CS294-73 Final Project: Multiphase Material Solid Mechanics

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Part I

Introduction

The project proposed for this class involves the calculation of the mechanical behavior of a multiphase material. The main equation being solved will be the balance of linear momentum in a static setting. The constitutive model for the mechanical behavior is based on the a paper by T.I. Zohdi and A.J. Szeri on a multiphase model of kidney stone fatigue. The detailed mathematics of the project will be outlined further below, yet it is important to note that the proposed problem will be solved on an unstructured grid in a 2-dimensional setting.

The differential equation being solved for this study is the balance of linear momentum

$$\nabla_x \boldsymbol{\sigma} + \mathbf{f} = \rho \frac{d^2\mathbf{u}}{dt^2}$$

in a time-independent setting, meaning $\frac{d^2\mathbf{u}}{dt^2} = 0$, resulting in

$$\nabla_x \boldsymbol{\sigma} + \mathbf{f} = 0$$

where σ represents the Cauchy stress, $\mathbf{f}$ represents body forces. When considering only infinitesimal deformations, we can approximate $\frac{d()}{dt} \approx \frac{\partial()}{\partial t}|X$ and $\nabla_{\mathbf{x}} = \nabla_{\mathbf{X}}$ where $\mathbf{x}$ is the current configuration and $\mathbf{X}$ is the reference configuration of the system. Now using a multiphase, elastic, isotropic constitutive law we can write

$$\boldsymbol{\sigma} = \mathbb{E}^* : (\boldsymbol{\epsilon})$$

where $\mathbb{E}^*$ represents the effective elastic tensor of the material. The effective elastic tensor for a multiphase material can be calculated using property derived from variational principles. In the case of two-phase materials, the following bounds can be written

- The bulk modulus κ, the lower and upper are respectively

$$\kappa^*_{(-)} = \kappa_1 + v_2\left(\frac{1}{\kappa_2 - \kappa_1} + \frac{3(1-v_2)}{3\kappa_1 + 4\mu_1}\right)^{-1}$$

$$\kappa^*_{(+)} = \kappa_2 + (1-v_2)\left(\frac{1}{\kappa_1 - \kappa_2} + \frac{3v_2}{3\kappa_2 + 4\mu_2}\right)^{-1}$$

- The shear modulus μ

$$\mu^*_{(-)} = \mu_1 + v_2\left(\frac{1}{\mu_2 - \mu_1} + \frac{6v_2(\kappa_2 + 2\mu_2)}{5\mu_1(3\kappa_1 + 4\mu_1)}\right)^{-1}$$

$$\mu^*_{(+)} = \mu_2 + (1-v_2)\left(\frac{1}{\mu_1 - \mu_2} + \frac{6v_2(\kappa_2 + 2\mu_2)}{5\mu_2(3\kappa_2 + 4\mu_2)}\right)^{-1}$$

The constitutive law can be written more compactly using Voigt notation

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{Bmatrix} = \begin{bmatrix} \mathbb{E}_{11} & \mathbb{E}_{12} & \mathbb{E}_{13} & \mathbb{E}_{14} & \mathbb{E}_{15} & \mathbb{E}_{16} \\ \mathbb{E}_{21} & \mathbb{E}_{22} & \mathbb{E}_{23} & \mathbb{E}_{24} & \mathbb{E}_{25} & \mathbb{E}_{26} \\ \mathbb{E}_{31} & \mathbb{E}_{32} & \mathbb{E}_{33} & \mathbb{E}_{34} & \mathbb{E}_{35} & \mathbb{E}_{36} \\ \mathbb{E}_{41} & \mathbb{E}_{42} & \mathbb{E}_{43} & \mathbb{E}_{44} & \mathbb{E}_{45} & \mathbb{E}_{46} \\ \mathbb{E}_{51} & \mathbb{E}_{52} & \mathbb{E}_{53} & \mathbb{E}_{54} & \mathbb{E}_{55} & \mathbb{E}_{56} \\ \mathbb{E}_{61} & \mathbb{E}_{62} & \mathbb{E}_{63} & \mathbb{E}_{64} & \mathbb{E}_{65} & \mathbb{E}_{66} \end{bmatrix} \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{12} \\ 2\epsilon_{23} \\ 2\epsilon_{31} \end{Bmatrix}$$

which can be rewritten in terms of the effective bulk modulus $\kappa*$ and the effective shear modulus $\mu*$

