

Nonlinear Elastodynamics with Radial Symmetry, Model and Qualitative Investigation.

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Abstract

This article deduces a model, stated as an integral equation, for a nonlinear elastic isotropic material undergoing a radially symmetric deformation. Such a model is useful in the study of an explosion, or a spherically symmetric impact. Determining the effects of nonlinear wave propagation, in relation to linear propagation, can be truly challenging in 3D dimensions. By reducing the system to a 1D radial partial integral equation numerical simulations are more accurate and manageable. Also, understanding the radially symmetric model sheds light on the qualitative behaviour of the full 3D nonlinear system. An emphasis is given on an intuitive understanding of the dynamics. After deducing the general integral model we present discontinuous jump conditions, and then discuss and substitute the Mooney-Rivlin approximation for the material. We point out how the model for the linearised material can approximate a Mooney-Rivlin material, and subsequently present the analytical solution to some important cases of the linearised material. The appendix attempts to be a rather complete exposition which departs from first principles, where the theoretical basis follows the axiomatic treatment of elasticity and the integral formulation of balance principles.

Summary

Throughout this article, we emphasize a qualitative understanding of stretch and the internal force. Technically difficult passages, such as giving a functional form to the

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Cauchy stress tensor are left to the Appendix, where we also briefly state the assumptions that are particular to elasticity in Appendix B, such as locality of the internal forces, and history independence. For the whole story on elastic constitutive theory see the books [5],[4] or [1].

To begin with, we introduce how to describe the motion of a body. For each time t , a body is a set of points $\mathcal{S} \subset \mathbb{R}^3$; for each point $x \in \mathcal{S}$ we define its initial position, at $t = 0$, as $X \in \mathbb{R}^3$. The set of all these initial positions is defined as $\mathcal{B} \subset \mathbb{R}^3$. We call \mathcal{B} the reference configuration which we will adopt as being the equilibrium configuration, that is, if at any given time, every $x \in \mathcal{S}$ is at its initial position X , with velocity $\dot{x} = 0$, then the body will remain still until disturbed by an outside force. We call \mathcal{S} the current configuration.

We can relate these two sets by means of a map $\phi : \mathcal{B} \rightarrow \mathcal{S}$ which tracks each particle $X \in \mathcal{B}$ to its current position at time t : $\phi(X, t) = x \in \mathcal{S}$, where we assume that ϕ is orientation preserving and invertible. In solid mechanics, when large deformations are present, it is convenient to use the equilibrium position X as a parameter for the state variables, rather than x . For example, the value $\rho(x, t)$ is the density of the material at some point x on the body, using ϕ we can locate x 's initial equilibrium position: $X = \phi^{-1}(x, t)$. Then we define the function ρ_{Ref} such that $\rho_{Ref}(X, t) = \rho(\phi(X, t), t)$. We say that ρ_{Ref} is the density described in the material system, using points $X \in \mathcal{B}$, while ρ is the density described in the spatial system, using points $x \in \mathcal{S}$.

The focus of our attention is a map $\phi^r : \mathbb{R}^2 \rightarrow \mathbb{R}$, such that if R is the radial equilibrium position of a particle, then $\phi^r(R, t)$ is the position of the particle at time t . Because the initial conditions are radially symmetric, and the material is homogeneous and isotropic, we know that every particle, with equilibrium position (R, Θ, Φ) , will be trapped in the line that joins it and the origin. In other words, the current position of the particle at time t is

$$\phi(R, \Theta, \Phi, t) = (\phi^r(R, t), \Theta, \Phi) = (r, \theta, \varphi), \quad (1)$$

where (r, θ, φ) is the current position, at time t , of a particle with equilibrium position (R, Θ, Φ) .

We then deduce a partial integral equation (PIE) (see equation (7)) that describes the evolution of r , after which we return to a qualitative understanding of how the internal forces are represented in the PIE.

The next natural step is to define a specific material. A material's behaviour is characterized by the internal free-energy per unit mass function $\Psi : \mathbb{R}^4 \rightarrow \mathbb{R}$. For a homogeneous isotropic material Ψ depends only on the eigenvalues of the Cauchy-Green stress tensor² \mathbf{C} and the temperature Θ . We then conclude that in our coordinate system Ψ depends only on $(\partial_R r)^2, (r/R)^2$ and Θ , where $\partial_R r$ is the partial derivative of r in relation to R . Notice that due to large displacement, we could not have approximated $r/R \approx 1$, therefore it was necessary to use the material description, i.e. the coordinates (R, t) . In isotropic linear theory, for the purely elastic case, we would need only two coefficients to define the material, in nonlinear theory we essentially need the whole function Ψ . It is important to note that the eigenvalues of \mathbf{C} are coordinate independent, therefore we can use experimental data from any coordinate system to determine the free-energy function Ψ . In euclidean coordinates these eigenvalues are $\{(\partial_X \phi^x)^2, (\partial_Y \phi^y)^2, (\partial_Z \phi^z)^2\}$, this association assists in the interpretation of what kind of stretch and contraction the body is undergoing in any coordinate system.

After deducing the general model, we suggest an approximation for Ψ which is valid for moderately nonlinear materials. With this material in mind, we argue that a model representing a linearised material is useful, moreover, we present solutions of some important cases of the linearised material.

Modelling with Radial Symmetry

Due to the radial symmetry of the deformation, we can reduce the problem to one dimension by using spherical coordinates, which is related to Euclidean coordinates by the following

$$(x, y, z) = r(\cos \theta \sin \varphi, \sin \theta \sin \varphi, \cos \varphi), \quad (2)$$

²a tensor which represents locally the stretch of the material and is defined in equation (B-5)

similarly for the reference coordinates,

$$(X, Y, Z) = R(\cos \Theta \sin \Phi, \sin \Theta \sin \Phi, \cos \Phi). \quad (3)$$

Based on the symmetry of the problem, that is radially symmetric initial conditions in an isotropic material, we know that the motion ϕ will be radially symmetric,

$$\phi(X, t) = (\phi^r(R, t), \phi^\theta(\Theta), \phi^\varphi(\Phi)) = (r, \Theta, \Phi). \quad (4)$$

The internal free-energy per unit mass function Ψ , also called internal potential energy, depends on the principle stretches, to be more precise: let $\mathbf{F} = \mathbf{D}\phi$ be the spatial differential³ of the map ϕ , and $\mathbf{C} = \mathbf{F}^T \mathbf{F}$. The principle stretches are respectively the square root of each of the eigenvalues λ_i 's of \mathbf{C} , which we call the Cauchy-Green stress tensor. In our case, $\lambda_1 = (\partial r / \partial R)^2$, $\lambda_2 = (r/R)^2$ and $\lambda_3 = (r/R)^2$.

A qualitative understanding of the dynamics in the spherical coordinate systems will be valuable. A good starting point for this understanding is to examine how the deformation of a finite volume element in spherical coordinates changes its internal free-energy. To simplify the matter, we shall consider the deformation in the direction of the base vectors \mathbf{e}_r and \mathbf{e}_φ ; the displacement in the \mathbf{e}_θ is analogous to that of \mathbf{e}_φ .

Note that any volume element originally in-between the angles φ_1 and φ_2 , will remain trapped on the rails defined by $\varphi = \varphi_1$ and $\varphi = \varphi_2$, see Figure 1. Now suppose some time has passed and the volume element originally at R_1 has been shifted upwards to $r(R_1, t)$ while maintaining $\Delta r = \Delta R$, thus λ_2 has increased while λ_1 has remained fixed, see Figure 1a. To accomplish this, the volume has been stretched in the \mathbf{e}_φ and \mathbf{e}_θ direction which has increased the internal free-energy.

Now we maintain $\lambda_2 = r^2/R^2$ fixed, i.e. $r(R_1, t) = R_1$ for every t , and vary $\lambda_1 = (\partial r / \partial R)^2$, which is exemplified by Figure 1b), where points originally close to R_1 , after time t , have been mapped further apart, hence $\Delta r / \Delta R \approx \partial r / \partial R > 1$ at R_1 , as a result the internal energy increased⁴. Also any combination of these displacements can occur, such

³More explicitly $F_A^a = \frac{\partial \phi^a}{\partial X^A}$ and for a vector $\mathbf{V} \in \mathbb{R}^3$, $\mathbf{F} \cdot \mathbf{V} = \mathbf{e}_a F_A^a V^A$.

⁴Figure 1b appears to be stretched in the \mathbf{e}_φ direction at one point, and compressed at another. This occurs because we are dealing with a finite volume, rather than the limit as $\Delta R \rightarrow 0$.

as Figure 1c, where the volume element has been compressed in both the \mathbf{e}_r direction and the \mathbf{e}_φ direction.

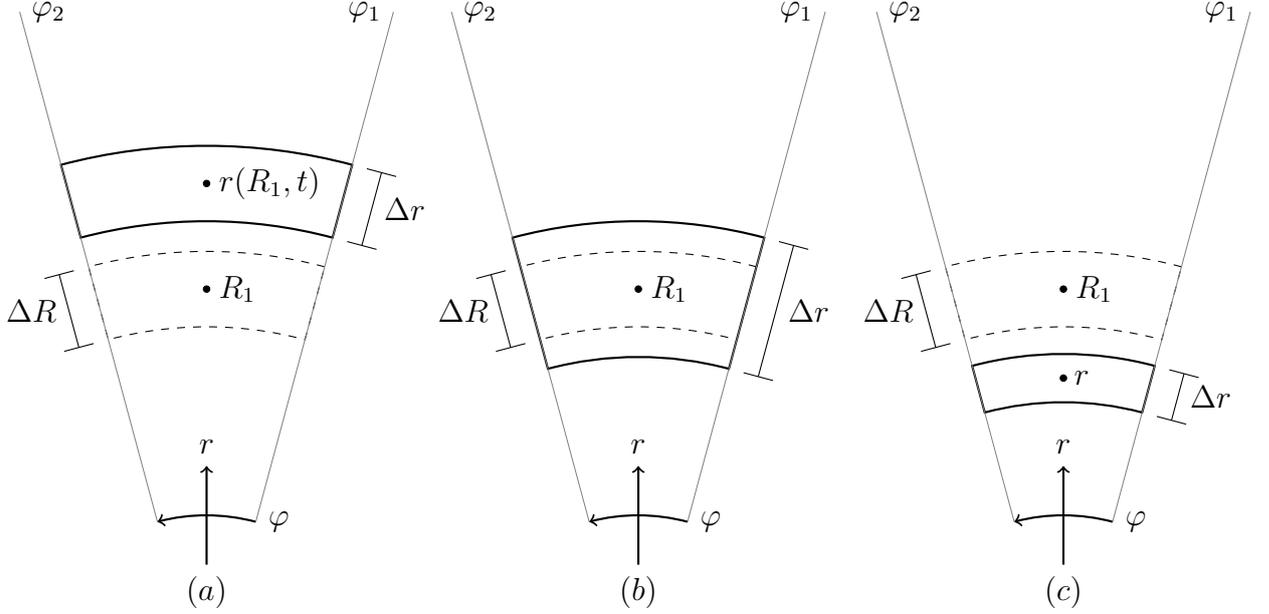


Figure 1: Representation of a finite volume element initially at its equilibrium position (dashed), which then at a later time occupies three distinct deformed states.

From this basic investigation we can already envision the qualitative behaviour of the system. A volume element will attain equilibrium in the radial direction \mathbf{e}_r and the angle direction \mathbf{e}_φ most likely at different times. While $\partial r / \partial R$ oscillates around its equilibrium value 1, so will r / R oscillate around 1, where both their cycles will manifest as a response of the internal stress in the radial direction. This change in the stress will determine the motion. In plain English, it is as if there are two modes of oscillation superimposed onto each other. However, they can not be separated because the solution is not a simple linear combinations of the modes. For instance, a compression in the \mathbf{e}_φ direction will effect the difficulty of compressing the material in the \mathbf{e}_r direction.

Knowing what qualitative behaviour to expect of the model is of vital importance when designing numerical approximations, on the grounds that we can use this understanding to rule out non-physical behaviour, such as eliminating artificial oscillations.

