

# A Collaborative Thick-Coupling Algorithm for True Multiscale Mechanical Problems

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**Résumé** — In this contribution, by using the most characteristic seminal Arlequin method idea, namely the volume/thick-models/scales coupling, relying on a superposition of subdomains pillar (see [1], [2]), we extend the Non-Intrusive-Global-Local Iterative (NIGLI) method, developed by Allix, Gosselet and their collaborators (see e.g. [3, 4]); an advanced, more robust and practically more interesting version of the Whitcomb's Iterative Global-Local method (see [5]), to solve true-complex problems requiring, for costs sustainability, the coupling of global coarse models and localized non-local-ones i.e. true-multiscale problems that can not be solved by the NIGLI method.

**Mots clés** — Collaborative-Algorithm, Non-Intrusive Method, Thick-Coupling, True Multiscale Problems

## 1 Introduction

We consider a static mechanical solid problem defined in a given bounded domain  $\Omega$ , encompassing a critical localized defect, denoted  $\chi$  (a hole, a crack, a local damage, a dislocation, a missing atom, ...), submitted to external loads and constraints. To solve numerically such problems with sufficient accuracy and affordable costs, one needs relatively very fine refinement in terms of models and/or scales (that could be atomistic, stochastic, etc.) in a very small local domain  $\Omega_l$ , with respect to  $\Omega \setminus \Omega_l$ ;  $\chi \subsetneq \Omega_l \subsetneq \Omega$  (observe here that one can consider several localized criticities  $\chi_i, i = 1, nb$ ). To achieve these goals, Global-non-Local modelling, and/or multiscale formulations, with associated appropriate computational method are mandatory, especially when the geometrically local model is physically a non-local one or when the problem is a true-multiscale one. As well-known, the Arlequin Method proved appropriate and efficient framework for the solution of these problems. However, looking to the softwares market, one could observe that there are well-established commercial softwares (say Abaqus, Nastran, Aster, Cast3m, Z-set, etc.) having required several decades, in terms of human's resources developments and tests, that solve efficiently Global and general industrial mechanical problems with rather complicated behaviours law, on the one hand, and so many local agile research laboratory softwares, developed for testing computational methods shaped to solve problems at very fine physical scales, on the other hand. Taking into account this ground reality, to achieve the highest resolution performance for the solution of true-multiscale, thus complex problems, it seems natural to establish a fair Dialogue to bridge iteratively Global Commercial and Local Laboratory Softwares; taking potentials of each of them to improve the solution efficiency of complex problems. In the Realm of surface coupling algorithms, one can mention the Global-Local Iterative algorithm, initiated by [5], (taking cue from the well-known Schwarz staggered algorithm). This algorithm was lately developed in a more robust way by Allix, Gosselet and their collaborators (see e.g. [3, 4]) and tested successfully for different localized phenomena (such as localized plasticity). This attests to the fact that the Iterative/Non-Invasive method is an interesting tool, allowing the communication between Global and Local softwares. However, relying on a specific surface domains decomposition couplings, it can not be used to couple two domains using, either a local and a non local model, or different scale, to solve, for instance, a problem using the coupling of a classical continuum model and a peridynamic one or an atomistic one. For the latters a thick/volume Arlequin Coupling is mandatory (see e.g. [6, 7, 8, 9]). Based on these observations and on the practical ease of implementation, provided by the Iterative/Non-Intrusive coupling methods, we propose a Non-Invasive-like Collaborative volume coupling method, following the path of Arlequin method's philosophy. This method is presented

in Section 2 and applied, in Section 3 to the case of the coupling of a particle model with non local interactions and a continuum one.

## 2 A Collaborative/Non-Invasive volume-coupling algorithm

To present the Collaborative/Non-Invasive volume coupling method, we first recall the classical Arlequin formulation of the static mechanical solid problem, previously mentioned.

We consider a solid  $\mathcal{B}$ , occupying the closure  $\overline{\Omega} \subset \mathbb{R}^d$  ( $d = 1 - 3$ ) of the bounded and sufficiently regular open domain  $\Omega \subset \mathbb{R}^d$  whose boundary  $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ ;  $\Gamma_D$ , verifying classical hypotheses. The domain  $\Omega$  is assumed to be partitioned into two subdomains : a global one  $\Omega_g$  and a local one  $\Omega_l$ , with an overlap  $\Omega_c = \Omega_g \cap \Omega_l$ , with  $d - measure > 0$  and non-zero thickness field  $e > 0$ . Moreover, we assume that a criticality  $\chi$  is strictly included in  $\Omega_l \setminus \Omega_c$  (cf. Figure 1b).

