

# A Jacobian-free Newton-Krylov method for cell-centred finite volume solid mechanics

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## Abstract

This work extends the application of Jacobian-free Newton–Krylov (JFNK) methods to higher-order cell-centred finite-volume formulations for solid mechanics. While conventional cell-centred schemes are typically restricted to second-order accuracy, we present third- and fourth-order formulations that employ local least-squares reconstructions for gradient evaluation combined with Gaussian quadrature at cell faces for flux integration. These schemes enable accurate resolution of complex stress and deformation fields in both linear and nonlinear solid mechanics, while retaining the flexibility and geometric generality of finite-volume methods. A novel contribution of this study is the development and assessment of a JFNK solution strategy for these higher-order formulations, which eliminates the need to assemble and store large Jacobian matrices explicitly. Instead, we demonstrate that a compact-stencil approximate Jacobian can be effectively employed as a preconditioner, mirroring the efficiency gains observed in second-order frameworks. The proposed methodology is benchmarked across a suite of two- and three-dimensional test problems involving elastic and nonlinear materials, where key performance metrics, including accuracy, computational cost, memory usage, and robustness, are systematically evaluated. Results confirm that the higher-order formulations deliver substantial accuracy improvements over second-order schemes, while the JFNK approach achieves strong performance and scalability with only minimal modifications to existing segregated frameworks. These findings underscore the potential of combining higher-order finite-volume methods with JFNK solvers to advance the state of the art in computational solid mechanics. The implementations are openly released in the solids4foam toolbox for OpenFOAM, supporting further exploration and adoption by the community.

**Keywords:** Jacobian-free Newton-Krylov, higher-order, cell-centred finite volume method, GMRES, solids4foam, OpenFOAM

# 1 Introduction

Potential structure of this section:

1. Higher-order discretisation in computational solid mechanics remains relatively underexplored compared to fluid dynamics, despite its potential for improving accuracy and efficiency. Comment on 'why' we should care about higher order: potentially cheaper to achieve the same mesh error; potential to reduce the amount of data when running large models on HPC systems (where data is the bottleneck).
2. Recent research has demonstrated that higher-order accuracy can be achieved in cell-centred formulations through gradient reconstruction (e.g. least-squares approaches) and face integration techniques (e.g. Gaussian quadrature); however, their efficiency and ease of implementation in an industrial code are unexplored.
3. The solution strategy is a crucial factor: segregated iterative solvers remain the standard in finite-volume solid mechanics but often suffer from slow convergence and limited robustness, and they are efficient for higher orders, as shown by Demirdzic. Jacobian-free Newton–Krylov (JFNK) methods have emerged as a promising alternative, avoiding the need for explicit Jacobian construction while enabling quadratic convergence through Krylov subspace acceleration. In addition, the JFNK approach is well-suited for integration into existing segregated frameworks.
4. Our previous work established the feasibility and efficiency of JFNK for second-order cell-centred formulations, where a compact-stencil approximate Jacobian proved highly effective as a preconditioner. This study extends JFNK to third- and fourth-order cell-centred finite-volume formulations for linear and nonlinear solid mechanics, combining least-squares gradient reconstruction with Gaussian quadrature integration.
5. We demonstrate that the proposed approach significantly improves accuracy while retaining computational efficiency, and we show that compact-stencil Jacobians remain effective as preconditioners in the higher-order setting.
6. The aim of this paper is therefore twofold: to contribute to the relatively sparse literature on higher-order cell-centred finite-volume methods for solids, and to explore the synergy between such methods and Jacobian-free Newton–Krylov solution strategies.

skica molekule na symmetry planeu skica molekule na dirichlet boundariu sve jedna slika na kojoj je desni rub dirichlet, dole je symmetry a gore je neumann rub!

Philip comment: we should mention the importance of using consistent areas and volumes, e.g when discretising the volumetric terms we should use the same cell decomposition as we use to calculate the cell volume; the same applies for the face area integrals. Ivan noted this is required for non-flat faces to get the expected order of accuracy, e.g. on the irregular hexahedra/polyhedra meshes.

