Solving Elliptic (and Hyperbolic) Equations in Nonlinear Viscoelasticity

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Abstract

The primary objective of this report is to put forth an integral equation formulation of the nonlinear PDEs arising in viscoelasticity. Motivated from [4], as a first application of practical relevance, the formulation is employed to solve a boundary value problem in hyperleasticity (with no dissipation). A (thick) spherical shell made up of a neohookean rubber, undergoing radially symmetric deformations, is considered. Since the underlying energy functional is quasi-convex, and ignoring inertial effects, the differential equations, from a mathematical perspective, are physically tractable. Moreover, due to the nonlinear nature of the problem, the integral equation representation of the PDE consists of volume integrals, much unlike classical Laplace, or Helmholtz, where only surface integrals need to be evaluated. Nyström discretization is used to discretize the resulting integral equation making it amenable to numerical calculations via standard *Newton-like* schemes.

1. Introduction

Rubber-like materials are highly deformable, and although within certain ranges of loadings they may be classified as hyperelastic, at an intrinsic level they are viscoelastic. The classical continuum approach has been to model their behavior using a hereditary-integral representation. More recently the *Generalized Standard Materials Framework* or the *Two-potential constitutive framework* has gained immense popularity among mathematicians. Owing to its practical relevance and high amenability to numerical calculations, the integral representation of the PDEs is restricted to the *Two-potential constitutive framework*. We briefly state the framework in section 2, and use it later to develop the formulation and corresponding equations. To put things in perspective, we present a brief overview of integral equations, for e.g. Laplace

$$\Delta u = 0, \quad \text{in} \quad \Omega \quad \text{with} \quad \begin{cases} u = g, & \text{in } \partial\Omega_x \\ \dfrac{\partial u}{\partial n} = h, & \text{in } \partial\Omega_t \end{cases} \quad : \ \partial\Omega = \partial\Omega_x \cup \partial\Omega_t \tag{1}$$

For the remainder of the note we restrict our attention to the pure Dirichlet case in which case the problem reduces to finding an integral representation of the harmonic function (u), for e.g. the double-layer representation

$$u = (D\varphi)(x) := \int_{\partial\Omega} \hat{n}_y \nabla_y G(x,y)\varphi(y)dy \qquad \text{where} \quad G := \Delta G = \delta \tag{2}$$

such that the unknown function $\varphi(x)$ (often called the density function) satisfies the integral equation (precisely of second kind)

$$(I/2 - D)\varphi = g \tag{3}$$

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More generally, for nonlinear PDEs it is difficult to approximate the solution as (2). Therefore the integral representation of the equation is of the form

$$\left(I + \tilde{D}\right)\varphi = \tilde{g}(x) \tag{4}$$

where the operator D, is any arbitrary nonlinear integral operator, and in general comprises of integrals over the surface and the volume

2. Problem

Consider a body (Ω_0), as in Fig.(1), in the undeformed stress-free configuration occupying a subset of the euclidean space ($\mathbb{R}^3$), with a Lipschitz continuous boundary ($\partial\Omega_0$). The mathematical problem in continuum mechanics amounts to finding a continuous mapping ($\boldsymbol{\chi}$) that maps every material point in the undeformed configuration to its corresponding location in the deformed configuration.

$$\exists \boldsymbol{\chi}(\mathbf{X}) \in C^2(\Omega_0) : \begin{cases} \mathbf{F} & = \boldsymbol{\nabla}\boldsymbol{\chi} \equiv F_{ij} = \dfrac{\partial \chi_i}{\partial X_j} = \dfrac{\partial x_i}{\partial X_j}, \qquad 1 \leq i, j \leq 3 \\ J & = \det\mathbf{F} > 0 \end{cases}$$

