

Asymptotic and numerical homogenization

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Homogenization is an important mathematical framework for developing effective models of differential equations with oscillations. We include in the presentation techniques for deriving effective equations, a brief discussion on analysis of related limit processes and numerical methods that are based on homogenization principles. We concentrate on first- and second-order partial differential equations and present results concerning both periodic and random media for linear as well as nonlinear problems. In the numerical sections, we comment on computations of multi-scale problems in general and then focus on projection-based numerical homogenization and the heterogeneous multi-scale method.

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1. Introduction

In this paper we present a very broad overview of the general subject of homogenization. The term homogenization is used in many areas for mechanisms that make a mixture or a process the same (homogeneous) throughout a domain. In mathematics the term is most commonly used in connection with the study of problems (differential equations) with rapidly variable coefficients. There are many variations and extensions, some purely theoretical and others of important practical value. Overall, the idea is to consider a complex multi-scale system, analyse its limit properties and approximate it by a simpler homogenized one.

Consider a general differential equation

$$F_\varepsilon(u^\varepsilon, x) = 0$$

depending on a small parameter ε with solution $u^\varepsilon : \mathbb{R}^d \rightarrow \mathbb{R}$. The natural mathematical questions are whether the family $(u^\varepsilon)_{\varepsilon>0}$ converges, as $\varepsilon \rightarrow 0$, in some topology to a limit u_0 , and if so, whether that limit satisfies a separate ‘homogenized’ equation

$$\bar{F}(u_0, x) = 0.$$

To give a flavour of the problem and to introduce some of the basic concepts, we consider first the very simple example of a two-point boundary value problem:

$$\begin{cases} -(a^\varepsilon(x)u_x^\varepsilon)_x = f & \text{in } (0, 1), \\ u^\varepsilon(0) = u^\varepsilon(1) = 0, \end{cases} \quad (1.1)$$

with

$$a^\varepsilon(x) = a(x/\varepsilon) > 0 \quad \text{and} \quad 1\text{-periodic in } y.$$

The coefficient a_ε is highly oscillatory when ε is small, because of the periodicity of a , and, as $\varepsilon \rightarrow 0$, converges weakly to its arithmetic mean.

It is straightforward to check, after integrating the differential equation in (1.1), dividing by a^ε and integrating again, that the solution u^ε of (1.1) is given by

$$u^\varepsilon(x) = - \int_0^x \left(a^\varepsilon(\xi)^{-1} \int_0^\xi f(\eta) \, d\eta + C^\varepsilon \right) d\xi,$$

with the constant of integration

$$C^\varepsilon = - \int_0^1 \left(a^\varepsilon(\xi)^{-1} \int_0^\xi f(\eta) \, d\eta \right) d\xi / \int_0^1 a^\varepsilon(\xi)^{-1} d\xi$$

determined by the boundary condition at $x = 1$.

Given this explicit formula of the solution, we now let $\varepsilon \rightarrow 0$ to find that

$$u^\varepsilon(x) \rightarrow u_0(x) = -a_H \int_0^x \left(\int_0^\xi f(\eta) d\eta + C \right) d\xi, \quad (1.2)$$

and

$$C^\varepsilon \rightarrow C = - \int_0^1 \left(\int_0^\xi f(\eta) d\eta \right) d\xi, \quad (1.3)$$

where

$$a_H = \left(\int_0^1 a(y)^{-1} dy \right)^{-1}.$$

It follows that u_0 satisfies the homogenized two-boundary value problem where a^ε is replaced by a_H , which is typically different from the arithmetic mean of a^ε ,

$$\begin{cases} -a_H u_{0xx} = f & \text{in } (0, 1), \\ u_0(0) = u_0(1) = 0. \end{cases} \quad (1.4)$$

The coefficient a_H can be seen as a homogenized or effective material coefficient, if a^ε represents an original material property, such as, for example, the conductivity of a composite material.

Problem (1.4) is of course much easier to analyse than the original (1.1). It is also much better suited for computations since any discretization does not need to resolve the small ε -scale of (1.1).

The problem can easily become more complicated. Consider, for example, the non-divergence-form two-point boundary value problem

$$\begin{cases} -u_{xx}^\varepsilon + \frac{1}{\varepsilon} b^\varepsilon(x) u_x^\varepsilon = f & \text{in } (0, 1), \\ u^\varepsilon(0) = u^\varepsilon(1) = 0, \end{cases} \quad (1.5)$$

where

$$b^\varepsilon(x) = b(x/\varepsilon) \quad \text{with } b \text{ 1-periodic and } \int_0^1 b(y) dy = 0. \quad (1.6)$$

As before, b^ε is highly oscillatory when ε is small, and converges weakly, as $\varepsilon \rightarrow 0$, to its arithmetic mean.

It is again an exercise, albeit slightly more elaborate, to check that the solution u^ε is given by

$$u^\varepsilon(x) = \int_0^x e^{B(y/\varepsilon)} dy C_\varepsilon - \int_0^x e^{B(y/\varepsilon)} \int_0^y e^{-B(z/\varepsilon)} f(z) dz, \quad (1.7)$$

with the constant of integration

$$C^\varepsilon = \left(\int_0^1 e^{B(\xi/\varepsilon)} dy \right)^{-1} \int_0^1 e^{B(x/\varepsilon)} \int_0^\xi e^{-B(y/\varepsilon)} f(y) dy d\xi$$

determined by the boundary condition at $x = 1$, and

$$B(y) = \int_0^y b(\xi) d\xi.$$

It is possible to check directly that, as $\varepsilon \rightarrow 0$, $u^\varepsilon \rightarrow u_0$, where u_0 solves the averaged boundary value problem

$$\begin{cases} -a_H u_{0xx} = f & \text{in } (0, 1), \\ u_0(0) = u_0(1) = 0, \end{cases} \quad (1.8)$$

with the homogenized coefficient a_H given by

$$a_H = \left[\int_0^1 e^{-B(y)} dy \int_0^1 e^{B(y)} dy \right]^{-1}. \quad (1.9)$$

Second-order equations in non-divergence form are closely related, via Itô's calculus, to solutions of stochastic differential equations (SDE for short). If $(W_t)_{t \in \mathbb{R}}$ is a standard Brownian motion, the SDE corresponding to (1.5) is

$$dX_t^\varepsilon = -\frac{1}{\varepsilon} b^\varepsilon(X_t^\varepsilon) dt + \sqrt{2} dW_t. \quad (1.10)$$

The asymptotics, as $\varepsilon \rightarrow 0$, of the solution of (1.10) are closely related to the behaviour, as $\varepsilon \rightarrow 0$, of the u^ε of (1.5). As a matter of fact there is a probabilistic proof which yields that, as $\varepsilon \rightarrow 0$, $X_t^\varepsilon \rightarrow X_t^0$, in the appropriate sense, where

$$dX_t^0 = \sqrt{2 a_H} dW_t \quad \text{with } X_0^0 = x, \quad (1.11)$$

with a_H given by (1.9).

In general it is not possible to derive closed-form expressions for the limiting solution, and other techniques must be used. It is also not always the case that the homogenized equations have the same form as the original solution, as can be seen in the homogenization of scalar conservation laws.

The general theory deals with more sophisticated homogenization problems in higher dimensions and more complicated linear and nonlinear equations in periodic, almost periodic and, more generally, random environments. In this paper we discuss only linear and fully nonlinear first- and second-order equations in periodic and random settings.

There are several approaches to the study of homogenization depending on the exact form of the problem at the level of the ε -scale, and the nature of the environment (periodic, random, *etc.*). In this paper we discuss a number of them, but not all. The first method, which is used most often,

especially at the formal level, is based on the construction of asymptotic expansions. This approach provides the homogenized equation but it is occasionally difficult to make rigorous due to lack of regularity. The second method, known as the energy method, is applied to problems which admit a variational formulation. A third method, known as two-scale convergence, is often used very effectively in variational problems and combines elements of the first two. A fourth method is based on probabilistic arguments and is used, of course, when the problem has a probabilistic interpretation. When dealing with nonlinear problems it is often necessary to adapt the general methodologies to accommodate the specific nonlinear structure. Some of the approaches used here include Γ -convergence, an effective tool for problems with variational formulation, and the perturbed-test function method typically used for (nonlinear) non-variational problems.

Even if some ideas in homogenization date further back, the early developments of the 1970s are fundamental. This is very well presented in the text from 1978 by Bensoussan, Lions and Papanicolaou (1978), which develops a systematic framework for asymptotic analysis. Influential contemporary contributions are the multi-scale analysis of Keller (1977), the homogenization techniques of Babuška (1976), the G -convergence theory of De Giorgi and Spagnolo (1973) and the analysis of Murat and Tartar (1997).

Lions, Papanicolaou and Varadhan (1983) were the first to consider the homogenization of first- and second-order fully nonlinear equations in the periodic setting. An influential contribution to the subject were the papers by Evans (1989, 1992). The literature for random homogenization is more limited. Papanicolaou and Varadhan (1979, 1981) and Kozlov (1985) were the first to consider the homogenization of uniformly elliptic linear divergence-form and non-divergence-form elliptic operators. The first nonlinear results in the variational setting were obtained by Dal Maso and Modica (1986) and in the non-variational setting by Souganidis (1999), Lions and Souganidis (2003), Kosygina, Rezakhanlou and Varadhan (2006) and Caffarelli, Souganidis and Wang (2005).

After the early period the development of homogenization has accelerated. In one direction there are many new results on nonlinear problems and stochastic equations, some of which are mentioned above. There is now also a wide literature on applications in solid and fluid mechanics. In another direction, theoretical tools developed in the context of homogenization, such as compensated compactness Γ -, G - and H -convergence, have been of great value in other areas of partial differential equations. Some of these later results will be discussed below but it is outside the scope of this paper to give an extensive review of the literature. We refer, for example, to the recent texts by Jikov, Kozlov and Oleinik (1991), Allaire *et al.* (1993), Cioranescu and Donato (2000), Marchenko and Khruslov (2006) and Pavliotis and Stewart (2007).

The purpose of this paper is to give easily accessible examples of the basic theory and recent progress. An important aspect is also the coupling of asymptotic and numerical methods. The first part (Sections 2 to 7) describes the general problem and is devoted to the analytic aspects of the theory, while the last three sections are devoted to numerical homogenization. In Section 2 we discuss the homogenization theory for linear divergence-form second-order elliptic partial differential equations (PDEs) in the periodic setting. Linear second-order elliptic PDEs in non-divergence form are discussed in Section 3. In Section 4 we consider nonlinear first- and second-order PDEs, in either divergence or non-divergence form, always in periodic media. In Section 5 we provide a general overview of the theory in the stationary ergodic environments, while in Section 6 we present results about rates of convergence. A few applications are given in Section 7 to illustrate the variety of homogenization results. In the second part (Sections 8 to 10) we start with a general discussion of numerical homogenization in Section 8, followed by two special techniques in Sections 9 and 10.

We conclude by remarking that homogenization is a very broad topic which cannot in all fairness be described in a few pages. The reader should keep in mind that here we only attempt to provide a short introduction and hope to stimulate further study of the subject. The same applies to the references. There are literally thousands of papers devoted to the different parts of the theory. Here we only refer to the ones which are relevant to the particular problems we discuss.

A final remark is that throughout the paper we will denote by C positive constants which are independent of ε .

2. Periodic homogenization for linear divergence-form second-order elliptic PDEs

We consider here the divergence-form elliptic boundary value problem

$$\begin{cases} -\operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)Du^\varepsilon\right) = f & \text{in } U, \\ u^\varepsilon = 0 & \text{on } \partial U, \end{cases} \quad (2.1)$$

which, using the summation convention, is rewritten as

$$\begin{cases} -\left(a_{ij}\left(\frac{x}{\varepsilon}\right)u_{x_j}^\varepsilon\right)_{x_i} = f & \text{in } U, \\ u^\varepsilon = 0 & \text{on } \partial U. \end{cases} \quad (2.2)$$

The matrix function $A = (a_{ij})_{1 \leq i, j \leq d}$ is assumed to be

$$\text{symmetric, continuous and } Y\text{-periodic,} \quad (2.3)$$

where Y is the unit cube, and

$$\begin{cases} \text{uniformly elliptic, i.e., there exist } \lambda, \Lambda > 0 \text{ such that,} \\ \text{for all } \xi, y \in \mathbb{R}^N, \quad \Lambda |\xi|^2 \geq a_{ij}(y) \xi_i \xi_j \geq \lambda |\xi|^2, \end{cases} \quad (2.4)$$

where $|\cdot|$ denotes the Euclidean norm and we have used the usual summation convention.

