Numerical Algorithms **32:** 141–161, 2003.

On the convergence of a non-incremental homogenization method for nonlinear elastic composite materials

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Received 27 September 2001; accepted 4 October 2002
Communicated by P.G. Ciarlet

In memory of François Devries

In order to simulate the nonlinear behaviour of elastomer composite materials, we use a homogenization technique which induces nonlinear problems. This paper presents a non-incremental solving method which allows the reduction of computational costs. In this paper the equivalence between the proposed solving method and a Newton-type method is proved, which allows us to prove the convergence under realistic assumptions. Numerical results on a composite illustrate the performances of this method.

Keywords: homogenization, nonlinear elastic behaviour, non-incremental solving methods, Newton-type methods

AMS subject classification: 65H10, 74G15

1. Introduction

Nowadays there is an increasingly widespread use of elastomer materials in automobile, space, aeronautic, railway or pneumatic industries for links in binding, damping or tightness processes. Reinforcements (e.g., fibers, carbon black, etc.) are traditionally used within these links to improve their mechanical properties. However, when dealing with the computation of the resulting mechanical behaviour, this association raises great difficulties which stem from the large number of heterogeneities and the nonlinear behaviour.

Elastomer materials and more generally nonlinear elastic materials have been widely studied as the literature reveals [1,2,10,20]. Different procedures may be used to compute the mechanical behaviour of such nonlinear composite materials. The first consists in determining bounds from the equivalent strain energy density [24–26] at low

numerical cost. However, this approach does not allow us to compute the sought behaviour of such materials accurately, and gives no information about stress and strain at the heterogeneity level. Such methods are thus inefficient for industrial applications.

Here we choose to use a homogenization technique [22], well suited for nonlinear elasticity problems and related to composites with periodic microstructures. This reduces the numerical cost of the simulations. In nonlinear elasticity, instability (such as buckling on the composite's microscale) could occur, due to the strain energy density not being a convex function of the deformation gradient. This homogenization technique would thus require us to consider variations which are periodic over a set of cells. However, in the case presented here where no such bifurcation phenomena are encountered, variations over only one period can be considered [18]. The technique in this case consists in solving microscopic and macroscopic problems, coupled to one another by mean relations. This allows us to compute the macroscopic and microscopic displacement fields and the first macroscopic and microscopic Piola–Kirchhoff stress tensors.

Since the behaviour induces nonlinearities, the problem requires a nonlinear solving method. An incremental algorithm has already been developed in [13,14]. However, since it converges too slowly [5], it requires too much CPU time. To reduce computational costs, we propose a non-incremental algorithm initially used for plastic and elastoplastic materials [19]. It consists in splitting up the equations into a group of nonlinear equations to be solved locally in space and a group of linear equations to be solved over the complete structure. In the case studied here, it thus consits in computing couples of microscopic and macroscopic strain and stress, alternatively satisfying the linear and nonlinear equations [7]. However, the convergence of this algorithm has not been proved yet. The purpose of this paper is to prove the convergence of the proposed solving method, when it is applied to the elastomer composite homogenization technique.

Section 2 of this paper presents the problem considered and the homogenization technique used. In section 3, the solving method is introduced. Let $\mathcal{L}$ (respectively $\mathcal{NL}$) be the set of strain and stress satisfying the linear equations (respectively nonlinear equations) and the transformation operator H^+ (respectively H^-). We assume that all continuous problems considered have a unique solution in some appropriate space which we do not define precisely. We use a classical finite element discretization and assume that the discrete problems considered have unique solution in the space of finite dimension defined by the discretization. We use the Euclidian norm in that space. Our main contribution is then the proof of the convergence of our algorithm. In section 4, we first prove that the particular choice of H^+ and H^- leads to a discrete method equivalent to a Newton-type method. Under classical assumptions, we can then derive a convergence proof. Section 5 is a study of a unidirectional composite with numerical results which highlight the efficiency of our algorithm.

2. The problem considered

2.1. The heterogeneous problem

We consider the heterogeneous nonlinear elastic structure $\mathcal{B}$ which occupies a domain denoted by Ω included in $\mathbb{R}^3$ with respect to its undeformed, stress-free state.

If we denote respectively by $\mathbf{T}^\varepsilon$, $\mathbf{F}^\varepsilon$, $\mathbf{U}^\varepsilon$, e^ε the heterogeneous first Piola–Kirchhoff stress tensor, deformation gradient tensor, displacement field and strain energy density, and assume that there are no body forces, the problem to be solved in Ω under the assumption of quasi-static deformation is written:

$$\begin{cases} \operatorname{div}_{\boldsymbol{x}} \mathbf{T}^\varepsilon = \mathbf{0}; & \mathbf{T}^\varepsilon = \dfrac{\partial \mathrm{e}^\varepsilon}{\partial \mathbf{F}}\big(\boldsymbol{x},\ \mathbf{F}^\varepsilon\big); & \mathbf{F}^\varepsilon = \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{U}^\varepsilon & \text{in } \Omega; \\ \mathbf{T}(\mathbf{N}) = \mathbf{g} & \text{on } \partial\Omega_g; & \mathbf{U} = \mathcal{U} & \text{on } \partial\Omega_u \end{cases} \tag{1}$$

where $\partial\Omega_u$ denotes the external boundary of Ω where displacement $\mathcal{U}$ is prescribed, $\partial\Omega_g$ the external boundary of Ω where stress $\mathbf{g}$ is prescribed, $\mathbf{N}$ the unit external normal to $\partial\Omega_g$, and $\operatorname{div}_{\boldsymbol{x}}$, $\nabla_{\boldsymbol{x}}$ respectively denote the divergence and the gradient operator with respect to the space variables (x_1, x_2, x_3).

Since we assume that each component is homogeneous and isotropic, the behaviour of the composite's components depends only on the principal invariants i_1, i_2, i_3 of the dilatation tensor $\mathbf{C}$ [23]. They are defined as follows:

$$\begin{cases} \mathbf{C} = {}^{\mathrm{t}}\mathbf{F}^\varepsilon\, \mathbf{F}^\varepsilon; \\ i_1 = \det(\mathbf{C}); \qquad i_2 = \dfrac{1}{2}\Big[\big(\det(\mathbf{C})\big)^2 - \det\big(\mathbf{C}^2\big)\Big]; \qquad i_3 = \operatorname{tr}(\mathbf{C}) \end{cases}$$

where ${}^{\mathrm{t}}\mathbf{F}^\varepsilon$, $\det(\mathbf{C})$ and $\operatorname{tr}(\mathbf{C})$ respectively denote the transpose of $\mathbf{F}^\varepsilon$, the determinant of $\mathbf{C}$ and the trace of $\mathbf{C}$ which leads to $\mathrm{e}^\varepsilon(\boldsymbol{x},\ \mathbf{F}^\varepsilon) = \mathrm{e}^\varepsilon(\boldsymbol{x}, i_1, i_2, i_3)$.

We assume that problem (1) has a unique solution in some appropriate space.

Remark. As illustrated in figures 1 and 2, elastomeric composite materials have in general a unique response and behavior under specific prescribed loadings or displacements. For this reason, assuming a unique solution makes sense according to the physics of the problem considered.

In order to solve (1), we must use a discretization technique such as a finite element method. We recall that the heterogeneities in the structure are much smaller than the size of the structure. In order to take into account all these heterogeneities, the finite element mesh should be very thin, in which case too many computations would result. To avoid such numerical overheads, it is now standard to introduce a homogenization technique [4,22].

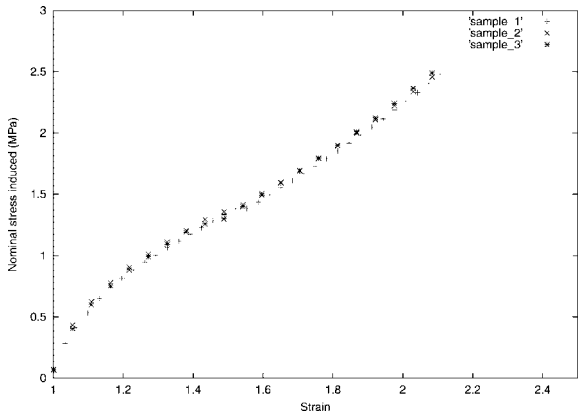

Figure 1. Response of test-tubes of naturel rubber reinforced by black of carbon under uni-axial tension test.

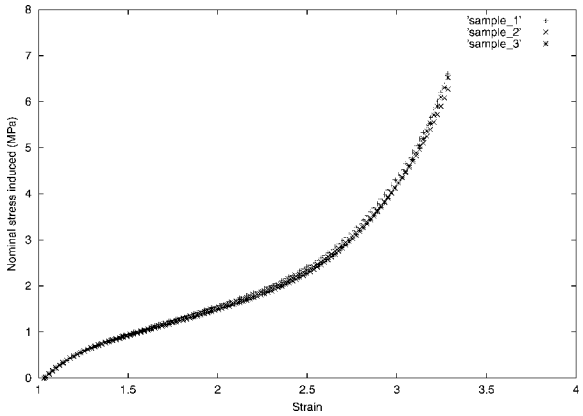

Figure 2. Response of test-tubes of naturel rubber reinforced by silica under uni-axial tension test.