Next we relate the internal forces embodied by the Cauchy stress tensor $\boldsymbol{\sigma}$, a second-order tensor of type $(0, 2)$, to Ψ using elastic constitutive hypothesis, balance principles and other fundamentals of continuum mechanics (see Appendix B),

$$\begin{aligned}\sigma^{rr} &= 2\rho_{Ref} \frac{\partial\Psi}{\partial\lambda_1} \frac{\partial r}{\partial R} \frac{R^2}{r^2}, \\ \sigma^{\theta\theta} &= 2\rho_{Ref} \frac{\partial\Psi}{\partial\lambda_2} \left(\frac{\partial r}{\partial R}\right)^{-1} \frac{1}{\sin^2\varphi r^2}, \\ \sigma^{\varphi\varphi} &= 2\rho_{Ref} \frac{\partial\Psi}{\partial\lambda_2} \left(\frac{\partial r}{\partial R}\right)^{-1} \frac{1}{r^2}.\end{aligned}\tag{5}$$

Note that only $\sigma^{\theta\theta}$ depends on one of the angle coordinates. This is to be expected, because although the motion is symmetric in the $\hat{\mathbf{e}}_\theta$ direction, the norm of the base vector \mathbf{e}_θ is $r \sin \varphi$. The article [2] by Jerrold Marsden and others, demonstrates that the Cauchy stress tensor may be taken to be a covector-valued differential two-form; The balance laws and other fundamental laws of continuum mechanics may be neatly rewritten in terms of this geometric stress.

In the next section, we use $\boldsymbol{\sigma}$ and balance of momentum to arrive at the general model for any elastic isotropic material. With the general model in hand, we will return to a qualitative understanding of the internal stress.

The Model

Returning to the equation of motion (4), and by deriving in time we conclude that $v^\theta = v^\varphi = 0$, where $\mathbf{v} = \partial_t \boldsymbol{\phi}$. To allow the possibility of discontinuities, we impose the integral formulation of balance of momentum (A-19). To do so, we must first choose a constant direction: $\mathbf{e}_{r_o} = \mathbf{e}_r(\theta_o, \varphi_o)$, in which θ_o and φ_o are constants. Then for any nice⁵ open set $\mathcal{U}_t \subset \mathcal{S}$, balance of momentum becomes,

$$\begin{aligned}\frac{d}{dt} \int_{\mathcal{U}_t} \rho \langle \mathbf{v}, \mathbf{e}_{r_o} \rangle dv &= \int_{\partial\mathcal{U}_t} \langle \langle \boldsymbol{\sigma}, \hat{\mathbf{n}} \rangle, \mathbf{e}_{r_o} \rangle da \implies \\ \frac{d}{dt} \int_{\mathcal{U}_t} \rho \mathbf{v}^r \langle \mathbf{e}_r, \mathbf{e}_{r_o} \rangle dv &= \int_{\partial\mathcal{U}_t} \sigma^{ab} \langle \mathbf{e}_b, \hat{\mathbf{n}} \rangle \langle \mathbf{e}_a, \mathbf{e}_{r_o} \rangle da,\end{aligned}$$

⁵By nice we mean the set has a piecewise smooth boundary.

where for the last term we sum over the indexes a and b , dv and da are the volume and area elements and $\hat{\mathbf{n}}$ is the outward unit normal. These equations state that the change in momentum is due to the internal forces exerted by the material outside of \mathcal{U}_t , acting on the boundary $\partial\mathcal{U}_t$.

The boundary $\partial\mathcal{U}_t$ can be divided into six regions, which are the six sides of a spherical volume element. These regions are defined by the surfaces $\theta = \theta_o + \delta\theta$ and $\theta = \theta_o - \delta\theta$ with respectively the unit normals $\hat{\mathbf{e}}_\theta$ and $-\hat{\mathbf{e}}_\theta$, $\varphi = \varphi_o \pm \delta\varphi$ with the unit normals $\pm\hat{\mathbf{e}}_\varphi$, $r = r_2$ and $r = r_1$ with respectively the unit normals \mathbf{e}_r and $-\mathbf{e}_r$. For each of these pairs of surfaces, we will calculate the integral, and then expand θ around θ_o and φ around φ_o . First we sum the surface integrals defined by $\theta = \theta_o + \delta\theta$ and $\theta = \theta_o - \delta\theta$,

$$\begin{aligned} \int \langle \langle \boldsymbol{\sigma}, \hat{\mathbf{n}} \rangle, \mathbf{e}_{r_o} \rangle r d\varphi dr &= \int \pm \sigma^{\theta\theta} \langle \mathbf{e}_\theta, \mathbf{e}_{r_o} \rangle r^2 \sin(\varphi) d\varphi dr \\ &= \int \sigma^{\theta\theta} \sin^2(\varphi) r^3 dr \int_{\varphi_o - \delta\varphi_o}^{\varphi_o + \delta\varphi_o} \langle \pm \hat{\mathbf{e}}_\theta, \mathbf{e}_{r_o} \rangle d\varphi \\ &= -4\delta\varphi \sin(\delta\theta) \sin(\varphi_o) \int \sigma^{\theta\theta} \sin^2(\varphi_o) r^3 dr. \end{aligned}$$

Summing the surface integrals defined by $\varphi = \varphi_o + \delta\varphi$ and $\varphi = \varphi_o - \delta\varphi$, gives us

$$\begin{aligned} \int \sigma^{\varphi\varphi} \langle \mathbf{e}_\varphi, \mathbf{e}_{r_o} \rangle \sin(\varphi) r d\theta dr &= \int \sigma^{\varphi\varphi} r^3 dr \int \langle \pm \hat{\mathbf{e}}_\varphi, \mathbf{e}_{r_o} \rangle \sin(\varphi) d\theta \\ &= \sin(2\delta\varphi) ((-\delta\theta - \sin(\delta\theta)) \sin(\varphi_o) + (\sin(\delta\theta) - \delta\theta) \sin(3\varphi_o)) \int \sigma^{\varphi\varphi} r^3 dr \\ &= -4\delta\theta\delta\varphi \sin(\varphi_o) \int \sigma^{\varphi\varphi} r^3 dr + \mathcal{O}(\delta\theta\delta\varphi). \end{aligned}$$

Finally, summing the surface integrals defined by $r = r_2$ and $r = r_1$, results in

$$\int \sigma^{rr} r^2 \langle \mathbf{e}_r, \mathbf{e}_{r_o} \rangle \sin(\varphi) d\theta d\varphi = 4\delta\theta\delta\varphi \sin(\varphi_o) \sigma^{rr} r^2 \Big|_{r_1}^{r_2} + \mathcal{O}(\delta\theta\delta\varphi).$$

Balance of momentum is valid for every value of $\delta\theta$ and $\delta\varphi$. Thus we can equate the terms of the same order and reduce balance of momentum to,

$$\frac{d}{dt} \int_{r_1}^{r_2} \rho \mathbf{v}^r \langle \mathbf{e}_r, \mathbf{e}_{r_o} \rangle dr = \sigma^{rr} r^2 \Big|_{r_1}^{r_2} - \int_{r_1}^{r_2} (\sigma^{\theta\theta} \sin^2 \varphi + \sigma^{\varphi\varphi}) r^3 dr. \quad (6)$$

If we assume that ρ, v^r, r are differentiable and r is regular we can use constitutive hypothesis for the stress tensor (5). When discontinuities appear in the solution we expect

them to be discrete, therefore if we assume that the state variables are differentiable and use constitutive theory, the value of the integrals above will not be altered. However, more investigation into the discontinuous jump will be necessary to actually track what happens at the discontinuity, this investigation is partly carried out in the section “Discontinuity Conditions”. Also, taking into account that r is monotonic and differentiable in R by parts, we can change variables and integrate in R ,

$$\int_{r_1}^{r_2} \rho v^r r^2 dr = \int_{R_1}^{R_2} \rho v^r r^2 \frac{\partial r}{\partial R} dR = \int_{R_1}^{R_2} \rho_{Ref} v^r R^2 dR,$$

where

$$\rho_{Ref}(R, t) = \rho(r, t) \frac{\partial r}{\partial R} \frac{r^2}{R^2}.$$

Substituting equations (5) into PIE (6), together with the above variable change, we arrive at

$$\frac{d}{dt} \int_{R_1}^{R_2} \frac{\partial r}{\partial t} R^2 dR = 2 \frac{\partial \Psi}{\partial \lambda_1} \frac{\partial r}{\partial R} R^2 \Big|_{R_1}^{R_2} - 4 \int_{R_1}^{R_2} \frac{\partial \Psi}{\partial \lambda_2} r dR. \quad (7)$$

Now we shall investigate qualitatively the origin of these terms. To facilitate compression, we shall exemplify the deformation and the forces on a finite spherical volume element, enclosed by the surfaces defined by $R = R_1, R = R_2, \varphi = \varphi_1, \varphi = \varphi_2, \theta = \theta_1$ and $\theta = \theta_2$ where, to simplify the analysis, we restrict our attention to the coordinates φ and r .

The PIE (7) states that the rate of change of momentum, in time, of the material between the points $r(R_1, t)$ and $r(R_2, t)$ is due to two phenomenons. The first is due to the deformation of the material in the radial direction, which manifests as a radial force on the surfaces defined by $R = R_1$ and $R = R_2$, expressed by the term

$$2 \frac{\partial \Psi}{\partial \lambda_1} \frac{\partial r}{\partial R} R^2 \Big|_{R_1}^{R_2}. \quad (8)$$

The term $\partial_R r$ is how much the material is locally stretched in the radial direction, and $\partial_{\lambda_1} \Psi$ is, in sense, how hard it is to further stretch the material in the radial direction, remembering that $\lambda_1 = (\partial_R r)^2$. The term R^2 is a geometric factor, brought about because the above expression represents the total force applied to the surface of a sphere. To

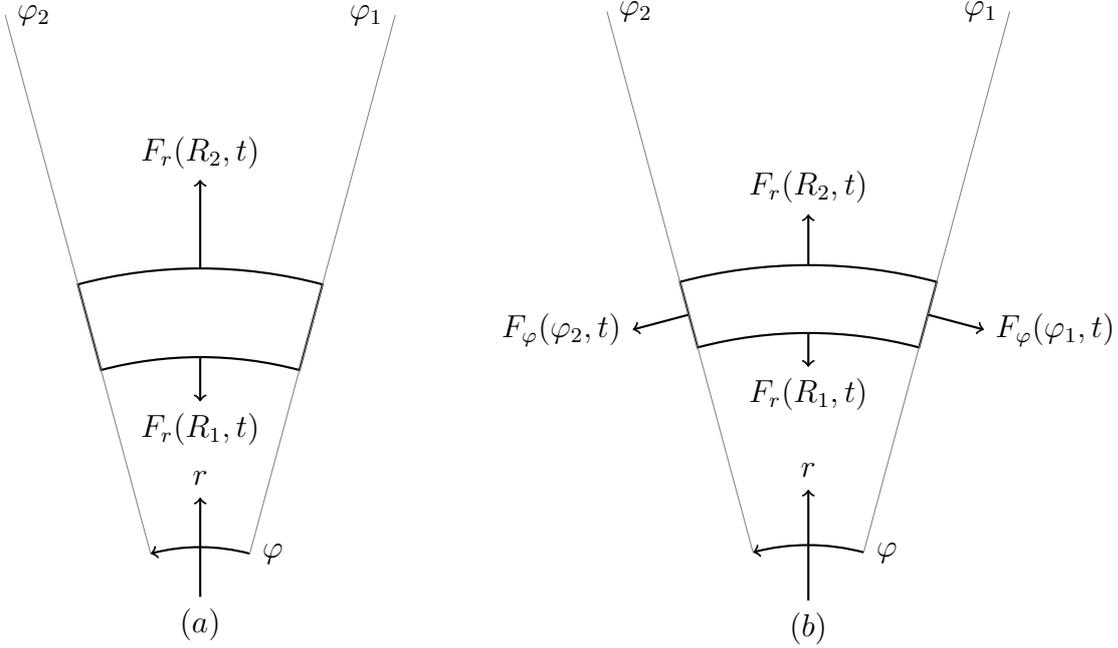


Figure 2: Figure (a) represents the difference of the radial forces $F_r(R_1, t)$ and $F_r(R_2, t)$ caused by the stretch in the radial direction \mathbf{e}_r . Figure (b) represents a state where all the surface forces cancel; $F_\varphi(\varphi_1, t)$ and $F_\varphi(\varphi_2, t)$ are the internal forces exerted on the surfaces defined by $\varphi = \varphi_1$ and $\varphi = \varphi_2$.

summarize, the term (8) contributes to the rate of change in radial momentum when there is a difference between the force applied on the surfaces $R = R_1$ and $R = R_2$, see Figure 2a.

The second contribution, in PIE (7), to the rate of change in momentum originates from the forces in the \mathbf{e}_θ and \mathbf{e}_φ directions. See the equilibrium state of this volume element represented in Figure 2b, where the sum of all the forces cancel. The integral on the right hand side of PIE (7) represents the radial projection of the force $F_\varphi(\varphi_1, t) + F_\varphi(\varphi_2, t)$. Notice that this force always acts to pull the volume element towards the origin, while the force $F(R_2, t) + F(R_1, t)$ tends to push the volume element away from the origin.

