Finite Element Analysis of Particle Reinforced Composites

Daniel Peterseim

Composite materials appear in many practical applications such as the approximation of effective properties of fiber materials, thermal management in electronics industry, and optimal design of electric capacitors; to mention only a few. All these problems have two characteristic features in common: Random microstructures on multiple scales and high contrast in physical properties. These properties are already present in the simple 2-dimensional model of a high contrast composite occupying the domain $Q^* := [-L_1, L_1] \times [-L_2, L_2]$. The (perfectly conducting) inclusions (filler), denoted by $B_i \subset Q^*$, $i = 1, \dots, N$, are assumed to be closed circles of radius r_i not intersecting each other. The so-called matrix (the perforated domain) is denoted by $Q := Q^* \setminus \bigcup_{i=1}^N B_i$. Let $Q^\pm := \{\mathbf{x} \mid x_2 = \pm L_2\}$ be the upper/lower boundary of Q and $Q^{\text{lat}} := \partial Q^* \setminus (\partial Q^+ \cup \partial Q^-)$ be the lateral boundary. We are interested in computing the effective conductivity

$$\hat{a} := \min_{v \in V} I[v] := \frac{1}{2|Q^*|} \int_Q |\nabla v|^2 d\mathbf{x}, \tag{1}$$

of the composite, where the space of admissible functions is given by

$$V := \{v \in H^1(Q) \mid \exists \mathbf{t} \in I\!R^N : \, v(\mathbf{x}) = t_i \text{ on } \partial B_i, \; v(\mathbf{x}) = \pm 1 \text{ on } \partial Q^\pm\}. \tag{2}$$

A minimizer $u \in V$ of (1) fulfills the corresponding Euler-Lagrange equations:

$$\begin{aligned} \Delta \mathbf{u} = 0, \text{ in } Q, \quad \mathbf{u}(\mathbf{x}) = \pm 1, \text{ on } \partial Q^\pm, \quad \tfrac{\partial \mathbf{u}}{\partial \boldsymbol{\nu}} = 0, \text{ on } Q^{\text{lat}} \\ \mathbf{u}(\mathbf{x}) = t_i, \text{ on } \partial B_i, \quad \textstyle\int_{\partial B_i} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\nu}} = 0, \quad i = 1, \dots, N. \end{aligned} \tag{3}$$

This model has been introduced in [2] and further been investigated in [3, 1]. Here, it will serve as a reference example for describing the mathematical challenges related to composite materials as well as the newly proposed prototype of solution method.

The main difficulty for a numerical approximation of problem (3) lies in the complexity of the underlying geometry, i.e. the perforated domain Q. Standard finite element methods will suffer from the fact that the computation of suitable

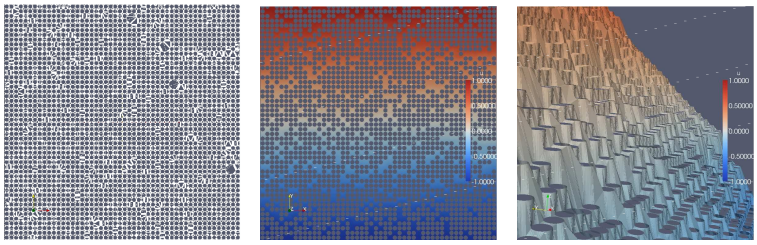

Figure 2. A generalized Delaunay mesh (left) and the corresponding generalized finite element approximation indicated by colors (middle, right).

