On the optimization of microstructurally motivated calculations in engineering mechanics *

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Abstract

One of principal research directions in computational mechanics is to describe and analyze multi-scale systems and phenomena where at least one macro- and one microscale has to be distinguished. Since such scales in realistic problems differ dramatically (often as meters and micrometers), the standard mesh refinement technique, well-known from the finite element analysis, is not available or leads to very slow and expensive calculations. This paper demonstrates on a model boundary problem how the mathematical two-scale convergence theory can help to bridge the gap between the macro- and microanalysis, using certain special iterative algorithm, with rather weak requirements to the method of interpolation. Some useful generalizations and references and comments to technical applications are presented, too.

1 Macro- and microanalysis in computational mechanics

In various engineering applications of the continuum mechanics the reliable analysis of behaviour of material samples, constructions, etc., cannot avoid information from the microstructural material analysis. Complex models "from nano-scale particles to terrestrial bodies" (as [19]) lead to very expensive numerical calculations – it is nearly impossible to cover two (or even more) scales by some unified family of decomposition to finite elements because the size of particles is typically between micro- and millimeters, but the size of the whole sample or construction is in meters: Figure 1 shows the structure of some commonly used building materials, including materials for special insulation layers, with various number, type, shape and size of

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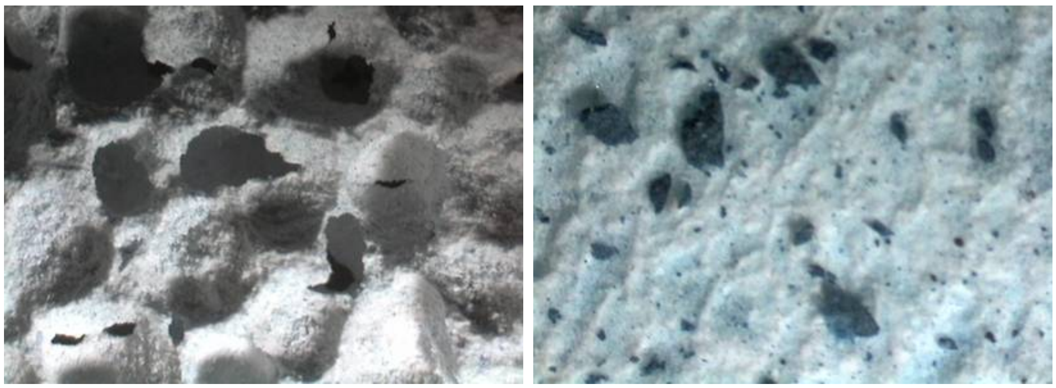
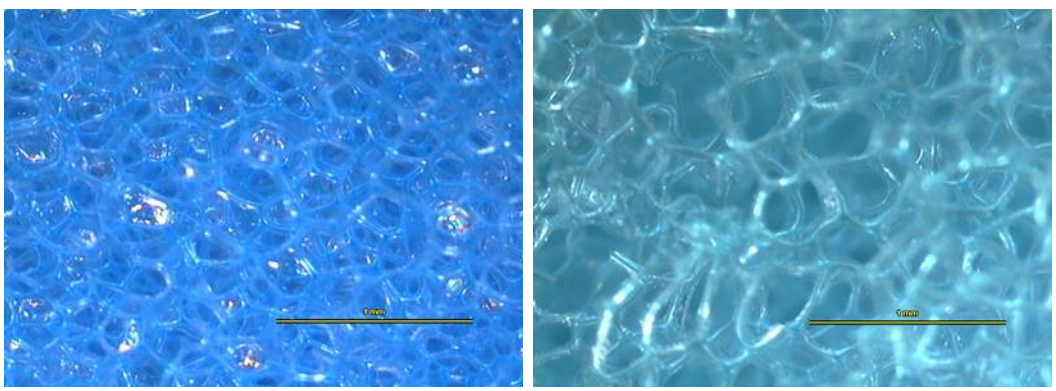
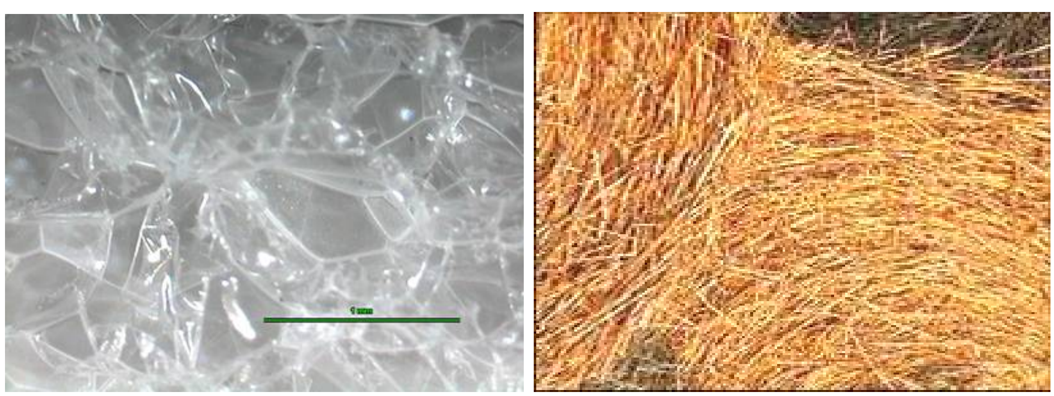
pores (which is substantial, e. g., for the numerical analysis of moisture and heat transfer in buildings). Figure 2 the structure of some advanced metal-based materials (important for the study of heat treatment of alloys, phase transformations, etc.). On the other side, most results of the separate microscale analysis can be naturally extended to the macroscale one only under very strong (often non-realistic) both physical and geometrical assumptions (on symmetry, exact periodicity, etc.).