2.2. *The homogenization problem*

The classic homogenization technique for the study of linear elastic Y-periodic composite structure, allows us to obtain a great deal of information at the level of structure $\mathcal{B}$ but also at the level of the heterogeneities. We assume that the material studied has a periodical (mechanical and geometrical) structure in such a way that the definition of its period (or representative volume element) allows it to be known. We also assume that Y does not contain holes, nor cracks and is undamaged. Moreover, denoting by H a representative length of the structure Ω, and by L one of the basic cells Y, we assume that the ratio

$$\varepsilon = \frac{L}{H} \tag{2}$$

is such that $\varepsilon \ll 1$. This parameter allows us to define the heterogeneity level.

The microscopic strain energy density is defined by

$$\boldsymbol{y} \to \mathrm{e}(\boldsymbol{y}, \mathbf{f}) \text{ Y-periodic in } \boldsymbol{y}, \quad \forall \boldsymbol{y} \in \mathrm{Y}. \tag{3}$$

Once Y has been defined, we can build the geometry and the behaviour of the structure $\mathcal{B}$. The geometric definition of $\mathcal{B}$ is defined by successive translations in the three spacial directions, and the strain energy density e^ε is given by

$$\mathrm{e}^\varepsilon(\boldsymbol{x}, \mathbf{F}) = \mathrm{e}\left(\frac{\boldsymbol{x}}{\varepsilon}, \mathbf{F}\right), \quad \forall \boldsymbol{x} \in \Omega. \tag{4}$$

In order to define the strain energy density E of the homogeneous equivalent materials, as ε converges to 0, which means that the heterogeneities are much smaller than the structure, let us introduce test functions $\mathbf{V}^\varepsilon \in \mathcal{U}_{\mathrm{ad}}$ [4] defined by

$$\begin{aligned} \mathcal{U}_{\mathrm{ad}} &= \left\{\mathbf{V} \mid \mathbf{V} = \mathcal{U} \text{ on } \partial\Omega_u\right\}, \\ \mathcal{U}_{\mathrm{ad}}^{\mathrm{Y}} &= \left\{\mathbf{v}(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{U}_{\mathrm{ad}} \ \forall \boldsymbol{y} \in \mathrm{Y} \text{ and } \mathbf{v}(\boldsymbol{x}, \boldsymbol{y}) \text{ Y-periodic in } \boldsymbol{y}\right\}, \end{aligned} \tag{5}$$

$$\mathbf{V}^\varepsilon(\boldsymbol{x}) = \mathbf{V}(\boldsymbol{x}) + \varepsilon \mathbf{v}\left(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}\right), \quad \mathbf{V} \in \mathcal{U}_{\mathrm{ad}} \text{ and } \mathbf{v} \in \mathcal{U}_{\mathrm{ad}}^{\mathrm{Y}}. \tag{6}$$

By setting $\boldsymbol{y} = \boldsymbol{x}/\varepsilon$, we introduce two different scales in the problem:

- a macroscopic scale of reference $(\mathrm{O}, \boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$, linked to the structure $\mathcal{B}$, in which the size of the heterogeneities are smaller than the unit;
- a microscopic scale of reference $(\mathrm{O}, \boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3)$ (with $y_i = x_i/\varepsilon$), linked to the basic cell Y, in which the size of the heterogeneities is related to unit size.

We assume that the strain energy density of the homogeneous equivalent material converges to the density E, which does not explicitely depend on $\boldsymbol{y}$, as ε converges to 0. This strain energy density E is defined by

$$\mathrm{E} = \inf_{k \in \mathbb{N}} \left\{ \min_{\mathbf{V},\, \mathbf{v}} \frac{1}{k^3} \frac{1}{|\mathrm{Y}|} \int_{k\mathrm{Y}} \mathrm{e}\big(\boldsymbol{y}, \mathbf{F}(\mathbf{V}) + \nabla_{\boldsymbol{y}} \mathbf{v}\big)\, \mathrm{d}y \right\}, \tag{7}$$

where $\mathbf{F}(\mathbf{V}) = \mathbf{1} + \nabla_x \mathbf{V}$ and $|\mathrm{Y}|$ is a measure of Y.

Remark. More precise informations of this result can be found in [22].

Here a minimisation on the number of basic cells can be noted. This allows us to take into account instability phenomena such as microscopic buckling. If we assume that such phenomena cannot happen then this minimisation step is not required, and $k = 1$ [18].

We have to solve the problem

$$\begin{cases} \text{Find } \mathbf{U} \in \mathcal{U}_{\mathrm{ad}} \text{ and } \mathbf{u} \in \mathcal{U}_{\mathrm{ad}}^{\mathrm{Y}} \text{ such as:} \\ \mathrm{E}(\mathbf{U},\ \mathbf{u}) = \min_{\mathbf{V},\, \mathbf{v}} \displaystyle\int_\Omega \frac{1}{|\mathrm{Y}|} \left(\int_{\mathrm{Y}} \mathrm{e}(\boldsymbol{y}, \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{V} + \nabla_{\boldsymbol{y}} \mathbf{v})\, \mathrm{d}y \right) \mathrm{d}\Omega, \end{cases} \tag{8}$$

denoting by **T**, **F** and **U** the macroscopic first Piola–Kirchhoff stress tensor, gradient tensor and displacement field respectively and by $\boldsymbol{\tau}$, **f** and **u** their microscopic equivalents. It is easy to prove that problem (8) is equivalent to the following:

Macroscopic problem.

$$\begin{cases} \operatorname{div}_{\boldsymbol{x}}\mathbf{T} = \mathbf{0}; & \mathbf{T} = \dfrac{\partial \mathrm{E}}{\partial \mathbf{F}}(\boldsymbol{x}, \mathbf{F}); \qquad \mathbf{F} = \mathbf{1} + \nabla_{\boldsymbol{x}}\mathbf{U} \quad \text{in } \Omega; \\ \mathbf{U} = \mathcal{U} \qquad \text{on } \partial\Omega_u; \qquad \mathbf{T}(\mathbf{N}) = \mathbf{g} \qquad \text{on } \partial\Omega_g. \end{cases} \tag{9}$$

Microscopic problem.

$$\begin{cases} \operatorname{div}_{\boldsymbol{y}}\boldsymbol{\tau} = \mathbf{0}; \qquad \boldsymbol{\tau} = \dfrac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f}); \qquad \mathbf{f} = \mathbf{F} + \nabla_{\boldsymbol{y}}\mathbf{u} \quad \text{in Y}; \\ \mathbf{u} \text{ Y-periodic}; \quad \boldsymbol{\tau}(\mathbf{n}) \text{ Y-antiperiodic} \end{cases} \tag{10}$$

where $\operatorname{div}_{\boldsymbol{y}}$ and $\nabla_{\boldsymbol{y}}$ denote the divergence and the gradient operator with respect to the space variables y_1, y_2, y_3, respectively, and where **n** is the unit external normal to Y. The microscopic strain energy density e is assumed to be known as we know the behaviour of each component. On the other hand, the macroscopic density E is implicitly defined by (11).

Microscopic–macroscopic relations. Finally, the macroscopic strain energy density E of the equivalent homogeneous material is defined by the following coupling relations,

$$\mathrm{E} = \langle \mathrm{e} \rangle_{\mathrm{Y}}, \qquad \mathbf{T} = \langle \boldsymbol{\tau} \rangle_{\mathrm{Y}}, \qquad \mathbf{F} = \langle \mathbf{f} \rangle_{\mathrm{Y}}, \tag{11}$$

with $\langle h \rangle_{\mathrm{Y}} = (1/|\mathrm{Y}|) \int_{\mathrm{Y}} h \, \mathrm{d}y$.

In the sequel, we describe our algorithm to solve these coupled nonlinear problems (9)–(11).

3. Non-incremental algorithm

Our non-incremental algorithm, is adapted from the method initially developed to study viscoplastic structures [11,19].

