_2}{\|Y\|_2} = C < \Gamma,$$

then the conclusion of Theorem 1 holds.

Proof. This follows immediately from the proof of Theorem 1. $\qquad Q.E.D.$

Observe that Theorem 2 is stronger than Theorem 1, but since Theorem 2 requires knowledge of Γ, Theorem 1 is easier to verify. The next two theorems, giving conditions on the right hand side $f(x, u, v)$ in (1), are what one would use in practice.

Theorem 3. If $f(x, u, v)$ in (1) is C^2 and bounded, then the conclusion of Theorem 1 holds.

Proof. $f(x, u, v)$ bounded and C^2 implies that $N(Y)$ is also bounded and C^2, and thus (8) holds with $C = 0$ and $\nu = 1/2$. Therefore the conclusion of Theorem 1 holds. $\qquad Q.E.D.$

Theorem 4. Let $f(x, u, v)$ in (1) be a C^2 mapping, and suppose there exist constants μ, ξ, and ν such that

$$\|f(x, u, v)\|_2 \leq \mu\big(\xi + (\|u\|_2 + \|v\|_2)^\nu\big), \quad 0 \leq \nu < 1,$$

for all $0 \leq x \leq 1$ and $u, v \in E^{\hat{n}}$. Then the conclusion of Theorem 1 holds.

Proof. Let

$$y_k(x) = \sum_{i=1}^{n} Y_{(k-1)n+i}\,\phi_i(x), \quad k = 1, \ldots, \hat{n}, \quad 0 \leq x \leq 1, \tag{10a}$$

and

$$z_k(x) = \sum_{i=1}^{n} Z_{(k-1)n+i}\,\phi_i(x), \quad k = 1, \ldots, \hat{n}, \quad 0 \leq x \leq 1. \tag{10b}$$

Since the basis functions ϕ_i are in V, it follows from the equivalence of norms in finite dimensional spaces that there exist constants $K_1 > 0$ and $K_2 < \infty$ such that

$$K_1(\alpha^t\alpha)^{1/2} \leq \left\|\sum_{i=1}^{n} \alpha_i\phi_i\right\|_{W_2^1[0,1]} \leq K_2(\alpha^t\alpha)^{1/2}, \tag{11}$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)^t$ is a real n-vector and $W_p^1[0,1]$ is the Sobolev space of functions whose (weak) derivatives lie in $L^p[0,1]$, and the Sobolev norms are (*cf.* [26])

$$\|v\|_{W_p^1[0,1]} = \left[\int_0^1 |v(x)|^p + |v'(x)|^p\, dx\right]^{1/p}, \quad 1 \leq p < \infty,$$

$$\|v\|_{W_\infty^1[0,1]} = \sup_{0 \leq x < y \leq 1} \left\{|v(x)|, \frac{|v(x) - v(y)|}{|x - y|}\right\}.$$

For instance, the constant K_2 corresponding to Example 1 in Section 2 has the form $K_2 = (\text{constant})/\sqrt{\min_j h_j}$.

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Now using (10), (11), the theorem hypothesis, the Cauchy-Schwarz inequality, Jensen's inequality, and the relation $(a + b)^2 \leq 2(a^2 + b^2)$ gives

$$\|N(Y)\|_2 = \sup_{\|Z\|_2=1} N(Y)^t Z = \sup_{\|Z\|_2=1} \sum_{m=1}^{\hat{n}} \langle f_m(\cdot, y, y'), z_m(\cdot) \rangle$$

$$\leq \sup_{\|Z\|_2=1} \sum_{m=1}^{\hat{n}} \|f_m(\cdot, y, y')\|_2 \|z_m(\cdot)\|_2$$

$$\leq \sup_{\|Z\|_2=1} \|f(\cdot, y, y')\|_2 \|z(\cdot)\|_2$$

$$\leq \sup_{\|Z\|_2=1} \left[\int_0^1 f_1(x, y(x), y'(x))^2 + \cdots + f_{\hat{n}}(x, y(x), y'(x))^2 \, dx \right]^{1/2} K_2 \|Z\|_2$$

$$\leq \mu K_2 \left[\int_0^1 \xi^2 + 2\xi \left(\|y(x)\|_2 + \|y'(x)\|_2 \right)^{\nu} \right.$$

