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Sensitivity analysis and Taylor expansions in numerical homogenization problems

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Summary. Two-scale numerical homogenization problems are addressed, with particular application to the modified compressible Reynolds equation with periodic roughness. It is shown how to calculate sensitivities of the homogenized coefficients that come out from local problems. This allows for significant reduction of the computational cost by two means: The construction of accurate Taylor expansions, and the implementation of rapidly convergent nonlinear algorithms (such as Newton's) instead of fixed-point-like ones. Numerical tests are reported showing the quantitative accuracy of low-order Taylor expansions in practical cases, independently of the shape and smoothness of the roughness function.

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1. Introduction

Most physical phenomena occur at several different length and time scales. Their modeling, in turn, differs from one scale to the other, from quantum mechanics at the atomic level to continuum mechanics at a more macroscopic one.

Focusing now within the domain of validity of continuum mechanics, a typical length range being $10^{-7} - 10^{3}$ meters, there is still plenty of space for the occurrence of multiple-scale phenomena. A good example is heat transfer and/or mechanical equilibrium in real materials. There is one length

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scale of the component itself (the wall thickness of a furnace, the length or width of a tool, etc.) on the one hand. On the other hand, no real material is homogeneous, and the size and shape of its heterogeneities define one or more additional length scales (the grain size in a metal or alloy, the distance between inclusions in a composite, the pore size in a porous medium, etc.).

Considering stationary two-scale phenomena, their predictive modeling implies the solution of a problem at a *global* scale L, whereas the material properties vary at a *local* scale ℓ. The complexity of the system grows as ε^{-d}, where $\varepsilon = \ell/L$ and d is the number of space dimensions. If $\varepsilon \ll 1$, some kind of approximation is needed. Such is the case of classical concepts like the effective thermal and elastic properties of materials such as wood, granite, or even steel. The underlying intuitive idea is that there exists a "global scale behaviour" that is governed by the geometry, the loads and the constraints, and that occurs at a length scale L. Each point of the global scale is not of zero diameter, but in fact an abstraction of a small elementary volume of diameter greater than ℓ. At each of these points, the response of the system comes from the small-scale or "local" behaviour, that is independent, or almost independent, of the global features.

The mathematical tools needed to add rigor to this intuitive idea come from homogenization theory. Under suitable assumptions, a partial differential equation (PDE) is found to hold on the global domain (denoted by Ω), that takes into account the small scale in an averaged sense. Its coefficients come from the solution of *local problems*, namely PDE problems defined on some unit cell (denoted by Y), representative of the small scale. This two-level structure cannot always be removed by the definition of "effective" homogeneous properties (e.g., in nonlinear cases), and it carries on to any numerical treatment of the problem.

In this article we consider the application of several tools from optimal design and bifurcation theory to the specific field of multiple-scale analysis. Though the arguments are quite general, the exposition is based on a specific problem. It consists of the flow of air between two surfaces in relative motion. The distance between the two surfaces is assumed to be very small ($\sim 10^{-6}\mathrm{m}$), so that lubrication hypotheses hold, rendering the problem two-dimensional. The small scale comes from assuming that the surfaces are rough, the typical scale of the roughness being much smaller than that of the surfaces themselves. The mathematical homogenization problem, of great technological interest, has been thoroughly studied in the incompressible case by Bayada and Faure [3], and in the compressible case by Jai [9]. We will focus on the latter, modeled by the so-called modified compressible Reynolds equation, that is nonlinear, and on its numerical treatment.

The main items addressed are:

1. The calculation of sensitivities of first and higher order at the local problem level, and their numerical approximation.
2. The construction and application of Taylor expansions as a way of significantly reducing the computational burden brought by local problems.
3. The use of first-order sensitivities at the local level to replace fixed-point iterations at the global level by Newton's method.
4. A brief discussion of extensions to optimal design homogenization problems

Our work is related to the literature as follows: The local problems introduced at each $x \in \Omega$ by homogenization depend on two parameters, one of them being the unknown value of the global solution at $x$on these parameters, a fact that occurs in many nonlinear problems [2,9]. We thus deal with a parametrized family of PDE problems at the local level, that in our specific case are linear but could well be nonlinear as in [6]. The approximation theory in this mathematical setting has been established in [4]. Intensive application of derivatives (mainly first order ones) with respect to parameters in the PDE can be found in the optimal design literature. However, perhaps due to the two-level structure discussed above, multiple-scale problems have received little attention. We can cite in this direction a recent paper on optimum composite materials by Haslinger and Dvorak [8]. They consider first derivatives with respect to the shape in linear elastic problems. The use of higher order derivatives and of Taylor expansions for finite element analysis has been proposed by Guillaume and Masmoudi [7] within the context of optimal shape design (without multiple-scale phenomena). Our work is oriented towards taking full profit of sensitivity analysis and Taylor expansions in the numerical approximation of homogenization problems, a task that is, to our knowledge, as yet unaccomplished.

2. Local problem and homogenized coefficients

2.1. Definitions and differentiability results

As discussed in the introduction, let Ω be a two dimensional domain, its points denoted by $x = (x_1, x_2)$ (the global variables). A global PDE problem, to be precised later, is assumed to be defined in Ω, its coefficients depending on the solution of local problems that we address in this Section. For this purpose, let Y be the unit cell, and let $y = (y_1, y_2)$ denote so-called local (or rapid) space variables defined in Y. For simplicity, we set $Y =]0,1[\times]0,1[$.

We consider the space of periodic functions

$$H^1_p(Y) = \left\{ v \in H^1(Y) / v \text{ takes equal values on opposite faces of } Y \right\}$$

and in particular its zero-mean subspace

$$H^1_m(Y) = \left\{ v \in H^1_p(Y) / \int_Y v = 0 \right\}$$

which is a Hilbert space under the norm

$$\|v\| = \left(\sum_{i=1}^{2} \left\| \frac{\partial v}{\partial y_i} \right\|^2_{L^2(Y)} \right)^{1/2}$$

We proceed to introduce a local problem in Y that depends on 2 parameters α_1, α_2 (we set $\alpha = (\alpha_1, \alpha_2)$ and extension to more parameters is straightforward). Let, for a given value of α within a suitable open set $\Xi \subset \mathbb{R}^2$, $B(\alpha)$ be the operator defined on $V = H^1_m(Y)$ by

$$B(\alpha).v = -\nabla_y.\,(d(\alpha; y).\nabla_y v) \tag{2.1}$$

where the subindices in differential operators refer to the (local or global) space variables and $d(\alpha; y)$ is of class C^m with respect to α, in the L^∞-norm, namely that

$$\sup_{y \in Y} \left\{ \left| \frac{\partial^{k_1+k_2} d}{\partial \alpha_1^{k_1} \partial \alpha_2^{k_2}} \right| (\alpha; y) \right\} \leq \beta \tag{2.2}$$

holds for some β (possibly depending on α) for all $k_1 + k_2 \leq m$. We also introduce the associated bilinear form

$$b(\alpha; u, v) = \int_Y d(\alpha; y) \nabla_y u.\nabla_y v dy \quad \forall u, v \in V \tag{2.3}$$

The function d is assumed to render b (strongly) V-elliptic, uniformly for all $\alpha \in \Xi$, i.e there exist a positive constant δ such that:

$$b(\alpha; u, u) \geq \delta \|u\|^2 \ \forall u \in V \tag{2.4}$$

In (2.1), $B(\alpha)$ is understood as an operator from V into its dual V', with the derivatives taken in the weak sense. In addition, let $U(\alpha; y)$ be a bounded vector field on Y, also of class C^m with respect to α in the sense of (2.2).

Local problem. For α given, find ω_i and χ_i, $i = 1, 2$, belonging to V as the (unique) solutions of

$$b(\alpha; \omega_i, v). = -\int_Y d(\alpha; y) \frac{\partial v}{\partial y_i} dy \qquad \forall v \in V \tag{2.5}$$

$$b(\alpha; \chi_i, v). = -\int_Y U_i(\alpha; y) \frac{\partial v}{\partial y_i} dy \qquad \forall v \in V \tag{2.6}$$

Remark 2.1 Existence and uniqueness for the local problem come from the V-ellipticity of b and from the Fredholm alternative.

The local problem is in fact an auxiliary problem introduced to calculate the so-called homogenized coefficients $A^*(\alpha)$ and $\Theta^*(\alpha)$, given by

$$A^*(\alpha) = \begin{bmatrix} A^*_{11}(\alpha) & A^*_{12}(\alpha) \\ A^*_{12}(\alpha) & A^*_{22}(\alpha) \end{bmatrix} = \widetilde{A}^*(\alpha, \omega_1(\alpha), \omega_2(\alpha)) \tag{2.7}$$

$$\Theta^*(\alpha) = \begin{bmatrix} \Theta^*_1(\alpha) \\ \Theta^*_2(\alpha) \end{bmatrix} = \tilde{\Theta}^*(\alpha, \chi_1(\alpha), \chi_2(\alpha)) \tag{2.8}$$

we suppose that the functions $\widetilde{A}^*(\alpha, \omega_1, \omega_2)$ and $\tilde{\Theta}^*(\alpha, \chi_1, \chi_2)$ satisfy the following:

(2.9) $\widetilde{A}^*$ and $\tilde{\Theta}^*$ are of class C^m with respect to their arguments.