This algorithm consists of computing couples $\mathrm{S} = ((\mathbf{U}, \mathbf{T});\ (\mathbf{u}, \boldsymbol{\tau}))$, alternatively belonging to the sets $\mathcal{L}$ and $\mathcal{NL}$, defined below. The method is defined by two operators, $\mathrm{H}^+ : \mathcal{L} \to \mathcal{NL}$ and $\mathrm{H}^- : \mathcal{NL} \to \mathcal{L}$ and by the iterations:

$$\mathrm{S}^0 \in \mathcal{L},$$

$$\mathrm{S}^{n+1/2} \in \mathcal{NL}, \text{ and } \mathrm{S}^{n+1/2} = \mathrm{H}^+\big(\mathrm{S}^n\big);\ \mathrm{S}^{n+1} \in \mathcal{L}, \text{ and } \mathrm{S}^{n+1} = \mathrm{H}^-\big(\mathrm{S}^{n+1/2}\big).$$

3.1. Choice of $\mathcal{L}$ and $\mathcal{NL}$

In order to split the equations, we assume that the macroscopic boundary conditions on $\partial\Omega$ are linear. We define the sets $\mathcal{L}$ and $\mathcal{NL}$ by

$$\mathcal{NL} = \left\{ \big((\mathbf{T}, \mathbf{U});\ (\boldsymbol{\tau}, \mathbf{u})\big) \text{ such that (14)} \big| \boldsymbol{\tau} = \frac{\partial \mathrm{e}}{\partial \mathbf{f}} \text{ in Y} \right\}, \tag{12}$$

$$\begin{aligned} \mathcal{L} = \big\{ \big((\mathbf{T}, \mathbf{U});\ (\boldsymbol{\tau}, \mathbf{u})\big) \text{ such that (14)} \big| \big\{ &\mathrm{div}_{\boldsymbol{x}} \mathbf{T} = \mathbf{0} \text{ in } \Omega;\ \mathbf{T}(\mathbf{N}) = \mathbf{g} \text{ on } \partial\Omega_g; \\ &\mathrm{div}_{\boldsymbol{y}} \boldsymbol{\tau} = \mathbf{0} \text{ in Y};\ \boldsymbol{\tau}(\mathbf{n}) \text{ Y-antiperiodic} \big\} \big\} \end{aligned} \tag{13}$$

where

$$\begin{cases} \mathbf{T} = \langle \boldsymbol{\tau} \rangle_{\mathrm{Y}}; \qquad \mathbf{F} = \langle \mathbf{f} \rangle_{\mathrm{Y}}; \qquad \mathbf{F} = \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{U} \quad \text{in } \Omega; \qquad \mathbf{U} = \mathcal{U} \quad \text{on } \partial\Omega_u \\ \mathbf{f} = \mathbf{F} + \nabla_{\boldsymbol{y}} \boldsymbol{u} \text{ in Y};\ \mathbf{u} \text{ Y-periodic}. \end{cases} \tag{14}$$

3.2. Computation of S^0

The first step of this algorithm consists in computing an initial approximation $\mathrm{S}^0 \in \mathcal{L}$, as cheaply as possible. To this end, we linearise the microscopic law near $\mathbf{f} = \mathbf{1}$, so that S^0 is defined by

$$\begin{cases} \mathrm{div}_{\boldsymbol{y}} \boldsymbol{\tau}^0 = \mathbf{0}; \qquad \boldsymbol{\tau}^0 = \mathbf{q}^0(\boldsymbol{y}) \big(\nabla_{\boldsymbol{x}} \mathbf{U}^0 + \nabla_{\boldsymbol{y}} \mathbf{u}^0 \big) \quad \text{in Y}, \\ \mathbf{u}^0 \text{ Y-periodic}; \quad \boldsymbol{\tau}^0(\mathbf{n}) \text{ Y-antiperiodic} \end{cases} \tag{15}$$

where

$$\mathbf{q}^0(\boldsymbol{y}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\, \partial \mathbf{f}}(\boldsymbol{y},\ \mathbf{f} = \mathbf{1}), \tag{16}$$

$$\begin{cases} \mathrm{div}_{\boldsymbol{x}} \mathbf{T}^0 = \mathbf{0}; & \mathbf{T}^0 = \mathbf{Q}^0 \nabla_{\boldsymbol{x}} \mathbf{U}^0 \quad \text{in } \Omega, \\ \mathbf{U}^0 = \mathcal{U} \quad \text{on } \partial\Omega_u; & \mathbf{T}^0(\mathbf{N}) = \mathbf{g} \qquad \text{on } \partial\Omega_g \end{cases} \tag{17}$$

where the homogenized stiffness tensor $\mathbf{Q}^0$ is implicitly defined by

$$\mathbf{T}^0 = \big\langle \boldsymbol{\tau}^0 \big\rangle_{\mathrm{Y}}; \qquad \mathbf{F}^0 = \big\langle \mathbf{f}^0 \big\rangle_{\mathrm{Y}}. \tag{18}$$

Thus, we get a coupled linear system, solved by a method similar to step $n + 1$ given in (3.4).

3.3. *Step $n + 1/2$: from $\mathcal{L}$ into $\mathcal{NL}$*

Let $B = \{(\boldsymbol{\tau},\ \mathbf{f})\}$, with $\boldsymbol{\tau}$ and $\mathbf{f}$ in some appropriate space. The operator H^+ we have chosen is defined by

$$\begin{aligned} &\mathrm{H}^+ : B \to \mathcal{NL}, \\ &\left(\boldsymbol{\tau}^n, \mathbf{f}^n\right) \to \left(\boldsymbol{\tau}^{n+1/2}, \mathbf{f}^{n+1/2}\right) \quad \text{with} \quad \begin{cases} \mathbf{f}^{n+1/2} = \mathbf{f}^n, \\ \boldsymbol{\tau}^{n+1/2} = \dfrac{\partial \mathrm{e}}{\partial \mathbf{f}}\left(\boldsymbol{y},\ \mathbf{f}^{n+1/2}\right). \end{cases} \end{aligned} \tag{19}$$

We make this choice because it is then easy to compute $\mathrm{S}^{n+1/2}$. Moreover, the equations we have to deal with are local in space. The iterate $\mathrm{S}^{n+1/2} = ((\mathbf{U}^{n+1/2}, \mathbf{T}^{n+1/2}),\ (\mathbf{u}^{n+1/2}, \boldsymbol{\tau}^{n+1/2}))$ is thus defined by

$$\begin{cases} \mathbf{T}^{n+1/2} = \left\langle \boldsymbol{\tau}^{n+1/2} \right\rangle_{\mathrm{Y}}; \qquad \mathbf{F}^{n+1/2} = \left\langle \mathbf{f}^{n+1/2} \right\rangle_{\mathrm{Y}} \qquad \text{in } \Omega; \\ \mathbf{U}^{n+1/2} \mid \nabla_x \mathbf{U}^{n+1/2} = \mathbf{F}^{n+1/2} - \mathbf{1} \quad \text{in } \Omega; \qquad \mathbf{U} = \mathcal{U} \qquad \text{on } \partial\Omega_u; \\ \boldsymbol{\tau}^{n+1/2} = \dfrac{\partial \mathrm{e}}{\partial \mathbf{f}}\left(\boldsymbol{y}, \mathbf{f}^{n+1/2}\right); \qquad \mathbf{f}^{n+1/2} = \mathbf{f}^n \quad \text{in Y}; \\ \mathbf{u}^{n+1/2} | \nabla_y \mathbf{u}^{n+1/2} = \mathbf{f}^{n+1/2} - \mathbf{F}^{n+1/2} \quad \text{in Y}; \qquad \mathbf{u}^{n+1/2}\ \text{Y-periodic}. \end{cases} \tag{20}$$

It may be noted that

$$\forall\, \mathbf{S} \in \mathcal{NL}, \quad \mathrm{H}^+(\mathbf{S}) = \mathbf{S}.$$

Also if $\mathrm{S}^\star$ is a solution of (9)–(11) then $\mathrm{H}^+(\mathrm{S}^\star) = \mathrm{S}^\star$.

3.4. *Step $n + 1$: from $\mathcal{NL}$ into $\mathcal{L}$*

In order to define H^-, we notice that there is no behaviour law connecting stress and strain. Then the operator H^- we have chosen is a "tangent" operator such that

$$\begin{aligned} &\mathrm{H}^- : B \to \mathcal{L}, \\ &\left(\boldsymbol{\tau}^{n+1/2}, \mathbf{f}^{n+1/2}\right) \to \left(\boldsymbol{\tau}^{n+1}, \mathbf{f}^{n+1}\right), \\ &\text{with } \boldsymbol{\tau}^{n+1} = \boldsymbol{\tau}^{n+1/2} + \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\, \partial \mathbf{f}}\left(\boldsymbol{y}, \mathbf{f} = \mathbf{f}^{n+1/2}\right)\left(\mathbf{f}^{n+1} - \mathbf{f}^{n+1/2}\right). \end{aligned} \tag{21}$$