$$\left. + \left(\|y(x)\|_2 + \|y'(x)\|_2 \right)^{2\nu} \, dx \right]^{1/2}$$

$$\leq \mu K_2 \left[\xi^2 + 2^{1+\nu/2}\xi \int_0^1 \left(\|y(x)\|_2^2 + \|y'(x)\|_2^2 \right)^{\nu/2} \, dx \right.$$

$$\left. + 2^{\nu} \int_0^1 \left(\|y(x)\|_2^2 + \|y'(x)\|_2^2 \right)^{\nu} \, dx \right]^{1/2}$$

$$\leq \mu K_2 \left[\xi^2 + 2^{1+\nu/2}\xi \|y\|_{W_2^1}^{\nu} + 2^{\nu} \|y\|_{W_2^1}^{2\nu} \right]^{1/2}$$

$$= \mu K_2 \left(\xi + 2^{\nu/2} \|y\|_{W_2^1}^{\nu} \right)$$

$$\leq \mu K_2 \left(\xi + 2^{\nu/2} K_2^{\nu} \|Y\|_2^{\nu} \right) \tag{12}$$

Therefore for $\epsilon > 0$ and $\|Y\|_2$ sufficiently large it follows from (12) that

$$\frac{\|N(Y)\|_2}{\|Y\|_2^{\nu}} \leq 2^{\nu/2} \mu K_2^{\nu+1} + \epsilon,$$

which is precisely the condition (8) in Theorem 1 for some constant

$$C \leq 2^{\nu/2} \mu K_2^{\nu+1}. \hspace{4cm} Q.E.D.$$

Even though the growth conditions on $f(x, u, v)$ in Theorems 3 or 4 do not hold, it may turn out that for some constant $K > 0$, the solution to (1) is the *same* as the solution to (1) with $f(x, u, v)$ replaced by

$$\hat{f}(x, u, v) = \begin{cases} f(x, u, v), & \text{if } \|u\|_2 \leq K \text{ and } \|v\|_2 \leq K, \\ f(x, \psi(u), \psi(v)), & \text{if } \|u\|_2 > K \text{ or } \|v\|_2 > K, \end{cases}$$

where $\psi : E^{\hat{n}} \to E^{\hat{n}}$ is C^2, bounded, and $\psi(u) = u$ for $\|u\|_2 \leq K$. Since the theorems apply to $\hat{f}(x, u, v)$, a globally convergent homotopy algorithm can still be successfully applied to the problem.

3. Algorithm. The general idea of the algorithm is apparent from Theorem 1: just follow the zero curve γ emanating from $(0, W)$ until a zero $\tilde{Y}$ of $F(Y)$ 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 for solving the nonlinear system of equations (7) is clear and simple. The homotopy map is

$$\rho_W(\lambda, Y) = \lambda F(Y) + (1 - \lambda)(Y - W),\tag{13}$$

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 $F(Y) = 0$. 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. Of course, methods have been developed [14–19, 23] to navigate turning points, but the method considered here does so automatically. The second important difference is that there are never any "singular points" which afflict 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 1 guarantees that γ cannot just "stop" at an interior point of $[0, 1) \times E^p$.

The zero curve γ of the homotopy map $\rho_W(\lambda, Y)$ in (13) can be tracked by many different techniques; refer to the excellent survey [1] and recent work by Rheinboldt and Burkhardt [23] and Mejia [18]. The numerical results in Section 4 were obtained with the software package HOM-PACK, currently under development at Sandia National Laboratories, General Motors Research Laboratories, Virginia Polytechnic Institute and State University, and the University of Michigan. HOMPACK is a suite of codes for tracking zero curves of probability one homotopy maps, and provides both high-level and low-level subroutines for three different approaches to tracking γ. The three algorithmic approaches provided by HOMPACK are: 1) an ODE-based algorithm derived from that in [47], with several refinements; 2) a predictor-corrector algorithm whose corrector follows the flow normal to the Davidenko flow (a "normal flow" algorithm); 3) a version of Rheinboldt's linear predictor, quasi-Newton corrector algorithm [23] (an "augmented Jacobian" method). There are qualitatively different algorithms for dense and sparse Jacobian matrices; only algorithms for dense Jacobian matrices are discussed here. See [56] for a discussion of sparsity in relation to homotopy methods.