Lemma 2.1 *Under assumptions (2.2), (2.4) and (2.9), the solutions $\omega_i(\alpha)$ and $\chi_i(\alpha)$, $i = 1, 2$, of the local problem, and the homogenized coefficients $A^*(\alpha)$ and $\Theta^*(\alpha)$ are of class C^m with respect to α.*

Proof. We remark that the functions $d(\alpha; y)$ and $U(\alpha; y)$ are such that the linear forms

$$\int_Y \frac{\partial^{k+l} d}{\partial \alpha_1^k \partial \alpha_2^l} \frac{\partial v}{\partial y_i}\, dy \qquad , \qquad \int_Y \frac{\partial^{k+l} U_i}{\partial \alpha_1^k \partial \alpha_2^l} \frac{\partial v}{\partial y_i}\, dy \tag{2.10}$$

are continuous (with respect to $v \in V$) for all $k + l \leq m$. Eqs. (2.5)-(2.6) thus admit the generic form

$$b(\alpha; z, v) = \langle f(\alpha), v \rangle \qquad \forall v \in V \tag{2.11}$$

where $b(\alpha; \cdot, \cdot) : V \times V \to \mathbb{R}$ and $f(\alpha) : V \to \mathbb{R}$ are, as bilinear and linear forms, respectively, of class C^m with respect to α. Moreover $b(\alpha; \cdot, \cdot)$, in view of its ellipticity, defines an isomorphism $B(\alpha)$ (of class C^m) from V to V' by $\langle B(\alpha)\, u, v \rangle = b(\alpha; u, v)$. Eq. (2.11) can thus be rewritten as $F(\alpha; u) \stackrel{\text{def}}{=} B(\alpha)u - f(\alpha) = 0$. We have by the implicit function theorem that the function $z(\alpha)$ defined by (2.11) is also of class C^m with respect to α. The result is thus established for $\omega_i(\alpha)$ and $\chi_i(\alpha)$. That for $A^*(\alpha)$ and $\Theta^*(\alpha)$ comes from the differentiability of composite functions. □

Remark 2.2 The previous lemma generalizes to the case where $b(\alpha; z, v)$ is nonlinear (but of class C^m) in z, provided that its differential defines an isomorphism, as is evident from above.

2.2. Specific application: modified compressible Reynolds equation

We consider a lubrication problem, specifically the flow of air (or other fluid) between two surfaces in relative motion. The distance between the surfaces, or air gap, is assumed to be very small ($\sim 10^{-6}\mathrm{m}$), given by a known function $h_\varepsilon(x)$. The subindex ε expresses that the surfaces are rough, with a roughness wavelength ε that is superposed to a mean value $H_0(x)$. An important technological application concerns computer magnetic storage devices, in which the gap between the reading head and the magnetic disk or tape is extremely small.

The mathematical model, due to Burgdorfer [5], is a modification of the classical Reynolds equation accounting for molecular slip at the surfaces. It reads

$$\nabla.\left[\left(h_\varepsilon^3 P_\varepsilon + \lambda h_\varepsilon^2\right)\nabla P_\varepsilon\right] = \Lambda \frac{\partial}{\partial x_1}\left(h_\varepsilon P_\varepsilon\right) \qquad x=(x_1,x_2)\in\Omega \tag{2.12}$$
$$P_\varepsilon(x) = 1 \qquad x\in\partial\Omega$$

where $P_\varepsilon = P_\varepsilon(x)$ is the normalized pressure between the two rough surfaces, $\Omega \subseteq \mathbb{R}^2$ is the region (with smooth boundary $\partial\Omega$) where the upper and lower bodies are in proximity. Except for normalization factors, λ is a physical constant (the Knudsen number) and Λ (the gas bearing number) depends on the relative velocity and on the minimal clearance.

Eq. (2.12) is a two-scale one as discussed in the introduction, v.g., its coefficients vary on a length scale ε assumed to be much smaller that the diameter of Ω. Let us now recall its treatment by homogenization techniques. The real gap is defined as an $\varepsilon-$periodic function around the average value $H_0(x)$ by

$$h(x,y) = H_0(x) + H_1(y)$$

where $H_1(y)$ is a given periodic function. In [9] it was shown, by way of the two scale convergence, that the (unique) weak positive solution of problem (2.12) converges to the homogenized solution P_0 of the following *homogenized system*:

$$\begin{cases} \nabla.\left(\left(A^*(H_0(x),P_0(x))\,\nabla P_0\right)\right. \\ \qquad \left. = \Lambda\nabla.\left(\Theta^*(H_0(x),P_0(x))P_0\right)\right) \quad \text{in} \quad \Omega \\ P_0 = 1 \quad \text{along} \quad \partial\Omega \end{cases} \tag{2.13}$$

where A^* and Θ^* are of the form given in (2.7) and (2.8) with

$$\text{(2.14)}\qquad \begin{cases} \alpha = (\alpha_1, \alpha_2) = (H_0(x), P_0(x)) \\ \widetilde{A}^*_{ii}(\alpha, \omega_1, \omega_2) = \int_Y d(\alpha; y) \left(\dfrac{\partial \omega_i}{\partial y_i} + 1 \right) dy \qquad i = 1, 2 \\ \widetilde{A}^*_{12}(\alpha, \omega_1, \omega_2) = \widetilde{A}^*_{21}(\alpha, \omega_1, \omega_2) = \int_Y d(\alpha; y) \dfrac{\partial \omega_2}{\partial y_1} dy \\ \widetilde{\Theta}^*_1(\alpha, \chi) = \int_Y \left(\alpha_1 + H_1(y) + d(\alpha; y) \dfrac{\partial \chi_1}{\partial y_1} \right) dy \\ \widetilde{\Theta}^*_2(\alpha, \chi) = \int_Y d(\alpha; y) \dfrac{\partial \chi_1}{\partial y_2} dy \end{cases}$$

and ω_i and χ_1 are solutions of the local problems (2.5) and (2.6) with the functions d and U given by

$$\text{(2.15)}\qquad \begin{cases} d(\alpha; y) = \left(\alpha_1 + H_1(y)\right)^3 \alpha_2 + \lambda \left(\alpha_1 + H_1(y)\right)^2 \\ U_1(\alpha; y) = H_1(y) \\ U_2(\alpha; y) = 0 \end{cases}$$

For the sake of clarity, we will systematically refer to this specific problem in the following sections.

Remark 2.3 As a consequence of Lemma 2.1 and of the C^∞-regularity of the functions d and U defined by (2.15), we know that ω_i, χ_1, A^* and Θ^* are C^∞ functions of α_1 (=$H_0(x)$) and α_2 (= $P_0(x)$).

Remark 2.4 A^* and Θ^* in (2.13) can be viewed, simply, as a function of x, but its regularity would depend on that of P_0. It is a crucial trick to get the C^∞-regularity to explicit that its dependence on x is through $H_0(x)$ and $P_0(x)$. Parametrized with respect to these two quantities, A^* and Θ^* can be differentiated up to an arbitrary order without regularity assumptions with respect to the global space variable x.

Remark 2.5 Local problems of the form (2.5)-(2.6) and homogenization formula like (2.7)-(2.8) are obtained by asymptotic expansion (with convergence under additional assumptions) of the general quasilinear convection-diffusion equation

$$\text{(2.16)}\qquad -\sum_{1\le i,j\le n} \partial_{x_i} \left(a^\varepsilon_{ij}(x, u^\varepsilon) \partial_{x_j} u^\varepsilon \right) + \sum_{1\le i\le n} \partial_{x_i} \left(b^\varepsilon_i(x, u^\varepsilon) u^\varepsilon \right) = f$$

3. Sensitivities and Taylor expansions

3.1. Taylor expansions

Any numerical treatment of (2.13) leads to multiple evaluations of A^*, Θ^* for many $\alpha_1 = H_0(x)$ and $\alpha_2 = P_0(x)$. It must be noticed, however, that each

evaluation needs the solution of a partial differential equation or, in practice, a numerical approximation of it by finite elements, finite differences, or other method. Considering that the global problem (2.13) involves generally some thousand discretisation points, a naif approach leads to the same number of numerical boundary value problems, times the number of local unknown fields (3 in our case, ω_1, ω_2 and χ), times the number of nonlinear iterations. Moreover, it is not obvious how to implement an iterative algorithm other than a fixed-point one in view of the implicit definition of $A^*(\alpha)$ and $\Theta^*(\alpha)$, and fixed-point algorithms are known to converge slowly.