## 2 Mathematical Model

For arbitrary body of volume  $\Omega$  bounded by surface  $\Gamma$  with outward facing unit normal  $\mathbf{n}$  the strong integral form of linear momentum in *total* Lagrangian form is:

$$\int_{\Omega_o} \rho_o \frac{\partial^2 \mathbf{u}}{\partial t^2} d\Omega_o = \oint_{\Gamma_o} (\mathbf{n}_o \cdot \mathbf{P}^T) d\Gamma_o + \int_{\Omega_o} \mathbf{f}_b d\Omega_o, \quad (1)$$

where  $\rho$  is density,  $\mathbf{u}$  is the displacement vector,  $\mathbf{P}$  is the first Piola–Kirchhoff stress tensor, and  $\mathbf{f}_b$  is a body force per unit volume, e.g.,  $\rho \mathbf{g}$ , where  $\mathbf{g}$  is gravity. Subscript  $o$  is used to indicate quantities in the initial reference configuration. Through Nanson's formula it is possible to relate the first Piola–Kirchhoff stress tensor with the Cauchy  $\boldsymbol{\sigma}$  stress tensor in the current configuration:

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^{-T}, \quad (2)$$

where  $\mathbf{F}$  is deformation gradient defined as  $\mathbf{I} + (\nabla_o \mathbf{u})^T$  and  $J$  is its determinant  $J = \det(\mathbf{F})$ .

This work also considers linear geometry formulation, i.e. small strain assumption:

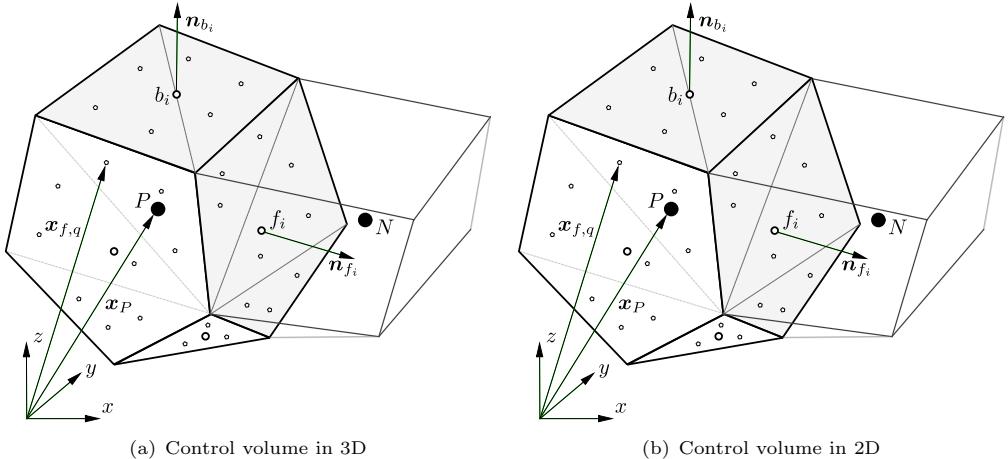
$$\int_{\Omega} \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} d\Omega = \oint_{\Gamma} \mathbf{n} \cdot \boldsymbol{\sigma}_s d\Gamma + \int_{\Omega} \mathbf{f}_b d\Omega, \quad (3)$$

where  $\boldsymbol{\sigma}_s$  is the engineering (small strain) stress tensor which coincide with Piola stress tensor.

Constitutive relation for Cauchy  $\boldsymbol{\sigma}$  stress in Equations 2 and 3 is given by a chosen mechanical law. Mechanical laws considered in this work (Hooke's law, St. Venant-Kirchhoff, Mooney–Rivlin, neo-Hookean, and Guccione) are briefly outlined in Appendix A. The governing equations are complemented by boundary conditions, with three types considered here: prescribed displacement, prescribed traction, and symmetry.

## 3 High-order Finite Volume Discretisation

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**Fig. 1** Representative convex polyhedral cell  $P$  and neighbouring cell  $N$ , which share a face  $f_i$

Sliku dekompozicije za volumni integral

### 3.1 Volume Integrals

### 3.2 Surface Integrals

### 3.3 Alpha Stabilisation

## 4 Solution Algorithm

### 4.1 Jacobian-free Newton-Krylov Algorithm

## 5 Test Cases

root mean square error

$$L_2 = \frac{1}{N_c} \sum_{i=1}^{N_c} |\Delta\phi_i|, \quad (4)$$

and infinity norm representing the maximum absolute error

$$L_{\infty} = \max_{1 \leq i \leq N_c} |\Delta\phi_i|, \quad (5)$$

where  $\Delta\phi_i$  is the difference between expected and predicted solutions and  $N_c$  is the overall number of computational points, i.e. cells. Both norms are calculated for displacement magnitude  $|\mathbf{u}| = \sqrt{u_x^2 + u_y^2 + u_z^2}$  and von Mises stress:

$$\sigma_{ekv} = \sqrt{\frac{1}{2} [(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2] + 3 (\sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{zx}^2)} \quad (6)$$