The approximation S^{n+1} is given by

$$\begin{cases} \mathrm{div}_{\boldsymbol{y}}\, \boldsymbol{\tau}^{n+1} = \mathbf{0}; \qquad \boldsymbol{\tau}^{n+1} = \mathbf{p}^{n+1/2} + \mathbf{q}^{n+1/2}\left(\nabla_{\boldsymbol{x}} \mathbf{U}^{n+1} + \nabla_{\boldsymbol{y}} \mathbf{u}^{n+1}\right) \quad \text{in Y}, \\ \mathbf{u}^{n+1}\ \text{Y-periodic}; \qquad \boldsymbol{\tau}^{n+1}(\mathbf{n})\ \text{Y-antiperiodic}, \end{cases} \tag{22}$$

$$\begin{cases} \mathrm{div}_{\boldsymbol{x}} \mathbf{T}^{n+1} = \mathbf{0}; \qquad \mathbf{T}^{n+1} = \dfrac{\partial \mathrm{E}}{\partial \mathbf{F}}\left(\boldsymbol{x}, \mathbf{F}^{n+1}\right); \quad \mathbf{F}^{n+1} = \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{U}^{n+1} \quad \text{in } \Omega, \\ \mathbf{U}^{n+1} = \mathcal{U} \quad \text{on } \partial\Omega_u; \qquad \mathbf{T}^{n+1}(\mathbf{N}) = \mathbf{g} \quad \text{on } \partial\Omega_g \end{cases} \tag{23}$$

where E is implicitly defined by

$$\mathbf{T}^{n+1} = \left\langle \boldsymbol{\tau}^{n+1} \right\rangle_{\mathrm{Y}}; \qquad \mathbf{F}^{n+1} = \left\langle \mathbf{f}^{n+1} \right\rangle_{\mathrm{Y}} \tag{24}$$

and where

$$\begin{aligned} \mathbf{q}^{n+1/2} &= \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\, \partial \mathbf{f}}\left(\boldsymbol{y}, \mathbf{f} = \mathbf{f}^{n+1/2}\right); \\ \mathbf{p}^{n+1/2} &= \boldsymbol{\tau}^{n+1/2} + \mathbf{q}^{n+1/2}\left(\mathbf{1} - \mathbf{f}^{n+1/2}\right). \end{aligned} \tag{25}$$

It may be noted that

$$\forall \mathbf{S} \in \mathcal{L}, \quad \mathrm{H}^{-}(\mathbf{S}) = \mathbf{S}$$

and also that $\mathrm{H}^{-}(\mathrm{S}^{\star}) = \mathrm{S}^{\star}$.

Finally, since $\boldsymbol{\tau}^{n+1}$ is a linear function of $\nabla_{\boldsymbol{x}} \mathbf{U}^{n+1}$, we split the microscopic fields as follows:

$$\mathbf{u}^{n+1} = \mathbf{v}^{n+1} - \boldsymbol{\chi}^{kl} \frac{\partial \mathrm{U}^{k}}{\partial x_l}, \qquad \boldsymbol{\tau}^{n+1} = \mathbf{t}^{n+1} + \boldsymbol{\sigma}^{kl} \frac{\partial \mathrm{U}^{k}}{\partial x_l}, \tag{26}$$

where the ten couples $(\mathbf{t}^{n+1}, \mathbf{v}^{n+1})$ and $(\boldsymbol{\sigma}^{kl}, \boldsymbol{\chi}^{kl})$ $((k, l) \in \{1, 2, 3\}^2)$ are solutions of

$$\begin{cases} \mathrm{div}_{\boldsymbol{y}} \mathbf{t}^{n+1} = \mathbf{0}; & \mathbf{t}^{n+1} = \mathbf{p}^{n+1/2} + \mathbf{q}^{n+1/2} \nabla_{\boldsymbol{y}} \mathbf{v}^{n+1} \quad \text{in Y}, \\ \mathbf{v}^{n+1} \text{ Y-periodic}; & \mathbf{t}^{n+1}(\mathbf{n}) \text{ Y-antiperiodic} \end{cases} \tag{27}$$

and

$$\begin{cases} \mathrm{div}_{\boldsymbol{y}} \boldsymbol{\sigma}^{kl} = \mathbf{0}; & \boldsymbol{\sigma}^{kl} = \mathbf{q}^{n+1/2}\left(\mathbf{1}^{kl} - \nabla_{\boldsymbol{y}} \boldsymbol{\chi}^{kl}\right) \quad \text{in Y}, \\ \boldsymbol{\chi}^{kl} \text{ Y-periodic}; & \boldsymbol{\sigma}^{kl}(\mathbf{n}) \text{ Y-antiperiodic} \end{cases} \tag{28}$$

where $(1^{kl})_{ij} = \delta_{ik}\delta_{kl}$.

These problems are linear and independent of the unknown macroscopic fields, so they are easy to solve.

We assume that problems (27), (28) have a unique solution.

Once problems (27) and (28) have been solved, we compute the macroscopic fields $\mathbf{T}^{n+1}$ and $\mathbf{U}^{n+1}$ by solving the following linear problem

$$\begin{cases} \mathrm{div}_{\boldsymbol{x}} \mathbf{T} = \mathbf{0}; & \mathbf{T} = \mathbf{P}^{n+1} + \mathbf{Q}^{n+1} \nabla_{\boldsymbol{x}} \mathbf{U}^{n+1} \quad \text{in } \Omega; \\ \mathbf{U}^{n+1} = \mathcal{U} \quad \text{on } \partial\Omega_u; & \mathbf{T}^{n+1}(\mathbf{N}) = \mathbf{g} \quad \text{on } \partial\Omega_g \end{cases} \tag{29}$$

with

$$\mathrm{Q}_{ijkl}^{n+1} = \left\langle \sigma_{ij}^{kl} \right\rangle_{\mathrm{Y}}; \qquad \mathrm{P}_{ij}^{n+1} = \left\langle \mathrm{t}_{ij}^{n+1} \right\rangle_{\mathrm{Y}}. \tag{30}$$

We assume that (30) has a unique solution.

Finally, we compute the microscopic fields using (26).

3.5. Convergence criterion

The solution $S^\star$ satisfies $S^\star \in \mathcal{L} \cap \mathcal{NL}$, so $H^+(S^\star) = H^-(S^\star) = S^\star$.

As usual, we define a stopping criterion based on the difference between two iterates. We choose a criterion using both microscopic and macroscopic energies defined by

$$\begin{cases} e^{n+1} = \dfrac{\|\boldsymbol{\tau}^{n+1}\colon \mathbf{f}^{n+1} - \boldsymbol{\tau}^{n+1/2}\colon \mathbf{f}^{n+1/2}\|_Y}{\|\boldsymbol{\tau}^{n+1/2}\colon \mathbf{f}^{n+1/2}\|_Y}; \\ \mathcal{E}^{n+1} = \dfrac{\|\mathbf{T}^{n+1} : \mathbf{F}^{n+1} - \mathbf{T}^{n+1/2}\colon \mathbf{F}^{n+1/2}\|_\Omega}{\|\mathbf{T}^{n+1/2}\colon \mathbf{F}^{n+1/2}\|_\Omega}; \qquad \text{rate}^{n+1} = \sup\left(e^{n+1}, \mathcal{E}^{n+1}\right) \end{cases}$$

with $\|\cdot\|_Y = \int_Y |\cdot| \,\mathrm{d}y$ and $\|\cdot\|_\Omega = \int_\Omega |\cdot| \,\mathrm{d}x$. The stopping test is then

$$\text{rate}^{n+1} < \varepsilon \tag{31}$$

where ε has to be specified.

3.6. Discretization

In order to compute S^{n+1}, we first give the variational formulation at step $n+1$, and then we discretize it.

Let us denote by u_{ad} the space of the microscopic admissible displacement field, defined by

$$u_{\text{ad}} = \{\mathbf{v} \mid \mathbf{v} \text{ Y-periodic}\}. \tag{32}$$

Let us introduce $\mathcal{U}_{\text{ad}}$, the space of the macroscopic admissible displacement fields, defined by

$$\mathcal{U}_{\text{ad}} = \{\mathbf{V} \mid \mathbf{V} = \mathcal{U} \text{ on } \partial\Omega_u\}, \tag{33}$$

and denote by $\mathcal{U}^0_{\text{ad}}$ the vectorial space associated to $\mathcal{U}_{\text{ad}}$, defined by

$$\mathcal{U}^0_{\text{ad}} = \{\mathbf{V} \mid \mathbf{V} = \mathbf{0} \text{ on } \partial\Omega_u\}. \tag{34}$$