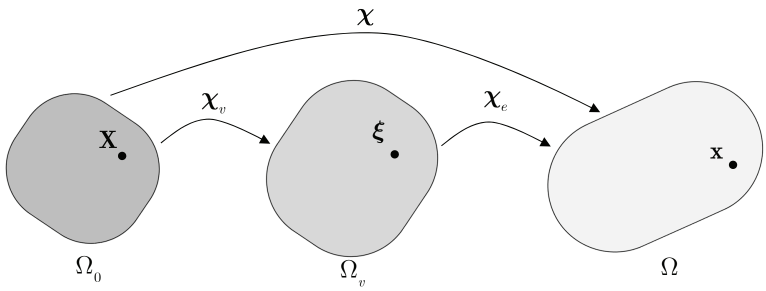


Figure 1: Schematic of the deformation mapping $\boldsymbol{\chi}$, showing material points in the undeformed configuration $\mathbf{X}$ and in the deformed configuration $\mathbf{x}$

In context of viscoelasticity, $\boldsymbol{\chi}$ can be shown to admit the multiplicative decomposition $\boldsymbol{\chi} = \boldsymbol{\chi}_e \circ \boldsymbol{\chi}_v$, and consequently we have $\mathbf{F} = \mathbf{F}^e\mathbf{F}^v$. Furthermore within continuum mechanics, we restrict our attention to problems where the *Cauchy's lemma* is satisfied, i.e. namely

$$\exists \mathbf{T} : \mathbf{t} = \mathbf{T}\mathbf{n} \quad \text{and} \quad \int_\Omega \mathbf{b}(\mathbf{x}, t) d\mathbf{x} + \int_{\partial\Omega} \mathbf{t}(\mathbf{x}, t) d\mathbf{x} = \int_\Omega \rho(\mathbf{x}, t) \ddot{\chi}(\mathbf{x}, t) d\mathbf{x} \tag{5}$$

where the second order tensor $\mathbf{T}$ is also called the Cauchy-stress tensor. It physically corresponds to the force per unit area in the deformed configuration of the body. The corresponding counterpart, in the undeformed configuration is called the First-piola kirchoff stress tensor (denoted by $\mathbf{S}$) and is given by

$$\mathbf{S} = J\mathbf{T}\mathbf{F}^{-T} \tag{6}$$

While for most problems, determining $\boldsymbol{\chi}$ amounts to solving a nonlinear PDE, several key simplifications can be utilized to reduce the number of independent dimensions in the system. This is elaborated in detail in Section (4).

2.1. Two potential Constitutive framework

The key idea behind the *Two-potential constitutive framework*[1] is to give a quantitative description of the storage and dissipation of energy by the means of two thermodynamic potentials *(i)* ψ : the free energy function, that describes the storage and *(ii)* ϕ: the dissipation potential, that describes the dissipation. To set the framework in an isothermal setting we consider the following:

$$\psi := \psi(\mathbf{F}, \mathbf{F}^v) \quad ; \quad \phi := \phi(\mathbf{F}, \mathbf{F}^v, \dot{\mathbf{F}^v}) \tag{7}$$

where $(\mathbf{F}^v)$ is an internal variable that serves to describe the dissipation of energy. constitutive model is given by

$$\begin{cases} \mathbf{S}(\mathbf{F}, \mathbf{F}^v) = \dfrac{\partial \psi}{\partial \mathbf{F}}(\mathbf{F}, \mathbf{F}^v) \\ \dfrac{\partial \psi}{\partial \mathbf{F}^v} + \dfrac{\partial \phi}{\partial \dot{\mathbf{F}}^v} = \mathbf{0} \end{cases} \quad \& \quad \underbrace{\mathrm{Div}\mathbf{S} + \mathbf{b} = \mathbf{0}}_{\mathrm{BLM}} \tag{8}$$

The system of equations in (8) can be efficiently solved numerically by a combination of Finite-Difference $(\mathbf{F}^v)$ and Finite Element/Boundary Element $(\mathbf{F})$.