A function $u^\varepsilon \in H_0^1(U)$, the Sobolev space of functions vanishing on the boundary ∂U which, together with their derivatives, are square-integrable in U , is defined to be a solution of (2.1) if, for all $v \in H_0^1(U)$,

$$a_\varepsilon(u^\varepsilon, v) = (f, v), \quad (2.5)$$

where, for $f \in L^2(U)$ and $u, v \in H_0^1(U)$,

$$(f, v) = \int_U f v \, dx \quad \text{and} \quad a_\varepsilon(u, v) = \int_U a_{ij} \left(\frac{x}{\varepsilon} \right) u_{x_j} v_{x_i} \, dx.$$

The problem is well defined in $H_0^1(U)$. For $f \in L^2(U)$, it admits a unique solution $u^\varepsilon \in H_0^1(U)$ satisfying the estimate

$$\|u^\varepsilon\|_{H_0^1(U)} \leq C \|f\|_{L^2(U)}. \quad (2.6)$$

The two-point boundary value problem (1.1) is a special case of (2.1). Its variational formulation is

$$\int_0^1 a \left(\frac{x}{\varepsilon} \right) u_x^\varepsilon v_x \, dx = \int_0^1 f v \, dx \quad \text{for all } v \in H_0^1(0, 1). \quad (2.7)$$

To explain the difficulties arising in the study of the behaviour, as $\varepsilon \rightarrow 0$, of (2.1), we proceed with (1.1). Taking $v = u^\varepsilon$ in (2.7), we find

$$\|u^\varepsilon\|_{H_0^1(0,1)} \leq C.$$

Therefore we may extract subsequences, still denoted by u^ε , such that, as $\varepsilon \rightarrow 0$,

$$u^\varepsilon \rightarrow u \quad \text{weakly in } H_0^1(0, 1).$$

Recall also that, as $\varepsilon \rightarrow 0$, we have weak $*$ convergence

$$a \left(\frac{\cdot}{\varepsilon} \right) \rightarrow \langle a \rangle = \int_0^1 a(y) \, dy \quad \text{in } L^\infty(0, 1).$$

It is therefore natural to expect that, in the limit $\varepsilon \rightarrow 0$, we have

$$-(\langle a \rangle u_x)_x = f \quad \text{in } (0, 1),$$

an equation which is *not* satisfied, as we already know from the discussion in the Introduction.

Next we present an argument that is not based on having an exact formula and yields the correct answer. To this end, let

$$\xi^\varepsilon = a^\varepsilon u_x^\varepsilon.$$

Since the a^ε s are bounded, it follows that the family $(\xi^\varepsilon)_{\varepsilon>0}$ is bounded in $L^2(0,1)$, and, since it satisfies

$$-\xi_x^\varepsilon = f,$$

is actually bounded in $H^1(0,1)$. Therefore, along subsequences $\varepsilon \rightarrow 0$,

$$\xi^\varepsilon \rightarrow \xi \text{ in } L^2(0,1) \quad \text{and} \quad \xi_x^\varepsilon \rightarrow \xi_x \text{ weakly in } L^2(0,1).$$

In view of the above,

$$\frac{1}{a^\varepsilon} \xi^\varepsilon \rightharpoonup \left\langle \frac{1}{a} \right\rangle \xi \text{ weakly in } L^2(0,1) \quad \text{and} \quad -\xi_x = f.$$

Since

$$\frac{1}{a^\varepsilon} \xi^\varepsilon = u_x^\varepsilon,$$

we conclude that

$$u_x = \left\langle \frac{1}{a} \right\rangle \xi \quad \text{and} \quad - \left(\left\langle \frac{1}{a} \right\rangle^{-1} u_x \right)_x = f.$$

We now present the method of the asymptotic expansion, which is very convenient and is a common technique for obtaining homogenized equations. The justification may need other general tools.

To study the asymptotic behaviour of the solutions of (2.1), we form a two-scale expansion in ε and then match terms of the same order in ε .

We begin with the *ansatz* that

$$u^\varepsilon(x) = u_0(x, x/\varepsilon) + \varepsilon u_1(x, x/\varepsilon) + \varepsilon^2 u_2(x, x/\varepsilon) + \cdots, \quad (2.8)$$

with $u_j(x, y)$ ($j = 0, 1, 2, \dots$) Y -periodic in y .

If we regard x and y as separate variables, applied to a function $\phi(x, x/\varepsilon)$, the differentiation operator D_x becomes $D_x + \frac{1}{\varepsilon} D_y$. Then, if

$$A^\varepsilon v = -\operatorname{div} \left(A \begin{pmatrix} x \\ \varepsilon \end{pmatrix} Dv \right),$$

we may write

$$A^\varepsilon = \varepsilon^{-2} A_1 + \varepsilon^{-1} A_2 + \varepsilon^0 A_3 + \cdots,$$

with

$$\begin{cases} A_1 = -\operatorname{div}_y(A(y)D_y), \\ A_2 = -\operatorname{div}_y(A(y)D_x) - \operatorname{div}_x(A(y)D_y), \\ A_3 = -\operatorname{div}_x(A(y)D_x). \end{cases} \quad (2.9)$$

Using the assumed expansion, the equation yields

$$\begin{cases} \text{(i)} & A_1 u_0 = 0, \\ \text{(ii)} & A_1 u_1 + A_2 u_0 = 0, \\ \text{(iii)} & A_1 u_2 + A_2 u_1 + A_3 u_0 = f. \end{cases} \quad (2.10)$$

The homogenized operator is then constructed from (2.10).

Before we continue with the analysis, we recall the classical Fredholm alternative argument, which states that

$$\begin{cases} B\phi = F & \text{in } Y, \\ \phi & Y\text{-periodic,} \end{cases} \quad (2.11)$$

where B is a general second-order operator in either divergence or non-divergence form, has a solution if and only if

$$\int_Y F(y)m(y) dy = 0,$$

where m is an invariant measure, *i.e.*, the unique solution of the adjoint equation

$$\begin{cases} B^*m = 0 & \text{in } Y, \\ m & Y\text{-periodic,} \end{cases} \quad (2.12)$$

with

$$m > 0 \quad \text{and} \quad \int_Y m(y) dy = 1. \quad (2.13)$$

We return now to the asymptotic analysis of (2.1).

Since the only periodic solutions of (2.10(i)) are constants in y , we have

$$u_0(x, y) = u(x),$$

and therefore (2.10(ii)) reduces to

$$\begin{cases} -\operatorname{div}_y(A(y)D_y u_1) = \operatorname{div}_y(A(y)D_x u_0) & \text{in } Y, \\ u_1 & Y\text{-periodic in } y, \end{cases} \quad (2.14)$$

which, in view of the previous discussion, admits a unique solution by Fredholm's alternative, up to addition of a constant. Indeed, here for (2.14) we can take $m \equiv 1$. It is then immediate that

$$\int_Y \operatorname{div}_y(A(y)D_x u_0)m dy = 0.$$

The special form of the right-hand side of (2.14) allows us to represent u_1 as

$$u_1(x, y) = w \cdot D_x u_0 + \tilde{u}(x), \quad (2.15)$$

where each component of $w = (w_1, \dots, w_d)$ is the unique (up to additive constants) solution of the cell problem

$$\begin{cases} -\operatorname{div}_y(A(y)D_y w_i) = \operatorname{div}_y(Ae_i) & \text{in } U, \\ w_i & Y\text{-periodic in } y. \end{cases} \quad (2.16)$$

Applying the Fredholm alternative once again to (2.10(iii)), recalling that the average of $f - A_2 u_1 - A_3 u_0$ over Y must be zero, and replacing u_1 by (2.15) leads to the homogenized equation

$$\begin{cases} -\operatorname{div}(\bar{A}D u_0) = f & \text{in } U, \\ u_0 = 0 & \text{on } \partial U, \end{cases} \quad (2.17)$$

with the effective matrix $\bar{A} = (\bar{a}_{ij})_{1 \leq i, j \leq d}$ given by

$$\bar{a}_{ij} = \int_Y a_{ij}(y)(D_y w_i + e_i)(D_y w_j + e_j) dy. \quad (2.18)$$

Notice that the matrix \bar{A} is uniformly elliptic. Moreover, since it is constant, (2.17) can also be written in the non-divergence form

$$\begin{cases} -\operatorname{tr} \bar{A} D^2 u_0 = f & \text{in } U, \\ u_0 = 0 & \text{on } \partial U. \end{cases}$$

Although the method of the asymptotic expansion is simple, it is often difficult to implement, since it is based on establishing the expansion (2.8). It is, however, very useful to guess the homogenized problem. A second step is then required to prove the actual convergence of the u^ε s to u_0 . The latter can be established by several methods, such as maximum principle, Γ - or G -convergence, *etc.* An effective method, known as the energy method, was introduced in Tartar (1977). It is based on the choice of appropriate test functions in the variational formulation (2.5) of (2.1) which says that, for all $v \in H_0^1(U)$,

$$\int_U \left(A \left(\frac{x}{\varepsilon} \right) D u^\varepsilon(x) \cdot D v(x) \right) dx = \int_U f(x) v(x) dx. \quad (2.19)$$

As already discussed in the one-dimensional case, it is not possible to pass to the limit $\varepsilon \rightarrow 0$ in the left-hand side of (2.19) for every v , since the families $(A(\frac{\cdot}{\varepsilon}))_{\varepsilon > 0}$ and $(D u^\varepsilon)_{\varepsilon > 0}$ are only weakly convergent. The idea of the energy method is to use an appropriate family v^ε of test functions to pass in the limit $\varepsilon \rightarrow 0$ taking advantage of the ‘compensated compactness’ which takes place. This family of test functions is given by

$$v^\varepsilon(x) = v(x) + \varepsilon \tilde{w} \left(\frac{x}{\varepsilon} \right) \cdot D v(x), \quad (2.20)$$

with v a smooth H_0^1 function and $\tilde{w} = (w_1, \dots, w_d)$ the solution of the adjoint cell problem

$$\begin{cases} -\operatorname{div}(A^*(y)(D_y \tilde{w}_i + e_i)) = 0 & \text{in } Y, \\ \tilde{w}_i & Y\text{-periodic in } y, \end{cases}$$

which, once again, exists in view of Fredholm's alternative. Inserting (2.20) in (2.19) allows us to eliminate the 'bad' terms and prove the convergence.

We next present an argument justifying the formal expansion (2.8) under the additional assumption that the coefficients, f and, hence, the solution u^ε are smooth. Under these assumptions it is possible to show that, as $\varepsilon \rightarrow 0$, $u^\varepsilon \rightarrow u$ uniformly in \bar{U} .

To this end, take u_1 as in (2.15) with $\tilde{u}_1 \equiv 0$ and set

$$z_\varepsilon = u^\varepsilon - (u + \varepsilon u_1 + \varepsilon^2 u_2).$$

It follows that

$$A^\varepsilon z_\varepsilon = -\varepsilon \tilde{z}_\varepsilon,$$

with

$$\tilde{z}_\varepsilon = A_2 w + A_3 u_1 + \varepsilon A_3 u_2.$$

If f is smooth, then u_0 , u_1 and u_2 are smooth, and hence

$$|\tilde{z}_\varepsilon| \leq C \quad \text{in } U.$$

On the boundary ∂U we have

$$z_\varepsilon = -(\varepsilon u_1 + \varepsilon^2 u_2),$$

and therefore

$$|z_\varepsilon| \leq C\varepsilon \quad \text{on } \partial U.$$

It follows from the maximum principle that

$$|z_\varepsilon| \leq C\varepsilon \quad \text{in } \bar{U}$$

and, finally,

$$|u^\varepsilon - u| \leq C\varepsilon \quad \text{in } \bar{U}.$$

The general result is as follows.

Theorem 2.1. Assume (2.3) and (2.4) and let u^ε and u_0 be, respectively, the solutions of (2.1) and (2.17). Then, as $\varepsilon \rightarrow 0$, $u^\varepsilon \rightarrow u_0$ weakly in H_0^1 . In addition, $u^\varepsilon - u_0 - \varepsilon u_1(\frac{\cdot}{\varepsilon}) \rightarrow 0$ strongly in H_0^1 , where u_1 is the solution of (2.14).

The proof of the weak convergence follows along the lines discussed earlier. The strong convergence without the correction εu_1 is not true. We refer to Bensoussan *et al.* (1978) for an extensive discussion and the detailed proof.

Next we describe briefly another method, known as two-scale convergence and developed in Nguetseng (1989) and Allaire (1992), which, in some sense, blends the asymptotic expansion and energy methods and yields the homogenization in one step.

To describe the method it is necessary to introduce some notation. We write $C_p^\infty(Y)$ for the functions in $C^\infty(\mathbb{R}^d)$ that are Y -periodic, while $C_p(Y)$ is the space of continuous Y -periodic functions. Finally, $C_c^\infty(U; C_p^\infty(Y))$ is the space of infinitely smooth and compactly supported functions with values in $C_p^\infty(Y)$.