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{Bmatrix} = \begin{bmatrix} \kappa^* + \frac{4}{3}\mu^* & \kappa^* - \frac{2}{3}\mu^* & \kappa^* - \frac{2}{3}\mu^* & 0 & 0 & 0 \\ \kappa^* - \frac{2}{3}\mu^* & \kappa^* + \frac{4}{3}\mu^* & \kappa^* - \frac{2}{3}\mu^* & 0 & 0 & 0 \\ \kappa^* - \frac{2}{3}\mu^* & \kappa^* - \frac{2}{3}\mu^* & \kappa^* + \frac{4}{3}\mu^* & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu^* & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu^* & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu^* \end{bmatrix} \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{12} \\ 2\epsilon_{23} \\ 2\epsilon_{31} \end{Bmatrix}$$

Furthermore, the strain tensor $\{\epsilon\}$ can be written in terms of spatial derivatives

$$\{\epsilon\} = \begin{Bmatrix} \frac{\partial u_1}{\partial x_1} \\ \frac{\partial u_2}{\partial x_2} \\ \frac{\partial u_3}{\partial x_3} \\ \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \\ \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \\ \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \end{Bmatrix}$$

which can be expressed in term of the finite element discretization

$$\frac{\partial u_i}{\partial x_j} = \sum_{A=1}^{N} a_i^A \frac{\partial \phi^A}{\partial x_j}$$

which makes it useful to define the following matrix $[T]$

$$[T] = \begin{Bmatrix} \frac{\partial}{\partial x_1} & 0 & 0 \\ 0 & \frac{\partial}{\partial x_2} & 0 \\ 0 & 0 & \frac{\partial}{\partial x_3} \\ \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} & 0 \\ 0 & \frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} & 0 & \frac{\partial}{\partial x_1} \end{Bmatrix}$$

which allows the strain tensor to rewritten as

$$\{\epsilon\} = [T] \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

Weak Form of Time-Dependent Balance of Linear Momentum

The first step in the finite element method is to derive the weak form of the equation by integrating the equation over the domain of the problem and multiplying the equation by a test function v:

$$\nabla_X \boldsymbol{\sigma} + \mathbf{f} = 0$$

$$\int_\Omega v \cdot (\nabla_X \boldsymbol{\sigma} + \mathbf{f}) \, d\Omega = 0 \quad \forall v \in H_{1(\Omega)}$$

This equation can be modified using the product rule of differentiation:

$$\int_\Omega \nabla \cdot (\boldsymbol{\sigma} \colon v)\, d\Omega = \int_\Omega v \cdot (\nabla \boldsymbol{\sigma})\, d\Omega + \int_\Omega \nabla v \colon \boldsymbol{\sigma}\, d\Omega \quad \forall v \in H_{1(\Omega)}$$

which leads to the following equation

$$\int_\Omega \nabla_X \cdot (\boldsymbol{\sigma} \colon v)\, d\Omega - \int_\Omega \nabla_X v \colon \boldsymbol{\sigma}\, d\Omega + \int_\Omega v \cdot \mathbf{f}\, d\Omega = 0 \quad \forall v \in H_{1(\Omega)}$$

Next the divergence theorem is applied

$$\int_\Omega \nabla_X \cdot (\boldsymbol{\sigma} \colon v)\, d\Omega = \int_{\partial\Omega} \boldsymbol{\sigma} \cdot \boldsymbol{n} \cdot v\, dS$$

yielding

$$\int_\Omega \nabla_X v \colon \boldsymbol{\sigma}\, d\Omega = \int_{\partial\Omega} \boldsymbol{\sigma} \cdot \boldsymbol{n} \cdot v\, dS + \int_\Omega v \cdot \mathbf{f}\, d\Omega \quad \forall v \in H_{1(\Omega)}$$

which applying the boundary condition becomes

$$\int_{\partial\Omega} \boldsymbol{\sigma} \cdot \boldsymbol{n} \cdot v\, dS = \int_{\Gamma_t} \boldsymbol{t} \cdot v\, dS \qquad \forall v \textit{ such that } v = 0 \textit{ on } \Gamma_d$$