2.2. Case of Hyperelasticity ($\phi = 0$)

To this end, leaving the dissipative properties aside ($\phi = 0$), we consider a body undergoing large deformations in absence of body forces ($\mathbf{b} = 0$). The constitutive model can be further simplified as

$$\mathbf{S}(\mathbf{F}) = \frac{\partial \psi}{\partial \mathbf{F}}(\mathbf{F}) \quad \text{and} \quad \mathrm{Div}\mathbf{S} = \mathbf{0} \tag{9}$$

and consequently the entire boundary value problem reduces to finding the deformation mapping $(\boldsymbol{\chi})$ or equivalently the deformation field $(\mathbf{u})$, such that the following boundary value problem is well posed

$$\mathrm{Div}\mathbf{S}(\mathbf{F}) = 0, \quad \Omega_0 \quad \text{subject to} \quad \mathbf{u}(\mathbf{X}) = \mathbf{g} \text{ in} \quad \partial\Omega_0 \tag{10}$$

The above model is amenable to numerical calculations (e.g. FEM) and this forms the starting point of our integral representation of (9). In particular for arbitrary geometry and Dirichlet boundary conditions we seek a representation of the form

$$\mathbf{u}(\mathbf{X}) = \left(\tilde{\mathbf{D}}\tilde{\mathbf{u}}\right)(\mathbf{X}) \tag{11}$$

and correspondingly the integral equation

$$\left(I + \tilde{D}\right)\tilde{\mathbf{u}} = \tilde{\mathbf{g}}(\mathbf{X}) \tag{12}$$

Since the fields are no longer scalar functions, like classical Laplace (or Helmholtz) but are vector fields (functions of the position vector $\mathbf{X}$ – therefore 3 components), the kernel $(\tilde{\mathbf{D}})$ is a second order tensor (9-components in eucledian space). (11)-(12) together serve as a useful basis for application of a plethora of numerical techniques. In the sequel we specialize the above formulation to a simple yet functionally rich BVP

3. Boundary Value Problem:

To begin with, we consider a quasi-convex free energy function ψ, which has shown to describe the behavior of compressible rubbers under a large range of deformation (notably in absence of strain hardening, in which case we resort to more complicated choices for ψ)

$$\psi = \frac{\mu}{2}(I_1 - 3) + \frac{\kappa}{2}(J - 1)^2 \tag{13}$$

where

$$I_1 = \mathrm{tr}\left(\mathbf{F}^T\mathbf{F}\right) = F_{ij}F_{ij} \tag{14}$$

and μ and κ are the lamè parameters, physically corresponding to the shear and bulk modulus of the material

$$\mathbf{S} = \frac{\partial \psi}{\partial \mathbf{F}} = \frac{\partial \psi}{\partial I_1}\frac{\partial I_1}{\partial \mathbf{F}} + \frac{\partial \psi}{\partial J}\frac{\partial J}{\partial \mathbf{F}} \tag{15}$$

the derivatives in the above equation are given by

$$\frac{\partial \psi}{\partial I_1} = \frac{\mu}{2} \quad ; \quad \frac{\partial \psi}{\partial J} = \kappa(J-1) \quad ; \quad \frac{\partial I_1}{\partial \mathbf{F}} = 2\mathbf{F} \quad ; \quad \frac{\partial J}{\partial \mathbf{F}} = J\mathbf{F}^{-T}$$

$$\implies \mathbf{S} = \mu\mathbf{F} + \kappa J(J-1)\mathbf{F}^{-T} \implies \mathrm{Div}\mathbf{S} = \mu\nabla^2\mathbf{u} + \kappa\nabla(J(J-1))\mathbf{F}^{-T} \tag{16}$$

which gives

$$\mu\nabla^2\mathbf{u} + \kappa\nabla(J(J-1))\mathbf{F}^{-T} = \mathbf{0}, \text{ in } \quad \Omega_0 \quad \text{subject to} \quad \mathbf{u} = \mathbf{g}, \text{ in } \partial\Omega_0 \tag{17}$$

4. Radially Symmetric case

4.1. Kinematics

In this section we consider the problem of radially symmetric deformation fields, for a spherical shell subjected to dirichlet data on the boundary. The geometry is described by

$$\mathbf{X} \in \Omega_0 \subset \mathbb{R}^3 : A \leq \sqrt{|\mathbf{X}\cdot\mathbf{X}|} \leq B \tag{18}$$

where A and B are the inner and outer radii in the undeformed stress free configuration. In particular we are interested in radially symmetric deformation mappings ($\boldsymbol{\chi}$) of the form

$$\boldsymbol{\chi} = f(R)\mathbf{X} \implies \mathbf{F} = (Rf'(R) + f)\underbrace{\frac{1}{R^2}\mathbf{X}\otimes\mathbf{X}}_{\mathcal{K}_1} + f\underbrace{\left(I - \frac{1}{R^2}\mathbf{X}\otimes\mathbf{X}\right)}_{\mathcal{K}_2} \tag{19}$$

where $\mathcal{K}_1$ and $\mathcal{K}_2$ are the orthogonal projection tensors.