We propose to replace A^* and Θ^* in (2.13) by their Taylor expansions of order $n \leq m$

$$T_{A_n^*}(\alpha) = A^*(\alpha^0) + \sum_{i=1}^{n} \frac{1}{i!} \left((\alpha_1 - \alpha_1^0) \frac{\partial}{\partial \alpha_1} + (\alpha_2 - \alpha_2^0) \frac{\partial}{\partial \alpha_2} \right)^i A^*(\alpha^0) \tag{3.1}$$

$$T_{\Theta_n^*}(\alpha) = \Theta^*(\alpha^0) + \sum_{i=1}^{n} \frac{1}{i!} \left((\alpha_1 - \alpha_1^0) \frac{\partial}{\partial \alpha_1} + (\alpha_2 - \alpha_2^0) \frac{\partial}{\partial \alpha_2} \right)^i \Theta^*(\alpha^0) \tag{3.2}$$

for a representative vector α^0, so that, once the coefficients of the expansions are known, no further solution of a local problem is needed to evaluate A^*, Θ^* for an arbitrary value of α.

For α^0 given in Ξ, we know from Lemma 2.1 that the Taylor expansion is well defined and that there exist $\eta > 0$ such that, if

$$\left\| \alpha - \alpha^0 \right\| < \eta$$

then

$$\left| A^*(\alpha) - T_{A_n^*}(\alpha) \right| = o\left(\left\| \alpha - \alpha^0 \right\|^n \right)$$
$$\left| \Theta^*(\alpha) - T_{\Theta_n^*}(\alpha) \right| = o\left(\left\| \alpha - \alpha^0 \right\|^n \right)$$

This local result is however not sufficient for the algorithm to be useful. It remains to show: *(i)* That for realistic intervals $H_{\min} \leq \alpha_1 \leq H_{\max}$, $P_{\min} \leq \alpha_2 \leq P_{\max}$, the Taylor expansions, with a reasonably low order n, provide a high enough accuracy to render valid the replacement of $A^*(\alpha)$, $\Theta^*(\alpha)$ by $T_{A_n^*}(\alpha)$, $T_{\Theta_n^*}(\alpha)$; *(ii)* that the numerical treatment of the local problems (by finite elements or other technique) does not interfere with the Taylor-expansion idea; *(iii)* that numerical approximations of the Taylor expansion coefficients can indeed be calculated at an affordable cost; and *(iv)* that the computer implementation of Taylor expansions is not too troublesome in what concerns programming. These questions will be discussed in the rest of the paper, some of them by means of numerical experiments.

3.2. Calculation of the Taylor-expansion coefficients

The derivatives intervening in (3.1)-(3.2) can be calculated by the so-called "direct" method, or by the "adjoint" method. In this case the former is more convenient, as the number of variables $(two : \alpha_1, \alpha_2)$ is smaller than the number of functions to be differentiated $(five : A^*_{11}, A^*_{22}, A^*_{12}, \Theta^*_1, \Theta^*_2)$. The direct method begins with the evaluation of the derivatives of the solutions ω_i, χ_i of (2.5)-(2.6) up to the order n. This evaluation proceeds as the following inductive sequence:

Let α^0 given in Ξ, and let k_1, k_2 be two nonnegative integers, with $k_1 + k_2 \leq m$, and set

$$Z(k_1, k_2) = \{(l, n) \in \mathbb{N} \times \mathbb{N} / \ 0 \leq l \leq k_1, \\ 0 \leq n \leq k_2, l + n < \ k_1 + k_2\}$$

Assume that $\dfrac{\partial^{l+n}\omega_i}{\partial\alpha_1^l \partial\alpha_2^n}, \dfrac{\partial^{l+n}\chi_i}{\partial\alpha_1^l \partial\alpha_2^n}$, $i = 1, 2$, *are known for all* $(l,n) \in Z(k_1, k_2)$. *The* (k_1, k_2) *derivatives then are the unique functions in* V *satisfying:*

$$b(\alpha^0; \frac{\partial^{k_1+k_2}\omega_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}, v) = -\int_Y \frac{\partial^{k_1+k_2} d}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \frac{\partial v}{\partial y_i} dy \\ - \sum_{(l,n)\in Z(k_1,k_2)} \binom{k_1}{l} \binom{k_2}{n} \frac{\partial^{k_1+k_2-l-n} b}{\partial\alpha_1^{k_1-l}\partial\alpha_2^{k_2-n}} \left(\alpha^0, \frac{\partial^{l+n}\omega_i}{\partial\alpha_1^l\partial\alpha_2^n}, v\right) \qquad \forall v \in V \tag{3.3}$$

$$b(\alpha^0; \frac{\partial^{k_1+k_2}\chi_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}, v) = -\int_Y \frac{\partial^{k_1+k_2} U_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \frac{\partial v}{\partial y_i} dy \\ - \sum_{(l,n)\in Z(k_1,k_2)} \binom{k_1}{l} \binom{k_2}{n} \frac{\partial^{k_1+k_2-l-n} b}{\partial\alpha_1^{k_1-l}\partial\alpha_2^{k_2-n}} \left(\alpha^0, \frac{\partial^{l+n}\chi_i}{\partial\alpha_1^l\partial\alpha_2^n}, v\right) \qquad \forall v \in V \tag{3.4}$$

where the derivatives of the bilinear form are given, as expected, by

$$\frac{\partial^{l+n} b}{\partial\alpha_1^l\partial\alpha_2^n}(\alpha; w, v) = \int_Y \frac{\partial^{l+n} d}{\partial\alpha_1^l\partial\alpha_2^n}(\alpha; y) \nabla_y w . \nabla_y v \quad dy \\ \forall w, v \in V \tag{3.5}$$

Remark 3.1 $\dfrac{\partial^{l+n} b}{\partial\alpha_1^l\partial\alpha_2^n}(\alpha; ., .)$ is a continuous bilinear form defined on V.

This is due to (2.2) which gives

$$\left| \frac{\partial^{l+n} b}{\partial\alpha_1^l\partial\alpha_2^n}(\alpha; w, v) \right| \leq \beta \ \|w\| \ \|v\| \qquad \forall w, v \in V \tag{3.6}$$

Once the computation of all derivatives of ω_i and χ_i up to order n has been finished, those of A^* and Θ^* are obtained from the chain rule. Instead of providing a general expression, that is quite involved, let us write down the first two derivatives of A^*_{kl}:

First derivatives of $A^*(\alpha) = \tilde{A}^*(\alpha, \omega_1(\alpha), \omega_2(\alpha))$ at $\alpha = \alpha^0$.

$$\frac{\partial A^*_{kl}}{\partial \alpha_i} = \frac{\partial \widetilde{A}^*_{kl}}{\partial \alpha_i} + \left\langle D_2 \tilde{A}^*_{kl}, \frac{\partial \omega_1}{\partial \alpha_i}(\alpha^0) \right\rangle + \left\langle D_3 \tilde{A}^*_{kl}, \frac{\partial \omega_2}{\partial \alpha_i}(\alpha^0) \right\rangle \qquad i = 1, 2$$

Second derivatives.

$$\begin{aligned}
\frac{\partial^2 A^*_{kl}}{\partial \alpha_i \partial \alpha_j} = {} & \frac{\partial^2 \widetilde{A}^*_{kl}}{\partial \alpha_i \partial \alpha_j} + \left\langle D_2 \left(\frac{\partial \widetilde{A}^*_{kl}}{\partial \alpha_j} \right), \frac{\partial \omega_1}{\partial \alpha_i} \right\rangle + \left\langle D_2 \left(\frac{\partial \widetilde{A}^*_{kl}}{\partial \alpha_i} \right), \frac{\partial \omega_1}{\partial \alpha_j} \right\rangle \\
& + D^2_{22} \tilde{A}^*_{kl} \left(\frac{\partial \omega_1}{\partial \alpha_i}, \frac{\partial \omega_1}{\partial \alpha_j} \right) + \left\langle D_2 \tilde{A}^*_{kl}, \frac{\partial^2 \omega_1}{\partial \alpha_i \partial \alpha_j} \right\rangle \\
& + D^2_{23} \tilde{A}^*_{kl} \left(\frac{\partial \omega_1}{\partial \alpha_i}, \frac{\partial \omega_2}{\partial \alpha_j} \right) + D^2_{23} \tilde{A}^*_{kl} \left(\frac{\partial \omega_1}{\partial \alpha_j}, \frac{\partial \omega_2}{\partial \alpha_i} \right) \\
& + \left\langle D_3 \left(\frac{\partial \widetilde{A}^*_{kl}}{\partial \alpha_j} \right), \frac{\partial \omega_2}{\partial \alpha_i} \right\rangle + \left\langle D_3 \left(\frac{\partial \widetilde{A}^*_{kl}}{\partial \alpha_i} \right), \frac{\partial \omega_2}{\partial \alpha_j} \right\rangle \\
& + D^2_{33} \tilde{A}^*_{kl} \left(\frac{\partial \omega_2}{\partial \alpha_i}, \frac{\partial \omega_2}{\partial \alpha_j} \right) + \left\langle D_3 \tilde{A}_{kl}, \frac{\partial^2 \omega_2}{\partial \alpha_i \partial \alpha_j} \right\rangle \quad 1 \le i, j \le 2
\end{aligned} \tag{3.7}$$

The derivatives of the homogenized convection vector Θ^* can be calculated analogously.