With theses notations and definitions, the VWP-based version of the Arlequin method, relying on i) a domain partition, ii) a partition of unity of Virtual Works and iii) a volume Coupling between two accommodated different models, reads as following : (see e.g. [10])

Find  $(\mathbf{u}_g, \mathbf{u}_l, \boldsymbol{\lambda}) \in \mathbf{W}_0(\Omega_g) \times \mathcal{W}(\Omega_l) \times \mathbf{M}$  such that :

$$a_g(\mathbf{u}_g, \mathbf{v}_g) + c(\boldsymbol{\lambda}, \mathbf{v}_g) = l_g(\mathbf{v}_g) \quad \forall \mathbf{v}_g \in \mathbf{W}_0(\Omega_g), \quad (1a)$$

$$a_l(\mathbf{u}_l, \mathbf{v}_l) - c(\boldsymbol{\lambda}, \Pi_l^g \mathbf{v}_l) = l_l(\mathbf{v}_l) \quad \forall \mathbf{v}_l \in \mathcal{W}(\Omega_l), \quad (1b)$$

$$c(\boldsymbol{\mu}, \mathbf{u}_g - \Pi_l^g \mathbf{u}_l) = 0 \quad \forall \boldsymbol{\mu} \in \mathbf{M}. \quad (1c)$$

where  $\mathbf{u}_g$ ,  $\mathbf{u}_l$  and  $\boldsymbol{\lambda}$  stand for the global and local displacement fields and the volume-Lagrange multiplier and where the bilinear and linear forms  $a_g$ ,  $a_l$ ,  $l_g$  and  $l_l$  have classical partitioned forms. The bilinear form  $c(\cdot; \cdot)$  defines the third classical Arlequin Framework ingredient which is the essential and characteristic volume-Arlequin coupling. It is given by :

$$c(\boldsymbol{\mu}, \mathbf{v}) = \int_{\Omega_c} (\kappa_1 \boldsymbol{\mu} \cdot \mathbf{v} + \kappa_2 \boldsymbol{\epsilon}(\boldsymbol{\mu}) : \boldsymbol{\epsilon}(\mathbf{v})) \, d\Omega, \quad \forall (\boldsymbol{\mu}, \mathbf{v}) \in \mathbf{M}^2 \quad (2)$$

with, in this context,  $\kappa_1 = E/e^2$  and  $\kappa_2 = E$ ,  $E$  being the solid Young modulus, and the mediator space  $\mathbf{M}$  taken equal to  $\mathbf{W}_0(\Omega_c)$ .

The fields  $\mathbf{u}_g$  and  $\mathbf{u}_l$  being different in nature, to impose their weak equality, it is necessary to make them comparable in a certain sense. This is done by introducing an accommodation operator, denoted  $\Pi_l^g$ .

We propose an extension of the NIGLI to the case of a volume coupling, in the philosophy of the AF. The setting up of the volume NIGLI strategy we propose is similar to those with a surface coupling. To implement it, we propose the following steps : (see [11])

1. The domain  $\Omega$  is partitioned into two overlapping subdomains ; a global subdomain  $\Omega_g$  and a local one  $\Omega_l$  ; the thickness  $e$  of the overlap domain, denoted  $\Omega_c = \Omega_g \cap \Omega_l$ , with  $e > 0$  (cf. Figure 1b). We assume that the criticality is strictly contained in  $\Omega_l \setminus \Omega_c$  and we define a **local problem**, denoted  $(\mathcal{P}_l)$ .
2. We carrying out simplifications on the local domain  $\Omega_l$  which can be of a geometrical nature but also physical. Here for example we remove the crack, forming a new domain, denoted  $\Omega_a$  and called auxiliary domain, see Figure 1c. On this domain we will define an **auxiliary problem**, denoted  $(\mathcal{P}_a)$ .
3. We construct a modified global domain, denoted  $\Omega_m$  such that :  $\Omega_m = \Omega_g \cup \Omega_a$ , see Figure 1c. On this domain we will define a **modified problem**, denoted  $(\mathcal{P}_m)$ .