Then, it is easy to prove that the variational formulation of (22), (23) and (24) is given by

$$\begin{aligned} &\mathbf{U}^{n+1} \in \mathcal{U}_{\text{ad}}, \quad \mathbf{u}^{n+1} \in u_{\text{ad}} \quad \text{such that} \\ &\begin{cases} a^{n+1}\left(\mathbf{u}^{n+1}, \mathbf{v}\right) = l^{n+1}(\mathbf{v}), & \forall \mathbf{v} \in u_{\text{ad}} \\ A^{n+1}\left(\mathbf{U}^{n+1}, \mathbf{V}\right) = L^{n+1}(\mathbf{V}), & \forall \mathbf{V} \in \mathcal{U}^0_{\text{ad}} \end{cases} \end{aligned} \tag{35}$$

with

$$\begin{cases} a^{n+1}(\mathbf{u}, \mathbf{v}) = \displaystyle\int_Y \mathbf{q}^{n+1/2} \nabla_y \mathbf{u} \nabla_y \mathbf{v} \,\mathrm{d}\boldsymbol{y}, \\ l^{n+1}(\mathbf{v}) = -\displaystyle\int_Y \left(\mathbf{p}^{n+1/2} + \mathbf{q}^{n+1/2} \nabla_{\boldsymbol{x}} \mathbf{U}^{n+1}\right) \nabla_y \mathbf{v} \,\mathrm{d}\boldsymbol{y} \end{cases} \tag{36}$$

and

$$\begin{cases} A^{n+1}(\mathbf{U},\mathbf{V}) = \displaystyle\int_\Omega \left(\int_Y \mathbf{q}^{n+1/2}\,\mathrm{d}\boldsymbol{y} \right) \nabla_{\boldsymbol{x}}\mathbf{U}\nabla_{\boldsymbol{x}}\mathbf{V}\,\mathrm{d}\boldsymbol{x}, \\ L^{n+1}(\mathbf{V}) = \displaystyle\int_{\partial\Omega_g} \mathbf{g}\mathbf{V}\,\mathrm{d}\boldsymbol{x} - \int_\Omega \left(\frac{1}{|Y|} \left(\int_Y \left(\mathbf{p}^{n+1/2} + \mathbf{q}^{n+1/2}\nabla_{\boldsymbol{y}}\mathbf{u}^{n+1} \right) \mathrm{d}\boldsymbol{y} \right) \right) \nabla_{\boldsymbol{x}}\mathbf{V}\,\mathrm{d}\boldsymbol{x}. \end{cases} \tag{37}$$

Problem (35) may be discretized by approximating u_{ad}, $\mathcal{U}_{\mathrm{ad}}$ and $\mathcal{U}^0_{\mathrm{ad}}$ by spaces of finite dimension, using a finite element method [9,15]. Let us introduce the subspaces u^h_{ad}, $\mathcal{U}^h_{\mathrm{ad}}$ and $\mathcal{U}^{0,h}_{\mathrm{ad}}$ of finite dimension with

$$\dim u^h_{\mathrm{ad}} = n_h; \qquad \dim \mathcal{U}^h_{\mathrm{ad}} = \dim \mathcal{U}^{0,h}_{\mathrm{ad}} = N_h.$$

By choosing for $\mathbf{V}$ and $\mathbf{v}$ the basis vectors $\boldsymbol{\Phi}^i$ and $\boldsymbol{\Psi}^i$ of $\mathbb{R}^{N_h}$ and $\mathbb{R}^{n_h}$, respectively, we get the following problem:

$$\begin{aligned} &\mathbf{U}^{n+1,h} \in \mathcal{U}^h_{\mathrm{ad}}, \quad \mathbf{u}^{n+1,h} \in u^h_{\mathrm{ad}} \quad \text{such that} \\ &\begin{cases} a^{n+1}\big(\mathbf{u}^{n+1,h}, \boldsymbol{\Psi}^i\big) = l^{n+1}\big(\boldsymbol{\Psi}^i\big), & \forall i = 1,\dots,n_h, \\ A^{n+1}\big(\mathbf{U}^{n+1,h}, \boldsymbol{\Phi}^i\big) = L^{n+1}\big(\boldsymbol{\Phi}^i\big), & \forall i = 1,\dots,N_h. \end{cases} \end{aligned} \tag{38}$$

4. Convergence of the algorithm

In order to prove convergence, we first write the variational formulation of problem (9)–(11), and discretize it. Then we prove that, with our choice of the sets $\mathcal{L}$, $\mathcal{NL}$ along with our choice of the operators H^+ and H^-, we get an algorithm which is equivalent to a Newton-type method. This result allows us to prove convergence.

4.1. Discretization

It is easy to prove that the variational formulation of the nonlinear problem (9)–(11) is given by

$$\begin{aligned} &\mathbf{U} \in \mathcal{U}_{\mathrm{ad}}, \quad \mathbf{u} \in u_{\mathrm{ad}} \quad \text{such that} \\ &\begin{cases} a'(\mathbf{u},\mathbf{v}) = 0, & \forall \mathbf{v} \in u_{\mathrm{ad}}, \\ A'(\mathbf{U},\mathbf{V}) = L'(\mathbf{V}), & \forall \mathbf{V} \in \mathcal{U}^0_{\mathrm{ad}} \end{cases} \end{aligned} \tag{39}$$

with

$$a'(\mathbf{u},\mathbf{v}) = \int_Y \frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y},\ \mathbf{f} = \mathbf{1} + \nabla_{\boldsymbol{x}}\mathbf{U} + \nabla_{\boldsymbol{y}}\mathbf{u})\nabla_{\boldsymbol{y}}\mathbf{v}\,\mathrm{d}\boldsymbol{y} \tag{40}$$

and

$$\begin{cases} A'(\mathbf{U},\mathbf{V}) = \displaystyle\int_\Omega \frac{1}{|\mathrm{Y}|}\Big(\int_\mathrm{Y} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y},\ \mathbf{f}=\mathbf{1}+\nabla_{\boldsymbol{x}}\mathbf{U}+\nabla_{\boldsymbol{y}}\mathbf{u})\,\mathrm{d}y\Big)\nabla_{\boldsymbol{x}}\mathbf{V}\,\mathrm{d}\boldsymbol{x}, \\ L'(\mathbf{V}) = \displaystyle\int_{\partial\Omega_g} \mathbf{g}\mathbf{V}\,\mathrm{d}\mathbf{S}. \end{cases} \tag{41}$$

We use the same finite element method as previously. The discrete problem is

$$\mathbf{U}^h \in \mathcal{U}^h_{\mathrm{ad}}, \quad \mathbf{u}^h \in u^h_{\mathrm{ad}} \quad \text{such that:} \quad F_i\big(\mathbf{U}^h,\mathbf{u}^h\big)=0, \quad \forall i=1,\dots,N_h+n_h, \tag{42}$$

where

$$\begin{cases} F_i\big(\mathbf{U}^h,\mathbf{u}^h\big) = a'\big(\mathbf{u}^h,\boldsymbol{\Psi}^i\big), & \forall i=1,\dots,n_h \\ F_i\big(\mathbf{U}^h,\mathbf{u}^h\big) = A'\big(\mathbf{U}^h,\boldsymbol{\Phi}^{i-n_h}\big) - L'\big(\boldsymbol{\Phi}^{i-n_h}\big), & \forall i=1+n_h,\dots,n_h+N_h. \end{cases} \tag{43}$$

In order to solve this problem, let us consider a Newton-type method.

4.2. Newton-type method

In the sequel, we omit the exponent h but all fields are discretized. The Newton method is defined by the iterations

$$\big(\mathbf{U}^{n+1},\ \mathbf{u}^{n+1}\big) = \big(\mathbf{U}^n,\mathbf{u}^n\big) + \big(\mathbf{W}^n,\mathbf{w}^n\big) \tag{44}$$

where

$$\boldsymbol{F}\big(\mathbf{U}^n,\mathbf{u}^n\big) + \boldsymbol{J}\big(\mathbf{U}^n,\mathbf{u}^n\big)\big(\mathbf{W}^n,\mathbf{w}^n\big) = 0 \tag{45}$$

and $J(\mathbf{U}^n,\mathbf{u}^n)$ is the Jacobian of $\boldsymbol{F}(\mathbf{U}^n,\mathbf{u}^n)$. Let us consider $\boldsymbol{J}(\mathbf{U}^n,\mathbf{u}^n)(\mathbf{W}^n,\mathbf{w}^n)$.

Lemma 1. Let $\mathbf{f}(\mathbf{u},\mathbf{U}) = \mathbf{1}+\nabla_{\boldsymbol{x}}\mathbf{U}+\nabla_{\boldsymbol{y}}\mathbf{u}$. Then

$$\frac{\partial}{\partial \mathbf{U}}\left(\frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y},\mathbf{f})\right)(\mathbf{W}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y},\mathbf{f})\nabla_{\boldsymbol{x}}\mathbf{W},$$
$$\frac{\partial}{\partial \mathbf{u}}\left(\frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y},\mathbf{f})\right)(\mathbf{w}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y},\mathbf{f})\nabla_{\boldsymbol{y}}\mathbf{w}.$$

Proof. As $\mathbf{f}$ is linear with respect to $\mathbf{U}$ and $\mathbf{u}$, we have

$$\frac{\partial \mathbf{f}}{\partial \mathbf{U}}(\mathbf{W}) = \nabla_{\boldsymbol{x}}\mathbf{W}; \qquad \frac{\partial \mathbf{f}}{\partial \mathbf{u}}(\mathbf{w}) = \nabla_{\boldsymbol{y}}\mathbf{w},$$

so

$$\frac{\partial}{\partial \mathbf{U}}\left(\frac{\partial \mathrm{e}}{\partial \mathbf{f}}\right)(\mathbf{W}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}\frac{\partial \mathbf{f}}{\partial \mathbf{U}}(\mathbf{W}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}\nabla_{\boldsymbol{x}}\mathbf{W},$$
$$\frac{\partial}{\partial \mathbf{u}}\left(\frac{\partial \mathrm{e}}{\partial \mathbf{f}}\right)(\mathbf{w}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}\frac{\partial \mathbf{f}}{\partial \mathbf{u}}(\mathbf{w}) = \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}\nabla_{\boldsymbol{y}}\mathbf{w}. \qquad \square$$

