APPLICATION OF THE PROPER GENERALIZED DECOMPOSITION METHOD TO POLYMER VISCOELASTICITY UNDER CYCLIC LOADING

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Abstract

In this work, the Proper Generalized Decomposition (PGD) method is used to simulate the cyclic loading of a polymer specimen. The viscoelastic behavior of the polymer is described by a Generalized Maxwell model which makes use of a relaxation times distribution. From a numerical point of view, a global model and several local models had to be solved. Within the PGD framework, the globalization of the local models is here investigated and consists in solving entirely all the problems (equilibrium equation and internal variables evolution) with the PGD method. As different times are considered, we here discuss the possibility to decrease the computation time by using adapted time discretizations. For this purpose, the link between the cycle time, the relaxation time and the time step is analyzed through different simulations according to the number of relaxation times and the relaxation times distribution.

1. Introduction

In order to model the linear viscoelastic behavior of polymer materials, a General Maxwell model is often used. This model consists in using internal variables and their associated relaxation times. The evolution of the internal variables are described by differential equations to represent the kinetic evolution of microscopic phenomena. According to the polymer material and the temporal domain of the simulation, a large number m of relaxation times have to be considered. As example, Cunat has demonstrated in 1991 [1] the necessity to consider 50 relaxation times for an accurate representation of a continuous distribution spread over 6 decades. To predict the response of these materials, the finite element method is classically used and consists in integrating the local models (m differential equations) at the Gauss points and then solving the global model. The nature of the differential equations can require a large computation time. Indeed, the solving of nonlinear differential equations requires the use of another temporal scheme, for example an adaptive Runge-Kutta. Moreover, for polymer materials, a large number of cycles has to be simulated to reach the the stabilized cycle which induces a large time domain. The prediction of the viscoelatic polymer under cyclic loading can be therefore time consuming.

To overcome this computation time, other numerical strategies can be investigated as for example the LArge Time INcrement method [2]. We here suggest the use of another alternative numerical method: the Proper Generalized Decomposition (PGD) method ([3]). This method consists in writing a space and time separated representation of the unknown fields. The basis functions are not known a priori like in the Proper Orthogonal Decomposition method but constructed within an iterative procedure. For a complete and recent review of this method, the reader can refer to [4] and the references therein. The coupling between global and local equations have already been investigated in the framework of the PGD with different strategies. For details, the reader can refer to [5]. In this paper, as the equations are strongly coupled, the adopted strategy consists in globalizing the solution of the local models. All the problems are solved entirely with the PGD method. The main inconvenient is that if the number of internal variables is high, the computation time becomes large, a space-time solver being applied for each species.
As in our aimed application, the number of internal variables can be large, we here suggest to decrease this computation time by considering adapted time discretizations. They are linked to the cycle time and the relaxation time. The purpose of this paper is to discuss this link.
In the first part of the paper, the numerical modeling within the PGD framework and the parameters of the simulation are presented. In the next section, the results are compared and discussed in terms of displacement accuracy and computation time according to the time step, the number of internal variables and the relaxation time. This section precedes the conclusions.

2. Numerical procedure

2.1. Simulation model

Let us consider a one-dimensional mechanical equation with a viscoelastic behavior described by internal variables z_j. The generic form of the problem can be written as follows:

$$\frac{\partial \sigma}{\partial x} + f = 0, \tag{1}$$

$$\frac{dz_j}{dt} + \frac{1}{\tau_j}\left(z_j - z_j^\infty\right) = 0 \qquad \forall \;\; 1 \leq j \leq m \tag{2}$$

where

$$\sigma = E_v \frac{\partial u}{\partial x} - \sum_{j=1}^{m} z_j, \tag{3}$$

$$z_j^\infty = E_{rj}^\infty \frac{\partial u}{\partial x} \qquad \forall \;\; 1 \leq j \leq m. \tag{4}$$

where z_j^∞ is the value at the equilibrium of the internal variables z_j, τ_j is the associated relaxation time, E_v is the vitreous modulus. The relaxed modulus at equilibrium E_{rj}^∞ generated by the process j is written as: $E_{rj}^\infty = p_j E_r \;\; \forall \;\; 1 \leq j \leq m$, where E_r represents the relaxed modulus and p_j the weights given by a distribution.
Equations ((1) and (2)) are assumed to be defined on the domain: $\Omega = \Omega_x \times \Omega_t$, where $\Omega_x = [0, L_x]$ and $\Omega_t = [0, L_t]$. The initial conditions are equal to zero for the displacement field and the internal variables and the boundary conditions are written as: $\underline{\underline{\sigma}}.\underline{n} = \underline{F}$ on $\partial\Omega_\sigma$ and $\underline{u} = \underline{0}$ on $\partial\Omega_u$.

