Journal of Computational Physics 330 (2017) 884–901

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A tightly-coupled domain-decomposition approach for highly nonlinear stochastic multiphysics systems

Søren Taverniers, 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 18 March 2016
Received in revised form 21 October 2016
Accepted 22 October 2016
Available online 27 October 2016

Keywords:
Noise propagation
Implicit coupling
Domain decomposition
Multiphysics
Hydrogen separation
Nonlinear diffusion

ABSTRACT

Multiphysics simulations often involve nonlinear components that are driven by internally generated or externally imposed random fluctuations. When used with a domain-decomposition (DD) algorithm, such components have to be coupled in a way that both accurately propagates the noise between the subdomains and lends itself to a stable and cost-effective temporal integration. We develop a conservative DD approach in which tight coupling is obtained by using a Jacobian-free Newton–Krylov (JfNK) method with a generalized minimum residual iterative linear solver. This strategy is tested on a coupled nonlinear diffusion system forced by a truncated Gaussian noise at the boundary. Enforcement of path-wise continuity of the state variable and its flux, as opposed to continuity in the mean, at interfaces between subdomains enables the DD algorithm to correctly propagate boundary fluctuations throughout the computational domain. Reliance on a single Newton iteration (explicit coupling), rather than on the fully converged JfNK (implicit) coupling, may increase the solution error by an order of magnitude. Increase in communication frequency between the DD components reduces the explicit coupling's error, but makes it less efficient than the implicit coupling at comparable error levels for all noise strengths considered. Finally, the DD algorithm with the implicit JfNK coupling resolves temporally-correlated fluctuations of the boundary noise when the correlation time of the latter exceeds some multiple of an appropriately defined characteristic diffusion time.

1. Introduction and motivation

High-performance computing facilitates the simulation of ever more complex phenomena comprising multiple physical, chemical and/or biological processes that take place on a wide range of spatiotemporal scales. Many of these problems involve constituent processes that occur in separate spatial domains and influence each other through the interfaces between these domains. One example is conjugate heat transfer across a fluid–solid interface [1], which manifests itself in applications as diverse as gas turbine cooling [2] and vehicle entry and re-entry in planetary atmospheres [3].

Construction of a single discrete operator containing the different components and their interactions yields a "tight" coupling, which guarantees temporal synchronization of state variables across inter-component interfaces. Yet, this "monolithic" [4] approach is intrusive (i.e., requires development of new software) and might become unfeasible for high-

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

http://dx.doi.org/10.1016/j.jcp.2016.10.052
0021-9991/

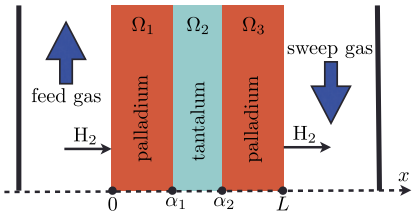

Fig. 1. A three-layer dense membrane configuration for hydrogen separation (not to scale).

dimensional systems. The alternative strategy of "component partitioning" or domain decomposition (DD) advances the components independently and employs a coupling method to exchange information at the interfaces. Deployment of DDs in high-performance computing facilitates an optimal distribution of the work load between the available processing cores (load balancing), while minimizing communication between cores acting on adjacent subdomains (communication scheduling) [5]. The DD approach is nonintrusive, i.e., allows for a "black-box" implementation of existing (legacy) codes, but requires an iterative coupling to avoid desynchronization of the state variables computed with the individual components,[1] which may significantly increase its computational cost.

Studies of the numerical properties of DD algorithms have led to nontrivial conclusions, which might be difficult to generalize. For instance, an otherwise unstable loose coupling used in one-dimensional simulations of fluid–solid-interactions can be made stable by enforcing Neumann boundary conditions for the structural calculation and Dirichlet boundary conditions for the fluid solver [9]; and the use of a small number of iterations in a coupled linear diffusion problem leads to conditional or unconditional stability in a nonintuitive way when using a backward Euler solver in the subdomains [10]. Random fluctuations inside or on the boundary of a computational domain further affect the accuracy and performance of DD methods [11,12].

We focus on a highly nonlinear multiscale diffusion problem driven by a temporally correlated boundary noise. A nonlinear dependence of the diffusion coefficient on the state variable (concentration) poses a host of challenges not encountered in linear [11,12] and weakly nonlinear [12] problems. A computational testbed problem described in Section 2—one-dimensional nonlinear diffusion in a composite solid forced by a truncated Gaussian noise at its left boundary—represents production of ultra-pure hydrogen gas [13]. Section 3 contains a description of our DD algorithm, which uses a Jacobian-free Newton–Krylov (JfNK) method to tightly couple two explicit Euler diffusion solvers. In Section 4 we analyze the stability of the time advancement scheme in the presence of a temporally fluctuating boundary noise. In Section 5 we conduct a series of computational experiments to elucidate the numerical properties of our algorithm. A summary of our findings is reported in Section 6.

2. Problem formulation

Consider a state variable $\rho(x,t)$ whose dynamics is governed by a one-dimensional nonlinear diffusion equation,

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

with the ρ-dependent diffusion coefficient D; this equation is defined on the simulation domain $\Omega \equiv (0,L)$ for times $t > 0$. While (1a) describes a large number of physical phenomena, we ground it in an application related to production of ultra-pure hydrogen gas [13]. Thus, $\rho(x,t)$ represents the concentration of atomic hydrogen (H) that diffuses through a dense composite metal membrane of thickness L. The latter is placed between streams of feed and sweep gases flowing in opposite directions in order to extract H_2 from the feed gas (for a typical configuration, see, e.g., [14] and Fig. 1). The membrane consists of a tantalum (Ta) layer Ω_2 sandwiched between two palladium (Pd) layers Ω_1 and Ω_3 [15]. Palladium's selective permeability to hydrogen [16] makes it suitable for use in hydrogen-separation membranes. To increase its structural stability, Pd has been alloyed with materials such as silver [17]. An alternative, and potentially superior approach, is the combination of Pd with refractory (group V) metals, such as Ta, into layered membranes [18]. Refractory metals have even higher bulk hydrogen permeabilities than Pd or its alloys [19], and are cheaper than Pd.

The diffusion coefficient of H in this composite is given by [20]

$$D(\rho,x) = \begin{cases} D_{\mathrm{Pd}} \equiv D_{\mathrm{Pd}}^{\mathrm{int}}\left[f_1(\beta) + f_2(\rho)V_{\mathrm{Pd}}\rho\dfrac{1-\rho V_{\mathrm{Pd}}}{k_B T}\right] & \text{for } x \in \Omega_1 \cup \Omega_3 \\ D_{\mathrm{Ta}} \equiv D_{\mathrm{Ta}}^{\mathrm{int}} & \text{for } x \in \Omega_2 \end{cases} \tag{1b}$$

[1] Examples of such a desynchronization due to the use of noniterative or "loosely" coupled algorithms, and methods to iteratively correct them, can be found in [6–8].