Physio-mechanical simulation of human's left ventricle using finite element method

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**PHYSIO-MECHANICAL SIMULATION OF HUMAN'S LEFT
VENTRICLE USING FINITE ELEMENT METHOD**

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SCHOOL OF CIVIL AND ENVIRONMENTAL ENGINEERING

2008

Physio-Mechanical Simulation of Human's Left Ventricle Using Finite Element Method

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School of Civil and Environmental Engineering

A thesis submitted to the Nanyang Technological University
in fulfilment of the requirement for the degree of
Doctor of Philosophy

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Summary

Heart diseases are the leading causes of death worldwide and most of these diseases happen in left ventricle (LV). So the study on LV's electro-mechanism is very helpful to doctors to make an appropriate diagnosis. The modeling LV muscle is crucially important as cardiac muscle is the main component of ventricle wall. In this thesis, based on physiological observation, LV muscle is assumed to be composed of two different materials: myocardium masses (MM) and myocardium fibers (MF). An isotropic Mooney-Rivlin material property is implanted into MM, and a Hill's fiber force model is developed for representing MF which relates the microscopic molecular electricity events to macroscopic LV muscle performance. This assumption simply but effectively implants real complex fiber structure into the LV model. The fluid-structure interaction between MM and cavity blood (CB) has been considered using penalty method. The mathematical model has been discretised into numerical model using finite element method (FEM). MM and MF are meshed by finite element, while CB is meshed by an Arbitrary Lagrangian Eulerian (ALE) finite element. Automatic mesh updating has been taken for large domain changes. The available FEM package LS-DYNA is used as the solver. The FEM results show good agreements with clinic report and other references. The model can be a powerful tool to diagnose cardiac abnormalities in future studies.

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List of Symbols

a, b, α, β	constants in Hill's fiber force model
A, B	Mooney-Rivlin constitutive parameters
$\mathbf{b}, \{b^i\}$	external body force vector
B_0, B	undeformed and deformed configurations, respectively
$\mathbf{C}, \{C_{MN}\}$	right Cauchy-Green tensor
C_2	intercept of the u_s - u_p curve in equation of state
E	internal energy per initial volume in CB
$\mathbf{E}, E_{MN}$	physical Green strain components
E_p	elastic constants of the parallel element
$\mathbf{f}, \{f^i\}$	acceleration vector
$\mathbf{F}, \{F_M^i\}$	deformation gradient tensor
$\{i_j\}, \{e_j\}, \{g_j^{(x)}\}$	base vectors for the rectangular Cartesian coordinate system
I_1, I_2, I_3	principal invariants of $\mathbf{C}$
I_{Na}	calcium current
J	Jacobian for coordinate transformations
L_{p0}, L_{s0}, L_{m0}	total initial length, initial lengths of contractile and series elements in Hill's fiber force model
$\hat{n}, \{\hat{n}_i\}$	unit normal vector to a given surface
p	hydrostatic pressure
$P_{(appl)}$	applied surface pressure
$\mathbf{r}$	position vector of a point $p(\mathbf{x})$ in B
$\mathbf{R}$	position vector of a point $P(\mathbf{X})$ in B_0
$\mathbf{R}, \{R_L^i\}$	orthogonal rotation tensor
$\mathbf{s}, \{s^i\}$	external stress vector

List of Symbols

$\mathbf{S}, \{s^{Mj}\}$	first Piola-Kirchhoff stress tensor
S_1, S_2, S_3	coefficients of the slope of u_s - u_p curve
$\mathbf{t}, \{t^i\}$	internal stress or traction vector
$\mathbf{T}, \{T^{MN}\}$	second Piola-Kirchhoff stress tensor
T_0	maximum force developed in muscle under isometric condition
T_m, T_s	forces in contractile and series elements in Hill's fiber force model
T_{tot}	total force in Hill's fiber force model
$\mathbf{u}$	displacement vector
$\mathbf{U}, \{U_M^L\}$	right stretch tensor
U_p^0, U_m^0, U_s^0	elongations of the parallel, contractile and series elastic elements
v	velocity of the muscle contraction
$\mathbf{v}, \{v^i\}$	velocity vector
$W, \bar{W}$	strain energy function
$\mathbf{x}\{x_i\}$	rectangular Cartesian coordinates of a point in B
$\mathbf{X}\{X_M\}$	material coordinates of the point $\mathbf{x}$ in B_0
$\{Y_j\}$	global rectangular Cartesian coordinate system
$\alpha_a(t)$	activation factor
γ_0	Gruneisen gamma in equation of state
$\delta v, \{\delta v_i\}$	virtual displacement vector
$\delta^{MN}, \delta_N^M, \delta_{MM}$	Kronecker delta
$\{\lambda_i\}$	principal extension ratios (eigenvalues of $\mathbf{U}$)
$\lambda_p, \lambda_m, \lambda_s$	stretches of the parallel, contractile and series elastic

List of Symbols

	elements
$\dot{\lambda}_{m0}$	strain rate
μ	volume compression in CB
ν_{mm}	Poisson's ratio for MM
$\{\xi_M\}$	finite element material coordinates
ρ, ρ_0	material densities for deformed and undeformed configurations, respectively
ρ_{mf}	density of fibers
$\sigma^{(ij)}$	physical Cauchy stress components
$\sum, \{\sigma^{ij}\}$	Cauchy stress tensor
ϕ	fraction of the muscle in the total volume
Ψ_i	Lagrange basis function

List of Acronyms

3D	three dimension
ALE	Arbitrary Lagrangian Eulerian
AP	atria pressure
AV	atrioventricular
CB	cavity blood
CPU	central processing unit
CT	tomography
DN	DiFrancesco-Noble
DTI	diffusion tensor imaging
ENO	essentially non-oscillatory
FE	finite element
FEM	finite element method
FSI	fluid-structure interaction
LAP	left atria pressure
LR	Luo-Rudy
LV	left ventricle
LVP	left ventricle pressure
MF	myocardium fibers
MM	myocardium masses
MRI	magnetic resonance imaging
MRT	magnetic resonance tomography
MUSCL	monotone upwind schemes for conservation laws
PC	personal computer
SAN	sinoatrial node
SPAMM	spatial modulation of magnetization
SUPG	streamline upwind Petrov-Galerkin

List of Acronyms

US ultrasonography

Chapter 1 Introduction

■ 1.1 Objective of the thesis

The primary objective of this study is to develop a new physio-mechanical model to describe total left ventricle⁽¹⁾ (LV) functions. How to create a mathematical model from physical model and how to discretise the mathematical model to finite element model (FEM) model are the focuses of the study. An investigation on anatomy and physiology of LV has been conducted to understand the basic biological processes of heart motion. Various approaches can be found in the literature reviews for heart mechanical modeling. Anisotropy, nonlinearity, electricity and fluid-structure interaction are the main issues to be addressed when modeling muscular tissue, and few models can be found that meet all these requirements. In this approach, based on physiological observation, LV muscle is assumed to be composed of two different materials: myocardium⁽²⁾ masses (MM) and myocardium fibers (MF). An isotropic Mooney-Rivlin material property is implanted into the MM, and a Hill's fiber force model is developed for representing the MF which relates the microscopic molecular electricity events to macroscopic LV muscle performance. The fluid-structure interaction between MM and cavity blood (CB) has been considered by using the penalty method. The mathematical model has been discretised into numerical model by using FEM.

■ 1.2 Layout of the thesis

In Chapter Two, reviews of heart physiology and different heart ventricle models are presented. It clearly shows the progresses researchers have made in these fields: ventricle geometry, material properties including passive one (passive material response and material parameters) and active one (from cell model to tissue and muscle model), residual stresses and fluid-structure interaction.

Chapter Three contains a new mathematical model of LV. In this chapter, the physical model of LV has been idealized to a mathematical model based on certain assumptions that together lead to differential equations governing the mathematical

model. The mathematical model of LV mainly includes five types of different materials: MM, MF, CB, valve and vessel. The equations that govern the motion of these materials can be derived in the following four steps: kinematic relations, stress equilibrium, constitutive relations and boundary conditions.

Chapter Four presents a finite element model which solves the governing equations of the mathematical model created in Chapter Three. MM, CB, valve and vessel are meshed by 3D elements while MF is meshed by line elements. Arbitrary Lagrangian-Eulerian (ALE) approach for CB and penalty method adopted for simulating CB-MM interaction are presented. All material parameters, boundary and initial conditions are defined in the FEM model according to Chapter 3. Finally, the available FEM package LS-DYNA is used as the solver.

Chapter Five describes the results and discussions. The volume and pressure curves, ejection fraction, the variations in LV wall thickness obtained from the simulation results are compared with clinical reports or other references. The results on movement of CB, deformation of MM, principal stresses and strains of MM, velocities and displacement of LV wall and twisting of MF are also presented.

Chapter Six presents the general conclusions and the finding of this study. Future works on simulating the LV and even the whole heart are also recommended here.

Note:

- (1) The **left ventricle** is one of four chambers (two atria and two ventricles) in the human heart. It receives oxygenated blood from the left atrium via the mitral valve, and pumps it into the aorta via the aortic valve.
- (2) **Myocardium** is the muscular tissue of the heart.

Chapter 2 Literature Reviews

Heart diseases (myocardial infarction⁽¹⁾, stenosis⁽²⁾, arrhythmias⁽³⁾, fibrillation⁽⁴⁾, heart block, valve leak et al) are leading causes of death worldwide. In order to gain insight into the mechanisms behind heart diseases and to determine their causes, the knowledge of the structure and electromechanical behavior of heart is important.

In recent years, advances in the biological sciences have increasingly relied on modeling and numerical simulation. Development of modern computers has paralleled the need for quantitative understanding of complex heart problems, and itself has enriched the understanding of heart phenomena. Modeling and numerical simulation have provided an essential step and a powerful tool in understanding the mechanism behind the heart behaviors. The study of ventricle mechanics has received much attention as a research topic. Hunter et al (2003) presents a very good review on modeling total heart function.

■ 2.1 Ventricular geometry

In the early age of studying ventricle mechanics, the analytical approach was usually adopted due to the absence of computers. Ventricle wall stresses were calculated based on the force balance relations of continuum mechanics between the loading conditions and generated stresses. To keep the problem mathematically tractable, simplified geometric shapes were usually assumed.

One of the earliest models is proposed by Woods (1892) who treated the LV as a simple thin walled sphere with uniform internal pressure. The result shows that the myocardial tension is proportional to the product of pressure and radius. Sandler and Dodge (1963) used a similar technique to model the LV as an axisymmetric

ellipsoid. They concluded that the ventricle wall stresses can be expressed in terms of wall thickness, the principal radii and the cavity pressure. Later on, Falsetti et al (1970) and Walker et al (1971) calculated ventricular wall stresses by using the similar thin walled models. In most of these models, Laplace's law is employed to characterize these balance relations, which states that the tension in a thin membrane structure is proportional to the pressure at the location but inversely proportional to the curvature radius at the location. The estimation of wall stresses from these models can be obtained by means of simple measurements of ventricular pressure and geometry. The biggest limitation to these models is that the thickness of the wall is assumed to be much less than the radii of curvature, and the material properties of the ventricle muscle have been ignored.

One of the first thick walled models was developed by Wong and Rautaharju (1968) who model LV by using an ellipsoidal geometry shape. Their result shows that transmural variations in myocardial stress are determined by ellipsoidal shells of compressible, isotropic, linearly elastic and homogeneous tissue. However, they used small-strain elasticity theory into the model which is not appropriate for the large deformation in LV.

Five years later, Mirsky (1973) used large deformation elasticity theory into his model, and the result shows that the nonlinear terms in the strain-displacement relationship produced a very high stress concentration at the endocardium of almost ten times that predicted by the linear model. This clearly indicates that small-strain elasticity is invalid.

Besides thick walled ellipsoids models (Wong and Rautaharju, 1968; Mirsky, 1969; Ghista and Sandler, 1969; Beyar and Sideman, 1986), researchers have also developed other shapes of LV geometry, such as thick walled cylinders (Arts et al,

1979; Chadwick, 1982; Ohayon and Chadwick, 1988a, b; Arts and Reneman, 1989; Guccione et al, 1991), thick walled spheres (Mirsky, 1973; Demiray, 1976b; Abe and Nakamura, 1982), non-circular cylinders (Janz et al, 1989), hollow conical shell with a constant shear modulus (Azhari, 1992) and even a kinematic model (Arts, 1992; Arts, 1993) combining the modes from spherical, prolate ellipsoidal and cylindrical models.

However, the shape of an LV is neither spherical nor cylindrical. Even a prolate ellipsoid is a gross simplification of the shape of an LV. The analyses performed by these models are based on simplifying assumptions about the material behavior of the heart muscle and the governing equations of motion.

When the realistic geometries are added into the model, closed form expressions for ventricular wall deformation and stress are not available any more and an appropriate numerical method is required. With the rapid developments of modern computer and computational methods, Finite Element Method (FEM) has become a promising and effective tool of modeling ventricular mechanics, in order to consider its complicated geometry, anisotropy, nonlinearity and fluid-structure interaction.

One of the first finite element (FE) models of ventricular mechanics was formulated by Gould, Ghista, Brombolich and Mirsky (1972). In their work, a realistic longitudinal cross-section of the LV wall was incorporated into an axisymmetric FE representation. The model was comprised of 13 elements with axisymmetric configuration and uniform thickness. Linear elasticity, isotropy and homogeneity of the material properties were also assumed. The results indicate that a linear stress distribution across the LV wall thickness reverses when one curvature of the wall changes signs, which means that instead of an endocardial to epicardial stress gradient in regions where the ventricle is concave inward, the opposite is obtained

where the wall is concave outward.

Four years later, Heethaar et al (1977) used 7000 tetrahedral elements to study the stress distribution in both a single left ventricle and in a combined right and left ventricle model. This model is more realistic than all previous models, since each chamber is not necessary by axisymmetric, and the effect of the right ventricle is included. The geometry data of the LV were obtained from multiple X-ray views of an isolated working dog heart, which pumps fluid containing radiopaque compound. The data were recorded from a dead heart filled with contrast fluid placed in X-ray field. The model assumed isotropic, homogeneous and linearly elastic material properties as well. The results show higher stresses at the endocardium for the diastolic LV. This model presents a true 3-D shape of the LV configuration.

Zhang .Y. and Bajaj C. (2004) constructed a very detailed tetrahedral heart model (more than 200,000 nodes) with some necessary components, such as aorta, veins, four chambers (left, right atriums and ventricles), heart valves, muscles, etc. The extended Dual Contouring method is used here to build the tetrahedral heart model from volumetric imaging data.

In the current study, a model is built based on a real geometry of LV, whose configuration is extracted from ultrasonic techniques (see Chapter 3) and is meshed by 3D finite elements (see Chapter 4).

■ 2.2 Architecture of myocardium and material properties

The appropriate constitutive law for soft tissue is crucial for building any successful ventricle models. The mechanical behavior of cardiac tissue can be modeled using a variety of material response functions which were based on detailed physiological observations of cardiac tissue. Usually, the material response in myocardium can be

split into two parts: passive one during diastole phase and active one during systole phase. In this thesis, the passive and active properties of myocardium are treated separately, which will be presented in detail in Chapter 3.

■ 2.2.1 Architecture of myocardium

The ventricular myocardium resides between endo- and epicardium and is the primary structural component of the wall. It consists of muscle bundles organized in overlapping sheets (Fig. 2.1). The sheets are oriented into a spiral when followed from base to apex of the heart. The muscle fibers in the ventricles are oriented and laminated (Streeter and Bassett, 1966). In the myocardium of human LV, the muscle fiber orientation varies from endo- (around 60°) to epicardium (around -60°). The change of angle from endo- to epicardium is nearly linear, with 0° in the mid-myocardium. A similar structure can be found in the canine myocardium (Fig. 2.2). Apart from containing muscle fibers, the ventricular myocardium consists of fibroblasts, nerve cells, connective tissue, etc., which build up the muscular structure. The muscle bundles are composed of myocytes enclosed by a membrane.

Studies (MacCallum 1900; Mall 1911; Robb and Robb 1942; Streeter and Bassett 1966; Streeter et al, 1969) of cardiac tissue have revealed that fiber structure has crucial determinant of its ventricular function.

Figure 2.1 Ventricular wall with sheet and fiber orientation (courtesy of Nash, 1998)

Figure 2.2 Reconstruction of fiber orientation of a canine left ventricle wall (courtesy of Katz, 1992)

The fiber orientation cannot yet be extracted directly from images acquired by medical imaging systems. However the diffusion tensor imaging (DTI)⁽⁵⁾ technique (a special magnetic resonance tomography technique) provides means to examine fibrous structures such as e. g. brain and heart (Zhukov and Barr, 2003; Köhler et al, 2003). DTI is used to acquire the anisotropic diffusion properties of water in a tissue at a spatial position within the probe. The mapping of fiber orientation is based on the presumption that diffusion of water along the cells is larger than transversal to it. The fibers can be reconstructed by examining the sum of the linear and planar tensor anisotropies of the diffusion tensor, followed by tracing the fibers along the principal eigenvector direction (Zhukov and Barr, 2003; Sachse et al, 2001). Zhukov and Barr (2003) extracted the fiber orientation of an extra corporal

canine heart, which rested in a contracted state (Fig. 2.3). Furthermore, manual assignment of fiber orientation of myocytes can be performed using e.g. pointwise definition of restrictions with manual and rule-based methods, interpolation of orientation and lamination by iterative averaging, assignment and validation (Sachse et al, 2004).

Figure 2.3 Reconstructed fiber orientation of a canine heart from MRI data
(courtesy of Zhukov and Barr, 2003)

■ 2.2.2 Passive material properties

■ 2.2.2.1 Passive material response

The myocardial tissue has been proven to be nonlinear, anisotropic and viscoelastic, which is common for most biological tissues. The change in volume due to

deformation is small and therefore an approximate incompressibility can be postulated.

The first attempt to implant anisotropy and non-homogeneity material property into the ventricle model was made by Mirsky (1970) who used a thick-walled prolate spheroid. Although its linear elastic and axisymmetric deformation assumption weakens its conclusion, the results indicate that in homogeneity must be carefully treated.

Another early attempt to incorporate material anisotropy and heterogeneity into the model was made by Janz and Grimm (1972). The myocardium at the base of the ventricle was assumed to be isotropic with properties comparable to those of collagen. The remainder of the ventricle was assumed to be composed of two layers: one that is transversely isotropic with stiffness like muscle, and the other that is isotropic with the muscle properties. The model consisted of 198 elements, and produced a close approximation to the actual state of deformation in arrested rat hearts in diastole. The results were questioned due to the small-strain elasticity theory adopted in the model. Two years later, Janz et al (1974) extended their early model to incorporate large deformation theory and their results showed that the small-strain elasticity was not appropriate.