First the ODE-based algorithm will be discussed. Assuming that $F(Y)$ is C^2 and W is such that Theorem 1 holds, the zero curve γ is C^1 and can be parametrized by arc length s. Thus $\lambda = \lambda(s)$, $Y = Y(s)$ along γ, and

$$\rho_W(\lambda(s), Y(s)) = 0\tag{14}$$

identically in s. Therefore

$$\frac{d}{ds}\rho_W(\lambda(s), Y(s)) = D\rho_W(\lambda(s), Y(s)) \begin{pmatrix} \dfrac{d\lambda}{ds} \\ \dfrac{dY}{ds} \end{pmatrix} = 0,\tag{15}$$

$$\left\| \left(\frac{d\lambda}{ds}, \frac{dY}{ds} \right) \right\|_2 = 1.\tag{16}$$

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If we take

$$\lambda(0) = 0, \quad Y(0) = W, \tag{17}$$

the zero curve γ is the trajectory of the initial value problem (15-17). When $\lambda(\bar{s}) = 1$, the corresponding $Y(\bar{s})$ is a zero of $F(Y)$. Thus all the sophisticated ODE techniques currently available can be brought to bear on the problem of tracking γ [27], [48].

ODE software requires $(d\lambda/ds, dY/ds)$ explicitly, and (15), (16) only implicitly define the derivative $(d\lambda/ds, dY/ds)$. This can be calculated by finding the kernel of the $p \times (p+1)$ Jacobian matrix

$$D\rho_W(\lambda(s), Y(s)),$$

which has full rank by Theorem 1. It is here that a substantial amount of computation is incurred, and it is imperative that the number of derivative evaluations be kept small. Once the kernel has been calculated, the derivative $(d\lambda/ds, dY/ds)$ is uniquely determined by (16) and continuity. Complete details for solving the initial value problem (15-17) and obtaining $Y(\bar{s})$ are in [47] and [51].

Remember that tracking γ was merely a means to an end, namely a zero $\tilde{Y}$ of $F(Y)$. Since γ itself is of no interest (usually), one should not waste computational effort following it too closely. However, since γ is the only sure way to $\tilde{Y}$, losing γ can be disastrous. The tradeoff between computational efficiency and reliability is very delicate, and a fool-proof strategy appears difficult to achieve. This is the reason HOMPACK provides several algorithms: no single algorithm is superior overall, and each of the three beats the other two (sometimes by an order of magnitude) on particular problems.

The normal flow algorithm due to Georg [11] has three phases: prediction, correction, and step size estimation. (13) and (14) are the relevant equations here. For the prediction phase, assume that several points $P^{(1)} = (\lambda(s_1), Y(s_1))$, $P^{(2)} = (\lambda(s_2), Y(s_2))$ on γ with corresponding tangent vectors $(d\lambda/ds(s_1), dY/ds(s_1))$, $(d\lambda/ds(s_2), dY/ds(s_2))$ have been found, and h is an estimate of the optimal step (in arc length) to take along γ. The prediction of the next point on γ is

$$Z^{(0)} = p(s_2 + h), \tag{18}$$

where $p(s)$ is the Hermite cubic interpolating $(\lambda(s), Y(s))$ at s_1 and s_2. Precisely,

$$p(s_1) = (\lambda(s_1), Y(s_1)), \quad p'(s_1) = (d\lambda/ds(s_1), dY/ds(s_1)),$$

$$p(s_2) = (\lambda(s_2), Y(s_2)), \quad p'(s_2) = (d\lambda/ds(s_2), dY/ds(s_2)),$$

and each component of $p(s)$ is a polynomial in s of degree less than or equal to 3.

Starting at the predicted point $Z^{(0)}$, the corrector iteration is

$$Z^{(n+1)} = Z^{(n)} - \left[D\rho_W\left(Z^{(n)}\right) \right]^\dagger \rho_W\left(Z^{(n)}\right), \quad n = 0, 1, \ldots \tag{19}$$

where $\left[D\rho_W\left(Z^{(n)}\right) \right]^\dagger$ is the Moore-Penrose pseudoinverse of the $p \times (p+1)$ Jacobian matrix $D\rho_W$. Small perturbations of W produce small changes in the trajectory γ, and the family of trajectories γ for varying W is known as the "Davidenko flow". Geometrically, the iterates given by (19)

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return to the zero curve along the flow normal to the Davidenko flow, hence the name "normal flow algorithm".

