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Short communication

Optimizing cardiac material parameters with a genetic algorithm

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Abstract

Determining the unknown material parameters of intact ventricular myocardium can be challenging due to highly nonlinear material behavior. Previous studies combining a gradient-search optimization procedure with finite element analysis (FEA) were limited to twodimensional (2D) models or simplified three-dimensional (3D) geometries. Here we present a novel scheme to estimate unknown material parameters for ventricular myocardium by combining a genetic algorithm (GA) with nonlinear finite element analysis. This approach systematically explores the domain of the material parameters. The objective function to minimize was the error between simulated strain data and finite element model strains. The proposed scheme was validated for a 2D problem using a realistic material law for ventricular myocardium. Optimized material parameters were generally within 0.5% of the true values. To demonstrate the robustness of the new scheme, unknown material parameters were also determined for a realistic 3D heart model with an exponential hyperelastic material law. When using strains from two material points, the algorithm converged to parameters within 5% of the true values. We conclude that the proposed scheme is robust when estimating myocardial material parameters in 2D and 3D models. © 2006 Elsevier Ltd. All rights reserved.

Keywords: Ventricular myocardium; Finite element analysis; Material parameter optimization; Three-dimensional heart model

1. Introduction

Cardiac wall stresses determine myocardial oxygen consumption and coronary blood flow (Suga, 1990; Jan, 1985), and are important indicators of dysfunction (Mann, 2004; DiNapoli et al., 2003). Since no experimental methods can measure ventricular wall stresses, investigators use a combination of experiments, mathematical models, and numerical techniques. These approaches require a strain-energy function with tissue-specific material parameters to develop stress–strain relationships for the ventricular wall. These parameters must thus be determined from experimental data as an inverse problem.

Due to the complex material behavior and threedimensional (3D) heart geometry, finite element analysis (FEA) is well suited to model cardiac wall mechanics. Guccione et al. (1991) implemented a gradient-search optimization using FEA to identify myocardial material

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parameters in a cylindrical geometry. Moulton et al. (1995) combined FEA with gradient-search optimization to determine material parameters in isotropic two dimensional (2D) geometries. When parameter estimates are initially far from the global minimum, gradient-search methods can fail by converging to local minima. Genetic algorithms (GA) are popular because they can identify the global minimum in highly nonlinear problems with multiple local minima (Pandit et al., 2005; Vigdergauz, 2001; Karr et al., 2000).

The objective of this study was to determine the feasibility of coupling a GA with nonlinear FEA to optimize material parameters of ventricular myocardium. GAs explore the solution space by testing parameter combinations simultaneously, helping to avoid local minima (Goldberg, 1989). Moreover, the GA does not require derivative or other auxiliary information.

In this study, a GA optimized material parameters by minimizing the error between the target response and the FEA-generated response. This approach was validated in 2D and 3D geometries with a realistic material model.

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2. Methods

2.1. Material model

Myocardium was modeled as transversely isotropic hyperelastic material using the strain-energy function (Guccione et al., 1991)

$$W = \frac{1}{2}C(e^{Q} - 1), \tag{1}$$

where

$$Q = b_1 E_{\rm ff}^2 + b_2 \left(E_{\rm rr}^2 + E_{\rm cc}^2 + 2E_{\rm rc}^2 \right) + 2b_3 \left(E_{\rm fr}^2 + E_{\rm fc}^2 \right), \tag{2}$$

W is the strain-energy density, and *C*, b_1 , b_2 , and b_3 are unknown material parameters. The Green's strain components, E_{ij} , were defined relative to local fiber (f), cross-fiber (c), and radial (r) directions. The second Piola–Kirchhoff stress tensor was obtained from

$$S = \frac{\partial W}{\partial E}.$$
(3)

The Cauchy stress tensor was computed as

$$T = [F][S][F]^{\mathrm{T}},\tag{4}$$

where F is the deformation gradient tensor. Stress equilibrium equations were solved using ABAQUS/Standard (ABAQUS Inc., 2004) with material parameters optimized using a GA.

2.2. 2D model of myocardium

A simulated slab of ventricular myocardium was subjected to three different loads: uniaxial stretch in the fiber direction, uniaxial stretch in the cross-fiber direction, or equibiaxial stretch. A state of plane stress was established by subjecting the slab to a stretch ratio of 1.25 in five steps. Experimentally, stresses in the stretched myocardial slab are measured using transducers (Lin and Yin, 1998). These stresses were treated as target stresses, generated by Eqs. (1)–(4) using parameters from Vetter and McCulloch (2000). The objective function was the root mean squared error (RMSE) between target and FEA-generated stresses. Since the parameter b_3 characterizes the response in shear, b_3 was held constant at 1.63 because shear loading was excluded in these 2D simulations.

