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Survey

Computational efficiency and accuracy of sequential nonlinear cyclic analysis of carbon nanotube nanocomposites

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ABSTRACT

The accuracy and efficiency of a numerical strategy for sequential nonlinear cyclic analyses of carbon nanotube nanocomposites are investigated. The computational approach resorts to a nonlinear 3D finite element implementation that seeks to solve the cyclic hysteretic response of the nanocomposite. A variant of the Newton-Raphson method within a time integration scheme is proposed whereby the elastic tangent matrix is chosen as iteration matrix without paying the price of its iterative update. This is especially rewarding in the context of the employed mechanical model which exhibits hysteresis manifested through a discontinuous change in the stiffness at the reversal points where the loading direction is reversed. Key implementation aspects – such as the integration of the nonlinear 3D equations of motion, the numerical accuracy/efficiency as a function of the time step or the mesh size – are discussed. In particular, efficiency is regarded as performing fast computations especially when the number of cyclic analyses becomes large. By making use of laptop CPU cores, a good speed of computations is achieved not only through parallelization but also employing a caching procedure for the iteration matrix.

1. Introduction

Designing new multiphase, multiscale materials such as nanostructured materials via a simulation-driven approach is typically regarded as extremely challenging due to the high computational cost and time. This is particularly true when the material behavior is nonlinear and hysteretic, and several optimization cycles are required. This justifies the development of numerical solution strategies that, coupled with efficient global optimization algorithms, can achieve high efficiency and accuracy.

The material here under investigation is a carbon nanotube nanocomposite. The employed mesoscale mechanical model for the nanocomposite was previously proposed and validated in [1,2] and regards the two-phase material (the isotropic hosting polymer and the carbon nanotubes introduced as inelastic cylindrical inclusions) as a homogenized inelastic continuum.

To compute the cyclic response of the nanocomposite, we modified a variant of the Newton-Raphson method within a time integration scheme. In the modified Newton–Raphson scheme the iteration matrix is frozen to the elastic tangent matrix and thus is assembled only once for an individual cyclic analysis as well as for the whole parametric analysis when the loading amplitude is changed. The reliability of the employed method is here supported by an extensive campaign of numerical tests aimed at comparing the baseline method performance with the same method in a parallel implementation.

The implementation of the finite element numerical strategy makes use of FEniCS [3], an open-source computing platform for solving partial differential equations. The core algorithm solves the equations of motion of the nanocomposite for a given loading program. On top of it an optimization algorithm is implemented according to the Differential Evolution method to optimize macroscopic material properties such as the damping ratio over a given range of strains.

An updated review of Differential Evolution methods can be found in [4,5], but the more general field of nonlinear optimization, which includes stochastic and randomized algorithms, is growing very steadily. Recent improvements to resolve dynamic optimization problems via meta-heuristic techniques can be found in [6], while recent advances in ant colony and particle swarm algorithms are discussed in [7] and [8], respectively. The present paper does not discuss the optimization problem which is instead reported in a recent paper [9]. Indeed, most of the computational cost of an optimization algorithm is associated with the numerical evaluation of the objective function [10–12],

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especially when, as in our case, this function is computed by solving several cyclic analyses of a highly nonlinear problem.

In this work our numerical strategy is shown to reduce considerably the computational time while preserving accuracy. Note that the implemented approach is not amenable to DE optimization only, but can also be extended to more sophisticated numerical strategies such as path-following.

Contribution. The main contribution is in the proposition of a variant of the Newton-Raphson scheme that makes use of the elastic matrix as iteration matrix which is thus assembled only once during a single cyclic analysis across which the tangent stiffness changes. This freezing of the iteration matrix works also for full parametric analyses when several cyclic responses are computed by changing the loading amplitude. The reliability of the employed method is corroborated by a rich campaign of numerical tests aimed at comparing the baseline method performance with the same method in a parallel implementation. The main objective of the numerical is to enable an overall multi-objective material optimization resorting to full 3D analyses at reasonable costs and computational time.

Outline. The manuscript is organized as follows. In Section 2 we summarize the nonlinear hysteretic model for CNT nanocomposite materials, while in Section 3 we describe both space and time discretizations, present a specialized Newton–Raphson time integration scheme, and we outline the caching mechanism that underlies our proposed numerical procedure. In Section 4 we discuss both the accuracy and efficiency of our methodology by a numerical campaign on both a beam- and a plate-like 3D nanocomposite sample.

2. Nanocomposite hysteretic model in a nutshell

The nanocomposite mesoscale hysteretic model here employed was proposed in [1,2,9]. In particular, the model is framed within the class of homogeneization methods, developed initially for linear elasticity. Such methods were referred to by Benveniste [13] as "Equivalent Inclusion–Average Stress" methods.