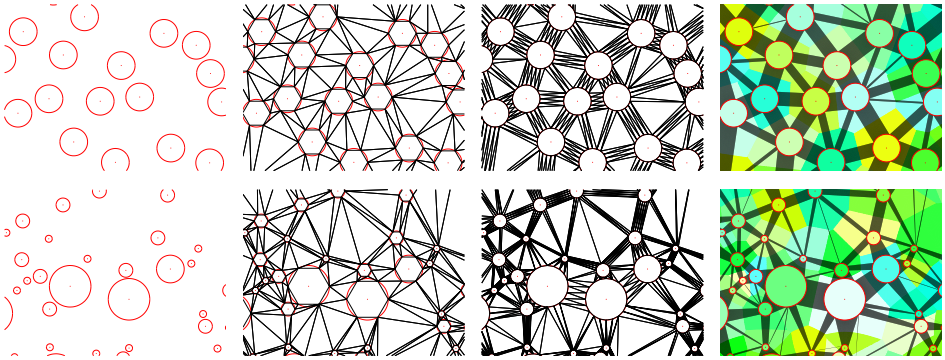

FIGURE 3. Construction of the generalized Delaunay mesh (from left to right): Part of domain Q (equally/non-equally sized inclusions above/below), approximation of Q by regular 6-gons and related Delaunay partition, approximation of Q by regular 20-gons and related Delaunay partition, generalized Delaunay partition and (generalized) Voronoi tessellation of the inclusions.

meshes is expensive, since every hole needs to be resolved by the triangulation in order to derive satisfactory results from standard finite element approximations; Figure 1 illustrates the problem for a model situation. This resolution condition forces even the coarsest available meshes to be very fine, i.e. it forces the minimal mesh size to be of order of the inclusion radii. Due to the shape regularity requirement the minimal number of nodes in the triangulation will further depend critically on the distribution of the inclusions and their distances. This is particularly disadvantageous since problem (3), typically, needs to be solved very often as a part of a statistical investigation of the material properties.

As a first step towards a new class of finite element models, in [4], we are currently developing a generalization of triangular meshes which allow to model the inclusions as weighted vertices. This approach is inspired by the work of Berlyand [2, 3, 1]. A typical generalized mesh $\mathcal{G}$ for equally sized inclusion is depicted in Figure 2. It is based on the Voronoi tessellation of the inclusions defining a neighborhood relation between the inclusions. $\mathcal{G}$ is a subdivision of Q^* into generalized vertices (circles), generalized edges (channels) and triangles. The subdivision reflects physics in the sense that the potential is mainly determined by fluxes between neighboring inclusions, whereas fluxes between inclusions of a certain distance can be neglected (cf. [3]). Such a subdivision can be derived by employing a convergent sequence of polygonal approximations to Q and its corresponding Delaunay triangulations with respect to the corners as it is illustrated in Figure 3.

Based on these new type of meshes a generalized nodal basis defining a generalized conforming Courant finite element space is introduced. A representative shape function is depicted in Figure 2 which shows the related Galerkin approximation to problem (3) for the composite from Figure 2. These shape functions,

similar the classical P1 finite element shape functions, are uniquely defined by their values at the vertices and to some extend linearly interpolated in between.

The new approach is optimal in the sense that the number of unknowns in the discrete problem (and the computational complexity) equals the number of unknowns t_i of the continuous problem (3). Note that additional (0-weighted) vertices can be introduced in the matrix Q to improve the approximation quality whereever necessary. Under additional mild assumptions on the hole distribution the classical a priori error bound on the error of the approximation $u_{\mathcal{G}}$

$$\|u - u_{\mathcal{G}}\|_{H^1(Q)} \leq Cd|u|_{H^2(Q)},$$

is proven in [4]. Here, d denotes the maximal distance between neighboring inclusions. Such an a priori result shows the potential of the new approach but it is only the very first step. Besides considering the 3-dimensional version of problem (3) and its approximation, which is rather straight forward, more general geometries with regard to the inclusions and more general differential equations need to be studied. Furthermore, the model needs to be investigated with respect to its asymptotic behavior regarding volume fraction and the interparticular distance.

References

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Exact sampling for highly oscillatory molecular systems

Petr Plecháč

(joint work with Mathias Rousset)

We present a new numerical method called *implicit mass-matrix penalization* (IMMP) for numerical integration and sampling large particle systems whose dynamics exhibits multiple time scales. The detailed description and numerical analysis of the IMMP method can be found in [PleRous].

In this contribution we describe the IMMP method applied to Langevin processes (Hamiltonian dynamics with stochastically perturbed forces) in order to obtain an efficient and accurate sampling from the *canonical distribution* at the inverse temperature $\beta = 1/kT$ associated with the separable Hamiltonian $H(p,q) = \frac{1}{2}p^T M^{-1} p + V(q)$. The potential is assumed to be of form $V(q) = U(q, \xi(q))$ with the "fast" degrees of freedom (fDOFs) $(\xi_1, .., \xi_n)$ explicitly given, and $q \in \mathbb{R}^d$,