Multiscale material design in construction

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Abstract. Classic R&D in material science was based on statistical modeling. However, large number of control factors and the absence of universal computational method that can be used for numerical investigation at all structural levels of constructional composite dictate the necessity of multiscale approach in computational material science. In the present work we are focusing on the description of spatial scales and primary types of interactions that take place in different layers of building materials. The five spatial scales are considered. Three of them allow using the simplest and universal modeling method that is based on the representation of composite as a particle system; still, modeling requires taking into account some extra types of pair forces and forces that are arising due to technological actions.

1 Introduction

The traditional way of R&D in material science of construction is based on experimental design, regression and further analysis of the obtained models; this well-known method is often denoted as "statistical modeling". Still, the necessity to design the advanced construction materials whose properties depend on large number of control factors renders real experiments too pricey, even in case of application of proper experimental design and planning. High level of confidence requires extra resource consumption and costly experimental setups. Because of this, the role of numerical studies becomes more and more important; modeling in material science has been constantly growing in recent decades. Thus, together with real experiments, the numerical design takes their place as the most productive method in day-to-day technological practice [1, 2]. A world of research papers, thesis and monographs on the subject are published; software for various models and algorithms are already developed.

However, no one single model and no one single computational method can be used for numerical investigation at all structural levels of heterogeneous multi-phase materials that are made of different binders, fine fillers, aggregates and admixtures; it is impossible to derive all physical behavior of matter from an as small as possible set of fundamental laws, e.g. relativistic quantum theory [3].

The gap between traditional and numerical experiments is due to the fact that no theoretical description of building material currently allows to derive a model for assured prediction of key operational properties of composite. At most, numerical studies are used for reduction of dimension and measure of control factor space, eliminating unacceptable

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designs of composition. But the proper selection of modeling methods and simulation software is not trivial, even for the aforesaid aim.

The key proposition that was made to facilitate the adoption of numerical methods for the design of materials is the proposition of multiscale modeling [1, 3-5].

2 Structural levels of building materials

To oversee the set of available modeling methods and computational software, we should consider the structural levels of building material in detail.

Representation of building material in terms of appropriate mathematical model is central to successful application of numerical methods. Building materials are heterogeneous dispersions that are formed during hardening of technological mix (such as fresh concrete); even constructional steel can be considered as a composite material. Both thermodynamics and physical chemistry of colloids are only of limited use during prediction of operational properties. The operational characteristics of building materials are usually found during experimental research and statistical modeling; the experiments require alteration of composition (specific surface of the filler, grain size distribution of aggregates, rheology of the binder) and technology (mode of laying, compaction and hardening). Composition and technology are tightly connected to each other and usually cannot be selected independently. The key point is that composition and technology are tightly connected to each other and usually cannot be selected independently; the connection is determined by predominant interaction – gravity, steric conditions, surface effects, etc. And what is most important, the same predominant interaction also determines the set of suitable modeling methods – quantum chemistry, classical mechanics, geometry modeling, probabilistic modeling, continuum mechanics (Table 1).

The first row of Table 1 may correspond to distinctive spatial levels and reflects the fact that in some circumstances heterogeneous structure of constructional composite may be ignored. This fact is the fundamental assumption for production-level software packages currently used for design in construction. If only macroscopic properties – strength, modulus, Poisson ratio – are considered, than a lot of discrete models developed in applied mathematics (finite difference, finite element, boundary element, finite volume) can be applied for investigation of stress-strain state, acoustics, conservative transfer (heat, mass), hydrodynamics and aeroelasticity. The phenomenological constitutive relations can also be improved by incorporating proper micromechanical relations that are also based on multiscale approach [6].

The next two structural levels – macro- and microstructure – are of great interest for material scientists [7]. Microstructure of the building material is the spatial level where structure formation is strongly affected by surface effects (free surface energy, surface tension and wetting). This level is formed when binder is combined with fine filler (specific surface of such filler is usually above 100 m^2/kg; corresponding particle size is below 10 um). Numerous processes take place during hardening of microstructure; cluster formation [8, 9] is one of such processes.

Macrostructure of the building materials is defined as a level where structure formation is primarily affected by weight of the structural units, steric effects and technological actions (pressure, vibration). Macrostructure is formed when coarse grained aggregates are combined with microstructure. Exact spatial boundary between macro- and microstructure is not strictly defined; it is near 100 um. Since at the macroscopic level the main types of interactions are caused by gravity force and steric effects, the motion equations for elements of the system are simple. These are equations of classical mechanics.

Table 1. Spatial scales, interactions and modeling software in material science.

Spatial scale	**Structural level**	**Theory, models, and modeling software**
~ 1 m	Homogeneous structure	Continuum mechanics, finite difference and finite element representations. Numerous production-quality computational tools are available.
> 0.1 mm	Macrostructure: gravitation and technological actions	Geometry of the system may be investigated with statistical simulation. Only a limited number of particle dynamics software is known. Computation tools for constructional material science either unavailable or unsuitable for productive R&D.
0.1-100 um	Microstructure: surface effects	Particle systems with classical mechanics and statistical simulation combined with analysis of ensemble geometry. Numerous production-quality computation tools are already developed. Specific software implementations for constructional material science still have to be developed.
1-100 nm	Nanostructure: size effects	Particle systems with classical mechanics. Theory is in active development; semi-empirical models are in use. Software tools for neighbor spatial scales can be utilized.
0.1-1 nm	Atomistic level: quantum effects	Quantum chemistry methods. Many computational tools are available.