Now the idea, as done in the surface version of the NIGLI strategy, is to introduce in the simplified model a volume density of forces, defined over the overlapping zone  $\Omega_c$ , denoted  $\boldsymbol{\phi}$ , allowing to reproduce the effect of the local criticality in the simplified modelling. The three problems formulations are given by :

— The modified problem  $(\mathcal{P}_m)$ , given by :

Given  $\boldsymbol{\phi} \in \mathbf{M}$ , find  $\mathbf{u}_m \in \mathbf{W}_0(\Omega_m)$ , such that :

$$a_m(\mathbf{u}_m, \mathbf{v}_m) = l_m(\mathbf{v}_m) - c(\boldsymbol{\phi}, \mathbf{v}_m) \quad \forall \mathbf{v}_m \in \mathbf{W}_0(\Omega_m). \quad (3)$$

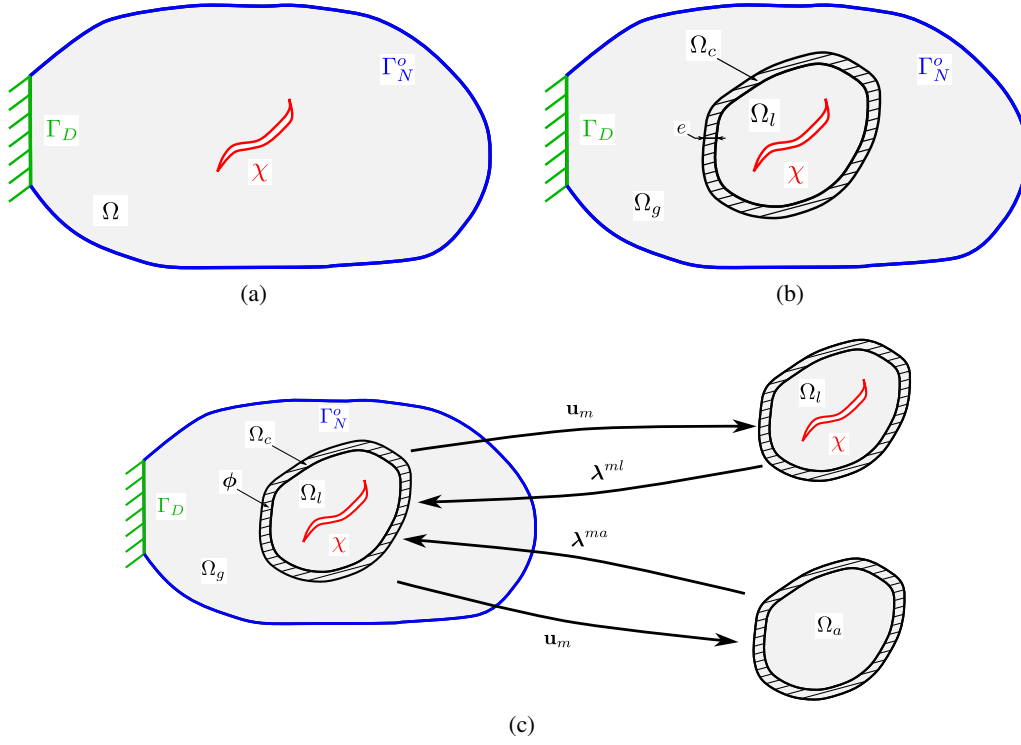


FIGURE 1 – A generic mechanical problem with a crack  $\chi$  in (a), a generic example of two domains decomposition for a global/local resolution of the mechanical problem with a volume coupling in (b) and the NIGLI algorithm principle in (c)

— The local problem ( $\mathcal{P}_l$ ), given by :

Given  $\mathbf{u}_m \in \mathbf{W}_0(\Omega_m)$ , find  $(\mathbf{u}_l, \boldsymbol{\lambda}^{ml}) \in \mathcal{W}(\Omega_l) \times \mathbf{M}$ , such that :

$$a_l(\mathbf{u}_l, \mathbf{v}_l) + c(\boldsymbol{\lambda}^{ml}, \Pi_l^g \mathbf{v}_l) = l_l(\mathbf{v}_l) \quad \forall \mathbf{v}_l \in \mathcal{W}(\Omega_l), \quad (4a)$$

$$c(\boldsymbol{\mu}, \Pi_l^g \mathbf{u}_l) = c(\boldsymbol{\mu}, \mathbf{u}_m) \quad \forall \boldsymbol{\mu} \in \mathbf{M}. \quad (4b)$$

