Stochastic bridging of scales in the Arlequin framework

Régis Cottereau, Hachmi Ben Dhia, Didier Clouteau

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R. Cottereau, H. Ben Dhia, D. Clouteau

Laboratoire MSSMat (École Centrale Paris, CNRS UMR 8579)
Grande voie des vignes, F-92295 Châtenay-Malabry, France
{regis.cottereau,hachmi.ben-dhia,didier.clouteau}@ecp.fr

Résumé — As the use of multiscale and multiphysics models spreads out, the need to use stochastic models increases. However the numerical costs associated with the resolution of such models is usually much larger than that of their deterministic counterpart. We present here a method, set in the Arlequin framework, to couple a probabilistic model with a deterministic one, therefore introducing randomness only where necessary to improve the reliability of our quantities of interest.

Mots clés — Multiscale modeling, Stochastic modeling, Coupling method, Arlequin method, Homogenization.

1 Introduction

Classical deterministic models provide global predictions that are satisfactory for many industrial applications. However, when one is interested in a very localized behavior or quantity, or when multiscale phenomena come into play, these models may not be sufficient. For instance, the limited heterogeneity of a material modeled as a continuum might have no influence on its behavior on a large scale, while the study of a local stress intensity factor would strongly depend on the local heterogeneity of the mechanical parameters. Likewise, the prediction of the outbreak of a fracture in a structure might be performed with homogeneous models, while the incorporation of atomic modeling would be necessary to follow the exact path of that fracture. Unfortunately, for these problems, the information necessary to parameterize the relevant, very complex, models is usually not available. Stochastic methods have therefore been proposed and now appear unavoidable in multiscale modeling.

Although the use of stochastic models and methods has expanded rapidly in the last decades, the related numerical costs are still often prohibitive. Hence, the application of these methods in a complex or industrial context remains limited. An important field of research is therefore concerned with the reduction of the costs associated with the use of stochastic methods, for example by using iterative methods specially adapted to the structure of the matrices arising in the Stochastic Finite Element (FE) method [8, 11], using reduced bases for the representation of random fields [6], or using special domain decomposition techniques for parallel resolution on clusters of computers [12].

The present paper proposes an alternative to these purely mathematical/numerical approaches through the coupling of two models : one deterministic and one stochastic. The general goal is that of modeling a global problem in a mean or homogeneous way where it yields sufficient accuracy, while retaining a stochastic model where needed. Hence, additional complexity is added in the model only where required, and the general approach is both more elegant and numerically cheaper than a global all-over stochastic model would be. Further, the cuts on computational costs mean that industrial applications come within reach.

More specifically, we discuss here the interaction and coupling of a classical continuum model with another continuum model with random parameters. The former model, deterministic, aims at representing a part of the domain where the local fluctuations of the parameters, such as Young's modulus, do not influence the output of interest in a significant manner, and where a homogenized model is sufficient to predict this output. The latter model, stochastic, stands for the part of the domain where the local behavior is of interest and the fluctuations of the parameters cannot be considered only in a homogenized way. The coupling of these models is performed in the Arlequin framework [1, 3, 2]. Note that the choice of two continuous models is by no means a restriction of the contents of this paper, and that the Arlequin method can accomodate different models [5]. However, considering corresponding models allows us to concentrate more particularly on the specific aspects of the coupling of a deterministic model with a stochastic one.

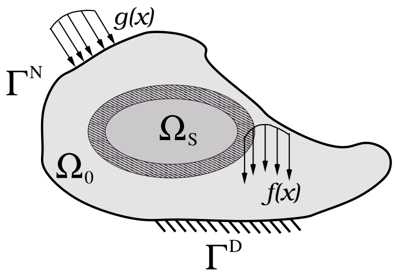
The framework of this paper is very different from that of classical micromechanics [19, 4] and homogenization [10]. In these, the objective is to find a mean, or homogenized, behavior for a material, that will allow its study on a higher scale. In our case, we wish to study the local behavior of a small subdomain of that material, while the influence of the rest of the domain is taken into account in some homogenized way. Even when homogenization techniques are embedded within a stochastic FE framework, with both scales actually represented, the coupling does not go both ways, and only the low scale influences the high one (see for instance [16]). This type of one-way coupling approach is also very classical in climate modeling [17], where the influence of the small, unresolved, details at the global scale are taken into account through stochastic models more or less tuned on a lower scale. Nevertheless, we will re-use some notions explored extensively in homogenization techniques. In particular the notion of size of a Representative Volume Element, with respect to the correlation length of the parameters of the medium and/or the number of realizations of that medium (see in particular [9, 10, 15, 18]) will be discussed in relation with the size of the coupling zone between our two models.

