Numerical Analysis of the Behaviour of Rubber-Like Polymers with Hyperbolic Models of Nonlinear Thermoelasticity

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R. V. N. Melnik[*], D. V. Strunin[†] and A. J. Roberts[‡]

Abstract

Desirable thermomechanical properties of rubber-like polymers at an economical cost made these materials a relatively cheap alternative to more traditional metallic materials in many applications in aircraft, automotive, and other industries. In this paper we study numerically a combined effect of hyperbolicity and nonlinearity on the dynamics of such materials. Modelling the thermomechanical behaviour of a ring-shaped body with the Lord-Shulman-type model, we demonstrate an intrinsic connection between nonlinear effects and hyperbolicity of the dynamics. In particular, we show that the vanishing relaxation time can lead to the suppression of nonlinearities.

Key words: models of coupled thermoelasticity with relaxation times, rubber-like polymers.

AMS subject classifications: 65M06, 73B30, 35M10.

1 Introduction

Many contributions to the numerical analysis in thermoelasticity theory have traditionally been devoted to linear models [4]. However, in many industrial applications we have to deal with the materials that exhibit typically nonlinear thermomechanical behaviour. Rubber-like polymers are, perhaps, one of the most cited examples of such materials. Although rubber-like polymers provide a classical example where nonlinear effects are essential in the adequate description of material dynamics [8, 5], only few recent papers discuss numerical results obtained for these materials with general nonlinear models of coupled thermoelasticity [2, 7] (see also references therein). In dealing with the nonlinear behaviour of such materials we must give a proper weight to the fact that nonlinearities in the dynamics of rubber-like materials are closely interwoven with the effect of thermal relaxation time [1]. In this paper we deal with rubber-like *solid* polymers that, in contrast to many other solid materials such as metals or ceramics, are energy elastic, and since they have relatively large thermal relaxation times, they demonstrate hyperbolic effects in a more pronounced fashion compared to "hard" solids. To our knowledge there have been virtually no attempts to apply hyperbolic models of nonlinear thermoelasticity to the description of the dynamics of rubber-like materials. To cover this gap, this paper reports some preliminary results on a combined effect of nonlinearity and thermal relaxation time in rubber-like polymers. A more detailed analysis will be published separately.

The motion of the material is described by the kinematic law

$$\mathbf{y} = \mathbf{x} + \mathbf{u}(\mathbf{x}, t), \tag{1}$$

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where $\mathbf{x} = (x_1, x_2, x_3)$ is the original and $\mathbf{y} = (y_1, y_2, y_3)$ is the deformed coordinate of a material point of the thermomechanical body, and $\mathbf{u} = (u_1(\mathbf{x}), u_2(\mathbf{x}), u_3(\mathbf{x}))$ is the displacement vector. The motion at each point of the body can be represented by the deformation gradient

$$(2) \qquad \mathbf{F} = \left[\frac{\partial y_i}{\partial x_j} \right]_{i,j=1,2,3} = \mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{x}},$$

where $\mathbf{I}$ is the second order identity tensor. Then, the Lagrangian equations of motion and energy balance have the form

$$(3) \qquad \rho_0 \ddot{\mathbf{y}} = \operatorname{div} \boldsymbol{\sigma}, \quad \rho_0 \dot{e} - \boldsymbol{\sigma}^T : (\nabla \mathbf{v}) + \rho_0 \operatorname{div} \mathbf{q} = 0,$$

where e is the internal energy, ρ_0 is the original density, $\mathbf{q}$ is the heat flux, $\boldsymbol{\sigma} = J[(\mathbf{F}^T)^{-1}]^T \mathbf{T}$ is the nominal stress tensor, $\mathbf{T}$ is the Cauchy (true) stress tensor, $J = \det \mathbf{F}$, and $\boldsymbol{\sigma}^T = J\mathbf{T}(\mathbf{F}^T)^{-1}$ is the first Piola-Kirchhoff stress tensor (e.g. [5], p. 153). This formulation is used as the basis for our computational experiments reported in Section 3. The stress tensor and the internal energy function are expressed in a conventional way through the free energy function which, in its turn, is represented in terms of temperature θ and displacements (for details see, e.g., [7]). The connection between the heat flux and the temperature is given by the Cattaneo-Vernotte (CV) equation implicating the relaxation time τ_0

