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 in order to compute the effective elastic properties of random materials.

Let us consider here heterogeneous elastic materials containing inclusions embedded in a matrix, where the typical scale of the inclusions is small with respect to the size of the domain occupied by the material. Let us assume in addition 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 is solved using appropriate boundary conditions (for instance, periodic). 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, the precision of the approximations given by quasi-analytic schemes (Hashin-Shtrikman bounds, self-consistent models, Mori-Tanaka approximation...) is 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 resaonable 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 to be used the), and when one considers realistic 3D problems.

In this project, the candidate will 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 can then be seen as a generalization of the Eshelby problem. In [1, 2], the advising team of the candidate, in collaboration with Benjamin Stamm (Aachen university, Germany), have shown how such auxiliary problems can be used to approximate the effective thermal conduction properties of heterogeneous materials.

The interest of considering such an alternative formulation lies in the fact that a very efficient numerical method can be used to solve these problems. The method is described in [3]. This aproach has been tested to compute the homogenized thermal diffusion coefficient of a material in the case when the inclusions are spherical, and when the materials composing the inclusions and the matrix are assumed to be isotropic. Th 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 encouraging numerical results were obtained with this method : a 3D computation has been solved in 10 minutes on a laptop for an elementary volume containing 100 000 inclusions ! Problems of this size can only be tackled with great difficulty by other methods. The efficiency of this 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 effective mechanical properties (elastic tensor) of microstructured materials ;
– compute effective properties of materials where inclusions are distributed in a polydisperse manner ;
– treat the case of anisotropic materials ;
– consider inclusions of more general shape (ellipsoids).

The fast numerical treatment of the type of auxiliary problem can also be used in conjunction with variance reduction methods to estimate the effective properties of a material composed of inclusions of arbitrary shape.

In this context, the candidate will be able to spend one month in Benjamin Stamm's group in Aachen university as an invited student. He or she will be able to discuss with research teams belonging to the Laboratoire Navier (mechanics lab of the Ecole des Ponts Paristech) and CERMICS (applied mathematics lab of Ecole des Ponts Paristech). The final aim of the project will be to run computations for realistic microstructures studied by experimentalists in the Laboratoire Navier.

The candidate will have a PhD, either in applied maths, computer science or computational mechanics. He or she should already have a strong experience in coding. Knowledge about boundary integral methods would be preferable, but not mandatory. The post-doctoral position will be financed by the Labex MMCD (gross salary 2500 euros/month + 1500 euros for missions).

Références

[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.

[3] E. Cancès, V. Ehrlacher, F. Legoll and B. Stamm, *Integral equation methods for solving corrector problems in stochastic homogenization*, in preparation.

[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).