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Monolithic Homotopy Continuation with Predictor Based on Higher Derivatives

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Abstract

The predictor component of a monolithic homotopy continuation algorithm is augmented with higher derivative information for use as an efficient, robust, and scalable continuation algorithm suitable for application to large sparse systems of nonlinear algebraic equations. Convergence of the algorithm is established analytically, and efficiency studies are performed by applying the method to a practical computational aerodynamics problem.

Keywords: homotopy, continuation, higher order predictor, globalization, Newton-Krylov, computational fluid dynamics

1. Introduction

Homotopy continuation methods are root-finding algorithms based on continuous deformations known as homotopies [1]. Some applications in the field of computational fluid dynamics (CFD) include the study systems where multiple solutions exist [29, 36] or where solutions may be unstable [18, 35]. Homotopy continuation has also been applied to facilitate the solution to CFD problems at high Reynolds numbers by solving the same problem at a lower Reynolds number and gradually increasing the Reynolds number [7].

Motivated (at least in some cases) by the increased demand for scalable CFD solvers, there has been interest in implementing homotopy continuation as an efficient equation solver for CFD problems in general [3, 14, 17] or with special focus on higher-order accurate spatial discretizations [34, 37]. By far the most common continuation method in CFD is pseudo-transient continuation, the computational cost of which scales super-linearly with mesh refinement due to the dependence on the Courant-Friedrichs-Lewy (CFL) number [22]. Homotopy continuation algorithms can fare better. For example, Hao *et al.* [14] found that computational cost scales linearly with mesh refinement for a homotopy continuation algorithm for some one- and two-dimensional problems for a third-order finite-difference WENO scheme [21], presumably using a direct solver. Brown and Zingg [6] similarly observed better performance scaling for some three-dimensional inviscid cases using a finite-difference SBP-SAT [8, 9, 12, 20] discretization with the Krylov linear solver FGMRES [30].

The present research programme follows from the work of Hicken *et al.* [15], who studied a non-physical homotopy based on adding a large amount of non-physical dissipation to the discrete governing equations and gradually removing it. Based on the promising results presented by the authors, we continued this approach using a predictor-corrector method [3], which was