Remark 3.2 For the specific case (2.14) we have for $k = 1, 2$

$$\begin{aligned}
\frac{\partial \tilde{A}^*_{ii}}{\partial \alpha_k}(\alpha^0, \omega_1(\alpha^0), \omega_2(\alpha^0)) &= \int_Y \frac{\partial d}{\partial \alpha_k}(\alpha^0; y) \\
&\quad \times \left(1 + \frac{\partial \omega_i}{\partial y_i}(\alpha^0; y) \right) dy \quad i = 1, 2 \\
\frac{\partial \tilde{A}^*_{12}}{\partial \alpha_k} = \frac{\partial \tilde{A}^*_{21}}{\partial \alpha_k} &= \int_Y \frac{\partial d}{\partial \alpha_k}(\alpha^0; y) \frac{\partial \omega_2}{\partial y_1}(\alpha^0; y)
\end{aligned}$$

$$\begin{aligned}
&\left\langle D_2 \tilde{A}^*_{11}(\alpha^0, \omega_1(\alpha^0), \omega_2(\alpha^0)), \frac{\partial \omega_1}{\partial \alpha_k}(\alpha^0) \right\rangle \\
&\qquad = \int_Y d(\alpha^0; y) \frac{\partial}{\partial y_1} \left[\frac{\partial \omega_1}{\partial \alpha_k}(\alpha^0; y) \right] dy \\
&\left\langle D_3 \tilde{A}^*_{11}(\alpha^0, \omega_1(\alpha^0), \omega_2(\alpha^0)), \frac{\partial \omega_2}{\partial \alpha_k}(\alpha^0) \right\rangle \\
&\qquad = \left\langle D_3 \tilde{A}^*_{22}(\alpha^0, \omega_1(\alpha^0), \omega_2(\alpha^0)), \frac{\partial \omega_1}{\partial \alpha_k}(\alpha^0) \right\rangle = 0
\end{aligned}$$

The expression for $\left\langle D_3\tilde{A}^*_{22}, \dfrac{\partial\omega_2}{\partial\alpha_k}\right\rangle$ is analogous to that for $\left\langle D_2\tilde{A}^*_{11}, \dfrac{\partial\omega_1}{\partial\alpha_k}\right\rangle$. It suffices to replace ω_1 by ω_2 and y_1 by y_2. The first derivative with respect to α_2 is obtained by replacing, in the previous formulae α_1 by α_2.

Remark 3.3 It is clear from (3.7) that the complexity grows rapidly with the order of differentiation. Fortunately, as will be shown in the next section, the computational procedures need not be programmed by hand, but instead be obtained by automatic differentiation.

4. Numerical approximation

Let V_h be a finite element subspace of $H^1_m(Y)$, made of piecewise polynomial functions of degree K. Discrete versions of ω_i and χ_i, that we will denote by ω_{ih}, χ_{ih} are defined as unique solutions in V_h to problems (2.5)-(2.6) restricted to V_h. Moreover, discrete versions $\left(\dfrac{\partial^{k_1+k_2}\omega_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h$ and $\left(\dfrac{\partial^{k_1+k_2}\chi_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h$ can be defined by induction restricting problems (3.3)-(3.4) to V_h and replacing exact derivatives in the right-hand side by their discrete versions. The same is done with A^*, Θ^* and their derivatives, every time ω_i, χ_i or their derivatives appear in their expressions, they are replaced by their discrete versions. Let A^*_h, Θ^*_h and $\left(\dfrac{\partial^{k_1+k_2}A^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h$, $\left(\dfrac{\partial^{k_1+k_2}\Theta^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h$ be the numerically obtained coefficients and their derivatives. Finally let $T^h_{A^*_n}$ and $T^h_{\Theta^*_n}$ be the discrete version of the Taylor expansions (3.1)-(3.2). The systematic replacement of each exact quantity by its discrete version throughout the process makes the following proposition hold:

Proposition 4.1 *For k_1, k_2 two nonnegative integers such that $k_1+k_2 \leq m$, we have*

$$\left(\frac{\partial^{k_1+k_2}\omega_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h = \frac{\partial^{k_1+k_2}\omega_{ih}}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \tag{4.1}$$

$$\left(\frac{\partial^{k_1+k_2}\chi_i}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h = \frac{\partial^{k_1+k_2}\chi_{ih}}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \tag{4.2}$$

Moreover,

$$\left(\frac{\partial^{k_1+k_2}A^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h = \frac{\partial^{k_1+k_2}A_h^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \tag{4.3}$$

$$\left(\frac{\partial^{k_1+k_2}\Theta^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}}\right)_h = \frac{\partial^{k_1+k_2}\Theta_h^*}{\partial\alpha_1^{k_1}\partial\alpha_2^{k_2}} \tag{4.4}$$

Proof. The proof of (4.1) or (4.2) is done by induction and can be found in [7]. (4.3) and (4.4) are an immediate consequence. □

Remark 4.1 Prop.4.1 implies that automatic differentiation, that provides us with computational procedures to evaluate the right-hand sides of (4.1)-(4.4), can indeed be used to get approximate derivatives (the left-hand sides of (4.1)-(4.4)) without any loss in accuracy. Formula (3.7), for example, was never programmed, and in fact it was first derived at the time of writing down this article. Implementation issues are, thus, nonexistent.

We now establish an approximation result. In fact, it is linked to previous results in [4] and [7], but the context is quite different.

Proposition 4.2 *Let k_1, k_2 be two given non-negative integers with $k_1 + k_2 \leq m$, and assume that*

$$\frac{\partial^{l+n}d}{\partial\alpha_1^l\partial\alpha_2^n}\,,\ \frac{\partial^{l+n}U_i}{\partial\alpha_1^l\partial\alpha_2^n}\ \in H^K(Y),\ i=1,2\ l+n\leq m \tag{4.5}$$

Then, under assumption (2.9), there exists a constant C independent of h (the mesh size) such that

$$\left\|\frac{\partial^{l+n}\omega_{ih}}{\partial\alpha_1^l\partial\alpha_2^n} - \frac{\partial^{l+n}\omega_i}{\partial\alpha_1^l\partial\alpha_2^n}\right\| \leq Ch^K \tag{4.6}$$

$$\left\|\frac{\partial^{l+n}\chi_{ih}}{\partial\alpha_1^l\partial\alpha_2^n} - \frac{\partial^{l+n}\chi_i}{\partial\alpha_1^l\partial\alpha_2^n}\right\| \leq Ch^K \tag{4.7}$$

for α_1, α_2 given and $0 \leq l \leq k_1, 0 \leq n \leq k_2$. In addition,

$$\left\|\left(\frac{\partial^{l+n}A^*}{\partial\alpha_1^l\partial\alpha_2^n}\right)_h - \frac{\partial^{l+n}A^*}{\partial\alpha_1^l\partial\alpha_2^n}\right\| \leq Ch^{2K} \tag{4.8}$$

$$\left\|\left(\frac{\partial^{l+n}\Theta^*}{\partial\alpha_1^l\partial\alpha_2^n}\right)_h - \frac{\partial^{l+n}\Theta^*}{\partial\alpha_1^l\partial\alpha_2^n}\right\| \leq Ch^{2K} \tag{4.9}$$

Proof. See Appendix A. □

Remark 4.2 From Proposition 4.2 it is clear that the homogenized coefficients (together with their derivatives), are calculated with an accuracy order that is twice the one attained for the local solutions ω_i , χ_i. This is true in a wide class of numerical homogenization problems.

5. Numerical results

In the previous sections we have addressed most of the questions posed in Sect. 3.1. It only remains to show that, for a practical application, the accuracy of the Taylor expansion is high enough to permit its use instead of the "exact" homogenized coefficient (the one obtained by solving the local problems). This will be addressed by means of a numerical example.

For the homogenized version of the modified compressible Reynolds equation, Eq. (2.13), it is known [9] that in practical cases the exact solution $P_0(x)$ may vary, in normalized units, between 1 and 10. The range of values of $H_0(x)$ depends on the actual form of the two surfaces. Again in normalized units, a realistic range is $1-10$. We need thus to calculate $A^*(\alpha_1,\alpha_2)$ and $\Theta^*(\alpha_1,\alpha_2)$ for $1 \le \alpha_1 \le 10$, $1 \le \alpha_2 \le 10$.

We consider three cases, the transverse-roughness situation, which has an explicit analytical solution given in [9], a general two-dimensional roughness function and finally a two-dimensional discontinuous roughness function.

The local domain Y is discretized by finite elements of degree $K=1$, and size $h=1/N$.