$$(4) \qquad \tau_0 \dot{\mathbf{q}} + \mathbf{q} = -\mathcal{K} \nabla \theta,$$

where $\mathcal{K}$ is the coefficient of thermoconductivity. This connection turns into the standard Fourier law $q = -\mathcal{K} \nabla \theta$ in the limit of vanishing relaxation time $\tau_0 \to 0^+$.

2 Governing Equations of Nonlinear Thermoelasticity: Dynamics of a Ring-Shaped Polymer Structure in the One-Dimensional Case

We consider elongational oscillations of a ring-shaped polymer structure assuming that it is subjected to periodic boundary conditions. Simplifying matters and omitting lengthy derivations, we present the resulting formulae which connect the internal energy, temperature, strain, and stress. These formulae are obtained for the rubber-like structure in the form of a ring by using leading terms of Taylor expansions under the assumption that $(\theta - \theta_0)/\theta_0 \ll 1$

$$(5) \qquad \dot{e} = \bar{c}\dot{\theta} + \gamma \theta_0 \frac{\partial \dot{u}}{\partial x}, \quad \sigma = \rho_0 \frac{k_0}{\theta_0} \theta \frac{\partial u}{\partial x} - \rho_0 \gamma (\theta - \theta_0),$$

where $\bar{c}$ is the heat capacity, γ and k_0 are constants, θ_0 is the reference temperature. Taking into account (5), equations (3), (4) can be written in the form

$$(6) \qquad \begin{cases} \rho_0 \ddot{u} = \dfrac{k_0}{\theta_0}\theta \dfrac{\partial^2 u}{\partial x^2} + \dfrac{k_0}{\theta_0}\dfrac{\partial \theta}{\partial x}\dfrac{\partial u}{\partial x} - \gamma \dfrac{\partial \theta}{\partial x}, \\[2mm] \bar{c}\dot{\theta} = -\dfrac{\partial q}{\partial x} + \dfrac{k_0}{\theta_0}\theta \dfrac{\partial u}{\partial x}\dfrac{\partial \dot{u}}{\partial x} - \gamma(\theta - \theta_0)\dfrac{\partial \dot{u}}{\partial x}, \\[2mm] \tau_0 \dfrac{\partial q}{\partial t} + q = -\mathcal{K}\dfrac{\partial \theta}{\partial x}. \end{cases}$$

Excluding the heat flux q from (6) by differentiating the CV equation with respect to x and substituting therein the derivative $\partial q / \partial x$ extracted from the energy balance equation we obtain that

$$\tau_0 \frac{\partial}{\partial t}\left(\frac{\partial q}{\partial x}\right) + \frac{\partial q}{\partial x} = -\mathcal{K}\frac{\partial^2 \theta}{\partial x^2},$$

and then

$$(7) \qquad \begin{cases} \rho_0 \ddot{u} = \dfrac{k_0}{\theta_0}\theta \dfrac{\partial^2 u}{\partial x^2} + \dfrac{k_0}{\theta_0}\dfrac{\partial \theta}{\partial x}\dfrac{\partial u}{\partial x} - \gamma \dfrac{\partial \theta}{\partial x}, \\[2mm] \tau_0 \bar{c}\ddot{\theta} + \bar{c}\dot{\theta} = \mathcal{K}\dfrac{\partial^2 \theta}{\partial x^2} + \tau_0 k_0 \left[\left(\dfrac{\partial \dot{u}}{\partial x}\right)^2 + \dfrac{\partial u}{\partial x}\dfrac{\partial \ddot{u}}{\partial x} \right] + k_0 \dfrac{\partial u}{\partial x}\dfrac{\partial \dot{u}}{\partial x} \\[2mm] \qquad - \gamma \tau_0 \dot{\theta}\dfrac{\partial \dot{u}}{\partial x} - \gamma \tau_0 \theta \dfrac{\partial \ddot{u}}{\partial x} - \gamma \theta \dfrac{\partial \dot{u}}{\partial x}. \end{cases}$$

