Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 289 (2015) 79–103
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Decreasing the temporal complexity for nonlinear, implicit reduced-order models by forecasting

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Received 27 October 2014; received in revised form 31 January 2015; accepted 9 February 2015
Available online 14 February 2015

Abstract

Implicit numerical integration of nonlinear ODEs requires solving a system of nonlinear algebraic equations at each time step. Each of these systems is often solved by a Newton-like method, which incurs a sequence of linear-system solves. Most model-reduction techniques for nonlinear ODEs exploit knowledge of a system's spatial behavior to reduce the computational complexity of each linear-system solve. However, the number of linear-system solves for the reduced-order simulation often remains roughly the same as that for the full-order simulation.

We propose exploiting knowledge of the model's temporal behavior to (1) forecast the unknown variable of the reduced-order system of nonlinear equations at future time steps, and (2) use this forecast as an initial guess for the Newton-like solver during the reduced-order-model simulation. To compute the forecast, we propose using the Gappy POD technique. The goal is to generate an accurate initial guess so that the Newton solver requires many fewer iterations to converge, thereby decreasing the number of linear-system solves in the reduced-order-model simulation.

Keywords: Nonlinear model reduction; Gappy POD; Temporal correlation; Forecasting; Initial guess

1. Introduction

High-fidelity physics-based numerical simulation has become an indispensable engineering tool across a wide range of disciplines. Unfortunately, such simulations often bear an extremely large computational cost due to the large-scale, nonlinear nature of many high-fidelity models. When an implicit integrator is employed to advance the solution in time (as is often essential, e.g., for stiff problems) this large cost arises from the need to solve a sequence of high-dimensional systems of nonlinear algebraic equations—one at each time step. As a result, individual simulations

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[3] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

http://dx.doi.org/10.1016/j.cma.2015.02.013
0045-7825/

can take weeks or months to complete, even when high-performance computing resources are available. This renders such simulations impractical for time-critical and many-query applications. For example, uncertainty-quantification applications (e.g., Bayesian inference problems) call for hundreds or thousands of simulations (i.e., forward solves) to be completed in days or weeks; in-the-field analysis (e.g., in-field data acquisition) requires near-real-time simulation.

Projection-based nonlinear model-reduction techniques have been successfully applied to decrease the computational cost of high-fidelity simulation while retaining high levels of accuracy. To accomplish this, these methods exploit knowledge of the system's dominant *spatial behavior* – as observed during 'training simulations' conducted *a priori* – to decrease the simulation's *spatial complexity*, which we define as the computational cost of each linear-system solve.[4] To do so, these methods (1) decrease the dimensionality of the linear systems by projection, and (2) approximate vector-valued nonlinear functions by sampling methods that compute only a few of the vector's entries (e.g., empirical interpolation [1,2], Gappy POD [3]). However, these techniques are often insufficient to adequately reduce the computational cost of the simulation. For example, Ref. [4] presented results for the GNAT nonlinear model-reduction technique applied to a large-scale nonlinear turbulent-flow problem. The reduced-order model generated solutions with sub-1% errors, reduced the spatial complexity by a factor of 637, and employed only 4 computing cores—a significant reduction from the 512 cores required for the high-fidelity simulation. However, the total number of linear-system solves required for the reduced-order-model simulation, which we define as the *temporal complexity*, remained large. In fact, the temporal complexity was decreased by a factor of only 1.5. As a result, the total computing resources (computing cores $\times$ wall time) required for the simulation were decreased by a factor of 438, but the wall time was reduced by a factor of merely 6.9. While these results are promising (especially in their ability to reduce spatial complexity), the time integration of nonlinear dynamics remains problematic and often precludes real-time performance.

The goal of this work is to exploit knowledge of the system's *temporal behavior* as observed during the training simulations to decrease the temporal complexity of reduced-order-model simulations. For this purpose, we first briefly review methods that exploit observed temporal behavior to improve computational performance.

Temporal forecasting techniques have been investigated for many years with a specific focus on reducing wall time in a stable manner with maximal accuracy. The associated body of work is large and a comprehensive review is beyond the scope of this paper. However, this work focuses on time integration for reduced-order models of highly nonlinear dynamical systems; several categories of specialized research efforts provide an appropriate context for this research.

At the most fundamental level of temporal forecasting, a variety of statistical time-series-analysis methods exist that exploit (1) knowledge of the temporal structure, e.g., smoothness, of a model's variables, and (2) previous values of these variables for the current time series or trajectory. The connection between these methods and our work is that such forecasts can serve as an initial guess for an iterative solver (e.g., Newton's method) at an advanced point in time. However, the disconnect between such methods and the present context is that randomness and uncertainty drive time-series analysis; as such, these forecasting methods are stochastic in nature (see Refs. [5–12]). In addition, the majority of time-series analyses have been applied to application domains (e.g., economics) with dynamics that are not generally modeled using partial differential equations. Finally, such forecasting techniques do not exploit a collection of observed, complete time histories from training experiments conducted *a priori*. Because such training simulations lend important insight into the spatial and temporal behavior of the model, we are interested in developing a technique that can exploit such data.

Alternatively, time integrators for ordinary differential equations (ODEs) employ polynomial extrapolations to provide reasonably accurate forecasts of the state or the unknown at each time step. Time integrators employ such a forecast for two purposes. First, algorithms with adaptive time steps employ interpolation to obtain solutions (and their time derivatives) at arbitrary points in time. Implicit time integrators for nonlinear ODEs, which require the iterative solution of nonlinear algebraic systems at each time step, use recent history (of the current trajectory) to forecast an accurate guess of the unknown in the algebraic system (see, e.g., Ref. [13]). Again, forecasting by polynomial extrapolation makes no use of the temporal behavior observed during training simulations.

Closely connected to time integration but specialized to leverage developments in high-performance computing, time parallel methods can offer computational speedup when integrating ODEs. Dating back to before the

[4] A sequence of linear systems arises at each time step when a Newton-like method is employed to solve the system of nonlinear algebraic equations.