2.3. Passive inflation heart model

A 3D cardiac ventricular geometry (Vetter and McCulloch, 2000) was discretized using hexahedral elements with a hybrid formulation for material incompressibility. Myofiber orientation and constitutive relations were implemented through user subroutines. Basal epicardium nodes were fixed, and basal left ventricle (LV) endocardial nodes were constrained to move in the circumferential–radial plane. The LV was inflated from 0 to 25 mmHg pressure in five equal steps.

In experiments, surface strains are computed from measured displacements of surface markers. For the 3D simulations, these target strains were simulated using material parameters from Vetter and McCulloch (2000), treated here as the actual parameters. The objective function was the RMSE between target strains and FEA-generated strains. Two scenarios were studied to evaluate computational effort and convergence. In Scenario A, the fiber, cross-fiber, and shear strains were computed at a single material point on the LV epicardial wall. In Scenario B, target strains were also computed at an epicardial point located 90° circumferentially from the first (Fig. 1).

Preliminary studies revealed that parameters from Vetter and McCulloch (2000) resulted in 10–15 h FEA simulations. Since our goal was to determine the feasibility of this scheme, parameter C was increased by a factor of 10, reducing the computational time to 15–20 min for each FEA simulation.



Fig. 1. The three-dimensional finite element heart model and material points used in the two optimization scenarios. In Scenario A, strains at only material point 1 were used in the optimization; Scenario B used strains from material points 1 and 2.

Table 1 Lower and upper bounds on the domains of the material parameters in Eqs. (1) and (2)

Parameter	С	b_1	b_2	<i>b</i> ₃	
Lower bound0.001Jpper bound0.100		0.100	0.100	0.100	
		100.0	100.0	100.0	

Large parameter domains were used to better characterize the ability of the algorithm to identify the correct parameter values. Smaller domains would reduce the computational time but also bias the algorithm toward the correct parameter values.

2.4. Genetic algorithm-based optimization

A real-encoded "simple genetic algorithm" was implemented with selection, recombination, and mutation operators (Pohlheim, 1996). An initial generation of chromosomes was created from a set of material parameters selected randomly within the specified bounds (Table 1). Each chromosome encoded four variables corresponding to parameters C, b_1 , b_2 , and b_3 . The GA used default fitness, selection, recombination, and mutation operators (Pohlheim, 1996). The objective function for each chromosome in a generation was evaluated using the FEA-generated response. Chromosomes were then ranked by the fitness operator and selected for mating. Recombination and mutation operators were applied to the selected chromosomes, creating the next generation. This procedure was repeated for each generation until a termination criterion was met. This approach was implemented as a MATLAB script that communicated with the FEA software by creating an input file from each chromosome. The script then extracted the FEA solution and evaluated the objective function for each chromosome. The GA then created the next generation. The optimization was terminated when stresses (2D case) or strains (3D case) were within 2% of target values.

3. Results

3.1. 2D slab

In 10 optimizations of the 2D problem, the GA identified the actual parameters within 0.57% in nine runs (Table 2). One run converged prematurely, suggesting the population size of 36 chromosomes was suboptimal. Stress versus

Table 2 Results of ten optimization runs in the 2D myocardial slab

Parameter	С	b_1	b_2	Objective function
Target value	0.001760	50.000	5.000	_
FEA run				
1	0.001761	49.990950	4.997732	0.469249
2	0.001762	49.988720	4.995002	0.766594
3	0.001759	50.005580	5.002000	0.371746
4	0.078822	1.897424	0.128267	926.370900
5	0.001757	49.992170	5.005049	2.696769
6	0.001762	49.988510	4.995293	0.762465
7	0.001753	50.051920	5.014194	2.821704
8	0.001751	50.078140	5.022122	3.958483
9	0.001750	50.055930	5.023951	4.00623
10	0.001762	49.984250	4.996222	0.847507
Mean	0.001757	50.015130	5.005729	
Standard deviation	4.93×10^{-6}	0.0363	0.0115	

Run 4 showed premature convergence, demonstrated by the high objective function value and dissimilarity of parameters compared to the other nine runs. The results of run 4 were excluded from the calculation of the mean and standard deviation of the parameters.