— The auxiliary problem ( $\mathcal{P}_a$ ), given by :

Given  $\mathbf{u}_m \in \mathbf{W}_0(\Omega_m)$ , find  $(\mathbf{u}_a, \boldsymbol{\lambda}^{ma}) \in \mathbf{W}(\Omega_a) \times \mathbf{M}$ , such that :

$$a_a(\mathbf{u}_a, \mathbf{v}_a) + c(\boldsymbol{\lambda}^{ma}, \mathbf{v}_a) = l_a(\mathbf{v}_a) \quad \forall \mathbf{v}_a \in \mathbf{W}(\Omega_a), \quad (5a)$$

$$c(\boldsymbol{\mu}, \mathbf{u}_a) = c(\boldsymbol{\mu}, \mathbf{u}_m) \quad \forall \boldsymbol{\mu} \in \mathbf{M}. \quad (5b)$$

where  $\mathbf{u}_m$ ,  $\mathbf{u}_l$  and  $\mathbf{u}_a$  stand for the modified, local and auxiliary displacement fields,  $\boldsymbol{\lambda}^{ml}$  and  $\boldsymbol{\lambda}^{ma}$  the local and auxiliary volume Lagrange multipliers.

The volume density of correction effort being *a priori* unknown and not being able/willing to solve directly the real problem, we propose to use the same iterative algorithm of resolution proposed in the surface coupling framework, called Non-Intrusive Fixed Point Solver in [12]. It consists in, solving the problem ( $\mathcal{P}_m$ ) to obtain  $\mathbf{u}_m^k$ , use it to solve, in parallel, the problems ( $\mathcal{P}_l$ ) and ( $\mathcal{P}_a$ ) to obtain  $(\mathbf{u}_l^k, \boldsymbol{\lambda}^{ml,k})$  and  $(\mathbf{u}_a^k, \boldsymbol{\lambda}^{ma,k})$ . The Lagrange multipliers are used to update the force density  $\phi^{k+1} = \boldsymbol{\lambda}^{ml,k} - \boldsymbol{\lambda}^{ma,k}$ . This procedure is repeated till the relative variation of the force density correction, given by :

$$\eta_{\text{rel}}^{k+1} = \frac{\|\phi^{k+1} - \phi^k\|}{\|\phi^{k+1}\|} \quad (6)$$

is lower than a given tolerance  $\varepsilon_{\text{tol}}$ .

With this algorithm, the NIGLI strategy allows each of the three problems to be treated by a different codes as long as the one treating the simplified problem can receive an external volume density of forces and the ones treating the local and auxiliary problems can receive an external displacement field. The classical configuration being to use for the simplified problem an industrial code and a more specialized one, of research type, for both local and auxiliary problems.

### 3 Application to an atomistic/continuum volume coupling

In this section we propose to apply the previously detailed method to the case of a coupling particle and continuum models. We base our presentation on the developments already realized in the AF, see e.g. [13, 14], and more particularly on two 1D problems. For each problem, we are willing to approximate the atomistic model in most of the domain and only keep it in a local zone.

#### 3.1 The model problems

We start by giving the two problems common parameters. The particle model rely on a set of  $N_p$  particles, denoted  $\mathcal{N}$ , distributed on a regular lattice in  $\mathbb{R}$  of mesh size  $l$ , occupying the closure of  $\Omega_l$ . The position of the particle  $i$  in the reference configuration is given by the coordinate  $p_i$ , such that :  $p_i = (i - 1) \times l$ . We consider here that each particle may interact with the others by means of harmonic pair potentials. The potential  $V_{ij}$  modelling the interaction between particles  $i$  and  $j$  is given by :

$$V_{ij}(z_i, z_j) = \frac{1}{2} k_{ij} (|p_j + z_j - p_i - z_i| - |p_j - p_i|)^2, \quad (7)$$

where  $z_i$  is the displacement of particle  $i$  and  $k_{ij}$  is the stiffness coefficient of potential  $V_{ij}$ . For the sake of simplicity, we introduce the global vector  $\mathbf{z} = [z_1, \dots, z_{N_p}]$  of all individual displacements  $z_i$ . In the following, we will assume that every particle  $i$  interacts only with the subset  $\mathcal{N}_i \subset \mathcal{N}$  of neighboring particles so that long-ranged interactions are neglected. This assumption is applied by simply setting the coefficients  $k_{ij}$  to zero whenever a particle  $j$  is not in  $\mathcal{N}_i$ .