A corrector step ΔZ is the unique minimum norm solution of the equation

$$[D\rho_W]\Delta Z = -\rho_W. \tag{20}$$

Fortunately ΔZ can be calculated at the same time as the kernel of $[D\rho_W]$, and with just a little more work. Normally for dense problems the kernel of $[D\rho_W]$ is found by computing a QR factorization of $[D\rho_W]$, and then using back substitution. By applying this QR factorization to $-\rho_W$ and using back substitution again, a *particular* solution v to (20) can be found. Let $u \neq 0$ be any vector in the kernel of $[D\rho_W]$. Then the minimum norm solution of (20) is

$$\Delta Z = v - \frac{v^t u}{u^t u} u. \tag{21}$$

Since the kernel of $[D\rho_W]$ is needed anyway for the tangent vectors, solving (20) only requires another $\mathcal{O}(p^2)$ operations beyond those for the kernel. The number of iterations required for convergence of (19) should be kept small (say < 4) since QR factorizations of $[D\rho_W]$ are expensive. The alternative of using $[D\rho_W(Z^{(0)})]$ for several iterations, which results in linear convergence, is rarely cost effective.

When the iteration (19) converges, the final iterate $Z^{(n+1)}$ is accepted as the next point on γ , and the tangent vector to the integral curve through $Z^{(n)}$ is used for the tangent–this saves a Jacobian matrix evaluation and factorization at $Z^{(n+1)}$. The step-size estimation described next attempts to balance progress along γ with the effort expended on the iteration (19).

Define a contraction factor

$$L = \frac{\|Z^{(2)} - Z^{(1)}\|}{\|Z^{(1)} - Z^{(0)}\|}, \tag{22}$$

a residual factor

$$R = \frac{\|\rho_W(Z^{(1)})\|}{\|\rho_W(Z^{(0)})\|}, \tag{23}$$

a distance factor $(Z^* = \lim_{n\to\infty} Z^{(n)})$

$$D = \frac{\|Z^{(1)} - Z^*\|}{\|Z^{(0)} - Z^*\|}, \tag{24}$$

and ideal values $\bar{L}$, $\bar{R}$, $\bar{D}$ for these three. Let h be the current step-size (the distance from Z^* to the previous point found on γ), and $\bar{h}$ the "optimal" step-size for the next step. The goal is to achieve

$$\frac{\bar{L}}{L} \approx \frac{\bar{R}}{R} \approx \frac{\bar{D}}{D} \approx \frac{\bar{h}^q}{h^q} \tag{25}$$

for some q. This leads to the choice

$$\bar{h} = \left(\min\{\bar{L}/L, \bar{R}/R, \bar{D}/D\}\right)^{1/q} h, \tag{26}$$

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a worst case choice. To prevent chattering and unreasonable values, constants $h_{\min}$ (minimum allowed step-size), $h_{\max}$ (maximum allowed step-size), $B_{\min}$ (contraction factor), and $B_{\max}$ (expansion factor) are chosen, and $\bar{h}$ is taken as

$$\bar{h} = \min\left\{\max\left\{h_{\min}, B_{\min}h, \hat{h}\right\}, B_{\max}h, h_{\max}\right\}. \tag{27}$$

There are eight parameters in this process: $\bar{L}$, $\bar{R}$, $\bar{D}$, $h_{\min}$, $h_{\max}$, $B_{\min}$, $B_{\max}$, q. HOMPACK permits the user to specify nondefault values for any of these. The choice of $\bar{h}$ from (27) can be refined further. If (19) converged in one iteration, then $\bar{h}$ should certainly not be smaller than h, hence set

$$\bar{h} := \max\{h, \bar{h}\} \tag{28}$$

if (19) only required one iteration.

To prevent divergence from the iteration (19), if (19) has not converged after K iterations, h is halved and a new prediction is computed. Every time h is halved the old value h_{old} is saved. Thus if (19) has failed to converge in K iterations sometime during this step, the new $\bar{h}$ should not be greater than the value h_{old} known to produce failure. Hence in this case

$$\bar{h} := \min\left\{h_{\text{old}}, \bar{h}\right\}. \tag{29}$$

Finally, if (19) required the maximum K iterations, the step-size should not increase, so in this case set

$$\bar{h} := \min\{h, \bar{h}\}. \tag{30}$$

The logic in (28–30) is rarely invoked, but it does have a stabilizing effect on the algorithm.