Hunter (1975) presented the first non-axisymmetric, large-deformation FE model of the LV. His model was based on the transmural distribution of fiber orientations, which was measured by Streeter et al (1969). An empirical one-dimensional constitutive equation was used for active contraction to estimate the generated force by myocardial fibers. The ventricular anatomy was measured by mounting silicone filled canine hearts onto a rig and using a probe to record the radial coordinates of the endocardial and epicardial surfaces at several pre-defined angular and axial

locations.

Two years later, Panda and Natarajan (1977) improved the LV model by taking the LV geometry as a thick-walled layered shell of revolution, and assuming the fiber orientations in the endocardial, middle and epicardial wall of 40° , -5° , -50° from the circumferential direction. They assumed that the material properties along the fiber direction are orthotropic. They found, from the layered model, that the maximum circumferential endocardial and epicardial stresses diminish and midwall stresses increase as the ratio of the longitudinal to transverse stiffness increased; however, the meridional stresses increase in both the endocardial and epicardial layers and diminish in the middle layer with increasing relative stiffness.

In accordance with the early quantitative studies of tissue organization (Streeter and Bassett, 1966; Streeter et al, 1969), the ventricle tissue can be considered as a continuum of myocardial fibers, with a smooth transmural variation of fiber orientations. Based on this theory, many works (Horowitz et al, 1988; Humphrey et al, 1990; Bovendeerd et al, 1992; Huyghe et al, 1992; Guccione et al, 1995) have been performed by incorporating transversely constitutive laws. One of them is the “pole-zero” law, which was introduced by Nash (1998). The parameters in the constitutive laws are derived in part from a model of the underlying distributions of collagen fibers. These distributions are based on the observations of the fibrous sheet laminar architecture of myocardial tissue. The main drawback is that the model is formulated in terms of too many parameters that require lots of processings .

■ 2.2.2.2 Passive material parameters

In a uniaxial passive material properties test, cardiac trabeculae exhibit viscoelastic and high-nonlinear properties. The stiffness is rather low when the sarcomere

lengths are in a range of 1.6-2.1 μm , but becomes much higher when the sarcomere length increase to a range of 2.1-2.3 μm (ter Keurs, 1995 and Hanley et al, 1999). There is a limiting extension for the sacromere lengths (Granzier and Irving, 1995).

The multiaxial relationship between force and length is fundamental for any computational models, especially when this relationship based on in vivo measurements. If in vivo constitutive parameter estimation can be validated, the computational models can have wide applications to medicine, surgery, and bioengineering.

The most common in-vitro experiment for non-contracting material properties is the biaxial test, which has been done on thin sections of cardiac muscle (Lanir, 1979; Demer and Yin, 1983; Humphrey and Yin, 1987; Shacklock, 1987; Yin et al, 1987; Nielsen et al, 1991). Usually, forces are applied at the two ends of cut edges of the sample and the results are used to fit in a pre-defined constitutive equation. The myocardial test specimens exhibit nonlinear, viscoelastic, anisotropic material properties and larger stiffness along the fiber direction. Experiments (Novak et al, 1994) also show that the differences between specimens from LV subepicardial, midwall and subendocardial sites are small. Although these tests have provided useful information for modeling left ventricle, the constitutive relationship must be treated with caution because the sample cutting from the ventricle wall, and the surrounding collagen structures have important effects on its elasticity.

Another problem in the above mentioned testing is that the shear deformations are hard to be obtained from a test, but they are also very important determinants for heart mechanics. In order to overcome this problem, Dokos, Young and Smail (2000) developed a triaxial device which helps to measure the compressive and shear deformations in small tissue volumes. The orthogonal forces also are measured.

They extended their work (Dokos et al, 2002) two years later, and found that the shear properties of passive LV myocardium were related to its laminar structure. Analysis shows that the shear stiffness in the passive myocardium is relatively small.

To overcome problems of tissue damage during myocardial deformation, recent non-invasive methods, such as LV angiography⁽⁶⁾, computed tomography⁽⁷⁾, ultrasonic, echocardiography⁽⁸⁾ and magnetic resonance imaging (MRI)⁽⁹⁾ have been used to track the movements of the muscle. Kong et al (1971) used biplane coronary cinéangiography⁽⁹⁾ and successfully recorded the bifurcations of superficial coronary arteries. Young, Hunter and Smail (1992) extended the method to a non-homogeneous strain analysis and an epicardial surface was included in the FE model. The disadvantage of cinéangiography measurement is that measurement is only performed on the epicardial surface. The MRI tagging technique (Zerhouni et al, 1988; Buchalter et al, 1990; Clark et al, 1991; Rademaker et al, 1994) is known as the spatial modulation of magnetization, which uses a sequence of non-selective radio frequency pulses separated by magnetic field gradients to generate orthogonal planes of magnetic saturation. In using this method, the movements of myocardial material landmarks can be tracked down during the whole heart cycle. Based on this technique, Axel and Dougherty (1989) created a non-homogeneous ventricle strain distribution model at several configurations during the whole heart cycle.

■ 2.2.3 Active material properties

For the contracting myocardium properties, ter Keurs (1995) gave a very good review on this topic. Active stresses generated during the heart cycle are a function of sarcomere length, velocity and also strain history. A thorough understanding of active myocardium material response properties from cardiac cell models to muscle models is necessary.

The components of the conduction system (Fig. 2.4) are explained in this way: the initial electrical stimulus in a normal heart is generated inside the sinoatrial node (SAN)⁽¹⁰⁾, the so called primary pacemaker cells. The cells have the ability to automatically depolarize and generate an action potential, which then propagates along the crista terminalis⁽¹¹⁾, pectinate muscles⁽¹²⁾ and to surrounding right atrial myocytes. Moreover, the Bachmann bundle transmits the activation to the left atria. The electrical stimulus reaches the atrioventricular node, whose slow conductive tissue delays the excitation to the ventricles to account for temporal synchronization of contraction. In a healthy heart, this tissue structure is the only electrical connection between atria and ventricles, due to the insulation of the cardiac skeleton. The pursuing structures are the atrioventricular bundle followed by the Tawara bundle, which splits into three branches. Two of the tree branches conduct the excitation to the left, the third to the right ventricle. They split into a subendocardial network of Purkinje fibers, which connects to myocytes and activates muscle contraction. The ventricles are excited from endo- to epicardium and from apex to base.

The action potential curve for each tissue type following the conduction system within the myocardium varies in length and shape. This is due to the cell structure, i.e. amount of channels, pumps and exchangers. The variation of conduction velocities results in a temporal and spatial excitation pattern, and hence in the most effective spatial and temporal contraction of myocytes for an optimal pumping functionality.

Figure 2.4 Intrinsic conduction system (courtesy of Elaine, 1996)

■ 2.2.3.1 Cell models

Based on the physiology of cells, Hodgkin and Huxley (1952) firstly developed the Hodgkin-Huxley model which describes the sodium, potassium and leakage ion channels in a squid axon and the time-dependent gates controlling the flow of ions across the membrane. From then on, a large number of cell models have been developed.

By adapting the equations of the original Hodgkin-Huxley squid axon model (1952), Noble published one of the first mathematical models of a cardiac cell. In this model, the long lasting action and pace-maker potentials of the Purkinje fibers of the heart are described. The sodium current equations are very similar to the previous model but the potassium-current equations are different from those of Hodgkin and Huxley in that the potassium ions are assumed to flow through two types of channel in the membrane. The main limitation of this model is that it only includes one voltage gated inward current, I_{Na} . Calcium currents were not yet been found, but there was a hint in the model that something is missing. The model can

only work under the condition that the voltage range of the sodium current must greatly be extended. In effect, the sodium current is introduced to serve the function of both the sodium and the calcium channels as far as the plateau is concerned. There is a clear experimental prediction: either sodium channels in the heart are quantitatively different from those in neurons, or other inward current-carrying channels must exist. Later works proved that both predictions are correct.

Following Noble's 1962 model of cardiac action potentials in Purkinje fibres, McAllister, Noble and Tsien (1975) published a paper, which formulated new ionic current equations based on new experimental data. This was a very important contribution to cardiac membrane modeling. Although the description of the kinetics of the currents was still based on the Hodgkin-Huxley model, the currents themselves incorporated some significant new changes: the total ionic current was broken down into nine discrete, individual ionic fluxes.

Compared to the earlier Purkinje fiber ionic current models of Noble (1962) and McAllister, Noble and Tsien (1975), Beeler and Reuter (1977) developed a simpler model to describe the mammalian ventricular action potential. In this model, not all the ionic currents of the Purkinje fiber model were presented in the ventricular tissue. The total ionic flux is divided into only four discrete, individual ionic currents. The Beeler-Reuter ionic current model could explain the intracellular calcium ion concentration.

Eight years later, DiFrancesco and Noble (1985) presented the DiFrancesco-Noble model of Purkinje fiber cell, which reproduced phenomena such as supernormality, shortening in action potential duration during pacing rate increases, alternation of duration with changes in rhythm, graded responses and 'all-or-none' repolarisation in a quantitatively realistic way. Each of these phenomena come from time and

space dependencies, not directly a part of the ionic current measurements on which the DN model is based. Cabo and Barr's (1992) experimental results showed that the DN equations correctly simulate these situations and support the goal of having a model that is broadly applicable to Purkinje tissue, including refractory period properties and response to electrical stimulation.

In 1991, Luo and Rudy updated the Beeler-Reuter mammalian ventricular model (1977) by introducing a new mathematical model of the ventricular cardiac action potential. This original model is the first of the two Luo-Rudy models, and it subsequently become to be known as the Luo-Rudy I model. This Luo-Rudy I model also uses Hodgkin-Huxley type equations to calculate ionic currents.

Three years later, Luo and Rudy (1994) further develop the Luo-Rudy II model by addressing some of the issues which were not studied in the model. In particular, the LR-II model incorporates a more thorough description of the processes which regulate intracellular calcium ion concentration and the movement of calcium ions through the cell to the sarcoplasmic reticulum. Although their mathematical model is based upon experimental data from guinea pig ventricular cells, it provides a framework for modeling other types of ventricular cells with appropriate modifications to account for its heterogeneity.

Noble et al (1998) extended the guinea-pig ventricular cell model (originally developed in 1991 by Noble et al) to further include accumulation and depletion of calcium in a diadic space between the sarcolemma and the sarcoplasmic reticulum, where the majority of calcium-induced calcium release is triggered. The model also includes rapid and slow components of the delayed rectifier current, with incorporating length and tension dependent changes in mechanical and electrophysiological processes. In this model, drug-receptor interactions have also started to be modeled using the sodium channel as an example. The results show

that the drugs used have the effect of blocking the inactivation h-gate of the fast sodium channel.

■ 2.2.3.2 Tissue and muscle models

Early attempts to incorporate cell models into tissue models has been tried by van Capelle and Durrer (1980), who used a model that treats each cell as a discrete unit. Later on, other researchers (Leon and Horacek, 1991; Trayanova, 1996; Rudy, 2000) created models either as a discrete set of cells or tissue bundles or a continuum. Usually, these models only included simple cell models (Rogers and McCulloch, 1994), while more advanced cellular models have been incorporated into the tissue models in recent years (Huiskamp, 1998; Buist and Pullan, 2001).

Hill (1970) firstly introduced a cardiac muscle model which develops active tension in the skeletal muscle. From then on, more cardiac muscle models have been developed based on various approaches. Bergel and Hunter (Bergel and Hunter, 1979) used a function of fading memory to fit the results from muscle response experiments. Allen and Kentish (1985) concluded that the active stresses generated in myocytes are less than in skeletal muscle but their sensitivity is greater. The maximum active force corresponds to a sarcomere length of $2.25\mu\text{m}$, and then decrease to 0 when the sarcomere length of $1.6\mu\text{m}$. There are a number of 1-D force generation models which incorporate different levels of molecular bases (Hunter et al, 1998, Rice and Hunter, 1999).

A new methodology of simulating the active force in systole was developed in 1986 by Perl et al. The active force was modeled as the load applied to the truss element residing in the LV finite element mesh. The active force is chosen so that the predicted numerical LV pressure and volume at each moment of the cardiac cycle match the experimental measurements. The model assumes: 1) really irregular

geometry of the left ventricle whose data are obtained from Ritman's group (Ritman et al, 1980); 2) anisotropy of the wall in which the fibers orient from -60° to $+60^{\circ}$ in endocardial to epicardial surface direction (Streeter, 1979); 3) large deformation that the LV undergoes during the cardiac cycle; 4) material nonlinearity of the myocardium in which the stress-strain relation from a uniaxial myocardial tissue in the passive state is given; and 5) mechanical activation of the heart muscle. In their model, the LV pressure and volume at each moment of the cardiac cycle match the experimental data.

Guccione and McCulloch (1993) proposed an active fiber force model based on a cross-bridge model where the force is determined by calcium transient. This is the so called "deactivation". In 1997, based on FitzHugh-Nagumo membrane kinetics and a monodomain model, Panfilov (1997) simulated a reentrant wave on an anatomically realistic model of a canine heart (Nielsen et al, 1991). One of the latest attempts was made by Nickerson, Smith and Hunter (2005), who are developing a strong coupled fiber length transients model, where the role of electrical heterogeneity in determining left ventricular function.

In this thesis, a Hill's fiber force model is employed for linking the electrical activity to the tissue mechanical performance. It will be presented in Chapter 3.

■ 2.3 Residual stress

In 1990, Omens and Fung (1990) cut an equatorial cross sectional ring (Fig. 2.5) which was from an isolated rat heart, and they observed that an angle opened after an radial cut. This gave a very important implication that the residual stresses must be incorporated into the models. The results from models (Boverdeerd et al, 1992; Demiray, 1976a; Feit, 1979; Huyghe et al, 1992; Mirsky, 1973) which use stress-free status must be treated with care for the lack of residual stresses. These

models (Demiray, 1976a; Feit, 1979; Mirsky, 1973) overestimate the magnitude of the stresses. Residual stresses give rise to more uniform distributions of end-diastolic myocardial stress (Guccione et al, 1991; Nevo and Lanir, 1994; Rodriguez et al, 1993). For systole, Guccione et al (1993) found that the residual stresses are negligible compared to the contracting stresses.

Recently, Omens et al (2003) have shown that significant residual stresses still exists in the ring after a radial cut is made in the mouse myocardium. Indeed, further stress is relieved by making a circumferential cut after the radial cut. A modeling analysis has shown that these secondary cuts reveal significantly different and possibly much more complex distributions of residual stress and strain than those predicted from models with a single cut.

Figure 2.5: Opening angle in an equatorial cross sectional slice

2.4 Fluid-structure interaction

Computational fluid dynamics (CFD) has already been highly developed in engineering. Even in cardiovascular field, the governing equations of blood have already been understood (Xu and Collins, 1999; Verdonck and Perktold, 2000; Roach, 1998). But less attention has been paid to the fluid-structure interaction

(FSI) between the blood and ventricle walls.

McQueen and Peskin (2000) proposed a comprehensive model of ventricular fluid flow by using the immersed boundary method. Later on Kovacs et al (2001) extended their model to study the relationship among fluid, wall and valves motion, and their results showed good agreements with the data from experiments. McQueen and Peskin used the perspective that the cardiovascular tissue is comprised of (essentially) incompressible tissue with essentially uniform mass density; therefore, the Navier-Stokes equations for an incompressible fluid, appropriately modified, can be applied to the four chambered heart and great vessels. The solution provides fluid, wall and valve motion as a function of space and time.

In the immersed boundary method, tissue representation is a rather coarse approximation of the heart's orthotropic fibrous-sheet structure (LeGrice et al, 1995; LeGrice et al, 1997). An alternating Lagrangian-Eulerian (ALE) mesh was proposed by Hughes et al (1981), which has the advantage because of the mesh adaptively of moving fluid. More recently, based on thin-shell theory, an axisymmetric, 2-D coupled fluid-structure model with nonlinear material property model was developed (Vierendeels et al, 2000), which gives useful information. Another try was made by Baccani et al (2002), who obtained interesting results concerning trans-mitral vortex formation using a relatively simple axisymmetric model in two space dimensions with fixed mitral valves. Watanabe and his colleagues (2004) built a FSI model using the ALE method, in which they set the ALE coordinates to be identical to the Lagrangian coordinates on the deformable interface.

In this thesis, the fluid is meshed by the ALE elements and the ventricle wall is meshed by finite elements. A penalty method is used to deal with the interaction

problem between fluid and structure (see Chapter 4).

Note:

- (1) **Myocardial infarction**, more commonly known as a heart attack, is a medical condition that occurs when the blood supply to a part of the heart is interrupted, most commonly due to rupture of a vulnerable plaque
- (2) A **stenosis** is an abnormal narrowing in a blood vessel or other tubular organ or structure.
- (3) Cardiac **arrhythmia** is any of a group of conditions in which the electrical activity of the heart is irregular or is faster or slower than normal.
- (4) **Fibrillation** is the rapid, irregular, and unsynchronized contraction of the muscle fibers of the heart.
- (5) **Diffusion MRI** is a specific Magnetic Resonance Imaging (MRI) modality that produces in vivo images of biological tissues weighted with the local microstructural characteristics of water diffusion.
- (6) **Angiography** is a medical imaging technique in which an X-ray picture is taken to visualize the inner opening of blood filled structures, including arteries, veins and the heart chambers.
- (7) **Computed tomography** (CT) is a medical imaging method employing tomography where digital geometry processing is used to generate a three-dimensional [image](#) of the internals of an object from a large series of two-dimensional X-ray images taken around a single axis of rotation.
- (8) An **echocardiogram** is an ultrasound of the heart. Also known as a cardiac ultrasound, it uses standard ultrasound techniques to image two-dimensional slices of the heart.
- (9) **Magnetic resonance imaging (MRI)** is a non-invasive method using nuclear magnetic resonance to render images of the inside of an object.
- (10) The **sinoatrial node** is the impulse generating (pacemaker) tissue located in the right atrium of the heart, and thus the generator of sinus rhythm.
- (11) The line of union between the right atrium and the right auricle is present on the interior of

the atrium in the form of a vertical crest, known as the **crista terminalis**.

(12) In the right atrium, behind the crest the internal surface of the atrium is smooth, while in front of it the muscular fibers of the wall are raised into parallel ridges resembling the teeth of a comb, and hence named the **pectinate muscles**.

Chapter 3 Fundamental Equations and Description of Left Ventricle

Mathematical models are fundamental to understand the complex mechanical behavior of LV. To predict LV wall motion and identify regions of abnormality or high mechanical stress, models must include realistic descriptions of cardiac geometry, material properties, fluid-structure interaction and boundary conditions. As reviewed in Chapter 2, mathematical models of the heart have ranged from simple axisymmetric shapes with isotropic, homogeneous myocardium (Wong and Rautaharju 1968) to accurate geometries (Nielsen et al, 1991) with detailed descriptions of the fibrous-sheet microstructure of myocardium (LeGrice 1992). In this chapter, a new mathematical model of LV is developed based on real geometry, composite material property, myocardial fiber's (MF) activation and interactions between myocardial masses (MM) and cavity blood (CB).