Now we can apply the constitutive law for the Cauchy stress

$$\boldsymbol{\sigma} = \mathcal{D}\,\mathbb{E}^{\boldsymbol{*}} : (\boldsymbol{\epsilon})$$

to obtain the equation

$$\int_\Omega \nabla_X v \colon (\mathcal{D}\,\mathbb{E}_{\boldsymbol{0}} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon_\theta} - \boldsymbol{\epsilon_p}))\, d\Omega = \int_{\partial\Omega} \boldsymbol{\sigma} \cdot \boldsymbol{n} \cdot v\, dS + \int_\Omega v \cdot \mathbf{f}\, d\Omega$$

which can be broken into the different strain integrals

$$\int_\Omega \nabla_X v \colon (\mathcal{D}\,\mathbb{E}^* : \boldsymbol{\epsilon})\, d\Omega = \int_{\partial\Omega} \boldsymbol{\sigma} \cdot \boldsymbol{n} \cdot v\, dS + \int_\Omega v \cdot \mathbf{f}\, d\Omega$$

Now the finite element discretization can be applied

$$u(x,y,z) = \sum_{A=1}^{N} a_A \phi_A(x,y,z) \qquad v(x,y,z) = \sum_{A=1}^{N} b_A \phi_A(x,y,z)$$

or

$$u_i(x,y,z) = \sum_{A=1}^{N} a_i^A \phi^A(x,y,z) \qquad v_i(x,y,z) = \sum_{A=1}^{N} b_i^A \phi^A(x,y,z) \quad i = 1,2,3$$

Now we define the matrix 3x24 $[\phi]$ as follows

$$[\phi] = \begin{array}{cccccccc} \phi_1 & \phi_2 & \phi_3 & \phi_4 & \phi_5 & \phi_6 & \phi_7 & \phi_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}$$

as the first block of eight columns

$$[\phi] = \begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \phi_1 & \phi_2 & \phi_3 & \phi_4 & \phi_5 & \phi_6 & \phi_7 & \phi_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}$$

as the second block of eight columns

$$[\phi] = \begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \phi_1 & \phi_2 & \phi_3 & \phi_4 & \phi_5 & \phi_6 & \phi_7 & \phi_8 \end{matrix}$$

as the third block of eight columns. All three blocks are put together to form the full matrix. This what done explicity here due to space limitations of the text processor. A similar appraoch will be used to express other large matrices. Now if we define the solution vector $\{a\}$ to be a 24x1 vector of the following form

$$\{a\} = \begin{Bmatrix} a_1^1 \\ a_2^1 \\ a_3^1 \\ a_1^2 \\ a_2^2 \\ a_3^2 \\ \vdots \\ a_3^8 \end{Bmatrix}$$

we can define the solution vector as

$$u(x) = [\phi]\{a\}$$

and the strain tensor as

$$\{\epsilon\} = [T][\phi]\{a\}$$

where $[T][\phi]$ is

$$[T][\phi] = \begin{bmatrix} \frac{\partial\phi^1}{\partial x_1} & 0 & 0 \\ 0 & \frac{\partial\phi^1}{\partial x_2} & 0 \\ 0 & 0 & \frac{\partial\phi^1}{\partial x_3} \\ \frac{\partial\phi^1}{\partial x_2} & \frac{\partial\phi^1}{\partial x_1} & 0 \\ 0 & \frac{\partial\phi^1}{\partial x_3} & \frac{\partial\phi^1}{\partial x_2} \\ \frac{\partial\phi^1}{\partial x_1} & 0 & \frac{\partial\phi^1}{\partial x_3} \end{bmatrix}$$

for the first block

$$[T][\phi] = \begin{bmatrix} \frac{\partial\phi^2}{\partial x_1} & 0 & 0 \\ 0 & \frac{\partial\phi^2}{\partial x_2} & 0 \\ 0 & 0 & \frac{\partial\phi^2}{\partial x_3} \\ \frac{\partial\phi^2}{\partial x_2} & \frac{\partial\phi^2}{\partial x_1} & 0 \\ 0 & \frac{\partial\phi^2}{\partial x_3} & \frac{\partial\phi^2}{\partial x_2} \\ \frac{\partial\phi^2}{\partial x_1} & 0 & \frac{\partial\phi^2}{\partial x_3} \end{bmatrix}$$