We say that a family $(u^\varepsilon)_{\varepsilon>0}$ in $L^2(U)$ is two-scale convergent to $u_0 \in L^2(U \times Y)$ if, for all $\psi \in C_c^\infty(U; C_p^\infty(Y))$,

$$\lim_{\varepsilon \rightarrow 0} \int_U u^\varepsilon(x) \psi\left(x, \frac{x}{\varepsilon}\right) dx = \int_U \int_Y u_0(x, y) \psi(x, y) dx dy. \tag{2.21}$$

We next summarize the key results on two-scale convergence. For each bounded family $(u^\varepsilon)_{\varepsilon>0}$ in $L^2(U)$ there exists a subsequence, still denoted by u^ε , and $u_0 \in L^2(U \times Y)$ such that, as $\varepsilon \rightarrow 0$, u^ε is two-scale convergent to u_0 . Moreover, as $\varepsilon \rightarrow 0$,

$$u^\varepsilon \rightarrow u = \int_Y u_0(\cdot, y) dy \text{ weakly in } L^2(U),$$

and, if u_0 is smooth, and, as $\varepsilon \rightarrow 0$,

$$\|u^\varepsilon\|_{L^2(U)} \rightarrow \|u_0\|_{L^2(U \times Y)},$$

then,

$$u^\varepsilon(\cdot) - u_0\left(\cdot, \frac{\cdot}{\varepsilon}\right) \rightarrow 0 \text{ strongly in } L^2(U).$$

Finally, if $(u^\varepsilon)_{\varepsilon>0}$ is bounded in $H^1(U)$, then there exist $u \in H^1(U)$ and $u_1 \in L^2(U; H_p^1(Y))$ such that, up to subsequences, u^ε and Du^ε are two-scale convergent, as $\varepsilon \rightarrow 0$, to u and $D_x u + D_y u_1$ respectively.

We now sketch how two-scale convergence can be used to study the asymptotic behaviour, as $\varepsilon \rightarrow 0$, of (2.1). All the arguments below work up to subsequences.

In view of (2.6) and our earlier general results on two-scale convergence, we know that there exist $u_0 \in H_0^1(U)$ and $u_1 \in L^2(U; H_p^1(Y))$ such that u^ε and Du^ε are two-scale convergent to u and $D_x u + D_y u_1$ respectively. The expectation is that u_ε should behave as $u + \varepsilon u_1(\cdot, \frac{\cdot}{\varepsilon})$.

Using test functions such as $\phi + \varepsilon \phi_1(\cdot, \frac{\cdot}{\varepsilon})$ in (2.19), with ϕ and ϕ_1 smooth and Y -periodic, yields

$$\begin{aligned} \int_U A\left(\frac{x}{\varepsilon}\right) Du^\varepsilon \cdot \left[D\phi(x) + D_y \phi_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon D_x \phi_1\left(x, \frac{x}{\varepsilon}\right) \right] dx \\ = \int_U f(x) \left[\phi(x) + \varepsilon \phi_1\left(x, \frac{x}{\varepsilon}\right) \right] dx. \end{aligned}$$

Passing to the limit, as $\varepsilon \rightarrow 0$, in the definition of two-scale convergence for Du_ε gives

$$\begin{aligned} & \int_U \int_Y A(y)[Du(x) + D_y u_1(x, y)] \cdot [D\phi(x) + D_y \phi_1(x, y)] \, dx \, dy \\ &= \int_U f(x)\phi(x) \, dx. \end{aligned} \quad (2.22)$$

A straightforward application of the Lax–Milgram theorem implies that there exists a unique solution (u, u_1) of (2.22) in $H_0^1(U) \times L^2(U; H_p^1(Y))$. Hence, the whole family u^ε and Du^ε are two-scale convergent to u and $D_x u + D_y u_1$, respectively. Moreover, it follows by integration that (2.22) is a variational formulation for the system

$$\begin{cases} -\operatorname{div}_y(A(y)(D_x u + D_y u_1)) = 0 & \text{in } U \times Y, \\ -\operatorname{div}_x \left[\int_Y A(y)(D_x u + D_y u_1) \, dy \right] = f & \text{in } U, \\ u = 0 & \text{on } \partial U, \\ u_1(x, \cdot) & Y\text{-periodic in } y, \end{cases} \quad (2.23)$$

which is equivalent to the usual homogenized and cell problem equations derived earlier.

To obtain the strong convergence result in Theorem 2.1 using the two-scale method, it suffices to observe that $u_1(x, \frac{x}{\varepsilon}) = Dw(\frac{x}{\varepsilon}) \cdot D_x u(x)$ is in $L^2(U)$ and can be used as a test function for two-scale convergence.

3. Periodic homogenization for linear second-order elliptic PDEs in non-divergence form

We next consider uniformly elliptic non-divergence-form equations and, in particular, the problem

$$\begin{cases} A^\varepsilon u^\varepsilon = -a_{ij} \left(\frac{x}{\varepsilon} \right) u_{x_i x_j}^\varepsilon + \frac{1}{\varepsilon} b_j \left(\frac{x}{\varepsilon} \right) u_{x_j}^\varepsilon = f & \text{in } U, \\ u^\varepsilon = 0 & \text{on } \partial U, \end{cases} \quad (3.1)$$

assuming in addition to (2.3) and (2.4) that

$$b \text{ is } Y\text{-periodic and bounded.} \quad (3.2)$$

Notice that, if $b_j = -(a_{ij})_{y_j}$, then (3.1) is the problem considered in the previous section.

The behaviour, as $\varepsilon \rightarrow 0$, of (3.1) can be studied using probabilistic methodology applied to homogenization (Bensoussan *et al.* 1978).

Since it requires considerable terminology, we choose here to present its PDE analogue. We again use the method of asymptotic expansions. We set

$$A^\varepsilon = \varepsilon^{-2}A_1 + \varepsilon^{-1}A_2 + \varepsilon^0A_3, \quad (3.3)$$

where

$$\begin{cases} A_1 = -a_{ij}(y)\partial_{y_i y_j}^2 + b_i(y)\partial_{y_i}, \\ A_2 = -a_{ij}(y)\partial_{y_i y_j}^2 - a_{ij}(y)\partial_{x_i y_j}^2 + b_i\partial_{x_i}, \\ A_3 = -a_{ij}(y)\partial_{x_i x_j}^2, \end{cases} \quad (3.4)$$

and use the *ansatz*

$$u^\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \cdots, \quad (3.5)$$

with u_0, u_1, u_2 periodic in $y = x/\varepsilon$, which leads to the equations

$$\begin{cases} \text{(i)} & A_1 u_0 = 0, \\ \text{(ii)} & A_1 u_1 + A_2 u_0 = 0, \\ \text{(iii)} & A_1 u_2 + A_2 u_1 + A_3 u_0 = f. \end{cases} \quad (3.6)$$

As in Section 2, it is immediate that, since u_0 is assumed to be periodic in y and A_1 is uniformly elliptic, we must have

$$u_0(x, y) = u_0(x). \quad (3.7)$$

Then (3.6(ii)) becomes

$$A_1 u_1 + b(y) \cdot Du_0 = 0. \quad (3.8)$$

We consider again the adjoint problem

$$\begin{cases} A_1^* m = -(a_{ij}(y)m)_{y_i y_j} - \operatorname{div}_y(bm) = 0 \quad \text{in } Y, \\ m \quad Y\text{-periodic,} \end{cases} \quad (3.9)$$

which has a unique solution m such that

$$m > 0 \quad \text{and} \quad \int_Y m(y) \, dy = 1. \quad (3.10)$$

Fredholm's alternative once again says that (3.8) has a periodic solution provided the b_i s satisfy, for each $i = 1, \dots, d$, the compatibility (centering) condition

$$\int b_i(y)m(y) \, dy = 0. \quad (3.11)$$

Assuming (3.11) and using the form of A_1 , we may assume that u_1 has the form

$$u_1(x, y) = -\chi^i(y)u_{0x_i} + \tilde{u}_1(x), \quad (3.12)$$

where, for each $i = 1, \dots, d$, χ^i satisfies

$$A_1 \chi^i + b_i(y) = 0 \quad \text{in } Y \quad \text{and} \quad \chi^i \text{ is } Y\text{-periodic.} \quad (3.13)$$

Then (3.6(iii)) can be rewritten as

$$A_1 u_2 = f + u_{0x_i x_j} \left(a_{ij} - a_{kj} \chi_{y_k}^i - a_{ki} \chi_{y_k}^j + \frac{1}{2} (b_i \chi^j + b_j \chi^i) \right). \quad (3.14)$$

We recall that it is possible to find a solution as long as the right-hand side of (3.14) is orthogonal to the invariant measure m . This leads to the homogenized equation

$$-\bar{a}_{ij} u_{x_i x_j} = f \quad \text{in } U, \quad (3.15)$$

with

$$\bar{a}_{ij} = \int_Y m(y) \left[a_{ij} - a_{kj} \chi_{y_k}^i - a_{kj} \chi_{y_k}^j + \frac{1}{2} (b_i \chi^j + b_j \chi^i) \right] dy.$$

Direct computations lead to the identity

$$\bar{a}_{ij} = \int m [a_{ij} + a_{k\ell} \chi_{y_k}^j \chi_{y_\ell}^i - a_{kj} \chi_{y_k}^i - a_{ij} \chi_{y_k}^j] dy. \quad (3.16)$$

Using the uniform ellipticity of the a_{ij} s it is now possible to show that the matrix $\bar{A} = (\bar{a}_{ij})_{1 \leq i, j \leq d}$ is also uniformly elliptic.

It is an instructive exercise, which we leave to the interested reader, to check that for the simple one-dimensional problem considered in the Introduction, (3.16) is the same as (1.9).

Theorem 3.1. Assume (2.3), (2.4), (3.2) and (3.11). Let u^ε and u_0 be the solutions of (3.1) and (3.15), respectively. If $f \in C^3(U)$, then

$$|u^\varepsilon - u_0| \leq C\varepsilon \quad \text{on } \bar{U}. \quad (3.17)$$

We briefly sketch the proof and refer to Bensoussan *et al.* (1978) for the details. To this end, we return to the issue of the solvability of (3.14). We take $\tilde{u}_1 = 0$ and write

$$u_2(x, y) = u_{0x_i x_j} \chi^{ij}(y), \quad (3.18)$$

where the periodic functions χ^{ij} solve, for $i, j = 1, \dots, d$,

$$A_1 \chi^{ij} = a_{ij} - a_{kj} \chi_{y_k}^i - a_{ki} \chi_{y_k}^j + \frac{1}{2} (b_i \chi^j + b_j \chi^i) - \bar{a}_{ij}. \quad (3.19)$$

With this choice it is easy to check that

$$A^\varepsilon \tilde{u}^\varepsilon = f + \varepsilon A_2 u_2 + \varepsilon A_3 u_1 + \varepsilon^2 A_3 u_2 = f + \varepsilon g_\varepsilon,$$

with

$$g_\varepsilon = -a_{ij} (\chi_{y_i}^{k\ell} u_{0x_j x_k x_\ell} + \chi_{y_j}^{k\ell} u_{0x_i x_k x_\ell}) \\ + b_i \chi^{k\ell} u_{0x_i x_k x_\ell} + a_{ij} \chi^\ell u_{0x_i x_j x_\ell} - \varepsilon a_{ij} \chi^{k\ell} u_{0x_i x_j x_k x_\ell}.$$

If f is sufficiently smooth, then the solution u of

$$\begin{cases} -\bar{a}_{ij}u_{0x_i x_j} = f & \text{in } U, \\ u_0 = 0 & \text{on } \partial U, \end{cases}$$

is also smooth, and thus

$$|g_\varepsilon| \leq C \quad \text{on } \bar{U}.$$

Therefore, if we set

$$z_\varepsilon = u^\varepsilon - \tilde{u}^\varepsilon,$$

we see that

$$A^\varepsilon z_\varepsilon = \varepsilon g_\varepsilon \quad \text{in } U \quad \text{with} \quad z_\varepsilon = -\varepsilon u_1 - \varepsilon^2 u_2 \quad \text{on } \partial U,$$

and hence

$$|z_\varepsilon| \leq C\varepsilon \quad \text{on } \bar{U}.$$

We conclude the discussion by remarking once again that the key step in the analysis was solving the cell problem. The necessary solvability solution then leads to the homogenized operator.

4. Nonlinear periodic homogenization

In this section we consider the homogenization of nonlinear equations both in the variational and non-variational settings. As before, we concentrate on second-order problems. The approach in the variational setting is based on the general method of Γ -convergence (see Dal Maso (1993) for the general theory). The theory for non-divergence-form equations is based on viscosity solutions and the so-called perturbed test function method (see Lions *et al.* (1983) for the first result, and then Evans (1989)).

We begin with the variational setting. The goal is to study the behaviour, as $\varepsilon \rightarrow 0$, of functionals of the form

$$F_\varepsilon(u) = \int_U f\left(\frac{x}{\varepsilon}, Du(x)\right) dx, \quad (4.1)$$

defined on, for example, $W^{1,p}(U)$ and their associated calculus of variations problems

$$\min\left\{\int_U f\left(\frac{x}{\varepsilon}, Du\right) dx : u \in W_0^{1,p}(U)\right\}. \quad (4.2)$$

Functionals and minimization problems like (4.1) and (4.2) model phenomena in continuum mechanics in the presence of micro-structures with ε the scale of the medium. The integrand f is, typically, the energy density. For example, F_ε may be the stored energy of an elastic material and u a

deformation, or u may be the difference of potential in a composed material occupying U .