Next, Taylor expansions $T^h_{A^*_n}$ and $T^h_{\Theta^*_n}$ were built, by developpement around $\alpha_1^0=5, \alpha_2^0=5$, for several values of n and N and for all values of α_1 and α_2 between 1 and 10 with intervals of 0.5.. It is clear that, as $N\to\infty$ $(h\to 0)$, $T^h_{A^*_n}\left(\alpha_1^0,\alpha_2^0\right)\to A^*\left(\alpha_1^0,\alpha_2^0\right)$ and $T^h_{\Theta^*_n}\left(\alpha_1^0,\alpha_2^0\right)\to \Theta^*\left(\alpha_1^0,\alpha_2^0\right)$. It is also clear that, in some neighbourhood of $\left(\alpha_1^0,\alpha_2^0\right)$, $T^h_{A^*_n}\to A^*$ and $T^h_{\Theta^*_n}\to\Theta^*$ as both $n,N\to\infty$. Let us investigate the actual accuracy of these approximations. For this purpose, we define

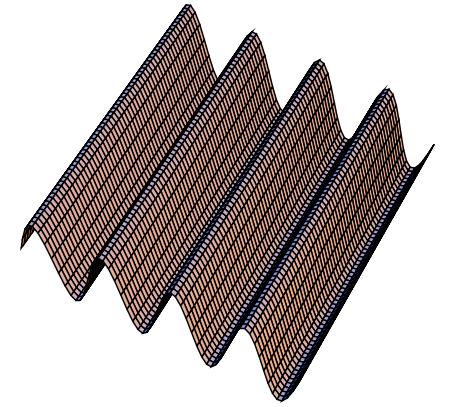
(5.1)

$$ERROR(n,N,A^*)=\frac{\sup_{1\le\alpha_1,\alpha_2\le 10}\left|T^h_{A^*_n}(\alpha_1,\alpha_2)-A^*(\alpha_1,\alpha_2)\right|}{\sup_{1\le\alpha_1,\alpha_2\le 10}\left|A^*(\alpha_1,\alpha_2)\right|}$$

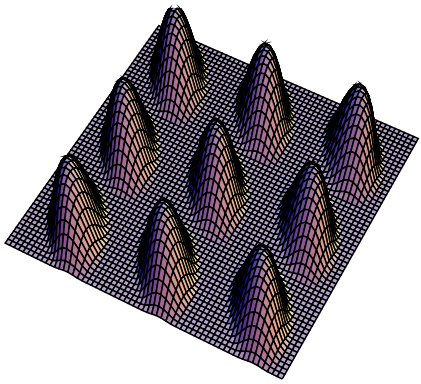
(5.2)

$$ERROR(n,N,\Theta^*)=\frac{\sup_{1\le\alpha_1,\alpha_2\le 10}\left|T^h_{\Theta^*_n}(\alpha_1,\alpha_2)-\Theta^*(\alpha_1,\alpha_2)\right|}{\sup_{1\le\alpha_1,\alpha_2\le 10}\left|\Theta^*(\alpha_1,\alpha_2)\right|}$$

where we have taken $|M|=\sup_{i,j}|M_{ij}|$ as norm for matrices, and the euclidian norm for vectors.



a



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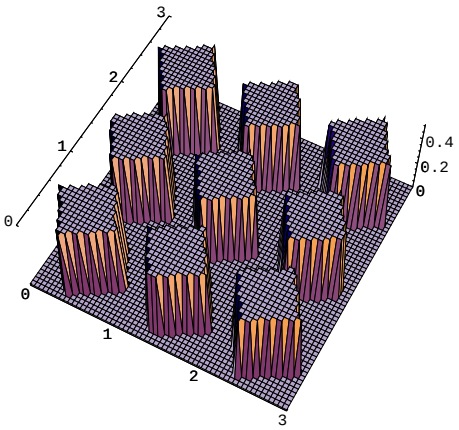

c

Fig. 1a–c. Different forms of the surface roughness. **a** Transverse roughness. **b** Two-dimensional continuous roughness. **c** Two-dimensional discontinuous roughness

Table 1. Errors between exact and Taylor's expansion of the homogenized coefficients in the transverse roughness case

a. Homogenized diffusion matrix

$ERROR(n, N, A^*)$	$N = 5$	$N = 10$	$N = 20$	$N = 40$
$n = 0$	0.9197712	0.9197712	0.9197712	0.9197712
$n = 2$	0.2831131	0.2831124	0.2831124	0.2831124
$n = 3$	0.0566187	0.0566187	0.0566187	0.0566187
$n = 4$	5.570×10^{-5}	4.648×10^{-5}	4.648×10^{-5}	4.648×10^{-5}

b. Homogenized convection vector

$ERROR(n, N, \Theta^*)$	$N = 5$	$N = 10$	$N = 20$	$N = 40$
$n = 0$	0.5052175	0.5052175	0.5052143	0.5052143
$n = 1$	1.699×10^{-2}	1.700×10^{-2}	1.700×10^{-2}	1×700.10^{-2}
$n = 2$	1.305×10^{-2}	1.309×10^{-2}	1.309×10^{-2}	1×309.10^{-2}
$n = 3$	9.821×10^{-3}	9.886×10^{-3}	9.886×10^{-3}	9×886.10^{-3}
$n = 4$	7.710×10^{-3}	7.788×10^{-3}	7.788×10^{-3}	7×788.10^{-3}

5.1. Transverse roughness

The roughness function H_1 depends only on $y_1$and the homogenized coefficients are expressed by (see [9]):

$$A^*_{11}(\alpha_1, \alpha_2) = \frac{1}{\int_0^1 \frac{dy_1}{(\alpha_1 + H_1(y_1))^2((\alpha_1 + H_1(y_1))\alpha_2 + \lambda)}}$$

$$A^*_{22}(\alpha_1, \alpha_2) = \int_0^1 (\alpha_1 + H_1(y_1))^2((\alpha_1 + H_1(y_1))\alpha_2 + \lambda)dy_1$$

$$\Theta^*_1(\alpha_1, \alpha_2) = \frac{\int_0^1 \frac{dy_1}{(\alpha_1 + H_1(y_1))((\alpha_1 + H_1(y_1))\alpha_2 + \lambda)}}{\int_0^1 \frac{dy_1}{(\alpha_1 + H_1(y_1))^2((\alpha_1 + H_1(y_1))\alpha_2 + \lambda)}} \tag{5.3}$$

$$A^*_{12}(\alpha_1, \alpha_2) = A^*_{21}(\alpha_1, \alpha_2) = \Theta^*_2(\alpha_1, \alpha_2) = 0$$

Choosing $H_1(y_1) = \sin(2\pi y_1)$ (see Fig 1a) it easy to calculate (with Mathematica) exact expressions for A^* and Θ^*. These are compared with the numerically obtained values (more precisely, with the values of the numerically obtained Taylor expansions around $\left(\alpha_1^0, \alpha_2^0\right) = (5, 5)$) in Tables 1a and 1b.

From Tables 1a and 1b one can remark the following:

1. The accuracy of the Taylor expansions seems to depend only on the order of expansion n. More precisely, for a given value of n the relative error

between the exact solution and the approximate one levels off around $N = 10$. This tells us that, to reduce the error, it is better to increase the order of the Taylor expansion than to refine the mesh in Y.

2. There is a jump of the error of A^* (resp.Θ^*) from $n = 3$ (resp. $n = 0$) to $n = 4$ (resp. $n = 1$). The dominant terms in the expansions of A^* (resp.Θ^*) are thus those of order $n \leq 4$ (resp. $n \leq 1$).
3. It is clear that, for $n = 4$ we have already an extremely accurate approximation. In fact, considering that there is an incertainty in the values of the physical data, even $n = 3$ would be acceptable.

5.2. Two-dimensional surface roughness

The need of efficient numerical methods is most evident when the roughness function $H_1(y)$ is two-dimensional, we have chosen the following reference function

(5.4)

$$H_1^0(y_1^0, y_2^0) = \begin{cases} -\beta \exp(\frac{1}{a^2}) \exp\left(-\left(a^2 - (y_1^0 - \frac{1}{2})^2 - (y_2^0 - \frac{1}{2})^2\right)^{-1}\right) \\ \qquad\qquad \text{if } a^2 > (y_1^0 - \frac{1}{2})^2 + (y_2^0 - \frac{1}{2})^2 \\ 0 \qquad\qquad \text{otherwise} \end{cases}$$

To introduce a surface roughness orientation we consider the following mapping:

(5.5)

$$\begin{cases} y_1 = \cos\theta \cdot y_1^0 + \sin\theta . y_2^0 \\ y_2 = \left(-\sin\theta \cdot y_1^0 + \cos\theta . y_2^0\right)/\gamma \end{cases}$$

from which we deduce the roughness function:

$$H_1(y_1, y_2) = H_1^0(\cos\theta y_1 - \sin\theta y_{2,}, \sin\theta y_1 + \cos\theta y_2)$$

So that the roughness corresponds, roughly speaking, to elliptic bumps of orientation θ and amplitude β. Let us select $\beta = 0.5$, $a = 0.6$, $\gamma = 4$, $\theta = \pi/3$. The form of the roughness function can be seen in Fig. 1b. It is a nontrivial case, as in fact the amplitude of the bumps is half the minimum air gap considered.