gas concrete fire-clay brick

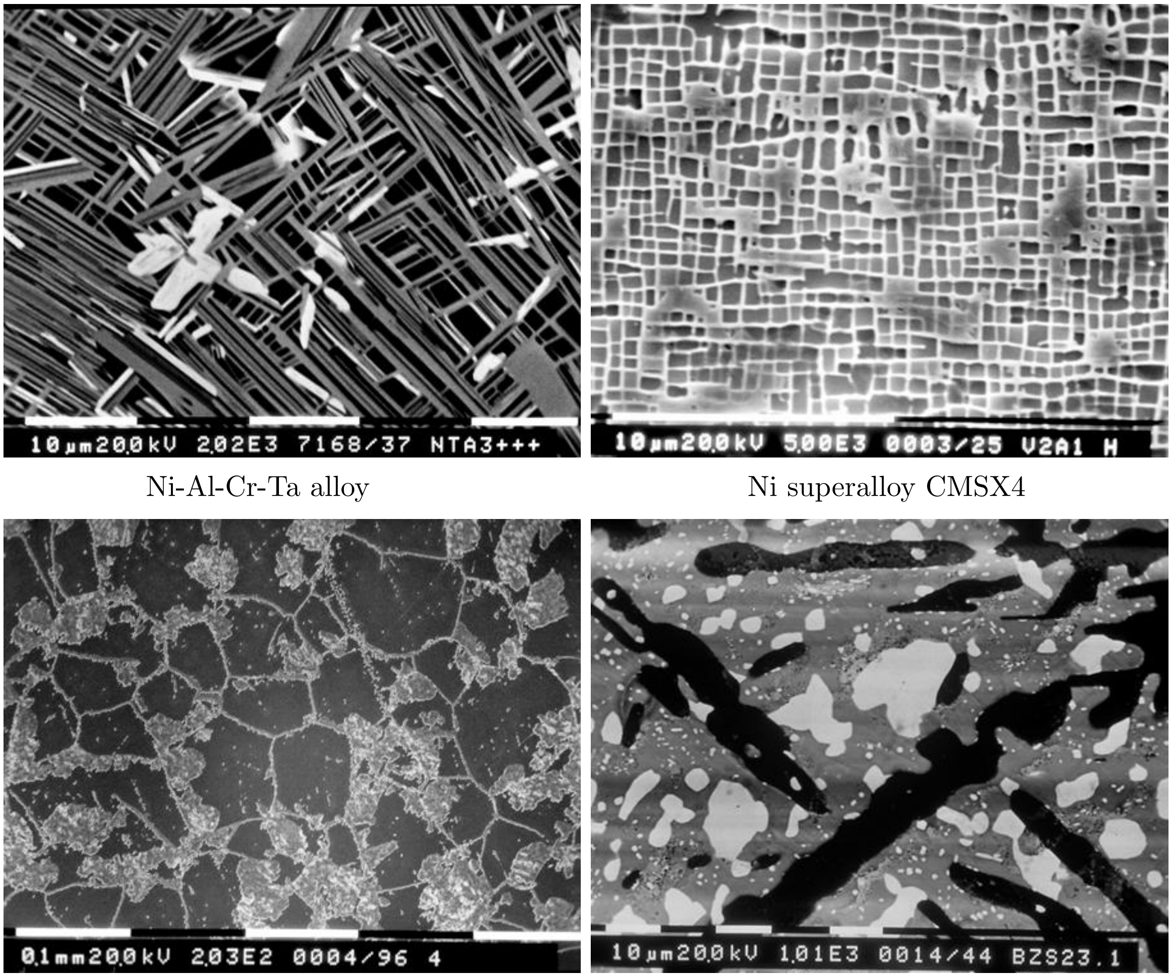


2 types of polyurethan-based insulation



foam polyethylen straw pannel Stramit

Figure 1: Structure of some porous building materials
(Laboratory of Building Physics, Faculty of Civil Engineering, Brno University of Technology)



Ni-Al-Cr-Ta alloy — Ni superalloy CMSX4

superaustenitic iron NICROFER — Bi-Sn-Zn alloy

Figure 2: Structure of some advanced alloys
(Institute of Physics of Materials in Brno, Academy of Sciences of the Czech Republic)

The aim of all two-scale (or even multi-scale) studies of problems from engineering mechanics is to bridge the gap between the micro- and macrostructural analysis and to optimize the hardware and software requirements of numerical implementation of corresponding models. Unfortunately, the term "two-scale problems" appears in at least two different senses in the literature. The first one (referenced by i) here) emphasizes that two levels of not necessarily nested grids are considered (often with no deeper analysis of microstructural phenomena), the second one (referenced by ii) here) makes use of the two-scale homogenization theory, based on the careful definition of the two-scale convergence (more general than the strong convergence, less general than the weak one). This paper tries to demonstrate how both these approaches are able to be combined to guarantee similar results as standard numerical (e. g.finite element) techniques.

