High-Speed Simulation of the 3D Behavior of Myocardium Using a Neural Network PDE Approach

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Abstract. The full characterization of three-dimensional (3D) mechanical behaviour of myocardium is essential in understanding their function in health and disease. The hierarchical structure of myocardium results in their highly anisotropic mechanical behaviors, with the spatial variations in fiber structure giving rise to heterogeneity. The optimal set of loading paths has been used to estimate the constitutive parameters of myocardium using a novel numerical-experimental approach with full 3D kinematically controlled (triaxial) experiments [1,2]. Due to the natural variations in soft tissue structures, the mechanical behaviors of myocardium can vary dramatically within the same organ. To alleviate the associated computational costs for obtaining responses of myocardium under a range of loading conditions with a given realization of structure, we developed a neural network-based method integrated with finite elements. The boundary conditions were parameterized. The neural network generated a corresponding trial solution of the underling hyperelasticity problem for each boundary condition. Thus, the neural network approximated the parameter-to-state map. A physics-informed approach was used to train the neural network. Due to their learnability characteristics, the neural network was able to predict solutions for a range of boundary conditions with given individual specimen fiber structures. The neural network was validated with finite element solutions. This method will provide efficient and robust computational models for clinical evaluation to improve patient outcomes.

Keywords: Cardiac simulation · Myocardium · Machine learning

1 Introduction

The full characterization of three-dimensional (3D) mechanical behavior soft tissues, such as myocardium, is essential in simulating organ function in health and

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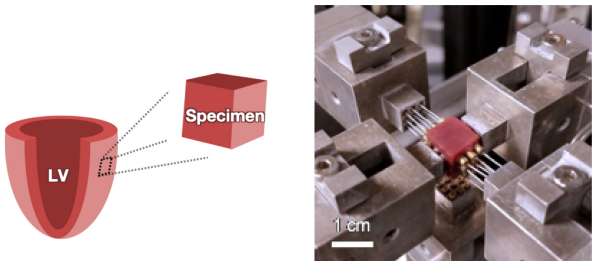
disease. The hierarchical structure of soft tissues dictates their highly anisotropic mechanical behaviors, with the spatial variations in fiber structure also giving rise to heterogeneity. To address these issues in a full 3D context, we have developed a novel numerical-experimental approach to determine the optimal model form and parameter estimation for continuum constitutive models of soft tissues, as applied to the myocardium [1, 2]. This approach utilized optimal experimental design of the full 3D kinematic (triaxial) experiments coupled to an inverse model that incorporated local fibrous structure to perform robust parameter estimation (Fig. 1). Due to the natural variations in soft tissue structures (Fig. 2), the mechanical behaviors of soft tissues can vary dramatically within the same organ. The set of optimal loading paths for a tissue specimen (Fig. 2) includes three pure shear and three simple shear loading conditions.



(a) (b)

Fig. 1. Tissue specimen of left ventricular myocardium for triaxial mechanical testing [2]

It becomes prohibitive to obtain the responses of heart-specific models under varying parameters, including boundary conditions and fibrous structures, in translational clinical time frames. To shift the computational cost ahead of prediction time, neural network (NN) representations of the parameter-to-state map have been proposed as surrogates for parametric partial differential equations (PDEs) due to the representation power of neural networks. Data-driven approaches that require training datasets of finite element (FE) solutions were developed to train the neural network surrogate models. For example, derivative-informed projected neural networks were developed to improve generalization accuracy [3], and machine learning methods were used to enhance reduced order models [5]. To avoid generating training dataset by solving numerous linear or nonlinear FE equations, physics-informed approaches have been developed. The densely connected neural networks were utilized to approximate the solutions of the governing equations trained by minimizing the L_2 norm of the residuals and penalizing the violation of boundary conditions [4]. The convolutional neural networks with a finite difference method estimating spatial gradients [6] is limited to regular domains.