2.2. Application of the Proper Generalized Decomposition method

To solve this problem with the PGD method, we first globalize the local models as suggested in [5] by considering the internal variables as functions of space and time. The solutions u and z of the coupled problem are sought under the form:
$u(x,t) \approx \sum_{i=1}^{N} A_i(x)B_i(t)$ and $z_j(x,t) \approx \sum_{i=1}^{N} C_{ij}(x)D_{ij}(t) \quad \forall \quad 1 \leq j \leq m.$
At enrichment step n of the PGD algorithm, the following approximations are already known:

$$u^n(x,t) = \sum_{i=1}^{n} A_i(x)B_i(t), \tag{5}$$

$$z_j^n(x,t) = \sum_{i=1}^{n} C_{ij}(x)D_{ij}(t) \qquad \forall \quad 1 \leq j \leq m \tag{6}$$

We wish to compute the next functional product $A_{n+1}(x)B_{n+1}(t)$ and $C_{(n+1)j}(x)D_{(n+1)j}(t) \quad \forall \quad 1 \leq j \leq m$ which is denoted by $R(x)S(t)$ and $V_j(x)W_j(t)$ $\forall 1 \leq j \leq m$ for alleviating the notation.

As the displacement and the internal variables are strongly coupled, all the unknowns could be computed at each enrichment step as in our previous paper in the case of thermoviscoelasticity [6]. Let us here remark that the displacement field and the internal variables are completely interrelated, but each internal variable depends only on the value of the displacement. We here suggest to compute alternatively the functional products $R(x)S(t)$ and $V_j(x)W_j(t)$ $\forall 1 \leq j \leq m$. At each enrichment step, it leads to solve $m+1$ nonlinear problems as described below.
Remark. In our simulations, $f = 0$ and the boundary conditions are as follows: $\sigma \cdot \vec{n} = F$ at $x = L_x$ where F depends only on time and $u = 0$ at $x = 0$. The following equations are related to these parameters.

1. Computing $R(x)S(t)$

The weak form related to Equation (1) reads:

$$\int_{\Omega} (div\sigma + f)\, u^* d\Omega + \int_{\partial\Omega_\sigma} \left(\sigma \cdot \vec{n} - F\right) u^* dS = 0 \tag{7}$$

for all test functions u^* selected in an appropriate functional space.
The stress σ being derived from Equation (3) with the values z_j^n, and the trial and test functions being written as follows:

$$u(x,t) = \sum_{i=1}^{n} A_i(x)B_i(t) + R(x)S(t), \tag{8}$$

$$u^*(x,t) = R^*(x)S(t) + R(x)S^*(t), \tag{9}$$

Equation (7) is a nonlinear problem with respect to $R(x)$ and $S(t)$ that must be solved by means

of a suitable iteration scheme. The simple iterative scheme is an alternating directions point fixed algorithm. Each iteration consists of two steps that are repeated until convergence. The first step assumes $S(t)$ known from the previous iteration and computes an update for $R(x)$. From the just-updated $R(x)$, the second step updates $S(t)$.
Remark. At *n=0*, $R(x)S(t)$ is solution of the related elastic problem (without any internal variable).

2. Computing $V_j(x)W_j(t)\ \forall 1 \leq j \leq m$

For each value of j, the weak form related to Equation (2) reads:

$$\int_\Omega \left(\frac{\partial z_j}{\partial t} + \frac{1}{\tau_j}\left(z_j - z_j^\infty\right)\right) z_j^* d\Omega = 0 \tag{10}$$

for all test functions z_j^* selected in an appropriate functional space.
The value of the internal variable at the equilibrium z_j^∞ being derived from Equation (4) with the value u^{n+1}, and the trial and test functions being written as follows:

$$z_j(x,t) = \sum_{i=1}^{n} C_{ij}(x)D_{ij}(t) + V_j(x)W_j(t), \tag{11}$$

$$z_j^*(x,t) = V_j^*(x)W_j(t) + V_j(x)W_j^*(t), \tag{12}$$

Equation (10) is a nonlinear problem with respect to $V_j(x)$ and $W_j(t)$. An alternating directions point fixed algorithm is used as previously for the displacement. Each iteration consists of two steps that are repeated until convergence. The first step assumes $W_j(t)$ known from the previous iteration and computes an update for $V_j(x)$. From the just-updated $V_j(x)$, the second step updates $W_j(t)$. This iterative procedure continues until reaching convergence. Then z^{n+1} is computed from the converged functions $V_j(x)$, $W_j(t)$.