The typical example of the original theoretical analysis of type i) is [5]; consequently in [6] a family of iterative method is studied to solve second-order elliptic system with two-scale data using two levels of grids (in the numerical example the Dirichlet problem for the Poisson equation). Another approach is presented in [23]: the aim is to prove good convergence properties near corners of planar domains with complicated shapes which is the reason for the construction of a two-scale grid (with very precise near-boundary triangular elements).

The fundamental definitions and lemmas of the theory ii) come from [20] and [1]. The extensive overview of standard homogenization methods for periodic material structures, including G-, H-, Γ- and two-scale convergence, with applications to linearized elasticity, heat and wave equations, can be found in [2]. The two-scale convergence technique is applicable even to strongly nonlinear elliptic problems (cf. [29]) and to rather general parabolic problems (cf. [7]); such parabolic problems can be analyzed numerically as sequences of elliptic problems with help of the method of Rothe (cf. [28]). Also the assumption of material periodicity can be weakened substantially (cf. [8]). Moreover, in last several years some authors systemize more general convergence concepts, avoiding the formal notion of the two-scale convergence: the "scale convergence" from [14] is based on the theory of (generalized) Young measures, [21] and [22] work with rather abstract "proper H-structures", etc. However, the motivation for the two-scale approach comes from problems of technical physics and engineering. Unlike some other homogenization methods, its fundamentals are both geometrically and physically transparent and contain no artificial or tricky choices of admissible test functions. General software packages for the analysis of problems of continuum mechanics typically ignore all advanced homogenization approaches; however, a lot of non-commercial numerical algorithms and software codes for special problems (not only for those discussed in [2]) has been developed yet. Some classical problems in mechanics (from linear elastostatics to local contact conditions and elastoplasticity with infinitesimal strain) are covered by the analysis [26], the equations of heat transfer are studied in details in [11], etc.

To demonstrate that it is possible to suggest rather simple algorithm to couple the micro- and macroanalysis and not to debase convergence properties of commonly used numerical methods, we shall formulate a linear elliptic model problem with homogeneous Dirichlet boundary conditions and explain the convergence of our approach for the special type of construction of finite-dimensional approximating spaces (e. g.for the linear finite element interpolation, discussed in the same context in [27], in particular on polyhedral domains). Then, removing some simplifications, we shall observe the consequences, sketch how to overcome corresponding difficulties and refer to relevant literature.

2 Iterative algorithm for a model problem

Let us consider a domain Ω in the real Euclidean space R^3 and a subspace V of the Sobolev space $W^{1,2}(\Omega)$ containing $W_0^{1,2}(\Omega)$ (Dirichlet boundary conditions are included here). Let Λ be some subdomain of Ω; in practice $\operatorname{vol}\Omega \gg \operatorname{vol}\Lambda$. Let us assume that the decomposition of Ω (well-known from the finite element theory) generates finite-dimensional spaces V_h and the decomposition of Λ finite-dimensional spaces V_δ; h and δ here are norms of such decompositions (for $h \gg \delta > 0$ the notation V_h and V_δ cannot be mismatched) and we expect $V_\delta \to V$ and $V_h \to V$ as $h, \delta \to 0$ is some reasonable sense. For simplicity, we shall now assume that V_h and V_δ are even subspaces of V; we just know that it is not realistic to assume some relation between V_h and V_δ a priori. Following [5], let us therefore introduce a new space (of higher finite dimension) $V_{h\delta} = V_h + V_\delta$. Since all above mentioned spaces are Hilbert ones, it is possible to define operators of orthogonal projections $P_h\, V_{h\delta} \to V_h$ and $P_\delta : V_{h\delta} \to V_\delta$, using an arbitrary bilinear, symmetric, continuous and coercive form $a : V \times V \to R$ (as $a(.,.)$ can be identified with a scalar product in V). These projections will be crucial for the design of the iterative algorithm, generating special sequences of approximate solutions of our model problem.

Let us consider some "external load" $f \in V^*$ (V^* is a dual space to V, $\langle .,. \rangle$ will denote the duality between V and V^*). We shall try to construct the bilinear form a from the formula

$$a(u,v) = \int_\Omega \widetilde{A}(x)\nabla u(x) \cdot \nabla v(x)\,\mathrm{d}x$$

for every $u, v \in V$. It is not quite easy because we do not know "homogenized material characteristics" $\widetilde{A}$ on Ω properly – at least on Λ (where we intend to analyze lower-scale phenomena) we have to obtain them by some homogenization process (via $\varepsilon \to 0$) from

$$a^\varepsilon(u^\varepsilon, v) = \int_\Omega A(x, x/\varepsilon)\nabla u^\varepsilon(x) \cdot \nabla v(x)\,\mathrm{d}x$$

where some "quasiperiodic material characteristics" A are prescribed in the Lebesgue space $L^\infty(\Omega \times R^3)$ such that its values are Y-periodic in the second variable, Y is a unit cell in R^3 (a representative volume element of paralleliped shape, often rescaled as $Y = [0,1]^3$) and $u^\varepsilon, v \in V$ again. To make the homogenization possible, we shall need