In constructional material science, transient problem of structure formation process reflects technology of preparation and laying of constructional mix. If this problem is out of scope for the research, then modeling is often preformed only to determine the final configuration of coarse aggregates. The corresponding problems are theoretical examination and statistical simulation of dense packing in polydisperse systems, as well as percolation problems for frame of aggregates (the results can be used for prediction of mechanical properties) and pores (properties of porous space affects permeability and coupled properties – water, chemical and frost resistance). These problems have long history (it was originated in the beginning of XX century [10, 11]). Theoretical aspects of packing problem for polydisperse spheres and particles with complex shape were discussed in many research works due to importance of method which allows to design an ideal particle size distribution for constructional mix. Various geometric models were proposed, and different methods from percolation theory applied during simulation of packing. But surprisingly, despite the great interest to the packing and percolation problems at the macroscopic level of constructional composite, there are no well known software tools for simulation in this area. Tools with quite limited functionality were created mostly by authors of algorithms; such tools often requires mutually incompatible formats of input and output data, and implementation of algorithms is not verified extensively. In no conditions such software tools can be considered as production-ready, even if some of them were proposed for commercial use.

The fourth row of Table 1 corresponds to nanoscale level. “Nanostructure” of constructional composite is the spatial level where properties of material are considerably affected by size effects. Submicrocrystalline structures of hardening inorganic binder and molecular globules of thermosetting polymers are examples of formations at the nanoscale level. Software tools for neighbor spatial scales can be utilized during investigation of nanostructure. For instance, modeling based on the analysis of the ensemble geometry can be used for solution of percolation problem at nanoscale level [12].

The last row of the Table 1 corresponds to atomistic scale. It is the domain of quantum mechanics: there are no particles; there are only waves and probability.

The hierarchies of physical models that are similar to one demonstrated in Table 1, though not related to the building materials, are presented in many sources, e.g. in [13].

3 Micro- and macrostructure as particle system

The pioneering works on particle system dynamics are dated back to the mid XX century [14, 15]. These works are primarily inspired by problems arising in astrophysics. Significant results were summarized in [16]; in particular, attention was made to integration schemes that are suitable for particle dynamics. Later, particle system dynamics is segregated into several areas with designated set of models – molecular dynamics, dynamics of complex and non-Newtonian fluids, smoothed particle hydrodynamics and more [17-22].

Representation in form of particle system has many advantages: simple underlying theory, natural representation of many building materials, ability to model arbitrary pair forces, possibility to investigate large and nonlinear deformations, crack propagation and contact interactions. The known disadvantage is tremendous amount of computational operations, especially for direct particle-particle models. Thus, the efficient parallel algorithms for particle-mesh schemes are quite important for the adoption of the method. At present there are already a lot of efficient algorithms and highly-optimized computer code for the purpose. The comprehensive list of resources concerning software suitable for *N*-body simulation can easily be found.

For example, the GROMACS [23] molecular dynamics package was originally developed in the University of Groningen in the early 1990s. The package was initially a part of the parallel hardware project. The hardware became out of date, while the simulation software is proven to be significant as a standalone entity. Features of the packages that are similar to the GROMACS make them suitable for almost every simulation in material science; however, in case of multiscale modeling of building materials, extra pair forces have to be taken into account. Such forces depend not only on distance between surfaces of particles and can not be handled by many existing ODE packages. The example of complex pair force is the force caused by solvation shells. The particle with solvation shell can be modeled as two concentric spheres composed with rigid (impenetrable) core and viscous shell; such model is general enough to represent both micro- and macrostructure level of constructional composite. The viscous force can be estimated as a value proportional to cross section of the shells (outer spheres). The direction of the force is collinear to the relative velocities of the particles but not to the vector that is drawn between particles. Such force can not be represented as a potential field. There are also other types of force fields (both pairwise and volumetric) that represent technological actions, e.g. external pressure and vibrating [24].

Because of the absence of ready to use software package that is suitable for the multiscale modeling of building materials, the decision was made to implement such software [25]. The designed particle system simulation software correctly represents both tangent and normal pair forces, along with forces caused by gravity, technology and steric conditions. This allows detailed study of the influence of composition and technology to the properties of both technological mix and constructional composite.

4 Summary

In the present work we have made the review of spatial scales and primary types of interactions at different structural levels of building materials. The five spatial scales are considered; at three of them the most simple and universal modeling method that is based on the representation of composite in form of particle system can be used.

Modeling the building materials requires to take into account some extra types of pair forces and forces that are due technological actions. Thus, despite the fact that there is

currently a lot of software suitable for *N*-body simulation, the new special-purpose software [25] is implemented.

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