Theorem 2.

$$\boldsymbol{J}\big(\mathbf{U}^n, \mathbf{u}^n\big)\big(\mathbf{W}^n, \mathbf{w}^n\big) = \big(A_i^n\big)_{1\leqslant i\leqslant n_h+N_h}$$

with

$$\begin{cases} \mathrm{A}_i^n = \displaystyle\int_{\mathrm{Y}} \mathbf{q}^n\big(\nabla_{\boldsymbol{x}}\mathbf{W}^n + \nabla_{\boldsymbol{y}}\mathbf{w}^n\big)\nabla_{\boldsymbol{y}}\boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y}, & 1 \leqslant i \leqslant n_h, \\ \mathrm{A}_i^n = \displaystyle\int_{\Omega} \frac{1}{|\mathrm{Y}|}\bigg(\int_{\mathrm{Y}} \mathbf{q}^n\big(\nabla_{\boldsymbol{x}}\mathbf{W}^n + \nabla_{\boldsymbol{y}}\mathbf{w}^n\big)\,\mathrm{d}\boldsymbol{y}\bigg)\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}^i \,\mathrm{d}\boldsymbol{x}, & n_h+1 \leqslant i \leqslant n_h+N_h \end{cases}$$

and with $\mathbf{q}^n = (\partial^2\mathrm{e}/(\partial\mathbf{f}\,\partial\mathbf{f}))(\boldsymbol{y},\ \mathbf{f} = \mathbf{1} + \nabla_{\boldsymbol{x}}\mathbf{U}^n + \nabla_{\boldsymbol{y}}\mathbf{u}^n)$.

Proof. By definition of F (43):

$$\begin{cases} F_i = \displaystyle\int_{\mathrm{Y}} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\nabla_{\boldsymbol{y}}\boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y}, \quad 1 \leqslant i \leqslant n_h, \\ F_i = \displaystyle\int_{\Omega} \frac{1}{|\mathrm{Y}|}\bigg(\int_{\mathrm{Y}} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\,\mathrm{d}y\bigg)\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}^{i-n_h}\,\mathrm{d}\boldsymbol{x} - \int_{\partial\Omega_g} \mathbf{g}\boldsymbol{\Phi}^{i-n_h}\,\mathrm{d}\mathbf{S}, \\ \quad n_h+1 \leqslant i \leqslant n_h+N_h, \end{cases}$$

where $(\partial \mathrm{e}/\partial\mathbf{f})(\boldsymbol{y}, \mathbf{f}) = (\partial \mathrm{e}/\partial\mathbf{f})(\boldsymbol{y},\ \mathbf{f} = \mathbf{1} + \nabla_{\boldsymbol{x}}\mathbf{U}^n + \nabla_{\boldsymbol{y}}\mathbf{u}^n)$. As

$$\boldsymbol{J}\big(\mathbf{U}^n, \mathbf{u}^n\big)\big(\mathbf{W}^n, \mathbf{w}^n\big) = \bigg(\frac{\partial F_i}{\partial \mathbf{U}}\big(\mathbf{U}^n, \mathbf{u}^n\big)\big(\mathbf{W}^n\big) + \frac{\partial F_i}{\partial \mathbf{u}}\big(\mathbf{U}^n, \mathbf{u}^n\big)\big(\mathbf{w}^n\big)\bigg)_{1\leqslant i\leqslant n_h+N_h}$$

for $1 \leqslant i \leqslant n_h$, we have by use of lemma 1

$$\begin{aligned} \frac{\partial F_i}{\partial \mathbf{U}}(\mathbf{u}, \mathbf{U})\big(\mathbf{W}^n\big) &= \int_{\mathrm{Y}} \frac{\partial}{\partial \mathbf{U}}\bigg(\frac{\partial \mathrm{e}}{\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\bigg)\big(\mathbf{W}^n\big)\nabla_{\boldsymbol{y}}\boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} \\ &= \int_{\mathrm{Y}} \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\nabla_{\boldsymbol{x}}\mathbf{W}^n\nabla_{\boldsymbol{y}}\boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} \end{aligned}$$

and

$$\frac{\partial F_i}{\partial \mathbf{u}}(\mathbf{u}, \mathbf{U})\big(\mathbf{w}^n\big) = \int_{\mathrm{Y}} \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\nabla_{\boldsymbol{y}}\mathbf{w}^n\nabla_{\boldsymbol{y}}\boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y}.$$

We can also prove that for $1 + n_h \leqslant i \leqslant n_h + N_h$:

$$\begin{aligned} \frac{\partial F_i}{\partial \mathbf{U}}(\mathbf{u}, \mathbf{U})\big(\mathbf{W}^n\big) &= \int_{\Omega} \frac{1}{|\mathrm{Y}|}\bigg(\int_{\mathrm{Y}} \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\,\mathrm{d}\boldsymbol{y}\bigg)\nabla_{\boldsymbol{x}}\mathbf{W}^n\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}^{i-n_h}\,\mathrm{d}\boldsymbol{x}, \\ &= \int_{\Omega} \frac{1}{|\mathrm{Y}|}\bigg(\int_{\mathrm{Y}} \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\nabla_{\boldsymbol{x}}\mathbf{W}^n\,\mathrm{d}\boldsymbol{y}\bigg)\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}^{i-n_h}\,\mathrm{d}\boldsymbol{x}, \\ \frac{\partial F_i}{\partial \mathbf{u}}(\mathbf{u}, \mathbf{U})\big(\mathbf{w}^n\big) &= \int_{\Omega} \frac{1}{|\mathrm{Y}|}\bigg(\int_{\mathrm{Y}} \frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\,\partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f})\nabla_{\boldsymbol{y}}\mathbf{w}^n\,\mathrm{d}\boldsymbol{y}\bigg)\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}^{i-n_h}\,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

Finally, by summation over i ($i \in \{1, \ldots, n_h + N_h\}$) of $(\partial F_i/\partial \mathbf{U})(\mathbf{u}, \mathbf{U})(\mathbf{W}^n)$ and $(\partial F_i/\partial \mathbf{u})(\mathbf{u}, \mathbf{U})(\mathbf{w}^n)$, we obtain the result. □

Therefore, problem (45) is equivalent to

$$
\begin{aligned}
&\mathbf{W}^n \in \mathcal{U}_{\mathrm{ad}}^h, \quad \mathbf{w}^n \in u_{\mathrm{ad}}^h \\
&\begin{cases}
\forall i,\ 1 \leqslant i \leqslant n_h, \\
\displaystyle\int_{\mathrm{Y}} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}\big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} + \int_{\mathrm{Y}} \mathbf{q}^n \big(\nabla_{\boldsymbol{x}} \mathbf{W}^n + \nabla_{\boldsymbol{y}} \mathbf{w}^n\big) \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} = 0, \\
\forall i,\ 1 + n_h \leqslant i \leqslant n_h + N_h, \\
\displaystyle\int_{\Omega} \frac{1}{|\mathrm{Y}|} \bigg(\int_{\mathrm{Y}} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}\big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) \,\mathrm{d}\boldsymbol{y} \bigg) \nabla_{\boldsymbol{x}} \boldsymbol{\Phi}^{i-n_h} \,\mathrm{d}\boldsymbol{x} - \int_{\partial \Omega_g} \mathbf{g} \boldsymbol{\Phi}^{i-n_h} \,\mathrm{d}S \\
\qquad \displaystyle + \int_{\Omega} \frac{1}{|\mathrm{Y}|} \bigg(\int_{\mathrm{Y}} \mathbf{q}^n \big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) \big(\nabla_{\boldsymbol{x}} \mathbf{W}^n + \nabla_{\boldsymbol{y}} \mathbf{w}^n\big) \,\mathrm{d}\boldsymbol{y} \bigg) \nabla_{\boldsymbol{x}} \boldsymbol{\Phi}^{i-n_h} \,\mathrm{d}\boldsymbol{x} = 0
\end{cases}
\end{aligned}
\tag{46}
$$

with $\mathbf{f}^n = \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{U}^n + \nabla_{\boldsymbol{y}} \mathbf{u}^n$.

Theorem 3. If the initial solution and the finite element method used are the same for the non-incremental method and the Newton-type method, if the discrete problems considered have a unique solution, the discretized non-incremental method (38) and the Newton-type method (46) are equivalent.