$$\lim_{\varepsilon \to 0} a^\varepsilon(u^\varepsilon, v) = a(u,v)\,. \tag{1}$$

To guarantee the validity of (1) is not trivial. The explicit form of $\widetilde{A}$ is known only in very special cases, as for layered materials (see [2], p. 98), including simple applications to heat propagation (cf. [11]). In most cases a deeper knowledge of the two-scale convergence theory is necessary. For simplicity, the symbol $\to$ will be reserved for the strong convergence, the symbol $\rightharpoonup$ for the weak convergence and the symbol $\rightharpoonup\!\!\rightharpoonup$ for the two-scale convergence in the following sense (by [2], p. 176): we say that a sequence $\{v^\varepsilon\}$, constructed for such positive ε that $\varepsilon \to 0$, two-scale converges to $v_0 \in L^2(\Lambda \times Y)$, briefly $v^\varepsilon \rightharpoonup\!\!\!\rightharpoonup v_0$, iff

$$\lim_{\varepsilon\to 0} \int_\Lambda v^\varepsilon(x)\psi(x, x/\varepsilon)\,\mathrm{d}x = (\mathrm{vol}\,Y)^{-1} \int_\Lambda \int_Y v_0(x,y)\psi(x,y)\,\mathrm{d}y\,\mathrm{d}x$$

for every $\psi \in C_0^\infty(\Lambda, C_\#^\infty(Y))$; the lower index $_\#$ here forces the Y-periodicity. Let us sketch the basic idea of the the two-scale homogenization now (much more details are presented in [2] – the crucial proof can be found in [2], p. 182, many generalizations are available). Since $\{u^\varepsilon\}$ is a bounded sequence in V (or at least in certain V^Λ, containing all restrictions of functions from V to Λ), $u^\varepsilon \rightharpoonup\!\!\!\rightharpoonup u_0$ holds for some $u_0 \in L^2(\Lambda \times Y)$ constant in the second variable, thus also $u^\varepsilon \to u_0$ (where the second variable is omitted) in $L^2(\Lambda)$. Moreover, $\nabla u^\varepsilon \rightharpoonup\!\!\!\rightharpoonup \nabla_x u_0 + \nabla_y u_1$ ($x \in \Lambda$, $y \in Y$); here an additional function $u_1 \in L^2(\Lambda, W_\#^{1,2}(Y))$ has the zero mean value

$$\int_Y u_1(.,y)\,\mathrm{d}y = 0$$

on Λ. Consequently also $A^\varepsilon(./\varepsilon)\nabla u^\varepsilon \rightharpoonup \widetilde{A}\nabla u_0$ in $L^2(\Lambda)^3$. Unfortunately, a corresponding $\widetilde{A} \in L^2(\Lambda)$, for a fixed $x \in \Lambda$ a constant elliptic matrix, cannot be determined in a simple way – its general derivation requires solving an auxiliary system of differential or integral equations (for details see [2], p. 112). Under some more regularity assumptions such expensive calculations can be avoided; the relevant discussion is contained in [17], [16], [15] and [4]. The alternative "multiresolutional homogenization" of [11] is based on the MAPLE-supported wavelet analysis.

Let us now introduce our model problem: find such $u \in V$ that

$$a(u,v) = \langle f, v\rangle \tag{2}$$

for all $v \in V$; some estimate of u, denoted by u^0 (not substantial for further considerations), is available. Its discrete analogy is: find such $u_{h\delta} \in V_{h\delta}$ that

$$a(u_{h\delta}, v_{h\delta}) = \langle f, v_{h\delta}\rangle \tag{3}$$

for all $v_{h\delta} \in V_{h\delta}$. In particular, (2) can be expressed as

$$a(u, v_{h\delta}) = \langle f, v\rangle \tag{4}$$

for all $v_{h\delta} \in V_{h\delta}$ (because V_h and V_δ are subspaces of V).

Let ω be certain real parameter, $0 < \omega < 2$. Following [5] (with slight modifications, coming from the two-scale analysis), let us suggest the following algorithm:

1. find such $w_\delta^\varepsilon \in V_\delta$ that
$$a^\varepsilon(w_\delta^\varepsilon, v_\delta) = \langle f, v_\delta\rangle - a^\varepsilon(u^0, v_\delta) \tag{5}$$
for all $v_\delta \in V_\delta$,

2. set $u^{\frac{1}{2}} = u^0 + \omega w^\varepsilon_\delta$,
3. find such $w_h \in V_h$ that
$$a(w_h, v_h) = \langle f, v_h \rangle - a(u^{\frac{1}{2}}, v_h) \tag{6}$$
for all $v_h \in V_h$,
4. set $u^1 = u^{\frac{1}{2}} + \omega w_h$.

The solvability of (2), (5) and (6) is evident from the standard Lax-Milgram theorem (cf. [2], p. 66). Similarly (using u^1 instead of u^0) $u^{\frac{3}{2}}$, u^2, etc., can be evaluated. We shall verify that in this way we receive a sequence of approximate solutions of (2) with good convergence properties, related to its exact solution u.

