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Optimization and identification in multiscale modelling

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This work is devoted to the general formulation of optimization and identification problems in multiscale modelling.
The multiscale modelling of materials and structures is very important and challenging area of research allowing to design new materials and products with better quality, strength and performance parameters. It allows to create reliable models taking into account products and material properties and topology in different length scales.
Several approaches have been elaborated for direct problems of multiscale modelling. The bridging and homogenization methods are the most popular. The bridging consists in connecting of scales on some boundaries; this method is especially important if some phenomenon occurs in a small part of the structure and should be taken into account. The example of the bridging method is connection between an atomic model and a continuum micro-model discretized by the finite or boundary element method for problems with the crack initialization and propagation. Another approach – the computational homogenization is used for analyzing models with a locally periodical microstructure. The computational homogenization allows to consider a complicated microstructure with nonlinearities like the elasto-plastic material, the contact with friction, wear or phase changes in the micromodel. This approach is used in the paper to solve direct problems in which transition from micro- to macro-scales and vice versa is performed.
Optimization problems, and generally speaking inverse problems considered in the paper, are much more complicated than direct problems.

Optimization in multiscale modelling allows to find structures with best performance or strength in one scale with respect to design variables in another scale. The identification problem is formulated as evaluation of some geometrical or material parameters of structures in one scale having measured information in another scale. This last problem can be formulated and considered as a special task of the optimization problem.

Problems considered in the paper tackle optimization and identification of microstructure parameters on the base of objective functionals and measured data (displacements, strains or natural frequencies) obtained for the macroscale level.
The proposed approach of identification is one of the most important stage of multiscale modelling because it enables to find some geometrical and/or material parameters of a micro-model in the rational and efficient way. Such parameters are necessary to formulate and solve the direct problems, in framework of the multiscale methodology, for engineering analysis of existed structures.

The global optimization algorithms based on bioinspired algorithms are applied in optimization and identification problems in the multiscale modelling. The most important advantages of bioinspired algorithms are their robustness, great probability of finding the global optimum and easy adaptation to new problems. The main disadvantage is long computation time due to the need of solving hundreds or thousands direct problems during optimization. To speed-up computations parallel and multi-subpopulation approaches are proposed.

Optimization and identification performed with the use of the evolutionary and immune algorithms and multiscale FEM models based on the computational homogenization are considered.
Several numerical examples of optimization and identification of composite and functionally graded engineering materials and bone tissues are presented.

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