■ 3.1 Physical model for LV motion

The heart is one of the vital organs in the human body. It is responsible for circulating blood and hence oxygen and nutrients to the body and itself. The adult heart is about the size of a clenched fist and consists of four muscular chambers: two atria and two ventricles (Fig.3.1). The atria are thin-walled chambers that receive blood from the large vein and deliver it to the ventricles. The walls of the ventricles are much thicker than those of atria, with the wall of LV being the thickest. The two ventricles are separated by a muscular sheet known as the interventricular septum. The contraction of the ventricles provides the force required to pump the blood round the pulmonary and systemic circulations. Septum is regarded as part of LV because it contracts at the same rhythms with LV. Most heart diseases happen in LV, and so it has become the objective of the study.

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■ 3.1.1 LV wall and cavity blood

The muscle of the heart is called myocardium. The ventricular myocardium resides between endo-⁽¹⁾ and epicardium⁽²⁾ and is the primary structural component of LV. It consists of muscle bundles organized in overlapping sheets (Fig. 3.2). The sheets are oriented into a spiral, when followed from base to apex of the heart. The muscle fiber orientation in the ventricles is oriented and laminated (Streeter and Bassett, 1966). In the human LV myocardium the muscle fiber orientation varies from endo-(around 60°) to epicardium(around -60°). The change of angle from endo- to epicardium is nearly linear, with 0° in the mid-myocardium.

Figure 3.1 Cross-section of the heart with cavities, valves and vessels (courtesy of Seeley et al, 2005)

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Figure 3.2 LV wall structure (courtesy of Nash, 1998)

Based on the physiology of LV, it is assumed the LV myocardium is composed by two different materials (Fig. 3.2): myocardium masses (MM) and myocardium fibers (MF). The LV cavity is filled up with blood, which is referred to cavity blood (CB) as shown in Fig. 3.3.

Figure. 3.3 Cavity blood in LV model

■ 3.1.2 Valves, pericardium and vessels

The atria are separated from the ventricles by a fibrous skeleton on which the four heart valves are located. The valves serve to ensure the unidirectional flow of blood from the ventricles into the pulmonary artery and the aorta. Back-flow of blood from the ventricles into the atria is prevented by the atrioventricular valves. On the

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right side of the heart, the atrioventricular valve (the tricuspid valve) consists of three roughly triangular flaps of fibrous connective tissue. On the left side, the atrioventricular valve consists of two such flaps and is known as the mitral valve. Back-flow of blood from the pulmonary artery into the right ventricle is prevented by the pulmonary valve, while back-flow of blood from the aorta into the left ventricle is prevented by the aortic valve. The pulmonary and aortic valves are also known as the semilunar valves. The valves and chambers of the heart are lined by a cellular layer known as the endocardium. The simulation of valves is not the concern of the study. To simplify the valves model, only one valve is used for modeling both mitral valve and aortic valve which connect to LV (Fig. 3.4, details are in Chapter 4).

The heart lies in a tough fibrous known as the pericardium which prevents it from expanding excessively due to overfillings with blood. The pericardium is attached to the diaphragm, so that the apex of the heart is relatively fixed. When the ventricles contract, the atria move towards the apex. This has the effect of expanding the atria as the ventricles contract.

Fig. 3.4 Simplified valve in model

Figure 3.5 Simplified vessel in model

The blood vessels connected to the LV are the aorta and pulmonary vessels. The walls of the larger blood vessels consist of three layers: the tunica intima, the tunica media, and the tunica adventitia – whose thickness varies according to the type of vessel. The modeling of the vessels is also not the focus of the study; so the vessel is simplified as a uniform cross-section pipe which connects with MM as shown in Fig. 3.5.

■ 3.2 Fundamental relations of solid and fluid

For modeling purpose, each part of the current model (including MM, MF, CB, valve and vessel) is assumed to be a continuum based on microstructure observations. Continuum mechanics deals with the motion of materials when subjected to applied forces. The motion of each part of model can be described by a continuous displacement field resulting from a set of forces acting on its body.

For solid materials (MM, MF, valve and vessel), the concepts of strain (a measure of length change and material distortion) and stress (the force per unit area on an infinitesimally small plane surface within the material) are of fundamental

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importance for finite deformation elasticity theory. For fluid materials (CB), the fluid velocity and pressure are the fundamental quantities entering the governing equations.

The equations that govern the motion of deformable materials (MM, MF, CB, valve and vessel) can be derived in the following four steps:

1. Kinematic relations, which define the components of the strain tensor in terms of displacement gradients.
2. Stress equilibrium, which is derived from the laws of conservation of linear momentum and conservation of angular momentum.
3. Constitutive relations or material properties for (i) solid material (MM, MF, valve and vessel), which express the relationship between stress and strain and must be established from experimental measurement, and for (ii) fluid material (CB), constitutive relations express the relationships among velocity, pressure and density.
4. Boundary conditions, which specify the external loads or displacement constraints acting on the deforming body.

■ 3.2.1 Kinematic relations

The key to analyzing strain in LV motion undergoing large displacements and deformation is to establish two coordinate systems and the relationship between them. The first is a material coordinate system (Lagrangian) and the second is a fixed spatial coordinate system (Eulerian). Deformation is quantified by expressing the spatial coordinates of a material particle in the deformed state, as a function of the coordinates of the same particle in the undeformed state. Length changes of material segments and material distortions can then be determined from the known displacement fields, and thus strain tensors can be calculated.

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To quantify the deformation of a material, it is necessary to consider the change in length of material segments and angle change between material segments. In Fig. 3.6, an infinitesimal material line segment, $d\mathbf{X}$, in the undeformed body, $\mathbf{B}_0$, has components dX^1, dX^2 and dX^3 with respect to global rectangular Cartesian coordinates (Y_1, Y_2, Y_3) . In the deformed body, B , the same material particles that constituted $d\mathbf{X}$ have reconfigured (due to applied loads) into $d\mathbf{x}$, which has components dx^1, dx^2 and dx^3 with respect to (Y_1, Y_2, Y_3) . The deformation is quantified by the deformation gradient tensor, which carries the line segment, $d\mathbf{X}$, into $d\mathbf{x} = \mathbf{F}d\mathbf{X}$, or in component form, $dx^i = F_M^i dX^M$. The deformation gradients $\mathbf{F}$ are defined in eqn (3.1).

Figure 3.6 The deformation gradient tensor, $\mathbf{F}$

$$F_M^i = \frac{\partial x_i}{\partial X_M} \quad (3.1)$$

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Any deformation of a continuum can be split into two parts: a rigid body rotation and a stretch. This polar decomposition can be represented mathematically by considering the deformation gradient tensor to be a product, $\mathbf{F} = \mathbf{R}\mathbf{U}$, of an orthogonal rotation tensor, $\mathbf{R}$, and a symmetric positive definite stretch tensor, $\mathbf{U}$. Thus the undeformed line segment components dX^M are deformed into $dy^L = U_M^L dX^M$ before being rotated into $dx^i = R_L^i dy^L$. Line segments also change directions, except the line segments in the principal direction of $\mathbf{U}$. Equivalently the line segment could be rotated first and then stretched. It is important to note here that the stretch tensor, $\mathbf{U}$, contains a complete description of the material strain, independent of any rigid body motion. Strain in a deforming body is determined by measuring segment length changes and changes of angles (distortion). Eqn (3.2) uses Pythagoras theorem to determine the arc length of the deformed segment $d\mathbf{x}$,

$$ds^2 = dx^i dx^i = d\mathbf{x}^T d\mathbf{x} = (\mathbf{F}d\mathbf{X})^T \mathbf{F}d\mathbf{X} = d\mathbf{X}^T \mathbf{F}^T \mathbf{F}d\mathbf{X} = d\mathbf{X}^T \mathbf{C}d\mathbf{X} \quad (3.2)$$

where

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = \left\{ \frac{\partial x_k}{\partial X_M} \frac{\partial x_k}{\partial X_N} \right\} \quad (3.3)$$

Eqn (3.3) defines the Green deformation tensor, which indicates how each component of the undeformed line segment $d\mathbf{X}$ contributes to the squared length of the deformed line segment $d\mathbf{x}$. Also, it defined the mentioned distortion. The deformation tensor $\mathbf{C}$ is related to the stretch tensor $\mathbf{U}$ in eqn (3.4), using the polar decomposition theorem.

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = (\mathbf{R}\mathbf{U})^T \mathbf{R}\mathbf{U} = \mathbf{U}^T \mathbf{R}^T \mathbf{R}\mathbf{U} = \mathbf{U}^T \mathbf{U} = \mathbf{U}^2 \quad (3.4)$$

since $\mathbf{R}$ is orthogonal ($\mathbf{R}^T = \mathbf{R}^{-1}$) and $\mathbf{U}$ is symmetric. Note that like $\mathbf{U}$, $\mathbf{C}$ is

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symmetric, and positive definite and that both $\mathbf{U}$ and $\mathbf{C}$ are expressed in terms of material coordinates. One method for computing the stretch tensor $\mathbf{U}$ from the deformation gradient tensor $\mathbf{F}$ is to first calculate $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, then calculate the eigenvalues $(\lambda_1)^2, (\lambda_2)^2$ and $(\lambda_3)^2$, and orthogonal eigenvectors $\mathbf{S}_1, \mathbf{S}_2$ and $\mathbf{S}_3$ of $\mathbf{C}$ using a similarity transformation. $\mathbf{U}$ may then be constructed using eqn (3.5):

$$\mathbf{C} = \mathbf{\Omega} \mathbf{\Lambda}^2 \mathbf{\Omega}^T = \mathbf{\Omega} \begin{bmatrix} (\lambda_1)^2 & 0 & 0 \\ 0 & (\lambda_2)^2 & 0 \\ 0 & 0 & (\lambda_3)^2 \end{bmatrix} \mathbf{\Omega}^T \quad \mathbf{U} = \mathbf{\Omega} \mathbf{\Lambda} \mathbf{\Omega}^T = \mathbf{\Omega} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \mathbf{\Omega}^T \quad (3.5)$$

where the columns of $\mathbf{\Omega}$ are the orthonormal eigenvectors of $\mathbf{C}$ and are the principal axes of stretch, and λ_i are the principal stretches.

The two orthogonal tensors $\mathbf{R}$ and $\mathbf{\Omega}$, derived from $\mathbf{F}$, have different physical interpretations. $\mathbf{R}$ describes the rigid body rotation component of the deformation with no information about the material stretching. On the other hand, the columns of $\mathbf{\Omega}$ are the orientations of the principal stretch axes relative to the material coordinates.

In three-dimensions, the deformation tensor is a 3×3 matrix. There are three invariants (scalar combinations of the components of $\mathbf{C}$), which remain unchanged under coordinate rotations at a given state of deformation. These principal invariants are given in eqn (3.6):

$$I_1 = \text{tr } \mathbf{C} \quad I_2 = \frac{1}{2}[(\text{tr } \mathbf{C})^2 - \text{tr } \mathbf{C}^2] \quad I_3 = \det \mathbf{C} \quad (3.6)$$

where the trace of $\mathbf{C}$, denoted by $\text{tr } \mathbf{C}$, is the sum of the diagonal terms, C_{MM} ; and

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the determinant of $\mathbf{C}$, $\det \mathbf{C}$, is a measure of volume change.

The similarity transformation of eqn (3.5) may be used to express the invariants of $\mathbf{C}$ in terms of the principal stretch ratios as in eqn (3.7):

$$\begin{aligned} I_1 &= (\lambda_1)^2 + (\lambda_2)^2 + (\lambda_3)^2 \\ I_2 &= (\lambda_1)^2(\lambda_2)^2 + (\lambda_2)^2(\lambda_3)^2 + (\lambda_3)^2(\lambda_1)^2 \\ I_3 &= (\lambda_1)^2(\lambda_2)^2(\lambda_3)^2 \end{aligned} \quad (3.7)$$

Eqn (3.8) is the additional kinematic constraint that must be imposed on the deformation field for incompressible materials:

$$\det \mathbf{C} = I_3 = (\lambda_1 \lambda_2 \lambda_3)^2 = 1 \quad (3.8)$$

Eqn (3.9) shows how the Lagrangian Green's strain tensor, with respect to rectangular Cartesian coordinates, is related to the right Cauchy-Green deformation tensor:

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) \quad (3.9)$$

■ 3.2.2 Stress equilibrium

Having established the kinematic framework for finite deformation analysis, the next step is to consider the governing force and momentum balances in LV structure, which follow from Newton's laws of motion. In large deformations (LV motion) theory, it is necessary to first define stress tensors.

■ 3.2.2.1 Stress tensors

To identify the high stresses in the LV structure, the concept of stress must be

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defined. Stress is defined as the force per unit area acting on an infinitesimally small plane surface. If the line of action of the force is normal to the plane then a normal or axial stress results, whereas a shear stress arises when the line of action of the force is tangential to the plane. The quantities of force and area can be referred either to the reference (undeformed) or deformed configurations, which leads to three important ways of representing stress in a deforming body, namely using the Cauchy, first or second Piola-Kirchhoff stress tensors.

1. The Cauchy stress tensor, denoted σ^{ij} , represents the force measured per unit deformed area acting on an element of surface in the deformed configuration. The first index indicates the direction of the normal to the surface on which σ^{ij} acts and the second index indicates the direction of the stress component.
2. The first Piola-Kirchhoff stress tensor, denoted by s^{Mj} , represents the force acting on an element of surface in the deformed configuration but measured per unit undeformed area. The first index is written in uppercase as it refers to the normal of the surface in the undeformed state, and is thus a material coordinate index. The second index denotes the direction of the force acting on the deformed material, and is a spatial coordinate index.
3. The second Piola-Kirchhoff stress tensor, denoted by T^{MN} , represents the force measured per unit undeformed area, $\mathbf{P}$, acting on an element of surface in the undeformed configuration. This force can be determined from the actual force, $\mathbf{p}$, in the same way that the undeformed material vector, $d\mathbf{X}$, is determined from the deformed material vector, $d\mathbf{x}$. Specifically $\mathbf{P} = \mathbf{F}^{-1}\mathbf{p}$ just as $d\mathbf{X} = \mathbf{F}^{-1}d\mathbf{x}$. The primary use of the second Piola-Kirchhoff stress tensor is for representing material behaviour at a point, independent of rigid body motion. Note that the second Piola-Kirchhoff stresses must be transformed into first Piola-Kirchhoff stresses for use in the equilibrium equations, which require a spatial frame of reference. Eqns (3.10) and (3.11) define the relationships between the second Piola-Kirchhoff, first

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Piola-Kirchhoff and Cauchy stress tensors.

$$S = JF^{-1}\Sigma \quad T = S(F^T)^{-1} = JF^{-1}\Sigma(F^T)^{-1}$$

$$s^{Mj} = J \frac{\partial X_M}{\partial x_i} \sigma^{ij} \quad T^{MN} = s^{Mj} \frac{\partial X_N}{\partial x_j} = J \frac{\partial X_M}{\partial x_j} = J \frac{\partial X_M}{\partial x_i} \sigma^{ij} \frac{\partial X_N}{\partial x_j} \quad (3.10)$$

or inversely

$$S = TF^T \quad \Sigma = \frac{1}{J}FS = \frac{1}{J}FTF^T$$

$$s^{Mj} = T^{MN} \frac{\partial x_j}{\partial X_N} \quad \sigma^{ij} = \frac{1}{J} \frac{\partial x_i}{\partial X_M} s^{Mj} = \frac{1}{J} \frac{\partial x_i}{\partial X_M} T^{MN} \frac{\partial x_j}{\partial X_N} \quad (3.11)$$

where J is the Jacobian of the transformation from reference to deformed coordinates, defined in Equation (3.12).

$$J = \det F = \sqrt{I_3} = \lambda_1 \lambda_2 \lambda_3 \quad (3.12)$$

■ 3.2.2.2 Conservation laws and the principle of virtual work

The conservation of mass principle relates the mass densities in the undeformed and deformed bodies (denoted by ρ_0 and ρ , respectively) given in eqn (3.13) .

$$\int_{V_0} \rho_0 dV_0 = \int_V \rho dV = \int_{V_0} \rho J dV_0 \quad (3.13)$$

Thus for arbitrary volumes, mass density for the undeformed and deformed bodies are related as

$$\rho_0 = J\rho = \sqrt{I_3} \rho \quad (3.14)$$

For a given set of particles, the time rate of change of the total linear momentum equates to the vector sum of all the external forces acting on the particles of the set.

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This is expressed mathematically in eqn (3.15), where $\mathbf{t}$ is the traction vector (external surface forces per unit area), $\mathbf{b}$ represents the body forces (per unit mass), and the rate of change of momentum is written in terms of the material derivative (d/dt) and the velocity vector $\mathbf{v}$:

$$\int_S \mathbf{t} dS + \int_V \rho \mathbf{b} dV = \frac{d}{dt} \int_V \rho \mathbf{v} dV \quad (3.15)$$

Cauchy's formula, defined in eqn (3.16), projects the components of a stress vector $\mathbf{t}$ (the force per unit area acting on some deformed surface dS , with unit normal $\hat{\mathbf{n}} = \hat{n}_j \mathbf{i}_j$) onto the set of orthogonal base vectors for the rectangular Cartesian reference coordinate system, $\mathbf{i}_j$:

$$\mathbf{t} dS = \sigma^{ij} \hat{n}_i \mathbf{i}_j dS \quad (3.16)$$

where σ^{ij} are components of the Cauchy stress tensor and are physical stresses, since $\mathbf{i}_j$ are unit vectors. Cauchy's formula is substituted into eqn (3.15) to form eqn (3.17), which is appropriate for a material with constant density. Note that eqn (3.17) is written in component form where the body force and velocity vectors have components $\mathbf{b} = b^j \mathbf{i}_j$ and $\mathbf{v} = v^j \mathbf{i}_j$, respectively.

$$\int_S \sigma^{ij} \hat{n}_i + \int_V \rho (b^j - \frac{dv^j}{dt}) dV = 0 \quad (3.17)$$

Applying the divergence theorem to eqn (3.17) yields:

$$\int_V [\frac{\partial \sigma^{ij}}{\partial x_i} + \rho b^j - \rho f^j] dV = 0 \quad (3.18)$$

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where $f^j = \frac{dv^j}{dt}$ are components of the acceleration vector.

■ 3.2.3 Constitutive relations

Constitutive equations are used to represent the behavior of a material through empirical relationships between experimentally observed stress and strain tensors. The most challenging part of modeling LV is to appropriately define the material properties of MM, MF, CB, valve and vessel.