The main physical question is whether the medium modelled by F_ε behaves, in the limit $\varepsilon \rightarrow 0$, as a homogeneous one. If this is the case, then there must exist an energy density f_0 , independent of x and U , such that the minima of (4.2) converge to the minima of

$$\min \left\{ \int_U f_0(Du(x)) \, dx : u \in W_0^{1,p}(U) \right\}. \quad (4.3)$$

The convergence of the minimum values and, perhaps, the minimizing functions of (4.2) are obtained as a consequence of the convergence, as $\varepsilon \rightarrow 0$, of (4.1) to the homogenized functional

$$F_0(u) = \int_U f_0(Du(x)) \, dx$$

in the sense of the Γ -convergence introduced by De Giorgi and Franzoni (1975). The book by Dal Maso (1993) is an excellent reference for the whole theory of Γ -convergence.

Next we briefly describe some of the basic facts. We begin with the definition of Γ -convergence on a metric space. Let $F_\varepsilon : X \rightarrow [0, \infty]$ be defined on a metric space (X, d) . The family $(F_\varepsilon)_{\varepsilon>0}$ Γ -converges to F , as $\varepsilon \rightarrow 0$, if:

- (i) for every $x \in X$ and every family $(x_\varepsilon)_{\varepsilon>0}$ such that $x_\varepsilon \rightarrow x$, as $\varepsilon \rightarrow 0$, we have $F(x) \leq \liminf_\varepsilon F_\varepsilon(x_\varepsilon)$, and
- (ii) for every $x \in X$ there exists a family $(x_\varepsilon)_{\varepsilon>0}$ such that $x_\varepsilon \rightarrow x$, as $\varepsilon \rightarrow 0$, and $F(x) = \lim_\varepsilon F_\varepsilon(x_\varepsilon)$.

The fundamental result of Γ -convergence says that if $(F_\varepsilon)_{\varepsilon>0}$ is d -equicoercive and Γ -converges on X to F , then

$$\min\{F(x) : x \in X\} = \liminf_\varepsilon \{F_\varepsilon(x) : x \in X\},$$

and, moreover, if x_ε is a minimizer of (4.2) and $x_\varepsilon \rightarrow x$, as $\varepsilon \rightarrow 0$, then x is a minimizer of (4.3).

We now concentrate on the Γ -convergence of functionals of the form (4.1). To this end, let U be a bounded subset of \mathbb{R}^d and $p > 1$. As far as the integrand $f : U \times \mathbb{R}^d \rightarrow \mathbb{R}$ is concerned, it is assumed that

$$\left\{ \begin{array}{l} \text{(i)} \quad \text{for every } \xi \in \mathbb{R}^d, f(\cdot, \xi) \text{ is measurable and } Y\text{-periodic,} \\ \text{(ii)} \quad \text{for almost every } y \in \mathbb{R}^d, f(y, \cdot) \text{ is convex in } \mathbb{R}^d, \\ \text{(iii)} \quad \text{for some } c > 0, \text{ almost every } y \in \mathbb{R}^d \text{ and every } \xi \in \mathbb{R}^d, \\ \quad \quad 0 \leq f(y, \xi) \leq c(|\xi|^p + 1) \quad \text{and} \quad f(y, 2\xi) \leq cf(y, \xi) + c. \end{array} \right. \quad (4.4)$$

For $\varepsilon > 0$ consider the functional $F_\varepsilon : L^p(U) \rightarrow [0, \infty]$ defined by

$$F_\varepsilon(u) = \begin{cases} \int_U f\left(\frac{x}{\varepsilon}, Du\right) dx & \text{if } u \in W^{1,p}(U), \\ +\infty & \text{otherwise,} \end{cases} \quad (4.5)$$

and let $f_0 : \mathbb{R}^d \rightarrow [0, +\infty)$ be defined by

$$f_0(\xi) = \inf_{v \in W_{\text{per}}^{1,p}(Y)} \int_Y f(y, \xi + Dv(y)) dy, \quad (4.6)$$

where $W_{\text{per}}^{1,p}(Y)$ denotes the set of all Y -periodic functions in $W_{\text{loc}}^{1,p}(\mathbb{R}^d)$.

Finally, consider $F_0 : L^p(\mathbb{R}^d) \rightarrow \mathbb{R}$ given by

$$F_0(u) = \begin{cases} \int_U f_0(Du) dx & \text{if } u \in W^{1,p}(U), \\ +\infty & \text{otherwise.} \end{cases} \quad (4.7)$$

Theorem 4.1. Assume that f satisfies (4.4) and let F_0 be defined by (4.7) for f_0 given by (4.6). Then, for every sequence $\varepsilon_n \rightarrow 0$, the sequence $(F_{\varepsilon_n})_{\varepsilon_n > 0}$ Γ -converges to F_0 .

We now turn our attention to non-variational homogenization problems. Before we enter into details we point out the main difference between linear and nonlinear theories. In the methods described in Sections 2 and 3, the key step was the solvability of the auxiliary cell problems obtained after expanding. This solvability was accomplished using Fredholm's alternative and the invariant measures, which are positive solutions of the adjoint operator. Cell problems also arise in nonlinear problems. In such settings, however, there is no notion of adjoint operator and Fredholm's alternative. It is therefore necessary to solve the cell problem directly.

For definiteness we consider the boundary value problem

$$\begin{cases} F\left(D^2u^\varepsilon, \frac{x}{\varepsilon}, x\right) = 0 & \text{in } U, \\ u^\varepsilon = 0 & \text{on } \partial U. \end{cases} \quad (4.8)$$

We assume that

$$F \in C(S^d \times \mathbb{R}^d \times U) \text{ is } Y\text{-periodic,} \quad (4.9)$$

and

$$\begin{cases} \text{uniformly elliptic, i.e., there exist } \lambda, \Lambda > 0 \text{ such that,} \\ \text{for all } (y, x) \in \mathbb{R}^d \times U \text{ and all } X, Y \in S^d \text{ with } Y \geq 0, \\ \lambda \|Y\| \leq F(X, y, x) - F(X + Y, y, x) \leq \Lambda \|Y\|, \end{cases} \quad (4.10)$$

where S^d denotes the space of $d \times d$ symmetric matrices.

Solutions of (4.8) are understood in the Crandall–Lions viscosity sense. For completeness we recall the definition below; for details we refer to Crandall, Ishii and Lions (1992).

Definition 4.2. An upper semi-continuous (respectively, lower semi-continuous) function u is a viscosity subsolution (respectively, supersolution) of $G(D^2u, Du, Du, u, x) = 0$ in U if, for all smooth ϕ and all local maximum (respectively, minimum) points x of $u - \phi$, we have $G(D^2\phi, D\phi, u(x), x) \leq 0$ (respectively, $G(D^2\phi, D\phi, u(x), x) \geq 0$). A continuous function is a solution, if it is both a subsolution and supersolution.

It turns out that viscosity solutions are the correct class of weak solutions for fully nonlinear (degenerate) elliptic second-order equations.

We return now to the homogenization of (4.8) and assume, for simplicity, that F is independent of x . We follow the asymptotic expansion approach and consider the *ansatz*

$$u^\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \cdots,$$

with u_0, u_1, u_2, \dots , periodic in y . Substituting in (4.8) we find

$$F\left(\frac{1}{\varepsilon^2} D_y^2 u_0 + \frac{1}{\varepsilon} (D_y^2 u_1 + D_{x,y}^2 u_0) + D_x^2 u_0 + D_{x,y}^2 u_1 + D_y^2 u_2 + \cdots, \frac{x}{\varepsilon}\right) = 0.$$

A heuristic argument based on the ellipticity of F yields that both u_0 and u_1 must be independent of y and, hence, the expansion reduces to

$$F\left(D_y^2 u_2 + D_x^2 u_0, \frac{x}{\varepsilon}\right) = 0.$$

The goal is then to find u_2 so that $F(D_y^2 u_2 + D_x^2 u_0, \frac{x}{\varepsilon})$ is a constant $\bar{F}(D_x^2 u_0)$ independent of $y = x/\varepsilon$. This leads to the cell problem

$$\left\{ \begin{array}{l} \text{for each } P \in S^d \text{ there exists a unique constant } \bar{F}(P) \\ \text{such that there exists a periodic solution } v \text{ of} \\ F(P + D_y^2 v, y) = \bar{F}(P) \text{ in } \mathbb{R}^d. \end{array} \right. \quad (4.11)$$

We recall the previous discussion on the fundamental difference between linear and nonlinear problems. In the linear setting the cell problem is solved using Fredholm's alternative, with the constant $\bar{F}(P)$ arising as the necessary compatibility condition for solvability. In the nonlinear problem, however, Fredholm's alternative has no meaning and it becomes necessary to solve (4.11) directly. The cell problem can be thought of as a nonlinear eigenvalue problem with $\bar{F}(P)$ the eigenvalue and the solution v , which is usually called the corrector, as the eigenfunction.

The cell problem is solved using the approximate problem

$$\alpha v_\alpha + F(D^2 v_\alpha + P, y) = 0 \quad \text{in } \mathbb{R}^d,$$

obtaining appropriate bounds and passing to the limit $\alpha \rightarrow 0$. The constant $\bar{F}(P)$ is obtained as the limit of $-\alpha v_\alpha(0)$. This step requires non-trivial arguments from the theory of viscosity solutions which are beyond the scope of this review. We refer to Lions *et al.* (1983), Evans (1989), *etc.*, for a discussion.

It is worth remarking that this approximate problem is not artificial. Indeed, if

$$v^\alpha(y) = \alpha v_\alpha\left(\frac{y}{\alpha^{1/2}}\right),$$

then

$$v^\alpha + F\left(D^2 v^\alpha + p, \frac{y}{\alpha^{1/2}}\right) = 0 \quad \text{in } \mathbb{R}^d.$$

If there is homogenization, then, as $\alpha \rightarrow 0$, $v^\alpha \rightarrow \bar{v}$ locally uniformly in \mathbb{R}^d , with

$$\bar{v} + \bar{F}(D^2 \bar{v} + P) = 0 \quad \text{in } \mathbb{R}^d,$$

in which case, since \bar{v} is bounded, we must have $\bar{v} = -\bar{F}(P)$.

To state the result we consider the boundary value problem

$$\begin{cases} \bar{F}(D^2 u_0) = 0 & \text{in } U, \\ u_0 = 0 & \text{on } \partial U. \end{cases} \quad (4.12)$$

The following was proved in Evans (1989).

Theorem 4.3. Let u^ε and u_0 be, respectively, the solutions of (4.8) and (4.12), with \bar{F} given by (4.11). Then, as $\varepsilon \rightarrow 0$, $u^\varepsilon \rightarrow u_0$ uniformly in \bar{U} .

The proof is relatively simple, therefore we briefly sketch its main steps.

It is not difficult to show, under some technical assumptions on F , that there exists $C > 0$ such that

$$|u^\varepsilon| \leq C \quad \text{on } \bar{U}.$$

We define next the so-called ‘relaxed’ half-limit, a very important tool in the theory of viscosity solutions, introduced by Barles and Perthame (1988). They are

$$u^*(x) = \limsup_{y \rightarrow x, \varepsilon \rightarrow 0} u^\varepsilon(y) \quad \text{and} \quad u_*(x) = \liminf_{y \rightarrow x, \varepsilon \rightarrow 0} u^\varepsilon(y).$$

It is of course immediate that $u_* \leq u^*$ in U . Next we show that u^* and u_* are, respectively, sub- and supersolution of (4.12). The comparison

property of viscosity solutions then yields that we must have $u^* \leq u_*$, and hence $u_0 = u_* = u^*$, a fact which yields that, as $\varepsilon \rightarrow 0$, $u^\varepsilon \rightarrow u_0$ in U .

We employ the so-called ‘perturbed test function’ method (Evans 1989) to show that u^* is a subsolution. The argument for u_* is similar. We would like to point out to the reader the similarity of the argument below to one used for linear equations. The main difference is that, due to the lack of higher regularity of solutions to fully nonlinear equations, it is not possible to justify the asymptotics directly. Instead this is done at the level of the test functions.

Let ϕ be a test function and suppose that $x_0 \in U$ is a strict local maximum of $u^* - \phi$ in $B(x_0, \delta)$ for some small $\delta > 0$. Moreover, we assume that $u^*(x_0) = \phi(x_0)$. We argue by contradiction and assume that

$$\bar{F}(D^2\phi(x_0)) = \sigma > 0.$$

Let ψ be the solution of the cell problem

$$F(D_y^2\psi + D^2\phi(x_0), y) = \bar{F}(D^2\phi(x_0)).$$

It follows¹ that the function

$$v^\varepsilon(x) = \phi(x) + \varepsilon^2\psi\left(\frac{x}{\varepsilon}\right)$$

is a supersolution of

$$F\left(D^2v^\varepsilon, \frac{x}{\varepsilon}\right) \geq 0 \quad \text{in } B(x_0, \delta).$$

The comparison of viscosity solutions then yields that

$$u^\varepsilon(x_0) - v^\varepsilon(x_0) \leq \max_{B(x_0, \delta)} (u^\varepsilon - v^\varepsilon) \leq \max_{\partial B(x_0, \delta)} (u^\varepsilon - v^\varepsilon).$$

Since $v^\varepsilon \rightarrow \phi$, as $\varepsilon \rightarrow 0$, we find

$$u^*(x_0) - \phi(x_0) \leq \max_{\partial B(x_0, \delta)} (u^* - \phi),$$

which is a contradiction, since $u^*(x_0) = \phi(x_0)$ and $\max_{\partial B(x_0, \delta)} (u^* - \phi) < 0$.

