Post-doctoral position: Domain decomposition method for the computation of the effective elastic tensor of random materials

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The aim of this project is to develop an efficient and original numerical method to compute the effective elastic properties of random heterogeneous materials.

We focus on heterogeneous elastic materials containing inclusions embedded in a matrix, where the typical size of the inclusions is small with respect to the size of the domain occupied by the material. We assume that these inclusions are randomly distributed in the material. The effective elastic properties of the material are then deterministic, and their computation by a full-field method requires the resolution of an auxiliary problem defined over the entire space. Classical methods consist in considering a large (but finite) statistical elementary volume, on which the auxiliary problem, complemented with appropriate boundary conditions (for instance, periodic boundary conditions), is solved. A full-field method is particularly interesting in situations where the volumic fraction of the inclusions in the material is significant. Indeed, in this case, approximations provided by quasi-analytic schemes (Hashin-Shtrikman bounds, self-consistent models, Mori-Tanaka approximation, ...) are not always sufficiently accurate.

The size of the elementary volume is the main limiting factor in the numerical resolution of these auxiliary problems, for instance with a standard finite element method. Indeed, this size must be sufficiently large to represent accurately the statistical properties of the distribution of the inclusions in the material. However, the number of degrees of freedom needed to perform a reasonable finite element computation increases very quickly with this size, especially when the contrast between the different phases composing the material is significant (a quite fine discretization mesh has then to be used), or when one considers realistic 3D problems.

In this project, we consider another type of auxiliary problem, defined over the whole space, where the statistical elementary volume is embedded in an exterior infinite homogeneous material. The new problem, which has initially been introduced in a completely different setting [4], can be seen as a generalization of the Eshelby problem. In [1, 2], we have shown, in collaboration with Benjamin Stamm (Aachen university, Germany), how such auxiliary problems can be used to approximate the effective thermal conduction properties.

The interest of considering such an alternative formulation lies in the fact that an efficient numerical method can be used to solve these problems. The method is described in [3]. The approach has been tested

to compute the homogenized thermal diffusion coefficient of a 3D material in the case when the inclusions are spherical, and when the materials composing the inclusions and the matrix are assumed to be isotropic. The main ingredients of the approach are:

- a boundary integral method to represent the solution of the problem;
- a domain decomposition method which enables to solve small local problems at the surface of each inclusion in parallel;
- a discretization of the problem using spherical harmonics.

Very promising numerical results have been obtained: a 3D computation has been performed in 10 minutes on a laptop for an elementary volume containing 100 000 inclusions. Problems of this size are difficult to address when using standard numerical approaches. The efficiency of our approach leads to promising perspectives for the treatment of large elementary volumes and complex microstructures.

In this project, the candidate will extend the range of application of the method in order to

- compute the effective properties of polydisperse materials (i.e. when the matrix contains inclusions of several sizes);
- compute the effective mechanical properties of microstructured materials; only thermal problems have been considered until now;
- consider the case of anisotropic materials, or anisotropic (e.g. non-spherical) inclusions.

The successfull candidate will be offered to spend one month in Benjamin Stamm's group in Aachen university. At Ecole des Ponts Paristech, he or she will be in contact with research teams of the Laboratoire Navier (mechanics lab) and of the CERMICS (applied mathematics lab). This project lies at the crossroads of computational mechanics and scientific computing, as its final aim is to compute the effective properties of realistic microstructures studied by experimentalists in the Laboratoire Navier.

The successfull candidate will hold a Ph.D. either in applied maths, computer science or computational mechanics. He or she should already have a strong experience in software development. Knowledge about boundary integral methods would be preferable, but not required. The post-doctoral position will be funded by the Labex MMCD (gross salary 2500 euros/month and a starting allowance of 1500 euros for conference participation).

References

[1] E. Cancès, V. Ehrlacher, F. Legoll and B. Stamm, *An embedded corrector problem to approximate the homogenized coefficients of an elliptic equation*, Comptes-Rendus Mathématiques, 353:801–806 (2015).

[2] E. Cancès, V. Ehrlacher, F. Legoll and B. Stamm, *Approximation of effective coefficients in stochastic homogenization using a boundary integral formulation*, in preparation.

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[4] F. Lipparini, B. Stamm, E. Cancès, Y. Maday and B. Mennucci, *Fast domain decomposition algorithm for continuum solvation models: Energy and first derivatives*, Journal of Chemical Theory and Computation, 9:3637–3648 (2013).