Since no exact solution in closed form exists, a reference calculation was carried out with $N = 100$, evaluating A^* and Θ^* for all values of α_1 and α_2 between 1 and 10 with intervals of 0.5. The cost of this calculations is enormous, 361 different 10000×10000-matrix are to be built and factorized, each one solved for 3 different right-hand sides. Its results will be considered "exact" values in what follows. Graphs of $A_{11}^*(\alpha_1, \alpha_2)$ and $\Theta_1^*(\alpha_1, \alpha_2)$ can be seen in Fig. 2.

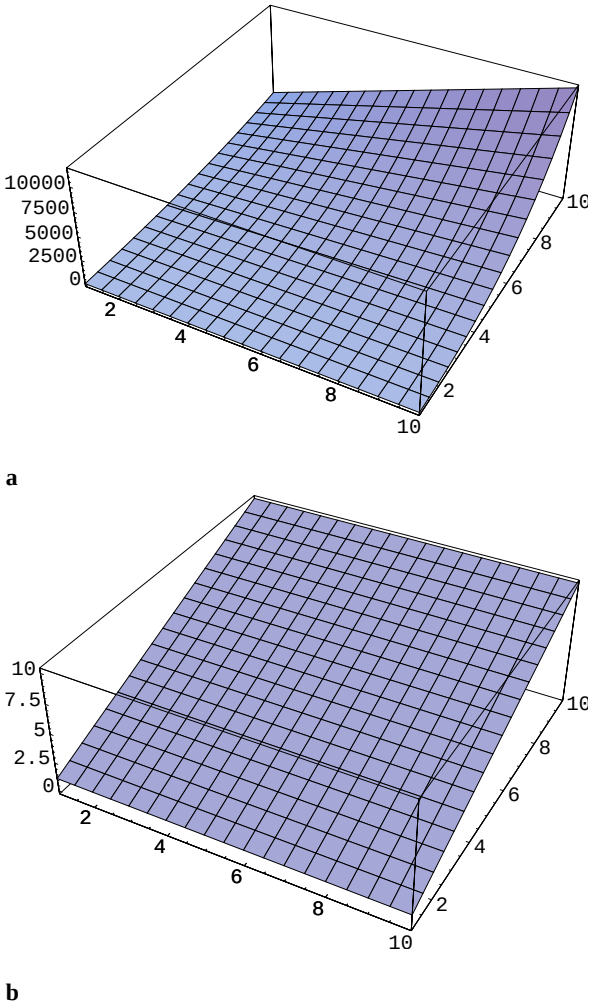

Fig. 2a,b. Behaviour of the homogenized coefficients. **a** Behaviour of A^*_{11}. **b** Behaviour of Θ^*_1

One gets approximately the same errors as in the transverse case (see Tables 2a and 2b, to be compared to Tables 1a and 1b, respectively). The same remarks as in Subsect. 5.1 apply. To give an idea of the accuracy of the Taylor expansion we plot in Fig. 3 the value of A^*_{11} as function of α_1 for $\alpha_2 = 10$. Also plotted are the Taylor expansions $A^*_{11}(n)$ up to order $n = 4$. It is clear that the approximation is excellent, even far away from $(5, 5)$.

Remark 5.1 Let us remark that, for the calculation of the Taylor expansions, only one matrix was assembled and factorized once and for all.. Depending on n, this matrix was then solved for $3\ (n = 0)$, $9\,(n = 1)$, $18\,(n = 2)$,

Table 2. Errors between exact and Taylor's expansion of the homogenized coefficients in the two-dimensional continuous surface roughness case

a. Homogenized diffusion matrix

$ERROR(n, N, A^*)$	$N = 5$	$N = 10$	$N = 20$	$N = 40$
$n = 0$	0.92170506	0.92174278	0.921744	0.921744
$n = 1$	0.65093702	0.65107469	0.651080	0.651079
$n = 2$	0.28711604	0.2872245	0.287225	0.287226
$n = 3$	0.0577645	0.057884	0.057872	0.057886
$n = 4$	2.864×10^{-4}	1.109×10^{-5}	1.219×10^{-6}	1.19×10^{-6}

b. Homogenized convection vector

$ERROR(n, N, \Theta^*)$	$N = 5$	$N = 10$	$N = 20$	$N = 40$
$n = 0$	0.5035976	0.5036178	0.5036195	0.5036198
$n = 1$	2.156×10^{-3}	2.132×10^{-3}	2.130×10^{-3}	2.129×10^{-3}
$n = 2$	1.793×10^{-3}	1.764×10^{-3}	1.762×10^{-3}	1.761×10^{-3}
$n = 3$	1.477×10^{-3}	1.446×10^{-3}	1.443×10^{-3}	1.442×10^{-3}
$n = 4$	1.232×10^{-3}	1.200×10^{-3}	1.196×10^{-3}	1.196×10^{-3}

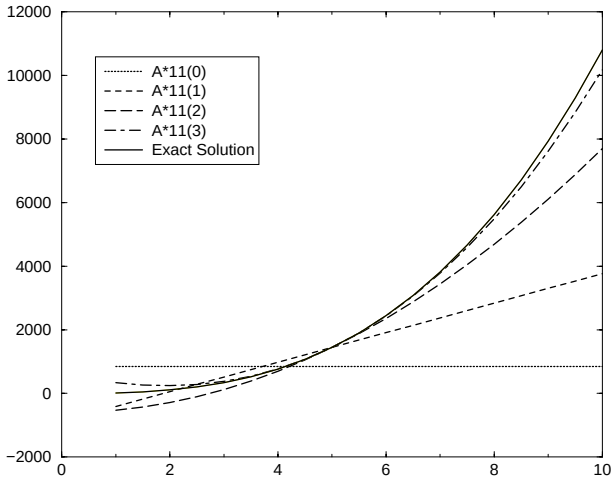

Fig. 3. Accuracy of Taylor expansion $A^*_{11}(n)$ with respect to α_1 with $\alpha_2 = 10$. The curve of the 4-th order expansion is not visible because it coincides (within resolution accuracy) with the exact solution

$30\,(n = 3)$ or $45\,(n = 4)$ different right-hand sides. The comparative efficiency with respect to solving local problems for numerous values of α_1 and α_2 (each involving a new matrix) is evident.

Table 3. Errors between exact and Taylor's expansion of the homogenized coefficients in the two-dimensional discontinuous surface roughness case

a. Homogenized diffusion matrix

$ERROR(n, N, A^*)$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
$n = 0$	0.917014	0.917027	0.917035	0.917035
$n = 1$	0.638754	0.638789	0.638812	0.638811
$n = 2$	0.275704	0.275750	0.275781	0.275780
$n = 3$	0.053911	.053956	0.053988	0.053987
$n = 4$	7.35×10^{-5}	2.76×10^{-5}	3.65×10^{-6}	2.52×10^{-6}

b. Homogenized convection vector

$ERROR(n, N, \Theta^*)$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
$n = 0$	0.492260	0.492288	0.492306	0.492306
$n = 1$	3.53×10^{-3}	3.48×10^{-3}	3.45×10^{-3}	3.45×10^{-3}
$n = 2$	2.72×10^{-3}	2.65×10^{-3}	2.62×10^{-3}	2.62×10^{-3}
$n = 3$	2.06×10^{-3}	1.98×10^{-3}	1.94×10^{-3}	1.94×10^{-3}
$n = 4$	1.60×10^{-3}	1.51×10^{-3}	1.47×10^{-3}	1.47×10^{-3}

5.3. Two-dimensional discontinuous surface roughness

We will end up by showing that the accuracy of the Taylor expansions does not depend on the regularity of the roughness function with respect to the spatial variables y_1, y_2. For this we choose a quite limit case, namely the following discontinuous function (see Fig 1c):

$$H_1(y_1 + \tfrac{1}{2}, y_2 + \tfrac{1}{2}) = \begin{cases} \beta & \text{if } |\cos\theta \cdot y_1 - \sin\theta \cdot_y 2| \\ & \leq a \text{ and } |\sin\theta \cdot y_1 + \cos\theta \cdot y_2| \leq a \\ 0 & \text{otherwise} \end{cases}$$

with $\beta = 0.5$ and $\theta = \pi/3$.

Considering the same errors given by (5.1)-(5.2) we obtain the results listed in Tables 3a and 3b. It is observed that the remarks in Subsect. 5.1 indeed apply, with the exception that the error now level off at $N \simeq 40$. Non-smooth roughness functions thus require finer meshes, but not higher order expansions.

6. Discussion

The previous sections have shown that accurate Taylor expansions for homogenization problems can indeed be calculated. The impact on the CPU cost of calculating local homogenized coefficients is evident. Only one matrix is to be assembled and factorized, and once the Taylor expansion is

known the solution of local problems is replaced by the simple evaluation of a polynomial expression. By the way, it has been shown that fourth order Taylor expansions are extremely accurate for the homogenization of the modified compressible Reynolds equation. Thus, rigorous homogenized coefficients can be evaluated at very low cost, and there is no need to approximate them by heuristic formulae.