Note that the linearised system (7) takes the form of the well-known Lord-Shulman model of hyperbolic thermoelasticity [3]. In applying the normalisation procedure to the system (7) we use seven dimensional parameters,

(8)
$$\rho_0 \left(\text{g cm}^{-3}\right), \quad k_0 \left(\text{g cm}^{-1}\,\text{s}^{-2}\right), \quad \theta_0(\text{K}), \quad \mathcal{K}\left(\text{g cm s}^{-3}\,\text{K}^{-1}\right),$$

$$\gamma \left(\text{g cm}^{-1}\,\text{s}^{-2}\,\text{K}^{-1}\right), \quad \tau_0(\text{s}), \quad \bar{c}\left(\text{g cm}^{-1}\,\text{s}^{-2}\,\text{K}^{-1}\right),$$

four of which have "independent" dimensionalities. Taking this quadruple as $(\rho_0, k_0, \theta_0, \mathcal{K})$, we obtain the following (dimensional) scale factors for our variables:

(9)
$$x_* = \frac{\rho_0^{1/2}\mathcal{K}\theta_0}{k_0^{3/2}}, \quad t_* = \frac{\rho_0\mathcal{K}\theta_0}{k_0^2}, \quad T_* = \theta_0.$$

Substituting $\ddot{u}$ from the momentum equation (see system (7)) into the energy balance equation and replacing θ by $\theta_0 + T$ we obtain the non-dimensional system

(10)
$$\begin{cases} \ddot{u} = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 \dot{u}}{\partial x^2} - \dfrac{C}{B}\dfrac{\partial T}{\partial x} + \dfrac{\partial T}{\partial x}\dfrac{\partial u}{\partial x} + T\dfrac{\partial^2 u}{\partial x^2}, \\[2mm] A\ddot{T} + \dot{T} = \left(B + \dfrac{AC^2}{B}\right)\dfrac{\partial^2 T}{\partial x^2} - AC\dfrac{\partial^3 u}{\partial x^3} - C\dfrac{\partial \dot{u}}{\partial x} + AB\left(\dfrac{\partial \dot{u}}{\partial x}\right)^2 \\[2mm] \qquad -2AC\,T\dfrac{\partial^3 u}{\partial x^3} - 2AC\dfrac{\partial T}{\partial x}\dfrac{\partial^2 u}{\partial x^2} - 2AC\dfrac{\partial^2 T}{\partial x^2}\dfrac{\partial u}{\partial x} + \dfrac{AC^2}{B}\,T\dfrac{\partial^2 T}{\partial x^2} \\[2mm] \qquad +AB\dfrac{\partial u}{\partial x}\dfrac{\partial^3 u}{\partial x^3} + B\dfrac{\partial \dot{u}}{\partial x}\dfrac{\partial u}{\partial x} - AC\,\dot{T}\dfrac{\partial \dot{u}}{\partial x} - C\,T\dfrac{\partial \dot{u}}{\partial x}, \end{cases}$$

where for simplicity we use the same variables' notations as before, and constants A, B, and C have the form

$$A = \frac{\tau_0 k_0^2}{\rho_0 \mathcal{K}\theta_0}, \quad B = \frac{k_0}{\theta_0\bar{c}}, \quad C = \frac{\gamma}{\bar{c}}.$$

Denoting $v = \dfrac{\partial u}{\partial t}$, $q = \dfrac{\partial T}{\partial t}$, we seek the solution to (10) in the form of Fourier series