for the second block

$$[T][\phi] = \begin{bmatrix} \frac{\partial\phi^3}{\partial x_1} & 0 & 0 \\ 0 & \frac{\partial\phi^3}{\partial x_2} & 0 \\ 0 & 0 & \frac{\partial\phi^3}{\partial x_3} \\ \frac{\partial\phi^3}{\partial x_2} & \frac{\partial\phi^3}{\partial x_1} & 0 \\ 0 & \frac{\partial\phi^3}{\partial x_3} & \frac{\partial\phi^3}{\partial x_2} \\ \frac{\partial\phi^3}{\partial x_1} & 0 & \frac{\partial\phi^3}{\partial x_3} \end{bmatrix}$$

for the third block, all of which assembled yield the full $[T][\phi]$.

Using these definitions, we can rewrite the weak form equation in matrix form

$$\underbrace{\int_\Omega ([T]\{v\})^T[\mathcal{D}\,\mathbb{E}_{\mathbf{0}}]([T]\{u\})d\Omega}_{[S]_1} = \underbrace{\underbrace{\int_\Omega \{v\}^T \cdot \mathbf{f}\, d\Omega}_{\{R\}_f} + \underbrace{\int_{\Gamma_t} v\{\bar{t}\} \cdot \boldsymbol{t}\, d\Gamma}_{\{R\}_t}}_{\{R\}}$$

Using the same discretization scheme as above,

$$u(x,y,z) = \sum_{A=1}^{N} a_A \phi_A(x,y,z) \qquad v(x,y,z) = \sum_{A=1}^{N} b_A \phi_A(x,y,z) \qquad \dot{u}(x,y,z) = \sum_{A=1}^{N} \dot{a}_A \phi_A(x,y,z)$$

leads to the following descretized weak form equation. For the left-hand-side strain terms:

$$\int_\Omega ([T]\{\sum_{A=1}^{N} b_A\phi_A\})^T [\mathcal{D}\,\mathbb{E}^*]([T]\{\sum_{A=1}^{N} a_A\phi_A\})d\Omega$$

and the right-hand-side

$$\int_\Omega \sum_{A=1}^{N} b_A\phi_A \cdot \mathbf{f}\, d\Omega + \int_{\Gamma_t} \sum_{A=1}^{N} b_A\phi_A \cdot \boldsymbol{t}\, d\Gamma$$

The b_A's are arbitrary and can be canceled out of the equation leading to the following stiffness matrix terms on the left-hand side

$$\sum_{A=1}^{N}\sum_{B=1}^{N} \underbrace{\int_\Omega ([T]\{\phi_A\})^T [\mathcal{D}\,\mathbb{E}^*]([T]\{\phi_B\})d\Omega}_{[S_1]} \underbrace{a_B}_{\{a\}}$$

and the following right-hand side

$$\underbrace{\sum_{A=1}^{N} \underbrace{\int_\Omega \phi_A \cdot \mathbf{f}\, d\Omega}_{\{R\}_f} + \underbrace{\int_{\Gamma_t} \phi_A \cdot \boldsymbol{t}\, d\Gamma}_{\{R\}_t}}_{\{R\}}$$

The weak then becomes the following matrix system of equations

$$([S_1])\{a(t)\} = \{R\}$$

Evaluation of the Weak Form

The mapping from the real space to the master element in three dimensions is defined as follows

$$x_1 = \sum_{i=1}^{8} X_{1i}\hat{\phi}_i = Map_{x_1}(\zeta_1,\zeta_2,\zeta_3)$$

$$x_2 = \sum_{i=1}^{8} X_{2i}\hat{\phi}_i = Map_{x_2}(\zeta_1,\zeta_2,\zeta_3)$$

$$x_3 = \sum_{i=1}^{8} X_{3i}\hat{\phi}_i = Map_{x_3}(\zeta_1,\zeta_2,\zeta_3)$$

In 3-D the shape function of the master element take on a different form. First, there are 8 distinct linear shape functions that define the isoparametric space