We should remark, however, that the concepts introduced above have wider, and perhaps more relevant applications. We will discuss two of them: They allow for the implementation of Newton-Raphson iterative methods in nonlinear homogenization, and they open the way towards systematic analysis of optimization and inverse problems.

6.1. Newton-Raphson iterations

Let us consider the homogenized nonlinear system (2.13). For its discretization, a finite-dimensional space $W_h \subset H^1(\Omega)$ is introduced. We set

$$W_h^D = \left\{ p_h \in W_h \diagup \quad p_{h|\partial\Omega} = 1 \right\}$$

and

$$W_h^0 = \left\{ p_h \in W_h \diagup \quad p_{h|\partial\Omega} = 0 \right\}$$

The discrete version of (2.13) thus reads: "Find $P_{0h} \in W_h^D$ such that

$$F(P_{0h}, q_h) = 0 \quad \forall q_h \in W_h^0 \tag{6.1}$$

where

$$F(P_{0h}, q_h) = \int_\Omega [A^*(H_0(x), P_{0h}(x)) \nabla P_{0h} . \nabla q_h \\ - \Lambda P_{0h}(x) \Theta^*(H_0(x), P_{0h}(x)) . \nabla q_h] dx$$

A Newton-Raphson iteration to solve (6.1) thus reads

$$\begin{cases} \text{1. Let } P_{0h}^n \text{ be given in } W_h^D \\ \text{2. Find } \delta^n \in W_h^0 \text{ satisfying the linear system} \\ D_1 F\left(P_{0h}^n, q_h\right) . \delta^n = -F\left(P_{0h}^n, q_h\right) \quad \forall q_h \in W_h^0 \\ \text{3. Set } P_{0h}^{n+1} = P_{0h}^n + \delta^n \text{ and go back to 1.} \end{cases} \tag{6.2}$$

where $D_1 F$ is the derivative of F with respect to $\alpha_2 (= P_0(x))$ and is given by

$$
\begin{aligned}
D_1 F\left(P_{0h}^n, q_h\right).\delta^n = & \int_\Omega A^*\left(H_0(x), P_{0h}^n(x)\right)\nabla\delta^n.\nabla q_h dx \\
& -\Lambda\int_\Omega \delta^n \Theta^*(H_0(x), P_{0h}^n(x)).\nabla q_h dx \\
& +\int_\Omega \delta^n \frac{\partial A^*}{\partial \alpha_2}\left(H_0(x), P_{0h}^n(x)\right)\nabla P_{0h}^n.\nabla q_h \\
& -\Lambda\int_\Omega \delta^n \frac{\partial \Theta^*}{\partial \alpha_2}(H_0(x), P_{0h}^n(x)) P_{0h}^n.\nabla q_h dx
\end{aligned}
$$

The matrix involved in (6.2), if $\left\{\varphi^I\right\}_{I=1,N}$ is a (e.g. finite-element) basis of W_h^0, is

$$
\begin{aligned}
M_{IJ} = & \int_\Omega \left[A^*\nabla\varphi^I.\nabla\varphi^J - \Lambda\Theta^*\varphi^J\nabla\varphi^I\right] dx \\
& +\int_\Omega \left[\varphi^J\frac{\partial A^*}{\partial P_0}\nabla P_{0h}^n.\nabla\varphi^I - \Lambda P_{0h}^n\varphi^J\frac{\partial\Theta^*}{\partial P_0}.\nabla\varphi^I\right]
\end{aligned}
$$

so that the derivatives of A^* and Θ^* with respect to P_0 are needed. At this point, if one has already constructed the Taylor expansions of A^* and Θ^*, one can simply differentiate them with respect to the second variable (α_2 in (3.1) and (3.2)) and in that way obtain the Taylor expansions of $\dfrac{\partial A^*}{\partial P_0}$ and $\dfrac{\partial\Theta^*}{\partial P_0}$.

Remark 6.1 Some readers may prefer calculate A^* and Θ^* for each value of $H_0(x)$ and $P_{0h}^n(x)$ by solving local problems instead of following the Taylor-expansion procedure we propose. That could be the case in massively parallel computers, as local problems are easily solved in parallel. In such a framework, the calculation of $\dfrac{\partial A^*}{\partial P_0}$ and $\dfrac{\partial\Theta^*}{\partial P_0}$ can indeed be done following the same procedures presented in Subsect. 3.2 to calculate first derivatives of the coefficients with respect to α_2. This is clear from the fact that the Newton-Raphson method is based upon a first-order Taylor expansion around P_{0h}^n.

6.2. Optimal design and inverse problems

In much the same way as the ability to differentiate the homogenized coefficients allows for the evaluation of Newton-Raphson matrices, it is possible to use them in optimal design problems. An immediate application, in the specific problem considered, is the determination of an optimal shape of the surface to surface gap $H_0(x)$. More generally, as the procedures described apply to any parameter that enters the local problems, it is not difficult to

attack the optimization of other local quantities, such as the orientation or shape of the inhomogeneities.. As details concerning this would need additional notation and numerous formulae, we will just provide an outline of the key facts below.

Equation (2.7), or more generally equation (2.11), lead after homogenization to problems of the form

$$-\nabla.\,(A^*\nabla u) + \nabla.\,(\Theta^* u) = f^* \tag{6.3}$$

where the coefficients A^* , Θ^* and f^* depend on the properties of inhomogeneities and, possibly, on the solution itself. Optimal design (or inverse) problems for (6.3) thus enter within the framework of optimization with respect to the coefficients of a partial differential equation (also called "optimization with respect to material parameters") of which several applications can be found, e.g., in [1]. The only difference is that A^* , Θ^* and f^* are not explicit functions of the shape and properties of inhomogeneities, but are implicitly defined through a local problem. However, as shown previously, this does not preclude their evaluation or differentiation, so that optimization techniques can indeed be applied.

7. Conclusions

In this article, it has been shown how to differentiate homogenized coefficients, defined by means of local problems, with respect to parameters involved in the differential operators of the local problems. An immediate application of this is the construction of Taylor expansions that, when accurate enough, significantly reduce the cost of the solution of nonuniform and/or nonlinear problems. In fact, it was shown that, for a technologically relevant lubrication problem, a fourth order Taylor formulae is very accurate, and thus that after the expansion is built, local problems can be replaced by the inexpensive evaluation of polynomials of degree four. As a by-product, Newton-Raphson iteration matrices are obtained that improve nonlinear convergence.

In a more general setting, the two-scale theory of optimal design is of wide applicability to two-scale problems, in particular in what concerns the determination of optimal characteristics of the inhomogeneities with respect to globally defined criteria. The differentiation procedures presented in this article allow for immediate application of optimal design techniques in an homogenization framework, a line of research that has been little explored.

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A. Proof of Proposition 4.2

We will use a continuous projection (or interpolation) operator $\pi_h : V \to V_h$ satisfying

$$\|\pi_h w - w\| \leq C_\pi h^K \qquad \forall w \in V \cap H^{K+1}(Y) \tag{A.1}$$

Let l be a nonnegative integer ($l \geq 1$), $W_l = V^l$ and $W_{l,h} = V_h^l$ and consider the following block-triangular bilinear form defined on W_l:

$$A((v^1, v^2, ..., v^l), (\xi^1, \xi^2, ..., \xi^l)) = \sum_{i=1}^{l} \sum_{j=1}^{i} b_{ij}(v^j, \xi^i) \tag{A.2}$$

where b_{ij} $(1 \leq i \leq l, 1 \leq j \leq i)$ are bilinear forms defined on V and satisfying the following:

There exists positive constants β_{ij}, δ_i such that

$$|b_{ij}(\varphi, \omega)| \leq \beta_{ij} \|\varphi\| \|\omega\| \qquad \forall\, (\varphi, \omega) \in V \times V \tag{A.3}$$

$$b_{ii}(\varphi, \varphi) \geq \delta_i \|\varphi\|^2 \qquad \forall \varphi \in V \tag{A.4}$$

We have the following lemma.