■ 3.2.3.1 Constitutive relations for MM

Eqn (3.19) defines the components of the second Piola-Kirchhoff stress tensor, when the strain energy W is expressed in terms of Green's strain components, E_{MN} , referred to X_M -material coordinates.

$$T^{MN} = \frac{1}{2} \left(\frac{\partial W}{\partial E_{MN}} + \frac{\partial W}{\partial E_{NM}} \right) \quad (3.19)$$

For isotropic materials (MM, MF, valve and vessel), the strain energy is constant for all orientations of the coordinate axes, or mathematically $W(C) = W(QCQ^T)$, where $\mathbf{Q}$ is any constant orthogonal tensor. Thus the strain energy is an invariant function of $\mathbf{C}$. It can be shown that any invariant function of $\mathbf{C}$ can be expressed as a function of the three principal invariants of $\mathbf{C}$, which are defined in eqn (3.6). This reduces the functional form of the strain energy function to $W = W(I_1, I_2, I_3)$.

For incompressible materials (MM, MF, valve and vessel) a further restriction on the form of the constitutive law can be imposed. In this case the additional kinematic constraint $I_3 = 1$ (eqn (3.8)) is applied. It is not sufficient to set $I_3 = 1$

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in the constitutive equation, since certain derivatives of W tend to infinity in the limiting case of an incompressible material. This problem is overcome by introducing an arbitrary Lagrange multiplier λ into the constitutive equation. The unspecified strain energy term $\bar{W}$ is thereby limited to be a function of I_1, I_2 only. Thus for isotropic, incompressible materials, eqn (3.20) shows the functional form of the strain energy function.

$$W = \bar{W}(I_1, I_2) + \lambda(I_3 - 1) \quad (3.20)$$

Eqn (3.20) can be substituted into eqn (3.19) and rearranged to give the components of stress with respect to X_M -material coordinates, expressed in eqn (3.21). Note that $\frac{\partial I_3}{\partial E_{MN}} = 2\delta^{MN}$, where δ^{MN} is the Kronecker delta, which is equal to one if the indices M and N are the same and zero otherwise. In addition, the arbitrary Lagrange multiplier is chosen to be $\lambda = -\frac{1}{2}p$ in the constitutive equation (eqn (3.30)) to ensure that the additional component in the diagonal terms of the stress tensor is a true hydrostatic stress.

$$T^{MN} = \frac{1}{2} \left(\frac{\partial \bar{W}}{\partial E_{MN}} + \frac{\partial \bar{W}}{\partial E_{NM}} \right) - p\delta^{MN} \quad (3.21)$$

where, for isotropic, incompressible materials

$$\frac{\partial \bar{W}}{\partial E_{MN}} = \frac{\partial \bar{W}}{\partial I_1} \frac{\partial I_1}{\partial E_{MN}} + \frac{\partial \bar{W}}{\partial I_2} \frac{\partial I_2}{\partial E_{MN}} \quad (3.22)$$

A suitable form of $\bar{W}(I_1, I_2)$ must then be chosen, based on experimental observations of the material. To characterize the properties of MM, the Mooney-Rivlin Rubber (Mohr, M. B et al, 2003 and Zoran B. P et al, 2004) model

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is adopted for the constitutive equation based on hyperelastic material theory. The simple isotropic Mooney-Rivlin strain-energy potential is a linear function of the first two principal invariants of the right Cauchy-Green deformation tensor. It has been widely used for large deformation analysis of nonlinear rubber elasticity. In the constrained formulation, the material is assumed to be incompressible, thus introducing the Lagrange multiplier p , which must be included as another dependent variable in the analysis. In the slightly compressible formulation, values for the bulk modulus, C_{compr} , in the order of 100 kPa produce nearly isochoric behavior at physiological stresses for typical soft biomaterials. In this model, the strain energy density function is defined as:

$$W = A(I_1 - 3) + B(I_2 - 3) + C_1(I_3^{-2} - 1) + D(I_3 - 1)^2 \quad (3.23)$$

where

$$\begin{aligned} C_1 &= 0.5A + B \\ D &= \frac{A(5\nu_{mm} - 2) + B(11\nu_{mm} - 5)}{2(1 - 2\nu)} \end{aligned} \quad (3.24)$$

ν_{mm} : Poisson's ratio for MM

$G = 2(A + B)$: Shear modulus of liner elasticity

I_1, I_2, I_3 : Invariant of right Cauchy – Green Tensor

■ 3.2.3.2 Constitutive relations for MF

Fibers play a crucial role in LV motion and their constitutive relations are fundamental important for its mechanical performance.

As introduced in Chapter 2, the heart beats spontaneously. It shows an inherent

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rhythmicity that is independent of any extrinsic nerve supply. Excitation is initiated by a group of specialized cells in the sinoatrial node that lies close to the point of entry of the great veins into the right atrium. A wave of depolarization is then conducted throughout the myocardium. From the sinoatrial node (SAN), excitation spreads first across both the atria. It then passes to the ventricles via the atrioventricular (AV)⁽³⁾ node, which forms the only bridge of conducting tissue between the atria and ventricles. The AV node consists of a narrow bundle of specialized cardiac fibers. These fibers are small-diameter cells which have relatively few gap junctions between adjacent cells. As a result, conduction through the AV node is relatively slow and the spread of excitation to the ventricles is delayed for around 0.1s at this point. This ensures that the atria have time to contract before the ventricle muscle is excited. Conduction through the remainder of the system is rapid (around 1m^{-1}) and is mediated by the left and right bundle branches supplying the left and ventricles. The bundles fibers are specialized large-diameter cardiac myocytes arranged end to end to permit the rapid conduction of the wave of excitation from the AV node to an extensive network of large fibers (Purkinje fibers) that lies just beneath the endocardium. These fibers then spread the excitation to the ventricular myocytes via gap junctions. Conduction spreads through the myocardium itself, with the result that all parts of the ventricles are excited at nearly the same time. In order to implant this physiology into the mechanical model, a Hill's fiber force model is developed in this section.

Based on the previous work done by Kojic et al (1998), there is a Hill's fiber force model developed for simulating the fibers. One of the most important relations in muscle mechanics is Hill's equation. It refers to a property of skeletal muscle in the tetanized condition. This equation is given as

$$(v + b)(T + a) = b(T_0 + a) \quad (3.25)$$

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where T represents tensional force in muscle, v is the velocity of the muscle contraction, and a , b and T_0 are constants. The constant T_0 is the maximum force developed in the muscle under isometric condition (function of the muscle length L_0). A dimensionless form of Hill's equation is

$$\frac{T}{T_0} = \frac{1 - (v/v_0)}{1 + c(v/v_0)} \quad (3.26)$$

where $c = T_0/a$. A graphical representation of eqn (3.26) is given in Fig. 3.7.

Figure 3.7: Graph of muscle force-velocity

Figure 3.8: Hill's material model

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Figure 3.9: Isometric tension-length curve of a muscle

Hill's fiber force model is composed by three elements (Fig. 3.8): CE is a contractile element, SEE is a series elastic element and PEE is a parallel elastic element.

The contractile element, whose behavior is described by Hill's equation and by the relation given in Fig. 3.8, is connected in series with a non-linear elastic element, for which the experimental force-stretch relation is given by (Kojic, 1998):

$$S = (S^* + \beta)e^{\alpha(\lambda - \lambda^*)} - \beta \quad (3.27)$$

where α and β are constants, and S^* is the force corresponding to stretch λ^* .

The series of the contractile and the non-linear elastic elements are coupled in parallel to the linear elastic element representing the surrounding connective tissue.

The following contents are the numerical algorithm for stress calculation.

The following relation is from the Fig. 3.8:

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$$L_{p0} + U_p^0 = L_{m0} + U_m^0 + L_{s0} + U_s^0 \quad (3.28)$$

where L_{p0} is the total initial length, while L_{m0} and L_{s0} are initial lengths of contractile and series elements; U_p^0 , U_m^0 and U_s^0 are elongations (displacements) of the corresponding elements. It is supposed that the relation between the lengths is given by

$$L_{s0} = kL_{m0} \quad (3.29)$$

where k is a constant.

Dividing (3.28) by L_{m0} and using (3.27) and $L_{p0} = L_{m0} + L_{s0}$, a relation for the stretches is obtained:

$$\lambda_m^0 = (1 + k)\lambda_p^0 - k\lambda_s^0 \quad (3.30)$$

Usually it is considered that the initial state corresponds to the undeformed configuration; hence $\lambda_p^0 = 1$ and then $\lambda_m^0 = 1$.

At an arbitrary time t , there is a following equation for lengths:

$${}^tL_p = L_{m0} + U_m^0 + \int_{t_a}^t v_m dt + L_{s0} + {}^tU_s = L_{p0} + {}^tU \quad (3.31)$$

where v_m is the rate of change of the muscle length, and t_a is activation time.

Dividing this equation by L_{m0} , the following equation is obtained:

$$(1 + k){}^t\lambda_p = \lambda_m^0 + \int_{t_a}^t \frac{v_m}{L_{m0}} dt + k{}^t\lambda_s \quad (3.32)$$

At the end of the contraction, this equation can be written as

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$$(1 + k)^{t+\Delta t} \lambda_p = {}^t\lambda_m + \Delta\lambda_m + k {}^t\lambda_s + k\Delta\lambda_s \quad (3.33)$$

with increment of stretches.

Contractile forces T_m and T_s in the contractile and the series elastic element must be equal at any time, hence

$${}^{t+\Delta t}T_m = {}^{t+\Delta t}T_s \quad (3.34)$$

According to Hill's eqn (3.34), it is obtained that:

$${}^{t+\Delta t}T_m = {}^tT_0 {}^{t+\Delta t}\alpha_a \frac{1 + \Delta\lambda_m / \Delta\lambda_{m0}}{1 - c\Delta\lambda_m / \Delta\lambda_{m0}} \quad (3.35)$$

where it is taken into account the condition that contractile velocity is considered negative. Force tT_0 is the force corresponding to stretch ${}^t\lambda_m$, according to Fig. 3.8. The activation function of the muscle is given as ${}^{t+\Delta t}\alpha_a$, which could be determined from experiments. Here $\Delta\lambda_{m0}$ is calculated as

$$\Delta\lambda_{m0} = \Delta t \dot{\lambda}_{m0} \quad (3.36)$$

where $\dot{\lambda}_{m0}$ is the strain rate which corresponds to maximum isometric tetanized force; this is a characteristic of the contractile element, taken as a known quantity in practical applications. The constitutive equation for the force ${}^{t+\Delta t}T_s$ follows from eqn (3.27):

$${}^{t+\Delta t}T_s = \beta [e^{\alpha({}^t\lambda_s - 1 + \Delta\lambda_s)} - 1] = e^{\alpha\Delta\lambda_s} ({}^tT_s + \beta) - \beta \quad (3.37)$$

where

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$${}^tT_s = \beta[e^{\alpha({}^t\lambda_s - 1)} - 1] \quad (3.38)$$

is the force corresponding to time t .

From eqn (3.33), it is obtained that:

$$\Delta\lambda_m = a_1 - k\Delta\lambda_s \quad (3.39)$$

where

$$a_1 = (1 + k)^{t+\Delta t} \lambda_p - {}^t\lambda_m - k {}^t\lambda_s \quad (3.40)$$

Finally, from eqn (3.34), (3.35), (3.37) and (3.39), the non-linear equation is obtained:

$$f(\Delta\lambda_s) = (a_2 + a_3\Delta\lambda_s)e^{\alpha\Delta\lambda_s} - a_4\Delta\lambda_s - a_5 = 0 \quad (3.41)$$

with one unknown $\Delta\lambda_s$, where

$$\begin{aligned} a_2 &= ({}^tT_s + \beta)(1 - \frac{ca_1}{\Delta\lambda_{m0}}), & a_3 &= ({}^tT_0 + \beta)\frac{kc}{\Delta\lambda_{m0}} \\ a_4 &= -\frac{{}^tT_0^{t+\Delta t}\alpha_a - \beta c}{\Delta\lambda_{m0}}, & a_5 &= {}^tT_0 + \beta + \frac{{}^tT_0^{t+\Delta t}\alpha_a - \beta c}{\Delta\lambda_{m0}}a_1 \end{aligned} \quad (3.42)$$

This equation is solved numerically by the standard Newton's method.

The force in the parallel elastic element ${}^{t+\Delta t}T^E$ is calculated as

$${}^{t+\Delta t}T^E = C^E {}^{t+\Delta t}T_s \quad (3.43)$$

where C^E is determined by the surrounding connective tissue. The total force

${}^{t+\Delta t}T_{tot}$ is expressed as

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$${}^{t+\Delta t}T_{tot} = {}^{t+\Delta t}T^E (1 - \phi) + \phi {}^{t+\Delta t}\alpha_a {}^{t+\Delta t}T_s \quad (3.44)$$

where ϕ is the fraction of the muscle in the total volume. The force ${}^{t+\Delta t}T_s$ has only one non-zero component- in the direction of the fiber. This is the force that will be implanted into the LV model.

■ 3.2.3.3 Constitutive relations for CB

CB's most important governing equation (Gruneisen formulation, Theory manual of LS-DYNA 970) is eqn (3.45) which describes the relationship between pressure and volume.

$$\bar{p} = \frac{\bar{\rho}_0 C_2^2 \mu [1 + (1 - \frac{\gamma_0}{2})\mu - \frac{a}{2}\mu^2]}{[1 - (s_1 - 1)\mu - s_2 \frac{\mu^2}{\mu + 1} - s_3 \frac{\mu^3}{(\mu + 1)^2}]} + (\gamma_0 + \alpha\mu)E \quad (3.45)$$

where E is the internal energy per initial volume, C_2 is the intercept of the u_s - u_p curve (which describes the relationship between pressure and volume in experiment), S_1 , S_2 , and S_3 are the coefficients of the slope of the u_s - u_p curve, γ_0 is the Gruneisen gamma, and a is the first order volume correction to γ_0 . Constants C_2 , S_1 , S_2 , S_3 , γ_0 , and a are all input parameters. The compression is defined in terms of the relative volume, V , as:

$$\mu = \frac{1}{V} - 1. \quad (3.46)$$

For expanded materials as the pressure is defined by:

$$p = \bar{\rho}_0 C_2^2 \mu + (\gamma_0 + \alpha\mu)E \quad (3.47)$$

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For fluid under normal temperature and small pressure (as pressure in LV), the fluid property parameters are usually reduced to bulkmodulus only, which gives the relation between the change of volume and the change of pressure. For CB the relation can be assumed linear:

$$p = \Delta V \cdot C_2^2 \quad (3.48)$$

where C_2 is the square root of the bulk modulus of CB.

■ 3.2.3.4 Constitutive relations for valve and vessel

Valve and vessel are not the focus of the study. They are simplified as rigid material which means the young's modulus is nearly infinite and they do not deform in the LV motion.

■ 3.2.4 Boundary constraints and surface tractions

LV model has quite a complex boundary conditions (constrains and external pressure), especially at the apex and the base level of LV. Reasonable boundary conditions are very important for mathematical models.

If external surface pressures are applied to the visual work equation, this integral must be evaluated for those portions of the boundary that sustain the loads. In the absence of boundary pressures, this term vanishes. Consider a deforming surface, with unit normal $\hat{n} = \hat{n}_j \mathbf{i}_j$. If the surface is loaded by a pressure, $p_{(appl)}$ (a physical stress); then the surface traction vector has components $\mathbf{s} = p_{(appl)} \hat{n}_j \mathbf{i}_j$ and is evaluated using eqn (3.49).

$$\int_{S_2} \mathbf{s} \cdot \delta \mathbf{v} dS = \int_{S_2} p_{(appl)} \hat{n}_j \delta v_j dS \quad (3.49)$$

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■ 3.3 Four phases model of LV motion**■ 3.3.1 Physiology**

The cardiac cycle can be separated into two major phases referred to as ventricular systole (which is the period of contraction) and ventricular diastole (during which the heart relaxes and fills ready for the next cycle). These phases can be differentiated according to pressure and volume change. The phases are:

- during systole: isovolumic contraction and ejection phase
- during diastole: isovolumic relaxation and passive fillings

These phases are marked by the opening and closing of valves (Fig. 3.10) and are furthermore explained for LV.

■ 3.3.1.1 Isovolumic contraction

Starting with the development of tension in the systole the rising of intraventricular pressure leads to a closure of the mitral valve. At this time, the aortic valve is still closed (Fig. 3.10, I). The ventricle performs an isometric contraction surrounding the incompressible fluid blood, and adapts towards a spherical shape. The spherical geometry is adopted since a sphere has a smaller surface surrounding a constant volume. Furthermore, the valve plane of the heart consisting of cytoskeleton, and the valves are pulled towards the apex. This isovolumic contraction results in a steep pressure increase without volume change. During a regular heart cycle (0.8s), this phase takes approx 40 ms.

■ 3.3.1.2 Ejection phases

The aortic valve opens as soon as the intraventricular pressure rises above the aortal diastolic pressure and blood is ejected into the arteries (Fig. 3.10, IIa). The intraventricular pressure rises until it reaches a peak and decreases with the end of the systolic phase (Fig. 3.10, IIb). From the blood volume of approx 130 ml for a

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normal heart beat only 70 ml are ejected, which is the so called stroke volume. A blood volume of 60 ml remains in the ventricle as end-systolic volume. The fraction of stroke volume to filling volume (end-diastolic) is called ejection fraction. The closure of the aortic valve marks the end of the systole. However, compared to the pressure curve it is slightly delayed. This is due to the kinetic energy of the blood flowing against the pressure gradient inside the aortic system for a short period of time.

■ 3.3.1.3 Isovolum relaxation

The isovolum relaxation commences after the end of the ejection, where the aortic valve closes (Fig. 3.10, III). The cavity relaxes to its regular shape and the pressure drops. As soon as the intraventricular pressure drops below the atrial pressure, the mitral valve opens and the filling phase starts.

■ 3.3.1.4 Passive fillings

During the passive filling phase, a quick (Fig. 3.10, IVa) and a slow filling phase (Fig. 3.10, IVb) can be differentiated. The blood from the atria generates the preload for the next contraction. During a normal heart cycle, the filling of the ventricle is mostly complete, when the atria systole commences (Fig. 3.10, IVc). The additional volume increase is only about 10%. During higher heart frequencies however, the atrial fraction of the filling volume increases, since the diastolic phase decreases more than the systolic phase.

