Journal of Computational Physics 313 (2016) 674–686

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Spatio-spectral concentration of convolutions

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ARTICLE INFO

Article history:
Received 18 December 2015
Received in revised form 25 February 2016
Accepted 29 February 2016
Available online 7 March 2016

Keywords:
Renormalisation group
Homogenisation

ABSTRACT

Differential equations may possess coefficients that vary on a spectrum of scales. Because coefficients are typically multiplicative in real space, they turn into convolution operators in spectral space, mixing all wavenumbers. However, in many applications, only the largest scales of the solution are of interest and so the question turns to whether it is possible to build effective coarse-scale models of the coefficients in such a manner that the large scales of the solution are left intact. Here we apply the method of numerical homogenisation to deterministic linear equations to generate sub-grid-scale models of coefficients at desired frequency cutoffs. We use the Fourier basis to project, filter and compute correctors for the coefficients. The method is tested in 1D and 2D scenarios and found to reproduce the coarse scales of the solution to varying degrees of accuracy depending on the cutoff. We relate this method to mode-elimination Renormalisation Group (RG) and discuss the connection between accuracy and the cutoff wavenumber. The tradeoff is governed by a form of the uncertainty principle for convolutions, which states that as the convolution operator is squeezed in the spectral domain, it broadens in real space. As a consequence, basis sparsity is a high virtue and the choice of the basis can be critical.

1. Introduction

In the early 1970s, a significant hurdle faced by particle physicists was the computation of partition functions that involved evaluating integrals over large ranges in wavenumbers. Ultimately, the only parameters of interest were at coarse scales of the systems under study. To compute these parameters, Kenneth Wilson introduced mode-elimination Renormalisation Group (RG) that enabled building low-wavenumber representations of fluctuating coefficients while succeeding in preserving the coarse-scale accuracy of the solutions. In other words, RG describes a means of projecting the small scales onto the large, and by degrees, integrating out rapid variations in the coefficients. This procedure has the potential to greatly reduce the computational burden. RG is perhaps the most celebrated instance of the concept of building coarse-scale models of inherently multi-scale phenomena, and has been widely used to model a range of phenomena. The application of mode-elimination RG to generate sub-grid-scale models of fluid turbulence, i.e. that convey the effect of scales smaller than the grid size, was suggested by Yakhot and Orszag [18] and studied in detail for passive-scalar advection by Avellaneda and Majda [1] (also see Smith and Woodruff [15] who compare these methods and Kraichnan's Direct Interaction Approximation, Kraichnan [10]). Yakhot and Orszag [18] suggested integrating over shells of wavenumbers, proceeding from the largest to the smallest, sequentially adding corrections to the coefficients of the turbulence model in question.

Independently, Kozlov [9] and Papanicolaou and Varadhan [13] studied solutions to the diffusion equation with random coefficients. Defining a small parameter ε to be the ratio of the correlation length-scale of the random coefficient to the

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http://dx.doi.org/10.1016/j.jcp.2016.02.068
0021-9991/

relevant coarse scale of the solution, Kozlov [9] and Papanicolaou and Varadhan [13] derived a two-scale asymptotic theory to estimate effective coefficients. The formulation is similar in concept to RG and produces a zero-wavenumber (constant) representation of the original random coefficient, and in the limit of vanishingly small ε, Papanicolaou and Varadhan [13] showed that the solution was accurate. Multi-scale coefficients however present a challenge and appropriately decimating these coefficients onto a coarser grid (not necessarily zero wavenumber) is of relevance in computational physics. In the finite-scale-cutoff scenario with non-random media, the method of numerical homogenisation is remarkably similar to RG. These techniques can be applied to build effective models of wavespeeds (whose spatial distributions can be complicated) in seismology, deriving coarse-scale descriptions of porosity coefficients in porous media etc. In this article, we will focus on these two scenarios.

A central goal of seismic studies of the Sun, stars and Earth is to infer the structural and dynamical properties of interiors using observations of their surface oscillations. The *forward problem*, critical to this effort, is the simulation of small-amplitude (linear) waves through the relevant media. Such media can comprise a wide spectrum of length scales, possibly much smaller than the wavelength. The problem thus becomes computationally stiff and very expensive to attempt. We are therefore interested in bringing to bear methods of homogenisation, which describe the coarse-scale behaviour of differential equations with rapidly varying coefficients, on these problems of wave propagation. We seek to replace the fine-scale structure with an effective sub-grid-scale model such that the coarse scales of the solution are accurately reproduced to within a specified tolerance.