Fig. 2. Stress-stretch relations for the 2D slab using actual parameters (Vetter and McCulloch, 2000) and those obtained using a genetic algorithm. Lines are known solutions; open circles and triangles show fiber stress and cross-fiber stress, respectively, using optimized parameters. Filled circles and triangles show the percent error in stress (right vertical axis) versus stretch ratio. Panel A: Stress versus stretch for uniaxial stretch in the fiber direction. Panel B: Stress versus stretch for equibiaxial stretch.

stretch plots (Fig. 2) using actual and optimized parameters show excellent agreement, confirming the proposed scheme can identify unknown myocardial constitutive parameters.



Fig. 3. Epicardial strains versus LV pressure for Scenario A using strains from only material point 1. Strains at material point 1 are accurate (panel A), but those at material point 2 show nearly 100% error (panel B). Lines are true strains, circles are fiber strain ($E_{\rm fr}$), triangles are cross-fiber strain ($E_{\rm cc}$), and squares are shear strain ($E_{\rm fc}$).

Table 3 Optimization results for 3D passive inflation scenarios

Parameter	С	b_1	b_2	<i>b</i> ₃	FEA runs	GA generations
Target value	0.0176	50.00	5.0	1.63	_	_
Scenario A (1 point) % Error	0.0140 -20.45	53.80 7.60	7.5 50.00	1.40 -14.11	7668	213
Scenario B (2 point) % Error	0.0171 -2.84	51.20 2.40	5.1 2.00	1.70 4.29	5400	150

3.2. 3D heart model

In Scenario A, the algorithm converged after 7668 FEA simulations with a RMSE in strain of 0.046. Fig. 3 shows simulated strains were in very good agreement with true strains at material point 1. At material point 2, however, the error in strains was nearly 100%. This and the resulting parameters (Table 3) clearly indicated the existence of a local minimum. In Scenario B, convergence was achieved after 5400 FEA simulations with a RMSE in strain of 0.0198. The additional strain information from the second material point accelerated the convergence rate and significantly improved the solution. Strain versus inflation



Fig. 4. Epicardial strains versus LV pressure for Scenario B, using strains from both material point 1 (panel A) and material point 2 (panel B). Including the second material point in the optimization significantly improved the resulting material parameters and accelerated the convergence of the genetic algorithm (Table 3). Lines are true strains, circles are fiber strain ($E_{\rm fr}$), triangles are cross-fiber strain ($E_{\rm cc}$), and squares are shear strain ($E_{\rm fc}$).

pressure plots (Fig. 4) show that the true strains were accurately reproduced using the optimized parameters, which are within 5% of the target parameters (Table 3).

4. Discussion

A new optimization scheme coupling a genetic algorithm with nonlinear FEA was developed to identify ventricular myocardium constitutive parameters and validated using 2D and 3D simulations. For the 2D case the algorithm converged to target stresses within the specified 2% tolerance (Table 2). The single premature convergence run was readily identifiable from its objective function value and variation in parameters from the converged runs. Although a larger population size would prevent premature convergence at a cost of increased computational time, the small standard deviation from the converged runs show that material parameters can be identified using this approach. Computation required 15–25 h on a desktop computer. Stress versus stretch plots show excellent agreement between the true and optimized values.

This is the first study to optimize myocardial material parameters in a realistic 3D cardiac geometry using a GA coupled with FEA. In the first scenario, the GA optimized material parameters using strains at a single material point; the solution, however, represented a local minimum. Including strains from a second point allowed the GA to identify the global minimum and increased the convergence rate. In both scenarios, strains analyzed by the algorithm were within 2% of the target strains. FEA simulations dominated the computation time, requiring 25-40 days on a desktop computer. The number of FEA simulations can be reduced by narrowing the parameter domain bounds. accelerating convergence of the GA. Smaller domains can be judiciously estimated using material parameters reported in the literature (Okamoto et al., 2000; Omens et al., 1993). Computational time can also be reduced through hybrid schemes that combine a GA with gradient-search techniques (Potty et al., 2000), or multiprocessor implementations to evaluate chromosomes in parallel (van Soest and Casius, 2003).

In our simulations the GA determined material parameters using FEA-simulated strains. This scheme can be applied to experimental measurements where strains are computed from epicardial surface marker or ultrasonic crystal displacements (Emery et al., 1997; Omens et al., 1993). Recently, Lorenzen-Schmidt et al. (2005) measured epicardial strains concurrently on the right ventricular wall and outflow tract of the heart; such data would allow for two-point optimizations like our Scenario B.

This study was limited to determining the feasibility of using a GA to optimize parameters of nonlinear myocardial material laws. Our GA utilized general operators recommended in the literature. Future studies should investigate how alternative genetic operators and hybrid schemes affect the convergence rate and solution accuracy.

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