Rheinboldt's augmented Jacobian algorithm together with step size strategies has been described very well elsewhere [2, 23], and will not be repeated here.

4. Numerical results. As a first example, consider Jeffery-Hamel flow [17] given by

$$y'' - 4y + 6y^2 = c,$$
$$y(0) = y(1) = 0,$$

where c is a constant. Using the piecewise linear basis functions $\{o_i\}_{i=1}^n$ described in Example 1 in Section 2, the Galerkin approximation for $y(x) \approx Y(x) = \sum_{i=1}^n Y_i o_i(x)$ is the nonlinear system of equations

$$\sum_{i=1}^{n} Y_i \langle \phi'_i, \phi'_k \rangle - \langle c - 4Y - 6Y^2, \phi_k \rangle = 0, \quad k = 1, \ldots, n.$$

The remark following Theorem 4 applies to this situation, and the homotopy algorithm can be applied with no difficulty. Rather than presenting numerical results for Jeffery-Hamel flow (which are well known, cf. [17]), we instead tackle a problem where y is a vector, the boundary conditions are unbalanced (so integration by parts does *not* give $\langle -A'', o_k \rangle = \langle A', o'_k \rangle$), the interval is $[0, \infty)$, and shooting and finite difference methods are known to have difficulty [25].

Consider the magneto-hydronamics (MHD) nonlinear two-point boundary value problem [25]:

$$H''' = H\,H'' - \frac{(H')^2}{2} + m\,H' + 2\,G^2 \qquad (31)$$

$$G'' = H\,G' - H'\,G + m\,G \qquad (32)$$

$$\theta'' = \Pr\,H\,\theta' \qquad (33)$$

with the boundary conditions

$$H(0) = -A, \quad H'(0) = 0, \quad G(0) = 1, \quad \theta(0) = 1, \qquad (34)$$

$$H'(\eta) \to 0, \quad G(\eta) \to 0, \quad \theta(\eta) \to 0 \quad \text{as } \eta \to \infty, \qquad (35)$$

where Pr denotes the Prandtl number and m is a magnetic parameter. Note that $H(\eta)$ and $G(\eta)$ are determined by equations (31) and (32) independent of $\theta(\eta)$, and thus $\theta(\eta)$ can be uncoupled from the system. Once $H(\eta)$ has been found from (31), (32), (34), and (35), $\theta(\eta)$ can be determined from the one-dimensional two-point boundary value problem constituted by (33) and the θ parts of (34), (35). The (routine) computation for $\theta(\eta)$ will not be discussed here.

In practice the boundary conditions (35) are replaced by

$$H'(\tau) = G(\tau) = \theta(\tau) = 0 \qquad (35a)$$

for some τ sufficiently large.

Let S_n be the finite dimensional vector space with basis $\left\{ B_{j,k,\mathbf{t}}(x) \right\}_{j=1}^{n}$, where $B_{j,k,\mathbf{t}}(x)$ is the j-th B-spline of order k (degree $\le k-1$) defined on the knot sequence $\mathbf{t} = (t_1, t_2, \ldots, t_{n+k})$. When there is no ambiguity $B_{j,k,\mathbf{t}}(x)$ is simply written as $B_j(x)$. For this problem the knot sequence $\mathbf{t}$ is based on the breakpoint sequence

$$\xi = (0, .25, .50, .75, 1.0, 1.25, 1.50, 1.75, 2.0, 2.25, 2.50, 2.75,$$

$$3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 7.0, 8.0, 9.0, 11.0, 13.0, 15.0,$$

$$18.0, 21.0, 24.0, 28.0, 32.0, 36.0, 41.0, 46.0, 51.0, 60.0,$$

$$70.0, 80.0, 90.0, 100.0),$$

following the convention

$$t_1 = t_2 = \cdots = t_k \qquad \text{and} \qquad t_{n+1} = t_{n+2} = \cdots = t_{n+k}.$$

Depending on the values of n and k, only an initial subsequence of ξ may be needed.

The approximations are

$$H(\eta) = \sum_{j=1}^{N+2} \alpha_j B_j(\eta), \qquad (36)$$

$$\alpha_1 = -A, \quad \alpha_2 = \frac{A\,B_1'(0)}{B_2'(0)}, \quad \alpha_{N+2} = \frac{-\alpha_{N+1} B_{N+1}'(\tau-)}{B_{N+2}'(\tau-)}, \qquad (37)$$

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Table 1.