$$\hat{\phi}_1(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1-\zeta_1)(1-\zeta_2)(1-\zeta_3) \qquad for\, \zeta_1,\zeta_2,\zeta_3 \in [-1,1]$$

$$\hat{\phi}_2(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1+\zeta_1)(1-\zeta_2)(1-\zeta_3) \qquad for\, \zeta_1,\zeta_2,\zeta_3 \in [-1,1]$$

$$\hat{\phi}_3(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1+\zeta_1)(1+\zeta_2)(1-\zeta_3) \qquad for\, \zeta_1,\zeta_2,\zeta_3 \in [-1,1]$$

$$\hat{\phi}_4(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1-\zeta_1)(1+\zeta)(1-\zeta_3) \qquad for\,\zeta_1,\zeta_2,\zeta_3\,\in\,[-1,1]$$

$$\hat{\phi}_5(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1-\zeta_1)(1-\zeta_2)(1+\zeta_3) \qquad for\,\zeta_1,\zeta_2,\zeta_3\,\in\,[-1,1]$$

$$\hat{\phi}_6(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1+\zeta_1)(1-\zeta_2)(1+\zeta_3) \qquad for\,\zeta_1,\zeta_2,\zeta_3\,\in\,[-1,1]$$

$$\hat{\phi}_7(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1+\zeta_1)(1+\zeta_2)(1+\zeta_3) \qquad for\,\zeta_1,\zeta_2,\zeta_3\,\in\,[-1,1]$$

$$\hat{\phi}_8(\zeta_1,\zeta_2,\zeta_3) = \frac{1}{8}(1-\zeta_1)(1+\zeta_2)(1+\zeta_3) \qquad for\,\zeta_1,\zeta_2,\zeta_3\,\in\,[-1,1]$$

Now we define the the $[F]$ matrix

$$[F] = \begin{bmatrix} \frac{\partial x_1}{\partial \zeta_1} & \frac{\partial x_1}{\partial \zeta_2} & \frac{\partial x_1}{\partial \zeta_3} \\ \frac{\partial x_2}{\partial \zeta_1} & \frac{\partial x_2}{\partial \zeta_2} & \frac{\partial x_3}{\partial \zeta_3} \\ \frac{\partial x_3}{\partial \zeta_1} & \frac{\partial x_3}{\partial \zeta_2} & \frac{\partial x_3}{\partial \zeta_3} \end{bmatrix}$$

The Jacobian of the transformation to the isoparametric space is

$$J = det\,|F| = \frac{\partial x_1}{\partial \zeta_1}(\frac{\partial x_2}{\partial \zeta_2}\frac{\partial x_3}{\partial \zeta_3} - \frac{\partial x_3}{\partial \zeta_2}\frac{\partial x_2}{\partial \zeta_3}) - \frac{\partial x_1}{\partial \zeta_2}(\frac{\partial x_2}{\partial \zeta_1}\frac{\partial x_3}{\partial \zeta_3} - \frac{\partial x_2}{\partial \zeta_1}\frac{\partial x_3}{\partial \zeta_3}) + \frac{\partial x_1}{\partial \zeta_3}(\frac{\partial x_2}{\partial \zeta_1}\frac{\partial x_2}{\partial \zeta_2} - \frac{\partial x_3}{\partial \zeta_1}\frac{\partial x_2}{\partial \zeta_2})$$

The differential relationships for the isoparametric mapping are

$$\frac{\partial}{\partial \zeta_1} = \frac{\partial}{\partial x_1}\frac{\partial x_1}{\partial \zeta_1} + \frac{\partial}{\partial x_2}\frac{\partial x_2}{\partial \zeta_1} + \frac{\partial}{\partial x_3}\frac{\partial x_3}{\partial \zeta_1}$$

$$\frac{\partial}{\partial \zeta_2} = \frac{\partial}{\partial x_1}\frac{\partial x_1}{\partial \zeta_2} + \frac{\partial}{\partial x_2}\frac{\partial x_2}{\partial \zeta_2} + \frac{\partial}{\partial x_3}\frac{\partial x_3}{\partial \zeta_2}$$

$$\frac{\partial}{\partial \zeta_3} = \frac{\partial}{\partial x_1}\frac{\partial x_1}{\partial \zeta_3} + \frac{\partial}{\partial x_2}\frac{\partial x_2}{\partial \zeta_3} + \frac{\partial}{\partial x_3}\frac{\partial x_3}{\partial \zeta_3}$$