■ 3.3.1.5 Initial phase in the model

Although it is an essential requirement for any ventricle models to determine the initial shape in an undeformed state under stress-free conditions (even exclude the residual stress), it is hard to know this stress-free state in a living human LV. Whether the stimulation starts at the beginning of isovolum contraction or at the

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Figure 3.10 Cardiac cycle (courtesy of Silbernagl and Despopoulos, 1991)

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beginning of isovolume relaxation, the stresses existing in the MM are difficult to determine. So the initial so called “undeformed” LV shape is created using these assumptions:

1. The cavity volume of an adult LV is around 130 ml (maximum LV cavity volume) when the LV is under fully relaxed condition (end of diastole). At this time, the ventricle wall is under tension.
2. At the end of systole, the cavity volume of LV is around 60 ml (minimum LV cavity volume) and the ventricle wall at this time is under contraction.
3. Therefore, a stress-free state (nominal one) is assumed to happen in the middle of during diastole (i.e. when the cavity volume is 95 ml); then the loads and boundary conditions are defined to process the analysis. The total fiber length (the sum of all the fibers length) is calculated at the same cavity volume (i.e.95ml) during the systole. If both of the fiber lengths are the same, then this cavity volume is taken as the initial volume of the LV. Otherwise, another cavity volume is tried. By this method, the cavity volume is determined to be 106 ml for the initial shape of the LV.

The whole mathematical model for LV in this study will be divided into 5 periods as show in Fig. 3.11 (Silbernagl and Despopoulos, 1991). Different material parameters in different phases will be explained in the following sections.

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Figure 3.11 Five periods of LV motion in the study

■ 3.3.2 Geometry in four phases model

The macroscopic model of the anatomy of the heart is created from 3D/4D image data taken in a clinical environment. The images are filtered, segmented and classified into tissue classes describing different tissue types and properties. Thus, a suitable model for simulation is gained. Several medical imaging modalities exist, which can be used to capture in-vivo images of the heart. Imaging systems in medical environments are ultrasonography (US), magnetic resonance tomography (MRT), and computed tomography (CT). Furthermore, all imaging techniques can also be used for in vitro investigations. The ultrasonography relies on the fact that acoustic waves from a transmitter are reflected or scattered depending on acoustic impedance of traversed tissue. The time a wave travels from a transducer into the material and back is measured and utilized to compute the penetration depth. The strength of the echo depends on the difference between acoustic impedances of the structures. When the transducer is mechanically or electrically swiveled, the received data can be used to reconstruct 2D or 3D images. The geometry in this study is taken from the ultrasonography (Uni. Of Auckland) as shown in Fig. 3.12. At this moment, the LV is at the end of relaxation and the cavity volume is maximum (130ml). The endocardium surface is extracted from Fig. 3.12 and has

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been proportionally modified to get its original volume which is 106ml as explained in section 3.2. This proportional method is based on these assumptions:

1. The longitude length of LV cavity keeps constant.
2. The vertical axis which points from base to apex is regarded as the center of each cross section.
3. The radius lengths (from endocardium to vertical axis) of each cross section are proportionally reduced in order to make the volume 130ml to 106ml. The initial shape of endocardium surface is shown in Fig. 3.13.

Once the initial geometry of LV has been determined, the starting geometry of other phases is the same configuration with the one at the end of the previous phase.

Figure 3.12: Ultrasonic image for ventricles

Figure 3.13: Initial shape of endocardium surface

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■ 3.3.3 Material parameters in four phases model

■ 3.3.3.1 Material parameters for MM

In all the phases, the isotropic Mooney-Rivlin material properties are implanted into MM. The parameters A and B in eqn (3.23) must be defined. Alternatively, the stress versus strain curve can be defined, instead of giving the values of A, B. It is shown in Fig. 3.14. (Johansson, T. et al, 2000) Possion's ratio set for this nearly incompressible material is 0.495 and density is $1.37 \times 10^3 \text{ kg/m}^3$.

Figure 3.14. Stress versus strain curve for MM

■ 3.3.3.2 Material parameters for MF

The representative values for the material parameters defined in MF are listed:

Elastic constants of the parallel element: $E_p = 1.0 \times 10^6 \text{ N/m}^2$, $\nu_p = 0.495$

Elastic constants of the series element: $\alpha = 9.4$, $\beta = 1.1 \times 10^5 \text{ N/m}^2$

Density of fibers: $\rho_{mf} = 1.37 \times 10^3 \text{ kg/m}^3$

Strain rate: $\dot{\lambda}_{m0} = 2 \text{ m/s}$

Fraction of the muscle in the total volume: $\phi = 0.7$

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Constants: $k = 0.3$, $a = 70 \times 10^3 \text{ N/m}^2$, $c = 0.15 - 0.25$

The maximum tetanized isometric force T_0 is determined according to each length of the fibers.

Normalized membrane potential and relative activation factor are shown in Fig. 3.15 (Gillian and Christopher, 2004). The activation factor $\alpha_a(t)$ is the important parameter to link the membrane potential of electricity to the fiber's mechanical force (Chapter 4). It varies from 0 to 1 in the four phases.

Figure 3.15: Normalized membrane potential and relative activation factor $\alpha_a(t)$

■ 3.3.3.3 Material parameters for CB

At any time, the LV cavity is filled with blood. The most important material property for CB in the left ventricle cavity is the equation of state as introduced in Section 3.2.3.3. With the equation-of-state, the behavior of a fluid like blood can be simulated. In this model, the fluid properties are defined by the bulk modulus, which is 250000 N/m^2 . It gives the relation between the change of volume and the change of pressure. Here, the relation is assumed linear. The density of CB is

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defined as $\rho = 1.067 \times 10^3 \text{ kg/m}^3$

■ 3.3.3.4 Material parameters for valve and vessel

As mentioned in Section 3.2.3.4, the valve and vessel are assumed as rigid body and they don't deform during the analysis.

■ 3.3.4 Boundary and initial conditions in four phases model

■ 3.3.4.1 Boundary condition at MM and vessel

The deformation simulations in virtual space need a reference point. In case of simulating a ventricle deformation, the apex was chosen to be fixed. This behavior is consistent with reality, as the heart apex is fixed to the pericardial sac, whereas the heart base with cytoskeleton and valves is pulled towards the apex. It is shown in Fig 3.16. The junction places (endocardium and middle myocardium) where vessel connects with MM are also fixed because the vessel is assumed as rigid body. The epicardium at the base level is assumed as fixed in x and y direction only and it can contract towards apex. It is a reasonable assumption comparing with the LV motion from clinical observation (Gillian P. and Christopher D. R., 2004).

Figure 3.16 Boundary conditions at MM and vessel

■ 3.3.4.2 Boundary condition at valve

In the four phases of LV motion, the opening and closing of valve are manually controlled due to the time. At the iso-volume contraction and iso-volume relaxation, the valve is closed which means it is fixed. At the passive fillings and ejection phases, the valve is opened which means it is free. And the pressure acting on valve is shown in Fig. 3.17 (Silbernagl and Despopoulos, 1991).

Figure 3.17. Input pressure on valve

■ 3.3.4.3 Residual stress in MF

As discussed in Chapter 2, the heart is not stress free in its unloaded state (Omen and Fung, 1990), and residual stress must be taken into account. Residual stress imposes prestretch on myofibers at the epicardium and compresses myofibers at the endocardium. In the current model, the residual strain in the inner fiber is supposed be to 0.05, in the outer fibers is supposed to be 0.05 and in the middle layer of fiber remains 0.05 too. The average values are taken due to the open angle test done by Omen and Fung (1990).

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Note:

- (1) The **endocardium** is the innermost layer of tissue that lines the chambers of the heart.
- (2) **Epicardium** describes the outer layer of heart tissue.
- (3) The **atrioventricular node** is an area of specialized tissue between the atria and the ventricles of the heart, which conducts the normal electrical impulse from the atria to the ventricles.

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The finite element method is used to solve physical problems in engineering analysis and design. Physical problem typically involve an actual structure or structural component subjected to certain loads. In chapter 3, the physical problem (LV motion) has been idealized to a mathematical model based on certain assumptions. This model can be discretized into finite elements. The finite element analysis solves this mathematical model. A typical process of finite element analysis is shown in Fig. 4.1. In this chapter, a finite element model for left ventricle has been built according to the mathematical model presented in Chapter 3.

■ 4.1 The finite element method for finite elasticity

To analyze wall stresses in LV structure undergoing large elastic deformation, the equations that govern finite deformation elasticity must be solved. For materials with regular geometries and simple material properties, this may be done analytically. However, for LV structure, materials behave nonlinearly and assume complex shapes. Irregular domains have to be discretised into a number of smaller regular elements, over which displacements of nodes are continuously approximated. There are two kinds of elements used in the thesis: 2-nodes line elements and 8-nodes 3D elements, as shown in Fig. 4.2 and 4.3.

Linear Lagrange basis functions for line and 3D elements are introduced in Section 4.1.1.

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Figure 4.1 The process of finite element analysis (Bathe,1996)

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Figure 4.2 Line element

Figure 4.3 3D element

For each element, the equations governing finite deformation elasticity are expressed in terms of known material properties and the unknown displacements of nodes. To formulate these equations many integrals must be evaluated and often this cannot be done analytically. Gaussian quadrature is a suitable numerical integration scheme for use with FE analysis.

Element contributions are assembled into a global system of equations to ensure that the solution is compatible across element boundaries. The system of nonlinear

equations are solved, subject to boundary constraints, to yield a set of deformed nodal coordinates from which deformation patterns are approximated using interpolation.

■ 4.2 Finite element mesh of initial LV shape

Based on the initial shape of left ventricle mentioned in chapter 3 (Fig. 3.12), a finite element mesh for MM is created following these steps: 1) an endocardium surface mesh is firstly generated (inner surface) from the ultrasonic image (from Uni. of Auckland) of an adult human LV; 2) it is modified as a whole LV in accordance with the out surface. (the average thickness of LV is around 10mm, Fig. 4.4). There are totally 741 nodes and 480 3D hexahedral (8 nodes each, Fig. 4.3)) elements created for representing MM.

It is known that the ventricle wall consists of multiple layers of muscle bundles which are named as MF. In the current model, the ventricle wall is divided into three layers from endocardium to epicardium, the MF directions in each layer are around -60° , 0° , and 60° (Fig. 4.5) respectively, relative to the plane perpendicular to the long axis of the LV. Line elements (Fig. 4.3) are used for meshing MF.

3D hexahedral elements are also used for meshing CB, valve and vessel, as shown in Fig. 4.8, 4.9, 4.10. Fig. 4.11 shows the total mesh of LV model. The FE nodes for MM and CB are not common nodes on surface.

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Figure 4.4: Mesh of myocardium masses from different views

Figure 4.5: Mesh of MF

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Figure 4.6 Mesh of CB

Figure 4.7 Mesh of valve

Figure 4.8 Mesh of vessel

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Figure 4.9 Total mesh of LV model

Actually the MF mesh is combined into the MM mesh which means the nodes of line element are also the nodes of 3D elements. Line elements are “lying” on the surface of 3D elements (Fig. 4.12). During the systole, the MF contract and become shorter which will “pull” the MM inward. The MM’s movement toward inside will cause the myocardium stresses and push the CB into the aorta.

Figure 4.10 Line elements connect with 3D elements

■ 4.3 Simplified ALE approach

■ 4.3.1 ALE formulation

The CB is meshed by 3D element and a simplified ALE formulation takes during the analysis. The ALE approach is a very effective alternative for simulating large deformation problems which performs automatic rezoning. Usually, manual rezoning can be performed by

- 1 . Stopping the calculation when the mesh is distorted,
2. Smoothing the mesh,
3. Remapping the solution from the distorted mesh to the smooth mesh.

An ALE formulation consists of a Lagrangian time step followed by a "remap" or "advection" step. The advection step performs an incremental rezone, where "incremental" refers to the fact that the positions of the nodes are moved only a small fraction of the characteristic lengths of the surrounding elements. Unlike a manual rezone, the topology of the mesh is fixed in an ALE calculation. An ALE calculation can be interrupted like an ordinary Lagrangian calculation and a manual rezone can be performed if an entirely new mesh is necessary to continue the calculation.

The accuracy of an ALE calculation is often superior to the accuracy of a manually rezoned calculation because the algorithm used to remap the solution from the distorted to the undistorted mesh is second order accurate for the ALE formulation while the algorithm for the manual rezone is only first order accurate.

In theory, an ALE formulation contains the Eulerian formulation as a subset. Eulerian codes can have more than one material in each element, but most ALE implementations are simplified ALE formulations which permit only a single

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material in each element (There is only the blood material defined in the ALE elements for this research). Primary advantage of a simplified formulation is its reduced cost per time step. When elements with more than one material are permitted, the number and types of materials present in an element can change dynamically. Additional data is necessary to specify the materials in each element and the data must be updated by the remap algorithms.

The range of problems that can be solved with an ALE formulation is a direct function of the sophistication of the algorithms for smoothing the mesh. Early ALE codes were not very successful largely because of their primitive algorithms for smoothing the mesh. In simplified ALE formulations, most of the difficulties with the mesh are associated with the nodes on the material boundaries. If the material boundaries are purely Lagrangian, i.e., the boundary nodes move with the material at all times, no smooth mesh maybe possible and the calculation will terminate. The algorithms for maintaining a smooth boundary mesh are therefore as important to the robustness of the calculations as the algorithms for the mesh interior.

The cost of the advection step per element is usually much larger than the cost of the Lagrangian step. Most of the time in the advection step is spent in calculating the material transported between the adjacent elements, and only a small part of it is spent on calculating how and where the mesh should be adjusted. Second order accurate monotonic advection algorithms are used in LS-DYNA (the commercial software package used in this thesis) despite their high cost per element because their superior coarse mesh accuracy which allows the calculation to be performed with far fewer elements than would be possible with a cheaper first order accurate algorithm.

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The overall flow of an ALE time step is:

- 1 . Perform a Lagrangian time step.
2. Perform an advection step.
 - a. Decide which nodes to move.
 - b. Move the boundary nodes.
 - c. Move the interior nodes.
 - d. Calculate the transport of the element-centered variables.
 - e . Calculate the momentum transport and update the velocity.

Each element solution variable must be transported. The total number of solution variables, including the velocity, is at least six and depends on the material models. For elements that are modeled with an equation of state (like CB), only the density, the internal energy, and the shock viscosity are transported. When the elements have strength, the six components of the stress tensor and the plastic strain must also be advected, for a total of ten solution variables.

The nodal velocities add an extra three solution variables that must be transported, and they must be advected separately from the other solution variables because they are centered at the nodes and not in the elements. In addition, the momentum must be conserved, and it is a product of the node-centered velocity and the element-centered density. This imposes a constraint on how the momentum transport is performed that is unique to the velocity field. A detailed consideration of the difficulties associated with the transport of momentum is deferred later.

The simplest strategy for minimizing the cost of the ALE calculations is to perform them only every few time steps. The cost of an advection step is typically two to five times than the cost of the Lagrangian time step. By performing the advection step only every ten steps, the cost of an ALE calculation can often be reduced by a

factor of three without adversely affecting the time step size. In general, it is not worthwhile to advect an element unless at least twenty percent of its volume will be transported because the gain in the time step size will not offset the cost of the advection calculations.

■ 4.3.2 Mesh smoothing algorithms

The algorithms for moving the mesh relative to the material control can be solved by an ALE formulation. The equipotential method which is used in LS-DYNA was developed by Winslow (1990). It has proven to be very successful in a wide variety of problems. "Equipotential" zoning (Winslow, 1963) is a method of making a structured mesh for finite difference or finite element calculations by using the solutions of Laplace equations (later extended to Poisson equations) as the mesh lines. The same method can be used to smooth selected points in an unstructured three-dimensional mesh provided that it is at least locally structured. This section presents a derivation of the three-dimensional equipotential zoning equations, taken from the references, and gives their finite difference equivalents in a form ready to be used for smoothing interior points. The well-known two-dimensional zoning equations will be reviewed and extended to three dimensions formulation.

In two dimensions, the curvilinear coordinates ξ, η satisfy Laplace's equation:

$$\nabla^2 \xi = 0 \quad (4.1a)$$

$$\nabla^2 \eta = 0 \quad (4.1b)$$

Eqns (4.1) can be solved for the coordinates $x(\xi, \eta)$ and $y(\xi, \eta)$ of the mesh lines: that is, the geometric coordinates x, y become the dependent variables and the curvilinear coordinates ξ, η the independent variables. By the usual methods of changing variables, Eqns (4.2) can be obtained:

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$$\alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} = 0 \quad (4.2a)$$

$$\alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} = 0 \quad (4.2b)$$

Where

$$\alpha \equiv x_{\eta}^2 + y_{\eta}^2, \quad \beta \equiv x_{\xi}x_{\eta} + y_{\xi}y_{\eta}, \quad \gamma \equiv x_{\xi}^2 + y_{\xi}^2 \quad (4.3)$$

Eqns (4.2) can be written in vector form

$$\alpha \vec{r}_{\xi\xi} - 2\beta \vec{r}_{\xi\eta} + \gamma \vec{r}_{\eta\eta} = 0 \quad (4.4)$$

Where

$$\vec{r} = x\vec{i} + y\vec{j}$$

Eqn (4.4) can be differenced and solved numerically by an iterative method, since they are nonlinear. In (ξ, η) space, a mesh is used whose curvilinear coordinates are straight lines which take on integer values corresponding to the usual numbering in a two-dimensional mesh. The numerical solution then gives the location of the "equipotential" mesh lines.

In three dimensions x, y, z , a third curvilinear coordinate ζ is added and a third Laplace equation

$$\nabla^2 \zeta = 0 \quad (4.5)$$

Inversion of the system of three eqns (4.1) and (4.5) by change of variable is rather complicated. It is easier, as well as more illuminating, to use the methods of tensor analysis pioneered by Warsi (1982). Let the curvilinear coordinates be represented by ξ^i ($i=1,2,3$). For a scalar function $A(x,y,z)$, Warsi shows that the transformation of its Laplacian from rectangular Cartesian to curvilinear coordinates is given by

$$\nabla^2 A = \sum_{i,j=1}^3 g^{ij} A_{\xi^i \xi^j} + \sum_{k=1}^3 (\nabla^2 \xi^k) A_{\xi^k} \quad (4.6)$$

where a variable subscript indicates differentiation with respect to that variable.

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Since the curvilinear coordinates are each assumed to satisfy Laplace's equation, the second summation in eqn (4.6) vanishes and

$$\nabla^2 A = \sum_{i,j=1}^3 g^{ij} A_{\xi^i \xi^j} \quad (4.7)$$

If $A = x, y,$ and z successively, the left-hand side of (4.7) vanishes in each case and three equations can be written in vector form

$$\sum_{i,j=1}^3 g^{ij} \vec{r}_{\xi^i \xi^j} = 0 \quad (4.8)$$

Eqn (4.8) is the three-dimensional generalization of eqns (4.5), and it only remains to determine the components of the contravariant metric tensor g^{ij} in three dimensions. These are defined to be

$$g^{ij} \equiv \vec{a}^i \cdot \vec{a}^j \quad (4.9)$$

where the contravariant base vectors of the transformation from (x,y,z) to (ξ^1, ξ^2, ξ^3) are given by

$$\vec{a}^i \equiv \nabla \xi^i = \frac{\vec{a}_j \times \vec{a}_k}{\sqrt{g}} \quad (4.10)$$

(i,j,k cyclic). Here the covariant base vectors, the coordinate derivatives, are given by

$$\vec{a}_i \equiv \vec{r}_{\xi^i} \quad (4.11)$$

Where

$$\vec{r} \equiv x\vec{i} + y\vec{j} + z\vec{k}$$

Also,

$$g \equiv \det g_{ij} = [\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)]^2 = J^2 \quad (4.12)$$

where g_{ij} is the covariant metric tensor given by

$$g_{ij} \equiv \vec{a}_i \cdot \vec{a}_j \quad (4.13)$$

And J is the Jacobian of the transformation.