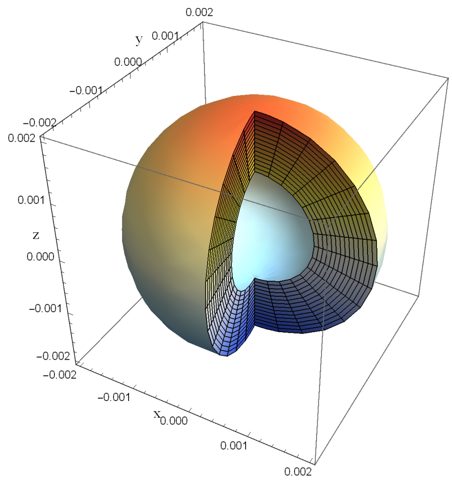


Figure 2: Schematic of the spherical shell for numerical calculations, with inner radius $A = 10^{-3}$ and $B = 2 \times 10^{-3}$

While (10) serves to describe a general Dirichlet problem in nonlinear Hyperelasticity, its specialization to the case of radially symmetric mappings reduces Eq. (17) to a nonlinear ODE, which can then be readily solved for the unknown function $f(R)$. Since the underlying stored energy function is isotropic the corresponding form of the stress tensor is given by

$$\mathbf{S} = \sigma_1 \underbrace{\frac{1}{R^2}\mathbf{X}\otimes\mathbf{X}}_{\mathcal{K}_1} + \sigma_2 \underbrace{\left(I - \frac{1}{R^2}\mathbf{X}\otimes\mathbf{X}\right)}_{\mathcal{K}_2} \tag{20}$$

where σ_1 and σ_2 are the singular values of $\mathbf{S}$ and $\lambda_1 = Rf' + f$ and $\lambda_2 = f$ are the singular values of $\mathbf{F}$ respectively such that in their spectral form, we can write

$$\mathbf{S} = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_2 \end{bmatrix} \qquad \mathbf{F} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_2 \end{bmatrix} \tag{21}$$

Plugging (20) into (10) yields

$$\begin{aligned}
\mathrm{Div}\mathbf{S} &= \frac{\partial}{\partial R}\Big(\frac{\sigma_1}{R^2}\Big)\frac{\partial R}{\partial X_j}X_iX_j + \frac{\sigma_1}{R^2}\frac{\partial (X_iX_j)}{\partial X_j} - \frac{\partial}{\partial R}\Big(\frac{\sigma_2}{R^2}\Big)\frac{\partial R}{\partial X_j}X_iX_j - \frac{\sigma_2}{R^2}\frac{\partial (X_iX_j)}{\partial X_j} + \frac{\partial \sigma_2}{\partial R}\frac{\partial R}{\partial X_i} = 0 && (22)\\
&= \Big(\frac{1}{R^2}\frac{\partial \sigma_1}{\partial R} - \frac{2}{R^3}\sigma_1\Big)\frac{X_j}{R}X_iX_j + \frac{4}{R^2}(\sigma_1 - \sigma_2)X_i - \Big(\frac{1}{R^2}\frac{\partial \sigma_2}{\partial R} - \frac{2}{R^3}\sigma_2\Big)\frac{X_j}{R}X_iX_j + \frac{X_i}{R}\frac{\partial \sigma_2}{\partial R} && (23)\\
&= \Big(\frac{1}{R^2}\frac{\partial \sigma_1}{\partial R} - \frac{2}{R^3}\sigma_1 + \frac{2}{R^3}\sigma_2\Big)RX_i + \frac{4}{R^2}(\sigma_1 - \sigma_2) - \frac{X_i}{R}\frac{\partial \sigma_2}{\partial R} + \frac{X_i}{R}\frac{\partial \sigma_2}{\partial R} && (24)\\
&= \Big(\frac{1}{R}\frac{\partial \sigma_1}{\partial R} + \frac{2}{R^2}(\sigma_1 - \sigma_2)\Big)X_i = 0 && (25)
\end{aligned}$$