A	m	k	$N+2$	$-H(\tau)$	$-H(\infty)$	NFE	CPU time	arc length
-1.0	1.0	6	12	-.80700	-.43166	29	13:28	1.309
-1.0	2.0	6	12	-.88173	-.78156	29	13:28	1.387
-1.0	4.0	6	12	-.94477	-.93015	30	14:37	1.518
0.0	1.0	6	12	.11991	.25331	25	11:13	1.067
0.0	2.0	6	12	.07372	.10858	25	11:24	1.103
0.0	4.0	6	12	.03558	.04078	20	9:07	1.198
1.0	1.0	6	12	1.06079	1.0898	21	9:38	1.141
1.0	2.0	6	12	1.03959	1.0481	20	8:57	1.187
1.0	4.0	6	12	1.02103	1.0225	15	6:42	1.272
2.0	1.0	6	12	2.02744	2.0318	18	8:00	1.257
2.0	2.0	6	12	2.01968	2.0213	24	10:38	1.296
2.0	4.0	6	12	2.01193	2.0123	15	6:37	1.365
4.0	1.0	6	12	4.00625	4.0064	18	7:58	1.471
4.0	2.0	6	12	4.00530	4.0054	18	7:58	1.491
4.0	4.0	6	12	4.00402	4.0041	15	6:38	1.530
-1.0	1.0	6	24	-.43877	-.43166	32	1:09:37	1.916
-1.0	2.0	6	24	-.78196	-.78156	27	58:20	1.604
-1.0	4.0	6	24	-.93019	-.93015	24	51:32	1.953
0.0	1.0	6	24	.25286	.25331	26	55:45	1.986
0.0	2.0	6	24	.10852	.10858	21	44:53	1.804
0.0	4.0	6	24	.04073	.04078	25	53:27	1.903
-1.0	1.0	6	32	-.43165	-.43166	33	2:15:48	2.765
-1.0	2.0	6	32	-.78158	-.78156	34	2:20:28	2.334
-1.0	4.0	6	32	-.93018	-.93015	27	1:52:50	2.752
-1.0	1.0	4	24	-.42854	-.43166	41	55:37	2.196
-1.0	2.0	4	24	-.78043	-.78156	38	51:12	1.810
-1.0	4.0	4	24	-.93062	-.93015	29	39:06	2.128

$$G(\eta) = \sum_{j=1}^{N+2} \beta_j B_j(\eta), \tag{38}$$

$$\beta_1 = 1, \quad \beta_{N+2} = 0. \tag{39}$$

The boundary conditions (34-35) force the equations (37) and (39). The Galerkin approximation is the nonlinear system of equations

$$\langle -H''' - H\,H'' - (H')^2/2 - m\,H' + 2\,G^2, \ B_i \rangle = 0, \qquad i = 3, \dots, N+1,$$

$$\langle -G'' + H\,G' - H'\,G + m\,G, \ B_i \rangle = 0, \qquad i = 2, \dots, N+1, \tag{40}$$

where

$$\langle u, v \rangle = \int_0^\tau u(\eta)v(\eta)\,d\eta.$$

Let $Y = (a_3, a_4, \dots, a_{N+1}, \beta_2, \beta_3, \dots, \beta_{N+1})^t$ and $F(Y) = 0$ be given by the $p = 2N - 1 = 2n - 5$ equations (40).

Table 1 shows some numerical results obtained by applying HOMPACK to (40). The values $H(\infty)$ are from [25], and τ can be inferred from n, k, and the breakpoint sequence ξ listed above. The integrals in (40) were computed by 10-point Gaussian quadrature over each subinterval, and are are thus essentially exact. NFE is the number of Jacobian matrix evaluations, and the format of the CPU time (on a VAX 11/780) is hh:mm:ss. The local curve tracking tolerance was 10^{-4} and the final accuracy (the end game tolerance [55]) was 10^{-6}.

Although the theory in Section 2 is not directly applicable to this MHD problem, these numerical results suggest that the homotopy algorithm is more widely applicable than the theory

indicates, and the accuracy is exactly what would be expected given the spline order and knot spacing.

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