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Substituting (4.10) into (4.9), and using the vector identity

$$(\vec{a} \times \vec{b}) \cdot (\vec{c} \times \vec{d}) \equiv (\vec{a} \cdot \vec{c})(\vec{b} \cdot \vec{d}) - (\vec{a} \cdot \vec{d})(\vec{b} \cdot \vec{c}) \quad (4.14)$$

The following can be obtained:

$$gg^{ii} = \vec{a}_j^2 \vec{a}_k^2 - (\vec{a}_j \cdot \vec{a}_k)^2 = g_{jj}g_{kk} - (g_{jk})^2 \quad (4.15a)$$

$$gg^{ij} = (\vec{a}_i \cdot \vec{a}_k)(\vec{a}_j \cdot \vec{a}_k) - (\vec{a}_i \cdot \vec{a}_j)\vec{a}_k^2 = g_{ik} - g_{ij}g_{kk} \quad (4.15b)$$

Before substituting (4.11) into (4.15a, b), original notation is used:

$$\xi \equiv \xi^1, \eta \equiv \xi^2, \zeta \equiv \xi^3 \quad (4.16)$$

Then, the following can be obtained by using eqn(4.11),:

$$gg^{11} = \vec{r}_\eta^2 \vec{r}_\zeta^2 - (\vec{r}_\eta \cdot \vec{r}_\zeta)^2 \quad (4.17a)$$

$$gg^{22} = \vec{r}_\zeta^2 \vec{r}_\xi^2 - (\vec{r}_\zeta \cdot \vec{r}_\xi)^2 \quad (4.17b)$$

$$gg^{33} = \vec{r}_\xi^2 \vec{r}_\eta^2 - (\vec{r}_\xi \cdot \vec{r}_\eta)^2 \quad (4.17c)$$

for the three diagonal components, and

$$gg^{12} = (\vec{r}_\xi \cdot \vec{r}_\zeta)(\vec{r}_\eta \cdot \vec{r}_\zeta) - (\vec{r}_\xi \cdot \vec{r}_\eta)\vec{r}_\zeta^2 \quad (4.18a)$$

$$gg^{23} = (\vec{r}_\eta \cdot \vec{r}_\xi)(\vec{r}_\zeta \cdot \vec{r}_\xi) - (\vec{r}_\eta \cdot \vec{r}_\zeta)\vec{r}_\xi^2 \quad (4.18b)$$

$$gg^{31} = (\vec{r}_\zeta \cdot \vec{r}_\eta)(\vec{r}_\xi \cdot \vec{r}_\eta) - (\vec{r}_\zeta \cdot \vec{r}_\xi)\vec{r}_\eta^2 \quad (4.18c)$$

for the three off-diagonal components of this symmetric tensor.

Eqns (4.17) are expressed in terms of the Cartesian coordinates, it can be written as

$$gg^{11} = (x_\eta y_\zeta - x_\zeta y_\eta)^2 + (x_\eta z_\zeta - x_\zeta z_\eta)^2 + (y_\eta z_\zeta - y_\zeta z_\eta)^2 \quad (4.19a)$$

$$gg^{22} = (x_\zeta y_\xi - x_\xi y_\zeta)^2 + (x_\zeta z_\xi - x_\xi z_\zeta)^2 + (y_\zeta z_\xi - y_\xi z_\zeta)^2 \quad (4.19b)$$

$$gg^{33} = (x_\xi y_\eta - x_\eta y_\xi)^2 + (x_\xi z_\eta - x_\eta z_\xi)^2 + (y_\xi z_\eta - y_\eta z_\xi)^2 \quad (4.19c)$$

It can be obtained by writing out eqns (4.18):

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$$\begin{aligned}
gg^{12} &= (x_\xi x_\zeta + y_\xi y_\zeta + z_\xi z_\zeta)(x_\eta x_\zeta + y_\eta y_\zeta + z_\eta z_\zeta) - (x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta)(x_\zeta^2 + y_\zeta^2 + z_\zeta^2) \\
gg^{23} &= (x_\eta x_\xi + y_\eta y_\xi + z_\eta z_\xi)(x_\zeta x_\xi + y_\zeta y_\xi + z_\zeta z_\xi) - (x_\eta x_\zeta + y_\eta y_\zeta + z_\eta z_\zeta)(x_\xi^2 + y_\xi^2 + z_\xi^2) \\
gg^{31} &= (x_\zeta x_\eta + y_\zeta y_\eta + z_\zeta z_\eta)(x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta) - (x_\zeta x_\xi + y_\zeta y_\xi + z_\zeta z_\xi)(x_\eta^2 + y_\eta^2 + z_\eta^2)
\end{aligned} \tag{4.20}$$

Hence finally eqns (4.9) can be written in the form

$$g(g^{11}\vec{r}_{\xi\xi} + g^{22}\vec{r}_{\eta\eta} + g^{33}\vec{r}_{\zeta\zeta} + 2g^{12}\vec{r}_{\xi\eta} + 2g^{23}\vec{r}_{\eta\zeta} + 2g^{31}\vec{r}_{\zeta\xi}) = 0 \tag{4.21}$$

where the gg^{ij} are given by eqns (4.19) and (4.20). Because eqns (4.8) are homogeneous, gg^{ij} can be used in place of g^{ij} as long as g is positive, as it must be for a nonsingular transformation. Positivity at each mesh point can be tested by using eqn(4.22):

$$\sqrt{g} = J = \begin{vmatrix} x_\xi & y_\xi & z_\xi \\ x_\eta & y_\eta & z_\eta \\ x_\zeta & y_\zeta & z_\zeta \end{vmatrix} \tag{4.22}$$

and requiring that $J > 0$.

To check that these equations reproduce the two-dimensional equations when there is no variation in one dimension, ξ is taken as the invariant direction, thus reducing eqn (4.21) to

$$gg^{11}\vec{r}_{\xi\xi} + 2gg^{12}\vec{r}_{\xi\eta} + gg^{22}\vec{r}_{\eta\eta} = 0 \tag{4.23}$$

If $\zeta = z$, then the covariant base vectors become

$$\vec{a}_1 = x_\xi \vec{i} + y_\xi \vec{j} \tag{4.24a}$$

$$\vec{a}_2 = x_\eta \vec{i} + y_\eta \vec{j} \tag{4.24b}$$

$$\vec{a}_3 = \vec{k} \tag{4.24c}$$

From (4.24), using (4.15), eqns(4.25) can be obtained:

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$$gg^{11} = x_{\eta}^2 + y_{\eta}^2 \quad (4.25a)$$

$$gg^{22} = x_{\xi}^2 + y_{\xi}^2 \quad (4.25b)$$

$$gg^{12} = -(x_{\xi}x_{\eta} + y_{\xi}y_{\eta}) \quad (4.25c)$$

Substituting eqn(4.25) into eqn(4.23) yields the two-dimensional equipotential zoning eqns (4.2).

Before differencing eqns (4.21), the notation can be simplified and be written in the form

$$\alpha_1 \bar{r}_{\xi\xi} + \alpha_2 \bar{r}_{\eta\eta} + \alpha_3 \bar{r}_{\zeta\zeta} + 2\beta_1 \bar{r}_{\xi\eta} + 2\beta_2 \bar{r}_{\eta\zeta} + 2\beta_3 \bar{r}_{\zeta\xi} = 0 \quad (4.26)$$

where

$$\begin{aligned} \alpha_1 &= (x_{\eta}y_{\zeta} - x_{\zeta}y_{\eta})^2 + (x_{\eta}z_{\zeta} - x_{\zeta}z_{\eta})^2 + (y_{\eta}z_{\zeta} - y_{\zeta}z_{\eta})^2 \\ \alpha_2 &= (x_{\zeta}y_{\xi} - x_{\xi}y_{\zeta})^2 + (x_{\zeta}z_{\xi} - x_{\xi}z_{\zeta})^2 + (y_{\zeta}z_{\xi} - y_{\xi}z_{\zeta})^2 \\ \alpha_3 &= (x_{\xi}y_{\eta} - x_{\eta}y_{\xi})^2 + (x_{\xi}z_{\eta} - x_{\eta}z_{\xi})^2 + (y_{\xi}z_{\eta} - y_{\eta}z_{\xi})^2 \\ \beta_1 &= (x_{\xi}x_{\zeta} + y_{\xi}y_{\zeta} + z_{\xi}z_{\zeta})(x_{\eta}x_{\zeta} + y_{\eta}y_{\zeta} + z_{\eta}z_{\zeta}) - (x_{\xi}x_{\eta} + y_{\xi}y_{\eta} + z_{\xi}z_{\eta})(x_{\zeta}^2 + y_{\zeta}^2 + z_{\zeta}^2) \\ \beta_2 &= (x_{\eta}x_{\xi} + y_{\eta}y_{\xi} + z_{\eta}z_{\xi})(x_{\zeta}x_{\xi} + y_{\zeta}y_{\xi} + z_{\zeta}z_{\xi}) - (x_{\zeta}x_{\eta} + y_{\zeta}y_{\eta} + z_{\zeta}z_{\eta})(x_{\xi}^2 + y_{\xi}^2 + z_{\xi}^2) \\ \beta_3 &= (x_{\eta}x_{\zeta} + y_{\eta}y_{\zeta} + z_{\eta}z_{\zeta})(x_{\xi}x_{\eta} + y_{\xi}y_{\eta} + z_{\xi}z_{\eta}) - (x_{\xi}x_{\eta} + y_{\xi}y_{\eta} + z_{\xi}z_{\eta})(x_{\zeta}^2 + y_{\zeta}^2 + z_{\zeta}^2) \end{aligned} \quad (4.27)$$

Eqns (4.26) can be differenced in a cube in the rectangular $\xi\eta\zeta$ space with unit spacing between the coordinate surfaces, using subscript i to represent the ξ direction, j the η direction, and k the ζ direction, as shown in Fig 4.11.

Figure 4.11 Rectangular $\xi\eta\zeta$ space

Using central differencing, the following finite difference approximations for the coordinate derivatives can be obtained:

$$\vec{r}_{\xi} = (\vec{r}_{i+1} - \vec{r}_{i-1}) \quad (4.28a)$$

$$\vec{r}_{\eta} = (\vec{r}_{j+1} - \vec{r}_{j-1}) \quad (4.28b)$$

$$\vec{r}_{\zeta} = (\vec{r}_{k+1} - \vec{r}_{k-1}) \quad (4.28c)$$

$$\vec{r}_{\xi\xi} = (\vec{r}_{i+1} - 2\vec{r} + \vec{r}_{i-1}) \quad (4.28d)$$

$$\vec{r}_{\eta\eta} = (\vec{r}_{j+1} - 2\vec{r} + \vec{r}_{j-1}) \quad (4.28e)$$

$$\vec{r}_{\zeta\zeta} = (\vec{r}_{k+1} - 2\vec{r} + \vec{r}_{k-1}) \quad (4.28f)$$

$$\vec{r}_{\xi\eta} = \frac{1}{4}[(\vec{r}_{i+1,j+1} + \vec{r}_{i-1,j-1}) - (\vec{r}_{i+1,j-1} + \vec{r}_{i-1,j+1})] \quad (4.28g)$$

$$\vec{r}_{\eta\zeta} = \frac{1}{4}[(\vec{r}_{j+1,k+1} + \vec{r}_{j-1,k-1}) - (\vec{r}_{j+1,k-1} + \vec{r}_{j-1,k+1})] \quad (4.28h)$$

$$\vec{r}_{\xi\zeta} = \frac{1}{4}[(\vec{r}_{i+1,k+1} + \vec{r}_{i-1,k-1}) - (\vec{r}_{i+1,k-1} + \vec{r}_{i-1,k+1})] \quad (4.28i)$$

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where for brevity subscripts i, j, or k (e.g., k+1 stands for i, j, k+1) have been omitted. Note that these difference expressions use only coordinate planes that pass through the central point, and therefore do not include the eight corners of the cube.

Substituting eqns (4.28) into (4.26,4.27) and collecting terms, eqn(4.29) can be obtained

$$\sum \omega_m (\vec{r}_m - \vec{r}) = 0 \quad (4.29)$$

where the sum is obtained over the 18 nearest (in the transform space) neighbours of the given point. The coefficients ω_m are given in Table 4.1.

Eqn (4.29) can be written

$$\vec{r} = \frac{\sum_m \omega_m \vec{r}_m}{\sum_m \omega_m} \quad (4.30)$$

expressing the position of the central point as a weighted mean of its 18 nearest neighbours. The denominator of eqn(4.30) is equal to $2(\alpha_1 + \alpha_2 + \alpha_3)$ which is guaranteed to be positive by eqn(4.27). This vector equation is equivalent to the three scalar equations

$$x = \frac{\sum_m \omega_m x_m}{\sum_m \omega_m} \quad (4.31a)$$

$$y = \frac{\sum_m \omega_m y_m}{\sum_m \omega_m} \quad (4.31b)$$

$$z = \frac{\sum_m \omega_m z_m}{\sum_m \omega_m} \quad (4.31c)$$

The same weights ω_m appear in each equation.

These equations are nonlinear, since the coefficients are functions of the coordinates.

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Therefore they can be solved by an iterative scheme. When applied to eqn(4.31a), for example, this gives for the $(n+1)^{\text{st}}$ iteration

$$x^{n+1} = (1 - f)x^n + f\left(\frac{\sum_m \omega_m x_m}{\sum_m \omega_m}\right) \quad (4.32)$$

where the over relaxation factor f must satisfy $0 < f < 2$. In (4.32) the values of x_m at the neighbouring points are the latest available values. The coefficients ω_m are recalculated before each iteration using Table 4.1 and eqns (4.27).

To smooth one interior point in a three-dimensional mesh, let the point to be smoothed be the interior point of Fig 4.11, assuming that its neighbourhood has the logical structure shown. Even though eqns(4.31) are nonlinear, the ω_m do not involve the coordinates of the central point, since the α 's and β 's do not. Hence eqns (4.31) can be simply solved for the new coordinates (x, y, z) , holding the 18 neighbouring points fixed, without needing to iterate.

If a group of interior points need to be smoothed, eqn(4.32) can be solved iteratively.

<u>m</u>	<u>index</u>	<u>ω_m</u>
1	i+1	α_1
2	i-1	α_1
3	j+1	α_2
4	j-1	α_2
5	k+1	α_3
6	k-1	α_3
7	i+1, j+1	$\beta_1/2$
8	i-1, j-1	$\beta_1/2$
9	i+1, j-1	$-\beta_1/2$
10	i-1, j+1	$-\beta_1/2$
11	j+1, k+1	$\beta_2/2$
12	j-1, k-1	$\beta_2/2$
13	j+1, k-1	$-\beta_2/2$
14	j-1, k+1	$-\beta_2/2$
15	i+1, k+1	$\beta_3/2$
16	i-1, k-1	$\beta_3/2$
17	i+1, k-1	$-\beta_3/2$
18	i-1, k+1	$-\beta_3/2$

Table 4.1 : 3D zoning weight coefficients

■ 4.3.3 Advection algorithms

LS-DYNA (the commercial software package used in the thesis) follows the SALE3D (a simplified ALE computer program for calculating three-dimensional fluid flow) strategy for calculating the transport of the element-centred variables (i.e., density, internal energy, the stress tensor and the history variables). The van

Leer MUSCL (monotone upwind schemes for conservation laws) scheme (van Leer 1977) is to calculate the values of the solution variables in the transport fluxes to achieve second order accurate monotonic results. To calculate the momentum transport, two algorithms have been implemented. The less expensive of the two is the one that is implemented in SALE3D, but it has known dispersion problems and may violate monotonicity (i.e., introduce spurious oscillations) (Benson, 1992a). As an alternative, a significantly more expensive method (Benson, 1992b), which can be shown analytically to not have either problem on a regular mesh, has also been implemented.

■ 4.3.3.1 Advection methods in one dimension

In this section the donor cell and van Leer MUSCL scheme are discussed. Both methods are one-dimensional and their extensions to multidimensional problems are presented later.

The remap step maps the solution from a distorted Lagrangian mesh on to the new mesh. The underlying assumptions of the remap step are 1) the topology of the mesh is fixed (a complete rezone does not have this limitation), and 2) the mesh motion during a step is less than the characteristic lengths of the surrounding elements. Within the fluids community, the second condition is simply stated as saying the Courant number, C , is less than one.

$$C = \frac{u\Delta t}{\Delta x} = \frac{f}{V} \leq 1 \quad (4.33)$$

Since the mesh motion does not occur over any physical time scale, Δt is arbitrary, and $u\Delta t$ is the transport volume, f , between adjacent elements. The transport volume calculation is purely geometrical for ALE formulations and it is not associated with any of the physics of the problem. The algorithms for performing the remap step are taken from the computational fluids dynamics community, and they are referred to as "advection" algorithms after the first order. Scalar

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conservation equation is frequently used as a model hyperbolic problem.

A good advection algorithm for the remap step is accurate, stable, conservative and monotonic. Although many of the solution variables, such as the stress and plastic strain, are not governed by conservation equations like momentum and energy, it is still highly desirable that the volume integral of all the solution variables remain unchanged by the remap step. Monotonicity requires that range of the solution variables does not increase during the remap. This is particularly important with mass and energy, where negative values would lead to physically unrealistic solutions.

Much of the research on advection algorithms has focused on developing monotonic algorithms with an accuracy that is at least second order. Not all recent algorithms are monotonic. For example, within the finite element community, the streamline upwind Petrov-Galerkin (SUPG) method developed by Hughes and coworkers (Brooks and Hughes, 1982) is not monotonic. Johnson *et.al.* (1984) has demonstrated that the oscillations in the SUPG solution are localized, and its generalization to systems of conservation equations works very well for the Euler equations. Mizukami and Hughes (1985) later developed a monotonic SUPG formulation. The essentially non-oscillatory (ENO) (Harten, 1989) finite difference algorithms are also not strictly monotonic, and work well for the Euler equations, but their application to hydrodynamics problems has resulted in negative densities (McGlaun, 1990). Virtually all the higher order methods that are commonly used were originally developed for solving the Euler equations, usually as higher order extensions to Godunov's method. Since the operator split approach is the dominant one in Eulerian hydrocodes, these methods are implemented only to solve the scalar advection equation.

The Donor cell algorithm.

