On the optimization of microstructurally motivated calculations in engineering mechanics

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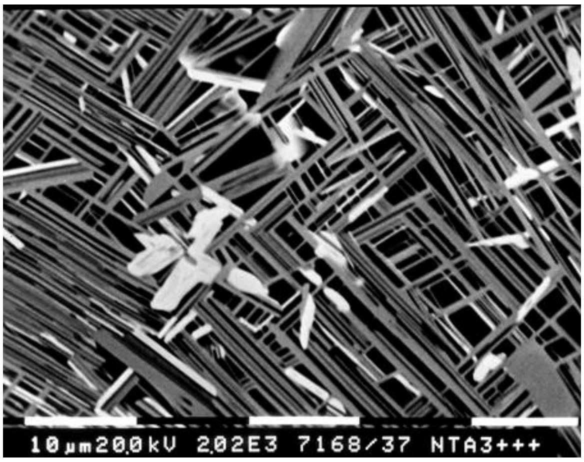

Example: structure of Ni-Al-Cr-Ta alloy (Institute of Physics of Materials, Brno)

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 nanoscale particles to terrestrial bodies" 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.... 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.).

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 emphasizes that two levels of not necessarily nested grids are considered (often with no deeper analysis of microstructural phenomena), the second one 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.

To avoid technical difficulties, 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 $W^{1,2}_0(\Omega)$ (some homogeneous Dirichlet boundary conditions can be prescribed). 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.

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^*). Let us 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 $u, v \in V$; this is not quite easy because we do not know "homogenized material characteristics" $\widetilde{A}$ on Ω properly – at least on Λ 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 and $u^\varepsilon, v \in V$ again.

Our model elliptic problem is: find such $u \in V$ that

$$a(u,v) = \langle f, v \rangle \text{ for all } v \in V\,.$$

Its numerical analysis is based on the following algorithm, started from some (e. g. macrocsale) estimate $u^0 \approx u$ with a real parameter ω:

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

etc. with shifted upper indices of $u^{\cdot}$. This algorithm creates a sequence $\{u^n\}_{n=0}^\infty$.

Using the properties of orthogonal projections of the space $V_{h\delta} = V_h + V_\delta$ into V_h and V_δ in case $0 < \omega < 2$, the extension theorems in Sobolev spaces and the homogenization step $\varepsilon \to 0$, under rather general assumptions on the interpolation properties of V_h and V_δ in V (in particular, under those from the famous Zlámal's article *On the finite element method* (1968)) it can be proved that a sequence of projections of $\{u^n\}_{n=0}^\infty$ to V has really a limit u. The detailed analysis on Λ can be done a posteriori with a finite positive ε.

The generalization of the presented algorithm to parabolic problems is based on the method of discretization in time and the analysis of convergence properties of Rothe sequences. Its practically important application is the two-scale analysis of thermal insulation and accumulation properties of building materials with a known porous structure.

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