Once the solutions $u^{n+1}$and all z_j^{n+1} are computed, the residuals are defined: Re_u, related to equation (1), and Re_{zj}, related to equation (2).

$$Re_u = \frac{\left(\int_\Omega \left(E_v \frac{\partial^2 u}{\partial x^2} - \sum_{j=1}^{m} \frac{\partial z_j}{\partial x} + f \right)^2 d\Omega \right)^{\frac{1}{2}}}{\|u\|}, \tag{13}$$

$$Re_{zj} = \frac{max_j \left(\int_\Omega \left(\frac{dz_j}{dt} + \frac{1}{\tau_j} z_j - \frac{E_{rj}^\infty}{\tau_j} \frac{\partial u}{\partial x} \right)^2 d\Omega \right)^{\frac{1}{2}}}{\|z_j\|}, \tag{14}$$

where $\|\ \|$ stands for the L^2 norm.

The iterative procedure stops when $max\ (Re_u, (Re_{zj},\ j = 1, .., n))$ is small enough. The solution of the coupled problem is then given by equation (5) for u and (6) for z_j. The details of the fixed point algorithm equations are given in [7].

2.3. Simulation parameters

The simulation test is a 5 mm long one-dimensional bar clamped at $x = 0$ and subject to a cyclic time load $F(t)$ which consists in 50 cycles with a cycle time of 20 s. The total simulation time equals 1000s. The material parameters are representative of a polypropylene material and are as follows: $E_r = 1000$ MPa, $E_v = 1140$ MPa. Different numbers of internal variables are investigated: 1 and 3. For each number of internal variables, the two degrees of freedom are : (a) the relaxation times with respect to the time cycle and (b) the associated time discretization.

3. Results

3.1. One internal variable

In the case of one internal variable, let us consider the following relaxation times: 1s (smaller than the time cycle), 10s (same than the time cycle) and 100s (larger than the time cycle), leading respectively to three different behaviors. The stabilized cycle is quickly reached in the case of the smaller relaxation time. In the case of the larger time cycle, this time domain is not large enough to capture the stabilized cycle, leading to a large computation time. Let us consider the influence of the time discretization on the accuracy of the displacement. The following time steps are investigated: 0.12s, 0.5s, 2s, 10s. The accuracy is computed by comparison with the prediction obtained with the finest time step. Figure 1 depicts the displacement for different time steps in the case of $\tau = 1s$. An accurate result is obtained with a time step smaller than 10s.
The different simulations show that when the relaxation time is greater (respectively smaller) than the time cycle, a coarse (respectively fine) scale is adequate to simulate the behavior of the polymer. The time basis can therefore be adapted to the relaxation time.

3.2. Three internal variables

Let us consider that the viscoelasticity is here described by three internal variables leading to three different relaxation times as follows:
- smaller than the cycle time [0.1 , 1 , 10]s,
- same order of the cycle time [1 , 10 , 100]s,
- greater than the cycle time [100 , 1000 , 10000]s

and for each triplet of relaxation times, the time step will take different values. An accurate displacement is obtained as expected in the case where the time step of the internal variable is adapted to the associated relaxation time. The relationship between these times follows the results obtained in the case of only one internal variable. The associated time steps are respectively [0.17, 0.25, 1]s, [0.25, 0.5, 2]s, [2, 5, 10]s for τ equals [0.1 , 1 , 10]s, [1 , 10 , 10]s, [100 , 1000 , 10000]s. Let us recall that the reference solution is the solution obtained with the finest time step for all the internal variables. Concerning the computation time, we observe that the gain ratio with adapted time steps increases with the relaxation times as depicted in Table 1.