Aside from its first order accuracy, it is everything a good advection algorithm should be: stable, monotonic, and simple. The value of $f_{j+1/2}^n$ is dependent on the sign of a at node j , which defines the upstream direction.

$$\phi_{j+1/2}^{n+1} = \phi_{j+1/2}^n + \frac{\Delta t}{\Delta x} (f_j^\phi - f_{j+1}^\phi) \quad (4.34a)$$

$$f_j^\phi = \frac{a_j}{2} (\phi_{j-1/2}^n + \phi_{j+1/2}^n) + \frac{|a_j|}{2} (\phi_{j-1/2}^n - \phi_{j+1/2}^n) \quad (4.34b)$$

The donor cell algorithm is a first order Godunov method applied to the advection equation. The initial values of ϕ to the left and the right of node j are $\phi_{j-1/2}^n$ and $\phi_{j+1/2}^n$, and the velocity of the contact discontinuity at node j is a_j .

The Van Leer MUSCL algorithm.

Van Leer (1977) introduced a family of higher order Godunov methods by improving the estimates of the initial values of left and right states for the Riemann problem at the nodes. The particular advection algorithm that is presented in this section is referred to as the MUSCL algorithm for brevity, although MUSCL really refers to the family of algorithms that can be applied to systems of equations.

The donor cell algorithm assumes that the distribution of ϕ is constant over an element. Van Leer replaces the piecewise constant distribution with a higher order interpolation function, $\phi_{j+1/2}^n(x)$ that is subject to an element level conservation constraint. The value of ϕ at the element centroid is regarded in this context as the average value of ϕ over the element instead of the spatial value at $x_{j+1/2}$.

$$\phi_{j+1/2}^n = \int_{x_j}^{x_{j+1}} \phi_{j+1/2}^n(x) dx \quad (4.35)$$

To determine the range of ϕ , $[\phi_{j+1/2}^{\min}, \phi_{j+1/2}^{\max}]$, for imposing the monotonicity

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constraint, the maximum and minimum values of $\phi_{j-1/2}^n, \phi_{j+1/2}^n$ and $\phi_{j+3/2}^n$ are used. Monotonicity can be imposed in either of two ways. The first is to require that the maximum and minimum values of $\phi_{j+1/2}^n(x)$ fall within the range determined by the three elements. The second is to restrict the average value of ϕ in the transport volumes associated with element $j + 1/2$. While the difference may appear subtle, the actual difference between the two definitions is quite significant even at relatively low Courant numbers. The second definition allows the magnitude of the ϕ transported to adjacent elements to be larger than the first definition. As a consequence, the second definition is better able to transport solutions with large discontinuities.

The first step up from a piecewise constant function is a piecewise linear function, where x is now the volume coordinate. The volume coordinate of a point is simply the volume swept along the path between the element centroid and the point. Conservation is guaranteed by expanding the linear function about the element centroid.

$$\phi_{j+1/2}^n(x) = S_{j+1/2}^n(x - x_{j+1/2}^n) + \phi_{j+1/2}^n \quad (4.36)$$

Letting $s_{j+1/2}^n$ be a second order approximation of the slope, the monotonicity limited value of the slope, $S_{j+1/2}^n$, according to the first limiting approach, is determined by assuming the maximum permissible values at the element boundaries.

$$S_{j+1/2}^n = \frac{1}{2}(\text{sgn}(s^L) + \text{sgn}(s^R)) \times \min(|s^L|, |s_{j+1/2}^n|, |s^R|) \quad (4.37a)$$

$$s^L = \frac{\phi_{j+1/2}^n - \phi_{j-1/2}^n}{\frac{1}{2}\Delta x_{j+1/2}} \quad (4.37b)$$

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$$s^R = \frac{\phi_{j+3/2}^n - \phi_{j+1/2}^n}{\frac{1}{2}\Delta x_{j+1/2}} \quad (4.37c)$$

The second limiter is similar to the first, but it assumes that the maximum permissible values occur at the centroid of the transport volumes. Note that as stated in eqns(4.37), this limiter still limits the slope at the element boundary even if the element is the downstream element at that boundary. A more compressive limiter would not limit the slope based on the values of ϕ at the downstream boundaries.

For example, if a_j is negative, only s^R would limit the value of s^n in eqns (4.37). If the element is the downstream element at both boundaries, then the slope in the element has no effect on the solution.

$$s^L = \frac{\phi_{j+1/2}^n - \phi_{j-1/2}^n}{\frac{1}{2}\Delta x_{j+1/2} - \frac{1}{2}\max(0, a_j\Delta t)} \quad (4.38a)$$

$$s^R = \frac{\phi_{j+3/2}^n - \phi_{j+1/2}^n}{\frac{1}{2}\Delta x_{j+1/2} + \frac{1}{2}\min(0, a_{j+1}\Delta t)} \quad (4.38b)$$

The flux at node j is evaluated using the upstream approximation of ϕ .

$$f_j^\phi = \frac{a_j}{2}(\phi_j^- + \phi_j^+) + \frac{|a_j|}{2}(\phi_j^- - \phi_j^+) \quad (4.39a)$$

$$\phi_j^+ = S_{j+1/2}^n(x^C - x_{j+1/2}^n) + \phi_{j+1/2}^n \quad (4.39b)$$

$$\phi_j^- = S_{j-1/2}^n(x^C - x_{j-1/2}^n) + \phi_{j-1/2}^n \quad (4.39c)$$

$$x^C = x_j^n + \frac{1}{2}\Delta t a_j \quad (4.39d)$$

The method for obtaining the higher order approximation of the slope is not unique. Perhaps the simplest approach is to fit a parabola through the centroids of the three adjacent elements and evaluate its slope at $x_{j+1/2}^n$. When the value of ϕ at the element centroids is assumed to be equal to the element average this algorithm

defines a projection.

$$s_{j+1/2}^n = \frac{(\phi_{j+3/2}^n - \phi_{j+1/2}^n)\Delta x_j^2 + (\phi_{j+1/2}^n - \phi_{j-1/2}^n)\Delta x_{j+1}^2}{\Delta x_j \Delta x_{j+1} (\Delta x_j + \Delta x_{j+1})} \quad (4.40a)$$

$$\Delta x_j = x_{j+1/2}^n - x_{j-1/2}^n \quad (4.40b)$$

■ 4.3.3.2 Advection methods in three dimensions

For programs that use a logically regular mesh, one-dimensional advection methods are extended to two and three dimensions by using a sequence of one-dimensional sweeps along the logically orthogonal mesh lines. This strategy is not possible for unstructured meshes because they don't have uniquely defined sweep directions through the mesh. CAVEAT (Addessio, *et. al.* 1986) uses one-dimensional sweeps in the spatial coordinate system, but their approach is expensive relative to the other algorithms and it does not always maintain spherical symmetry, which is an important consideration in underwater explosion calculations.

The advection in LS-DYNA is performed isotropically. The fluxes through each face of element A are calculated simultaneously, but the values of ϕ in the transport volumes are calculated using the one-dimensional expressions developed in the previous sections.

$$\phi_A^{n+1} = \frac{1}{V_A^{n+1}} (V_A^n \phi_A^n + \sum_{j=1}^6 f_j^\phi) \quad (4.41)$$

The disadvantage of isotropic advection is that there is no coupling between an element and the elements that are joined to it only at its corners and edges (i.e., elements that don't share faces). The lack of coupling introduces a second order error that is significant only when the transport is along the mesh diagonals.

The one-dimensional MUSCL scheme, which requires elements on either side of the element whose transport is being calculated, can not be used on the boundary elements in the direction normal to the boundary. Therefore, in the boundary

elements, the donor cell algorithm is used to calculate the transport in the direction that is normal to the boundary, while the MUSCL scheme is used in the two tangential directions.

It is implicitly assumed by the transport calculations that the solution variables are defined per unit current volume. In LS-DYNA, some variables, such as the internal energy, are stored in terms of the initial volume of the element. These variables must be rescaled before transport, then the initial volume of the element is advected between the elements, and then the variables are rescaled using the new "initial" volumes.

■ 4.4 Penalty method

The method which is taken to simulate interaction between CB and MM is penalty method. The forces generated between contact surfaces are determined by the depth of penetrating and young's modulus of each contact materials. It acts like putting elastic springs between contact surfaces. Interfaces can be defined in three dimensions by listing in arbitrary order all triangular and quadrilateral segments that comprise each side of the interface. One side of the interface is designated as the slave side (CB), and the other is designated as the master side (MM, Fig. 4.12). Nodes lying in those surfaces are referred to as slave and master nodes, respectively. In the symmetric penalty method, this distinction is irrelevant, but this method consists of placing normal interface springs between all penetrating nodes and the contact surface. With the exception of the spring stiffness matrix which must be assembled into the global stiffness matrix, the implicit and explicit treatments are similar. The penalty method approach is found to excite little if any mesh hourglassing. This lack of noise is undoubtedly attributable to the symmetry of the approach. Momentum is exactly conserved without the necessity of imposing impact and release conditions. Furthermore, no special treatment of intersecting interfaces is required, greatly simplifying the implementation. The interface

stiffness is chosen to be approximately the same order of magnitude as the stiffness of the interface elements normal to the interface. Consequently the computed time step size is unaffected by the existence of the interfaces. However, if interface pressures become large, unacceptable penetration may occur. By scaling up the stiffness and scaling down the time step size, such problems can still be solved by using penalty approach.

Figure 4.12 Interaction between slave surface and master surface

■ 4.4.1 Slave search

The slave search is common to all interface algorithms implemented in DYNA3D. This search finds for each slave node its nearest point on the master surface. Lines drawn from a slave node to its nearest point will be perpendicular to the master surface, unless the point lies along the intersection of two master segments, where a segment is defined to be a 3- or 4-node element of a surface.

Consider a slave node, n_s , sliding on a piecewise smooth master surface and assume that a search of the master surface has located the master node, m_s , lying nearest to n_s . Fig 4.13 depicts a portion of a master surface with nodes m_s and n_s labelled. If m_s and n_s do not coincide, n_s can usually be shown to lie in a segment s_i via the following tests:

$$(c_i \times s) \cdot (c_i \times c_{i+1}) > 0 \quad (4.42a)$$

$$(c_i \times s) \cdot (s \times c_{i+1}) > 0 \quad (4.42b)$$

where vector c_i and c_{i+1} are along edges of s_i and point outward from m_s .

Vector s is the projection of the vector beginning at m_s , ending at n_s , and denoted by $\mathbf{g}$, onto the plane being examined (see Fig 4.14).

$$s = g - (g \cdot m)m \quad (4.43)$$

Figure 4.13 Four master segments can harbor slave node n_s , given that m_s is the nearest master node.

Figure 4.14 Projection of $\mathbf{g}$ onto master segment s_i .

where for segment s_i

$$m = \frac{c_i \times c_{i+1}}{|c_i \times c_{i+1}|} \quad (4.44)$$

Since the sliding constraints keep n_s , close but not necessarily on the master surface and since n_s may lie near or even on the intersection of two master segments, the inequalities of eqns (4.42) may be inconclusive, i.e., they may fail to be satisfied or more than one may give positive results. When this occurs n_s is assumed to lie along the intersection which yields the maximum value for the quantity

$$\frac{\mathbf{g} \cdot \mathbf{c}_i}{|\mathbf{c}_i|} \quad i = 1, 2, 3, 4 \quad (4.45)$$

When the contact surface is made up of badly shaped elements, the segment apparently identified as containing the slave node actually may not, as shown in Fig 4.15.

Figure 4.15 When the nearest node fails to contain the segment that harbors the slave node, segments numbered 1-8 are searched in the order shown.

Assume that a master segment has been located for slave node n_s and that n_s is not identified as lying on the intersection of two master segments. Then the identification of the contact point, defined as the point on the master segment which is nearest to n_s , becomes nontrivial. Each master surface segment, s_i is given the parametric representation of eqn (4.46), repeated here for clarity:

$$r = f_1(\xi, \eta)i_1 + f_2(\xi, \eta)i_2 + f_3(\xi, \eta)i_3 \quad (4.46)$$

Where

$$f_i(\xi, \eta) = \sum_{j=1}^4 \phi_j x_i^j \quad (4.47)$$

Note that r_i is at least once continuously differentiable and that

$$\frac{\partial r}{\partial \xi} \times \frac{\partial r}{\partial \eta} \neq 0 \quad (4.48)$$

Thus $\mathbf{r}$ represents a master segment that has a unique normal whose direction depends continuously on the points of s_i .

Let $\mathbf{t}$ be a position vector drawn to slave node n , and assume that the master surface segment s_i has been identified with n_s . The contact point coordinates (ξ_c, η_c) on s_i must satisfy

$$\frac{\partial r}{\partial \xi}(\xi_c, \eta_c) \cdot [\mathbf{t} - \mathbf{r}(\xi_c, \eta_c)] = 0 \quad (4.49a)$$

$$\frac{\partial r}{\partial \eta}(\xi_c, \eta_c) \cdot [\mathbf{t} - \mathbf{r}(\xi_c, \eta_c)] = 0 \quad (4.49b)$$

Figure 4.16 Location of contact point when n_s lies above master segment.

The physical problem is illustrated in Fig.4.16 which shows n_s lying above the master surface. Eqns (4.49a) and (4.49b) are readily solved for ξ_c and η_c . One way to accomplish this is to solve Equation (4.49a) for ξ_c , in terms of η_c , and substitute the results into Equation (4.49b). This yields a cubic equation in η_c , which is presently solved numerically in LS-DYNA.

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The equations are solved numerically. When two nodes of a bilinear quadrilateral are collapsed into a single node for a triangle, the Jacobian of the minimization problem is singular at the collapsed node. Fortunately, there is an analytical solution for triangular segments since three points define a plane. Newton-Raphson iteration is a natural choice for solving these simple nonlinear equations. The method diverges with distorted elements unless the initial guess is accurate.

Three iterations with a least-squares projection are used to generate an initial guess:

$$\xi_0 = 0, \eta_0 = 0, \quad (4.50a)$$

$$\begin{bmatrix} r_{,\xi} \\ r_{,\eta} \end{bmatrix} \begin{bmatrix} r_{,\xi} & r_{,\eta} \end{bmatrix} \begin{Bmatrix} \Delta\xi \\ \Delta\eta \end{Bmatrix} = \begin{bmatrix} r_{,\xi} \\ r_{,\eta} \end{bmatrix} \{r(\xi_i, \eta_i) - t\} \quad (4.50b)$$

$$\xi_{i+1} = \xi_i + \Delta\xi, \eta_{i+1} = \eta_i + \Delta\eta \quad (4.50c)$$

followed by the Newton-Raphson iterations which are limited to ten iterations, but which usually converges in four or less.

$$[H] \begin{Bmatrix} \Delta\xi \\ \Delta\eta \end{Bmatrix} = - \begin{Bmatrix} r_{,\xi} \\ r_{,\eta} \end{Bmatrix} \{r(\xi_i, \eta_i) - t\}, \quad (4.51a)$$

$$[H] = \begin{Bmatrix} r_{,\xi} \\ r_{,\eta} \end{Bmatrix} \begin{bmatrix} r_{,\xi} & r_{,\eta} \end{bmatrix} + \begin{bmatrix} 0 & r \cdot r_{,\xi\eta} \\ r \cdot r_{,\xi\eta} & 0 \end{bmatrix}, \quad (4.51b)$$

$$\xi_{i+1} = \xi_i + \Delta\xi, \eta_{i+1} = \eta_i + \Delta\eta \quad (4.51c)$$

In concave regions, a slave node may have isoparametric coordinates that lie outside of the $[-1, +1]$ range for all of the master segments, yet still have penetrated the surface. A simple strategy is used for handling this case, but it can fail. The contact segment for each node is saved every time step. If the slave node contact point defined in terms of the isoparametric coordinates of the segment, is just outside of the segment, and the node penetrated the isoparametric surface, and no other segment associated with the nearest neighbor satisfies the inequality test, then

the contact point is assumed to occur on the edge of the segment. In effect, the definition of the master segments are extended so that they overlap by a small amount. In the hydrocode literature, this approach is similar to the slide line extensions used in two dimensions. This simple procedure works well for most cases, but it can fail in situations involving sharp concave comers.

■ 4.4.2 Sliding with closure and separation

In applying this penalty method, each slave node is checked for penetration through the master surface. If the slave node does not penetrate, nothing is done. If it does penetrate, an interface force is applied between the slave node and its contact point. The magnitude of this force is proportional to the amount of penetration. This may be thought of as the addition of an interface spring.

Penetration of the slave node n_s through the master segment which contains its contact point is indicated if

$$l = n_i \cdot [t - r(\xi_c, \eta_c)] < 0 \quad (4.52)$$

Where

$$n_i = n_i(\xi_c, \eta_c)$$

is normal to the master segment at the contact point.

If slave node n_s , has penetrated through master segment s_i , an interface force vector f_s is added

$$f_s = -lk_i n_i \quad \text{if} \quad l < 0 \quad (4.53)$$

to the degrees of freedom corresponding to n_s and

$$f_m^i = \phi_i(\xi_c, \eta_c) f_s \quad \text{if} \quad l < 0 \quad (4.54)$$

to the four nodes ($i = 1, 2, 3, 4$) that comprise master segment s_i . The stiffness factor k_i for master segment s_i is given in terms of the bulk modulus K_i , the volume V_i , and the face area A_i of the element that contains s_i as

$$k_i = \frac{f_{si} K_i A_i^2}{V_i} \quad (4.55)$$

for brick elements and

$$k_i = \frac{f_{si} K_i A_i}{\max(\text{shell diagonal})} \quad (4.56)$$

for shell elements where f_{si} is a scale factor for the interface stiffness and is normally defaulted to 0.1. Larger values may cause instabilities unless the time step size is scaled back in the time step calculation.

■ 4.5 Material properties in FEM model

■ 4.5.1 Material properties of 3D element for MM

The material properties of 3D elements for MM are: density $1.37 \times 10^3 \text{ kg/m}^3$, Poisson's ratio 0.495 and stress-strain curve defined in Fig. 3.14.

■ 4.5.2 Material properties of line element for MF

MF are filled up in the whole LV wall, and it is supposed that the density of MF in LV wall are constant. So the cross-section area of each line elements is determined by the volume of each element which the line element are "lying" and the length of the line element. The average cross section area is around $6.5 \times 10^{-4} \text{ m}^2$. At the apex area, the 3D elements reduced to 5 surfaces only and the cross section area of line elements are reduces also.

The density of line element for MF is the same with MM: $1.37 \times 10^3 \text{ kg/m}^3$.

Possion's ratio keeps 0.495 and Young's modulus is $0.5 \times 10^6 \text{ N/m}^2$.

Based on the mathematical model created in Chapter 3, the acting forces generated in Hill's fiber force model during the whole heart cycle can be described as Fig. 4.17.

