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**Mechanics and Material Properties of the Heart
using an Anatomically Accurate
Mathematical Model**

by Martyn Nash

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and Associate Professor Bruce Smaill**

**A thesis submitted in partial fulfilment of the requirements for the degree of
Doctor of Philosophy at the University of Auckland**



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Abstract

Global and regional mechanics of the cardiac ventricles were investigated using an anatomically accurate computational model formulated from concise mathematical descriptions of the left and right ventricular wall geometries and the non-homogeneous laminar microstructure of cardiac muscle. The finite element method for finite deformation elasticity was developed for the analysis and included specialised coordinate systems, interpolation schemes and parallel processing techniques for greater computational efficiency.

The ventricular mechanics model incorporated the fully orthotropic pole-zero constitutive law, based on the three-dimensional architecture of myocardium, to account for the nonlinear material response of resting cardiac muscle, relative to the three anatomically relevant axes. A fibre distribution model was introduced to reconcile some of the pole-zero constitutive parameters with direct mechanical properties of the tissue (such as the limiting strains estimated from detailed physiological observations of the collagen helices that surround myofibres), whilst other parameters were estimated from *in-vitro* biaxial tension tests on thin sections of myocardium. A non-invasive approach to *in-vivo* myocardial material parameter estimation was also developed, based on a magnetic resonance imaging technique to effectively tag ventricular wall tissue.

The spatially non-homogeneous distribution of myocardial residual strain was accounted for in the ventricular mechanics model using a specialised growth tensor. A simple model of fluid shift was formulated to account for the changes in local tissue volume due to movement of intramyocardial blood. Contractile properties of ventricular myofibres were approximated using a quasi-static relationship between the fibre extension ratio, intracellular calcium concentration and active fibre stress, and the framework has been developed to include a more realistic model of active myocardial mechanics, which could be coupled to a realistic description of the time-varying spread of electrical excitation throughout the ventricular walls. Simple volumetric cavity models were incorporated to investigate the effects of arterial impedance on systolic wall mechanics.

Ventricular mechanics model predictions of the cavity pressure versus volume relationships, longitudinal dimension changes, torsional wall deformations and regional distributions of myocardial strain during the diastolic filling, isovolumic contraction and ejection phases of the cardiac cycle showed good overall agreement with reported observations derived from experimental studies of isolated and *in-vivo* canine hearts. Predictions of the spatial distributions of mechanical stress at end-diastole and end-systole are illustrated.

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Glossary of Symbols

$\{Y_j\}$	global rectangular cartesian coordinate system
$\{\mathbf{i}_j\}, \{\mathbf{e}_j\}, \{\mathbf{g}_j^{(x)}\}$	base vectors for the rectangular cartesian coordinate system
B_0, B	undeformed and deformed configurations, respectively
$\mathbf{x}, \{x_i\}$	rectangular cartesian coordinates of a point in B
$\mathbf{X}, \{X_M\}$	material coordinates of the point \mathbf{x} in B_0
$\mathbf{F}, \{F_M^i\}$	deformation gradient tensor
$\mathbf{R}, \{R_L^i\}$	orthogonal rotation tensor
$\mathbf{U}, \{U_M^L\}$	right stretch tensor
$\mathbf{C}, \{C_{MN}\}$	right Cauchy-Green or Green deformation tensor
$\{\lambda_i\}$	principal extension ratios (eigenvalues of \mathbf{U})
I_1, I_2, I_3	principal invariants of \mathbf{C}
$\mathbf{E}, \{E_{MN}\}$	Lagrangian or Green strain tensor
$E_{(MN)}$	physical Green strain components
$\Sigma, \{\sigma^{ij}\}$	Cauchy stress tensor
$\sigma^{(ij)}$	physical Cauchy stress components
$\mathbf{S}, \{s^{Mj}\}$	first Piola-Kirchhoff stress tensor
$\mathbf{T}, \{T^{MN}\}$	second Piola-Kirchhoff stress tensor
J	Jacobian for coordinate transformations
ρ, ρ_0	material densities for deformed and undeformed configurations, respectively
$\mathbf{t}, \{t^i\}$	internal stress or traction vector
$\mathbf{b}, \{b^i\}$	external body force vector
$\mathbf{v}, \{v^i\}$	velocity vector
$\mathbf{f}, \{f^i\}$	acceleration vector
$\hat{\mathbf{n}}, \{\hat{n}_i\}$	unit normal vector to a given surface
$\delta\mathbf{v}, \{\delta v_i\}$	virtual displacement vector
$\mathbf{s}, \{s^i\}$	external stress vector

