Journal of Computational Physics 337 (2017) 154–174

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Good coupling for the multiscale patch scheme on systems with microscale heterogeneity

J.E. Bunder [a,*], A.J. Roberts [a], I.G. Kevrekidis [b]

[a] School of Mathematical Sciences, University of Adelaide, South Australia 5005, Australia
[b] Department of Chemical and Biological Engineering and PACM, Princeton University, Princeton, NJ 08544, USA

ARTICLE INFO

Article history:
Received 23 June 2016
Received in revised form 13 January 2017
Accepted 2 February 2017
Available online 16 February 2017

Keywords:
Multiscale computation
Equation-free methods
Patch dynamics
Diffusion

ABSTRACT

Computational simulation of microscale detailed systems is frequently only feasible over spatial domains much smaller than the macroscale of interest. The 'equation-free' methodology couples many small patches of microscale computations across space to empower efficient computational simulation over macroscale domains of interest. Motivated by molecular or agent simulations, we analyse the performance of various coupling schemes for patches when the microscale is inherently 'rough'. As a canonical problem in this universality class, we systematically analyse the case of heterogeneous diffusion on a lattice. Computer algebra explores how the dynamics of coupled patches predict the large scale emergent macroscale dynamics of the computational scheme. We determine good design for the coupling of patches by comparing the macroscale predictions from patch dynamics with the emergent macroscale on the entire domain, thus minimising the computational error of the multiscale modelling. The minimal error on the macroscale is obtained when the coupling utilises averaging regions which are between a third and a half of the patch. Moreover, when the symmetry of the inter-patch coupling matches that of the underlying microscale structure, patch dynamics predicts the desired macroscale dynamics to any specified order of error. The results confirm that the patch scheme is useful for macroscale computational simulation of a range of systems with microscale heterogeneity.

1. Introduction

Across all fields of science and engineering there are many systems which are only realistically described by mathematical models on multiple spatial and temporal scales, where each scale is critical to the model and must be accounted for in any numerical solution [1–3, e.g.]. Such multiscale systems are notoriously complex and computationally demanding, with computational methods of solution generally requiring enormous reductions in complexity and careful control of errors. One major challenge of multiscale modelling is how to transfer and represent information between different scales, particularly when the different scales are governed by different physics (for example, discrete and continuous, or deterministic and stochastic). A typical scenario is that a macroscale description of the system is required for practical applications, but essential to the system are fine details on microscales which are substantially smaller than the macroscale of interest. One important aim of multiscale modelling schemes is to be sufficiently accurate to reduce the need for expensive and time

* Corresponding author.
E-mail addresses: judith.bunder@adelaide.edu.au (J.E. Bunder), anthony.roberts@adelaide.edu.au (A.J. Roberts).

http://dx.doi.org/10.1016/j.jcp.2017.02.004
0021-9991/

consuming experiments; for example, in the design of metamaterials with novel properties for new metadevices [4]. This article derives good designs for the computational multiscale modelling scheme of patch dynamics [5–7, e.g.].

The multiscale computational technique of patch dynamics is 'equation-free' in the sense that it makes no attempt to derive a macroscale closed algebraic model from the original microscale system [8,6,9,10,7, for reviews]. Numerical resolution of the macroscale dynamics are obtained on demand by computing the microscale system on small discrete patches, with each patch centred about one macroscale grid point. A major advantage of this technique is that it is the original microscale system which is computed, and not an approximation. Unlike many other multiscale modelling techniques [11,12, e.g.], no assumptions are made regarding the relative importance of the various components of the microscale system since patch dynamics requires no such simplification. Two crucial, previously unresolved, questions in multiscale modelling when applying the patch method to systems with microscale heterogeneity are: (a) how to couple the discrete patches across space so that the unsimulated regions between the patches are best accounted for? and (b) how to appropriately design patches to capture relevant microscale characteristics? This article answers these questions.

A full implementation of patch dynamics involves discretising both space and time [13,14,8,15]. Here we concentrate on the spatial aspects of the patch scheme. Spatial patch dynamics, also known as the gap-tooth scheme, was successfully applied to various models, including Burgers' equation [16], a generalised advection–diffusion equation [17] and a Ginzburg–Landau model [18], and the resultant macroscale evolution was shown to be effectively independent of both patch width and patch coupling conditions [19]. However, these analyses all invoked systems where the microscale structures are smooth.