Using (3) and (5) and the projection operator P_δ, we can analyze the first step of the algorithm. We obtain

$$\begin{aligned}
a(w^\varepsilon_\delta - P_\delta(u_{h\delta} - u^0), v_\delta) &= a^\varepsilon(w^\varepsilon_\delta - P_\delta(u_{h\delta} - u^0), v_\delta) \\
&\quad +(a - a^\varepsilon)(w^\varepsilon_\delta - P_\delta(u_{h\delta} - u^0), v_\delta) \\
&= \langle f, v_\delta \rangle - a^\varepsilon(u^0, v_\delta) - a^\varepsilon(P_\delta(u_{h\delta} - u^0), v_\delta) \\
&\quad +(a - a^\varepsilon)(w^\varepsilon_\delta - P_\delta(u_{h\delta} - u^0)) \\
&= \langle f, v_\delta \rangle - a^\varepsilon(u^0, v_\delta) - a(P_\delta(u_{h\delta} - u^0), v_\delta) \\
&\quad +(a - a^\varepsilon)(P_\delta(u_{h\delta} - u^0)) + (a - a^\varepsilon)(w^\varepsilon_\delta - P_\delta(u_{h\delta} - u^0)) \\
&= \langle f, v_\delta \rangle - a^\varepsilon(u^0, v_\delta) - a(u_{h\delta} - u^0, v_\delta) + (a - a^\varepsilon)(w^\varepsilon_\delta, v_\delta) \\
&= \langle f, v_\delta \rangle - a^\varepsilon(u^0, v_\delta) - \langle f, v_\delta \rangle - a(u^0, v_\delta) + (a - a^\varepsilon)(w^\varepsilon_\delta, v_\delta) \\
&= (a - a^\varepsilon)(w^\varepsilon_\delta - u^0, v_\delta)\,;
\end{aligned}$$

this yields
$$w^\varepsilon_\delta = P_\delta(u_{h\delta} - u^0) + e_\delta \tag{7}$$
where e_δ is a solution (by the Lax-Milgram theorem again) of an equation
$$a(e_\delta, v_\delta) = (a - a^\varepsilon)(w^\varepsilon_\delta - u^0, v_\delta)$$
for an arbitrary $v_\delta \in V_\delta$; this can be expressed also in form
$$a(e_\delta, v_\delta) = (a(w^\varepsilon_\delta, v_\delta) - a^\varepsilon(w^\varepsilon_\delta, v_\delta)) - (a(u^0, v_\delta) - a^\varepsilon(u^0, v_\delta))\,,$$
more transparent for the understanding of two-scale convergence properties.

Similarly, using (3) and (6) and the projection operator P_h, we can analyze the third step of the algorithm. We obtain

$$\begin{aligned}
a(w_h - P_h(u_{h\delta} - u^{\frac{1}{2}}), v_h) &= \langle f, v_h \rangle - a(u^{\frac{1}{2}}, v_h) - a(P_h(u_{h\delta} - u^{\frac{1}{2}}), v_h) \\
&= \langle f, v_h \rangle - a(u^{\frac{1}{2}}, v_h) - a(u_{h\delta} - u^{\frac{1}{2}}, v_h) \\
&= \langle f, v_h \rangle - a(u^{\frac{1}{2}}, v_h) - \langle f, v_h \rangle + a(u^{\frac{1}{2}}, v_h) = 0\,;
\end{aligned}$$

this yields (unlike the previous case, without any "ε-corrections" here)

$$w_h = P_h(u_{h\delta} - u^{\frac{1}{2}})\,. \tag{8}$$

Let us study the distance between $u_{h\delta}$ and u^1 in V. Let I be an identity mapping. Applying (8) and (7), we have

$$\begin{aligned} u_{h\delta} - u^1 &= u_{h\delta} - u^{\frac{1}{2}} - \omega w_h \\ &= (I - \omega P_h)(u_{h\delta} - u^{\frac{1}{2}}) \\ &= (I - \omega P_h)(u_{h\delta} - u^0 - \omega w_\delta^\varepsilon) \\ &= (I - \omega P_h)(I - \omega P_\delta)(u_{h\delta} - u^0) - \omega(I - \omega P_h)e_\delta\,. \end{aligned}$$

For simplicity, let us supply the Hilbert space V by the norm $\|.\| = \sqrt{a(.\,,.)}$; similar norms are admissible in finite-dimensional subspaces of V, too. The norm of $(I-\omega P_h)(I-\omega P_\delta)$ is always (under the assumption $0 < \omega < 2$) lesser than 1; this result, derived in [5] for each couple of orthogonal projectors in a finite-dimensional Hilbert space, comes from the strengthened Cauchy-Buniakowskiĭ-Schwarz inequality and from the spectral analysis of linear operators. Thus for some positive α and β where $\beta < 1$ we can conclude

$$\begin{aligned} \|u_{h\delta} - u^1\| &\le \beta\|u_{h\delta} - u^0\| + \alpha\|e_\delta\|\,, \\ \|u_{h\delta} - u^2\| &\le \beta^2\|u_{h\delta} - u^0\| + (1+\beta)\alpha\|e_\delta\|\,, \end{aligned}$$

etc., and for an integer n finally

$$\|u_{h\delta} - u^n\| \le \beta^n\|u_{h\delta} - u^0\| + \frac{1-\beta^n}{1-\beta}\alpha\|e_\delta\|\,. \tag{9}$$