Discontinuity Conditions

We will assume that the material will not fracture, that no rip appears, hence $\phi^r = r$ is at least continuous. With this in mind, we apply the results for discontinuous jump conditions from Appendix A, which assumes the existence of a moving surface $\Sigma(t) \subset \mathcal{B}$, on which the state variables are discontinuous, but elsewhere are differentiable. We will employ the following notation: the vector $\mathbf{W}(Y, t)$ is the material velocity of $\Sigma(t)$ at $Y \in \Sigma(t)$, let f be some function defined on \mathcal{B} then the brackets $[f]$ denotes the discontinuous jump in value of f across $\Sigma(t)$, in other words $[f] = f^+ - f^-$ where f^+ is the limiting value of f approaching $\Sigma(t)$ from the “forward moving” side, and analogously for f^- and

$$\omega^r = \frac{\partial r}{\partial R} W^R.$$

Each balance principle imposes a different discontinuous jump condition. For conservation of mass, using equations (A-17) and (A-18):

$$\begin{aligned} [\rho\omega^r] = 0 &\implies \rho^- \omega^{r-} = \rho^+ \omega^{r+} \\ &\implies \rho_{Ref} \left(\frac{\partial r^-}{\partial R} \right)^{-1} \left(\frac{r}{R} \right)^2 \frac{\partial r^-}{\partial R} W^R = \rho_{Ref} \left(\frac{\partial r^+}{\partial R} \right)^{-1} \left(\frac{r}{R} \right)^2 \frac{\partial r^+}{\partial R} W^R, \end{aligned}$$

which is satisfied a priori because of the continuity of ϕ^r . For Balance of Momentum, using equation (A-20):

$$\rho^- \omega^{r-} [v^r] = -[\sigma^{rr}] \implies W_N [V^r] = -2 \left[\frac{\partial \Psi}{\partial \lambda_1} \frac{\partial r}{\partial R} \right].$$

For Conservation of Energy, using equation (A-27):

$$[\rho e] = -\frac{1}{2}(\sigma^{rr+} + \sigma^{rr-})[v^r],$$

if we assume that the temperature Θ is constant, and that $\partial \Psi / \partial \Theta = 0$, then entropy η is constant throughout the material, and the discontinuous jump condition becomes

$$[\rho \psi] = -\frac{1}{2}(\sigma^{rr+} + \sigma^{rr-})[v^r] \implies \left[\left(\frac{\partial r}{\partial R} \right)^{-1} \Psi \right] = -\left(\frac{\partial \Psi^+}{\partial \lambda_1} \frac{\partial r^+}{\partial R} + \frac{\partial \Psi^-}{\partial \lambda_1} \frac{\partial r^-}{\partial R} \right) [V^r].$$

For the Entropy Production Inequality, using equation (A-27):

$$[\rho\eta\omega^r] \leq -\left[\frac{q^r}{\Theta}\right].$$

If we consider that temperature does not change, then this equation becomes

$$\eta^+ \leq \eta^-,$$

which states that the entropy on the side where the surface has already passed through, is larger than the entropy of the other side.

This set of basic jump conditions are not enough to define both the velocity of the shock, or in our case a kink, and how r^+ and r^- change in time and space. More assumptions need to be made to uniquely define the shock in motion.

Moderate Nonlinearity

To specify the material we must choose how the internal energy explicitly depends on the eigenvalues of the Cauchy-Green tensor $\lambda_1 = (\partial_R r)^2$ and $\lambda_2 = (r/R)^2$, see equation (B-5).

For our purpose, we want a model for Ψ which is as simple as possible, but still captures prototypically nonlinear phenomena and can be fitted to available experimental data. One most convincing choice would be to use Spline interpolation, however data is often to scarce for this. A more manageable choice would be to approximate Ψ close to the equilibrium point $(\lambda_1, \lambda_2, \lambda_2) = (1, 1, 1)$, such as,

$$\begin{aligned} \Psi(\lambda_1, \lambda_2, \lambda_2) = & \tag{9} \\ \Psi + \frac{\partial\Psi}{\partial\lambda_1}(\lambda_1 - 1) + \frac{\partial\Psi}{\partial\lambda_2}(\lambda_2 - 1) + \frac{\partial\Psi}{\partial\lambda_3}(\lambda_3 - 1) + \frac{\partial^2\Psi}{\partial\lambda_1\partial\lambda_1}(\lambda_1 - 1)^2 + 2\frac{\partial^2\Psi}{\partial\lambda_1\partial\lambda_2}(\lambda_1 - 1)(\lambda_2 - 1) \\ + 2\frac{\partial^2\Psi}{\partial\lambda_1\partial\lambda_3}(\lambda_1 - 1)(\lambda_3 - 1) + 2\frac{\partial^2\Psi}{\partial\lambda_2\partial\lambda_3}(\lambda_2 - 1)(\lambda_3 - 1) + \frac{\partial^2\Psi}{\partial\lambda_3\partial\lambda_3}(\lambda_3 - 1)^2 + \frac{\partial^2\Psi}{\partial\lambda_2\partial\lambda_2}(\lambda_2 - 1)^2 \\ + \mathcal{O}(\lambda_1 - 1)^2 + \mathcal{O}(\lambda_2 - 1)^2 + \mathcal{O}(\lambda_3 - 1)^2, \end{aligned}$$

when left unspecified Ψ is evaluated at $(1, 1, 1)$. The value for $\Psi(1, 1, 1)$ is arbitrary, since only the rate of change of Ψ in relation to the stretch influences the dynamics, so we adopt $\Psi(1, 1, 1) = 0$. To clean up the approximation, we remind ourselves of

some of the inherit symmetries of isotropic materials: $\Psi(\gamma, 1, 1) = \Psi(1, \gamma, 1) = \Psi(1, 1, \gamma)$ and $\Psi(\gamma, \gamma, 1) = \Psi(1, \gamma, \gamma) = \Psi(\gamma, 1, \gamma)$ for every $\gamma > 0$. Therefore we can rename the following,

$$\eta = \frac{\partial \Psi}{\partial \lambda_1} = \frac{\partial \Psi}{\partial \lambda_2} = \frac{\partial \Psi}{\partial \lambda_3}, \quad \mu = \frac{\partial^2 \Psi}{\partial \lambda_1 \partial \lambda_1} = \frac{\partial^2 \Psi}{\partial \lambda_2 \partial \lambda_2} = \frac{\partial^2 \Psi}{\partial \lambda_3 \partial \lambda_3},$$

$$\nu = 2 \frac{\partial^2 \Psi}{\partial \lambda_1 \partial \lambda_2} = 2 \frac{\partial^2 \Psi}{\partial \lambda_1 \partial \lambda_3} = 2 \frac{\partial^2 \Psi}{\partial \lambda_2 \partial \lambda_3}.$$

Substituting these equations in equation (9),

$$\begin{aligned} \Psi(\lambda_1, \lambda_2, \lambda_3) = & \eta(\lambda_1 + \lambda_2 + \lambda_3 - 3) + \mu(\lambda_1 - 1)^2 + \mu(\lambda_3 - 1)^2 + \mu(\lambda_2 - 1)^2 \\ & + \nu(\lambda_1 - 1)(\lambda_2 - 1) + \nu(\lambda_1 - 1)(\lambda_3 - 1) + \nu(\lambda_2 - 1)(\lambda_3 - 1) \\ & + \mathcal{O}(\lambda_1 - 1)^2 + \mathcal{O}(\lambda_2 - 1)^2 + \mathcal{O}(\lambda_3 - 1)^2 \implies \end{aligned}$$

$$\begin{aligned} \Psi(\lambda_1, \lambda_2, \lambda_3) = & \kappa(\lambda_1 + \lambda_2 + \lambda_3 - 3) + \mu(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3) + \nu(\lambda_1 \lambda_2 + \lambda_1 \lambda_3 + \lambda_2 \lambda_3 - 3) \\ & + \mathcal{O}(\lambda_1 - 1)^2 + \mathcal{O}(\lambda_2 - 1)^2 + \mathcal{O}(\lambda_3 - 1)^2, \end{aligned}$$

where $\kappa = (\eta - 2\mu - 2\nu)$. To interpret this approximations recall that in Euclidean coordinates $\lambda_1 = (\partial_X \phi^x)^2$, $\lambda_2 = (\partial_Y \phi^y)^2$ and $\lambda_3 = (\partial_Z \phi^z)^2$. Hence only the term multiplying ν represents how the material responds when deformed simultaneously in two directions, such as \mathbf{e}_x and \mathbf{e}_y . An approximation which is simpler, captures this simultaneous deformation response, can be fitted to abundant available data and has had success in representing materials in a prototypical manner, is called the Mooney-Rivlin material, where

$$\Psi(\lambda_1, \lambda_2, \lambda_3) \approx \kappa(\lambda_1 + \lambda_2 + \lambda_3 - 3) + \nu(\lambda_1 \lambda_2 + \lambda_1 \lambda_3 + \lambda_2 \lambda_3 - 3),$$

where κ and ν must both be positive to guarantee that Ψ increases together with λ_1, λ_2 and λ_3 . For each material, the constants κ and ν are determined through experimental data. For radial symmetry $\lambda_2 = \lambda_3$, thus for this type of material

$$\partial_{\lambda_1} \Psi = \kappa + 2\nu\lambda_2 \text{ and } \partial_{\lambda_2} \Psi = \kappa + \nu(\lambda_1 + \lambda_2),$$

substituting these equations in to our general model (7), we conclude that

$$\frac{d}{dt} \int_{R_1}^{R_2} \frac{\partial r}{\partial t} R^2 dR = 2(\kappa + 2\nu \frac{r^2}{R^2}) \frac{\partial r}{\partial R} R^2 \Big|_{R_1}^{R_2} - 4 \int_{R_1}^{R_2} (\kappa + 2\nu (\frac{\partial r}{\partial R} + \frac{r^2}{R^2})) r dR. \quad (10)$$

Assume for time being that the following initial conditions $\overset{\circ}{\phi}(R) = \phi(R, 0)$. Then when $R \gg \|\overset{\circ}{\phi}\|_\infty$ the function $\partial_{\lambda_1}\Psi$ can be approximated by a constant. In this region the model locally behaves qualitatively like the model of a linearised material, i.e. with a linear stress to strain relation, this is specifically true for the First Piola-Kirchhoff stress tensor. Also the model linearised around the equilibrium state represents a physically viable material, hence its solution will exhibit “reflection” from $R = 0$. What this means exactly will be clarified in the next section, where we linearise the material and present the analytical solution for some important cases.

The Linear Model

First we write the localized form of PIE (10), to do so, we assume that $\partial_t r$ and $\partial_R r$ are differentiable. Then, in conservation form

$$\frac{\partial^2 r}{\partial t^2} R^2 - \frac{d}{dR} \left(V^2 \frac{\partial r}{\partial R} R^2 \right) + 2W^2 r = 0, \quad (11)$$

where

$$V^2 = 2 \frac{\partial \Psi}{\partial \lambda_1}, \text{ and } W^2 = 2 \frac{\partial \Psi}{\partial \lambda_2},$$

this renaming also serves to suggest that these quantities represent velocities, in some sense. We will consider that these velocities are constants, and expand equation (11)

$$\frac{\partial^2 r}{\partial t^2} = V^2 \frac{\partial^2 r}{\partial R^2} + \frac{2V^2}{R} \frac{\partial r}{\partial R} - 2W^2 \frac{r}{R^2} \implies \frac{\partial^2(Rr)}{\partial t^2} = V^2 \frac{\partial^2(Rr)}{\partial R^2} - 2W^2 \frac{Rr}{R^2},$$

or,

$$\frac{\partial^2 u}{\partial t^2} = V^2 \frac{\partial^2 u}{\partial R^2} - 2W^2 \frac{u}{R^2}, \quad (12)$$

where $u = Rr$. We can solve the above system for certain cases, but first, an easy task is to find the stationary configurations, where

$$\frac{\partial^2 u}{\partial R^2} = \frac{2W^2}{V^2} \frac{u}{R^2}, \text{ with } u(0, t) = 0 \text{ and } \partial_R u(0, t) = r(0, t) = 0,$$

then the stationary solution is

$$u(R, t) = R^{1/2 + \sqrt{1 + 8W^2/V^2}/2}. \quad (13)$$

For the nonlinear case we know that rest can only be achieved for $r(R, t) = R$ or $u(R, t) = R^2$. Assuming uniqueness for the stationary solution, for the nonlinear model, is similar to assuming that the internal free-energy Ψ is a convex function. It is not a necessary assumption for constitutive elastic theory, however it is commonly seen in experiments conducted in an approximate elastic regime.

Returning to our previous discussion, we conclude from the stable configurations (13) that the only linear model which oscillates around the equilibrium of the nonlinear model is such that $V = W$. This in part is the reason why only this linear model exhibits “reflection” from the origin.