Here we explore a discrete, one dimensional, diffusion system, specified in Section 2. In contrast to earlier studies [19, 18, e.g.], we invoke microscale heterogeneity in the diffusion coefficients. We assume that the diffusivity coefficient varies rapidly with some periodicity over the microscale lattice—in many applications one period is called a cell. This diffusion model with fine scale roughness in the diffusivity coefficient generalises previous research into the special case where the diffusion coefficient was limited to two values [20]. The importance of such a discrete microscale diffusion is that it is in the same universality class as a host of other microscale systems. We conjecture that our results apply to a wide variety of microscale systems whose emergent macroscale dynamics are effectively that of diffusive mixing. Consequently, our results describe how to design patch schemes for multiscale modelling of a wide range of problems with microscale heterogeneity.

Multiscale modelling of materials with microscale heterogeneous compositions has broad applications, including the analysis of contact interaction and wear [21], avoiding damage in composite materials [22,23], modelling of nanostructures [24], and predicting flow in porous media [25]. These problems are often tackled with some spatial averaging or homogenisation, but for these techniques the method of solution varies from problem to problem and is typically reliant on heuristic approximations or trial-and-error [26–28]. Furthermore, their application becomes a daunting tasks when faced with complicated phenomena including nonlinearity [11,27]. Our aim with patch dynamics is to develop a multiscale modelling method with broad applicability which is straightforwardly adaptable to large families of problems.

Section 2 introduces the patch dynamics scheme and discusses how microscale heterogeneity complicates the choice of patch size and placement: a patch must capture a sufficient range of diffusivities without giving preference to any diffusivity value. We address these issues with an ensemble average over several configurations of the variable diffusivity coefficient [14]. Section 4 further develops the patch dynamics scheme and presents a method for coupling neighbouring patches and extracting the required macroscale solutions from averages of microscale fields within each patch. Patch dynamics is dependent on several parameters, such as the patch width and how many microscale fields to average over when calculating the macroscale field. These parameters can be freely chosen: our aim is to determine an optimal choice.

Our results are as yet the only analytic based results for determining optimal patch coupling parameters in a system with microscale heterogeneity. To determine the best choice of parameters we compare the macroscale closure of patch dynamics with that of the microscale solution on the entire microscale domain. Section 3 uses an eigenvalue analysis to analytically derive the macroscale closure over the entire microscale domain and Section 5 derives the patch dynamic macroscale closure and details the parameter recommendations for optimum results. We find that it is useful to account for the underlying microscale, cell, structure when constructing a patch. When this structure is well known, patch parameters can be chosen to *exactly* reproduce the correct macroscale closure—an ensemble average is unnecessary. However, when the microscale structure is not well known, the ensemble average is useful for better approximating the correct macroscale closure. Section 6 presents numerical simulations which confirm the optimum patch conditions determined from the analysis in Section 5. Section 6 also presents numerical simulations for cases which are not accessible by analysis.

For simplicity, we concentrate on diffusion in one dimensional space, but the scheme is adaptable to higher dimensions. Section 4 briefly discusses the two dimensional case. Knapek [29] developed a homogenisation-based coarse-graining method for a two dimensional diffusion model with heterogeneous diffusion which showed varying degrees of success. Fig. 1 (top, mesh) shows a two dimensional simulation of discrete diffusion with fine scale heterogeneity in the diffusion coefficient; the variability in diffusion results in a jagged field across the entire domain. The patch dynamics simulation, indicated by the shaded (coloured) regions in Fig. 1, is constructed with six patches in both the x and y directions, providing a total of 36 patches. The patch simulation using a single configuration (top) produces a jagged structure, similar to that of the entire domain solution, but the patch simulation with an ensemble average (bottom) produces a smooth field which interweaves between the jagged entire domain solution. In this simulation we use optimum patch parameters determined from the one dimensional analysis and find that they are also suitable for two dimensions.

Herein we address only linear autonomous dynamics because of the fundamental role of linear systems to nonlinear and/or controlled non-autonomous systems. Firstly, a Hartman–Grobman theorem [30] assures us that generic nonlinear