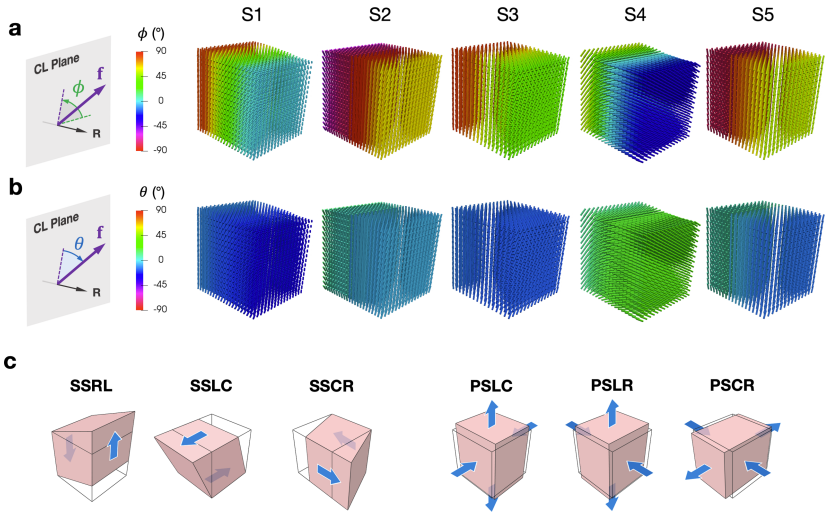


Fig. 2. Spatially varying fiber orientations on the cuboid domain for 4 different specimens, including (a) circumferential angle, and (b) out of plane angle. (c) Optimal loading paths for material parameter estimation including simple shear (SS) and pure shear paths in longitudinal (L), circumferential (C), and radial (R) directions. [2]

In-silico implementation of such complex 3D continuum soft tissue constitutive models to obtain the responses of varying boundary conditions and fibrous structures requires the solution of the associated hyperelasticity problem, which remains impractical in translational clinical time frames. To alleviate the associated substantial computational costs at the time of simulation, we have developed a neural network-based method that can simulate the 3D mechanical behavior of soft tissues. A physics-informed approach was employed to train the neural network (NN) surrogate model to give physically correct solution for a range of loading conditions by minimizing the potential energy without any training dataset generated by finite element (FE) solver. The FE discretization of the solution field is applicable to problems defined with complex geometry and boundary conditions such as ventricular simulations and it enables strong enforcement of the Dirichlet boundary conditions in a natural manner.

2 Methods

We aim to develop an efficient neural network representation of the solutions of parametric PDEs that describe heart-specific cardiac models. To this end, we streamline the neural network-based surrogates and finite elements in an end-to-end pipeline. The neural network generates the corresponding FE nodal values for a trial solution with a given realization of parameters. We construct the corresponding trial solution using finite element basis functions. The neural

network-based surrogate is trained by minimizing the sum of the energy functional for a set of sampled parameters.

We denote the reference configuration $\mathbf{X}$, the current configuration $\mathbf{x}$, the displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$, the deformation gradient $\mathbf{F} = \nabla \mathbf{u}$, the right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$. The unimodular right Cauchy-Green tensor is defined as $\bar{\mathbf{C}} = J^{-2/3}\mathbf{C}$, where $J = \det \mathbf{F}$. We modeled the myocardium as a hyperelastic nearly incompressible material using a recently developed strain invariant form as the strain energy function Ψ in the full 3D kinematic space [2]. The first isotropic invariant of $\bar{\mathbf{C}}$ is

$$\bar{I}_1 = \mathrm{Tr}(\bar{\mathbf{C}}). \tag{1}$$

Two pseudo-invariants of $\mathbf{C}$ for the squared fiber stretches in each fiber directions are defined using

$$I_{4f} = \mathbf{f}_0 \cdot \mathbf{C} \cdot \mathbf{f}_0,\ I_{4s} = \mathbf{s}_0 \cdot \mathbf{C} \cdot \mathbf{s}_0, \tag{2}$$

where $\mathbf{f}_0$ is the myofiber orientation of myocardium, $\mathbf{s}_0$ is the orthogonal direction within the tangent plane of the laminar sheet, and $\mathbf{n}_0$ is the normal direction to the sheet. Three pseudo-invariants of $\mathbf{C}$ for coupling effects are

$$I_{8fs} = \mathbf{f}_0 \cdot \mathbf{C} \cdot \mathbf{s}_0,\ I_{8fn} = \mathbf{f}_0 \cdot \mathbf{C} \cdot \mathbf{n}_0,\ I_{8sn} = \mathbf{s}_0 \cdot \mathbf{C} \cdot \mathbf{n}_0. \tag{3}$$

The constitutive model for myocardium consists of three exponentially stiffening terms, given by

$$\begin{aligned} \Psi = & \frac{a}{2b}\left(\exp\left(b\left(\bar{I}_1 - 3\right)\right) - 1\right) \\ & + \sum_{i=\mathrm{f,s}} \frac{a_i}{2b_i}\left(\exp\left(b_i\left(I_{4i} - 1\right)^2\right) - 1\right) \\ & + \sum_{i,j=\mathrm{f,s,n}\ i\neq j} \frac{a_{ij}}{2b_{ij}}\left(\exp\left(b_{ij} I_{8ij}^2\right) - 1\right) \\ & + \kappa\left(J - 1 - \ln J\right) \end{aligned} \tag{4}$$

where the first term is for isotropic extracellular matrix (ECM), the second term for fiber families within the sheet, the third term for coupling interactions, and the fourth term for enforcing incompressibility condition weakly.