It is plain from (25) that $X_i \neq 0$ and hence (10) is reduced to an ODE in R

$$\frac{\partial \sigma_1}{\partial R} + \frac{2}{R}(\sigma_1 - \sigma_2) = 0 \tag{26}$$

In light of the constitutive model given by (13), and the kinematic relations (19)-(20) σ_1 and σ_2 are given by

$$\begin{aligned}
\sigma_1 &= \mu(Rf' + f) + \kappa f^2\big((Rf' + f)f^2 - 1\big)\\
\sigma_2 &= \mu f + \kappa f(Rf' + f)\big((Rf' + f)f^2 - 1\big)
\end{aligned} \tag{27}$$

Substituting (27) in (26) we formulate the BVP in terms of an ODE in R and Dirichlet data on the boundary points (A, B)

$$4\big(\mu + \kappa f^4\big) + 2R\kappa f^3 f'^2 + R\big(\mu + \kappa f^4\big)f'' = 0 \qquad \text{subject to} \qquad \begin{cases} f(A) &= 1 \\ f(B) &= 2 \end{cases} \tag{28}$$

5. Integral representation

It proves useful to rewrite (28) as

$$\int_A^R \Big(f''(\xi) + 2\kappa\frac{f^3(\xi)f'^2(\xi)}{\mu + \kappa f^4(\xi)} + \frac{4}{\xi}\Big)d\xi = 0 \tag{29}$$

Given that $f \in C(A, B)$, integrals in (29) are classical Lebesgue integrals and can be carried out readily to result in the following integral equation

$$f(R) + 2\kappa \int_A^R K(R, f'(\xi), \xi)\ \mathcal{F}(f(\xi))\ d\xi = \mathcal{G}(R) \tag{30}$$

where

$$\mathcal{G}(R) = 1 + c(R - A) - 4R\left(\log\left(\frac{R}{A}\right) - 1\right) \tag{31}$$

$$K(R, f'(\xi), \xi) = (R - \xi) f'^2(\xi) \tag{32}$$

$$\mathcal{F}(f(\xi)) = \frac{f^3(\xi)}{\mu + \kappa f^4(\xi)} \tag{33}$$

$$c = f'(A) = 1 + 4B\left(\log\left(\frac{B}{A}\right) - 1\right) + 2\kappa \int_A^B K(B, f'(\xi), \xi)\mathcal{F}(f(\xi))\, d\xi \tag{34}$$

It is worth noting that (30) is in many ways similar to the integral equations that arise in the case classical Laplace (or Helmholtz) PDE, except that the kernel (K) is nonlinear and the integral unlike a layer potential, is over the entire volume (in $1D$ a volume integral is simply the line integral over the domain). Having formulated the integral equation for the BVP, we now proceed to solve (30) numerically

6. Numerical Implementation

A variety of numerical techniques can be used to solve (30). Before proceeding with the numerical implementation, the following remarks are in order

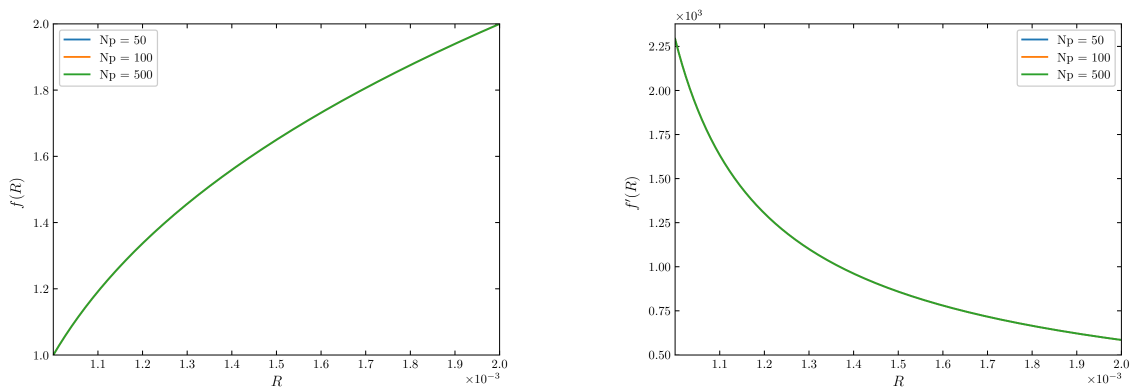
- The kernel K is nonlinear function of f' and hence an approximation of f' is required to evaluate the kernel K and the integral. For this we use a first order (backward) finite difference approximation