At this point we remark that, if the corrector v is not periodic, which will be the case in general, it is necessary for the above argument to work as well as for the uniqueness of $\bar{F}(P)$ to obtain correctors which are strictly subquadratic at infinity. This is not always possible: see Lions and Souganidis (2003).

We also remark that the approach described above can be used to study the homogenization of several variants of (4.8), including completely degenerate (Hamilton–Jacobi) equations.

¹ This argument, which is non-rigorous since ψ is not necessarily smooth, can be justified using arguments from the theory of viscosity solutions.

5. The random setting

In this section we outline several recent developments to the theory of fully nonlinear first- and second-order partial differential equations in stationary ergodic settings. The general problem is the almost sure (a.s. for short) behaviour, as $\varepsilon \rightarrow 0$, of the solution of u^ε of equations of the general form

$$\begin{cases} F\left(D^2u^\varepsilon, \varepsilon D^2u^\varepsilon, Du^\varepsilon, u^\varepsilon, x, \frac{x}{\varepsilon}, \omega\right) = 0 & \text{in } U, \\ u^\varepsilon = g & \text{on } \partial U, \end{cases} \quad (5.1)$$

where F and g satisfy all the necessary assumptions for (5.1) to have, for each $\varepsilon > 0$ and $\omega \in \Omega$, the underlying probability space, a unique viscosity solution $u^\varepsilon(\cdot, \omega) \in C(\bar{U})$. The key assumptions for the homogenization are that

$$F \text{ is stationary with respect to } (y, \omega), \quad (5.2)$$

and

$$\begin{cases} \text{the underlying measure-preserving transformation} \\ \tau_y : \Omega \rightarrow \Omega \text{ is ergodic.} \end{cases} \quad (5.3)$$

Recall that a random field ξ is stationary if, for any finite set of points $x_1, \dots, x_k \in \mathbb{R}^d$ and any $h \in \mathbb{R}^d$, the distribution of the random vector

$$\xi(x_1 + h), \dots, \xi(x_k + h)$$

does not depend on h . If $\xi : \mathbb{R}^d \times \Omega \rightarrow \mathbb{R}$ is a stationary random field, where (Ω, μ) is the underlying probability space, then it can be represented in the form

$$\xi(x, \omega) = \tilde{\xi}(\tau_x \omega),$$

for some fixed random variable $\tilde{\xi} : \Omega \rightarrow \mathbb{R}$ and a measure-preserving transformation $\tau_x : \Omega \rightarrow \Omega$ with $x \in \mathbb{R}^d$.

A measure-preserving transformation $(\tau_x)_{x \in \mathbb{R}^d}$ is ergodic if all translation-invariant subsets of Ω have probability either zero or one. We shall also say that a stochastic process is stationary ergodic if it is stationary and the measure-preserving group is ergodic.

Stationary ergodic media are rather general. The classical periodic and almost periodic settings can be thought of as special cases. But the general setting includes other configurations, such as random chessboards with tiles of arbitrary random size.

The goal is to show that there exists an effective first- or second-order (depending only on the particular form of F in (5.1)) nonlinearity \bar{F} such

that, if $u_0 \in C(\bar{U})$ solves

$$\begin{cases} \bar{F}(D^2u_0, Du_0, u_0, x) = 0 & \text{in } U, \\ u_0 = g & \text{on } \partial U, \end{cases} \quad (5.4)$$

then, as $\varepsilon \rightarrow 0$ and a.s. in ω , $u^\varepsilon(\cdot, \omega) \rightarrow u_0$.

We recall that most of the results in periodic homogenization are based on the fact that it is possible to solve the associated macroscopic (cell) problem. In the almost periodic and random settings the macroscopic problem is set in the whole space. The inherited lack of compactness then creates several difficulties. In the almost periodic case these difficulties can be overcome using the fact that such a setting is essentially compact. Exact solutions of the macroscopic cell problems can be replaced by approximate ones (see Ishii (1999), Lions and Souganidis (2005a)). The situation is, however, quite different in the random setting. In general, it is not possible to solve either exactly or approximately the macroscopic problem. To overcome this very serious difficulty, it is necessary to develop and follow a different strategy which makes use of the ergodic theorem and its nonlinear version (the sub-additive ergodic theorem).

Papanicolaou and Varadhan (1979, 1981), Kozlov (1985), Zhikov (1993) and Yurinskii (1980, 1982) (see also Jikov *et al.* (1991)) were the first to consider the problem of homogenizing linear, uniformly elliptic/parabolic operators. The first nonlinear result in the variational setting was obtained by Dal Maso and Modica (1986). The homogenization of fully nonlinear, convex, first-order (Hamilton–Jacobi) equations was considered in Souganidis (1999) and Rezakhanlou and Tarver (2000). Lions and Souganidis (2005a) studied the homogenization of, possibly degenerate, viscous Hamilton–Jacobi equations and Kosygina *et al.* (2006) considered the same problem but in the uniformly elliptic/parabolic setting. Lions and Souganidis (2003, 2005a) showed that the associated macroscopic problems do not have solutions. The homogenization of fully nonlinear, uniformly elliptic equations was studied by Caffarelli *et al.* (2005). Finally, Caffarelli and Souganidis (2008) recently obtained uniform error estimates for the homogenization of uniformly elliptic problems, which are described in Section 6.

The first problem we consider here is the viscous Hamilton–Jacobi equation

$$-\varepsilon \operatorname{tr} A\left(\frac{y}{\varepsilon}, \omega\right) D^2u^\varepsilon + H\left(Du^\varepsilon, \frac{x}{\varepsilon}, \omega\right) + u^\varepsilon = 0 \quad \text{in } \mathbb{R}^d, \quad (5.5)$$

where

$$\begin{cases} A(\cdot, \omega) \in C(S^d) \quad \text{and} \quad H(\cdot, \cdot, \omega) \in C(\mathbb{R}^d \times \mathbb{R}^d) \\ \text{are stationary ergodic} \end{cases} \quad (5.6)$$

and

$$A \text{ is degenerate elliptic and } H \text{ is coercive and convex.} \quad (5.7)$$

Since A is assumed to be degenerate elliptic, the next theorem yields as a special case the homogenization of Hamilton–Jacobi equations of the form

$$H\left(Du^\varepsilon, \frac{x}{\varepsilon}, \omega\right) + u^\varepsilon = 0 \text{ in } \mathbb{R}^d. \quad (5.8)$$

The main result is as follows.

Theorem 5.1. There exists $\bar{H} \in C(\mathbb{R}^d)$ coercive and convex such that, if u_0 is the solution of $u_0 + \bar{H}(Du_0) = 0$ in \mathbb{R}^d , then, as $\varepsilon \rightarrow 0$ and a.s., $u^\varepsilon(\cdot, \omega) \rightarrow u_0$ in $C(\mathbb{R}^d)$. Moreover,

$$\bar{H}(p) = \inf_{\phi \in \mathcal{S}} \sup_y [-\varepsilon \operatorname{tr} A(y, \omega) D^2 \phi + H(D\phi + p, y, \omega)],$$

where \mathcal{S} is the set of continuous random fields ψ that are a.s. strictly sub-linear at infinity.

The proof of the theorem in Lions and Souganidis (2005a) is based strongly on the (stochastic) control interpretation of (5.6), which is available due to the assumptions that H is convex and A independent of Du , and the use of the (sub-additive) ergodic theorem. For $A = I$ another proof and different formula for \bar{H} were obtained in Kosygina *et al.* (2006). For general A , even completely degenerate, this formula is generalized in Lions and Souganidis (2005b). It should be noted that convexity plays absolutely no role in the periodic/almost periodic settings. What happens without convexity in the random setting is an open problem. Recently Lions and Souganidis (2008) obtained a simple proof of Theorem 5.2 which, although it relies on the convexity of H , does not use the control interpretation at all.

Consider next the boundary value problem

$$\begin{cases} F\left(D^2 u^\varepsilon, Du^\varepsilon, x, \frac{x}{\varepsilon}, \omega\right) = 0 & \text{in } U, \\ u^\varepsilon = g & \text{on } \partial U, \end{cases} \quad (5.9)$$

where

$$F \text{ is stationary ergodic and uniformly elliptic.} \quad (5.10)$$

The main result obtained in Caffarelli *et al.* (2005) is as follows.

Theorem 5.2. There exists a uniformly elliptic $\bar{F} \in C(S^d)$ such that, if $u_0 \in C(\bar{U})$ is the solution of $\bar{F}(D^2 u_0, x) = 0$ in U and $u_0 = g$ on ∂U , then, as $\varepsilon \rightarrow 0$, and a.s. in ω , $u^\varepsilon(\cdot, \omega) \rightarrow u_0$ in $C(\bar{U})$.

Moreover, for each $(P, x) \in S^d \times U$,

$$F(P, x) = \lim_{R \rightarrow \infty} \inf_{\psi} \sup_{|y| \leq R} F(D^2\psi, x, y, \omega),$$

with the infimum taken over functions which are strictly subquadratic at infinity.

The proof of Theorem 5.2 is completely different from that of Theorem 5.1. It is based on identifying, for each level $\mu \in \mathbb{R}$, all the matrices $P \in C(S^D)$ such that $\bar{F}(P) \leq \mu$ or $\bar{F}(P) \geq \mu$. This is accomplished using the obstacle problem with quadratic obstacles and studying the ergodic properties of the contact set.

6. Rates of convergence

We describe here a number of results concerning rates of convergence for the homogenization of first- and second-order equations.

We begin with periodic Hamilton–Jacobi equations and, in particular, the problem

$$u^\varepsilon + H\left(Du^\varepsilon, \frac{x}{\varepsilon}, x\right) = 0 \quad \text{in } \mathbb{R}^d. \quad (6.1)$$

The following result was proved by Capuzzo-Dolcetta and Ishii (2001).

Theorem 6.1. Assume that H is convex, coercive and periodic and let $u^\varepsilon, u_0 \in C^{0,1}(\mathbb{R}^N)$ be the solutions of (6.1) and the homogenized equation, respectively. There exists a constant $C > 0$, depending only on H , such that

$$|u^\varepsilon - u_0| \leq C \varepsilon^{1/3}.$$

The rate of convergence for the periodic homogenization of

$$\begin{cases} F\left(D^2u^\varepsilon, \frac{x}{\varepsilon}\right) = f & \text{in } U, \\ u^\varepsilon = g & \text{on } \partial U, \end{cases} \quad (6.2)$$

was obtained recently by Caffarelli and Souganidis (2008).

Theorem 6.2. Assume that F is uniformly elliptic and periodic and let $u^\varepsilon \in C(\bar{U})$ and $u_0 \in C^{0,1}(\bar{U})$ be, respectively, the solutions of the oscillating and homogenized equations. There exist $\alpha \in (0, 1)$ depending on the ellipticity constants and the dimension, and $C > 0$ depending, in addition, on the Lipschitz constant of u_0 , such that

$$|u^\varepsilon - u_0| \leq C \varepsilon^\alpha \quad \text{in } \bar{U}.$$

The proof of Theorem 6.1 is based on classical arguments from the theory of viscosity solutions, while Theorem 6.2 is based on a general methodology, developed in Caffarelli and Souganidis (2007), which is based on regularity results concerning viscosity solutions of uniformly elliptic PDEs and the notion of δ -viscosity solutions.

We turn now to the random setting. Here it is necessary to introduce a *rate of mixing* somewhere in the assumptions. To this end, we assume that the nonlinearity F is strongly mixing with algebraic rate, *i.e.*, we assume that

$$\left\{ \begin{array}{l} \text{there exists } \phi : [0, \infty) \rightarrow [0, \infty) \text{ such that } \phi(r)r^{-\alpha} \rightarrow 0 \\ \text{for some } \alpha > 0 \text{ and for all } P \in S^d \text{ and } x, y \in \mathbb{R}^d \\ |E(F(P, x, \cdot)F(P, y, \cdot)) - (EF(P, x, \cdot))(EF(P, y, \cdot))| \\ \leq \phi(|x - y|)(EF^2(P, x, \cdot))^{1/2}(EF^2(P, y, \cdot))^{1/2}, \end{array} \right. \quad (6.3)$$

where E denotes the expectation in the probability space.

The following result on the linear equation

$$\left\{ \begin{array}{l} -a_{ij} \left(\frac{x}{\varepsilon}, \omega \right) u_{x_i x_j}^\varepsilon = f \text{ in } U, \\ u^\varepsilon = g \text{ on } \partial U, \end{array} \right. \quad (6.4)$$

was proved in Yurinskii (1982).