One can immediately see that the limit passage $n \to \infty$ in (9) yields

$$\lim_{n\to\infty}\|u_{h\delta} - u^n\| \le \frac{\alpha}{1-\beta}\|e_\delta\|\,.$$

Thanks to (1) the homogenization step $\varepsilon \to 0$ gives

$$\lim_{n\to\infty}\|u_{h\delta} - u^n\| = 0\,.$$

However, we have not verified the expected limit relation between solutions $u_{h\delta}$ of (3) and u of (2) yet. Let us compare (3) with (4); the first simple result is

$$a(u - u_{h\delta}, v_{h\delta}) = 0\,. \tag{10}$$

To support the macro- and microscale view to Ω, let us introduce such extension operator E for functions defined on $\Omega \setminus \overline{\Lambda}$ to Λ that for every $v \in V$ corresponding $\widehat{v}$ defined as $\widehat{v} = v$ on $\Omega \setminus \overline{\Lambda}$ and $\widehat{v} = Ev$ on Λ belongs to V again.

Let r_h and r_δ be standard interpolants from V to its finite-dimensional subspaces V_h and V_δ, respectively. Let us assume that the global interpolation criterion

$$\lim_{h \to 0} \|\widehat{v} - r_h \widehat{v}\| = 0 \tag{11}$$

and the local interpolation criterion

$$\lim_{\delta \to 0} \|(v - \widehat{v}) - r_\delta(v - \widehat{v})\| = 0 \tag{12}$$

are satisfied for an arbitrary $v \in V$. Then in (10) we can set $v_{h\delta} = u_{h\delta} - \widetilde{u}_{h\delta}$ where $\widetilde{u}_{h\delta} = r_h \widetilde{u} + r_\delta(u - \widetilde{u})$. We obtain

$$a(u - \widetilde{u}_{h\delta}, v_{h\delta}) = a(u_{h\delta} - \widetilde{u}_{h\delta}, v_{h\delta}) = a(v_{h\delta}, v_{h\delta})$$

and consequently the estimate

$$\|v_{h\delta}\|^2 \leq \|u - \widetilde{u}_{h\delta}\| \|v_{h\delta}\| \,.$$

Thus we receive (if $\widetilde{u}_{h\delta} \neq u_{h\delta}$)

$$\|u_{h\delta} - \widetilde{u}_{h\delta}\| \leq \|u - \widetilde{u}_{h\delta}\|$$

and also

$$\|u - u_{h\delta}\| \leq \|u - \widetilde{u}_{h\delta}\| + \|u_{h\delta} - \widetilde{u}_{h\delta}\| \leq 2\|u - \widetilde{u}_{h\delta}\| \,.$$

The final conclusion

$$\lim_{h,\delta \to 0} \|u - \widetilde{u}_{h\delta}\| = 0$$

follows from the estimate

$$\|u - \widetilde{u}_{h\delta}\| = \|\widehat{u} + (u - \widehat{u}) - r_h \widehat{u} - r_\delta(u - \widehat{u})\| \leq \|\widehat{u} - r_h \widehat{u}\| + \|(u - \widehat{u}) - r_\delta(u - \widehat{u})\|$$

and from the global and local interpolation criteria (11) and (12).

The classical finite element convergence result is a very special case of (11) and (12); for details see [27]; under additional regularity assumptions the better convergence quality can be attached. The same paper explains the construction of the extension operator E by means of extension theorems in Sobolev spaces. However, much more numerical approaches can be included here – cf. wavelet Galerkin methods in [3], various meshfree techniques in [12], [13] and [18], etc.

3 Generalizations and examples of technical applications

Up to now, we have supposed that V_δ, V_h are subspaces of V. This may be violated in many configurations: if Ω is not convex then its finite element approximation Ω_h usually contains points outside Ω; the same argument can be repeated for certain approximation Λ_δ of Λ. Let us sketch the main arguments, how to preserve our results. We shall believe that both a^ε and a (thanks to the properties of A) are allowed to be extended from Ω to Ω_h and Λ_δ; instead of a^ε in (5) we obtain some $a^\varepsilon + a^\varepsilon_\delta$ and instead of a in (6) some $a + a_h$; a_h is defined on $\Omega_h \setminus \Omega$ and a^ε_δ on $\Lambda_\delta \setminus \Omega$. In the same way we can extend a from Ω to obtain $a_{h\delta}$ on $(\Omega_h \cup \Lambda_\delta) \setminus \Omega$; the equation (3) then contains $a + a_{h\delta}$ instead of simple a. In the analysis of the first step of our iterative algorithm we obtain an additive right-hand side term $a^\varepsilon_\delta(w^\varepsilon_\delta - u^0, v_\delta) - a_{h\delta}(u_{h\delta}, v_\delta)$, in the analysis of its second step similarly $a_h(w_h - u^{\frac{1}{2}}, v_h) - a_{h\delta}(u_{h\delta}, v_h)$. We must verify that for their bounded arguments all such bilinear forms vanish if $h, \delta \to 0$; this can be done e. g.using the Lebesgue dominated convergence theorem. In more details: we obtain some additive term $\widetilde{e}_\delta$ in (7) (not only e_δ) and d_h in (8) whose norms $\|\widetilde{e}_\delta\|$ and $\|d_h\|$ will disturb the derivation of (9); we must guarantee their convergence to zero for $h, \delta \to 0$. The other difficulty is that (4) is not an exact consequence of (2) of now; disturbing terms have to be removed in the limit case again, using the arguments from the preceding discussion.