$$f'(\xi_i) = \frac{f(\xi_i) - f(\xi_{i-1})}{(\xi_i) - (\xi_{i-1})}$$

- Nyström discretization followed by the method of successive approximation results in a nonlinear system of algebraic equations which can be efficiently solved via any nonlinear solver of choice (e.g. *Newton*)

- In order to evaluate the line integral, we choose a standard *N-point* Gauss-Legendre quadrature (in this case $N = 100$). The nonlinear algebraic equations are then solved using *Scipy's* `newton-krylov` with the iterative solver `lgmres` for solving linear system at each iteration

In order to assess the accuracy of the numerical method used to solve (30), sample results corresponding to the following choice of material parameters (μ) and (κ) for (28) are presented. These correspond to collocation method, directly applied on the PDE, with different number of collocation points (N_p) over the domain (A, B). The results are fairly accurate with $N_p \sim 50$



(a) $f(R)$ vs R

(b) $f'(R)$ vs R

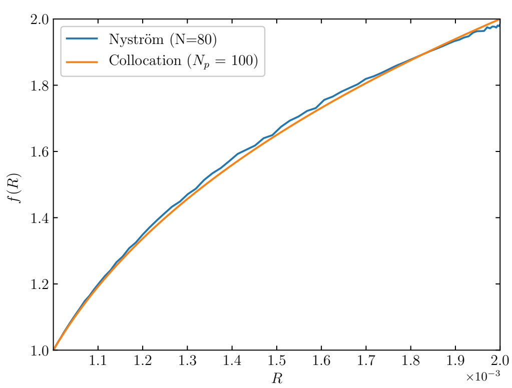
Discretizing (30) results in the following system of nonlinear algebraic equations

$$f_n^{(k+1)}(R_i) = \mathcal{G}_n^{(k)}(R_i) - 2\kappa \sum_{j=1}^{N} \omega_j K\Big(R_i, f_n'^{(k)}(\xi_j), \xi_j\Big)\mathcal{F}\Big(f_n^{(k)}(\xi_j)\Big) \tag{35}$$

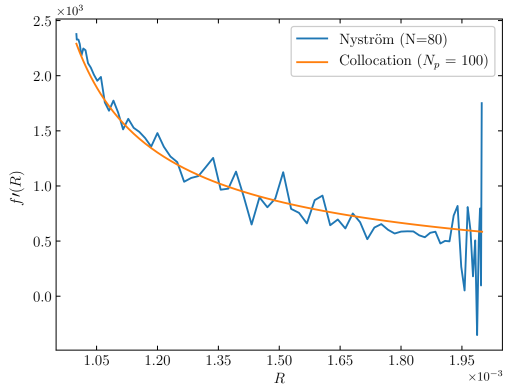
where ω_j and ξ_j are the quadrature weights and points respectively and k denotes the iteration number. Although (35) appears as a fixed-point iteration scheme, it is indeed, at an intrinsic level, a *Newton-like* scheme.

7. Sample results

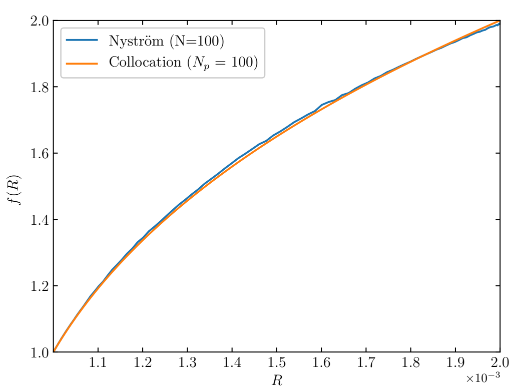
In this section we confront the results obtained using IE-Nyström to those obtained directly from PDE-Collocation. The plotted solution ()