Theorem 6.3. Assume that the matrix $A = (a_{ij})_{1 \leq i, j \leq d}$ is uniformly elliptic, stationary and strongly mixing. Let u^ε, u_0 be the solutions of (6.4) and the homogenized equation respectively. There exist $\alpha \in (0, 1)$, depending only on the ellipticity constant, and $C > 0$ depending on the ellipticity constants and the Lipschitz constant of u_0 , such that

$$|u^\varepsilon - u_0| \leq C \varepsilon^\alpha \text{ on } \bar{U}.$$

Finally, concerning the fully nonlinear equation

$$\left\{ \begin{array}{l} F \left(D^2 u^\varepsilon, \frac{x}{\varepsilon}, \omega \right) = f \text{ in } U, \\ u^\varepsilon = g \text{ on } \partial U, \end{array} \right. \quad (6.5)$$

the following was proved in Caffarelli and Souganidis (2008).

Theorem 6.4. Assume that F is uniformly elliptic, stationary and strongly mixing with algebraic rate. Let $u^\varepsilon \in C(\bar{U})$ and $u_0 \in C^{0,1}(\bar{U})$ be the solutions of (6.5) and the homogenized equation, respectively. There exist

positive constants C and c depending on the ellipticity, the Lipschitz constant of F , the dimension, the mixing rate and F , but not ε , such that, for all $\varepsilon \in (0, 1)$, there exist $A_\varepsilon \subset \Omega$ such that

$$\mu(A_\varepsilon) \leq C \varepsilon^{c|\ln \varepsilon|^{-1/2}} \quad \text{and} \quad |u^\varepsilon - u_0| \leq C \varepsilon^{c|\ln \varepsilon|^{-1/2}} \quad \text{in } \Omega \setminus A_\varepsilon.$$

7. Applications

We briefly discuss here a few applications of the homogenization results presented earlier.

The first application concerns motion of interfaces in random media. A typical problem is the evolution of the boundary Γ_t of an open subset Ω_t of \mathbb{R}^N with velocity V in the direction of the normal vector n given by

$$V = -\varepsilon \delta \operatorname{tr} Dn + v\left(n, \frac{x}{\varepsilon}\right).$$

Using the level set formulation for generalized front propagation, the problem reduces to the study of the a.s. behaviour, as $\varepsilon \rightarrow 0$, of the solution $u^\varepsilon(\cdot, \omega)$ of the corresponding level set PDE:

$$\begin{cases} u_t^\varepsilon - \varepsilon \delta \operatorname{tr}(I - \widehat{Du}^\varepsilon \otimes \widehat{Du}^\varepsilon) D^2 u^\varepsilon + v\left(\widehat{Du}^\varepsilon, \frac{x}{\varepsilon}, \omega\right) |Du^\varepsilon| = 0 \\ \quad \text{in } \mathbb{R}^N \times (0, \infty), \\ u^\varepsilon = u_0 \quad \text{on } \mathbb{R}^N \times \{0\}, \end{cases} \quad (7.1)$$

where $\Omega_0 = \{u_0 > 0\}$ and, for $p \in \mathbb{R}^N \setminus \{0\}$, $\hat{p} = |p|^{-1}p$.

There is no known result in the random case for (7.1) if $\delta \neq 0$. The reason is that, in view of the dependence on the gradient, the results of Lions and Souganidis (2005b) do not apply here. The behaviour of (7.1) for $\delta > 0$ in the periodic/almost periodic setting was analysed in Lions and Souganidis (2005b). More recently, Cardaliaguet, Lions and Souganidis (2008) looked at special cases of (7.1) and studied in detail what happens when the assumptions of Lions and Souganidis (2005b) are not satisfied. Finally, some related results were obtained by Dirr, Karali and Yip (2007).

The only known result in the random case obtained in Souganidis (1999) and Lions and Souganidis (2003) is as follows.

Theorem 7.1. Let $\delta = 0$. Assume that the map $p \mapsto v(\hat{p}, y)|p|$ is convex and $|v| \geq v_0 > 0$. There exists a convex $\bar{H} \in C(\mathbb{R}^N)$ such that, if $u_0 \in UC(\mathbb{R}^N \times [0, \infty))$ is the unique solution of $u_0 + \bar{H}(Du_0) = 0$ in $\mathbb{R}^N \times [0, \infty)$, then, as $\varepsilon \rightarrow 0$ and a.s. in ω , $u^\varepsilon(\cdot, \omega) \rightarrow u_0$ in $C(\mathbb{R}^N \times [0, \infty))$. In particular, as $\varepsilon \rightarrow 0$, and a.s. in ω , $\Gamma_t^\varepsilon \rightarrow \Gamma_t^0$ in the Hausdorff metric, where Γ_t^0 is moving with normal velocity $V = -\bar{H}(n)$.

An interesting question is what happens when the velocity v vanishes and changes sign. Mathematically this is a very challenging problem, since the positivity of v is critical, at the technical level, for obtaining the necessary estimates.

The typical problem is the equation

$$\begin{cases} u_t^\varepsilon + v\left(\frac{x}{\varepsilon}\right)|Du^\varepsilon| = 0 & \text{in } \mathbb{R}^d \times (0, \infty), \\ u^\varepsilon = g & \text{on } \mathbb{R}^d, \end{cases} \quad (7.2)$$

which is the level set PDE giving the evolution of $\Omega_0 = \{x \in \mathbb{R}^d : u_0(x) > 0\}$ with normal velocity

$$V = v\left(\frac{x}{\varepsilon}\right).$$

As far as the velocity v is concerned we assume that

$$v \text{ is } Y\text{-periodic and changes sign.} \quad (7.3)$$

The following was proved in Cardaliaguet *et al.* (2008). We refer to Craciun and Bhattachayra (2003) for related numerical results.

Theorem 7.2. Assume (7.3). Then, for every $R, T > 0$, as $\varepsilon \rightarrow 0$, we have $u^\varepsilon \rightarrow u_0$, and

$$u^\varepsilon \rightarrow u_0 = \theta g + (1 - \theta)u_1,$$

in the weak $*$ convergence sense in $L^\infty(B_R \times (\theta, T))$, where $\theta = |\{v < 0\} \cap Y|$ and u_1 is the solution of the homogenized equation with velocity v^+ .

The heuristics behind the result is that the front cannot penetrate the $\{v < 0\}$ region while it keeps propagating in all places. As a result it wraps around $\{v = 0\}$ and eventually keeps going ‘leaving a piece behind’. This latter phenomenon is characterized by the weak convergence.

The next example is about large deviations of diffusion processes in random environments. This is a very general topic, which cannot be discussed in any generality here. Instead we present a special case. Giving any references is beyond the scope of this paper.

Consider the diffusion process $(X_t^\varepsilon)_{t \geq 0}$ which evolves according to the SDE

$$\begin{cases} dX_t^\varepsilon = b\left(\frac{X_t^\varepsilon}{\varepsilon}, \omega\right) + \sqrt{2\varepsilon}\Sigma\left(\frac{X_t^\varepsilon}{\varepsilon}, \omega\right) dB_t & (t > 0), \\ X_0^\varepsilon = x, \end{cases}$$

where $(B_t)_{t \geq 0}$ is a standard M -dimensional Brownian motion on a different probability space (Ω_0, F_0, P_0) , b is a Lipschitz-continuous stationary ergodic vector field and Σ is a Lipschitz-continuous and stationary ergodic $d \times M$ matrix.

The medium is modelled by the stationary ergodic potential $V : \mathbb{R}^d \times \Omega \rightarrow [0, \infty)$ and the behaviour of the diffusion is governed by the weighted probability

$$Q_{t,\omega}^\varepsilon(d\omega_0) = S_{t,\omega}^{-1} \exp \left\{ -\varepsilon^{-1} \int_0^t V \left(\frac{X_s^\varepsilon}{\varepsilon}, \omega \right) \right\} P_0(d\omega_0),$$

where $S_{t,\omega}$ is a normalizing factor.

To formulate a typical large-deviation result it is necessary to consider, for $v_0 \in BUC(\mathbb{R}^N)$, the initial value problem

$$\begin{cases} v_t^\varepsilon - \varepsilon \operatorname{tr}(\Sigma \Sigma^T) \left(\frac{x}{\varepsilon}, \omega \right) D^2 v^\varepsilon + H(Du^\varepsilon, \frac{x}{\varepsilon}, \omega) = 0 & \text{in } \mathbb{R}^N \times (0, \infty), \\ v^\varepsilon = v_0 & \text{on } \mathbb{R}^N \times \{0\}, \end{cases}$$

where, for $(p, y, \omega) \in \mathbb{R}^N \times \mathbb{R}^N \times \Omega$,

$$H(p, y, \omega) = \operatorname{tr}((\Sigma \Sigma^T)(y, \omega) p \otimes p) - b(y, \omega) \cdot p - V(y, \omega). \quad (7.4)$$

Theorem 5.1 applied to this equation yields the existence of $\bar{H} : \mathbb{R}^N \rightarrow \mathbb{R}$ such that, if $\bar{v} \in BUC(\mathbb{R}^N \times [0, \infty))$ solves $\bar{v}_t + \bar{H}(D\bar{v}) = 0$ in $\mathbb{R}^N \times [0, \infty)$ with $\bar{v} = v_0$ on \mathbb{R}^N , then, as $\varepsilon \rightarrow 0$ and a.s. in ω , $v^\varepsilon \rightarrow \bar{v}$ in $C(\mathbb{R}^N)$.

As a consequence the following large-deviation principle holds.

Theorem 7.3. Let \bar{L} be the convex dual of the effective Hamiltonian \bar{H} corresponding to (7.4). For any Borel subset A of \mathbb{R}^N with interior A^0 and a.s. in ω ,

$$\begin{aligned} -t \inf_{A^0} \bar{L}(t^{-1}(x - y)) &\leq \liminf_{\varepsilon \rightarrow 0} \varepsilon \log Q_{t,\omega}(X_t^\varepsilon \in A) \\ &\leq \limsup_{\varepsilon \rightarrow 0} \varepsilon \log Q_{t,\omega}(X_t^\varepsilon \in A) \leq -t \inf_{y \in A} [\bar{L}(t^{-1}(x - y)).] \end{aligned}$$

Another application is related to combustion and the propagation of fronts arising as asymptotic limits of reaction–diffusion equations in a random environment. The particular problem of interest is the a.s. asymptotics, as $\varepsilon \rightarrow 0$, of the solution u^ε of the KPP-type equation

$$\begin{cases} u_t^\varepsilon - L^\varepsilon u^\varepsilon = \varepsilon^{-1} f \left(u^\varepsilon, \frac{x}{\varepsilon}, \omega \right) & \text{in } \mathbb{R}^N \times (0, T), \\ u^\varepsilon = g & \text{on } \mathbb{R}^N \times \{0\}. \end{cases}$$

Here L^ε is a general second-order uniformly elliptic operator

$$L^\varepsilon v = -\varepsilon \operatorname{tr} A \left(\frac{x}{\varepsilon}, \omega \right) D^2 v + b \left(\frac{x}{\varepsilon}, \omega \right) \cdot Dv,$$

with $A(\cdot, \omega) \in C^{0,1}(S^d)$ and $b(\cdot, \omega) \in C^{0,1}(\mathbb{R}^d)$ stationary ergodic and $f(\cdot, \cdot, \omega) \in C^{0,1}(\mathbb{R} \times \mathbb{R}^d)$.

The nonlinearity f is assumed to be of KPP-type, *i.e.*,

$$\begin{cases} f(0, y, \omega) = f(1, y, \omega) = 0, \quad f(u, y, \omega) > 0 \quad \text{if } u \in (0, 1), \quad \text{and} \\ f(u, y, \omega) \leq c(y, \omega)u \quad \text{with } c(y, \omega) = f_u(0, y, \omega). \end{cases}$$

Theorem 7.4. There exists \bar{H} such that, as $\varepsilon \rightarrow 0$ and a.s. in ω , locally uniformly in $\mathbb{R}^N \times (0, \infty)$ and exponentially fast,

$$u^\varepsilon(x, t, \omega) \rightarrow \begin{cases} 1 & \text{in int}\{\bar{v} = 0\}, \\ 0 & \text{in } \{\bar{v} > 0\}, \end{cases}$$

where \bar{v} is the unique viscosity solution of the variational inequality

$$\begin{cases} \min[\bar{v}_t + \bar{H}(D\bar{v}, x), \bar{v}] = 0 & \text{in } \mathbb{R}^N \times (0, \infty), \\ \bar{v} = \begin{cases} 0 & \text{in } \{g > 0\}, \\ +\infty & \text{in } \{g < 0\}. \end{cases} \end{cases}$$

We conclude with an example concerning the homogenization of a linear transport equation. Although we did not discuss such equations, we include this discussion here as an example of the fact that the homogenized equation may develop features not existing at the level ε of the oscillations. In particular we present a simple hyperbolic example where the homogenized equation contains an integral term describing a memory effect.

Consider the 2D-linear advection equation

$$u_t^\varepsilon(x, y, t) + a^\varepsilon(y)u_x^\varepsilon(x, y, t) = 0,$$

with initial conditions $u(x, y, 0) = g(x, y)$ and a^ε bounded. This simple model helps in explaining certain fingering effects of flow in layered subsurface reservoirs (Hou 2003)

It is easy to write the solution explicitly,

$$u^\varepsilon(x, y, t) = g(x - a^\varepsilon(y), t, y),$$

but not as simple to derive the homogenized solution for the weak limit u^0 of u^ε .