To solve the PDE (11) we convert it into an ODE by applying the Fourier Transform in time on both sides of the equation. then using a series substitution, and after some technical details related to the PDE’s dependence on the initial condition, we were able to solve analytically the cases where

$$\frac{W^2}{V^2} = \frac{(2n + 1)^2 - 1}{8},$$

for $n \in \mathbb{N}$. For the case $V = W$, we have that

$$\begin{aligned} u(R, t) = & \frac{1}{2}u(|R - Vt|, 0) + \frac{1}{2}u(R + Vt, 0) + \int_{|R-Vt|}^{R+Vt} \frac{-Vt}{2RP} u(P, 0) dP \\ & + \int_{|R-Vt|}^{R+Vt} \frac{(P^2 + R^2 - V^2t^2)}{4VRP} \frac{\partial u}{\partial t}(P, 0) dP. \end{aligned} \quad (14)$$

Through symmetry the origin of the spatial map $R = 0$ should remain still, i.e. $r(0, t) = 0$, spherically symmetric forces do not cause translation. Let us now check this property, i.e. does the limit $\lim_{R \rightarrow 0} r(R, t) = 0$?

Theorem 1 *The map r governed by the equation (14) satisfies the following limit,*

$$\lim_{R \rightarrow 0} r(R, t) = 0.$$

Proof: For any given t choose $\delta(t) > 0$ small enough so that

$$|R| < \delta \implies |R - Vt| = Vt - R,$$

then there exists $\bar{R} > 0$ where $|\bar{R} - Vt| < \delta$ such that

$$\frac{-Vt}{2R} \int_{|R-Vt|}^{R+Vt} \frac{1}{P} u(P, 0) dP = \frac{-Vt}{2R} u(\bar{R}, 0) \int_{Vt-R}^{R+Vt} \frac{dP}{P} = \frac{-Vt}{2R} u(\bar{R}, 0) \ln \left(\frac{Vt+R}{Vt-R} \right),$$

rewriting the function \ln as a second order truncated taylor series implies that,

$$\begin{aligned} \frac{-Vt}{2R} \int_{|R-Vt|}^{R+Vt} \frac{1}{P} u(P, 0) &= \frac{-Vt}{2R} u(\bar{R}, 0) \left(\frac{2R}{Vt} + \mathcal{O}(R^3) \right) \\ &= -u(\bar{R}, 0) (1 + \mathcal{O}(R^2)) = -u(Vt, 0) + \mathcal{O}(R). \end{aligned}$$

Upon taking the limit $\delta \rightarrow 0$ which implies that $R \rightarrow 0$, the above term will cancel with the terms

$$\frac{1}{2} u(Vt - R, 0) + \frac{1}{2} u(R + Vt, 0) = u(Vt, 0) + \mathcal{O}(R^2).$$

The remaining term tends to zero faster than R , where we repeat the argument that there exists \bar{R}_2 such that

$$\begin{aligned} &\int_{|R-Vt|}^{R+Vt} \frac{(P^2 + R^2 - V^2 t^2)}{4VRP} \frac{\partial u(P, 0)}{\partial t} dP \\ &= \frac{\partial u(\bar{R}_2, 0)}{\partial t} \int_{|R-Vt|}^{R+Vt} \frac{(P^2 + R^2 - V^2 t^2)}{4VRP} dP \\ &= \frac{1}{4VtR} \frac{\partial u(\bar{R}_2, 0)}{\partial t} \left(2VtR - (R^2 - V^2 t^2) \left(\frac{-2R}{Vt} + \mathcal{O}(R^2) \right) \right) \\ &= \frac{R^2}{2Vt} \frac{\partial u(\bar{R}_2, 0)}{\partial t} + \mathcal{O}(R^2), \end{aligned}$$

therefore $\lim_{R \rightarrow 0} r(R, t) = \lim_{R \rightarrow 0} u(R, t)/R = 0$. □

Theoretically, we can now impose the boundary condition $u(0, t) = 0$ and the solution will continue monotonic and continuous, a seemingly trivial imposition for the linear model but vital for the numerical simulation of the nonlinear model. Below we show qualitatively this “reflection” from the origin for the initial data, $u(R, 0) = R^2 + R^2 e^{-10(R-0.5)^2}$, and $V = 2$. To facilitate, we plot $u - R^2$, since u oscillates around R^2 , see Figure (3).

Repeating the same process for the case $n = 2$ and $W/V = \sqrt{7/2}$, which will not

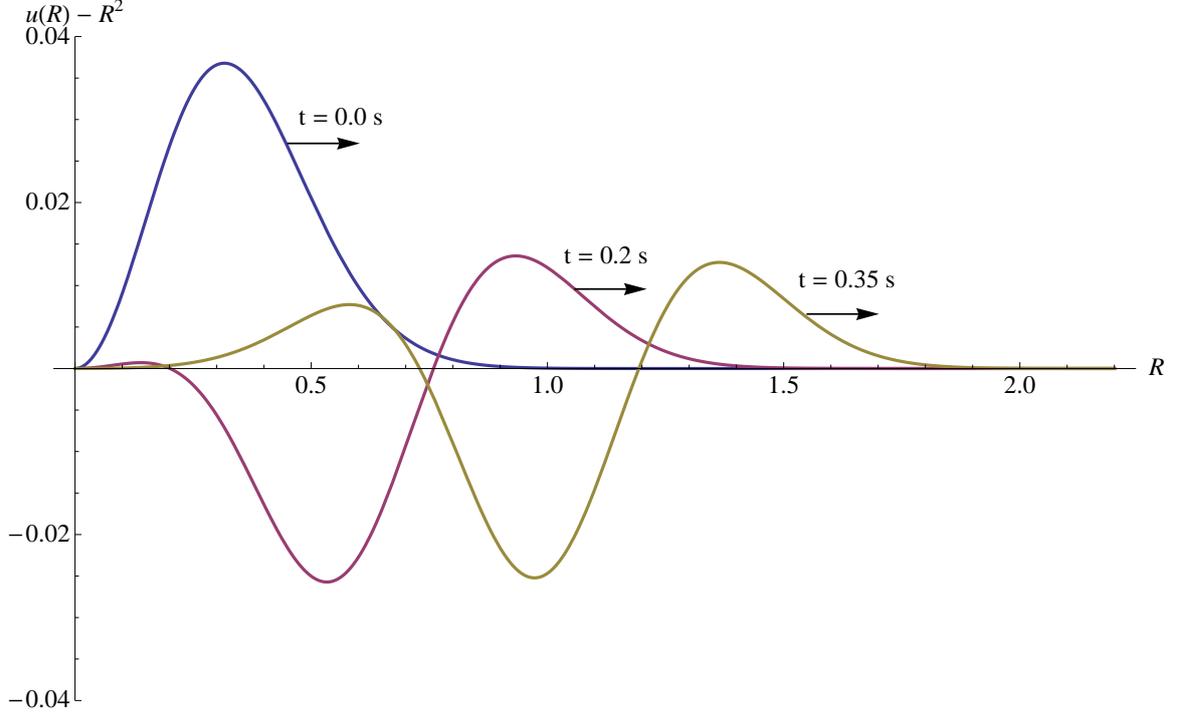


Figure 3: Reflection from origin.

exhibit reflection from the spatial origin⁶. The solution is

$$\begin{aligned}
u_2(R, t) = & \frac{1}{2}u(|R - Vt|, 0) + \frac{1}{2}u(R + Vt, 0) \\
& + \int_{|R-Vt|}^{R+Vt} \frac{(3Vt(V^2t^2 - P^2 - R^2))}{4P^2R^2} u(P, 0) dP \\
& + \int_{|R-Vt|}^{R+Vt} \left(\frac{3P^2 + 2(R^2 - 3V^2t^2)}{16VR^2} + \frac{3(R^2 - V^2t^2)^2}{16VP^2R^2} \right) \frac{\partial u(P, 0)}{\partial t} dP.
\end{aligned}$$

The solution to the limiting case $n = 0$ and $W/V = 0$ is well known,

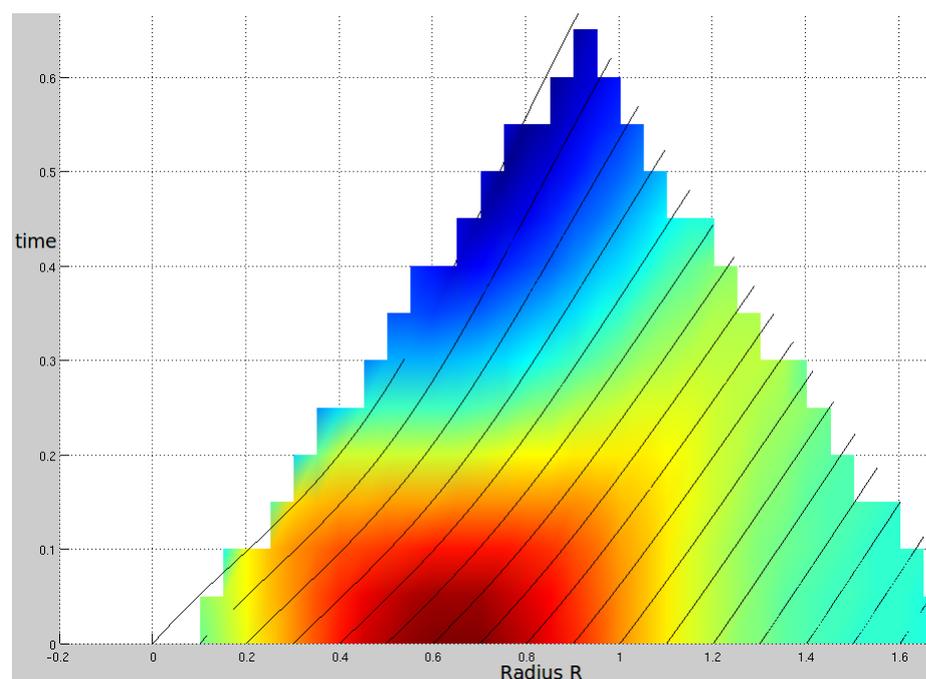
$$u_0(R, t) = \frac{1}{2}u(|R - Vt|, 0) + \frac{1}{2}u(R + Vt, 0) + \frac{1}{2V} \int_{|R-Vt|}^{R+Vt} \frac{\partial u(P, 0)}{\partial t} dP.$$

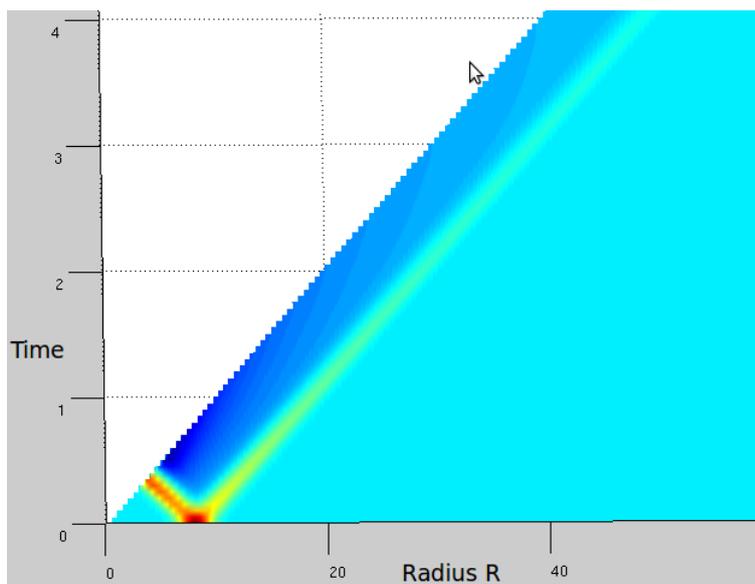
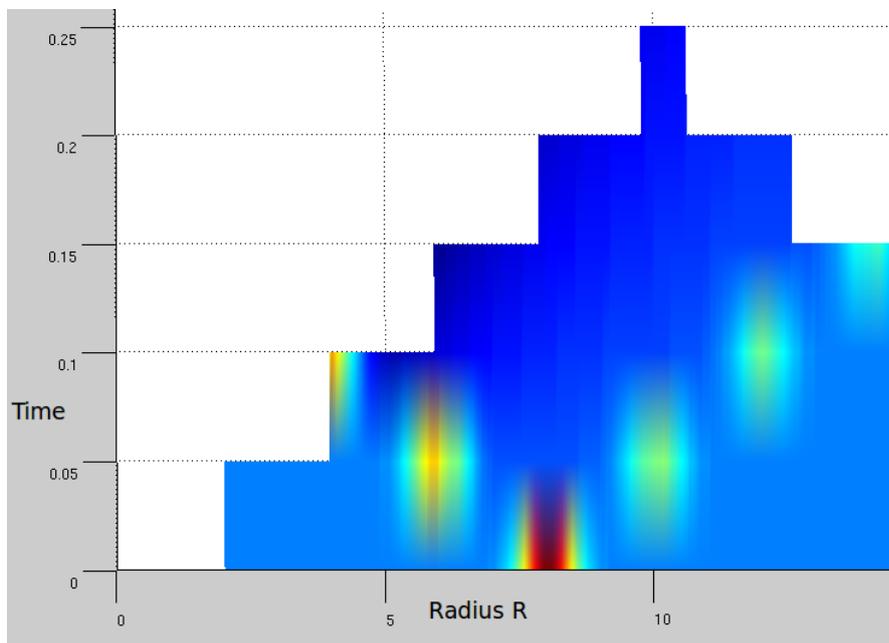
The comun structure of the solutions of these case do suggest a base of functions that we could use to approximate the general linear solution. Also, physically, solutions for intermediate values of W/V should behave similarly, numerical simulations based on the series solution in the frequency domain confirm this.