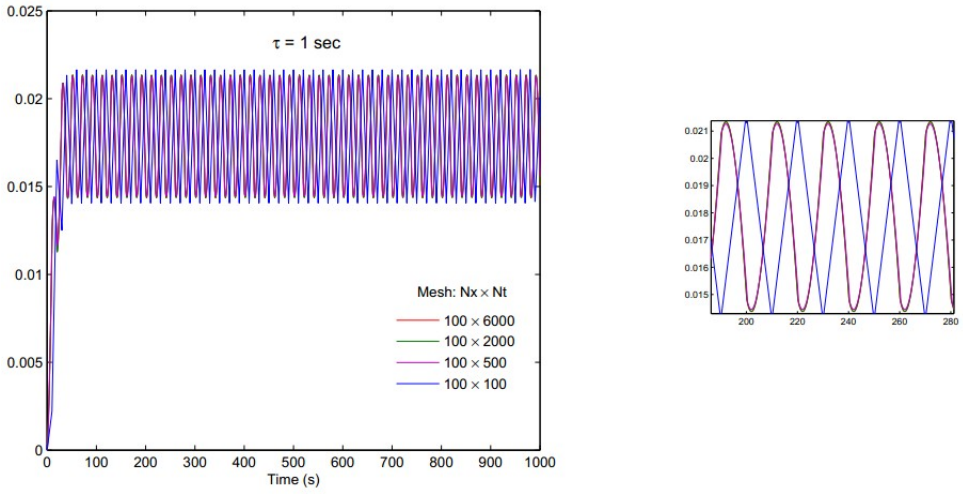

Figure 1. Displacement (mm) with respect to time for different time steps: [0.12,0.5,2,10]s which correspond to $Nt = [6000, 2000, 500, 100]$

Triplet of relaxation times (s)	Gain ratio	Number of PGD modes
[0.1 , 1 , 10]	3	8
[1 , 10 , 100]	5	12
[100 , 1000 , 10000]	8	3

Table 1. Gain ratio and number of PGD modes in the case of adapted discretizations for different triplets of relaxation times.

4. Conclusions

Within the PGD framework, the globalization of the local models allows to predict accurately the viscoelastic behavior of the polymer under cyclic loading. As the number of local models can be large, the computation time can become large. In this paper, the case with one internal variable has shown that it exists a link between the relaxation time, the cycle time and the time step to have accurate results. A coarse mesh is efficient with a large relaxation time whereas a finer mesh is mandatory with a relaxation time smaller than the cycle time. The same conclusions have been validated in the case of 3 internal variables. Adapted discretizations for each internal variable have reduced the computation time by a factor 8 in the case of three relaxation times larger than the time cycle. This factor decreases when the relaxation times are smaller than the time cycles. This way offers an opportunity to reduce computation time of viscoelasticity within the PGD framework. The future work consists in dealing with more realistic number of internal variables and more complex behaviors like non linear viscoelasticity.

References

[1] Ch Cunat. A thermodynamic theory of relaxation based on a distribution of non-linear processes. *Journal of Non-Crystalline Solids*, 131-133, Part 1:196 – 199, 1991.

[2] P Ladeveze. The large time increment method for the analysis of structures with non-linear behavior described by internal variables. *Comptes Rendus de l'Acadmie des Sciences. Serie II*, 309(11):1095–1099, 1989.

[3] A Ammar, B Mokdad, F Chinesta, and R Keunings. A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids. *Journal of Non-Newtonian Fluid Mechanics*, 139(3):153 – 176, 2006.

[4] F Chinesta, P Ladeveze, and E Cueto. A short review on model order reduction based on proper generalized decomposition. *Archives of Computational Methods in Engineering*, 18(4):395–404, 2011.

[5] F Chinesta, A Ammar, and E Cueto. Proper generalized decomposition of multiscale models. *International Journal for Numerical Methods in Engineering*, 83(8-9):1114 –1132, 2010.

[6] M Beringhier, M Gueguen, and J. C Grandidier. Solution of strongly coupled multiphysics problems using space-time separated representations-application to thermoviscoelasticity. *Archives of Computational Methods in Engineering*, 17(4):393 – 401, 2010.

[7] M Hammoud, M Beringhier, and J. C Grandidier. Application of the proper generalized decomposition method to a viscoelastic mechanical problem with a large number of internal variables and a large spectrum of relaxation times. In *4th International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS)*, pages 570–577, 2011.