Using the Laplace transform, Tartar (1989) showed that the weak limit satisfies the initial value problem

$$\begin{aligned} u_t^0 + a(y)u_x^0 &= \int_0^t \int_{-\infty}^\infty \frac{\partial^2}{\partial x^2} u^0(x - \lambda(t - s), y, s) \, d\mu_y(\lambda) \, ds, \\ u^0(x, y, 0) &= g(x, y), \end{aligned}$$

where $a(y)$ is the weak limit of $a^\varepsilon(y)$ and μ_y is the Young measure of $a^\varepsilon(y)$, as $\varepsilon \rightarrow 0$.

8. Numerical homogenization

Very often there is no known closed form of the homogenized or effective equations but we may still be in a situation where such an equation exists. The option is then to use numerical techniques to generate the homogenized equation or the effect of using a homogenized equation. The goal would typically be that of numerically solving a differential equation, which involves a wide range of scales. If the range of scales is very large the computational cost of direct numerical solution is prohibitive and some approximation is needed.

Let us briefly comment on the computational complexity. Consider a differential equation with the size of the domain of the independent variables of order one. Let the problem be of the type discussed in this paper, where material fluctuations with wave length $O(\varepsilon)$ produce a solution that also has oscillations with wave length $O(\varepsilon)$.

We also know from the asymptotic analysis of the earlier sections that the detailed interaction of oscillations is essential for the structure of the homogenized equation. This means that a direct numerical method must accurately represent the oscillations. From the Shannon sampling theorem (Shannon 1949), we then see that the number of unknowns must at least be of order $O(\varepsilon^{-d})$, where d is the dimension of the space of independent variables.

There are basically four classes of numerical multi-scale methods:

- (1) the classical numerical multi-scale methods that aim to solve the full problem efficiently,
- (2) generation of the effective equation by numerical solutions of cell problems,
- (3) techniques that start from the original full problem and generate a reduced model,
- (4) methods that on the finest scale only sample the original problem in order to reduce the overall computational complexity.

In class (1) we have, for example, the well-established methods of multi-grid and the fast multi-pole method. The discretized full problem with all scales is solved efficiently such that the computational cost is essentially proportional to the number of unknowns. There is a weak relation to homogenization in multi-grid methods in that the coarse-grid operator should approximate the homogenized differential equation (Engquist and Luo 1997). For the fast multi-pole method the far-field interaction is described by low-dimensional operators for which averaging plays a role. These methods are, however, not as closely related to homogenization as the methods we will focus on, and they will not be further discussed here.

For class (2) we assume it is known that there exists a homogenized equation based on the solution of cell problems. If there is no explicit formula for the cell problem solution it is natural to approximate that solution numerically. If the material properties are periodic this technique obviously applies. For more general settings it is still practically useful, as in the work of Durlafsky on homogenization or upscaling in oil reservoir modelling. See, for example, the discussion in Durlafsky (1998). The computational domain is divided into subdomains and a local cell problem is solved in each subdomain. The cell problems are solved by fine discretizations that resolve any oscillation and the solution is then used to define a global effective equation, which can be solved numerically on a coarser grid.

In class (3) the computational cost is at least as large as in (1), but the goal is now to generate a simplified problem that can then efficiently be solved many times. This simplified problem can have significance in itself or it can be used, for example, in control applications. The so-called model reduction techniques belong to this class.

A typical model reduction problem starts by a system of ordinary differential equations describing the state $x(t)$ and output $y(t)$ for a given input or control signal $u(t)$:

$$\begin{aligned} \frac{dx(t)}{dt} &= Ax(t) + Bu(t), & x \in \mathbb{R}^n, u \in \mathbb{R}^m \\ y(t) &= Cx(t) + Du(t), & y \in \mathbb{R}^p, n \gg m, p. \end{aligned}$$

The $n \times n$ matrix A is assumed to be very large and the goal is to replace this system with a reduced one. The reduced system should have a much lower dimension n but approximately the same relation between u and y for a relevant set of u -values. The large size of A typically originates from a discretization of a differential operator in space that may describe a multi-scale problem of the type discussed in this paper. For this type and related problems there is extensive literature: see, for example, Obinata and Anderson (2001).

The multi-scale finite element method (MSFEM) also belongs to this class. It was originated by Babuška (see, for example, Babuška, Caloz and Osborn (1994)), and further refined by Hou (see, for example, Hou (2003)). In this approach a numerical cell problem is not used to determine an effective equation but to generate new finite element basis functions. These basis functions cover a domain of several oscillations. Hou and others have successfully applied MSFEM to oil reservoir modelling problems (Hou 2003).

Projection-based numerical homogenization, which is briefly discussed in the next section, is another technique that belongs to this class.

In class (4) the computational cost for direct solution of the full problem is too large and resolution of the finest scale can only be done in selected

domains. The heterogeneous multi-scale method, or HMM (Engquist *et al.* 2007), is a framework for this class, and HMM is presented in Section 10. Another similar strategy is the equation-free technique by Kevrekidis *et al.* (2003). Both these methods rely on refined numerical approximation over sampled domains.

It should be pointed out that there is a strong similarity between the analytical homogenization described in the earlier sections and some of the numerical methods below. For example, projection-based numerical homogenization uses averaging, and adds a high-frequency correction term. The solution of cell problems is central to the heterogeneous multi-scale method and to some of the methods briefly mentioned above.

9. Projection-based numerical homogenization

In projection-based homogenization the fully discretized problem is projected onto a lower-dimensional space. The number of unknowns will be lower and the relevant operator condensed. Early work along these lines using wavelets were presented in Beylkin and Brewster (1995), Dorobantu and Engquist (1998) and Gilbert (1998), but we will follow the development as given in Andersson, Engquist, Ledfelt and Runborg (1999) and Engquist and Runborg (2001, 2001). Consider first the simple two-point boundary value problem that was introduced in Section 1,

$$\begin{cases} -(a^\varepsilon(x)u_x^\varepsilon)_x = f & \text{in } (0, 1), \\ u^\varepsilon(0) = u^\varepsilon(1) = 0, \end{cases} \quad (9.1)$$

$$a^\varepsilon(x) = a(x/\varepsilon) > 0, \quad a(y) \text{ is 1-periodic.}$$

Let us approximate this problem by centred divided differences,

$$L_h^\varepsilon u_h^\varepsilon = \frac{1}{h} \left(a^\varepsilon(x_{j+1/2}) \frac{u_{j+1} - u_j}{h} - a^\varepsilon(x_{j-1/2}) \frac{u_j - u_{j-1}}{h} \right) = f_h, \quad (9.2)$$

for $j = 1, 2, \dots, J-1$,

where $u_0 = u_J = 0$ and

$$x_j = jh, \quad j = 0, 1, \dots, J \quad \text{and} \quad Jh = 1.$$

Here

$$u_{\varepsilon,h} = (u_1, u_2, \dots, u_{J-1})^T \quad \text{and} \quad f_h = (f(x_1), f(x_2), \dots, f(x_{J-1}))^T,$$

and the linear operator $L_{\varepsilon,h}$ can be viewed as a finite difference operator or as a $(J-1) \times (J-1)$ matrix.

Our goal, as in general model reduction, is to transform (9.2) into a lower-dimensional problem that is easier to solve. In the example above the best way would be to use the homogenized equation (9.1) and discretize that.

The stepsize h could then be chosen without consideration of the small wave length ε in the oscillations.

In general we do not have access to an explicit homogenized form of the equation and a fully numerical process is needed. We first outline a projection process for homogenization of the original ∞ -dimensional problem that easily can be adjusted to finite-dimensional applications, for example of the form (9.2).

Consider an equation $Lu = f$ where L is a linear operator, f a right-hand side and u a solution that contains fine scales. Let P be a projection operator onto a subspace where the fine scales in the original solution do not exist. Our objective is to find the (projection-generated) *homogenized* operator \bar{L} such that $\bar{L}Pu = f$ for all f such that $Pf = f$. (When $Pf \neq f$ we also need to find the homogenized right-hand side \bar{f} .) We confine ourselves to the case of Hilbert spaces.

Let X be a Hilbert space of functions, typically a Sobolev space. Let $X_0 \subset X$ be a closed subspace representing the coarse part of the functions, and denote by P_x the orthogonal (and symmetric) projection operator in X onto X_0 . Let the spaces X_0 and X_0^\perp inherit the inner product and norm of X , so that $\|u\|_X = \|u\|_{X_0}$ and $(u, v)_X = (u, v)_{X_0}$ when $u, v \in X_0$, and similarly for X_0^\perp . In addition, set $Q_x = I_x - P_x$, where I_x is the identity operator in X , and introduce the unitary operator \mathcal{W}_x on X defined by

$$\mathcal{W}_x : X \mapsto X_0^\perp \times X_0, \quad \mathcal{W}_x u = \begin{pmatrix} Q_x u \\ P_x u \end{pmatrix}. \quad (9.3)$$

In the same way, define the corresponding operators P_y , Q_y and \mathcal{W}_y for another Hilbert space Y with subspace Y_0 . Let $\mathcal{L}(X, Y)$ be the set of bounded linear maps from X to Y . For an operator $L \in \mathcal{L}(X, Y)$, we have

$$\begin{aligned} \mathcal{W}_y L \mathcal{W}_x^* \begin{pmatrix} u \\ v \end{pmatrix} &= \mathcal{W}_y L (P_x + Q_x)(u + v) = \begin{pmatrix} Q_y L (P_x + Q_x)(u + v) \\ P_y L (P_x + Q_x)(u + v) \end{pmatrix} \\ &= \begin{pmatrix} Q_y L (P_x v + Q_x u) \\ P_y L (P_x v + Q_x u) \end{pmatrix} \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \end{aligned} \quad (9.4)$$

where

$$\begin{aligned} A &= Q_y L Q_x \in \mathcal{L}(X_0^\perp, Y_0^\perp), & B &= Q_y L P_x \in \mathcal{L}(X_0, Y_0^\perp), \\ C &= P_y L Q_x \in \mathcal{L}(X_0^\perp, Y_0), & D &= P_y L P_x \in \mathcal{L}(X_0, Y_0). \end{aligned} \quad (9.5)$$

When A is invertible the following definition can be stated.

Definition 9.1. Suppose $L \in \mathcal{L}(X, Y)$ and $f \in Y$. When A in (9.4), (9.5) is invertible (one-to-one and onto), we define the *homogenized* operator $\bar{L} : X_0 \mapsto Y_0$ as the Schur complement with respect to the decomposition in (9.4),

$$\bar{L} = D - CA^{-1}B, \quad (9.6)$$

and the homogenized right-hand side as

$$\bar{f} = P_y f - CA^{-1}Q_y f. \quad (9.7)$$

We will write \bar{L}_{X,X_0} and \bar{f}_{X,X_0} when there is a need to display explicitly between which spaces the homogenization step is made. From Definition 9.1 we immediately have the following result.

Lemma 9.2. Suppose $Lu = f$, where $L \in \mathcal{L}(X, Y)$, $u \in X$ and $f \in Y$. If A^{-1} exists,

$$\bar{L}P_x u = \bar{f}. \quad (9.8)$$

Proof. Since $Lu = f$, we get

$$\mathcal{W}_y L \mathcal{W}_x^* \mathcal{W}_x u = \mathcal{W}_y f \Rightarrow \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} Q_x u \\ P_x u \end{pmatrix} = \begin{pmatrix} Q_y f \\ P_y f \end{pmatrix}. \quad (9.9)$$

Moreover, since A is invertible, this system can be reduced with Gaussian elimination. It yields (9.8). \square

The homogenized operator expressed in terms of projections takes the form

$$\bar{L} = D - CA^{-1}B = PLP - PLQ(QLQ)^{-1}QLP.$$

In the elliptic case, there is a striking similarity between the Schur complement in Definition 9.1 and the classical homogenized operator in (2.18), repeated here for convenience:

$$PLP - PLQ(QLQ)^{-1}QLP, \quad (9.10)$$

$$\nabla \left(\int_{I_d} G(y) dy \right) \nabla - \nabla \left(\int_{I_d} G(y) \frac{d\chi(y)}{dy} dy \right) \nabla. \quad (9.11)$$

Both are written as the average of the original operator minus a correction term, which is computed in a similar way for both operators. For the analytic case, a local elliptic cell problem is solved to get $G\partial_y\chi$, while in the projection case, a positive operator $A = QLQ$ defined on a subspace is inverted to obtain $LQA^{-1}B$. The average over the terms is obtained by integration in the analytical case, and by applying P in the projection case.

In the practical and computational setting L and u are finite-dimensional as in the model problem (9.2). A natural way to define the projections discussed above is to use a wavelet basis. Discrete and coarse scales are well defined and the localization properties of wavelets are also practical (Beylkin and Brewster 1995, Engquist and Runborg 2001). In the definition of \bar{L} above, B , C and D are sparse matrices approximating differential operators. The matrix A^{-1} is dense but well approximated by a sparse matrix (Beylkin, Coifman and Rokhlin 1991). This means that \bar{L} is an approximation of a sparse matrix and can be seen as a numerical homogenization.