This work is closely related to previous works in the literature [13, 5]. However, in [13], the theoretical basis, different from the Arlequin formulation, is less general. In particular, it is only aimed at coupling a deterministic Boundary Element method with a stochastic FE method. In the recent work [5], the authors aim at coupling two stochastic models, one continuous, and one atomistic. However, many theoretical questions are left out. In particular, the coupling is performed between realizations of the stochastic operators, while we try to describe here the coupling at the level of the stochastic operators.

2 Description of the problem

Let us consider a domain Ω_0 of $\mathbb{R}^d$, with smooth boundary $\partial\Omega_0$ separated into Dirichlet and Neumann boundaries Γ_D and Γ_N, such that $\Gamma_D \cup \Gamma_N = \partial\Omega_0$, $\Gamma_D \cap \Gamma_N = \emptyset$, and $\Gamma_D \neq \emptyset$ (figure 1). A bulk loading field $f(\boldsymbol{x})$ is defined on Ω_0 and a subdomain Ω_s of Ω_0 is selected, supposing for simplicity that $\partial\Omega_s \cap \Gamma_D = \emptyset$ and $\boldsymbol{f}(\boldsymbol{x} \in \Omega_s) = \boldsymbol{0}$.

We then introduce the field of mechanical parameter K. We will concurrently consider two models of that parameter, namely a deterministic one, K_0, supposed constant on the domain, and a stochastic one, $\boldsymbol{K}(x)$, modeled as a random field on Ω_s. We further suppose that $\boldsymbol{K}(x)$ is perfectly known, and that $\mathrm{E}[\boldsymbol{K}(\boldsymbol{x})] = K_0$, with $\mathrm{E}[\cdot]$ the mathematical expectation. For the purpose of the applications, we will use the model developed by Soize [14], that ensures solvability of the associated weak formulation of the mechanical problem.



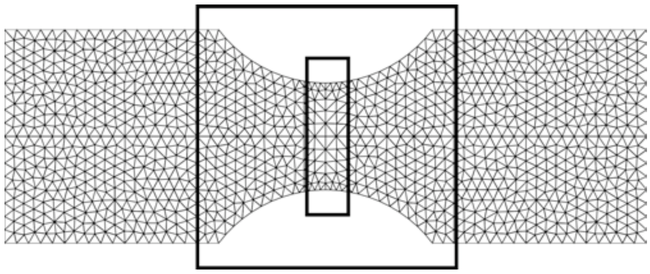


Figure 1 – Description of the model problem (left), and example of application (right), with the outermost square indicating the limit of Ω_s

3 The continuous Arlequin formulation

We first introduce a functional space for the functions corresponding to the deterministic model :

$$\mathcal{V}_0 = \{v \in \mathcal{H}^1(\Omega), v_{|\Gamma_N} = 0\},$$

equipped with the inner product $(v,w)_0 = \int_\Omega (\nabla_x v, \nabla_{\boldsymbol{x}} w) d\Omega$, and norm $\|v\|_0 = (v,v)_0^{1/2}$, $v,w \in \mathcal{V}_0$. We then define a complete probability space $(\Theta, \mathcal{T}, P)$, where Θ is a set of outcomes, $\mathcal{T}$ is a σ-algebra of events, and P is a probability mesure ($P : \mathcal{T} \to [0,1]$). The functions corresponding to the stochastic model are defined in

$$\mathcal{V}_s = \mathcal{L}^2(\Theta, \mathcal{V}_0),$$

the tensor Hilbert space of the second-order random variables defined on the probability space $(\Theta, \mathcal{T}, P)$, and with values in $\mathcal{V}_0$. That space is equipped with the inner product $(\boldsymbol{v}, \boldsymbol{w})_s = \mathrm{E}[(\boldsymbol{v}, \boldsymbol{w})_0]$, and corresponding norm $\|v\|_s = (v, \boldsymbol{v})_s^{1/2}$. Note that $\forall v \in \mathcal{V}_s$, $\mathrm{E}[v] \in \mathcal{V}_0$.