The variational problem for hyperelasticity of myocardium can be describe solved by a minimization problem. Given the body force $\mathbf{f}$ and the traction $\mathbf{t}$ on the Neumann boundary, find the displacement $\mathbf{u}$ ($\mathbf{u} \in \mathcal{V}_0^h$) that minimize the energy functional (potential) Π. The displacement $\hat{\mathbf{u}}(\mathbf{x})$ is discretized using

$$\hat{\mathbf{u}}(\mathbf{x}) = \mathbf{U}\mathbf{N}(\mathbf{x}) \tag{5}$$

where $\mathbf{U} \in \mathbb{R}^{3\times d_u}$ is the nodal values for the displacement, and $\mathbf{N}$ represents trilinear basis functions for the Q_1 Lagrange element on a hexahedral mesh of d_u nodes. We choose the Q_1 element since it is sufficient for the present study. The present method is not limited to the element we use.

For each instance of varying loading condition parameterized by a d_m-D vector $\mathbf{M}^{(i)} \in \mathbb{R}^{d_m}$, a nonlinear FE equation drived from the stationary conditons for the potential minimization problem needs to be solve to obtain the FE solution $\mathbf{U}^{(i)} \in \mathbb{R}^{d_u}$. To avoid prohibitive computational cost for numerous evaluation the parameter-to-state map $\mathbf{U}(\mathbf{M})$, we use a neural network surrogate model $\hat{\mathbf{U}} = f_{\text{NN}}(\mathbf{M}; \theta)$ to approximate the FE solutions for a range of $\mathbf{M}$ where θ parametrize the neural network.

The NN surrogate model $f_{\text{NN}}(\mathbf{M}; \theta)$ is trained by the optimization problem

$$\min_{\theta} \qquad \sum_{i=1}^{N} \Pi(\hat{\mathbf{u}}^{(i)}), \tag{6}$$

where the objective function is the aggregated potential on the sampled loading conditions $\mathbf{M}^{(i)}$. The nodal values for the corresponding trial solution $\hat{u}^{(i)}$ is $\hat{\mathbf{U}}^{(i)} = f_{\text{NN}}(\mathbf{M}^{(i)})$. Then, the Dirichlet boundary condition is enforced strongly. The potential is

$$\Pi(\mathbf{u}) \stackrel{\text{def}}{=} \int_{\Omega} \Psi(\mathbf{u}) \mathrm{d}x - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} \mathrm{d}x - \int_{\Gamma_N} \mathbf{t} \cdot \mathbf{u} \mathrm{d}s. \tag{7}$$

In the case of parameterized Dirichlet boundary conditions, $\mathbf{M}$ is a collection of prescribed nodal values for the fixed displacements. In the case of parameterized Neumann boundary conditions, $\mathbf{M}$ is a collection of prescribed nodal values for the loads.

In this work, we use fully connected network (FCN) which can be described as a sequence of composite functions of nonlinear functions and affine functions. For a FCN with L hidden layers, we have

$$f_{NN} = A_L \circ \phi \circ \cdots A_1 \circ \phi \circ A_0 \tag{8}$$

where A_i $(i = 0, \ldots, L)$ are affine functions, ϕ is a element-wise activation function. Using the FCN as an approximator of the parameter-to-state map, we can substitute the corresponding trial function into the potential.

To demonstrate the learnability of the neural network surrogate model, we considered the triaxial simulations parameterized by its Dirichlet boundary conditions on a cuboid domain (Fig. 3). The marked facets with aligned normal directions on two opposite sides of the cube has a single parameter dictates the magnitude of the fixed boundary condition. The Dirichlet boundary condition is $\mathbf{u} = \mathbf{n}M_i$ for the i-th pair of facets with normal directions $\mathbf{n} = \pm\mathbf{e}_i$ $(i = 1, \ldots, 3)$ where $\mathbf{e}_i$ is the Cartesian basis. Thus, the boundary conditions are parametrized by $\mathbf{M} \in \mathbb{R}^3$. We use low-discrepancy Halton sequence to sample N realizations of $\mathbf{M}$. The material parameters of the myocardium are listed in the Table 1. We trained the neural network for four different specimens to demonstrate the learnability of the neural networks.

