Nonlinear Elastomers: Modeling and Estimation *

H. T. Banks † N. J. Lybeck† B. C. Muñoz ‡ L. C. Yanyo‡

Abstract

We report on our efforts to model nonlinear dynamics in elastomers. Our efforts include the development of computational techniques for simulation studies and for use in inverse or system identification problems.

1 Introduction

A problem of fundamental interest and great importance in modern material sciences is the development of both passive and active ("smart") vibration devices constructed from polymer (long molecular chains of covalently bonded atoms often having cross-linking chains) composites such as elastomers filled with carbon black and/or silica or with active elements (i.e., piezoelectric, magnetic or conductive particles). These rubber based products (even without active elements) involve very complex viscoelastic materials that are not at all like metals (where large deformations lead to permanent material changes) and do not satisfy the usual, well-developed linear theory of (infinitesimal) elasticity for deformable bodies. They typically exhibit mechanical properties that combine elastic (purely reversible) and hysteretic (irreversible) phenomena. In considering macroscopic behavior, one finds that the usual constitutive relationships (e.g., Hooke's law) or rheological equations of state for pure elastics are not applicable. Indeed, one finds a number of factors that contribute to difficulty in modeling mechanical behavior: (i) deformations are sensitive to environmental temperatures as well as the strain level, strain history and rate of loading; (ii) one observes nonlinearities in both material and geometric behavior - in general, there is a nonlinear relationship between stress and strain even for small strains; (iii) deformations in the range of practical interest are large and infinitesimal based theories break down; (iv) deformations are not reversible; (v) the anisotropic nature of polymers can be important in certain types of deformations - for example, the amount and type of filler affects mechanical response in a nontrivial manner.

In spite of all these difficulties, there is a substantial literature on modeling of rubber-like elastomers (see [F, T, W] for basic texts), predominantly based on one of the two rather distinct approaches: (i) molecular (polymer chain) statistical thermodynamic formulations (ii) phenomenological (usually continuum) formulations involving stored energy or strain energy functions(SEF) and/or finite strain (FS) theories. In the phenomenological approach (which will be the basis of our efforts) most investigators begin with an isotropic material under homogeneous strain.

Strain energy function theories typically embody only elastic properties of elastomers or rubbers and hence are mostly used in static (equilibrium) finite element analysis (e.g. see [CYT]) of materials (e.g. natural gum rubbers) that exhibit little or no hysteretic behavior. SEF material models, such as those of Mooney-Rivlin, Ogden, Treloar and numerous others, are based on strain invariants I_i, where $I_1 = \lambda_1^2+\lambda_2^2+\lambda_3^2$, $I_2 = \lambda_2^2\lambda_3^2+\lambda_1^2\lambda_3^2+\lambda_1^2\lambda_2^2$ and $I_3 = \lambda_1^2\lambda_2^2\lambda_3^2$ and the λ_i are the principal extension ratios (deformed length of unit vectors along directions parallel to the principal axes i.e. the axes of zero shear strain). For example, the Mooney SEF is given by $U = C_1(I_1 - 3) + C_2(I_2 - 3)$, or more generally, the modified expression $U = C_1(I_1-3)+f(I_2-3)$, where f has certain qualitative properties, and is most appropriate for components where the rubber is not tightly confined and where the assumption of absolute incompressibility (implying $\lambda_1\lambda_2\lambda_3 = 1$ or $I_3 = 1$) is a reasonable approximation. The more general Rivlin SEF $U = \sum_{i+j\geq 1}^{N} C_{ij}(I_1-3)^i(I_2-3)^j$ and its generalization for near incompressibility (see [CYT]) allow higher order dependence of the SEF on the invariants.