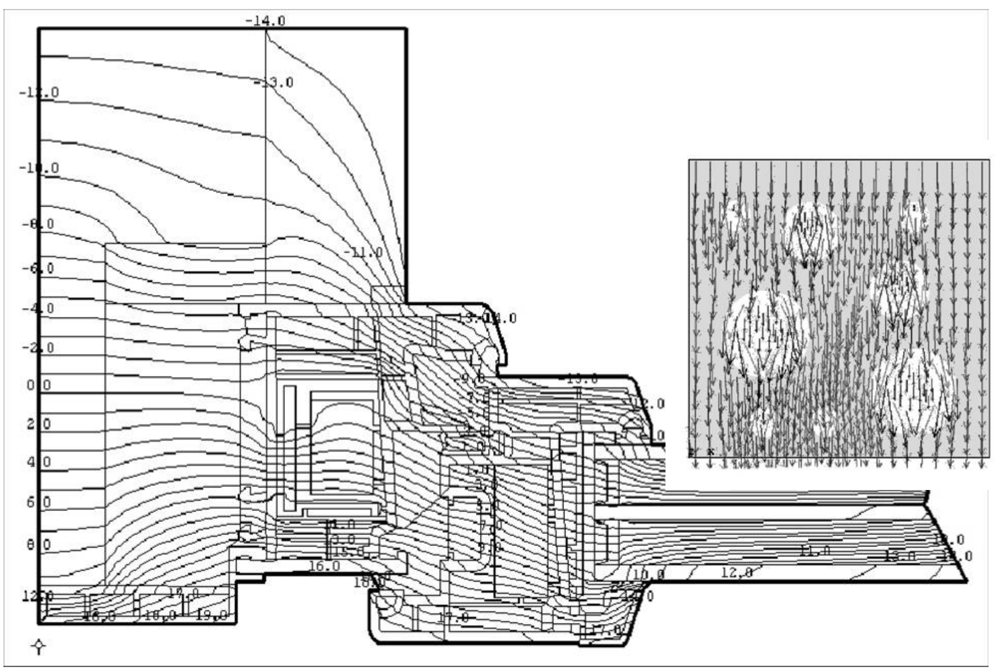


Figure 3: ANSYS-based calculations with "effective values" of heat conduction factors in porous rubber insulation layers (Department of Technology of Building Materials and Components, Faculty of Civil Engineering, Brno University of Technology)

Let us remind that our basic equation (2) occurs e. g.in the theory of stationary heat transfer with an unknown temperature field. Figure 3 demonstrates how the construction of homogenized bilinear forms a instead of discrete forms a^ε can be applied in the ANSYS-supported thermal design of new types of windows; its detail shows the thermal flows in a perforated rubber-based layer. However, such calculations can incorporate insulation material properties, but not accumulation ones. This is a motivation for the development of the same method for time-dependent parabolic problems that can be decomposed back (step-by-step) to elliptic ones, using the method of discretization in time, based on the analysis of convergence properties of Rothe sequences; principal ideas for such access can be taken from [28]. Another useful generalization leads to the (rather weak) nonlinearity of a; in fact, heat conduction factor is temperature-dependent. Unfortunately, such analysis brings technical difficulties that cannot be removed easily in general: the two-scale homogenization process, substituting a^ε by a, may be correct, but some formal generalization of the above presented algorithm may give bad results. If strong nonlinearities occur then the two-scale limit can exist even in case that no "effective" a is available and rather general measures (instead of classical Lebesgue and Hausdorff ones) are taken into consideration – cf. [29].

The macroscopic equations of heat transfer from the previous example belong to classical knowledge of mechanical and civil engineers; thus it was not very difficult to identify them with two-scale limit forms of similar equations at certain microstructural level. Unfortunately, in the analysis of more complicated physical processes in the microstructure the final macroscopic differential or integral formulation are typically not known a priori; consequently the construction of two-scale limits is complicated and no simple (linearized) numerical algorithm can be applied. One problem of this type is the analysis of the diffusive phase transformation in the substitutional multicomponent Fe-rich alloys. Nevertheless, the results of MATLAB-based numerical modelling of fields of molar fractions in this case can naturally explain some phenomena observed in the macroscopic world, as demonstrated in [25] where relevant references to both mathematical and physical studies can be found.

We have demonstrated that (at least for a sample problem) the general two-scale approach, combined with a relatively simple iterative algorithm, can be helpful to simplify formulations of mathematical models of engineering problems and to reduce all numerical computations without substantial loss of their validity (not identical with the "verification" of such models, incorporating the existence and uniqueness of solution, the convergence of numerical methods, etc., in practice). In this sense the "optimization" from the title may be understood, although no exact cost function(al) and / or precise requirements related to properties of above mentioned models have been presented. However, most questions of such "scale bridging" are still open and offer a large space for intensive research activities in the near future.

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References

[1] G. Allaire. Homogenization and two-scale convergence. *SIAM Journal on Mathematical Analysis*, **23**: 1482-1518, 1992.

[2] D. Cioranescu, P. Donato. *An Introduction to Homogenization.* Oxford University Press, 1999.