By considering the nanocomposite made of two material phases, namely, the hosting polymer matrix (here and henceforth denoted by subscript "m") and the carbon nanotube (denoted by subscript "c") modelled as cylindrical solid inclusions [14,15], the Mori-Tanaka approach allows us to consider the nanocomposite stresses and strains as averaged continuum tensors of the two phases treated themselves as two continuum media. In particular, the rates of stress and strain obey to the following equations:

$$\dot{\boldsymbol{T}} = \phi_{\mathrm{m}}\,\dot{\boldsymbol{T}}_{\mathrm{m}} + \phi_{\mathrm{c}}\,\dot{\boldsymbol{T}}_{\mathrm{c}}, \quad \dot{\boldsymbol{E}} = \phi_{\mathrm{m}}\,\dot{\boldsymbol{E}}_{\mathrm{m}} + \phi_{\mathrm{c}}\,\dot{\boldsymbol{E}}_{\mathrm{c}} \tag{1}$$

where the scalar ϕ_{c} is the CNT volume fraction, while ϕ_{m}: $=1-\phi_{\mathrm{c}}$ is its complementary part describing the volume fraction occupied by the hosting matrix. According to [2], the matrix phase can be represented as a linear elastic continuum, while the CNT phase as an inelastic continuum which can describe through its inelastic response the stick-slip phenomenon:[1]

$$\dot{\boldsymbol{T}}_{\mathrm{m}} = \boldsymbol{L}_{\mathrm{m}}\colon \dot{\boldsymbol{E}}_{\mathrm{m}}, \quad \dot{\boldsymbol{T}}_{\mathrm{c}} = \boldsymbol{L}_{\mathrm{c}}\colon (\dot{\boldsymbol{E}}_{\mathrm{c}} - \dot{\boldsymbol{E}}^{\mathrm{p}}) \tag{2}$$

indicating with $\boldsymbol{L}_{\mathrm{m}}$ and $\boldsymbol{L}_{\mathrm{c}}$ the fourth-order tensor of elastic coefficients of the two material phases: in particular, such phases are modelled as isotropic materials, thus $\boldsymbol{L}_{\mathrm{m}}$ and $\boldsymbol{L}_{\mathrm{c}}$ collect the well-known stiffness coefficients depending on Young's moduli (E_{m}, E_{c}) and Poisson ratios (ν_{m}, ν_{c}), respectively.

A key aspect of the here employed modeling is that the stick-slip-induced displacement/strain/stress discontinuity across the interfaces is circumvented by accounting for the CNTs inelastic eigenstrains which provide additional localized strains responsible for interface stress discontinuitiies driving the interfacial energy dissipation.

Moreover, the CNTs are considered perfectly and uniformly aligned, in the sense specified in the numerical tests. This is clearly a simplification of real nanocomposites which can never exhibit perfectly aligned and dispersed CNTs due to local entangling and agglomerations. However, consideration of composites with aligned or randomly oriented nanotubes and with various CNT lengths and volume fractions does not change the modeling framework of "Equivalent Inclusion–Average Stress" method here adopted [13,14]. Moreover, the macroscopic mechanical chararcterization of the nanocomposite turns out to be in good agreement with experimental evidences [2,14,16].

The hysteretic model is obtained in terms of the following incremental constitutive law relating the stress rate $\dot{\boldsymbol{T}}$ with the strain rate $\dot{\boldsymbol{E}}$:

$$\dot{\boldsymbol{T}} = \boldsymbol{L}_{\mathrm{e}}\colon \dot{\boldsymbol{E}} - \boldsymbol{L}_{\mathrm{p}}\colon \dot{\boldsymbol{E}}^{\mathrm{p}}, \tag{3}$$

where $\boldsymbol{L}_{\mathrm{e}}$ and $\boldsymbol{L}_{\mathrm{p}}$ are fourth order tensors collecting the elastic and tangent (plastic) coefficients, respectively, and $\dot{\boldsymbol{E}}^{\mathrm{p}}$ is the inelastic strain rate which very much affects the nonlinear, hysteretic response of the model. In particular, the fourth order tensors are related to the Eshelby tensor $\boldsymbol{S}$, regulating the strain transformations at the CNT-matrix interface according to the Eshelby theory of equivalent inclusion [13], and to the elastic mismatch $\boldsymbol{L}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{m}}$ between the nominal (isotropic) elastic tensors of the two phases:

$$\boldsymbol{L}_{\mathrm{e}} = \boldsymbol{L}_{\mathrm{m}}\colon [\boldsymbol{I} + \phi_{\mathrm{c}}\,\boldsymbol{B}\colon (\boldsymbol{L}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{m}})], \tag{4a}$$

$$\boldsymbol{L}_{\mathrm{p}} = \phi_{\mathrm{c}}\,\boldsymbol{L}_{\mathrm{m}}\colon \boldsymbol{B}\colon \boldsymbol{L}_{\mathrm{c}}, \tag{4b}$$

in which the following fourth order tensor was introduced:

$$\boldsymbol{B}\colon = [\boldsymbol{L}_{\mathrm{m}} + \phi_{\mathrm{m}}\,(\boldsymbol{L}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{m}})\colon \boldsymbol{S}]^{-1}. \tag{5}$$