The finite strain elastic theory of Rivlin [R, W] is developed with a generalized Hooke's law in an analogy to infinitesimal strain elasticity but makes no "small deformation" assumption and includes higher order exact terms in its formulation. Moreover, finite stresses are defined relative to the deformed body and hence are the "true stresses" as opposed to the "nominal" or "engineering" stresses (relative to the

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undeformed body) one usually encounters in the infinitesimal linear elasticity used with metals. This Eulerian measure of strain (relative to a coordinate system convected with the deformations) - as opposed to the usual Lagrangian measure (relative to a fixed coordinate system for the undeformed body) - is an important feature of any development of models for use in analytical/computation/experimental investigations of rubber-like material bodies. The finite strain elasticity of Rivlin can be directly related to the strain energy function formulations through equations relating the finite strains $\tilde{e}_{xx}, \tilde{e}_{yy}, \tilde{e}_{zz}$ to the extension ratios $\lambda_1, \lambda_2, \lambda_3$ used to define the SEF. For example, in homogeneous pure tensile strain we have $\lambda_1^2 = 1 + 2\tilde{e}_{xx}, \lambda_2^2 = 1 + 2\tilde{e}_{yy}, \lambda_3^2 = 1 + 2\tilde{e}_{zz}$ and $\tilde{e}_{yz} = \tilde{e}_{zx} = \tilde{e}_{xy} = 0$.

Whether one begins with a choice of the SEF or with Rivlin's finite strain formulation, one can use these along with standard material independent force and moment balance derivations (the Timoshenko theory [TYW, CP]) as the basis of dynamical models. To illustrate this we take the simplest example: an isotropic, incompressible ($\lambda_1\lambda_2\lambda_3 = 1$) rubber-like rod under simple elongation with a finite applied stress in the principal axis direction x_1. The finite stress theory (or the Mooney theory with SEF $U = C_1(I_1 - 3)$) leads to a true stress $\sigma = \frac{E}{3}(\lambda_1^2 - \frac{1}{\lambda_1})$ or an engineering or nominal stress for what are termed neo-Hookean materials

$$\sigma_{\text{eng}} = \frac{\sigma}{\lambda_1} = \frac{E}{3}(\lambda_1 - \frac{1}{\lambda_1^2}) \tag{1}$$

where in terms of deformation u in the $x_1 = x$ direction we have (since deformations in the y and z directions are negligible)

$$\begin{aligned} \lambda_1^2 &= 1 + 2\tilde{e}_{xx} = 1 + 2\frac{\partial u}{\partial x} + \left(\frac{\partial u}{\partial x}\right)^2 \\ &= \left(1 + \frac{\partial u}{\partial x}\right)^2 . \end{aligned} \tag{2}$$

Here E is a generalized modulus of elasticity.

This can be used in the Timoshenko theory for longitudinal vibrations of a rubber bar to obtain (ρ = mass density, F = applied external force)

$$\rho A\frac{\partial^2 u}{\partial t^2} - \frac{\partial S}{\partial x} = F \tag{3}$$

where S, the internal (engineering) stress resultant, is given by

$$S = \frac{AE}{3}(\lambda_1 - \frac{1}{\lambda_1^2}) = \frac{AE}{3}g\left(\frac{\partial u}{\partial x}\right) \tag{4}$$

with $g(\xi) = 1+\xi-(1+\xi)^{-2}$and A is the cross sectional area. This leads to the nonlinear partial differential equation

$$\rho A\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}\left(\frac{EA}{3}g\left(\frac{\partial u}{\partial x}\right)\right) = F \tag{5}$$

for dynamic longitudinal displacements of a neo-Hookean material rod in extension. Since a series expansion of g yields $g(\xi) = 3\xi - 3\xi^2 + 4\xi^3 - \ldots$, this is readily seen, in the case of small displacements, to reduce to the usual longitudinal deformation equation for Hookean materials.

The neo-Hookean or simple Mooney expression for the SEF yielding the form of g in (4) has only limited practical application since it is inadequate in describing most filled elastomers. In general, one would employ equations such as (5) with a more general nonlinearity g which should be estimated from dynamical experiments. Moreover, one must also include hysteresis in the nonlinear integropartial differential equations (see [F, SC, RHN, C, P]).