The particle lattice is approximated by a linear elastic beam of modulus  $E$ , occupying the closure of the global domain  $\Omega_m \times S_c$  with  $S_c$  its cross-section of area  $A$ . For simplicity, we will implicitly take  $A$  equal to unity. The material is supposed to obey Hooke's law  $\boldsymbol{\sigma} = E\boldsymbol{\varepsilon}$ , with  $\boldsymbol{\sigma}$  and  $\boldsymbol{\varepsilon}$  the beam's stress and strain. The strain is related to beam displacement  $u_g$  by :  $\boldsymbol{\varepsilon} = u_g'$ , where  $'$  stands for derivation  $\frac{d}{dx_1}$ .

Now, we detail each problems features :

- ( $\mathcal{P}_1$ ) – The problem geometry is depicted on Figure 2a. The beam is embedded at its left border ( $x_1 = 0$ ) and the particle  $P_c$  at the right border ( $x_1 = L$ ) is submitted to a traction effort  $F$ . We denote  $z_c$  the displacement of  $P_c$ . We consider a periodic distribution of springs with two springs stiffness constants  $k_1 = 100$  and  $k_2 = 1$ . We have for  $N_p$  odd :

$$\begin{aligned} k_{2j-1} &= k_1 & j &= 1, \dots, \frac{N_p - 1}{2} \\ k_{2j} &= k_2 & j &= 1, \dots, \frac{N_p - 1}{2} \end{aligned} \quad (8)$$

We define the following geometries and discretizations :  $\Omega_m = (0, 3)$ ,  $\Omega_l = (1, 3)$ ,  $\Omega_a = (1, 3)$ ,  $\Omega_c = (1, 2)$ ,  $N_p = 9$  and  $N^e = 4$ . The equilibrium length of the springs is equal to  $l = 0.25$  and the mesh size  $h_g = 2l = 0.5$ . The Young's modulus, using a representative cell (or Representative Volume Element, RVE) made of two consecutive springs, is given by :

$$E = \frac{k_1 k_2}{k_1 + k_2} 2l = \frac{100}{101} 0.5 = 0.49505 \quad (9)$$

The force  $F$  is chosen such that the displacement of the fully atomistic problem is equal to unity, i.e.  $F = E \times A / L$ .

- ( $\mathcal{P}_2$ ) – The problem geometry is depicted on Figure 2b. The beam is embedded at both ends ( $x_1 = 0$  and  $x_1 = L$ ). We consider a distribution of springs with a uniform stiffness constant  $k = 100$ . We have :

$$k_j = k \quad j = 1, \dots, N_p - 1 \quad (10)$$

The chain is submitted to a unit force  $F = 1$ , applied to the particle  $P_c$  at the center of  $\Omega_l$ . We suppose that the particle lattice is subjected to a defect consisting to a locally stiffness coefficient weakening of few bonds centered in a particle  $P_d$ . We denote by  $p_d$  the position of  $P_d$  in the reference configuration. The distribution of the bond stiffness coefficient  $k_{ij}$  between neighboring particles  $i$  and  $j$  is given in terms of  $k$  as :

$$k_{ij} = g(p_{ij}), \text{ with } g(x) = \frac{1}{1 + 10\exp^{-2x^2}}, \text{ and } p_{ij} = p_d - \frac{p_i - p_j}{2}. \quad (11)$$

We consider the following geometries and discretizations :  $\Omega_m = (0, 8.8)$ ,  $\Omega_l = (2.4, 7.4)$ ,  $\Omega_a = (2.4, 7.4)$ ,  $\Omega_c = (2.4, 3) \cup (7, 7.4)$ ,  $N_p = 8$ ,  $N^e = 4$  and  $z_d = 5.4$ . The equilibrium length of the springs is equal to  $l = 0.1$  and the mesh size  $h_g = 4l = 0.4$ . The Young's modulus is given by  $E = kl = 10$ .