We define the Arlequin problem as : find $(u_0, \boldsymbol{u}_s, \Phi) \in \mathcal{V}_0 \times \mathcal{V}_s \times \mathcal{V}_0$

$$\begin{cases} a_0(u_0, v) + C(\Phi, v) = \ell_0(v), & \forall v \in \mathcal{V}_0 \\ \mathcal{A}_s(u_s, v) - C(\Phi, \mathrm{E}[\boldsymbol{v}]) = 0, & \forall v \in \mathcal{V}_s \\ C(\Psi, u_0 - \mathrm{E}[u_s]) = 0, & \forall \Psi \in \mathcal{V}_0 \end{cases} . \tag{1}$$

The bilinear operators $a_0, C : \mathcal{V}_0 \times \mathcal{V}_0 \to \mathbb{R}$ and $\mathcal{A}_s : \mathcal{V}_s \times \mathcal{V}_s \to \mathbb{R}$, are defined by

$$a_0(u,v) = \int_\Omega \alpha_0 K_0 \nabla_{\boldsymbol{x}} u \cdot \nabla_x v \, d\Omega,$$

$$\mathcal{A}_s(u, \boldsymbol{v}) = \mathrm{E}\left[\int_{\Omega_s} \alpha_s \boldsymbol{K} \, \nabla_{\boldsymbol{x}} \boldsymbol{u} \cdot \nabla_{\boldsymbol{x}} v \, d\Omega\right],$$

and

$$C(u,v) = \int_{\Omega_0 \cap \Omega_s} (\kappa_0 uv + \kappa_1 \nabla_{\boldsymbol{x}} u \cdot \nabla_x v) \, d\Omega,$$

where the fields $\alpha_0(\boldsymbol{x})$ and $\alpha_s(\boldsymbol{x})$ are defined on Ω_0, such that $\alpha_0(\boldsymbol{x}) + \alpha_s(\boldsymbol{x}) = 1$ and $\alpha_s(\boldsymbol{x} \notin \Omega_s) = 0$, and κ_0 and κ_1 are normalization constants.

4 The discretized Arlequin formulation

The general idea here is to use a classical FE approach to discretize the first and third equations of the Arlequin system (1) and a stochastic FE method for the second one. It should be noted that a Monte Carlo resolution of this formulation is not straightforward because the coupling equation (the third one) works on the mean of $\boldsymbol{u}_s$, which is not available when one considers only one realization of that random field.

We therefore associate to the domain Ω a mesh $\mathcal{T}$, composed of elements E, and look for approximate functions of the elements of $\mathcal{V}_0$ in the functional space

$$\mathcal{V}_0^H = \{v \in P_1(E), v_{|\Gamma_N} = 0\},$$

composed of linear functions on each of the elements of the mesh. We then choose a basis $\{\mathrm{v}_\ell(x)\}_{1\le \ell \le m}$ for the functions in $\mathcal{V}_0^H$, for example the classical linear FE basis, and we introduce the matrices A_0 and C, with elements

$$\mathrm{A}_{0,ij} = \int_{\Omega_0} \alpha_0 K_0 \nabla_{\boldsymbol{x}} \mathrm{v}_i \cdot \nabla_{\boldsymbol{x}} \mathrm{v}_j \, d\Omega,$$

and

$$\mathrm{C}_{ij} = \int_{\Omega_0} \left(\kappa_0 \mathrm{v}_i \mathrm{v}_j + \kappa_1 \nabla_{\boldsymbol{x}} \mathrm{v}_i \cdot \nabla_{\boldsymbol{x}} \mathrm{v}_j\right) \, d\Omega.$$

For the space $\mathcal{V}_s$, we choose an approximating space as the span of the polynomial chaos basis [7], of order n and degree p, in conjunction with the previous basis for the spatial dimension. We denote this space $\mathcal{V}_s^{H,n,p}$ and the elements of its basis $\{\mathrm{w}_\ell(\boldsymbol{x})\}_{1\le \ell \le mN}$, where N is the number of elements in the polynomial chaos basis, which depends both on n and p. We expand both the parameter field $\boldsymbol{K}(x)$, and the solution $u_s(x)$ in that basis, and finally obtain the matrix $\mathbb{A}$ for the stochastic part of the Arlequin system as

$$\mathbb{A}_{j\ell,JL} = \sum_{i=1}^{N} c_{ijJ} \int_{\Omega_s} \alpha_s(\boldsymbol{x}) k_i(\boldsymbol{x}) \nabla_x \mathrm{w}_\ell(\boldsymbol{x}) \cdot \nabla_{\boldsymbol{x}} \mathrm{w}_L(\boldsymbol{x}) \, d\Omega,$$

where $c_{ijJ} = \mathrm{E}\left[\hat{\Gamma}_i[\boldsymbol{\xi}]\hat{\Gamma}_j[\xi]\hat{\Gamma}_J[\xi]\right]$, $k_i(x) = \mathrm{E}[K(x)\hat{\Gamma}_i(\boldsymbol{\xi})]$. Note that the double indices (j,ℓ) and (J,L) each correspond to only one index in the matrix form of the system. We further denote

$$\underline{\mathbb{A}} = \mathbb{A}_{0\ell,0L} = \int_{\Omega_0} \alpha_s K_0 \nabla_{\boldsymbol{x}} \mathrm{w}_i \cdot \nabla_{\boldsymbol{x}} \mathrm{w}_j \, d\Omega,$$