and the inverse differential relationships are

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial \zeta_1}\frac{\partial \zeta_1}{\partial x_1} + \frac{\partial}{\partial \zeta_2}\frac{\partial \zeta_2}{\partial x_1} + \frac{\partial}{\partial \zeta_3}\frac{\partial \zeta_3}{\partial x_1}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial}{\partial \zeta_1}\frac{\partial \zeta_1}{\partial x_2} + \frac{\partial}{\partial \zeta_2}\frac{\partial \zeta_2}{\partial x_2} + \frac{\partial}{\partial \zeta_3}\frac{\partial \zeta_3}{\partial x_2}$$

$$\frac{\partial}{\partial x_3} = \frac{\partial}{\partial \zeta_1}\frac{\partial \zeta_1}{\partial x_3} + \frac{\partial}{\partial \zeta_2}\frac{\partial \zeta_2}{\partial x_3} + \frac{\partial}{\partial \zeta_3}\frac{\partial \zeta_3}{\partial x_3}$$

Therefore

$$\begin{Bmatrix} dx_1 \\ dx_2 \\ dx_3 \end{Bmatrix} = \underbrace{\begin{bmatrix} \frac{\partial x_1}{\partial \zeta_1} & \frac{\partial x_1}{\partial \zeta_2} & \frac{\partial x_1}{\partial \zeta_3} \\ \frac{\partial x_2}{\partial \zeta_1} & \frac{\partial x_2}{\partial \zeta_2} & \frac{\partial x_2}{\partial \zeta_3} \\ \frac{\partial x_3}{\partial \zeta_1} & \frac{\partial x_3}{\partial \zeta_2} & \frac{\partial x_3}{\partial \zeta_3} \end{bmatrix}}_{F} \begin{Bmatrix} d\zeta_1 \\ d\zeta_2 \\ d\zeta_3 \end{Bmatrix}$$

and

$$\begin{Bmatrix} d\zeta_1 \\ d\zeta_2 \\ d\zeta_3 \end{Bmatrix} = \underbrace{\begin{bmatrix} \frac{\partial \zeta_1}{\partial x_1} & \frac{\partial \zeta_1}{\partial x_2} & \frac{\partial \zeta_1}{\partial x_3} \\ \frac{\partial \zeta_2}{\partial x_1} & \frac{\partial \zeta_2}{\partial x_2} & \frac{\partial \zeta_2}{\partial x_3} \\ \frac{\partial \zeta_3}{\partial x_1} & \frac{\partial \zeta_3}{\partial x_2} & \frac{\partial \zeta_3}{\partial x_3} \end{bmatrix}}_{F^{-1}} \begin{Bmatrix} dx_1 \\ dx_2 \\ dx_3 \end{Bmatrix}$$

Now the matrices in the weak form need to be expressed in terms of the master domain coordinates $\zeta_1, \zeta_2, \zeta_3$

$$[T(\phi(x_1, x_2, x_3)] = [\hat{T}(\hat{\phi}(Map_{x_1}(\zeta_1, \zeta_2, \zeta_3), Map_{x_2}(\zeta_1, \zeta_2\zeta_3), Map_{x_3}(\zeta_1, \zeta_2, \zeta_3)))]$$

Now we define $[\hat{T}]$ to be

$$[\hat{T}] = \begin{bmatrix} \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \\ 0 \\ 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \end{bmatrix}$$

for the first column

$$[\hat{T}] = \begin{bmatrix} 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \\ 0 \end{bmatrix}$$

for the second column

$$[\hat{T}] = \begin{bmatrix} 0 \\ 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \\ 0 \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ \frac{\partial}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \end{bmatrix}$$

