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Design and evaluation of homotopies for efficient and robust continuation

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ABSTRACT

Homotopy continuation, in combination with a quasi-Newton method, can be an efficient and robust technique for solving large sparse systems of nonlinear equations. The homotopy itself is pivotal in determining the efficiency and robustness of the continuation algorithm. As the homotopy is defined implicitly by a nonlinear system of equations to which the analytical solution is by assumption unknown, many properties of the homotopy can only be studied using numerical methods. The properties of a given homotopy which have the greatest impact on the corresponding continuation algorithm are traceability and linear solver performance. Metrics are presented for the analysis and characterization of these properties. Several homotopies are presented and studied using these metrics in the context of a parallel implicit three-dimensional Newton–Krylov–Schur flow solver for computational fluid dynamics. Several geometries, grids, and flow types are investigated in the study. Additional studies include the impact of grid refinement and the application of a coordinate transformation to the homotopy as measured through the traceability and linear solver performance metrics.

1. Introduction

Consider a curve segment defined implicitly by the system of equations

$$\mathcal{H}(\mathbf{q}(\lambda), \lambda) = \mathbf{0}, \tag{1}$$

$\mathcal{H}: \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}^N$, $\mathbf{q} \in \mathbb{R}^N$, $\lambda \in \mathbb{R}$ on some interval $\lambda \in \Lambda$, $\Lambda \subset \mathbb{R}$. Without loss of generality, let $\Lambda = [0, 1]$. In this paper we assume that $\mathcal{H}$ is at least C^1 differentiable, invertible, and that the curve is regular on Λ. As such, the curve derivatives cannot vanish and no bifurcations are present. While bifurcation analysis has been of practical interest to many researchers, including several in computational fluid dynamics [33,36,44,45], the application of interest in this paper is the design of efficient homotopy continuation algorithms, for which the construction of bifurcated curves should be avoided as such curves are difficult and computationally expensive to trace numerically.

The curve defined implicitly by equation (1) can also be interpreted as a deformation. If the deformation is continuous, it is called a homotopy [1]. In the case where $\mathcal{H}(\mathbf{q}, 1) = \mathbf{0}$ is easy to solve numerically and $\mathcal{H}(\mathbf{q}, 0) = \mathbf{0}$ is difficult to solve numerically, solving $\mathcal{H}(\mathbf{q}, 1) = \mathbf{0}$ for $\mathbf{q}$ and approximately tracing the curve numerically from $\lambda = 1$ to $\lambda = 0$ can be an efficient and robust strategy [4,6,13,14,16,43,46] for acquiring an approximation to the solution to $\mathcal{H}(\mathbf{q}, 0) = \mathbf{0}$, where $\mathcal{R}(\mathbf{q}) = \mathcal{H}(\mathbf{q}, 0)$ is a system of equations for which the solution is of interest. This is referred to as homotopy continuation [1].

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The use of homotopy continuation for its efficiency and robustness is a recent research area in computational fluid dynamics. Part of the attraction of homotopy continuation for large-scale scientific computing is the performance scalability as the number of degrees of freedom in the calculation increases. This is particularly attractive for future applications as the average problem size continues to increase, precipitated by the increasing availability and power of computational hardware. Performance scaling with grid refinement or discretization order has been investigated numerically by several authors [6,13,46] and is further investigated in this paper.

There are unlimited different ways in which to construct a regular homotopy $\mathcal{H}(\mathbf{q},\lambda)=\mathbf{0}$ satisfying $\mathcal{H}(\mathbf{q},0)=\mathcal{R}(\mathbf{q})$ for a given $\mathcal{R}(\mathbf{q})$. For our application of interest, the homotopy should be constructed to maximize the efficiency and robustness of the curve-tracing algorithm. Homotopies targeting this application have so far been designed with little to ensure that the curve will be easy to trace or result in an efficient algorithm.