In this lecture we report on our efforts to develop such a class of finite strain dynamic models to be used in design of rubber based elastomers. We develop a mathematical framework for well-posedness and approximation in the context of identification or inverse problems. Computational results as well as our use of these techniques with experiments will be discussed.

2 Variational Formulation

Our immediate interest is in the design of dynamic experiments to use in determining the strain function g in models such as (5). In one type of dynamic experiments a slender rod is suspended vertically with the top end ($x = 0$) fixed, as shown in Figure 1. Let

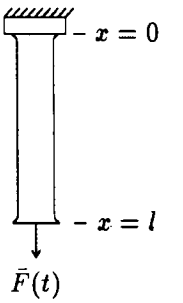

Figure 1: Experimental setup

$u(t, x)$ denote the deformation at time t of the cross section that was located at a distance x from the top when the rod was free hanging (with no applied load). Thus $u(t, 0) = 0$ for all t. The end $x = l$ of the rod is attached to a motor which supplies a force $\bar{F}(t)$ to produce some prescribed movement or deformation $u(t, l) = \Delta(t)$, $t > 0$. Hence the applied force F in

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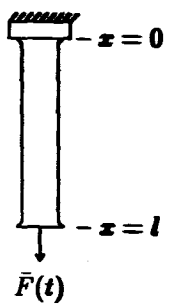

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3 Numerical Approximations

The ultimate goal of solving an inverse problem to determine the nonlinearity g must be considered when developing a numerical scheme to solve the forward problem (6). The presence of the prescribed deformation $u(t,l) = \Delta + d(t)$ indicates that a Tau-Galerkin method would be a convenient method for solving the weak formulation (6). The theory developed in [BW] shows further that a Tau-Galerkin method is an appropriate choice in the context of solving least-squares parameter estimation problems.

For a given g we use a Tau-Galerkin method with linear splines for the spatial discretization, and a Fehlberg fourth-fifth order Runge-Kutta method in time. We therefore seek an approximate solution to (6) of the form

$$u^N(t,x) = \sum_{j=1}^{N} w_j(t) L_j(x)$$

where the L_j are linear splines (given below), and w_j are unknown functions of time. In the Tau method, we impose the boundary condition $u(t,l) = \Delta + d(t)$ on the trial solutions u^N, not on the individual basis elements. The boundary condition $u(t,0) = 0$ is treated as an essential boundary condition and is imposed directly on each of the basis elements L_j.

Let $h = \frac{l}{N}$ denote the grid spacing. Let $x_j = jh$, $j = 1, \ldots, N$ be the grid points. The usual linear splines are defined for $1 \le j \le N-1$ by

$$L_j(x) = \begin{cases} 0\,, & 0 \le x \le (j-1)h \\ x/h - (j-1)\,, & (j-1)h \le x \le jh \\ -x/h + j + 1\,, & jh \le x \le (j+1)h \\ 0\,, & x \ge (j+1)h \end{cases},$$

with

$$L_N(x) = \begin{cases} 0\,, & 0 \le x \le (N-1)h \\ x/h - N + 1\,, & x \ge (N-1)h \end{cases}.$$

In order to use the Runge-Kutta method, (6) must be rewritten as a first order system in time. To accomplish this, let

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} u \\ \dot{u} \end{bmatrix}.$$

Then

$$\begin{bmatrix} \dot{u}_1 \\ \dot{u}_2 \end{bmatrix} = \begin{bmatrix} u_2 \\ \ddot{u} \end{bmatrix}.$$

Restate the weak formulation (6) as

$$\dot{u}_1 = u_2 \tag{10}$$

and for each $\phi \in H_0^1(0,l) \subsetneq V \equiv H_L^1(0,l)$

$$\int_0^l \dot{u}_2 \rho A \phi dx = -\int_0^l \phi' \frac{AE}{3} g\left(\frac{\partial u_1}{\partial x}\right) dx\,. \tag{11}$$