Proof. As a result of (19) and (25) we have

$$\frac{\partial^2 \mathrm{e}}{\partial \mathbf{f}\, \partial \mathbf{f}}\big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) = \mathbf{q}^{n+1/2}$$

and also $\nabla_{\boldsymbol{x}} \mathbf{W}^n + \nabla_{\boldsymbol{y}} \mathbf{w}^n = \mathbf{f}^{n+1} - \mathbf{f}^n$.

The first equation of (38) is equivalent to

$$\int_{\mathrm{Y}} \frac{\partial \mathrm{e}}{\partial \mathbf{f}}\big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} + \int_{\mathrm{Y}} \mathbf{q}^{n+1/2} \big(\mathbf{f}^{n+1} - \mathbf{f}^n\big) \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} = 0, \quad 1 \leqslant i \leqslant n_h.$$

Because of (19) and (25) it follows that

$$\mathbf{p}^{n+1/2} = \frac{\partial \mathrm{e}}{\partial \mathbf{f}}\big(\boldsymbol{y},\ \mathbf{f} = \mathbf{f}^n\big) + \mathbf{q}^{n+1/2} \big(\mathbf{1} - \mathbf{f}^n\big)$$

and since

$$\mathbf{f}^{n+1} = \mathbf{1} + \nabla_{\boldsymbol{x}} \mathbf{U}^{n+1} + \nabla_{\boldsymbol{y}} \mathbf{u}^{n+1}$$

we have finally

$$\int_{\mathrm{Y}} \mathbf{q}^{n+1/2} \nabla_{\boldsymbol{y}} \mathbf{u}^{n+1} \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} + \int_{\mathrm{Y}} \big(\mathbf{p}^{n+1/2} + \mathbf{q}^{n+1/2} \nabla_{\boldsymbol{x}} \mathbf{U}^{n+1}\big) \nabla_{\boldsymbol{y}} \boldsymbol{\Psi}^i \,\mathrm{d}\boldsymbol{y} = 0,$$

for $1 \leqslant i \leqslant n_h$.

The first set of equations of (46) and (38) are equivalent. The proof is similar for the second set of equations. Thus if the initial solution and the finite element method used are the same for both methods, then they are equivalent. □

Finally, we conclude that our specific choice of H^+ and H^- implies that the non-incremental method proposed is equivalent to a Newton-type method.

4.3. Convergence

In order to prove the convergence of our method, we need to make a few more assumptions.

- $\mathcal{H}_1$: $\exists \beta \in \mathbb{R}^+$ such as

$$\left\| \left(\frac{\partial^2 e}{\partial \mathbf{f} \, \partial \mathbf{f}} \right)^{-1} \right\| \leqslant \beta \quad \text{with } \|\mathbf{q}\| = \max_{\|\mathbf{f}\|=1} \|\mathbf{q}\mathbf{f}\| \text{ and } \mathbf{q} = \frac{\partial^2 e}{\partial \mathbf{f} \, \partial \mathbf{f}}$$

  and $\|\mathbf{f}\| = \sum_{i=1,\,j=1}^{3} \|f_{ij}\|$.

- $\mathcal{H}_2$: $\partial^2 e/(\partial \mathbf{f} \, \partial \mathbf{f})$ is such that $\exists \alpha \in \mathbb{R}^+$ such as

$$\left\| \frac{\partial^2 e}{\partial \mathbf{f} \, \partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f}_1) - \frac{\partial^2 e}{\partial \mathbf{f} \, \partial \mathbf{f}}(\boldsymbol{y}, \mathbf{f}_2) \right\| \leqslant \alpha \|\mathbf{f}_1 - \mathbf{f}_2\|.$$

These assumptions lead to the following theorem.

Theorem 4. We assume that all discrete problems considered have a unique solution and that $\mathcal{H}_1 - \mathcal{H}_2$ hold. Then the non-incremental method converges locally and quadratically.

Proof. Under our assumptions, the nonlinear discrete problem to solve has a unique solution and our non incremental method is equivalent to a Newton-type method.

Assumptions $\mathcal{H}_1$ and $\mathcal{H}_2$ guarantee the convergence [12]. □

5. Numerical application

In order to assess the performance of our non-incremental algorithm presented above, we use it here in the case of unidirectional composites. This case requires, a priori, the use of a finite element method for the solution of the microscopic problems, as well as for the macroscopic problem. In the case of prescribed loadings such that heterogeneous distribution of deformations is obtained at the macroscopic scale, the computation of the macroscopic problem indeed requires the use of an adapted numerical scheme. Thus we consider, in the sequel, only macroscopic loadings inducing homogeneous distributions of macroscopic deformations, such as defined in table 1. The structure considered is parallelipedic.

Table 1
Macroscopic loadings prescribed ($\mathbf{T}_t$: tangential component of $\mathbf{T}(\mathbf{N})$; $\mathbf{U}_N$: normal displacement).

Uniaxial tension on (O, x_i)	$\mathbf{U}_N = \pm U$, $\mathbf{T}_t = 0$ on $\lvert x_i\rvert = L_i$ $\mathbf{T}(\mathbf{N}) = \mathbf{0}$ on $\partial\Omega \mid \lvert x_i\rvert = L_i$
Biaxial tension on (O, x_i, x_j)	$\mathbf{U}_N = \pm U_i$, $\mathbf{T}_t = 0$ on $\lvert x_i\rvert = L_i$ $\mathbf{U}_N = \pm U_j$, $\mathbf{T}_t = 0$ on $\lvert x_j\rvert = L_j$ $\mathbf{T}(\mathbf{N}) = \mathbf{0}$ on $\partial\Omega \lvert (\lvert x_i\rvert = L_i \cup \lvert x_j\rvert = L_j)$
Pure shear on (O, x_i, x_j) and (O, x_i)	$\mathbf{U}_n = U_i$, $\mathbf{T}_t = 0$ on $\lvert x_i\rvert = L_i$ $\mathbf{T}(\mathbf{N}) = \mathbf{0}$ on $\lvert x_j\rvert = L_j$ $\mathbf{U}_N = 0$, $\mathbf{T}(\mathbf{N}) = \mathbf{0}$ on $\partial\Omega \lvert (\lvert x_i\rvert = L_i \cup \lvert x_j\rvert = L_j)$

5.1. *Choice of the basic cell*

The reinforcements of the chosen unidirectional composite are assumed to be all aligned in the same direction (O, y_3) (parallel to (O, x_3)) with circular section. Moreover, they are assumed to be distributed at the corners of a regular square mesh. The components of the basic cell are assumed to be homogeneous and isotropic in such a way that, because of these properties and the geometry of the basic cell, the homogeneous equivalent behaviour is orthotropic. Because of the nature of the composite considered, it is shown that the problem requires only a two-dimensional study [21].

The strain energy densities of the components of the basic cell have been chosen as follows:

- matrix: Harth–Smith modified [20]

$$\mathrm{e}(\mathrm{I}_1, \mathrm{I}_2, \mathrm{I}_3) = \mathrm{E}_1 \int_3^{\mathrm{I}_1} e^{\mathrm{E}_3(\mathrm{I}_1-3)^2}\,\mathrm{dI}_1 + \int_3^{\mathrm{I}_2} \frac{\mathrm{E}_2}{\mathrm{I}_2^{\mathrm{E}_4}}\,\mathrm{dI}_2 + \mathrm{E}_5(\mathrm{I}_3 - 1) - \mathrm{B}\ln \mathrm{I}_3$$

with

$$\begin{cases} \lambda = 4\left(\mathrm{E}_5 + \dfrac{\mathrm{E}_2}{3^{\mathrm{E}_4}}\left(1 - 4\dfrac{\mathrm{E}_4}{3}\right)\right), \\ \mu = 2\left(\mathrm{E}_1 + \dfrac{\mathrm{E}_2}{3^{\mathrm{E}_4}}\right), \quad \mathrm{E}_i \geqslant 0,\ \forall i \in \{1, \ldots, 5\}, \\ (\lambda,\ \mu\text{: Lamé's coefficients}), \\ \mathrm{B} = \mathrm{E}_1 + 2\dfrac{\mathrm{E}_2}{3^{\mathrm{E}_4}} + \mathrm{E}_5 \end{cases}$$

where we have chosen

$$\mathrm{E}_1 = 3 \cdot 10^5 \text{ Pa}, \qquad \mathrm{E}_2 = 10^6 \text{ Pa}, \qquad \mathrm{E}_3 = 0.03,$$
$$\mathrm{E}_4 = 0.63, \qquad \mathrm{E}_5 = 5 \cdot 10^5 \text{ Pa},$$

which leads to a Young's modulus (E) and a Poisson ratio (ν), respectively, equal to

$$\mathrm{E} = 1.5 \cdot 10^6 \text{ Pa}, \qquad \nu = 0.42,$$

- fiber: Ciarlet–Geymonat [10]:

$$\mathrm{e}(\mathrm{I}_1, \mathrm{I}_2, \mathrm{I}_3) = \frac{\mathrm{E}_1}{2}(\mathrm{I}_1 - 3) + \frac{\mathrm{E}_2}{2}(\mathrm{I}_2 - 3) + \frac{\mathrm{E}_3}{2}(\mathrm{I}_3 - 3) - \mathrm{B} \ln \mathrm{I}_3$$

with

$$\begin{cases} \mathrm{E}_2 = \mu - \mathrm{E}_1, \\ \mathrm{E}_3 = \dfrac{\lambda}{2} - \mathrm{E}_2, \quad \mathrm{E}_i \geqslant 0, \ \forall i \in \{1, \ldots, 3\}, \\ (\lambda, \mu\text{: Lamé's coefficients}), \\ B = \mathrm{E}_1 + 2\mathrm{E}_2 + \mathrm{E}_3 \end{cases}$$

where $\mathrm{E}_1 = 1.16 \cdot 10^8$ Pa, $\mathrm{E} = 1.10^9$ Pa, $\nu = 0.3$.