Table 1. The material parameters for the myocardium specimens.

	a (Pa)	b	a_f (Pa)	b_f	a_s (Pa)	b_s	a_{fs} (Pa)	b_{fs}	a_{fn} (Pa)	b_{fn}	a_{sn} (Pa)	b_{sn}
S1	4.81	5.05	1175	0.276	1665	6.93	135.5	0.024	3440	2.01	3278	20.4
S2	0.100	0.346	2936	0.045	989.1	0.190	548.6	0.0020	384.0	1.47	6397	0.004
S3	6.07	4.90	2892	0.0300	178.2	0.0500	1553	0.78	4174	40.3	1791	44.6
S4	1.05	12.0	2964	3.10	496.0	0.0870	369.0	0.011	1712	68.8	547.7	1.17

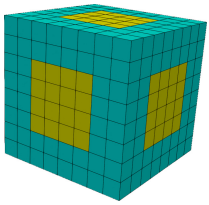


Fig. 3. A cuboid domain with side lengths of 1 cm is discretized using hexahedron elements. Dirichlet boundary conditions are imposed on the yellow facets. (Color figure online)

3 Results

We consider a cuboid domain with side lengths of 1 cm. The domain is discretized by trilinear elements. The number of DOFs is $3 \times 9^3 = 2187$. The 2-th order Gaussian quadrature is used. There are six pads on each facet where we apply the Dirichlet boundary conditions. The training range for sampling all components of $\mathbf{M} = (M_1, M_2, M_3)$ is $[-0.2, 0.2]$ cm. We restrict $\mathbf{M}$ to be unimodular using $(1+M_1)\times(1+M_2)\times(1+M_3) = 1$ to respect the incompressibility condition. The training range is incrementally expanded in 8 steps. The number of $\mathbf{M}$ samples generated using Halton sequence is 400. The NN has 1 hidden layer of 10 neurons with hyperbolic tangent function as the activation function.

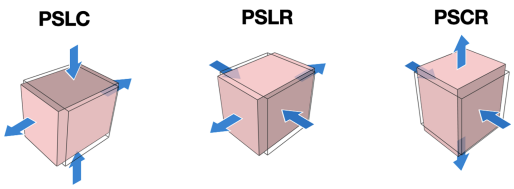
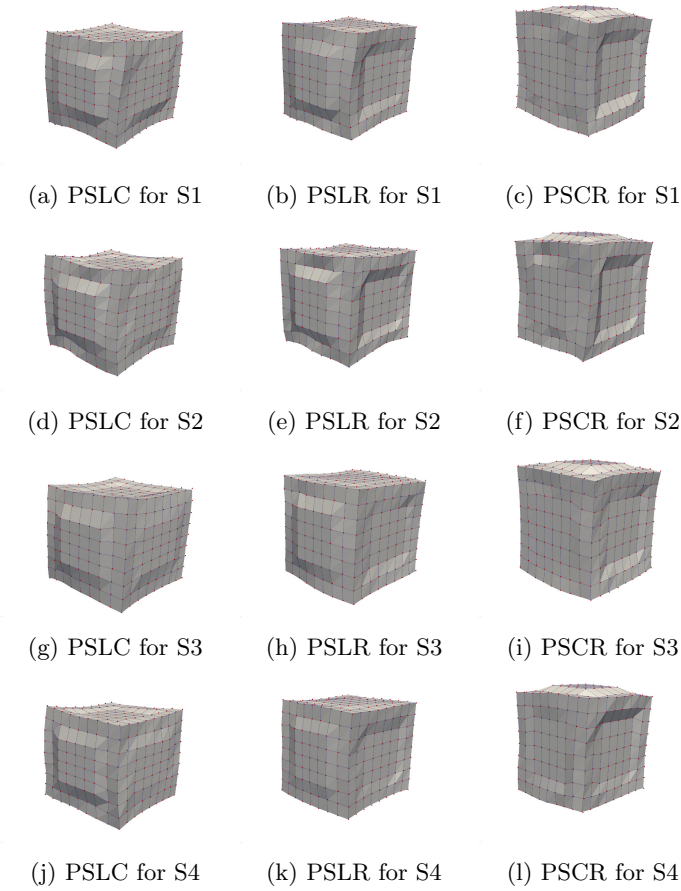


Fig. 4. Protocols for generating validation datasets.