The approximate solutions of (10) and (11) are given by

$$u_1^N(t,x) = \sum_{j=1}^{N-1} w_j(t) L_j(x) + (\Delta + d(t)) L_N(x)\,,$$

and

$$u_2^N(t,x) = \sum_{j=1}^{N-1} \psi_j(t) L_j(x) + \dot{d}(t) L_N(x)\,.$$

Substituting the approximate solutions into (10) we obtain equations

$$\dot{w}_j(t) = \psi_j(t)\,,\ j = 1\,, \ldots\,, N-1\,.$$

Substituting the approximate solutions into (11), and choosing $\phi = L_k$, we find

$$\int_0^l \left(\sum_{j=1}^{N-1} \dot{\psi}_j L_j + \ddot{d} L_N\right) \rho A L_k dx =$$

$$-\int_0^l L_k' \frac{AE}{3} g\left(\sum_{j=1}^{N-1} w_j L_j' + (\Delta + d) L_N'\right) dx\,.$$

For fixed t the discrete system is achieved by allowing k to vary between 1 and $N-1$. The following notation is necessary to write down the discrete system. Define the (symmetric) tridiagonal mass matrix M with entries

$$[M_{i,i}] = \int_0^l \rho A L_i^2 dx\,,$$

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$$\vec{G}_{N-1} = -\int_0^l L_{N-1}' \frac{AE}{3} g\left(\sum_{j=1}^{N-1} w_j L_j' + (\Delta + d) L_N'\right)$$

$$-\ddot{d} \rho A L_N L_{N-1} dx\,.$$

The first order discrete system is then given by

$$\begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} \dot{\vec{w}} \\ \dot{\vec{\psi}} \end{bmatrix} = \begin{bmatrix} 0 & I \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \vec{w} \\ \vec{\psi} \end{bmatrix} + \begin{bmatrix} \vec{0} \\ \vec{G}(\vec{\psi}) \end{bmatrix},$$

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4 Numerical Studies

We have used the numerical scheme outlined above in numerical simulation studies to aid in design of experiments. We describe briefly here some of our findings.

The first question to be addressed in using the approximation schemes is related to their accuracy. One can prove convergence results: as $N \to \infty$, the approximate solutions u^N converge to the solution u of (6). However, this does not answer the question of the value of N that we fix to use in our calculations. To aid in this matter, we performed a series of eigenvalue calculations with the approximate system in the case of a Hookean material ($g(\xi) = 3\xi$ in (5)). For a rod of length $l = 15$ cm, and constant cross section, one finds that the eigenvalues are given by $\lambda_n = n\pi/l\sqrt{E/\rho}$. Choosing material parameters $E = 2.1 \times 10^7$ dyn/cm^2, $\rho = .92$ g/cm^3, we obtain the corresponding natural frequencies $f_n = \lambda_n/(2\pi)$ given by $f_n = 159.25n$. Eigenvalue calculations with the approximate systems demonstrated good approximation of the first eight natural frequencies at $N = 64$. For example, at $N = 48$ and 64 we obtained $f_1^{48} = 159.28$, $f_1^{64} = 159.27$ to approximate $f_1 = 159.25$ while $f_7^{48} = 1124.55$, $f_7^{64} = 1120.28$ approximate $f_7 = 1114.75$. Similar approximates are found for the other frequencies. Based on these eigenvalue studies for the linear systems (of course, the ideas of eigenvalues and modes are not useful for the neo-Hookean system) we used $N = 48$ in our calculations, including those reported on here.

We considered a number of questions in support of our experimental design questions and we list several of these. (i)What shape ($l, A = A(x)$, etc.) should be used that will provide ample information about the material and yet be easily constructed? (ii) If additional observations (say of displacement) are possible, where should these be taken to maximize the differences between Hookean and neo-Hookean material responses? (We know, for example, that displacement sensors near nodal points for a linear system is not an intelligent choice!) (iii) What type of input signals will sufficiently distinguish the Hookean and neo-Hookean responses so as to enhance our possibilities for identifying g from vibration response data? (iv) How should we test damping? The linear version of equation (6) is undamped (does the nonlinearity g itself provide some type of damping of input energy?), while the experimental responses will definitely exhibit significant damping.