and $\mathbb{A}_c = \mathbb{A}_{0\ell,JL}$ the sub-matrices that correspond to the mean part of the unknown field, and $\mathbb{A}_s = \mathbb{A}_{j\neq 0\,\ell,JL}$ that corresponding to the fluctuating part. We finally get the form of the matrix system for the Arlequin problem (1) :

$$\begin{bmatrix} \mathrm{A}_0 & 0 & 0 & \mathrm{C} \\ 0 & \underline{\mathbb{A}} & \mathbb{A}_c & -\mathrm{C} \\ 0 & \mathbb{A}_c^T & \mathbb{A}_s & 0 \\ \mathrm{C}^T & -\mathrm{C}^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathrm{U}_0 \\ \underline{\mathrm{U}} \\ \mathrm{U}_s \\ \Phi \end{bmatrix} = \begin{bmatrix} \mathrm{F} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \tag{2}$$

where the coordinates of the vector F are defined by $\mathrm{F}_i = \ell_0(\mathrm{v}_i)$, and U_0, $\underline{\mathrm{U}}$, U_s, and Φ are the vectors of coordinates of u_0, $\mathrm{E}[\boldsymbol{u}_s]$, $\boldsymbol{u}_s - \mathrm{E}[\boldsymbol{u}_s]$, and Φ, in the bases of $\mathcal{V}_0^H$, $\mathcal{V}_0^H$, $\mathcal{V}_s^{H,n,p} \backslash \mathcal{V}_0^H$, and $\mathcal{V}_0^H$, respectively. Note that the controlling parameters for the size of that matrix are n and p, and that in most cases, $\mathbb{A}_s$ will be a very large matrix, much larger than the other ones appearing in the equation (2). However, it is much smaller than the matrix that would be obtained by applying directly a stochastic FE approach to the entire model.

5 Example of application

For illustrative purposes, we consider the indented plate of figure 1, with $-3 < x < 3$ and $-1 < y < 1$, with a neck in the zone around $x = 0$, $f(x,y) = 1$ in the zone $2 < x < 3$ (right side of the plate), and homogeneous Dirichlet boundary conditions on the left side of the plate. The boundary conditions read :

$$\begin{cases} u = 0, & x = -3 \\ \nabla_{\boldsymbol{x}} u = \mathbf{0}, & \text{on } \partial\Omega \backslash \{x = -3\} \end{cases}$$

We plot on figure 2 the stress field $|K\nabla u|$, along the line $y = 0$, corresponding to the solution of the Arlequin system (1) for these boundary conditions The stresses corresponding to u_0 and $\mathrm{E}[\boldsymbol{u}_s]$ are both plotted, showing the fact that the coupling works well, and we also plot three realizations of the stresses corresponding to $\boldsymbol{u}_s$.

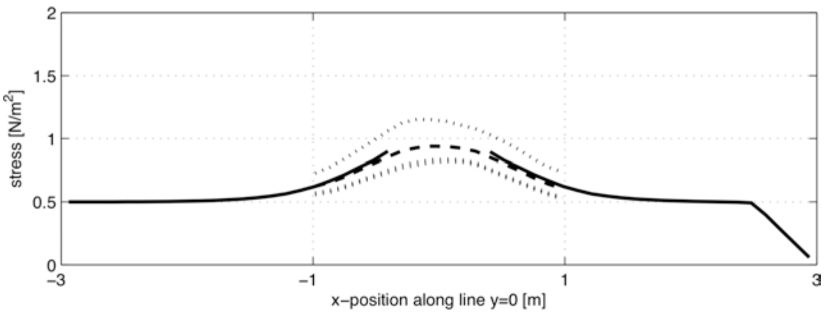


Figure 2 – Stresses $|K\nabla u|$ corresponding to the displacement fields u_0 (solid line), $\mathrm{E}[u_s]$ (dashed line), and three realizations corresponding to $\boldsymbol{u}_s$ (dotted lines)

6 Conclusion

We have shown here a method for coupling a probabilistic model of continuum mechanics with a deterministic one. The numerical costs associated with the resolution of a probabilistic model are heavily lowered, which renders its use in an industrial setting reasonable. The framework that was described here can very easily be extended to other problems, be it with different physics (continuum mechanics, molecular dynamics, nonlinear constitutive relation), using the available literature on the Arlequin method, or involving two probabilistic models. During the talk, we will discuss further the particularities of the method, and in particular the definition of the size of the coupling zone with respect to the definition of representative volume elements in homogenization techniques [9, 10, 15, 18].

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