(a) PSLC for S1 (b) PSLR for S1 (c) PSCR for S1

(d) PSLC for S2 (e) PSLR for S2 (f) PSCR for S2

(g) PSLC for S3 (h) PSLR for S3 (i) PSCR for S3

(j) PSLC for S4 (k) PSLR for S4 (l) PSCR for S4

Fig. 5. Validation results for the prediction of the neural network (black wireframe) with the finite element solutions (red points) for pure shear (PS) deformations in longitudinal (L), circumferential (C), radial (R) directions for specimen S1–S4. (Color figure online)

To demonstrate the performance of the neural networks, we examine the relative L_2 error, defined as

$$e = \frac{\sum_i ||u_{NN}^{(i)} - u_{FE}^{(i)}||_2}{\sum_i ||u_{FE}^{(i)}||_2}. \tag{9}$$

The validation dataset includes three loading protocols: (1) $M_1 \in [0, 0.2]$ cm, $M_2 \in [-0.167, 0]$ cm, $M_3 = 0$; (2) $M_1 \in [0, 0.2]$ cm, $M_2 = 0$, $M_3 \in [-0.167, 0]$ cm; (3) $M_1 = 0$, $M_2 \in [0, 0.2]$ cm, $M_3 \in [-0.167, 0]$ cm as shown in Fig. 4. Each loading protocol has 10 uniformly spaced steps. The results obtained with present NN matched closely with the finite element solutions (Fig. 5). The relative L_2

errors for four different specimen with different set of material parameters are listed in Table 2. We also examine the average responses (Fig. 6) for the first loading protocol using the first specimen as an example. The neural network predictions and the finite element solutions have a good agreement.

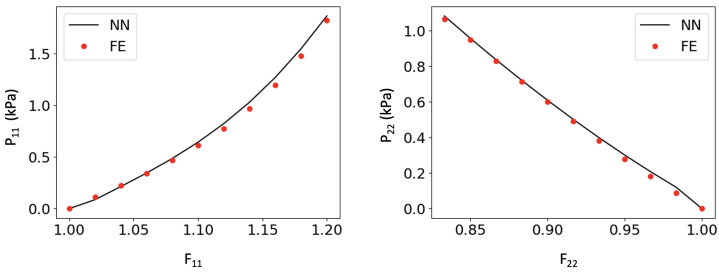


Fig. 6. The average first Piola-Kirchhoff stress on the boundary vs the deformation of the FE solutions and NN predictions.

Table 2. The relative L_2 error of neural network predictions using the corresponding FE solutions as ground truth on the validation datasets.

	S1	S2	S3	S4
e	6.2064%	6.9889%	6.9068%	7.6440%

The computation time for one prediction of the neural network surrogate model was 0.02236 s, while the FE solver takes 6.5762 s for assembly and solution for one step using a serial program, which is a speed-up of 294.1. The predictions of the neural network surrogate model and the FE solution were generated on using a Intel(R) Core(TM) i9-9920X on a System 76 Thelio Major computer. The average time needed to train the neural network surrogate model is 19 min 42.25 s on a NVIDIA(R) GeForce RTX 2080 Ti. The neural network surrogate model can give predictions in parallel while the FE solver needs a stepping scheme to incrementally obtain the solution for the fully loaded state which would multiply the cost with the number of steps. The number of steps is 10 in the present case.

4 Discussion

In this work, we have developed a high fidelity neural network surrogate model that is trained in a physics-informed approach to give a direct solution of 3D soft tissue hyperelasticity in-silico. The present method was found to be an order of 10^2 time faster than the equivalent FE model using the same mesh on the same machine. With the learnability of the neural networks, the architecture of the NNs can incorporate attributes such as spatially varying fiber structures.

By shifting the computation expense from FE solutions to NN training, the NN surrogate model can be used to give significantly fast atiredictions of complex 3D deformations in full kinematic space with given fiber structures by forward propagation in the neural network. More detailed studies on the error analysis of the NN surrogate model are reserved for the future. The future strategies for improving the accuracy of the NN surrogate models include efficient sampling method, scalable training algorithms, and advanced neural networks with improved representation power. One natural extension is to apply the present method to a ventricular model which has more complex geometry and boundary conditions. This method will pave the way for building an efficient template model of hearts with add-on heart-specific attributes, with neural network-based surrogates for fast predictions to evaluate the need to conduct high-fidelity simulations. The ultimate goal is to provide efficient and robust computational models for clinical evaluation to improve patient outcomes.

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