The elemental shape function matrix $[\hat{\phi}]$ has the following form

$$[\hat{\phi}] = \begin{matrix} \hat{\phi}_1 & \hat{\phi}_2 & \hat{\phi}_3 & \hat{\phi}_4 & \hat{\phi}_5 & \hat{\phi}_6 & \hat{\phi}_7 & \hat{\phi}_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}$$

for the first block of eight columns

$$[\hat{\phi}] = \begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hat{\phi}_1 & \hat{\phi}_2 & \hat{\phi}_3 & \hat{\phi}_4 & \hat{\phi}_5 & \hat{\phi}_6 & \hat{\phi}_7 & \hat{\phi}_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}$$

for the second block of eight columns

$$[\hat{\phi}] = \begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hat{\phi}_1 & \hat{\phi}_2 & \hat{\phi}_3 & \hat{\phi}_4 & \hat{\phi}_5 & \hat{\phi}_6 & \hat{\phi}_7 & \hat{\phi}_8 \end{matrix}$$

for the third block of eight columns, resulting in a 3x24 matrix. The product $[\hat{T}][\hat{\phi}]$ then becomes a 6x24 matrix

$$[\hat{T}][\hat{\phi}] = \begin{bmatrix} \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1} + \frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1} + \frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2} + \frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2} + \frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3} + \frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3} + \frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \end{bmatrix}$$

for the first block of eight columns

$$[\hat{T}][\hat{\phi}] = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

for the second block of eight columns

$$[\hat{T}][\hat{\phi}] = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_3}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_3}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_2}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_2}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_2} \\ \frac{\partial\hat{\phi}_1}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_1}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_1}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \frac{\partial\hat{\phi}_2}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_2}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_2}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} & \dots & \dots & \dots & \dots & \dots & \frac{\partial\hat{\phi}_8}{\partial\zeta_1}\frac{\partial\zeta_1}{\partial x_1}+\frac{\partial\hat{\phi}_8}{\partial\zeta_2}\frac{\partial\zeta_2}{\partial x_1}+\frac{\partial\hat{\phi}_8}{\partial\zeta_3}\frac{\partial\zeta_3}{\partial x_1} \end{bmatrix}$$

Applying Gaussian Quadrature

Now that all the matrices are defined, quadrature is applied to evaluate the expressions numerically. This leads to the following expressions

$$S^e_{ij} = \underbrace{\sum_{q=1}^{g}\sum_{r=1}^{g}\sum_{s=1}^{g} w_q w_r w_s ([\hat{T}]\{\hat{\phi}_i\})^T [\hat{\mathbb{E}}]([\hat{T}]\{\phi_j\})\,|F|}_{standard\,[S]\,term}$$

for the stiffness matrix, where g is the number of Gauss Points and $|F_s|$ is the Jacobian of the surface integral transformation. Elements that are not subject to the Dirichlet boundary conditions will only have the standard contribution to the stiffness matrix and elements with Dirichlet boundary conditions will be implemented by modifying the corresponding stiffness matrix accordingly. The load vector then becomes

$$R^e_i = \underbrace{\sum_{q=1}^{g}\sum_{r=1}^{g}\sum_{s=1}^{g} w_q w_r w_s [\hat{\phi}_i]^T \{f\}\,|F|}_{standard\,\{R\}\,term}$$

$$+\underbrace{\sum_{q=1}^{g}\sum_{r=1}^{g} w_q w_r [\hat{\phi}_i]^T \{t\}\,|F_s|}_{for\,\Gamma_t\cap\Omega_e\neq 0}$$

Elements that are not subject to the Dirichlet or the traction boundary conditions, i.e are not on the surface of Γ_t or Γ_d, are only subject to the standard contribution to the load vector. Elements that are subject to the traction boundary condition, i.e. are on the surface defined by Γ_t will have a contribution from the second sum. Elements that are subject to the Dirichlet boundary conditions, i.e. are on the surface defined by Γ_d will be modified to account for the Dirichlet boundary terms.

The transformation factor for the surface integral can be found using Nanson's formula

$$\mathbf{n}d\mathbf{\Gamma} = JF^{-T}\mathbf{N}\,d\Gamma_\zeta$$

which for an expression inside a surface integral yields

$$\mathbf{n}\cdot\mathbf{n}\,d\Gamma = J\sqrt{\mathbf{N}\cdot F^{-1}F^{-T}\cdot\mathbf{N}}d\Gamma_\zeta$$

as the transformation factor for surface integrals. The finite element approximation of the weak form is defined in the space of $H_1(\Omega)$.