5.2. *Results*

Figure 3 presents a comparison between the non-incremental method and an incremental one [13,14]. As the number of iterations N in the incremental method increases, the result obtained approaches that of the non-incremental method. Moreover, as the in-

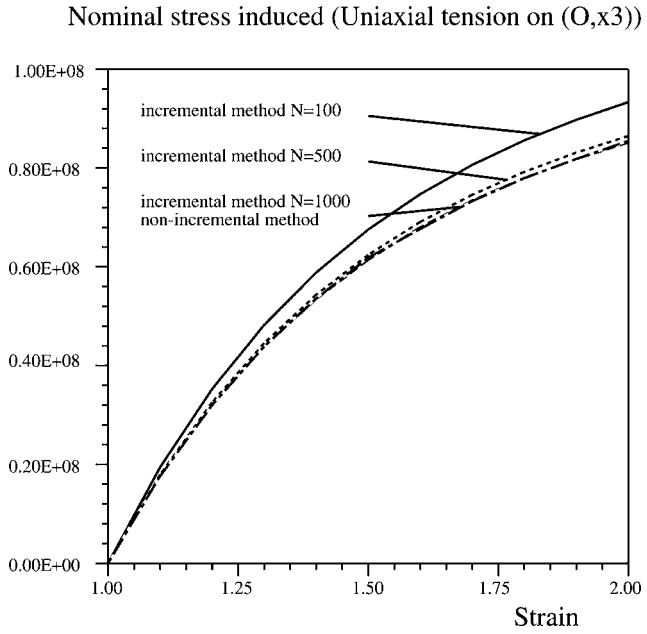

Figure 3. Comparison of the result of a non-incremental and an incremental method.

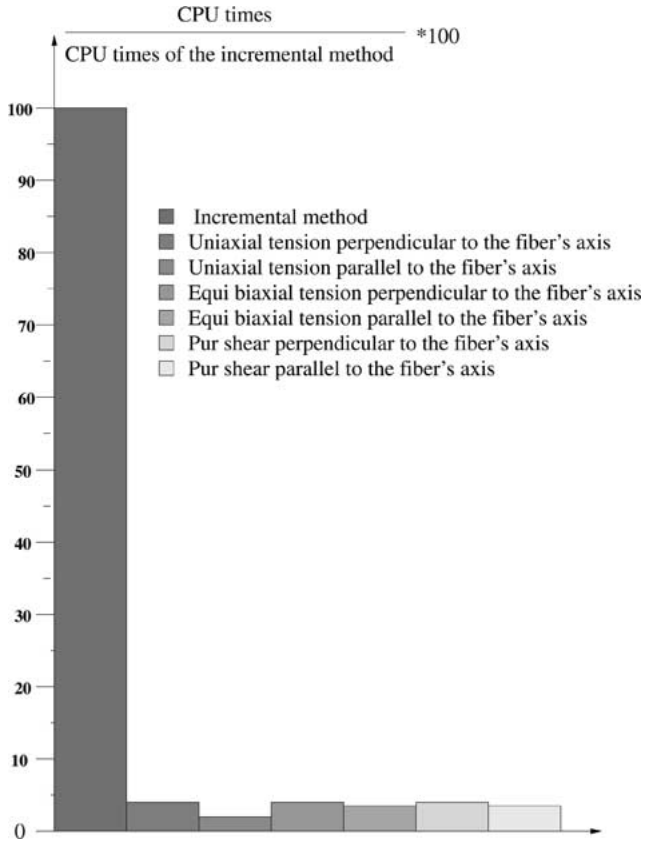

Figure 4. CPU times comparison.

cremental method leads to accurate results [14], we conclude that our new method is efficient for simulating the behaviour of such composites.

Figure 4 compares the CPU times required for both methods. First of all, let us note that CPU times of the incremental method do not depend on the loading conditions but only on the number of iterations. An impressive reduction of CPU time of about 95% is obtained.

Figure 5 presents the various convergence behaviours. As expected, the convergence rate is quadratic.

Finally, in order to analyse the influence of the initial solution, figure 6 shows the convergence curves in the case of uniaxial tension on (O, x_1) which induces a 50% deformation. This result highlights the local convergence of the proposed algorithm.

6. Conclusion

In this paper we presented a non-incremental method to solve nonlinear problems induced by a homogenization technique for elastomer composite materials. The method

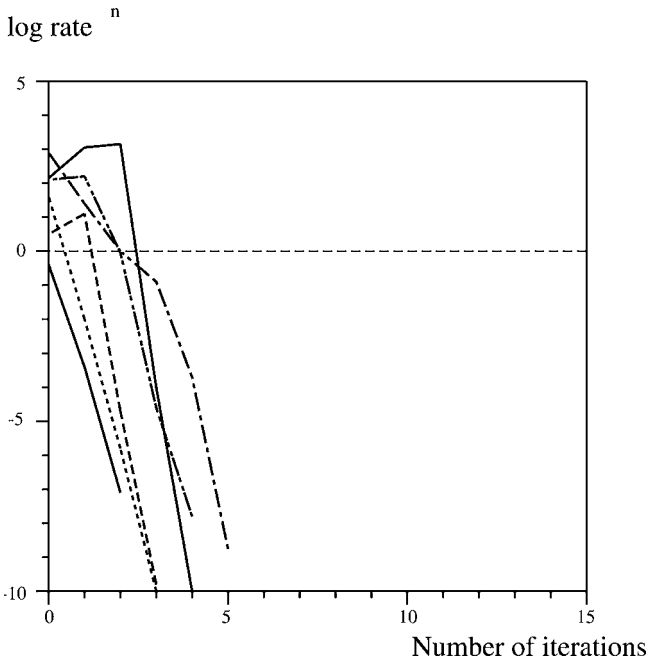

Figure 5. Convergence rate.

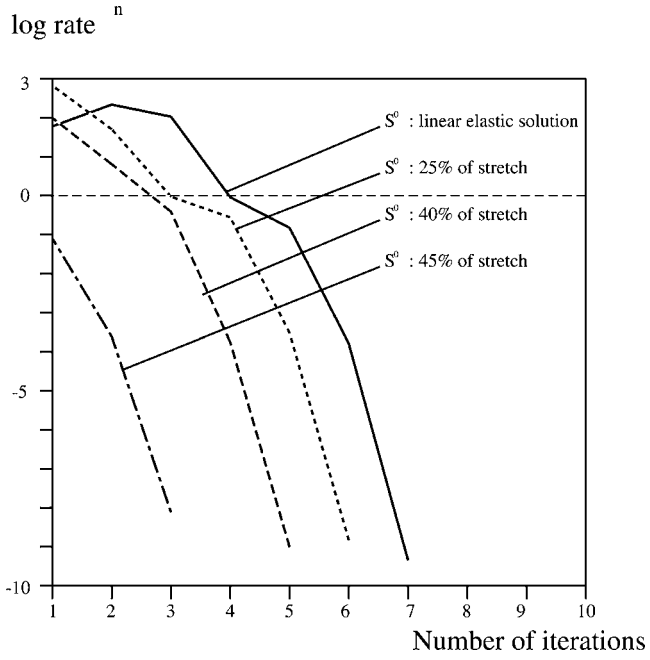

Figure 6. Influence of the initial solution.

relies on a judicious splitting of the different difficulties into two different groups, and on operators H^+ and H^- iterating from one group into the other. Each iteration then requires to solve either nonlinear problems which are local in space or problems which are global in space but linear.

The main result of this paper is the proof that this method is equivalent to a Newton-type method. It is thus easy to conclude that there is local quadratic convergence.

In order to assess the global convergence, we plan to investigate Newton methods with backtracking or continuation methods such as incremental Newton.

Our choice of operators and subspaces lead to the Newton method. We are also looking for new operators or splitting wich could speed-up the method.

Another way to reduce the CPU time is to design parallel algorithm. The local step is easy to parallelize and the global linear step can be parallelized by a substructuring method. We have implemented a parallel version of our method, so that we can deal with complex composite structures [6,8].

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