As developed in [13], the weak equality between  $\mathbf{z}$  and  $u$  is imposed by converting the discrete displacement  $\mathbf{z}$  into a displacement field  $\Pi_l^g \mathbf{z}$ , where  $\Pi_l^g$  is e.g. the linear interpolation operator and defining an energy coupling operator  $c$ , given by :

$$c(\lambda, u_g) = \int_{\Omega_c} \beta_1 \lambda u_g + \beta_2 \lambda' u_g' dx_1 \quad (12)$$

with, in this context,  $\beta_1 = E$  and  $\beta_2 = E/e$ . We uniformly mesh the domain  $\Omega_g$ , with a mesh size  $h$ , imposing the mesh compatibility between the continuum model and the particle lattice.

We are finally able to write the modified, local and auxiliary problems, which we won't detail here. To solve the problem we use exactly the same algorithm as before.

## 3.2 Results

We consider the fully atomistic problem solution as a reference one, where the domain  $\Omega$  is occupied by  $N_p^{\text{ref}}$  particles.

### 3.2.1 First problem

The displacement fields we obtain are represented in Figure 3a with in black the reference solution, in blue the simplified problem solution and in red the local one. These solutions are obtained for a convergence criteria taken as  $\varepsilon_{\text{tol}} = 10^{-10}$ . If we consider as quantity of interest the displacement value of the particle at the right border, we obtain a relative error value of 8.7% which is the expected value for this Arlequin atomistic-continuum configuration see [13].

### 3.2.2 Second problem

The displacement fields we obtain are represented in Figure 3b with in black the reference solution, in blue the simplified problem solution and in red the local one. These solutions are obtained for a convergence criteria taken as  $\varepsilon_{\text{tol}} = 10^{-10}$ . If we consider as quantity of interest the displacement value of the particle  $P_c$ , we obtain a relative error value of 0.56%.

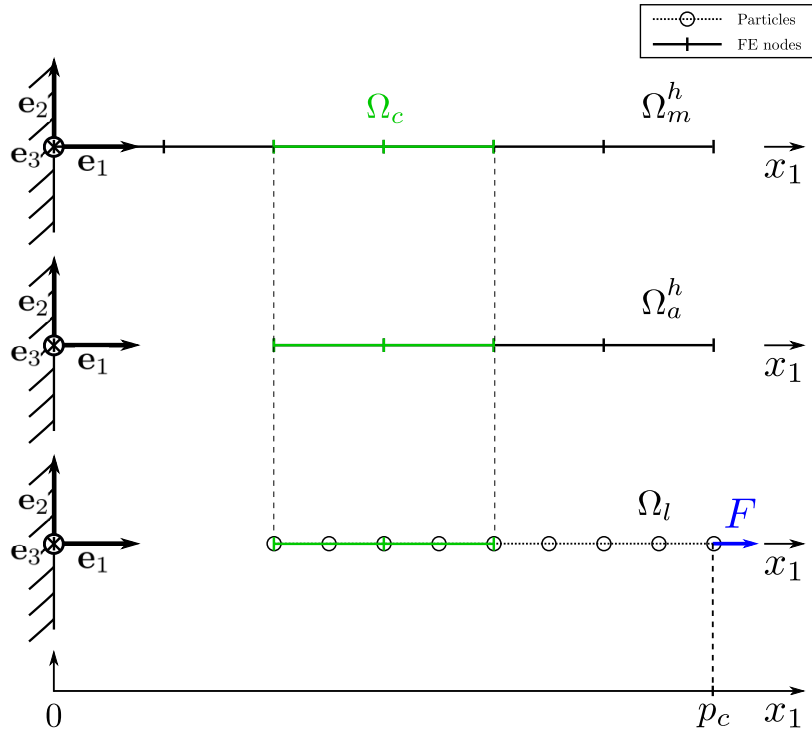
## 4 Conclusion

In this communication, we elaborated a collaborative algorithm with a thick coupling, taking cue from Iterative and Non-intrusive methods. We firstly applied it to the case of a classical mechanical problem i.e. the coupling of two macroscopic continuum models. Secondly, we demonstrate its feasibility and effectiveness to solve « true » multiscale problem by applying it to the coupling of atomistic and continuum models. More substantial examples will be shown during the presentation.