Integrals for Balance of Linear Momentum

Given the procedure outlined, the balance of linear differential equation requires the following integrals:

Integral 1

$$[S_1] = \int_{\Omega} ([T]\{\phi_A\})^T [\mathcal{D}\,\mathbb{E}_0]([T]\{\phi_B\}) d\Omega = \sum_{e=1}^{N_e} \int_{\Omega_e} ([T]\{\phi_A\})^T [\mathcal{D}\,\mathbb{E}_0]([T]\{\phi_B\}) d\Omega_e$$

$$[S_1]^e_{AB} = \iiint_{-1}^{1} \underbrace{([\hat{T}]\{\hat{\phi}_i\})^T [\mathcal{D}\,\mathbb{E}_0]([\hat{T}]\{\phi_j\}) \cdot |F| \, d\zeta_1 \, d\zeta_2 \, d\zeta_3}_{f_1(\zeta_1,\zeta_2,\zeta_3)}$$

which can using Gaussian Quadrature becomes

$$[S_1]^e_{AB} = \sum_{I=1}^{NP_1} \sum_{J=1}^{NP_2} \sum_{K=1}^{NP_3} w_I w_J w_K f_1(\zeta_1,\zeta_2,\zeta_3)$$

If the material properties change with time or temperature, then this integral has to be computed at each time-step. If they remain constant, then it has to be computed only once.

Integral 2

$$\{R\}_f = \int_{\Omega} \phi_A \cdot \mathbf{f} \, d\Omega = \sum_{e=1}^{N_e} \int_{\Omega_e} \phi_A \cdot \mathbf{f} \, d\Omega_e$$

$$\{R_f\}^e_A = \iiint_{-1}^{1} \underbrace{(\{\hat{\phi}_i\}^T \mathbf{f}) \cdot |F| \, d\zeta_1 \, d\zeta_2 \, d\zeta_3}_{f_5(\zeta_1,\zeta_2,\zeta_3)}$$

which can using Gaussian Quadrature becomes

$$\{R_f\}^e_A = \sum_{I=1}^{NP_1} \sum_{J=1}^{NP_2} \sum_{K=1}^{NP_3} w_I w_J w_K f_5(\zeta_1,\zeta_2,\zeta_3)$$

This integral has to be computed only once.

Integral 3

$$\{R\}_t = \int_{\Omega} \phi_A \cdot \boldsymbol{t} \, d\Omega = \sum_{e=1}^{N_e} \int_{\Omega_e} \phi_A \cdot \boldsymbol{t} \, d\Omega_e$$

$$\{R_t\}^e_A = \iint_{-1}^{1} \underbrace{(\{\hat{\phi}_i\}^T \boldsymbol{t}) \cdot |F| \, \sqrt{\mathbf{N} \cdot F^{-1} F^{-T} \cdot \mathbf{N}} \, |_{\zeta_i=-1,1} \; d\zeta_2 \, d\zeta_3}_{f_6(a,\zeta_2,\zeta_3)}$$

which can using Gaussian Quadrature becomes

$$\{R_t\}^e_A = \sum_{I=1}^{NP_1} \sum_{J=1}^{NP_2} w_I w_J f_6(a,\zeta_2,\zeta_3)$$

where a is a constant that represents the surface normal. The surface normal can be placed on any ζ_i depending on the specific boundary conditions. This integral has to be computed only once.

Applying the Boundary Conditions

Since this problem is a linear problem, the boundary conditions by forcing $v = 0 \quad on\,\Gamma_d$, which was applied as follows in the program:

Dirichlet Boundary Conditions

1. Find the rows of $[S]$, $[M]$, corresponding to the boundary nodes using the connectivity table

(a) Make the rows of the boundary nodes in $[S]$, $[M]$ equal to 0

(b) Make the diagonal element corresponding to that row equal to 1.

2. Find the rows of $\{R\}$ corresponding to the same boundary nodes using the connectivity table

   (a) Make the rows of the interior nodes in $\{R\}$ equal to $\bar{u}$.

This procedure ensures that each of the interior nodes always has the solution $u = \bar{u}$. Another method of ensuring this is to make the interior nodes of $\{a(t)\}$ equal to $u = \bar{u}$ for each time-step.

Neumann Boundary Conditions

The flux condition was applied by using the surface integral of the flux term and adding it to the load vector.