(11)
$$u = \sum_{n=-\infty}^{\infty} U_n(t)e^{inkx}, \quad v = \sum_{n=-\infty}^{\infty} V_n(t)e^{inkx}, \quad T = \sum_{n=-\infty}^{\infty} T_n(t)e^{inkx}, \quad q = \sum_{n=-\infty}^{\infty} Q_n(t)e^{inkx},$$

where k is the wave number ($k = 2\pi/L$, and L is the perimeter of the ring). Finally, substituting (11) into (10) and equating coefficients near $\exp(ink_0 x)$ leads to an infinite system of coupled ordinary differential equations for the amplitudes of the Fourier modes:

(12)
$$\begin{cases} dU_n/dt = V_n, \\[2mm] dV_n/dt = -(nk)^2 U_n - (nk)^2 V_n - \dfrac{C}{B}inkT_n \\[2mm] \qquad -k^2 \sum_{m=-\infty}^{\infty} m(n-m)T_m U_{n-m} - k^2 \sum_{m=-\infty}^{\infty} m^2 U_m T_{n-m} \\[2mm] dT_n/dt = Q_n, \\[2mm] AdQ_n/dt = -Q_n - \left(B + \dfrac{AC^2}{B}\right)(nk)^2 T_n + ACi(nk)^3 U_n - CinkV_n \\[2mm] \qquad -ABk^2 \sum_{m=-\infty}^{\infty} m(n-m)V_m V_{n-m} + 2ACik^3 \sum_{m=-\infty}^{\infty} m^3 U_m T_{n-m} \\[2mm] \qquad +2ACik^3 \sum_{m=-\infty}^{\infty} m(n-m)^2 T_m U_{n-m} + 2ACik^3 \sum_{m=-\infty}^{\infty} m(n-m)^2 U_m T_{n-m} \\[2mm] \qquad -\dfrac{AC^2}{B}k^2 \sum_{m=-\infty}^{\infty} (n-m)^2 T_m T_{n-m} + ABk^4 \sum_{m=-\infty}^{\infty} m(n-m)^3 U_m U_{n-m} \\[2mm] \qquad -Bk^2 \sum_{m=-\infty}^{\infty} m(n-m)V_m U_{n-m} - ACik \sum_{m=-\infty}^{\infty} mV_m Q_{n-m} - Cik \sum_{m=-\infty}^{\infty} mV_m T_{n-m}. \end{cases}$$
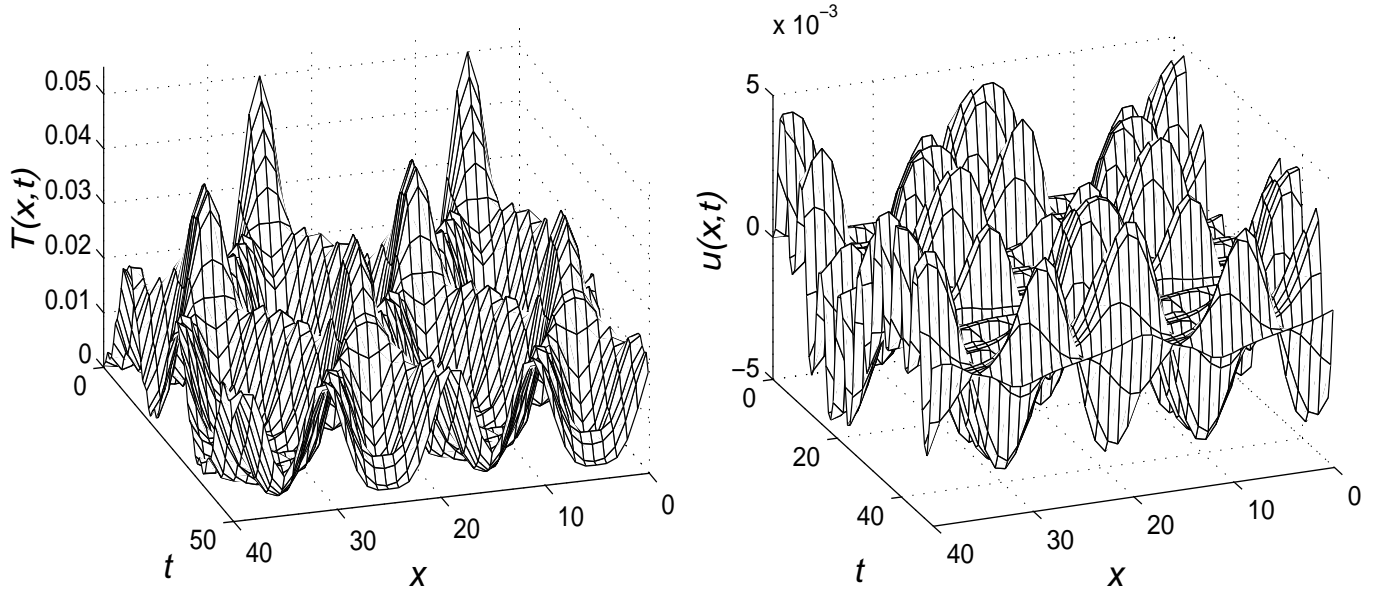
Figure 1: Dynamics of temperature and displacement for $\tau_0 = 10^{-12}$ s, $k = 1$, $t_1 = 50$.