Figure 4.17 Normalized acting forces generated in MF

■ 4.5.3 Material properties of 3D element for CB

The density of 3D elements for CB is $1.067 \times 10^3 \text{ kg/m}^3$ and the bulk modulus is 250000 N/m^2 for the fluid in normal temperature and low pressure.

■ 4.5.4 Material properties of 3D element for valve and vessel

The young's modulus of 3D element for valve and vessel is assumed as infinite and here it is defined as rigid body. The possion's ratio is defined as 0.495.

■ 4.6 Boundary conditions and initial conditions in FEM model

■ 4.6.1 Boundary condition at MM and vessel

As described in section 3.3.4.1, the apex is fixed. At the apex part of LV model, there are 3 nodes (node 241, 1241, 2241) and all of them are fixed. At the

connecting part between MM base and vessel, the nodes (from node 1 to node 20, and from node 1001 to node 1020) are also fixed. At the epicardium of MM base, the nodes (from node 2001 to 2020) are fixed in x and y directions, it can contract towards apex.

■ 4.6.2 Boundary condition at valve

At the iso-volume contraction and iso-volume relaxation, the nodes of 3D elements for valve are fixed. At the passive fillings and ejection phases, these nodes are set to free. The pressure shown in Fig. 3.17 is acting on the surface of 3D elements for valve.

■ 4.6.3 Residual stress in FEM

At the beginning, the pre-strain in line elements at endocardium position are set be to 0.05 and the pre-strain in line elements at epicardium position are set be 0.05 and pre-strain in line elements at the middle layer are set to be 0.05.

■ 4.7 FEM simulation

One cycle of LV motion is simulated for a heart rate (HR) of 75 beats per minute (one cardiac cycle: 0.8s). The above boundary and initial conditions are set during the cardiac cycle. The open and closing of valves are simulated by constraining or freeing nodes which represent valve. The starting point is filling phase when cavity volume is 106ml. The LV cavity volume keeps rising until the end of diastole. At that time, iso-volume contraction (around 40ms) starts. During this period, both the mitral and aortic valves are closed so that the flow normal velocity is zero at the valves place. The MF are activated by the excitation-contraction mechanism to increase the left ventricle pressure (LVP). When LVP exceeds the aortic pressure (AP), the aortic valve opens, during the ejection period (around 260ms), the mitral valve remains closed. When the AP is higher than LVP, the aortic valve closes and

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isovolumic relaxation (around 60ms) begins. Both of aortic valve and mitral valve close and LVP decreases. When the LVP falls below the left atrium pressure (LAP), the mitral valve opens, and the filling period (around 460ms) continues.

In the process of modeling LV motion, the available package LS-DYNA is used and it is an explicit finite element code which is widely applied in industry for modeling dynamic events. The advantages of this finite element code comparing with others are on fluid-structure interaction and the definition of user-defined material models. All the information about the LV geometry, myocardial material properties, fluid properties, fluid-structure interactions and boundary conditions etc. are converted into the input file. The program is running on PC under Windows operation system.

Chapter 5 Results and Discussions

Using the available FE package LS-DYNA (version 970), the FEM model has been successfully run on a PC (Intel Xeon processor, windows XP operation system). The CPU (central processing unit) times and maximum increment time for five phases (Fig 3.11) are shown in Table 5.1. The attentions will be put on the following results:

- a. Cavity pressure and ejection fraction
- b. Movement of CB and contraction of MF
- c. Deformations of LV wall
- d. Principal stresses in MM
- e. Principal strains in MM and MF
- f. Velocities and displacement of MM towards apex
- g. Twisting of MF

Periods	CPU time	Max. increment time
1	686 s	0.909E-06
2	556 s	0.178E-06
3	5921 s	0.399E-05
4	1021 s	0.399E-05
5	2373 s	0.399E-05
Table 5.1 CPU times and maximum increment time for five simulation periods		

■ 5.1 Cavity pressure and ejection fraction

In the results, the LV cavity pressure (average results taken from the elements at the middle position of the LV cavity) and cavity volume are compared with the data

taken from physiology book (Gillian and Christopher, 2004). The comparisons (Fig. 5.1 & 5.2) show good agreements with each other.

Fig. 5.1 & 5.2 illustrate the major events occurring during a single cardiac cycle. In a resting individual, the heart rate is around 75 beat per minute and each cardiac cycle lasts for about 0.8 s, where systole lasts for 0.3 s and diastole 0.5 s.

In Fig. 5.1 & 5.2, the starting point is the filling phase of LV. Blood flows continually from the veins into the left atrium, and most of it flows directly into the left ventricle (point 'A' to 'B'). Both the pressure and volume of LV increase during this period. Due to the resistance of myocardium and sac, the blood filling becomes very slow in the later period of filling (from point 'B' to 'C'). But during the contraction of the left atrium (point 'C' to 'D'), the pressure keeps rising in the left

Figure 5.1 LV pressure comparison

Figure 5.2 LV volume comparison

atrium, so it pumps some blood into the LV. There is a ‘bump’ in volume which can be observed in Fig. 5.2.

Ventricle contraction starts after the filling phase. For a short time (40ms) the valves at the entrance to the aorta and also the left atrium are shut, so that this is a period of isovolume contraction – the intraventricular pressure rises but the volume does not change. This can be seen (from point ‘D’ to ‘E’) in Fig. 5.2. The ejection phase of ventricular systole (from point ‘E’ to ‘F’) begins when the aortic valve opens (the point at which left ventricular pressure exceeds aortic pressure). There is a period of rapid ejection followed by a period of rather slow emptying. During the rapid ejection phase, both ventricular and aortic pressures rise steeply. For about the last quarter of ventricular systole very little blood flows from the ventricles to the aorta even though the ventricular fibers remains contracted.

At the end of end of ventricular systole, the LV begins to relax so that intraventricular pressures fall rapidly. The higher pressure in the aorta causes the

aortic valve to close, preventing back-flow of blood into the ventricle. There then follows a brief period of isovolume relaxation (from point 'F' to 'G'), during which the ventricular fibers continues to relax (with a concomitant fall in ventricular pressure) but the ventricular volume remains constant because the aortic and mitral valves are not yet open. This phase lasts for 60 ms before the ventricular pressures fall below those of the atria and the mitral valve opens. Ventricular relaxation continues but now blood enters the ventricle from the atria and ventricular volume increases quickly. This (from point 'G' to 'H') can be seen clearly in Fig. 5.2.

The ejection fraction is a very important measurement of the heart's efficiency in clinic and can be used to estimate the function of the left ventricle, which pumps blood to the rest of the body. The left ventricle pumps only a fraction of the blood it contains. The ejection fraction is the amount of blood pumped divided by the amount of blood the ventricle contains. If the heart becomes enlarged, even if the amount of blood being pumped by the left ventricle remains the same, the relative fraction of blood being ejected decreases. If heart infarction happens, the myocardium Young's modulus becomes stiffer which means the ejection fraction decreases also. According to the volume curve in Fig.5.2, the ejection fraction is calculated as 53.8% which means it is at the edge of unhealthy.

▪ 5.2 Movement of CB and contraction of MF

After establishing the finite element model based on appropriate composite material properties, 3 dimensional movement of CB from diastole to systole and back to diastole again can be clearly plotted using the post processor module: LSTC/LSPOST. The entire movement of CB from diastole to systole and back to diastole again is divided into 21 frames and there is 0.04s as an interval between each frame. The filling phase ends at time 0.35s. Then an isovolume contraction continues until time 0.39s. The ejection phase begins until time 0.65s. The end of

isovolume relaxation happens at time 0.69s and filling phase then follows. Fig. 5.3 shows the movement of CB during the whole cardiac cycle. Because MF are filled up in the whole LV cavity, so the MF are surrounding CB, from the Fig. 5.3, the contraction of MF can also be observed. In systole (time 0.35s to 0.69s), it clearly shows the contraction force generated in MF push the CB out of the LV cavity. Because of the apex keeping fixed, the MF contract towards apex and LV cavity inwards.

a. Time 0.0s

b. Time 0.04s

c. Time 0.08s

d. Time 0.12s

e. Time 0.16s

f. Time 0.2s

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g. Time 0.24s

h. Time 0.28s

i. Time 0.32s

j. Time 0.36s

k. Time 0.4s

l. Time 0.44s

m. Time 0.48s

n. Time 0.52s

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Figure. 5.3 Movement of CB and contraction of MM

■ 5.3 Deformations of LV wall

Deformations of LV wall (Fig. 5.4) are another important concern for doctors. With the development of modern imaging techniques (ultrasonic, echocardiography, MRI), LV wall motion can be recorded during the whole cycle. Then the results from simulation can be compared with the data from imaging techniques in order to valid the model and provide the insight for doctors. Fig. 5.4 also presents 21 frames of LV wall deformations during the whole cycle. The time interval between each frame is 0.04s.

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e. Time 0.16s

f. Time 0.2s

g. Time 0.24s

h. Time 0.28s

i. Time 0.32s

j. Time 0.36s

k. Time 0.4s

l. Time 0.44s

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m. Time 0.48s

n. Time 0.52s

o. Time 0.56s

p. Time 0.6s

q. Time 0.64s

r. Time 0.68s

s. Time 0.72s

t. Time 0.76s

u. Time 0.8s

Figure 5.4 Deformations of LV wall

The LV wall deformations in Fig. 5.4 are compared with the magnetic tagging data from Jinah (1996). Although the initial shapes of LV are different, the comparison clearly shows the trend of LV wall getting thicker from the end of diastole to the end of systole and also the LV wall shortening along the long-axis (Figs. 5.5, 5.6, 5.7).

The variations of wall thickness at the midventricular region of the LV are compared (Fig. 5.8) between the reference data (Watanbe et al. 2004) and FEM results (wall thickness between nodes '48' and '2048'). It shows during the whole cardiac cycle, the LV wall thickness changes from 11.0mm to 14.5mm (FEM model) which is close to most of the clinical reports.

Figure 5.5 MRI-SPAMM data points from long-axis view image planes (Jinah, 1996)

(a) Time 1 (b) Time 2 (c) Time 3 (d) Time 4 (e) Time 5
(ED) (ES)

Figure 5.6 Fitted models during systole with SPAMM data points and material points (Jinah, 1996)

(a) Time 1 (b) Time 2 (c) Time 3 (d) Time 4 (e) Time 5
(ED) (ES)

Figure 5.7 LV wall motion during the cardiac cycle in the model

Figure 5.8 Wall thickness comparison between reference (Watanbe et al, 2004) and FEM results

■ 5.4 Principal stresses in MM

The diagnosis of the highest stresses in MM is helpful to doctors to make a judgment. The principal stresses of all the elements in the finite element configuration of the model can be printed out from the model output file. Physically, they indicate the maximum tension that an individual element could generate at each phase. In a 3D finite element model, there are three principal stresses, maximum (tensile if the value is positive), minimum (compressive if the value is negative) and median stress. Principal stresses are shown in Fig. 5.9. The average maximum principal stresses at the endocardium are much higher (even approximately 10 times) than that the stresses at the epicardium. The endocardium suffers much more tension than in the epicardium. And the maximum principal stresses happen at the apex part what is the most complex place of fibers orientations.

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a. Time 0.0s

b. Time 0.04s

c. Time 0.08s

d. Time 0.12s

e. Time 0.16s

f. Time 0.20s

g. Time 0.24s

h. Time 0.28s

Chapter 5 Results and Discussions

i. Time 0.32s

j. Time 0.36s

k. Time 0.4s

l. Time 0.44s

m. Time 0.48s

n. Time 0.52s

o. Time 0.56s

p. Time 0.6s

Figure 5.9 Principal Stresses in MM during the whole cardiac cycle

Table 5.2 shows the average Von-mises stresses from ventricular base (level 1) to ventricular apex (level 12) at the end of systole ($t = 0.65s$). The results are compared with other reference and they are very close. The stresses distribution at the apex area is much higher than other areas. The reason may be due to the fixation of the apex point.

Positions	Average Von-Mises stresses (edocardium) kPa	Avergae Von-Mises stresses (epicardium) kPa	Von-Mises stresses (Kerckhoffs et al, 2003) kPa
Level 1 (LV base)	19.77	24.75	22.9 ± 2.68 (Equator)
Level 2	24.73	24.52	
Level 3	27.51	25.63	
Level 4	26.90	25.01	
Level 5	25.02	22.81	
Level 6 (Equator)	22.61	20.05	
Level 7	18.90	17.54	
Level 8	21.02	17.03	
Level 9	25.05	19.60	
Level 10	35.66	26.49	
Level 11	44.75	33.63	
Level 12 (LV apex)	44.00	34.00	
Table 5.2 Von-Mises stresses distribution at the end of systole (t = 0.65s)			

■ 5.5 Principal strains in MM and MF

The distribution of principal strains in MM is shown in Fig. 5.10. The whole cardiac cycle is also divided into 21 frames and each interval is 0.04s. The principal stresses is hard to compared with the clinic data. But the data of principal strains in MM can be extracted from the deformation of LV wall using the kinematic relationship between displacement and strain. So if the clinic imaging data can be obtained, it can be used to validate the FEM model.

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a. Time 0.0s

b. Time 0.04s

c. Time 0.08s

d. Time 0.12s

e. Time 0.16s

f. Time 0.20s

g. Time 0.24s

h. Time 0.28s

Chapter 5 Results and Discussions

i. Time 0.32s

j. Time 0.36s

k. Time 0.4s

l. Time 0.44s

m. Time 0.48s

n. Time 0.52s

o. Time 0.56s

p. Time 0.6s

Figure 5.10 Principal strains in MM

MF strains (around LV equator area) in endocardium, middle layer and epicardium during the whole cycle are plotted in Fig 5.11. The results are compared with Kerckhoffs et al's (2003) results. The tensile strains in the endocardium are much larger than the tensile strains in the epicardium at the end of diastole.

a. Fiber strains (near equator area) in endocardium

b. Fiber strains (near equator area) in middle layer

c. Fiber strains (near equator area) in epicardium

5.11 MF strains

■ 5.6 Velocities and displacement of MM towards the apex

The velocity vectors acquired by the FEM results show a locally different velocity distribution throughout the whole cardiac cycle (Fig. 5.12). The results in this figure show that during diastole, the velocities of MM change very slowly but during systole, the velocities change dramatically. This is also the reason why most of heart diseases happen in systole.

a. Time 0.0s

b. Time 0.04s

Chapter 5 Results and Discussions

c. Time 0.08s

d. Time 0.12s

e. Time 0.16s

f. Time 0.2s

g. Time 0.24s

h. Time 0.28s

i. Time 0.32s

j. Time 0.36s

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k. Time 0.4s

l. Time 0.44s

m. Time 0.48s

n. Time 0.52s

o. Time 0.56s

p. Time 0.6s

q. Time 0.64s

r. Time 0.68s

Figure 5.12 Velocities of MM towards the apex

If integrating the velocity of MM, the maximum displacements of equator area can be shown in Fig. 5.13, which are compared with the reference (Fan. L et al, 2003).

Figure 5.13 Maximum displacements of MM near the equator area

■ 5.7 Twisting of MF

During the cardiac cycle, besides the thickening and shorting of LV geometry, twisting or rotation of MF relative to apex can also be clearly observed as well. From Fig. 5.14, during the diastole, the MF twisting is slow and smooth, but during the systole, the MF twisting is violent (angle variations maximum up to 20°). At the endocardium surface, the MF twisting is larger than at the epicardium. In Fig. 5.14a, the change of MF angle at the base of endocardium is much larger than the other locations. This may due to the fixed boundary conditions at the base of endocardium. The real change of MF angle may not be so larger if the atrium motion is considered.

a. change of MF angle near the base of endocardium

b. change of MF angle near the equator of endocardium

c. change of MF angle near the apex of endocardium

d. change of MF angle near the base of epicardium

e. change of MF angle near the equator of epicardium

f. change of MF angle near the apex of epicardium

Figure 5.14 Twisting of MF

Chapter 6 Conclusions and Future Works

■ 6.1 Conclusions

To simulate the dynamic motion of LV, a MM plus MF FEM model is developed which incorporate fluid-structure interaction. The model successfully establishes a link between electricity activity at microscopic level and LV wall mechanical motion at macroscopic level through Hill's fiber force model. A good representation of non-linear, anisotropic, and incompressible characteristics of myocardial tissue was achieved. The results show good agreements with clinical observations. With further improvements, this model will be a powerful tool to analyze heart abnormality and diseases.

■ 6.2 Future works

Although a complete FEM model is presented on left ventricular motion, there are still many aspects which can be improved in the current model.

1. Boundary conditions

1) One disadvantage in the model is that: for simplicity, only one valve is used in the model instead of two respective valves. The pressure acting on the valve is manually changed instead of putting two pressure curves acting on two valves. Separation of the mitral valve and aortic valve will be taken into account in the future study.

2) Fixation of the apex point is artificial and is not the realistic situation. Although the apex nearly keeps static during the whole heart cycle, it is not fixed in a point. This assumed fixation may introduce the wrong stresses distribution near apex area.

3) Further focus must be set on the exact boundary conditions inherent in the heart. Pericardium sac plays an important role in constraining the over-expanding of LV during passive filling phase. Fixation of the ventricle to the pericardial sac (may be modeled in using spring elements), the influence of the cytoskeleton forming the valve place, the movement of the septum, and the influence of the right ventricle must be examined and considered in the model. In addition, the blood flow and its influence on mechanical deformation must be examined.

2. To deal with the residual stresses, the average residual stresses are implanted into the MF. This is a simplified assumption. It is hard to put the exact residual stresses into the myocardium because the detailed experimental data is not available yet.

3. The fibers orientations at the apex are complicated, and in this model straight line elements are used to connect the upper nodes with apex node which will introduce high stress concentration at the apex point. So the realistic fiber orientation near apex must be considered in the future study.

4. The fluid property accepted here is simple (as the viscous property of fluid has not been considered). Viscosity is an important characteristic of blood. This property needs to be further considered in the next study.

5. Fluid structure interaction can be further improved. In this model, ALE formulation and penalty method are taken for simulating the MM and CB interaction. CB is meshed by ALE element which may not fully describe the fluid property of the CB. Much attention has been paid to FSI during these years. MPCCI is a recent developed interface which can provide multidisciplinary simulations through code coupling. Basically, the Lagrangian FEM code (like LS-DYNA, ABAQUS, ANSYS et al.) can coordinate with Euler FEM code (like CFD,

FLUENT et al.) through MPCCI. It may be a promising tool for further studying the MM and CB interaction.

6. Improvement of the model should include adding more layers radically in the LV wall. This will give people more detailed stress distribution pattern from endocardial surface to epicardial surface. More accurate 3-D geometric data of LV can be added to the model as it becomes available.

A successful FE model must be combined with the recent non-invasive imaging tools (like MRI) to have more detailed geometry data (like fiber orientation, blood velocity, movement of pericardium sac and the contraction of other three heart chambers et al) and material property data. Doctors and FE analyst should have tighter cooperation.

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