⁶There can only be reflection if the material undulates around the state of rest $V = W$, ergo, reflection does not occur for the model linearised around a state that is not in equilibrium.

Future Research

The next step is to numerically simulate the model (10), to do so, we change to a coordinate system which follows the domain of dependency. Devising a numerical scheme appropriately in this coordinate system not only guarantees extracting information from the correct domain, but also attempts to capture the way in which information is spread in the domain of dependence. Physical characteristics such as being TVD, total variation diminishing, and obeying the discontinuous jump conditions are taken into account. The model behaves much like the linearised model far from the origin. Close to the origin difficulties arise, and at the moment we are working on a solution. Below are some figures that shows wave propagation far from the origin for several materials. The colour represents the value $r - R$.





Appendices

A Appendix

Coordinate Independent Balance Principles

This section presents the basic dynamical equations, in the form of balance laws, for continuum mechanics. All of which originate from an integral equation in the spatial

picture⁷ and are then translated to the material picture. These laws are used to give functional form to stress tensor, and to acquire the discontinuous jump conditions.

Transport Theorem

All classical balance laws involve equating an extensive quantity⁸ in any domain with a flux through the boundary, to do so, we will need the theorems below.

Theorem 2 (Transport Theorem) *Let $f(x, t)$ be a given C^1 scalar function of time t and position $x \in \mathcal{W}(t) \subset \mathcal{S}$, where $\mathcal{W}(t)$ is a moving open set. Suppose that $\partial\mathcal{W}(t)$ is moving with velocity $\mathbf{w}(x, t)$ at $x \in \mathcal{W}(t)$. Then,*

$$\boxed{\frac{d}{dt} \int_{\mathcal{W}(t)} f dv = \int_{\mathcal{W}(t)} \frac{\partial f}{\partial t} dv + \int_{\partial\mathcal{W}(t)} f w_n da} \quad (\text{A-1})$$

where w_n is the normal outward component of the velocity field \mathbf{w} on $\partial\mathcal{W}(t)$.

Proof: Using appendix C, this can be restated as

$$\frac{d}{dt} \int_{\mathcal{W}(t)} f dv = \int_{\mathcal{W}(t)} \frac{df}{dt} + f \left(\frac{d\mathbf{v}}{dx^m} \right)^m dv,$$

then by extending \mathbf{w} to a vector field from which we can define the flow⁹ $\psi(\mathcal{W}_0, t) = \mathcal{W}(t)$, i.e. $\mathbf{w}(x, t) = \dot{\psi}_t \circ \psi_{-t}(x)$, we can apply the results from appendix C.

Theorem 3 (Discontinuous Transport Theorem) *Let $f(x, t)$ be given. Suppose $f(x, t)$ and $\phi(X, t)$ have a jump discontinuity across a surface¹⁰ $\sigma(t) \subset \mathcal{S}$, but both are C^1 and $\phi(t)$ is regular elsewhere. Let us track this surface in the material system: $\phi(\Sigma(t), t) = \sigma(t)$, where $\Sigma(t) \subset \mathcal{B}$ possible varies in time. Assume that $\mathcal{L}_v f$ and $\partial f / \partial t$ are integrable on $\phi(\mathcal{U}, t)$. Then for a nice open set $\mathcal{U} \subset \mathcal{B}$,*

$$\boxed{\frac{d}{dt} \int_{\phi(\mathcal{U}, t)} f dv = \int_{\phi(\mathcal{U}, t)} \frac{\partial f}{\partial t} dv + \int_{\partial\phi(\mathcal{U}, t)} f v_n da + \int_{\phi(\mathcal{U}, t) \cap \phi(\Sigma(t), t)} [f(v_n + \omega_n)] da} \quad (\text{A-2})$$

⁷Using $x \in \mathcal{S}$ and t as the parameters for the state variables.

⁸A quantity directly proportional to the system size or the amount of material in the system.

⁹To define the flow uniquely it is sufficient that $w(x, t)$ be Lipschitz in x .

¹⁰Which divides $\phi_t(\mathcal{U})$ into two pieces.

the brackets $[*]$ denote the discontinuous jump in value across $\sigma(t)$. If one of the sides of $\sigma(t)$ is the boundary of the material (such a boundary can appear after a rip) the value f is to be considered zero on this side. Also, v_n is the normal component of \mathbf{v} , and ω is defined for every $Y \in \Sigma(t)$ as

$$\omega(x, t) = \frac{\partial \phi(Y, t)}{\partial X^A} W^A(Y, t),$$

where $\mathbf{W}(Y, t)$ is the material velocity of $\Sigma(t)$ at $Y \in \Sigma(t)$.

Proof: Divide $\mathcal{U}_t = \phi(\mathcal{U}, t) = \mathcal{U}_t^+ \cup \mathcal{U}_t^-$, where \mathcal{U}_t^+ is on the "forward moving" side of $\sigma(t)$, and let $\partial \mathcal{U}_t^+ = (\partial \mathcal{U}_t \cap \mathcal{U}_t^+) \cup \sigma(t)$, and analogously for $\partial \mathcal{U}_t^-$. Let $\hat{\mathbf{n}}$ be the outward normal vector for $\partial \mathcal{U}_t^+$. To apply the results of Theorem 2 we need the velocity of the boundary $\sigma(t)$, let $Y \in \Sigma(t)$, then

$$\frac{d\phi(Y, t)}{dt} = \frac{\partial \phi(Y, t)}{\partial t} + \frac{\partial \phi_t(Y, t)}{\partial X^A} W^A(Y, t) = \mathbf{v} + \omega = \mathbf{w}.$$

Now using Theorem 2 we conclude that

$$\frac{d}{dt} \int_{\mathcal{U}_t^+} f dv = \int_{\mathcal{U}_t^+} \frac{\partial f}{\partial t} dv + \int_{\partial \mathcal{U}_t \cap \mathcal{U}_t^+} f v_n da + \int_{\phi(\Sigma(t), t)} f^+ (v_n^+ + \omega_n^+) da, \quad (\text{A-3})$$

where f^+ is the limiting value of f approaching $\phi(\Sigma(t), t)$ from \mathcal{U}_t^+ , analogously for v_n^+ and ω_n^+ . Repeating the above reasoning with \mathcal{U}_t^- we get

$$\frac{d}{dt} \int_{\mathcal{U}_t^-} f dv = \int_{\mathcal{U}_t^-} \frac{\partial f}{\partial t} dv + \int_{\partial \mathcal{U}_t \cap \mathcal{U}_t^-} f v_n da - \int_{\phi(\Sigma(t), t)} f^- (v_n^- + \omega_n^-) da, \quad (\text{A-4})$$

noting that for \mathcal{U}_t^- the outward normal at σ_t is $-\hat{\mathbf{n}}$, then summing equations (A-3) and (A-4) we conclude theorem 3. \square

Corollary 1 *Discontinuous Transport Theorem (3) in the material system becomes*

$$\boxed{\frac{d}{dt} \int_{\mathcal{U}} F J dV = \int_{\mathcal{U}} \frac{\partial F}{\partial t} J dV + \int_{\partial \mathcal{U}} F V_N J da + \int_{\mathcal{U} \cap \Sigma_t} [F(V_n + W_n)] J da}, \quad (\text{A-5})$$

where $F = f \circ \phi_t$, $\mathbf{W} = d\phi^{-1} \mathbf{w}$, $\mathbf{V} = d\phi^{-1} \mathbf{v}$ and J , the Jacobian, is the determinant of the linear transformation $D\phi$,

$$D\phi = e^a \frac{\partial \phi^a}{\partial X^A} dX^A, \text{ and } J = \frac{\partial(\phi^1, \dots, \phi^n)}{\partial(X^1, \dots, X^n)} \sqrt{\frac{\det g_{ab}}{\det G_{AB}}}.$$

Proof: This is established by means of a pull-back of the Discontinuous Transport Theorem¹¹, and using results and notation from appendix C,

$$\begin{aligned} \frac{d}{dt} \int_{\phi(\mathcal{U},t)} f dv &= \frac{d}{dt} \int_{\mathcal{U}} F J dV = \int_{\mathcal{U}} \frac{\partial F}{\partial t} J dV + \int_{\partial \mathcal{U}} F \phi_t^*(\mathbf{i}_v d\mathbf{v}) + \int_{\mathcal{U} \cap \Sigma(t)} [F \phi_t^*(\mathbf{i}_v d\mathbf{v} + \mathbf{i}_w d\mathbf{v})] \\ &= \int_{\mathcal{U}} \frac{\partial F}{\partial t} J dV + \int_{\partial \mathcal{U}} F V_N J dv + \int_{\mathcal{U} \cap \Sigma(t)} [F(V_N + W_N)] J dA, \end{aligned}$$

where we used that ϕ_t is regular¹², implying that $\partial\phi(\mathcal{U}, t) = \phi(\partial\mathcal{U}, t)$ and assume that $\Sigma(t) \subset \mathcal{U}$ which implies that $\phi(\mathcal{U}, t) \cap \phi(\Sigma(t), t) = \phi(\mathcal{U} \cap \Sigma(t), t)$.

Balance Principles

All balance principles can be written in the form of the master balance principal below.

Definition 1 Let $f(x, t)$, $h(x, t)$ be scalar functions defined for $x \in \phi(\mathcal{B}, t)$ for every t in some open interval, and $\mathbf{u}(x, t)$ a given vector field on $\phi(\mathcal{B}, t)$. We say that f , h and \mathbf{u} satisfy the master balance law if, for every nice open set $\mathcal{U} \in \mathcal{B}$ the following integral equation holds

$$\boxed{\frac{d}{dt} \int_{\phi(\mathcal{U},t)} f dv = \int_{\phi(\mathcal{U},t)} h dv + \int_{\partial\phi(\mathcal{U},t)} \langle \mathbf{u}, \hat{\mathbf{n}} \rangle da.} \quad (\text{A-6})$$

where $\hat{\mathbf{n}}$ is the unit outward normal to $\partial\phi(\mathcal{U}, t)$. If the above equality is replaced by the inequality

$$\boxed{\frac{d}{dt} \int_{\phi(\mathcal{U},t)} f dv \geq \int_{\phi(\mathcal{U},t)} h dv + \int_{\partial\phi(\mathcal{U},t)} \langle \mathbf{u}, \hat{\mathbf{n}} \rangle da.} \quad (\text{A-7})$$

we say that f , h and \mathbf{u} satisfy the master balance inequality.

In the material picture this balance law becomes,

$$\boxed{\frac{d}{dt} \int_{\mathcal{U}} F J dV = \int_{\mathcal{U}} H J dV + \int_{\partial \mathcal{U}} \langle \mathbf{U}, \hat{\mathbf{N}} \rangle dA.} \quad (\text{A-8})$$

¹¹A less concise but more evident proof would be to use a material version of Transport Theorem (2), and then repeat an analogous argument to the one used for Discontinuous Transport Theorem.

¹²The map ϕ_t being regular implies points in the domain can not be mapped to the same point in the image, because if this were so, then in \mathbb{R}^n there would be a point whose direction derivative would be zero.

where $\hat{\mathbf{N}}$ is the outward unit normal to ∂U in the material system, and again the map ϕ_t must be regular for $\partial\phi_t(\mathcal{U} = \phi_t(\partial\mathcal{U}))$, and so that the material functions are well defined as

$$\begin{aligned} F(X, t)JdV &= \phi_t^*(fdv)(X, t) = f(\phi(X, t), t)J(X, t)dV(X), \\ H(X, t)JdV &= \phi_t^*(hdv)(X, t) = h(\phi(X, t), t)J(X, t)dV(X), \\ \mathbf{i}_U dV &= \phi_t^*(\mathbf{i}_u dv) = \mathbf{i}_{\phi_t^* \mathbf{u}} \phi_t^* dv = \mathbf{i}_{\phi_t^* \mathbf{u}} J dV = \mathbf{i}_{J\phi_t^* \mathbf{u}} dV \\ &\implies \mathbf{U}(X, t) = \frac{\partial\phi_t^{-1}}{\partial x^a}(x, t)u^a(\phi_t(X), t)J(X, t). \end{aligned}$$

For more details on notation see appendix C. Much like a physical law, f , h and \mathbf{u} must satisfy this balance principle everywhere, that is for every nice $\mathcal{U} \subset \mathcal{B}$. Using this, we shall simplify the discontinuity conditions.