The system (12) was truncated to a finite number of modes and integrated in time using the fourth order Runge-Kutta method.

3 Numerical Experiments: Combined Effects of Nonlinearities and Thermal Relaxation

Computational experiments reported in this section have been performed for a polyisoprene (natural rubber) ring. In this case typical values of parameters (8) are

(13)
$$\rho_0 = 0.913\,\text{g cm}^{-3}, \quad k_0 = 2270\,\text{MPa} = 2.27 \cdot 10^{10}\,\text{g cm}^{-1}\,\text{s}^{-2}, \quad \theta_0 = 293\,\text{K},$$

$$\mathcal{K} = 0.134\,\text{W m}^{-1}\,\text{K}^{-1} = 1.34 \cdot 10^{4}\,\text{g cm s}^{-3}\,\text{K}^{-1},$$

$$\gamma = 11.8 \cdot 10^{5}\ \text{N m}^{-2}\,\text{K}^{-1} = 1.18 \cdot 10^{7}\,\text{g cm}^{-1}\,\text{s}^{-2}\,\text{K}^{-1},$$

$$\bar{c} = 1905\,\text{J kg}^{-1}\,\text{K}^{-1} \cdot 0.913\,\text{g cm}^{-3} = 1.74 \cdot 10^{7}\,\text{g cm}^{-1}\,\text{s}^{-2}\,\text{K}^{-1},$$

Substituting these values into (9), we find typical spatial and time scales for our model (10) applied to the description of thermomechanical behaviour of rubber-like materials

$$x_* = 1.1 \cdot 10^{-9}\,\text{cm}, \quad t_* = 6.9 \cdot 10^{-15}\,\text{s}.$$

Initial conditions for the model (10) are chosen in the following form

(14)
$$T(x,0) = R\left(1 + \frac{5}{2}\sin(kx)\right)^4, \quad u(x,0) \equiv 0, \quad \left(\frac{\partial T}{\partial t}\right)_{t=0} \equiv 0, \quad \left(\frac{\partial u}{\partial t}\right)_{t=0} \equiv 0,$$

where the factor R in (14) is chosen in such a way that the maximal initial temperature is equal to the melting temperature of the material T_m. For natural rubber $T_m = 35\,$C, consequently the corresponding non-dimensional temperature equals to 0.05 which is provided by $R = 10^{-3}/3$.