We discuss briefly some of our findings related to two of these questions. First the question of damping is a difficult one that we are still pursuing. However, as the graphs in Figure 2 reveal, the Hookean model, as expected, has no inherent damping. Each graph in Figure 2 corresponds to a simulation with zero initial displacement but with the same nonzero initial velocity (this simulates a structure that has been excited with the same energy input at $t = 0$ and afterwards allowed to freely oscillate). The neo-Hookean response suggests that there is some inherent energy reduction in the nonlinear system but it clearly is not damping in the traditional sense we understand. It also does not correspond to the rapid dissipation we see in oscillating rubber samples.

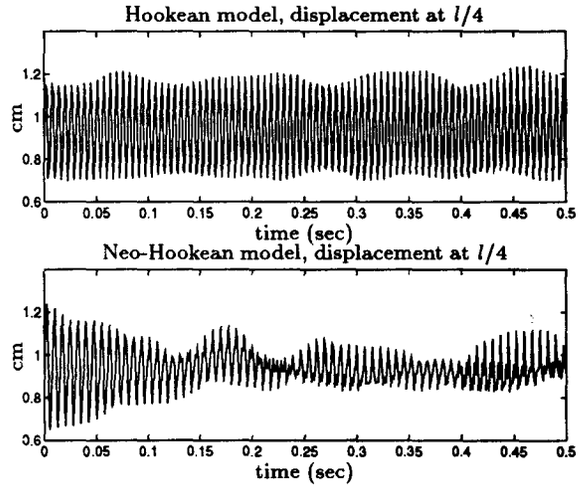

Figure 2: Damping experiment for both a Hookean and a neo-Hookean model

The question of type of input signal to use has yielded quite nicely to our numerical investigations. We have considered persistent sinusoidal inputs $d(t) = a \sin \omega t$ with the driving frequency of $f = \omega/(2\pi)$ near and far from resonance for the linear system. We also considered periodic triangular inputs (a "sawtoothed" sinusoidal that is between a square wave and a smooth sinusoidal). In many numerical experiments, it was observed that the driving frequency dominated the responses with varying levels of energy exciting the natural structural modes of the Hookean system. In FFT's of the neo-Hookean responses, one sees energy concentrations but not so sharply as in systems with modes. One important constraint on the periodic input signals is the frequency range for f possible in the experimental test equipment. While a frequency sweep (say between 0 and 500 Hz) would reveal significant information, we are physically restricted to excitations in the $0 - 25$ Hz range. These (in the range of displacements allowed) do not yield really substantial excitation in frequencies much beyond the first natural frequency of the Hookean model. Our most promising results to date suggest that a simulated "impulse" for the system might sufficiently distinguish the Hookean and neo-Hookean responses when working in the frequency/displacement ranges dictated by our experimental equipment. In Figures 3 and 4 we plot the in-

put signal (a triangular displacement approximating an impulse input) and the FFT of the corresponding displacement at $x = l/4$ in the rod for an input possible with frequency set at 15 Hz. Figure 3 contains the Hookean response while Figure 4 is the neo-Hookean. In Figures 5 and 6 we give similar plots for an input signal corresponding to $f = 25$ Hz.

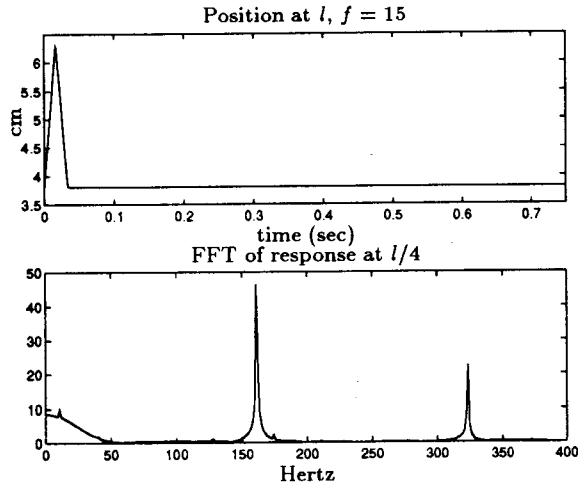

Figure 3: Hookean response at 15 Hz.