Similarly, in porous media, the permeability of the medium, a tensor quantity, is finely sampled at a large number of spatial points. The goal is to coarsen the grid and appropriately average these tensor coefficients. Effective coarse-grained models of fine-scale tensor coefficients will necessarily mix various components. Here we will derive a formal theory that describes how to mix various terms. Classical homogenisation primarily addresses problems in which the coefficients periodically vary [3], with the sub-grid model being a zero-wavenumber representation (e.g., by the harmonic mean). However, in a number of real-world applications, the rapid variations are aperiodic and a more general theory to attempt such problems is required. Along these lines, multi-resolution analysis in the aid of numerical homogenisation of aperiodic media has been developed (e.g. [4,7,8,12]). More recently, e.g., Capdeville et al. [5], have posed the problem of terrestrial seismic wave propagation through aperiodic heterogeneous media in the language of classical homogenisation.

In this article, we follow the methodology of [7] and [8], which is well laid out and from which details may be intuited. Numerical homogenisation affords two major advantages: significant reduction in spatial complexity and a less restrictive Courant condition on the timestep. Here, we use the spatial Fourier and Haar-wavelet bases to investigate the accuracy of numerical homogenisation on three different wave equations, each gaining complexity over the previous. The Fourier basis lends itself to elegant interpretation but produces dense matrices whose inverses may not be easy to compute. In contrast sparse matrix inversion techniques may be easily extended to homogenisation in the Haar basis. The demonstrable success of the method encourages a more complete exploration of its possibilities.

2. Numerical homogenisation in 1D

Consider the 1D operator $\mathcal{L}$ acting on a function u defined by $\mathcal{L}u = \partial_x(a\,\partial_x u)$, where $a = a(x) > 0$ is a coefficient, ∂_x is the spatial derivative with respect to the x coordinate. The wave equation corresponds to $\partial_t^2 u - S = \mathcal{L}u$, where t is time, $S = S(x,t)$ is a source and the equation takes on a hyperbolic character. The time-independent porous-flow equation, identical to the diffusion equation, is given by $\mathcal{L}u = 0$ and is elliptic in character.

The product in real space between $a(x)$ and $\partial_x u$ is a convolution in Fourier domain, resulting in the mixing of coarse and fine scales. In other words, the Fourier transform of this term (we do not add extra symbols to denote the transformed quantity) is

$$\mathcal{L}u(k) = -\sum_{k'} kk' a(k-k')\,u(k'), \tag{1}$$

and this results in a mixing between low and high wavenumbers. Thus to obtain the low-wavenumber representation of u, one must solve the equation over the full set of wavenumbers, which can be computationally expensive. The goal then is to create a sub-grid-scale model of a such that the coarse scales of u are well reproduced. Let us consider the projection of a function in the Fourier basis. Define a projection operator $\mathcal{F}$ that transforms a function in real space to the Fourier basis, producing a set of Fourier coefficients which may subsequently be characterised as "coarse" or "fine". Denoting the forward transform by $\mathcal{F}$, and given an $N \times 1$ vector v, the projection is written as $\mathcal{F}v = \begin{pmatrix} P \\ Q \end{pmatrix} v$, where P is a $k_p \times N$ matrix that projects v on to the coarse set of coefficients (of size $k_p \times 1$) and the $(N - k_p) \times N$-sized matrix Q projects v on to the fine coefficients. We note that $\mathcal{F}^{-1}\mathcal{F} = \mathcal{F}\mathcal{F}^{-1} = \mathbf{I}_N$, where the subscript denotes the size of the identity matrix ($N \times N$). Since we use the orthogonal Fourier basis, the inverse transform is $\mathcal{F}^{-1} = (P^* \;\; Q^*)$, where the $*$ denotes conjugate transpose (the Hermitian transpose) and the associated identities are satisfied

$$P P^* = \mathbf{I}_P, \;\; Q\,Q^* = \mathbf{I}_Q, \;\; P\,Q^* = \mathbf{0}, \;\; Q\,P^* = \mathbf{0}, \;\; P^*P + Q^*Q = \mathbf{I}_N. \tag{2}$$

Note that $\mathbf{I}_P$ is of size $k_p \times k_p$ and $\mathbf{I}_Q$ of size $k_q \times k_q$ (where $k_q = N - k_p$). With no loss of generality, this method may also be extended to other orthogonal and bi-orthogonal systems. Note that the sizes of the zero matrix $\mathbf{0}$ in the two identities