Some studies have been performed of homotopies in the context of efficient continuation. Hicken and Zingg [16] calculated eigenvalues along the continuation path to give an idea of the performance of the nonlinear and linear system solvers as a function of λ. For a simple one-dimensional problem, Hao et al. [13] plotted the solution field at several values of λ to give some intuitive visualization of the homotopy. For more complex three-dimensional systems, Brown and Zingg [6] tracked functionals as surrogates for the homotopy curve. However, even combining all of these approaches gives an incomplete profile of the homotopy and important information pertinent to continuation algorithm performance is still lacking.

Timing comparisons are not performed in this paper as they have been performed previously by Brown and Zingg [6], who found performance to be competitive or superior to the popular pseudo-transient continuation algorithm over an extensive suite of computational aerodynamics test cases. The focus of this paper is on identifying and quantifying features of homotopies which affect the performance of the continuation algorithm and in improving our understanding of why some homotopies lead to better algorithm performance. This knowledge will improve our ability to design effective homotopy continuation algorithms. The methodology is demonstrated by considering some candidate homotopies for the external aerodynamic flow solver of Hicken and Zingg [15] and Osusky and Zingg [29].

2. Homotopy

2.1. Homotopy continuation

Consider the so-called convex homotopy [1] which is defined as the (presumably) continuous solution $\mathbf{q}(\lambda)$ to

$$\mathcal{H}(\mathbf{q},\lambda)=(1-\lambda)\,\mathcal{R}(\mathbf{q})+\lambda\mathcal{G}(\mathbf{q})=\mathbf{0}, \tag{2}$$

$$\mathcal{H}:\mathbb{R}^N\times\mathbb{R}\to\mathbb{R}^N,\ \mathcal{G}:\mathbb{R}^N\to\mathbb{R}^N,\ \mathcal{R}:\mathbb{R}^N\to\mathbb{R}^N,\ \lambda\in\mathbb{R}.$$

A continuation method can be developed from this homotopy by discretizing in λ to form a sequence of nonlinear equations:

$$\mathcal{H}(\mathbf{q},\lambda_k)=(1-\lambda_k)\,\mathcal{R}(\mathbf{q})+\lambda_k\mathcal{G}(\mathbf{q})=\mathbf{0}, \tag{3}$$

$$k\in[0,m]\,,\ \lambda_k\in\mathbb{R},\ \lambda_0=1,\ \lambda_m=0,\ \lambda_{k+1}<\lambda_k.$$

In the context of the studies in this paper, $\mathcal{R}(\mathbf{q})$ is the discrete flow residual and $\mathcal{G}(\mathbf{q})$ a system of equations of our own design which we refer to as the homotopy system.

Another form of homotopy continuation, known as global or Newton homotopy continuation due to its original formulation as a globally convergent generalization of Newton's method [1,7,26], is performed by sequentially solving

$$\mathcal{H}(\mathbf{q},\lambda_k)=\mathcal{R}(\mathbf{q})-\lambda_k\mathcal{R}(\mathbf{q}_0)=\mathbf{0}, \tag{4}$$

$$k\in[0,m]\,,\ \lambda_k\in\mathbb{R},\ \lambda_0=1,\ \lambda_m=0,\ \lambda_{k+1}<\lambda_k,$$

$$\mathcal{H}:\mathbb{R}^N\times\mathbb{R}\to\mathbb{R}^N,\ \mathcal{R}:\mathbb{R}^N\to\mathbb{R}^N.$$

The vector $\mathbf{q}_0\in\mathbb{R}^N$ can be any vector of choice; for the computational aerodynamics examples presented in this paper, this vector is populated with the far-field boundary conditions.

2.2. Predictor–corrector algorithm for homotopy continuation

As the name suggests, the predictor–corrector algorithm consists of two phases: the predictor phase and the corrector phase. The two phases are applied repeatedly until traversing is complete.

The objective of the predictor phase is to obtain a suitable starting guess for the $k+1$st sub-problem using the estimated solution at the k-th sub-problem, a trajectory, and a distance (step-length) to travel along that trajectory. A common choice of predictor is the Euler predictor, for which the update at the kth step is given by