In principle, once the shape and amplitude of the initial conditions are specified, we are left with only one free parameter in our model, namely, the wave number k. However, since the thermal relaxation time is a difficult-to-measure characteristic, in all practical applications it can be given only approximately. Taking this into account, we vary this characteristic within a reasonable range of values in order to demonstrate its importance for the nonlinear
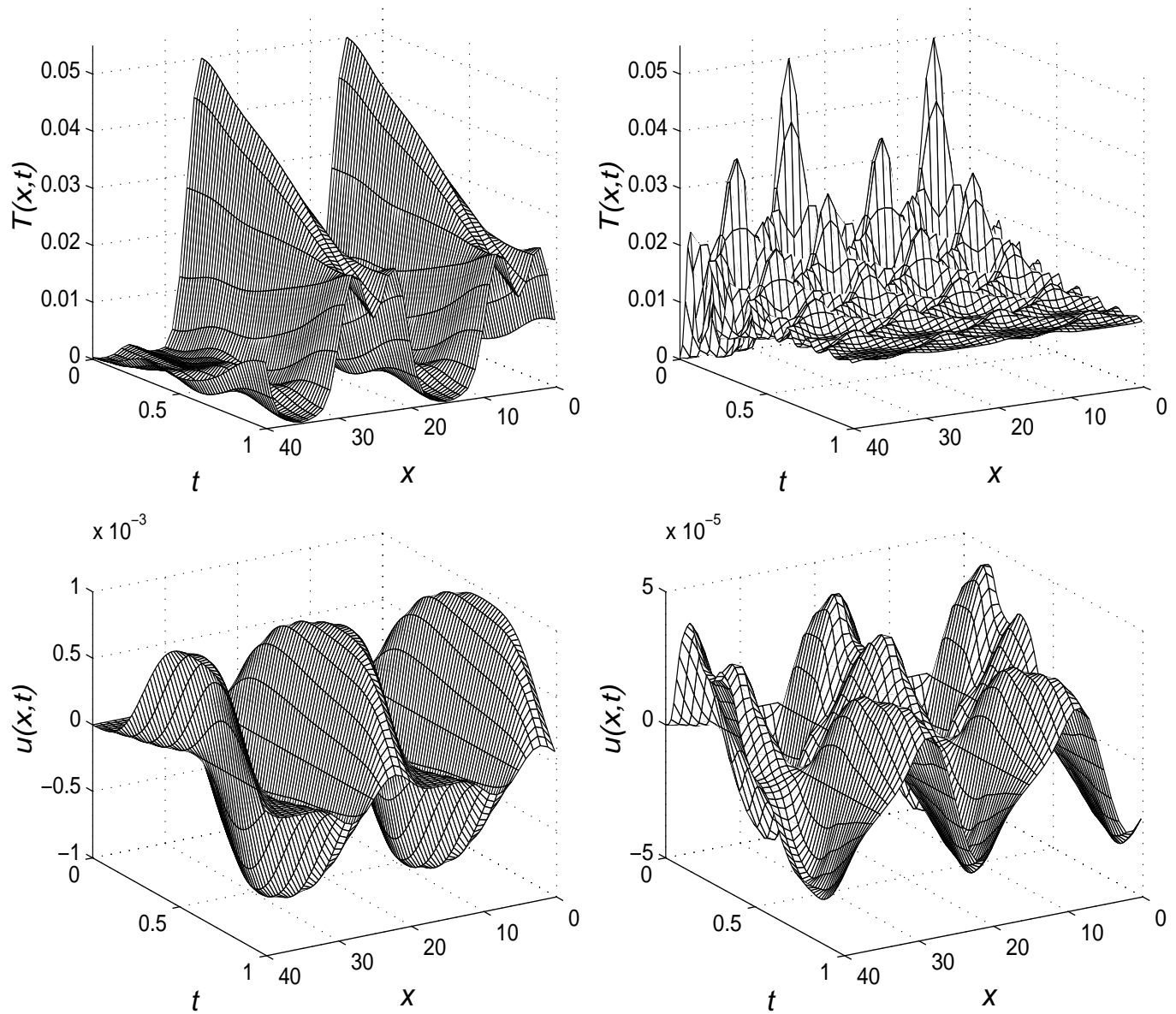
Figure 2: Dynamics of temperature and displacement for $\tau_0 = 10^{-12}$ s (left column) and $\tau_0 = 10^{-15}$ s (right column). In both cases $k = 5$.