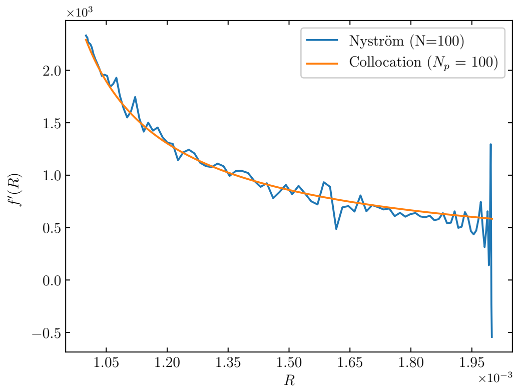
(a) $f(R)$ vs R, $N = 80$



(b) $f'(R)$ vs R, $N = 80$



(c) $f'(R)$ vs R, $N = 100$



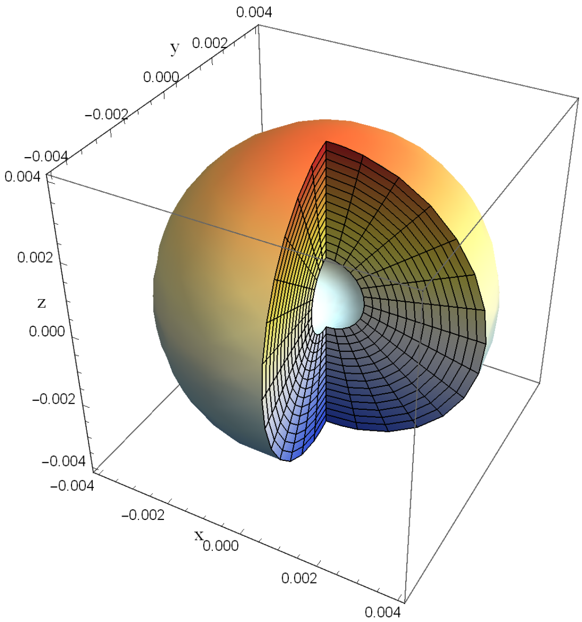
(d) $f'(R)$ vs R, $N = 100$

Figure 4: (a) and (c) correspond to the numerical solution ($f(R)$) using 80 and 100 gauss-points respectively to discretize the integral in (30), (b) and (d) correspond to the finite difference (first-order) approximation of the derivative obtained from the solution consists of the values of $f(R)$ evaluated at the quadrature-points. The boundary conditions are directly taken into account in the formulation, as seen in Appendix B

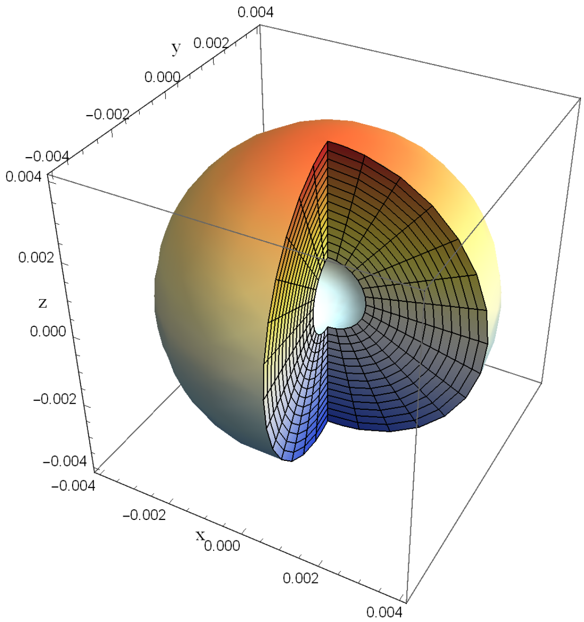
It is plain from the above plots that the first-order finite difference approximation for the derivative ($f\prime(R)$) is particularly inaccurate towards the end ($R = B$). This can be improved upon by using a higher order discretization at the ends to impose the Dirichlet data.