The inelastic strain rate actually models the stick-slip phenomenon at the CNT-matrix interface according to a Bouc-Wen-like evolution law, see [2,9]. The corresponding stress rate, namely $\dot{\boldsymbol{T}}^{\mathrm{p}}$: $=\boldsymbol{L}_{\mathrm{c}}\colon \dot{\boldsymbol{E}}^{\mathrm{p}}$, is expressed as

$$\dot{\boldsymbol{T}}^{\mathrm{p}} = 3\mu_{\mathrm{c}}\,\hat{h}_2\,(\Phi(\hat{\boldsymbol{T}})/S_{\mathrm{o}})^{(\mathrm{n}-2)}\,[(\hat{\boldsymbol{T}}^{\mathrm{dev}}/S_{\mathrm{o}}) \otimes (\hat{\boldsymbol{T}}^{\mathrm{dev}}/S_{\mathrm{o}})]\colon \dot{\boldsymbol{E}}_{\mathrm{c}}, \tag{6}$$

where $\mu_{\mathrm{c}} = E_{\mathrm{c}}/[2(1+\nu_{\mathrm{c}})]$ is the CNT shear modulus, S_{o} is the interfacial shear strength,

$$\hat{h}_2 = 1 + \gamma\,(\mathrm{sign}(\dot{\Phi}(\hat{\boldsymbol{T}})) - 1), \quad \Phi(\hat{\boldsymbol{T}}) = \left(\tfrac{3}{2}\,\hat{\boldsymbol{T}}^{\mathrm{dev}}\colon \hat{\boldsymbol{T}}^{\mathrm{dev}}\right)^{1/2}, \tag{7}$$

the stress discontinuity $\hat{\boldsymbol{T}}$ is introduced as

$$\hat{\boldsymbol{T}} = (\boldsymbol{L}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{m}})\colon (\boldsymbol{E}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{c}}^{-1}\colon \boldsymbol{T}^{\mathrm{p}}), \tag{8}$$

and the CNT strain rate $\dot{\boldsymbol{E}}_{\mathrm{c}}$ is associated with the nanocomposite strain rate $\dot{\boldsymbol{E}}$, *i.e.*:

$$\dot{\boldsymbol{E}}_{\mathrm{c}} = \boldsymbol{A}_{\mathrm{c}}^{-1}\colon \dot{\boldsymbol{E}}, \quad \boldsymbol{A}_{\mathrm{c}}\colon = [\boldsymbol{I} + \phi_{\mathrm{m}}\,\boldsymbol{S}\colon \boldsymbol{L}^{-1}\colon (\boldsymbol{L}_{\mathrm{c}} - \boldsymbol{L}_{\mathrm{m}})]. \tag{9}$$

The piece-wise function $\hat{h}_2$ governs the loading/unloading direction while $\Phi(\hat{\boldsymbol{T}})$ is the von Mises function of the interfacial stress discontinuity $\hat{\boldsymbol{T}}$ whose deviatoric part is denoted by $\hat{\boldsymbol{T}}^{\mathrm{dev}}$. Finally, $n \geq 2$ and $0 < \gamma < 1$ are the Bouc-Wen parameters, governing (inversely) the smoothness of the loading curve up to the yield stress S_{o} and the smoothness of the loading/unloading phases, respectively.

By substituting (9) into (6), and considering (8), the inelastic stress rate $\dot{\boldsymbol{T}}^{\mathrm{p}}$ is expressed as a highly nonlinear function of the displacement field $\boldsymbol{u}$ (through its corresponding linearized strain $\boldsymbol{E}$), the velocity $\dot{\boldsymbol{u}}$ (through $\dot{\boldsymbol{E}}$) and the stress discontinuity $\hat{\boldsymbol{T}}$ itself. Therefore, the incremental constitutive law (3) can be finally recast as

[1] We adopt Gibbs notation for vector and tensor fields. The dot and cross products of the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ are denoted by $\boldsymbol{u}\cdot\boldsymbol{v}$ and $\boldsymbol{u}\times\boldsymbol{v}$, respectively. The image of vector $\boldsymbol{u}$ under the application of tensor $\boldsymbol{A}$ is expressed as $\boldsymbol{A}\cdot\boldsymbol{u}$. On the other hand, the tensor product between vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ is denoted by $\boldsymbol{u}\otimes\boldsymbol{v}$. The same notation $\boldsymbol{A}\otimes\boldsymbol{B}$ is employed to indicate the tensor product between second-order tensors $\boldsymbol{A}$ and $\boldsymbol{B}$. Their inner product is expressed as $\boldsymbol{A}\colon\boldsymbol{B} = \mathrm{tr}(\boldsymbol{A}^{\top}\cdot\boldsymbol{B}) = A_{ij}B_{ij}$, where $\boldsymbol{A}^{\top}$ indicates the transpose of $\boldsymbol{A}$.