dynamics of rubber-like materials. Numerical results in Fig.2, obtained for $k = 1$ and $\tau_0 = 10^{-12}$s, demonstrate main features of this dynamics. We display two periods of temperature and displacement profiles for viewing convenience. The coordinate x is indicated in conditional units showing the number of points that were used to plot the curves. We note that longer calculations, performed beyond the limit $t_1 = 50$ (which is shown in Fig. 2), demonstrate that nonlinear effects eventually drive the profiles towards the formation of shock-type waves. This result confirms a theoretical analysis of nonlinear models of coupled thermoelasticity [6].

The role of nonlinearities in the system dynamics cannot be regarded without its intrinsic connection with the thermal relaxation time. Indeed, almost all nonlinear terms in system (10) involve the thermal relaxation time included into the system via the parameter A. In order to support our claim we carried out an experiment for $k = 5$ using different values of the relaxation time. The result is displayed in Fig.3. By switching from the case $\tau_0 = 10^{-12}$s to the case $\tau_0 = 10^{-15}$s we decrease τ_0, and therefore, suppress system nonlinearities. In the right column of Fig. 3 we observe a linear dissipation of temperature to some uniform distribution. When such a distribution is achieved, displacements continue to oscillate in an uncoupled manner, according to the equation of motion. A qualitatively different situation is demonstrated by the left column in Fig. 3. The dramatic contrast between the two cases cannot be explained just by different roles of nonlinearities in these two cases. It is a result of a combined effect of nonlinearities and the thermal relaxation time on the dynamics of our thermomechanical system.

Of course, the processes discussed above occur on extremely short time intervals and have very short spatial scales. However, the thermal relaxation time can play an important role on larger scales. To show this, we roughly estimate the terms involved in the determination of the effective coefficient of temperature dissipation, $B + AC^2/B$. For our data it can be found that $AC^2/B = 0.0026$ and $B = 0.00076$. This clearly indicates that despite the smallness of the relaxation time for rubber-like materials, the combination AC^2/B can be comparable in value with B. Therefore, in modelling dynamic behaviour of rubber-like polymer systems, the interplay between nonlinearity and hyperbolic features of the material dynamics is an important factor that influences thermomechanical properties of the systems. Accounting for industrial trends in moving from the simpler homogeneous polymers to more complex composite materials this factor will play an increasingly important role in many engineering applications.

4   Acknowledgements

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$$\rho\left[\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right] = -\vec{\nabla}p + \mu\vec{\nabla}^2\vec{v} + \rho\vec{f}$$

$$\rho\left[\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right] = -\vec{\nabla}p + \rho\vec{f}$$

$$p + \rho gz + \rho\frac{v^2}{2} = C$$

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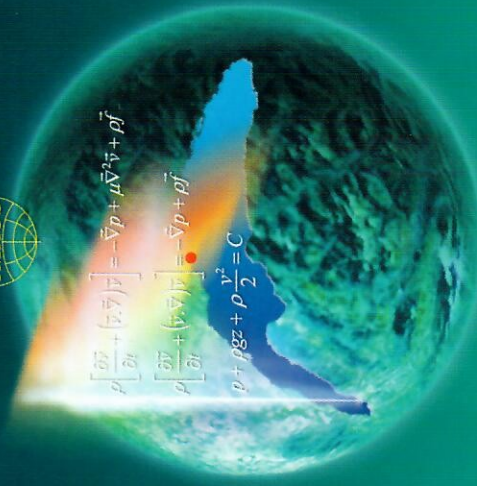Mario Romanò
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