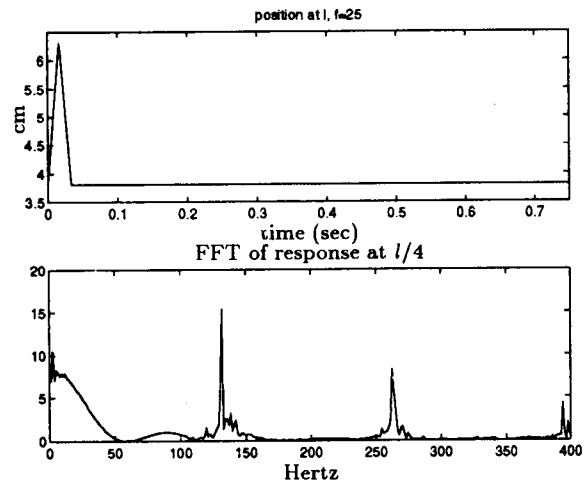

Figure 4: Neo-Hookean response at 15 Hz.

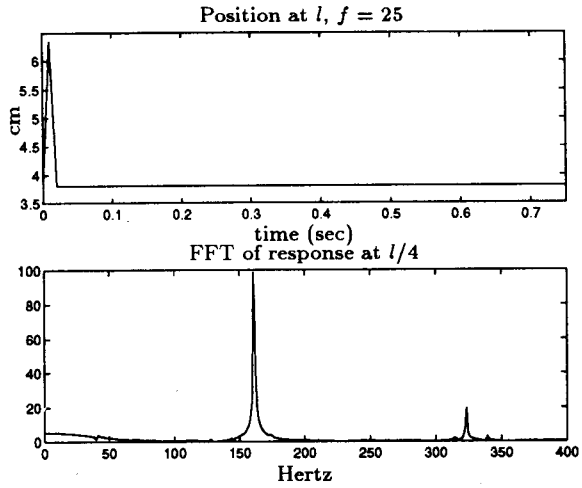

Figure 5: Hookean response at 25 Hz.

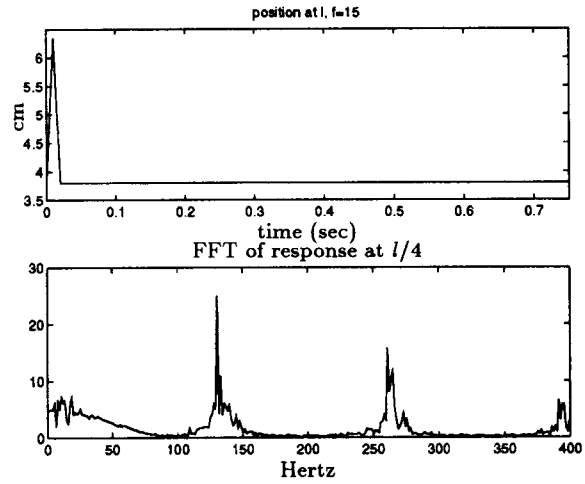

Figure 6: Neo-Hookean response at 25 Hz.

5 Concluding Remarks

In the discussions above we have outlined some of our initial efforts on the intellectually stimulating but difficult problems related to the understanding of the dynamics of filled elastomers. We are currently beginning experiments and developing computational techniques for the estimation of g in (6) from vibration response data. Moreover, in related studies [BMZ] we are developing models and computational schemes to treat hysteresis as well as damping in composite material structures containing viscoelastic components.

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