8. Conclusion

The formulation developed in the context of hyperelastic deformation of a spherical shell is fairly accurate except at the boundaries, where a higher order FD discretization is needed to accurately determine $(f'(R))$. The deformed geometries for the two cases $(N = 80, 100)$ are plotted below



(a) $N = 80$



(b) $N = 100$

The present scheme can be massively improved upon by a higher order discretization for $f'(R)$, particularly towards the ends, as well as tweaking the nonlinear solution algorithm. I plan to continue on the present work in the future, to improve the accuracy of the Dirichlet case, and then extend it to a general BVP in 3D

A. Existence of Solution to nonlinear integral equations

In this appendix, we briefly state the conditions required to prove the existence of solutions to nonlinear integral equations (in particular, for 1D). Consider a general nonlinear integral equation in 1D of the following form

$$u(x) - \int_0^x G(x, y, u(y)) \, dy = f(x) \tag{36}$$

The specific conditions under which a solution exists for the above nonlinear integral equation are

- The function $f(x)$ on the RHS is Lebesgue integrable (and bounded over an interval $(0, x)$)
- The function $f(x)$ must satisfy the Lipchitz condition in the interval (a, b). This means that

$$\|f(\xi_1) - f(\xi_2)\| < k\|\xi_1 - \xi_2\| \quad \forall \{\xi_1, \xi_2\} \in (a, b)$$

- The functional $G(x, y, u(y))$ is integrable and bounded. $G(x, y, u(y)) < K$ for all $\{x, y\} \in (a, b)$
- The functional $G(x, y, u(y))$ satisfies Lipchitz condition

$$\|G(x, y, \xi_1) - G(x, y, \xi_2)\| < M\|\xi_1 - \xi_2\|$$

In the above equation, $u'(y)$ does not appear as an argument in the nonlinear functional $G(x, y, u(y))$. Hence the derivation cannot be unconditionally extended to prove the existence of solution to (30). As an ad-hoc extension, the derivative can be considered as

$$u'(\xi) = \lim_{h \to 0} \frac{u(\xi_1 + h) - u(\xi_1)}{h} \tag{37}$$

For kernels exhibiting stronger singularity $u''(\xi) \to \pm\infty$, for some $\xi \in (a, b)$ the conditions required to prove existence of the solution may be more complicated and is out of the scope of this report. However I look forward to working on it in the future

B. Derivation of the integral equation directly from the PDE

The ODE can be directly written as

$$\begin{aligned}
&f'' + 2\kappa \frac{f^3 f'^2}{\mu + \kappa f^4} + \frac{4}{R} = 0 \\
&f'(\xi) - f'(A) + 2\kappa \int_A^\xi \frac{f^3(\eta) f'^2(\eta)}{\mu + \kappa f^4(\eta)} \, d\eta + 4 \log\left(\frac{\xi}{A}\right) = 0 \\
&f'(\xi) = f'(A) - 2\kappa \int_A^\xi \frac{f^3(\eta) f'^2(\eta)}{\mu + \kappa f^4(\eta)} \, d\eta - 4 \log\left(\frac{\xi}{A}\right) \\
&f(R) - \underbrace{f(A)}_{=1} = c(R - A) - 2\kappa \int_A^R \int_A^\xi \frac{f^3(\eta) f'^2(\eta)}{\mu + \kappa f^4(\eta)} \, d\eta d\xi - 4A\left(\frac{R}{A}\left(\log\left(\frac{R}{A}\right) - 1\right) + 1\right) \\
&f(R) = 1 + c(R - A) - 2\kappa \int_A^R (R - \xi) \frac{f^3(\xi) f'^2(\xi)}{\mu + \kappa f^4(\xi)} \, d\xi - 4A\left(\frac{R}{A}\left(\log\left(\frac{R}{A}\right) - 1\right) + 1\right)
\end{aligned}$$

Here $c = f'(A)$ can be directly determined from the other boundary condition ($f(B) = 2$) to give

$$c = f'(A) = \frac{1}{B - A}\left(1 + 2\kappa \int_A^B (B - \xi) \frac{f^3(\xi) f'^2(\xi)}{\mu + \kappa f^4(\xi)} \, d\xi + 4A\left(\frac{B}{A}\left(\log\left(\frac{B}{A}\right) - 1\right) + 1\right)\right)$$

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