W, \bar{W}	strain energy function
$\delta^{MN}, \delta_N^M, \delta_{MN}$	Kronecker delta (1 for $M = N$; 0 otherwise)
p	hydrostatic pressure (scalar) field
c_1, c_2	Mooney-Rivlin constitutive parameters
$P_{(appl)}$	applied surface pressure (physical stress)
r	position vector of a point $p(\mathbf{x})$ in B
R	position vector the same material point $P(\mathbf{X})$ in B_0
u	displacement vector ($\mathbf{u} = \mathbf{r} - \mathbf{R}$)
$\{\theta^k\}$	spatial curvilinear reference coordinates
$\{\mathbf{g}_i^{(\theta)}\}, \{\mathbf{g}^j_{(\theta)}\}$	covariant and contravariant base vectors for the θ_k -reference coordinate system
$\{g_{ij}^{(\theta)}\}, \{g^{ij}_{(\theta)}\}$	covariant and contravariant metric tensors for the θ_k -reference coordinate system
$\{v_\alpha\}$	microstructural material coordinates with respect to anatomically relevant axes
$\{\mathbf{A}_\alpha^{(v)}\}, \{\mathbf{A}^\alpha_{(v)}\}$	covariant and contravariant base vectors for undeformed v_α -material coordinates
$\{\mathbf{a}_\alpha^{(v)}\}, \{\mathbf{a}^\alpha_{(v)}\}$	covariant and contravariant base vectors for deformed v_α -material coordinates
$\{A_{\alpha\beta}^{(v)}\}, \{A^{\alpha\beta}_{(v)}\}$	covariant and contravariant metric tensors for undeformed v_α -material coordinates
$\{a_{\alpha\beta}^{(v)}\}, \{a^{\alpha\beta}_{(v)}\}$	covariant and contravariant metric tensors for deformed v_α -material coordinates
$u _\alpha$	covariant derivative of u with respect to the v_α -material coordinate
$\Gamma^i_{j\alpha}$	Christoffel symbol of the second kind
$\{\xi_M\}$	finite element material coordinates $0 \leq \xi_M \leq 1$
$\{\mathbf{G}_M^{(\xi)}\}, \{\mathbf{G}^M_{(\xi)}\}$	covariant and contravariant base vectors for undeformed ξ_M -material coordinates
$\{\mathbf{g}_M^{(\xi)}\}, \{\mathbf{g}^M_{(\xi)}\}$	covariant and contravariant base vectors for deformed ξ_M -material coordinates
$\{G_{MN}^{(\xi)}\}, \{G^{MN}_{(\xi)}\}$	covariant and contravariant metric tensors for undeformed ξ_M -material coordinates
$\{g_{MN}^{(\xi)}\}, \{g^{MN}_{(\xi)}\}$	covariant and contravariant metric tensors for deformed ξ_M -material coordinates
Ψ_i	Lagrange basis function
Ψ_n^i	Hermite basis function

$\left(\frac{ds_i}{d\xi_i}\right)_n$	scale factor between the arc-length, s_i , and the finite element coordinate, ξ_i , at element node n (no sum on i)
$(R, \Theta, Z), (r, \theta, z)$	cylindrical polar coordinates of a material point in B_0 and B , respectively
$\mathbf{g}_r, \mathbf{g}_\theta, \mathbf{g}_z$	base vectors for the cylindrical polar coordinate system
$(\Lambda, M, \Theta), (\lambda, \mu, \theta)$	prolate spheroidal coordinates of a material point in B_0 and B , respectively
d	focus for the prolate spheroidal coordinate system
$\mathbf{g}_\lambda, \mathbf{g}_\mu, \mathbf{g}_\theta$	base vectors for the prolate spheroidal coordinate system
$\xi^{(i)}, w_i$	Gaussian quadrature points and weights, respectively
δv_i^n	virtual nodal displacements
Ψ_n^p	hydrostatic pressure interpolation functions
p_n^e	element parameters for the hydrostatic pressure field
$\mathbf{J}(\mathbf{x})$	Jacobian of derivatives of residuals with respect to the solution variables
α, β, γ	fibre, imbrication and sheet angles, respectively
$(\mathbf{a}, \mathbf{b}, \mathbf{c})$	orthonormal vectors aligned with the undeformed microstructural material coordinate axes
$(\mathbf{f}, \mathbf{g}, \mathbf{h})$	orthonormal base vectors for the wall coordinate system
a_{11}, a_{22}, a_{33}	limiting strains or poles for axial modes of deformation
a_{12}, a_{13}, a_{23}	limiting strains or poles for shear modes of deformation
$k_{\alpha\beta}$	linear weighting coefficients for terms of the pole-zero strain energy function
$b_{\alpha\beta}$	curvature parameters for terms of the pole-zero strain energy function
$\mathbf{F}_g, \{F_{gNM}\}$	growth tensor used to define the residually stressed state
$\lambda_f^0, \lambda_s^0, \lambda_n^0$	initial extension ratios for the fibre, sheet and sheet-normal axes, respectively
T	active tension developed by myocardial fibres
$[\text{Ca}^{2+}]_i$	intracellular calcium concentration
$[\text{Ca}^{2+}]_o$	extracellular calcium concentration
T_0	actively developed isometric tension
T_{ref}	isometric tension at resting length and saturating $[\text{Ca}^{2+}]_i$
β	slope of the λ - T_0 relation, normalised by the resting isometric tension ($T_0 _{\lambda=1}$)
c_{50}	$[\text{Ca}^{2+}]_i$ at which T_0 is 50% of its maximum
h	Hill coefficient for the sigmoidal dose-response relation
$[\text{Ca}^{2+}]_{\text{max}}$	$[\text{Ca}^{2+}]_i$ at which activation is maximal
Ca_{actn}	activation parameter to determine $[\text{Ca}^{2+}]_i$
E_{ff}, E_{ss}, E_{nn}	fibre, sheet and sheet-normal axial Green strains, respectively