Lemma A.1 *Let* $u, \chi \in \left(H^{K+1}(Y)\right)^l \subset W_l$ *and define* u_h *and* $\chi_h \in W_{l,h}$ *by*

$$A(u - u_h, \xi) = 0 \qquad \forall \xi \in W_{l,h} \tag{A.5}$$

$$A(v, \chi - \chi_h) = 0 \qquad \forall v \in W_{l,h} \tag{A.6}$$

Then there exists a positive constant C *such that*

$$\|u - u_h\|_{W_l} \leq Ch^K \tag{A.7}$$

$$\|\chi - \chi_h\|_{W_l} \leq Ch^K \tag{A.8}$$

Proof. We begin by the proof of (A.7). It suffices to prove by induction that

$$\|e_{h,i}\| = \left\|u^i - u_h^i\right\| \leq Ch^K \qquad \text{for } 1 \leq i \leq l. \tag{A.9}$$

By setting $\xi = \left(\xi^1, 0, ..., 0\right)$ in equation (A.5) we obtain

$$b_{11}(u^1 - u_h^1, \xi^1) = 0 \qquad \forall \xi^1 \in V_h$$

and the desired estimate for $i = 1$ is classical. Suppose now that (A.9) is valid for $i = 1, ..., j-1$ $(j \leq l)$. By taking, in equation (A.5), ξ such that $\xi^i = 0$ for $i \neq j$ and $\xi^j \in V_h$ we obtain

$$\sum_{i=1}^{j} b_{ji}(u^i - u_h^i, \xi^j) = 0 \qquad \forall \xi^j \in V_h \tag{A.10}$$

Using Eq. (A.10), the continuity of b_{ij} (A.3), the strong coercivity of b_{ii} (A.4) and (A.1) we obtain the following:

$$\begin{aligned}
\|e_{h,j}\|^2 &\leq \frac{1}{\delta_j} b_{jj}\left(e_{h,j}, e_{h,j}\right) \\
&= \frac{1}{\delta_j} b\left(e_{h,j}, u^j - \pi_h\left(u^j\right)\right) + \frac{1}{\delta_j} b_{jj}\left(e_{h,j}, \pi_h e_{h,j}\right) \\
&\leq \frac{C_\pi \beta_{jj}}{\delta_j} \|e_{h,j}\| h^K + \frac{1}{\delta_j} \left| \sum_{i=1}^{j-1} b_{ji}\left(e_{h,j}, \pi_h e_{h,i}\right) \right| \\
&\leq \frac{C_\pi \beta}{\delta_j} \|e_{h,j}\| \left\{ \beta_{jj} h^K + \beta_{ji} \sum_{j=0}^{j-1} \|e_{h,j}\| \right\}
\end{aligned}$$

Now from the induction hypothesis we obtain $\|e_{h,j}\| \leq Ch^K$ and the proof of (A.7) is complete.

The proof of (A.8) is analogous, but in this case the induction is made in the opposite sense; i.e., the proof begins by showing that $\left\|\chi^l - \chi_h^l\right\| \leq Ch^K$ (this is done taking, in (A.6), $v^1 = v^2 = ... = v^{l-1} = 0$ and $v^l \in V_h$ arbitrary). □

Remark A.1 Lemma A.1 can be generalized to the case where, instead of the strong coercivity (2.4), we have the weak discrete coercivities

$$\inf_{\varphi\in V_h}\sup_{\psi\in V_h}\frac{b_{ii}(\varphi,\psi)}{\|\varphi\|\,\|\psi\|}\geq\delta_i$$
$$\inf_{\psi\in V_h}\sup_{\varphi\in V_h}\frac{b_{ii}(\varphi,\psi)}{\|\varphi\|\,\|\psi\|}\geq\delta_i$$

but the proof is of course different.

Lemma A.2 *Let $F:W_l\to\mathbb{R}$ be a C^2-function and assume that, for some $u\in\left(H^{K+1}(Y)\right)^l\subset W_l$, $J=DF(u)$ is such that the solution χ of*

$$A(v,\chi)=J(v)\qquad\forall v\in W_l \tag{A.11}$$

belongs to $\left(H^{K+1}(Y)\right)^l$, where A is as in Lemma A.1. We define $u_h\in W_h$ by

$$A(u-u_h,\xi)=0\qquad\forall\xi\in W_h \tag{A.12}$$

Then

$$|F(u)-F(u_h)|\leq Ch^{2K} \tag{A.13}$$

Proof. Since F is of class C^2, there exists a positive constant c such that

$$|F(u)-F(u_h)|\leq|J(u-u_h)|+c\,\|u-u_h\|_{W_l}^2$$

Let χ_h be a discrete solution to problem (A.11). Then we have

$$A(v,\chi-\chi_h)=0\qquad\forall v\in W_{l,h}$$

From Lemma A.1, we get

$$\|u-u_h\|_{W_l}\leq Ch^K$$
$$\|\chi-\chi_h\|_{W_l}\leq Ch^K$$

Now from (A.11) and (A.12) we have

$$\begin{aligned}|J(u-u_h)|&=|A(u-u_h,\chi-\chi_h)|\\&\leq C.\,\|u-u_h\|_{W_l}\,\|\chi-\chi_h\|_{W_l}\\&\leq Ch^{2K}\end{aligned}$$

□

Proof of Proposition 4.2. We will sketch the proof of the "scalar" case, namely when $\alpha \in \mathbb{R}$. No additional difficulty is posed by $\alpha \in \mathbb{R}^2$. Let us come back to the generic form (2.11).For l a nonnegative integer ($\leq m$) The i-th ($i \leq l$) order derivative of z and of its discrete approximation z_h at α^0 are given, respectively, by

$$b(\alpha^0; \frac{\partial^i z}{\partial \alpha^i}, v) = \left\langle \frac{\partial^i f}{\partial \alpha^i}, v \right\rangle - \sum_{j=0}^{i-1} \binom{i}{j} \frac{\partial^{i-j} b}{\partial \alpha^{i-j}} \left(\alpha^0, \frac{\partial^j z}{\partial \alpha^j}, v \right)$$

(A.14) $\forall v \in V$

$$b(\alpha^0; \frac{\partial^i z_h}{\partial \alpha^i}, v) = \left\langle \frac{\partial^i f}{\partial \alpha^i}, v \right\rangle - \sum_{j=0}^{i-1} \binom{i}{j} \frac{\partial^{i-j} b}{\partial \alpha^{i-j}} \left(\alpha^0, \frac{\partial^j z_h}{\partial \alpha^j}, v \right)$$

(A.15) $\forall v \in V_h$

where $\dfrac{\partial^j b}{\partial \alpha^j}$ are defined in (3.5).

Let $e_{h,i}$ be the error in the i-th order derivative

$$e_{h,i} = \frac{\partial^i z}{\partial \alpha^i} - \frac{\partial^i z_h}{\partial \alpha^i} \qquad i = 1, 2, ..., l$$

Consider the following bilinear form in W_{l+1} (we omit the parameter α, that is fixed $\alpha = \alpha^0$),

$$A((v^1, v^2, ..., v^{l+1}), (\xi^1, \xi^2, ..., \xi^{l+1})) = \sum_{i=1}^{l+1} \sum_{j=1}^{i} \binom{i-1}{j-1} \frac{\partial^{i-j} b}{\partial \alpha^{i-j}} (v^j, \xi^i)$$

also, let $L : W_{l+1} \to \mathbb{R}$ be defined by

$$L(\xi^1, \xi^2, ..., \xi^{l+1}) = \sum_{i=1}^{l+1} \left\langle \frac{\partial^i f}{\partial \alpha^i}, \xi^i \right\rangle$$

We have thus, from (A.14)-(A.15), and by setting $u = (z, \dfrac{\partial z}{\partial \alpha}, ..., \dfrac{\partial^l z}{\partial \alpha^l})$ $\in W_{l+1}$ and $u_h = (z_h, \dfrac{\partial z_h}{\partial \alpha}, ..., \dfrac{\partial^l z_h}{\partial \alpha^l}) \in W_{l+1,h}$:

$$A(u, \xi) = L(\xi) \qquad \forall \xi \in W_{l+1}$$
$$A(u_h, \xi) = L(\xi) \qquad \forall \xi \in W_{l+1,h}$$

and thus

$$A(u - u_h, \xi) = 0 \qquad \forall \xi \in W_{l+1,h}$$

Moreover the bilinear form A is of the form given in (A.2) with

$$b_{ij}(\varphi,\omega)=\frac{\partial^{i-j}b}{\partial\alpha^{i-j}}(\varphi,\omega)\qquad\forall(\varphi,\omega)\in V\times V$$

As the periodicity assumption precludes any singularity coming from the domain shape, from (A.14) and (4.5) we have $\dfrac{\partial^i z}{\partial\alpha^i}\in H^{K+1}(Y)$, and then $u\in W_{l+1}\cap\left(H^{K+1}(Y)\right)^{l+1}$. The hypotheses of continuity and coercivity (A.3) and (A.4) follow from (3.6) and (2.4). Thus all hypotheses of Lemma A.1 are satisfied and we have:

$$\left\|\frac{\partial^i z}{\partial\alpha^i}-\frac{\partial^i z_h}{\partial\alpha^i}\right\|\leq Ch^K\qquad i=1,2,...,l$$

Let us now show (4.8)-(4.9). Notice that, from hypothesis (2.9) and for α fixed, $\tilde{A}^*$ and $\tilde{\Theta}^*$ and all of their derivatives of order up to $k=m-2$, are in fact C^2-functions defined on W_{l+l} (the $k-th$ order derivatives of $\tilde{A}^*$ and $\tilde{\Theta}^*$ depend on the derivatives of ω_i and χ_i up to the order k). Thus we get the error estimation (4.8) and (4.9) in $\tilde{A}^*$ and $\tilde{\Theta}^*$ and all of their derivatives from Lemma A.2. $\square$