[3] W. Dahmen, A. Kunoth, R. Schneider. Wavelet least squares methods for boundary value problems. *SIAM Journal on Numerical Analysis*, **39**: 1985–2013, 2002.

[4] P. Fraunhofer, Ch. Schwab, R. A. Todor. Finite elements for elliptic problems with stochastic coefficients. *Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik*, research report **2004-12**, 2004.

[5] R. Glowinski, J. He, A. Lozinski, J. Rappaz, J. Wagner. Finite element approximation of multi-scale elliptic problems using patches of elements. *Numerische Mathematik*, in print.

[6] R. Glowinski, J. He, J. Rappaz, J. Wagner. A multi-domain method for solving numerically multi-scale elliptic problems. *Comptes Rendus de l'Acadèmie des Sciences Paris*, **I 338**: 741-746, 2004.

[7] A. Holmbom. Homogenization of parabolic equations: an alternative approach and some corrector-type results. *Applications of Mathematics*, **42**: 321-400, 1997.

[8] A. Holmbom, J. Silfver, N. Svanstedt, N. Wellander. On the two-scale convergence and related sequential compactness topics. *Applications of Mathematics*, in print.

[9] T. Y. Hou, X.-H. Wu, Z. Cai. Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients. *Mathematics of Computation*, **68**: 913-943, 1999.

[10] T. Y. Hou, X.-H. Wu, Z. Cai. Removing the cell resonance error in the multiscale finite element method via a Petrov-Galerkin formulation. *Communications in Mathematical Sciences*, **2**: 185-205, 2004.

[11] M. Kamiński. Homogenization-based finite element analysis of unidirectional composites by classical and multiresolutional techniques. *Computer Methods in Applied Mechanics and Engineering*, in print.

[12] P. Krysl, T. Belytschko. Element-free Galerkin method: convergence of the continuous and discontinuous shape functions. *Computer Methods in Applied Mechanics and Engineering*, **148**: 257-277, 1997.

[13] W. K. Liu, S. Jun, Y. F. Yhong. Reproducing kernel particle methods. *International Journal for Numerical Methods in Fluids*, **20**: 1081-1106, 1995.

[14] M. L. Mascarenhas, A.-M. Toader. Scale convergence in homogenization. *Numerical Functional Analysis and Optimization*, **22**: 127-158, 2001.

[15] A.-M. Matache. Sparse two-scale FEM for homogenization problems. *Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik*, research report **2001-09**, 2001.

[16] A.-M. Matache, Ch. Schwab. Two-scale FEM for homogenization problems. *Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik*, research report **2001-06**, 2001.

[17] A.-M. Matache, Ch. Schwab. Generalized FEM for homogenization problems. *Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik*, research report **2001-03**, 2001.

[18] V. Mošová. Meshless method RKHPU and its applications. *3rd IMACS Conference Modelling 2005 in Pilsen*, Abstracts: 44, Proceedings: to appear.

[19] A. Munjiza. From nano-scale particles to terrestrial bodies. *10th Conference Numerical Methods in Continuum Mechanics in Žilina*, Abstracts: 99-100, CD-ROM Proceedings: 9 pp., 2005.

[20] G. Nguetseng. A general convergence result for a functional related to the theory of homogenization. *SIAM Journal of Mathematical Analysis*, **20**: 608-623, 1989.

[21] G. Nguetseng, H. Nnang. Homogenization of nonlinear monotone operators beyond the periodic setting. *Electronic Journal of Differential Equations*, **2003-36**: 1-24, 2003.

[22] G. Nguetseng, J. L. Woukeng. Deterministic homogenization on parabolic monotone operators with time dependent coefficients. *Electronic Journal of Differential Equations*, **2004-82**: 1-23, 2004.

[23] M. Rech, S. Sauter, A. Smolianski. Two-scale composite finite element method for the Dirichlet problem on complicated domains. *Universität Zürich, Mathematisch-naturwissenschaftliche Fakultät, Institut für Mathematik*, preprint **2003-17**, 2003.

[24] S. Šťastník. Thermal insulation properties of new constructions of windows. *4th Matemathical Workshop in Brno*, to be published here.

[25] J. Svoboda, J. Vala, E. Gamsjäger, F. D. Fischer. Modelling of diffusive and massive phase transformations in substitutional alloys. *Acta Materialia*, to appear.

[26] K. Terada, H. Kikuchi. A class of general algorithms for multi-scale analysis of heterogeneous media. *Computer Methods in Applied Mechanics and Engineering*, **190**: 5427-5464, 2001.

[27] J. Vala. On the two-scale finite element method in engineering mechanics, *10th Conference Numerical Methods in Continuum Mechanics in Žilina*, Abstracts: 131-132, CD-ROM Proceedings: 10 pp., 2005.

[28] J. Vala. The method of Rothe and two-scale convergence in nonlinear problems. *Applications of Mathematics*, **48**: 587-606, 2003.

[29] J. Vala. Two-scale limits in some nonlinear problems of engineering mechanics. *Mathematics and Computers in Simulation*, **61**: 177-185, 2003.

[30] J. Vala, S. Šťastník. On the two-scale finite element method for the heat transfer in buildings. *3rd IMACS Conference Modelling 2005 in Pilsen*, Abstracts: 69, Proceedings: to appear.