Discontinuous Balance Principle

Let f , h , \mathbf{u} satisfy the master balance principal, assume the existence of a surface $\sigma(t) = \phi(\Sigma(t), t)$ on which f , h , \mathbf{u} and ϕ are discontinuous, but elsewhere $f \in C^1$, $h, \mathbf{u} \in C^0$ and ϕ for t fixed is regular. Divide the nice open domain in the same manner as the Discontinuous Transport Theorem, that is $\phi(\mathcal{U}_0, t) = \mathcal{U}_t = \mathcal{U}_t^- \cup \sigma_t \cup \mathcal{U}_t^+$, then this theorem states that

$$\frac{d}{dt} \int_{\mathcal{U}_t} f dv = \int_{\mathcal{U}_t} \frac{\partial f}{\partial t} dv + \int_{\partial\mathcal{U}_t} f v_n da + \int_{\mathcal{U}_t \cap \sigma(t)} [f(v_n + \omega_n)] da,$$

where v_n is the outward normal component of $\mathbf{v} = d\phi/dt$, and $\boldsymbol{\omega}(y, t)$ is the velocity of $y \in \sigma(t)$ relative to the particle at y , or simply

$$\boldsymbol{\omega}(y, t) = \frac{\partial\phi}{\partial X^A}(Y, t)W^A(Y, t),$$

where $y = \phi(Y, t)$ and \mathbf{W} is the material velocity of the discontinuous surface as defined in Theorem 3. Substituting the above equation in the master balance principal (A-6),

$$\int_{\mathcal{U}_t} \frac{\partial f}{\partial t} dv + \int_{\partial\mathcal{U}_t} f v_n da + \int_{\mathcal{U}_t \cap \sigma_t} [f(v_n + \omega_n)] da = \int_{\mathcal{U}_t} h dv + \int_{\partial\mathcal{U}} \langle \mathbf{u}, \hat{\mathbf{n}} \rangle da, \quad (\text{A-9})$$

the functions f , h , \mathbf{u} satisfy the master balance principal for the open sets $\mathcal{W}^+ \subset \mathcal{U}_t^+$ and $\mathcal{W}^- \subset \mathcal{U}_t^-$ separately, resulting in¹³,

$$\frac{d}{dt} \int_{\mathcal{W}^+} f dv = \int_{\mathcal{W}^+} \frac{\partial f}{\partial t} dv + \int_{\partial \mathcal{W}^+} f v_n da = \int_{\mathcal{W}^+} h dv + \int_{\partial \mathcal{W}^+} \langle \mathbf{u}, \hat{\mathbf{n}} \rangle da, \quad (\text{A-10})$$

and

$$\frac{d}{dt} \int_{\mathcal{W}^-} f dv = \int_{\mathcal{W}^-} \frac{\partial f}{\partial t} dv + \int_{\partial \mathcal{W}^-} f v_n da = \int_{\mathcal{W}^-} h dv + \int_{\partial \mathcal{W}^-} \langle \mathbf{u}, \hat{\mathbf{n}} \rangle da. \quad (\text{A-11})$$

Now subtract both equations (A-10) and (A-11) from equation (A-12). Then take the limits \mathcal{W}^+ to \mathcal{U}_t^+ , and \mathcal{W}^- to \mathcal{U}_t^- , resulting in

$$\int_{\mathcal{U}_t \cap \sigma(t)} [f \omega_n] da = - \int_{\mathcal{U}_t \cap \sigma(t)} [\langle \mathbf{u}, \hat{\mathbf{n}} \rangle] da. \quad (\text{A-12})$$

This statement is valid for every \mathcal{U} . Because $\mathbf{u}_n, f, \omega_n$ on $\mathcal{U}_t \cap \sigma(t)$ are at least continuous everywhere except $\mathcal{U}_t \cap \sigma(t)$, then we can conclude that

$$[f \omega_n] = -[\langle \mathbf{u}, \hat{\mathbf{n}} \rangle]. \quad (\text{A-13})$$

Theorem 4 (Localized Theory) *If $f, \phi_t, \mathbf{u} \in C^1$, ϕ_t is regular and $h \in C^0$, then they satisfy the master balance law iff*

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \left(\frac{d(f\mathbf{v})}{dx^a} \right)^a = h + \left(\frac{d\mathbf{u}}{dx^a} \right)^a}. \quad (\text{A-14})$$

They satisfy the master balance inequality iff

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \left(\frac{d(f\mathbf{v})}{dx^a} \right)^a \leq h + \left(\frac{d\mathbf{u}}{dx^a} \right)^a}. \quad (\text{A-15})$$

The proof of this theorem is a direct application of Transport Theorem. The material version of these localized theorems are:

$$\boxed{\frac{\partial(FJ)}{\partial t} = HJ + \left(\frac{d\mathbf{U}}{dX^A} \right)^A \quad \text{and} \quad \frac{\partial(FJ)}{\partial t} \leq HJ + \left(\frac{d\mathbf{U}}{dX^A} \right)^A}. \quad (\text{A-16})$$

¹³The Balance Principle does not necessarily hold on $\bar{\mathcal{U}}^+$, which would result in an equation similar to equation (A-3), because $\bar{\mathcal{U}}^+$ is closed. For balance of momentum this would be like demanding that two plates in contact both exert no force upon each other so that total force balances.

Conservation of Mass

States that the total mass of the set $\phi(\mathcal{U}, t)$ does not change in time,

$$\frac{d}{dt} \int_{\phi_t(\mathcal{U})} \rho dv = 0.$$

To find the discontinuity conditions substitute $\rho = f$ in equation (A-13), resulting in

$$\rho^+ \omega_n^+ = \rho^- \omega_n^-, \quad (\text{A-17})$$

if ρ and J are smooth, then by changing variables to the material system, we conclude that

$$\rho_{Ref}(X) = \rho(x, t) J(X, t), \quad (\text{A-18})$$

where

$$J(X, t) = \frac{\partial(\phi^1, \phi^2, \phi^3)}{\partial(X^1, X^2, X^3)} \frac{\sqrt{\det g_{ab}(x)}}{\sqrt{\det G_{AB}(X)}}.$$

Balance of Momentum

The integral form of momentum balance is subject to an important criticism: it is not form invariant under general coordinate transformations, although the dynamical equations themselves are. One way to work around this in \mathbb{R}^3 is as follows.

Given a constant vector $\mathbf{w} \in \mathbb{R}^3$, then momentum balances in the fixed \mathbf{w} direction,

Definition 2 (Balance of Momentum) *Given ϕ_t a regular map, $\rho(x, t)$ the density, $\mathbf{t}(x, t, \hat{\mathbf{n}})$ the internal stress, and an external force $\mathbf{b}(x, t)$ we say that balance of momentum holds if for every fixed $\mathbf{w} \in \mathbb{R}^3$ and every nice open set $\mathcal{U} \subset \mathcal{B}$,*

$$\frac{d}{dt} \int_{\phi(\mathcal{U}, t)} \rho \langle \mathbf{v}, \mathbf{w} \rangle dv = \int_{\phi(\mathcal{U}, t)} \rho \langle \mathbf{b}, \mathbf{w} \rangle dv + \int_{\partial\phi(\mathcal{U}, t)} \langle \mathbf{t}, \mathbf{w} \rangle da \quad (\text{A-19})$$

where \mathbf{t} is evaluated with the outward normal $\hat{\mathbf{n}}$ to $\partial\phi(\mathcal{U}, t)$.

Using Cauchy's theorem on stress (see theorem 2.2 p.134 in [5]), we can substitute the internal stress with the Cauchy stress tensor which depends on the outward unit normal

of the boundary $\partial\phi_t(\mathcal{U})$, in other words: $\mathbf{t} = \boldsymbol{\sigma}^n$. To acquire the discontinuous jump conditions we use equation (A-12) with

$$f = \rho \langle \mathbf{v}, \mathbf{w} \rangle, h = \rho \langle \mathbf{b}, \mathbf{w} \rangle \quad \text{and} \quad \langle \mathbf{u}, \mathbf{n} \rangle = \langle \boldsymbol{\sigma}^n, \mathbf{w} \rangle = \langle \boldsymbol{\sigma}^w, \mathbf{n} \rangle,$$

resulting in the conditions,

$$[\rho \langle \mathbf{v}, \mathbf{w} \rangle \omega_n] = -[\langle \boldsymbol{\sigma}^n, \mathbf{w} \rangle],$$

which together with the discontinuity conditions for conservation of mass (A-17), and noting that the above is valid for every fixed \mathbf{w} , results in

$$\rho^- \omega_n^- [\mathbf{v}] = -[\boldsymbol{\sigma}^n], \quad (\text{A-20})$$

this can be interpreted as the mass flow times the velocity difference accounts for the difference in internal forces at the discontinuity.

In a domain \mathcal{U} , where the quantities involved are continuous and ϕ_t is regular and C^1 then

$$\frac{d}{dt} \int_{\phi_t(\mathcal{U})} \rho \langle \mathbf{v}_t, \mathbf{w} \rangle dv = \int_{\phi_t(\mathcal{U})} \frac{\partial \rho}{\partial t} \langle \mathbf{v}_t, \mathbf{w} \rangle dv + \int_{\phi_t(\mathcal{U})} \rho \langle \frac{\partial \mathbf{v}_t}{\partial t}, \mathbf{w} \rangle dv \quad (\text{A-21})$$

$$+ \int_{\partial\phi_t(\mathcal{U})} \rho \langle \mathbf{v}_t, \mathbf{w} \rangle \operatorname{div} \mathbf{v} dv. \quad (\text{A-22})$$

using the conservation of mass $\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0$, then balance of momentum becomes

$$\int_{\phi_t(\mathcal{U})} \rho \langle \frac{d\mathbf{v}_t}{dt}, \mathbf{w} \rangle dv = \int_{\phi_t(\mathcal{U})} \langle \rho \mathbf{b}_t, \mathbf{w} \rangle dv + \int_{\partial\phi_t(\mathcal{U})} \langle \boldsymbol{\sigma}^n, \mathbf{w} \rangle da, \quad (\text{A-23})$$

the material balance of momentum becomes

$$\int_{\mathcal{U}} \rho_{Ref} \langle \frac{d\mathbf{V}_t}{dt}, \mathbf{w} \rangle dV = \int_{\mathcal{U}} \langle \rho_{Ref} \mathbf{B}_t, \mathbf{w} \rangle dV + \int_{\partial\mathcal{U}} \langle \mathbf{P}^N, \mathbf{w} \rangle dA, \quad (\text{A-24})$$

where $\mathbf{V} = \mathbf{v} \circ \phi_t$, $\mathbf{B} = \mathbf{b} \circ \phi_t$, \mathbf{N} is normal to $\partial\mathcal{U}$, \mathbf{n} is normal to $\partial\phi_t(\mathcal{U})$ and \mathbf{P} is the first Piola-Kirchhoff stress tensor.

Conservation of Energy

Let \mathcal{B} be a simply body in $\mathcal{S} = \mathbb{R}^3$, ϕ_t a regular differentiable motion of \mathcal{B} in \mathcal{S} , $h(x, t, \hat{\mathbf{n}})$ the heat flux across a surface with unit normal $\hat{\mathbf{n}}$, and $e(x, t)$ the internal energy function per unit mass.

Definition 3 (Conservation of Energy) *Given $\phi(X, t), \rho(x), \mathbf{t}(x, t, \mathbf{n}), e(x, t), \mathbf{b}(x, t)$ and $h(x, t, n)$, we say that conservation of energy holds provided that for every nice open set $\mathcal{U} \subset \mathcal{B}$,*

$$\boxed{\frac{d}{dt} \int_{\phi(\mathcal{U}, t)} \rho \left(e + \frac{1}{2} \langle \mathbf{v}, \mathbf{v} \rangle \right) dv = \int_{\phi(\mathcal{U}, t)} \rho \langle \mathbf{b}, \mathbf{v} \rangle dv - \int_{\partial\phi(\mathcal{U}, t)} \langle \boldsymbol{\sigma}^n, \mathbf{v} \rangle q^n da,} \quad (\text{A-25})$$

where we have used Cauchy's theorem to substitute $t = \langle \boldsymbol{\sigma}, \hat{\mathbf{n}} \rangle = \boldsymbol{\sigma}^n$ and $h(x, t, \hat{\mathbf{n}}) = -q^n(x, t)$.

