Journal of Computational Physics 313 (2016) 400–414

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Conservative tightly-coupled simulations of stochastic multiscale systems

Søren Taverniers, Alexander Y. Pigarov, Daniel M. Tartakovsky *

Department of Mechanical and Aerospace Engineering, University of California, San Diego, 9500 Gilman Drive, MC 0411, La Jolla, CA 92093, United States

ARTICLE INFO

Article history:
Received 23 March 2015
Received in revised form 29 January 2016
Accepted 1 February 2016
Available online 24 February 2016

Keywords:
Noise propagation
Implicit coupling
Domain decomposition
Hybrid
Multiphysics

ABSTRACT

Multiphysics problems often involve components whose macroscopic dynamics is driven by microscopic random fluctuations. The fidelity of simulations of such systems depends on their ability to propagate these random fluctuations throughout a computational domain, including subdomains represented by deterministic solvers. When the constituent processes take place in nonoverlapping subdomains, system behavior can be modeled via a domain-decomposition approach that couples separate components at the interfaces between these subdomains. Its coupling algorithm has to maintain a stable and efficient numerical time integration even at high noise strength. We propose a conservative domain-decomposition algorithm in which tight coupling is achieved by employing either Picard's or Newton's iterative method. Coupled diffusion equations, one of which has a Gaussian white-noise source term, provide a computational testbed for analysis of these two coupling strategies. Fully-converged ("implicit") coupling with Newton's method typically outperforms its Picard counterpart, especially at high noise levels. This is because the number of Newton iterations scales linearly with the amplitude of the Gaussian noise, while the number of Picard iterations can scale superlinearly. At large time intervals between two subsequent inter-solver communications, the solution error for single-iteration ("explicit") Picard's coupling can be several orders of magnitude higher than that for implicit coupling. Increasing the explicit coupling's communication frequency reduces this difference, but the resulting increase in computational cost can make it less efficient than implicit coupling at similar levels of solution error, depending on the communication frequency of the latter and the noise strength. This trend carries over into higher dimensions, although at high noise strength explicit coupling may be the only computationally viable option.

1. Introduction

Many, if not most, problems of practical importance deal with complex systems that involve multiple physical (as well as chemical and biological) processes, which occur on a wide range of spatial and/or temporal scales. These processes can either spatially coexist or occur in adjacent regions of space. We focus on the latter class of multiphysics phenomena, in which different processes take place in separate spatial domains and affect each other at the interfaces between these

* Corresponding author.
E-mail address: dmt@ucsd.edu (D.M. Tartakovsky).

http://dx.doi.org/10.1016/j.jcp.2016.02.047
0021-9991/

domains. Conjugate heat transfer across a fluid–solid interface [1] is an illustrative example of such phenomena. It is central to applications as diverse as satellite cold gas propulsion systems [2] and spacecraft re-entry into Earth's atmosphere [3].

Following the terminology established in the field of fluid–structure interactions (FSI), one can subdivide solution strategies for interfacially coupled multiphysics systems into two modeling frameworks: "monolithic" [4] and "component partitioning" [5]. The former combines all the different physics components and their interactions into a single discrete operator, which is then advanced in time. This "tight coupling" ensures temporal synchronization of all the state variables and hence possesses excellent robustness, accuracy and stability properties. However, it is computationally demanding and "intrusive", i.e., requires development of new codes. The second framework, which is also known as domain decomposition (DD), advances solutions of each physics component independently from the others, using additional solvers to exchange information at the interfaces through a coupling algorithm. It is "nonintrusive", i.e., allows for a "black-box" implementation of the physics components which can be done with existing ("legacy") codes. This operational expediency comes at a cost of reduced accuracy and stability when the physics components involved are "loosely coupled", leading to desynchronization of the state variables in the different components by one time step or a fraction of a time step [6]. Iterative coupling techniques can be used to achieve a tight coupling, which eliminates this time shift [7,8,6].

Despite the widespread use of DD approaches, there is a dearth of systematic studies of their numerical properties. Most studies deal with the coupling of deterministic components, which are typically represented by deterministic partial differential equations (PDEs). Representative examples include an analysis of the stability of an interfacial coupling in one-dimensional fluid–structure thermal diffusion [9], an analysis of predictor–corrector staggered schemes for simulating FSI [6], an investigation of the stability of a coupling algorithm based on mixed interface conditions for conjugate heat transfer simulations [10], and a demonstration of the effects of a non-converged iterative coupling on the stability of a coupled linear diffusion problem [11]. These and other similar studies have led to nontrivial conclusions, which are likely to be problem-specific and demonstrate the algorithmic complexity of coupling nonlinear solvers. For example, an otherwise unstable loose coupling used in FSI simulations can be made stable by enforcing Neumann boundary conditions for the structural calculation and Dirichlet boundary conditions for the fluid solver [9]; and standard staggered schemes for FSI simulations need to be modified by several iteratively made corrector steps to ensure conservation of energy [7,8,6].

When random fluctuations are generated by one of the constituent solvers, conclusions drawn from numerical studies of fully-deterministic systems may need to be modified. Currently, a systematic analysis of how random noise or stochasticity of one of the constituent solvers affects the numerical performance of both the other (possibly deterministic) solvers and an algorithm used to couple them is largely missing. Such studies are needed to gain confidence in the ever-growing number of multiphysics and hybrid simulations that combine deterministic and stochastic solvers [12–15]. The analysis presented below contributes to this area of research by studying the effects of random noise on numerical properties (coupling convergence, stability and accuracy) of a domain-decomposition algorithm which tightly couples a deterministic and stochastic subdomain solver. A complementary challenge, the need for adding a random source term to a (deterministic) PDE solver coupled to a stochastic solver whose microscopic fluctuations drive the macroscopic system dynamics (e.g., in highly nonlinear problems involving phase transitions), has been addressed in [16–19].

In Section 2 we formulate a computational testbed problem, one-dimensional diffusion in a composite material one segment of which contains a Gaussian white-noise forcing. Section 3 contains a description of our DD approach to solving this problem, which tightly couples the deterministic (explicit Euler) and stochastic (Euler–Maruyama) diffusion solvers using Newton's or Picard's iteration. Section 4 presents a stability analysis of our algorithm using fully-converged Picard's iteration. In Section 5 we conduct a series of numerical experiments to explore the performance of our algorithm. These findings are summarized in Section 6.

2. Problem formulation

Consider a one-dimensional linear diffusion equation,

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial \rho}{\partial x}\right] + f, \qquad x \in \Omega \equiv (-L/2, L/2), \quad t > 0, \tag{1a}$$

which describes the evolution of concentration $\rho(x,t)$ in space, x, and time, t. The diffusion coefficient $D(x)$ is piecewise constant,

$$D(x) = \begin{cases} D_1 & \text{for } x \in \Omega_1 \equiv (-L/2, 0) \\ D_2 \gg D_1 & \text{for } x \in \Omega_2 \equiv [0, L/2), \end{cases} \tag{1b}$$

and the source term $f(x,t)$ is defined as

$$f(x,t) = \begin{cases} 0 & \text{for } x \in \Omega_1 \\ \xi(x,t) & \text{for } x \in \Omega_2, \end{cases} \tag{1c}$$

where $\xi(x,t)$ is a zero-mean Gaussian space–time white noise with covariance

$$\mathbb{E}[\xi(x,t)\xi(y,\tau)] = \sigma_\xi^2 \delta(x-y)\delta(t-\tau), \quad x, y \in \Omega_2; \quad t, \tau > 0 \tag{1d}$$