10. The heterogeneous multi-scale method

The heterogeneous multi-scale method (HMM) is a framework for developing and analysing numerical techniques that couple different models with different ranges of scales in the same simulation. It was first introduced by E and Engquist (2003a). See also the shorter and less technical presentation in E and Engquist (2003b) and the more extensive survey in Engquist *et al.* (2007).

Let us turn to the structure of HMM. The general setting is as follows. We are given a microscopic system whose state variable is denoted by u , together with a micro-model, which can be abstractly written as

$$f(u, d) = 0, \quad (10.1)$$

where d is the data given by auxiliary conditions, such as initial and boundary conditions for the problem. We are not interested in the microscopic details of u , but rather the macroscopic state of the system, which we denote by U . It satisfies some abstract macroscopic equation:

$$F(U, D) = 0, \quad (10.2)$$

where D stands for the macroscopic data that are necessary for the model to be complete. We could here view (10.1) as the original problem with an ε -scale and view (10.2) as the effective or homogenized equation. Note that F does not need to be known.

Let Q denote the compression operator that maps u to U , and let R be any operator that reconstructs u from U , that is,

$$Qu = U, \quad RU = u. \quad (10.3)$$

Thus Q and R should satisfy $QR = I$, where I is the identity operator. Q is called a compression operator instead of a projection operator since it can be more general than projection, *e.g.*, it can be a general coarse-graining operator, as in bio-molecular modelling. The terminology of reconstruction operator is adopted from Godunov schemes for nonlinear conservation laws (LeVeque 1990) and gas-kinetic schemes (Xu and Prendergast 1994). Compression and reconstruction operators are similar to the projection and prolongation operators used in multi-grid methods, or the restriction and lifting operators in Kevrekidis *et al.* (2003).

Examples of Q and R were in given in E and Engquist (2003a). The goal of HMM is to compute U using the abstract form of F and the micro-scale model. It consists of two main components.

1. Selection of a macroscopic solver

Even though the macroscopic model is not available completely or is invalid on part of the computational domain, any available knowledge of the form of F is used to select a suitable macroscopic solver.

2. *Estimating the missing macro-scale data D using the micro-scale model*

This is typically done in two steps.

- (a) *Constrained micro-scale simulation.* At each point where some macro-scale data are needed, perform a series of constrained microscopic simulations. The micro-scale solution needs to be constrained so that it is consistent with the local macroscopic state, *i.e.*, $d = d(U)$. In practice, this is often the most important technical step.
- (b) *Data processing.* Use the micro-scale data generated from the microscopic simulations to extract the needed macro-scale data.

Data estimation can be performed either ‘on the fly’ or in a pre-processing step. The latter is often advantageous if the needed data depend on very few variables. Before we turn to concrete examples, we should emphasize that HMM is not a specific method: it is a framework for designing methods. For any particular problem, there is usually a considerable amount of work, such as designing the constrained microscopic solvers, that is necessary to turn HMM into a specific numerical method. In the remainder of this section, we will discuss examples of how HMM can be used for some relatively simple problems.

Let us first discuss the elliptic problem of Section 3. Consider the 2D case,

$$\begin{cases} -\left(a_{ij}\left(\frac{x}{\varepsilon}\right)u_{x_j}^\varepsilon\right)_{x_i} = f & \text{in } U, \\ u^\varepsilon = 0 & \text{on } \partial U. \end{cases} \quad (10.4)$$

Here ε is a small parameter that signifies explicitly the multi-scale nature of the coefficients. It is the ratio between the scale of the coefficient and the scale of the computational domain D . Here we present an approach based on the finite volume method. This is a simplified version of the methods presented in Abdulle and E (2003). Similar ideas can also be found in Durlfisky (1991).

As the macro-scale solver, we choose a finite volume method on a macro-scale grid, and we will let $\Delta x, \Delta y$ be the grid size. The grid points are at the centre of the cells, and the fluxes are defined at the boundaries of the cells. The macro-scale scheme is simply that on each cell, the total fluxes are balanced by the total source or sink terms,

$$-J_{i-\frac{1}{2},j} + J_{i+\frac{1}{2},j} - J_{i,j-\frac{1}{2}} + J_{i,j+\frac{1}{2}} = \int_{K_{i,j}} f(x) dx. \quad (10.5)$$

Here K denotes the (i, j) th cell.

The data that need to be estimated are the fluxes. This is done as follows. At each point where the fluxes are needed, we solve the original micro-scale

model (10.4) on a square domain of size δ , with the following boundary condition: $u^\varepsilon(x) - U(x)$ is periodic, where $U(x)$ is a linear function constructed from the macro-state at the two neighbouring cells; *e.g.*, for computing $J_{i+1,j}$, we have

$$U(x, y) = \frac{1}{2}(U_{j,k} + U_{j+1,k}) + \frac{U_{j+1,k} - U_{j,k}}{\Delta x}(x - x_{j+\frac{1}{2}}) + \frac{U_{j+1,k+1} - U_{j,k+1} - (U_{j+1,k-1} - U_{j,k-1})}{4\Delta y}(y - y_k). \quad (10.6)$$

We then use

$$J_{j+\frac{1}{2},k} = \frac{1}{\delta^2} \int_{I_\delta} j_1^\varepsilon dx, \quad J_{j,k+\frac{1}{2}} = \frac{1}{\delta^2} \int_{I_\delta} j_2^\varepsilon dx, \quad U_{j+1,k} - U_{j,k}, \quad (10.7)$$

where $(j_1^\varepsilon(x), j_2^\varepsilon(x)) = (a_{1k}u_{x_k}^\varepsilon, a_{2k}u_{x_k}^\varepsilon)$, to compute an approximation to the needed flux. The periodic boundary condition for the micro-scale problem is not the only choice: other boundary conditions might be used. A more thorough discussion is found in Yue and E (2008). To reduce the influence of the boundary conditions, a weight function can be inserted in (10.7).

To implement this idea, note that the J s are linear functions of $\{U_{i,j}\}$. Therefore to compute the fluxes, we first solve the local problems with U replaced by the nodal basis functions: $\Phi_{\ell,m}$ is the nodal basis function (vector) associated with the (ℓ, m) th cell if $\Phi_{\ell,m}$ is zero everywhere except at the (ℓ, m) th cell where it is 1. For each such basis function, there are only a few local problems that need to be solved, since the basis function vanishes on most cells. Since U can be written as a linear combination of these nodal basis functions, the fluxes corresponding to U can also be written as a linear combination of the fluxes correspond to these nodal basis functions. In this way, (10.5) is turned into a system of linear equations for U .

Now how do we choose δ ? Clearly the smaller the δ , the less costly the algorithm. If the original problem (10.4) has scale separation, *i.e.*, the micro-scale length ε is much smaller than $O(1)$, then we can choose δ such that $\varepsilon \ll \delta \ll 1$. This results in savings of cost for HMM, compared with solving the original micro-scale problem on the whole domain D .

The correctors in the homogenization theory describe the low-frequency contribution from interaction of highly oscillatory functions. That interaction is represented by the micro-scale problems in the δ -domains. There is a natural correspondence to the analytic cell problems.

We chose to use a finite volume method for our standard elliptic equation as the first example because it gives a good background for the following examples: a finite element method for the elliptic equation and a finite volume method for nonlinear conservation laws.

In the finite element approximation of (10.4), the macro-scale solver can be chosen simply as the standard C^0 piecewise linear finite element method

over a macroscopic triangulation \mathcal{T}_H of mesh size H . We will denote by X_H the macroscopic finite element space which could be the standard piecewise linear finite elements over \mathcal{T}_H .

The data that need to be estimated from the micro-scale model are contained in the stiffness matrix on \mathcal{T}_H : $A = (A_{ij})$, where

$$A_{ij} = \int_{\Omega} \nabla \Phi_i(\mathbf{x}) \bar{A}(\mathbf{x}) \nabla \Phi_j(\mathbf{x}) \, d\mathbf{x}. \quad (10.8)$$

Here $\bar{A}(\mathbf{x})$ is the homogenized conductivity tensor and $\{\Phi_i(\mathbf{x})\}$ are the basis functions for X_H . Had we known $\bar{A}(\mathbf{x})$, we could have evaluated A_{ij} simply by numerical quadrature: if $f_{ij}(\mathbf{x}) = \nabla \Phi_i(\mathbf{x}) \bar{A}(\mathbf{x}) \nabla \Phi_j(\mathbf{x})$, then

$$A_{ij} = \int_{\Omega} f_{ij}(\mathbf{x}) \, d\mathbf{x} \simeq \sum_{T \in \mathcal{T}_H} |T| \sum_{\mathbf{x}_k \in T} \omega_k f_{ij}(\mathbf{x}_k), \quad (10.9)$$

where $\{\mathbf{x}_k\}$ and $\{\omega_k\}$ are the quadrature points and weights respectively, while $|T|$ is the area of the element T .

In the absence of explicit knowledge of $\bar{A}(\mathbf{x})$, our problem reduces to the approximation of the values of $\{\bar{A}(\mathbf{x}_k)\}$. This will be done by solving the original micro-scale model locally around each quadrature point $\{\mathbf{x}_k\}$.

Let $I_{\delta}(\mathbf{x}_k) \ni \mathbf{x}_k$ be a square of size δ . Consider

$$-\left(a_{ij} \left(\frac{x}{\varepsilon} \right) \phi_{x_j}^{\varepsilon} \right)_{x_i} = 0, \quad \mathbf{x} \in I_{\delta}(\mathbf{x}_k). \quad (10.10)$$

The main objective is to probe efficiently the micro-scale behaviour under the constraint that the average gradient of the solution ϕ^{ε} is fixed to be a given constant vector. Having solutions to this local problem, we can define the effective conductivity tensor at \mathbf{x}_k by the relation

$$\left\langle A \left(\frac{x}{\varepsilon} \right) \nabla \phi^{\varepsilon} \right\rangle_{I_{\delta}} = \bar{A}(\mathbf{x}_k) \langle \nabla \phi^{\varepsilon} \rangle_{I_{\delta}}, \quad (10.11)$$

where $\langle v \rangle_{I_{\delta}} = (1/|I_{\delta}|) \int_{I_{\delta}} v(\mathbf{x}) \, d\mathbf{x}$. The basis of this procedure is the theory of Section 2. The homogenization theorems allow us to define the effective (or homogenized) conductivity tensor, by considering the infinite volume limit of the solutions of the micro-scale problem subject to the constraint that the average gradient remains fixed. The effective tensor is defined by an average relation of the type (10.11) in the infinite volume limit, *i.e.*,

$$L = \frac{\delta}{\varepsilon} \rightarrow \infty.$$

In the special case when the micro-structure is periodic, the infinite volume problem reduces to a periodic problem.

Let us now consider the coupling between gas dynamics on the macro-scale and molecular dynamics (MD) on the micro-scale. The macroscopic

equations are the usual conservation laws of density, momentum and energy. In one dimension, it can be expressed in a generic form:

$$\partial_t \mathbf{u} + \partial_x \mathbf{f} = 0. \quad (10.12)$$

Here \mathbf{f} is the flux. Traditional gas dynamics models assume that \mathbf{f} is a known function of \mathbf{u} . Here we do not make that assumption. Instead we will extract \mathbf{f} from an underlying atomistic model, namely, molecular dynamics (MD).

As the macro-scale solver, we select a finite volume method. One example is the Lax–Friedrichs scheme on a staggered grid:

$$\mathbf{u}_{j+1/2}^{n+1} = \frac{\mathbf{u}_j^n + \mathbf{u}_{j+1}^n}{2} - \frac{\Delta t}{\Delta x} (\mathbf{f}_{j+1}^n - \mathbf{f}_j^n). \quad (10.13)$$

The data that need to be estimated from MD are again the fluxes. This is done by performing a constrained MD simulation locally at the cell boundaries, which are the cell centres for the previous time step. The constraints are that the average density, momentum and energy of the MD system should agree with the local macro-state at the current time step n . This is realized by initializing the MD with such constraints and applying the periodic boundary condition afterwards. Using the Irving–Kirkwood formula, which relates the fluxes to the MD data, we can then extract the macro-scale fluxes by time-averaging the MD data. Ensemble averaging may also be used.

In this way we can rely on the more fundamental equations of molecular dynamics rather than on a flux function based on an empirical equation of state. Note that the micro-scale solver here plays the role of a Riemann solver in a standard conservation law scheme.

Remark. Recall the connection between projection-based and analytic homogenization. In both methods the homogenized operators were derived from a direct averaging and a correction for the high-frequency interaction. The correction involved the solution of a cell problem in the analytic case and the solution of a system of linear equations for the wavelet-based methodology. Here with HMM there is no such decomposition into averaging and correction, but the notion of a cell problem is quite clear. It is in the localized micro-scale problem where the high-frequency interaction is resolved and then transmitted to the model for the coarse scale. The compression steps typically include averaging, but that averaging step is taken after the local or cell problem is solved.

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