To obtain the discontinuous jump conditions we use equation (A-12) with

$$f = \rho \left(e + \frac{1}{2} \langle \mathbf{v}, \mathbf{v} \rangle \right), \text{ and } \langle \mathbf{u}, \hat{\mathbf{n}} \rangle = \langle \boldsymbol{\sigma}^n, \mathbf{v} \rangle - q^n$$

resulting in the conditions,

$$[\rho \left(e + \frac{1}{2} \langle \mathbf{v}, \mathbf{v} \rangle \right) \omega_n] = -[\langle \boldsymbol{\sigma}^n, \mathbf{v} \rangle], \quad (\text{A-26})$$

which together with the discontinuity condition (A-20) results in,

$$\boxed{[\rho e] = -\frac{1}{2} \langle \boldsymbol{\sigma}^{n+} + \boldsymbol{\sigma}^{n-}, [\mathbf{v}] \rangle.} \quad (\text{A-27})$$

The Entropy Production Inequality

The second law of thermodynamics is frequently shrouded in mysterious physical jargon, and my education was no exception. The results needed are given a concise mathematical treatment. This ‘‘law’’ is vital in elasticity, for with it we can uniquely define the internal stress in terms of the internal free-energy ψ , where $e = \psi + \eta$ and $\eta(x, t)$ is the

specific entropy¹⁴ per unit mass. Also assume there is function $\theta(x, t) > 0$, the absolute temperature.

Definition 4 (Clausius-Duhem inequality) *The functions in the inequality below are said to obey the entropy production inequality or the Clausius-Duhem inequality if, for all nice $\mathcal{U} \subset \mathcal{B}$ we have*

$$\boxed{\frac{d}{dt} \int_{\phi(\mathcal{U}, t)} \rho \eta \, dv \leq - \int_{\partial\phi(\mathcal{U}, t)} \frac{q^n}{\theta} \, da,} \quad (\text{A-28})$$

where we have used Cauchy's theorem to substitute $h(x, t, \mathbf{n}) = -q^n(x, t)$.

the discontinuous jump condition is

$$\boxed{[\rho \eta \omega_n] \leq [\frac{q^n}{\theta}].} \quad (\text{A-29})$$

B Appendix

Assumptions of Elasticity

This appendix will briefly summarize the assumptions which are particular to elastic theory. From this, we hope the reader can visualize what elastic theory attempts to capture.

The constitutive function $\hat{\Psi}$ is a map that given a motion ϕ and temperature field Θ returns a function for the internal free-energy Ψ . Below we informally define a constitutive function for thermoelasticity.

Definition 5 *A constitutive function for thermoelasticity*

$$\hat{\Psi} : (\phi, \Theta) \mapsto \Psi$$

¹⁴For a more advanced mathematical treatment, in which entropy is regarded as a measure of disorder and its origins in statistical mechanics via the Boltzmann's equation can be found in Ruelle [7] and [8]

is called local and history independent if for any open set $\mathcal{U} \subset \mathcal{B}$ and any two motions ϕ_1 and ϕ_2 and temperature fields Θ_1 and Θ_2 , such that $\phi_1(X, t) = \phi_2(X, t)$ and $\Theta_1(X, t) = \Theta_2(X, t)$ for every $X \in \mathcal{U}$, then $\hat{\Psi}(\phi_1, \Theta_1)$ and $\hat{\Psi}(\phi_2, \Theta_2)$ agree on \mathcal{U} .

The idea of using locality as a basic postulate is due to Noll[1958]. However, it must be emphasized, that this does not stop us from imposing nonlocal constraints, such as incompressibility.

Example 1 Nonlocal operator:

$$f : C^0[0, 1] \rightarrow C^0[0, 1] \text{ by } f(\phi)(x) = \int_0^x \phi(s) ds.$$

the functions ϕ_1 and ϕ_2 can agree on a ball around x and have that $f(\phi_1)(x)$ is not equal to $f(\phi_2)(x)$ on this same ball.

Axiom 1 (Axiom of Locality) *Constitutive functions for thermoelasticity are assumed to be local.*

Axiom 2 (Axiom of History Independence) *Constitutive functions for thermoelasticity do not depend on all past histories, but only on the current map, ϕ for t fixed, and temperature distribution, Θ for t fixed.*

These assumptions capture the essence of elasticity, for instance a consequence from¹⁵ axiom 2 is that the internal free-energy Ψ depends on how much the material is stretched, i.e. on \mathbf{C} , and not on the rate the material is being stretched. Independent of what has happened to the material, upon returning to the same spatial configuration the internal free-energy will be the same. This also excludes plasticity.

Using these axioms we can uniquely relate internal free energy and stress by assuming the entropy production inequality holds for all regular motions and temperature configurations. We achieve this by varying independently ϕ and Θ .

¹⁵Together with many other typical axioms employed in continuum mechanics and physical balance laws.

Axiom 3 (Axiom of Entropy Production) For any regular motion and temperature configuration of \mathcal{B} , the thermoelastic constitutive functions are assumed to satisfy the entropy production inequality:

$$\rho_{Ref}(\hat{N} \frac{\partial \Theta}{\partial t} + \frac{\partial \hat{\Psi}}{\partial t}) - \hat{P} : \frac{\partial \mathbf{F}}{\partial t} + \frac{1}{\Theta} \langle \hat{Q}, \nabla \Theta \rangle \leq 0.$$

Theorem 5 (Coleman and Noll) [1963] Suppose the axioms of locality and entropy production hold. Then $\hat{\Psi}$ depends only on the variables X , F , and Θ . Moreover, we have

$$\hat{N} = -\frac{\partial \hat{\Psi}}{\partial \Theta} \text{ and } \hat{P} = \rho_{Ref} \mathbf{g}^\# \frac{\partial \hat{\Psi}}{\partial \mathbf{F}}, \text{ that is, } \hat{P}_a^A = \rho_{Ref} \frac{\partial \hat{\Psi}}{\partial F_A^a}, \quad (\text{B-1})$$

where the derivatives are taken in the Fréchet sense, and the entropy production inequality reduces to

$$\langle \mathbf{Q}, \nabla \Theta \rangle \leq 0.$$

Proof: see p.190 Marsden [5]. □

It can shown (see p.217 from [5]) by using material frame indifference, that for an isotropic material Ψ depends only on the eigenvalues of $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and temperature Θ . Recall that the eigenvalues of \mathbf{C} are the principle stretches squared.

Now by using the above theorem, and that Ψ depends on \mathbf{C} only through its eigenvalues λ_i 's, we can relate the cauchy stress tensor $\boldsymbol{\sigma}$ with the motion ϕ and Ψ ,

$$\sigma^{ab} = P^{aA} \frac{\partial \phi^b}{\partial X^A} J^{-1} = \rho_{Ref} \mathbf{g}^{ab} \frac{\partial \hat{\Psi}}{\partial F_A^a} \frac{\partial \phi^b}{\partial X^A} J^{-1} = \rho_{Ref} \mathbf{g}^{ab} \frac{\partial \hat{\Psi}}{\partial \lambda_j} \frac{\partial \lambda_j}{\partial F_A^a} \frac{\partial \phi^b}{\partial X^A} J^{-1}, \quad (\text{B-2})$$

where the metric \mathbf{g} and \mathbf{G} , for the current and reference configuration coordinate systems, respectively, are defined by

$$g_{ab} = \langle \mathbf{e}_a, \mathbf{e}_b \rangle, \quad G_{AB} = \langle \mathbf{E}_A, \mathbf{E}_B \rangle,$$

where the vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$ are the base vectors of the spatial and reference configuration coordinate systems, and

$$J(X, t) = \frac{\partial(\phi^x, \phi^y, \phi^z)}{\partial(X, Y, Z)} \frac{\sqrt{\det g_{ab}(x)}}{\sqrt{\det G_{AB}(X)}}.$$

Spherical Coordinates Constitutive Equation

Let us develop the above constitutive equation for the Cauchy stress tensor $\boldsymbol{\sigma}$ in spherical coordinates both for the material body and current body. The same coordinate system used in the section *Modelling with Radial Symmetry*.

Using the above formula for the determinant of the Jacobian \mathbf{J} ,

$$J(X, t) = \frac{\partial(\phi^r, \phi^\theta, \phi^\varphi)}{\partial(R, \Theta, \Phi)} \frac{\sqrt{\det g_{ab}(x)}}{\sqrt{\det G_{AB}(X)}} = \frac{\partial r}{\partial R} \frac{r^2}{R^2},$$

the density $\rho_{Ref}(X)$ is a given constant function, and the metrics for spherical coordinates is

$$g_{rr} = 1, \quad g_{\theta\theta} = (r \sin \varphi)^2, \quad g_{\varphi\varphi} = r^2. \quad (\text{B-3})$$

similarly for the reference coordinate system,

$$G_{RR} = 1, \quad G_{\Theta\Theta} = (R \sin \Phi)^2, \quad G_{\Phi\Phi} = R^2. \quad (\text{B-4})$$

We also need the Cauchy-Green tensor \mathbf{C} , which in coordinates is defined by

$$C_{AB} = g_{ab} F_C^a F_B^b G^{AC},$$

the tensor G^{AB} is the inverse of G_{AB} , in other words $G_{CD} G^{CB} = \delta_C^B$, which is one if $C = B$ and zero otherwise. With the above tensors we can attain the Cauchy-Green tensor \mathbf{C} , which can be represented by the following matrix,

$$(C_{AB})_{AB} = \begin{pmatrix} (F_R^r)^2 & 0 & 0 \\ 0 & (F_\Theta^\theta)^2 \left(\frac{r}{R}\right)^2 & 0 \\ 0 & 0 & (F_\Phi^\varphi)^2 \left(\frac{r}{R}\right)^2 \end{pmatrix}. \quad (\text{B-5})$$

Although F_Θ^θ and F_Φ^φ are both the identity map for our application, they have been explicitly left because the constitutive equation, which relates the internal forces $\boldsymbol{\sigma}$ and the internal energy Ψ , uses the general dependence that Ψ has on the eigenvalues of \mathbf{C} in this coordinate system, in other words, $\hat{\Psi}$ is uniquely defined by $\lambda_1 = (F_R^r)^2$, $\lambda_2 = (F_\Theta^\theta)^2 \left(\frac{r}{R}\right)^2$, $\lambda_3 = (F_\Phi^\varphi)^2 \left(\frac{r}{R}\right)^2$ and temperature Θ .

Substituting the relevant quantities in equation (B-2), then the Fréchet derivative evaluated at this systems configuration, i.e. $F_{\Phi}^{\varphi} = F_{\Theta}^{\theta} = 1$, results in,

$$\begin{aligned}\sigma^{rr} &= 2\rho_{Ref} \frac{\partial \Psi}{\partial \lambda_1} \frac{\partial r}{\partial R} \frac{R^2}{r^2}, \\ \sigma^{\theta\theta} &= 2\rho_{Ref} \frac{\partial \Psi}{\partial \lambda_2} \left(\frac{\partial r}{\partial R} \right)^{-1} \frac{1}{\sin^2 \varphi r^2}, \\ \sigma^{\varphi\varphi} &= 2\rho_{Ref} \frac{\partial \Psi}{\partial \lambda_3} \left(\frac{\partial r}{\partial R} \right)^{-1} \frac{1}{r^2}.\end{aligned}$$

C Appendix

Results from Differential Geometry

Lie Derivative

Before defining this object we show where it appears in our application. In all balance principles, integrals of the following form will be present,

$$\frac{d}{dt} \int_{\psi_t(\mathcal{P})} \boldsymbol{\alpha},$$

where ψ_t is a function $\mathcal{S} \rightarrow \mathcal{B}$, and $\psi_t(x) = \psi(x, t)$. This notation will be adopted bellow when we only wish to deal with the spatial parameters x , and maintain t fixed. In regions in which we assume $\boldsymbol{\alpha}$ is differentiable we can recast this integral in another form,

$$\begin{aligned}\frac{d}{dt} \int_{\psi_t(\mathcal{P})} \boldsymbol{\alpha} &= \frac{d}{dt} \int_{\mathcal{P}} \psi_t^* \boldsymbol{\alpha} = \int_{\mathcal{P}} \frac{d}{dt} (\psi_t^* \boldsymbol{\alpha}) = \int_{\psi_t(\mathcal{P})} \psi_{t*} \frac{d}{dt} (\psi_t^* \boldsymbol{\alpha}) = \\ &= \int_{\psi_t(\mathcal{P})} \left(\psi_{s*}^{-1} \frac{d}{dt} (\psi_t^* \boldsymbol{\alpha}) \right) \Big|_{s=t} = \int_{\psi_t(\mathcal{P})} \left(\frac{d}{dt} (\psi_{t,s}^* \boldsymbol{\alpha}) \right) \Big|_{s=t} = \int_{\psi_t(\mathcal{P})} \mathbf{L}_v \boldsymbol{\alpha},\end{aligned}\quad (\text{C-1})$$

where $\psi_{t,s}(x) = \psi(\psi^{-1}(x, s), t)$, above the last equality is the definition of Lie Derivative,

Definition 6 Let \mathbf{w} be a C^1 , time dependent, vector field on the manifold \mathcal{M} , and let $\psi_{t,s}$ denote its flow, i.e. $(d\psi_{t,s}/dt)|_{s=t} = \mathbf{w}_t$. If \mathbf{T} is a C^1 tensor field on \mathcal{M} , then the Lie Derivative of \mathbf{T} with respect to \mathbf{w} is defined by

$$\mathbf{L}_{\mathbf{w}} \mathbf{T} = \left(\frac{d}{dt} \psi_{t,s}^* \mathbf{T}_t \right) \Big|_{s=t}. \quad (\text{C-2})$$

Example 2 Let $f \in C^1$ be a time dependent scalar function, then

$$\mathbf{L}_{\mathbf{w}}(f \mathbf{d}x^k) = \left(\frac{d}{dt} \psi_{t,s}^* f \mathbf{d}x^k \right) \Big|_{s=t} = \left(\frac{d}{dt} f(\psi_{t,s}(x), t) \frac{\partial \psi_{t,s}^k(x)}{\partial x^j} \mathbf{d}x^j \right) \Big|_{s=t},$$

we use bold \mathbf{d} when we wish to emphasize that the term is a differential form. In this last expression every x that appears is in the image of ψ_s which does not change in time.