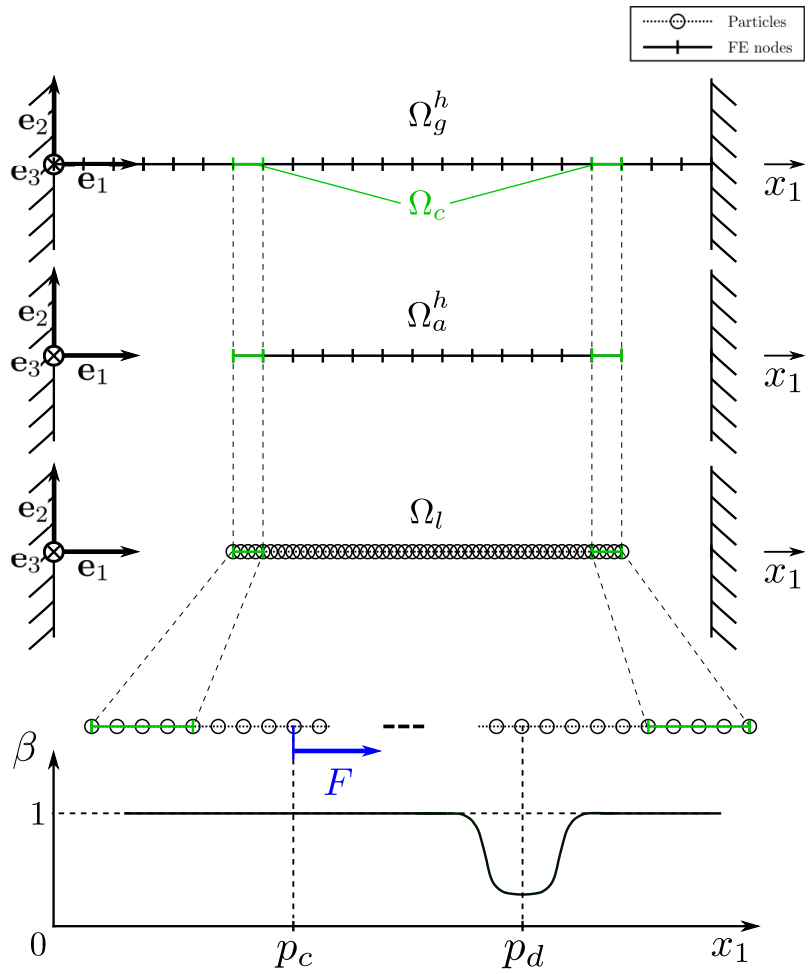
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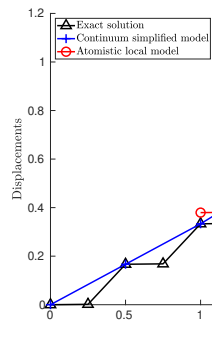


(a)

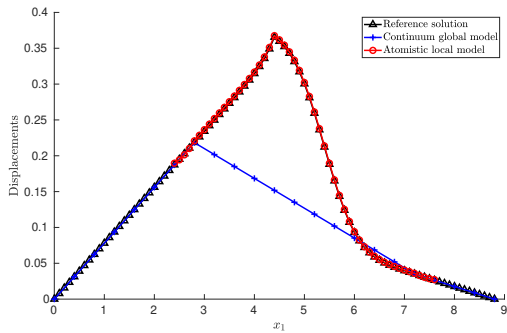


(b)

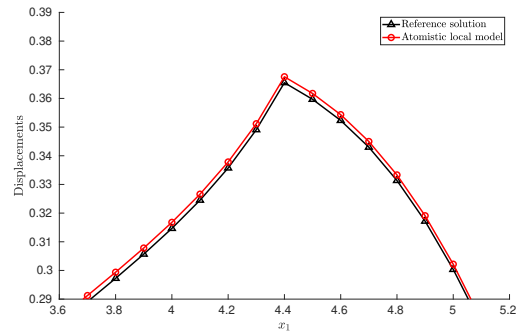
FIGURE 2 – Scheme of the continuum simplified and auxiliary domains and of the atomistic local one for the problem  $(\mathcal{P}_1)$  in (a) and for the problem  $(\mathcal{P}_2)$  in (b).



(a)



(b)



(c)

FIGURE 3 – Displacement fields obtained when convergence is reached in (a) for the problem  $\mathcal{P}_1$ , (b) for the problem  $\mathcal{P}_2$  with a zoom on the particle  $P_d$  in (c).