Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.2011.m12si04

Vol. **5**, No. 1, pp. 62-84
February 2012

Newton-Multigrid for Biological Reaction-Diffusion Problems with Random Coefficients

Eveline Rosseel[1], Nico Scheerlinck[1] and Stefan Vandewalle[1,*]

[1] *Computer Science Department, Katholieke Universiteit Leuven, Celestijnenlaan 200A, B-3001 Leuven, Belgium.*

Received 11 January 2011; Accepted (in revised version) 05 May 2011

Available 21 December 2011

Abstract. An algebraic Newton-multigrid method is proposed in order to efficiently solve systems of nonlinear reaction-diffusion problems with stochastic coefficients. These problems model the conversion of starch into sugars in growing apples. The stochastic system is first converted into a large coupled system of deterministic equations by applying a stochastic Galerkin finite element discretization. This method leads to high-order accurate stochastic solutions. A stable and high-order time discretization is obtained by applying a fully implicit Runge-Kutta method. After Newton linearization, a point-based algebraic multigrid solution method is applied. In order to decrease the computational cost, alternative multigrid preconditioners are presented. Numerical results demonstrate the convergence properties, robustness and efficiency of the proposed multigrid methods.

AMS subject classifications: 35K57, 35Q92, 65M55, 65N35

Key words: Multigrid, stochastic Galerkin finite element method, reaction-diffusion problems, implicit Runge-Kutta method and PDEs with random coefficients.

1. Introduction

Stochastic Galerkin finite element methods are being applied to a wide range of stochastic applications, e.g., to elasticity problems [10], heat transfer problems [21], in fluid-structure interactions [31] and in computational fluid mechanics [14]. In most cases, linear partial differential equations with random coefficients are considered. The extension to nonlinear problems is generally not straightforward for stochastic Galerkin methods [18]. The stochastic Galerkin projection may not be computed analytically, except for polynomial nonlinearities. Also, the stochastic Galerkin method transforms a stochastic problem into high-dimensional deterministic systems, for which special solvers need to be designed.

*Corresponding author. *Email addresses:* eveline.rosseel@cs.kuleuven.be (E. Rosseel), nico.scheerlinck@cs.kuleuven.be (N. Scheerlinck), stefan.vandewalle@cs.kuleuven.be (S. Vandewalle)

As an alternative to the stochastic Galerkin finite element method, so-called stochastic collocation methods were proposed [1, 17]. These methods enable a black-box reuse of deterministic simulation codes and do not require modifications for solving nonlinear stochastic problems. Although very good results can be obtained with the stochastic collocation method, its convergence rate is typically somewhat slower than the stochastic Galerkin convergence, in terms of the number of deterministic PDEs to be solved [7, 24]. In terms of computational cost, the success of the stochastic Galerkin method depends on the solution method for the high-dimensional deterministic Galerkin systems. For linear stochastic problems, efficient solvers can easily be designed [8, 22, 25]. This paper explores the construction of a multigrid solution approach for stochastic Galerkin discretizations of systems of nonlinear PDEs.

The stochastic Galerkin solution of a set of nonlinear, time-dependent reaction-diffusion equations is considered. We focus on a particular application, namely the conversion of starch into sugars in growing fruit. The accuracy of the simulation depends on the accuracy of a large set of parameters which model the chemical composition and shape of the fruit under consideration. Many of these parameters are inherently variable; hence a stochastic simulation is needed.

In the case of linear, time-dependent partial differential equations (PDE) with random coefficients, efficient multigrid methods exist for the systems resulting from a stochastic Galerkin finite element discretization combined with an implicit Runge-Kutta (IRK) time discretization [23]. The implicit Runge-Kutta method guarantees a high-order and stable time discretization and enables one to take larger time steps than with explicit time discretization schemes. In this paper we investigate whether such multigrid approaches can be extended to systems of nonlinear, stochastic PDEs.

This paper is structured as follows. In Section 2, the model equations are presented. Section 3 details the discretization of the set of nonlinear, stochastic PDEs. Section 4 proposes an algebraic multigrid (AMG) method to solve the high-dimensional discretized systems efficiently. Some implementation issues are addressed in Section 5. The biological application that motivated this research is detailed in Section 6. The properties of the AMG method are demonstrated by numerical experiments in Section 7. Section 8 summarizes the main conclusions of this paper.

2. Model description

The stochastic reaction-diffusion problem that we consider in this paper, can be described by the following set of equations:

$$\begin{cases} \partial_t u_1(x,t,\omega) = \nabla\cdot(a_1(x,\omega)\nabla u_1(x,t,\omega) + R_1(u_1(x,t,\omega),u_2(x,t,\omega)), \\ \partial_t u_2(x,t,\omega) = \nabla\cdot(a_2(x,\omega)\nabla u_2(x,t,\omega) + R_2(u_1(x,t,\omega),u_2(x,t,\omega)), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{in } D\times[0,T_f]\times\Omega, \\ \vec{n}\cdot\nabla u_1(x,t,\omega) = 0 \quad \text{and} \quad \vec{n}\cdot\nabla u_2(x,t,\omega) = 0 \qquad \text{in } \partial D\times[0,T_f]\times\Omega. \end{cases} \tag{2.1}$$