E_{fs}, E_{fn}, E_{sn}	fibre/sheet, fibre/sheet-normal and sheet/sheet-normal shear Green strains, respectively
k	impedance parameter for ventricular cavity models
$\sigma_{ff}, \sigma_{ss}, \sigma_{nn}$	fibre, sheet and sheet-normal axial Cauchy stresses, respectively
V_0	unloaded ventricular cavity volume
ΔA -B length	change in the apex-to-base dimension
γ	ventricular torsion parameter
α_{mv}	angle of ventricular rotation about the long axis at the mitral valve level
α_{lp}	angle of ventricular rotation about the long axis at the low papillary muscle level
h	distance between mitral valve and low papillary muscle levels
E_1, E_2, E_3	principal values (eigenvalues) of Green's strain tensor
ϕ_1, ϕ_2, ϕ_3	Euler (principal) angles for the axes of principal strain
$(\mathbf{w}_c, \mathbf{w}_l, \mathbf{w}_r)$	base vectors for the local cardiac coordinate system
E_{cc}, E_{ll}, E_{rr}	circumferential, longitudinal and radial axial Green strains, respectively
E_{cl}, E_{cr}, E_{lr}	in-wall-plane and the two transverse shear Green strains with respect to cardiac coordinates, respectively
ε_z	base-to-apex natural strain
ε_v	natural volume strain
$\Delta\Theta$	ventricular circumferential rotation about the long axis relative to the end-diastolic state
P_p	coronary perfusion pressure
$\Delta V_{\text{fluid}}, \Delta V_{\text{solid}}$	normalised changes in the local volumes of intramyocardial fluid and solid matrix, respectively
\mathbf{v}_f	intramyocardial fluid velocity
\dot{V}_{fluid}	normalised intramyocardial fluid volume flux
Δt	time step for fluid shift model
k	permeability of the solid matrix
V_s, v_s	undeformed and deformed solid volumes, respectively

Glossary of Acronyms

CIRC	circumflex artery
ECG	electrocardiogram
EF	ejection fraction
FE	finite element
FEM	finite element method
GMRES	generalised minimum residual
LA	left atrium
LAD	left anterior descending artery
LCA	left coronary artery
LV	left ventricle
LVEDP	left ventricular end-diastolic pressure
LVEDV	left ventricular end-diastolic volume
LVP	left ventricular pressure
MRI	magnetic resonance imaging
PDA	posterior descending artery
RA	right atrium
RCA	right coronary artery
RV	right ventricle
RVEDP	right ventricular end-diastolic pressure
RVEDV	right ventricular end-diastolic volume
RVP	right ventricular pressure
SD	standard deviation
SEM	standard error of the mean
SG	Silicon Graphics
SL	sarcomere length
SPAMM	spatial modulation of magnetisation

Notation

- This thesis uses the Einstein summation convention, where repeated indices implies summation over the individual components. For example a vector dot product, in N dimensions, may be written:

$$a_i b_i = \mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^N a_i b_i$$

If an index is in parenthesis then summation is not implied. For example:

$$a_i b_{(i)} = \begin{cases} a_1 b_1 & \text{if } i = 1 \\ a_2 b_2 & \text{if } i = 2 \end{cases}$$

- Mathematical variables represented by bold lowercase letters generally refer to vector quantities, while bold uppercase letters refer to tensor quantities, except where noted.
- In general, this thesis uses lowercase indices when dealing with coordinates in the deformed state and uppercase for coordinates in the undeformed reference state. Moreover, Roman letters generally refer to spatial coordinates, while Greek characters refer to material coordinates.