Therefore

$$\begin{aligned} \mathbf{L}_{\mathbf{w}}(f \mathbf{d}x^k) &= \left(\frac{\partial f}{\partial t} \frac{\partial \psi_{t,s}^k(x)}{\partial x^j} + \frac{\partial f}{\partial x^j} w^j \circ \psi_s^{-1} \frac{\partial \psi_{t,s}^k(x)}{\partial x^j} + f \frac{\partial w^k}{\partial x^j} \circ \psi_s^{-1} \mathbf{d}x^j \right) \Big|_{s=t} \\ &= \frac{\partial f}{\partial t} \mathbf{d}x^k + \frac{\partial f}{\partial x^j} w^j \mathbf{d}x^k + f \frac{\partial w^k}{\partial x^j} \mathbf{d}x^j, \end{aligned}$$

where we have used that $(\psi_{t,s})_{s=t}$ is the identity map.

To interpret the Lie Derivative it helps to separate it in the following manner. If we hold t fixed in \mathbf{T}_t , we obtain the *autonomous Lie derivative*:

$$\boxed{\mathcal{L}_{\mathbf{w}} T = \left(\frac{d}{dt} \psi_{t,s}^* \mathbf{T}_s \right) \Big|_{s=t}.}$$

Hence $\mathbf{L}_{\mathbf{w}} \mathbf{T} = \mathcal{L}_{\mathbf{w}} T + \partial T / \partial t$. In the integral equation (C-1), if $\boldsymbol{\alpha} = f \mathbf{d}v$, the volume form, then the autonomous Lie derivative can be interpreted as how much the integral (C-1) changes in time because of the motion of the boundary $\partial \psi_t(\mathcal{P})$. This motivates us to investigate if a surface integral of the flux is equal to the volume integral of $\mathcal{L}_{\mathbf{w}}(f \mathbf{d}v)$,

$$\int_{\partial \psi_t(\mathcal{P})} f w_n \mathbf{d}a = \int_{\psi_t(\mathcal{P})} \mathcal{L}_{\mathbf{w}}(f \mathbf{d}v), \quad (\text{C-3})$$

where w_n is the component of \mathbf{w} in the direction of the outward unit normal to the boundary $\partial \psi_t(\mathcal{P})$, and using the definition of lie derivative, we have that in coordinates

$$\mathbf{L}_{\mathbf{w}}(f \mathbf{d}v) = \frac{\partial f}{\partial t} \mathbf{d}v + \mathcal{L}_{\mathbf{w}}(f \mathbf{d}v) = \frac{\partial f}{\partial t} \mathbf{d}v + \left(\frac{\partial f}{\partial x^m} w^m + f \left(\frac{d\mathbf{w}}{dx^m} \right)^m \right) \mathbf{d}v. \quad (\text{C-4})$$

If we show that the exterior derivative $d(f w_n \mathbf{d}a) = \mathcal{L}_{\mathbf{w}}(f \mathbf{d}v)$, then by the generalized Stokes' theorem equation (C-3) can be established. To see how this is calculated classically see the section "Classical Transport Theorem" at the end of this appendix. What follows will be used to demonstrate the equality $d(f w_n \mathbf{d}a) = \mathcal{L}_{\mathbf{w}}(f \mathbf{d}v)$.

Definition 7 If \mathbf{w} is a vector field on \mathcal{M} and $\boldsymbol{\alpha}$ is a k -form, the contraction of \mathbf{w} with the first index of $\boldsymbol{\alpha}$ is called the interior product and is denoted by $\mathbf{i}_{\mathbf{w}}\boldsymbol{\alpha}$. Thus $\mathbf{i}_{\mathbf{w}}\boldsymbol{\alpha}$ is a $(k - 1)$ -form, given by

$$\boxed{(\mathbf{i}_{\mathbf{w}}\boldsymbol{\alpha})(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{k-1}) = \boldsymbol{\alpha}(\mathbf{w}, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{k-1}).}$$

A geometric interpretation for this contraction is given in the following proposition.

Proposition 1 Let $\hat{\mathbf{n}}$ be the unit outward normal to $\partial\mathcal{M}$ and \mathbf{w} a vector field on \mathcal{M} . Then on $\partial\mathcal{M}$, $\langle \mathbf{w}, \hat{\mathbf{n}} \rangle \mathbf{d}\mathbf{a} = \mathbf{i}_{\mathbf{w}}\mathbf{d}\mathbf{v}$, where $\mathbf{d}\mathbf{a}$ is the area element of $\partial\mathcal{M}$.

Proof: The equation we wish to prove is composed of coordinate independent quantities. Hence without loss of generality we choose coordinates $\{x^a\}$ for \mathcal{M} in which $\partial\mathcal{M}$ is the plane $x^1 = 0$, \mathcal{M} is defined by $x^1 < 0$ and $\hat{\mathbf{n}} = (1, 0, \dots, 0)$ is the unit normal to $\partial\mathcal{M}$. This way

$$\mathbf{i}_{\mathbf{w}}\mathbf{d}\mathbf{v} = \mathbf{i}_{\mathbf{w}}\sqrt{g_{ab}}\mathbf{d}x^1 \wedge \dots \wedge \mathbf{d}x^n = \sqrt{g_{ab}}(-1)^{1-i}w^i \underbrace{\mathbf{d}x^1 \wedge \dots \wedge \mathbf{d}x^n}_{\text{missing } \mathbf{d}x^i},$$

If we evaluate this expression on the domain of $\partial\mathcal{M}$, $x^1 = 0$, we are left with only the first term

$$\mathbf{i}_{\mathbf{w}}\mathbf{d}\mathbf{v} = \sqrt{g_{ab}}w^1\mathbf{d}x^2 \wedge \dots \wedge \mathbf{d}x^n = \langle \mathbf{w}, \hat{\mathbf{n}} \rangle \mathbf{d}\mathbf{a}$$

□

Now for the final theorem we need before our main result.

Theorem 6 The theorem is to establish the following identity,

$$\mathcal{L}_v(\mathbf{d}\mathbf{v}) = \frac{1}{\sqrt{\det g_{ab}}} \frac{\partial}{\partial x^m} (v^m \sqrt{\det g_{ab}}) \mathbf{d}\mathbf{v} = \left(\frac{d\mathbf{v}}{dx^m} \right)^m \mathbf{d}\mathbf{v}. \quad (\text{C-5})$$

Proof: Let γ_{ab}^c be the Christoffel symbols, then the identity is demonstrated by a direct calculation,

$$\begin{aligned} \frac{\partial}{\partial x^m} (v^m \sqrt{\det g_{ab}}) &= \frac{\partial v^m}{\partial x^m} \sqrt{\det g_{ab}} + \frac{v^m}{2\sqrt{\det g_{ab}}} \frac{\partial g_{ab}}{\partial x^m} (\text{Cof}g)^{ab} \\ &= \frac{\partial v^m}{\partial x^m} \sqrt{\det g_{ab}} + \frac{v^m}{2\sqrt{\det g_{ab}}} (g_{kb}\gamma_{ad}^k v^d + g_{ak}\gamma_{bd}^k v^d) (\text{Cof}g)^{ab}, \end{aligned}$$

in the last expression, we shall simplify the term: $v^m g_{kb} \gamma_{ad}^k v^d (Cofg)^{ab}$, fix a , in other words looking at the line a , now summing over b results in the determinant of some matrix. Notice all the lines, except the a -th, of this matrix are equal to the lines of the matrix $(g_{ab})_{ab}$. The a -th line has other lines of $(g_{ab})_{ab}$ summed to it, that is, for each k we sum another line of $(g_{ab})_{ab}$ to the a -th. Summing repeated lines contributes nothing to the determinant, this implies that setting $k = a$ does not change the value of the determinant. An analogous argument works for the other term. As a result we have,

$$\begin{aligned} v^m (g_{kb} \gamma_{ad}^k v^d + g_{ak} \gamma_{bd}^k v^d) (Cofg)^{ab} &= \frac{\partial v^m}{\partial x^m} \sqrt{\det g_{ab}} + v^m (g_{ab} \gamma_{ad}^a v^d + g_{ab} \gamma_{bd}^b v^d) (Cofg)^{ab} \\ &= v^m (\gamma_{ad}^a v^d + \gamma_{bd}^b v^d) \det g_{ab} = 2v^m \gamma_{ad}^a v^d \det g_{ab}, \end{aligned}$$

substituting this above results in

$$\begin{aligned} \frac{\partial}{\partial x^m} (v^m \sqrt{\det g_{ab}}) &= \frac{\partial v^m}{\partial x^m} \sqrt{\det g_{ab}} + v^m \gamma_{ad}^a v^d \sqrt{\det g_{ab}} \implies \\ \frac{1}{\sqrt{\det g_{ab}}} \frac{\partial}{\partial x^m} (v^m \sqrt{\det g_{ab}}) &= \left(\frac{d\mathbf{v}}{dx^m} \right)^m. \end{aligned}$$

Theorem 7 *The exterior derivative $\mathbf{d}(fi_{\mathbf{w}}\mathbf{d}v)$ is equal to the lie derivative $\mathcal{L}_{\mathbf{w}}(f\mathbf{d}v)$.*

Proof:

$$\begin{aligned} \mathbf{d}(fi_{\mathbf{w}}\mathbf{d}v) &= \mathbf{d}(f \sqrt{\det g_{ab}} (w^1 \mathbf{d}x^2 \wedge \mathbf{d}x^3 - w^2 \mathbf{d}x^1 \wedge \mathbf{d}x^3 + w^3 \mathbf{d}x^1 \wedge \mathbf{d}x^2)) \\ &= \left(\frac{\partial f}{\partial x^m} w^m + \frac{1}{\sqrt{\det g_{ab}}} \frac{\partial}{\partial x^m} (w^m \sqrt{\det g_{ab}}) \right) \mathbf{d}v = \mathcal{L}_{\mathbf{w}}(f\mathbf{d}v). \end{aligned}$$

Classical Transport Theorem

We define the divergence as

$$\operatorname{div} v = \left(\frac{d\mathbf{v}}{dx^m} \right)^m,$$

then classically Transport Theorem is shown by the following,

$$\begin{aligned} \frac{d}{dt} \int_{\psi_t(W_0)} f(x, t) dv &= \frac{d}{dt} \int_{W_0} f(\psi_t(X), t) J(X, t) dV = \\ & \int_{W_0} J(X, t) \frac{d}{dt} f(\psi_t(X), t) + f(\psi_t(X), t) \frac{d}{dt} J(X, t) dV = \\ & \int_{W_0} J \frac{\partial f}{\partial x^a} w^a + J \frac{\partial f}{\partial t} + f J \operatorname{div} w dV = \int_{W_0} J \frac{\partial f}{\partial t} + J \operatorname{div}(fw) dV = \\ & \int_{\psi_t(W_0)} \frac{\partial f}{\partial t} dv + \int_{\partial\psi_t(W_0)} fw_n da. \end{aligned}$$

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