## 5.1 Case 1: Order Verification via the Manufactured Solution Procedure

The first test case consists of a  $0.2 \times 0.2$  m square or  $0.2 \times 0.2 \times 0.2$  m cube with linear elastic ( $E = 200$  GPa,  $\nu = 0.3$ ) properties. A manufactured solution for displacement (Figure 8(a)) is employed in the form of polynomial, trigonometric [1] or mixed form [2]:

- 2D

$$\mathbf{u} = \begin{pmatrix} e^{x^2} \sin(y) \\ \ln(3+y) \cos(x) + \sin(y) \\ 0. \end{pmatrix} \quad (7)$$

- 3D - polynomial

$$\mathbf{u} = \begin{pmatrix} a_x(x^3 + xy^2) \\ a_y(y^3 + yz^2) \\ a_z(z^3 + zx^2) \end{pmatrix} \quad (8)$$

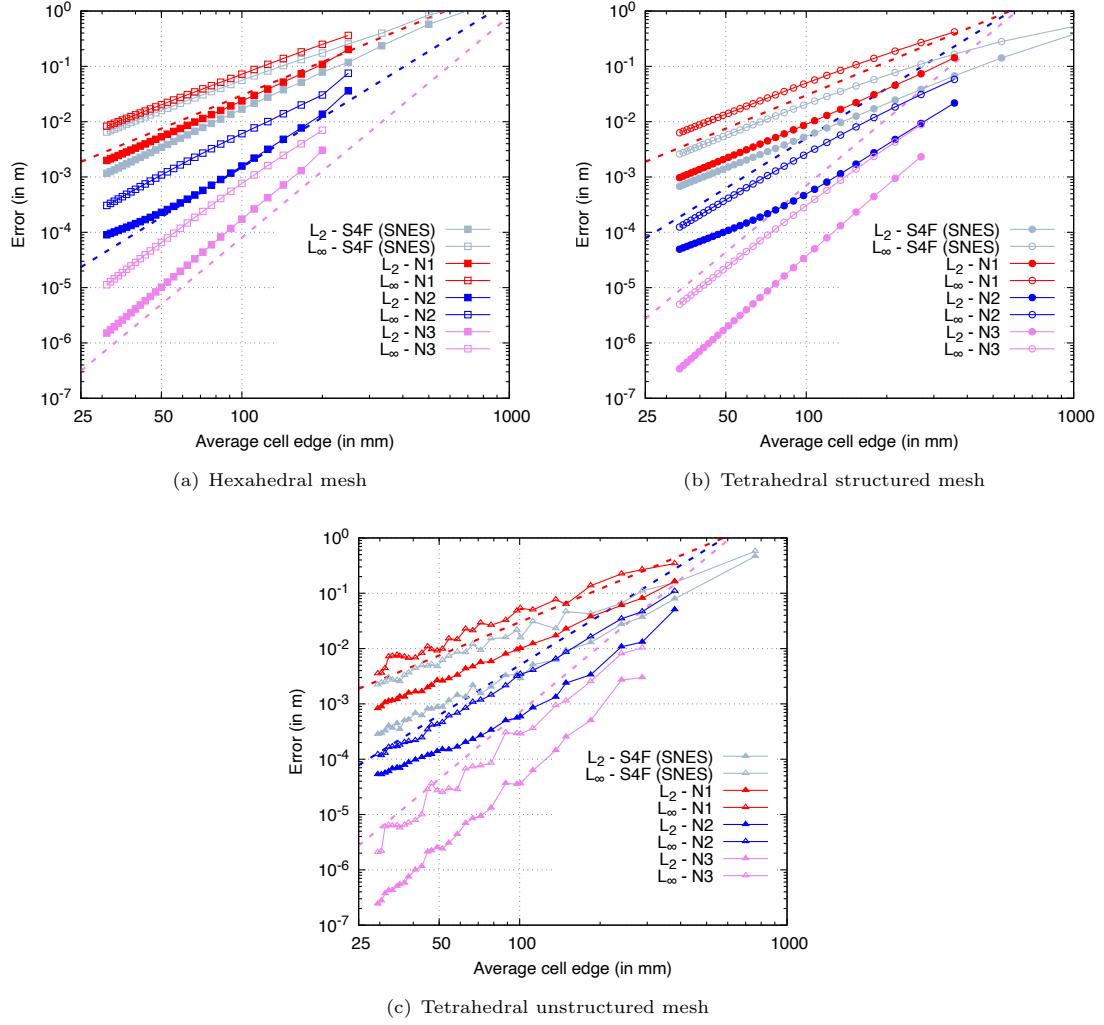
where  $a_x = 1 \mu\text{m}$ ,  $a_y = 1 \mu\text{m}$ , and  $a_z = 1 \mu\text{m}$ .

- 3D - trigonometric

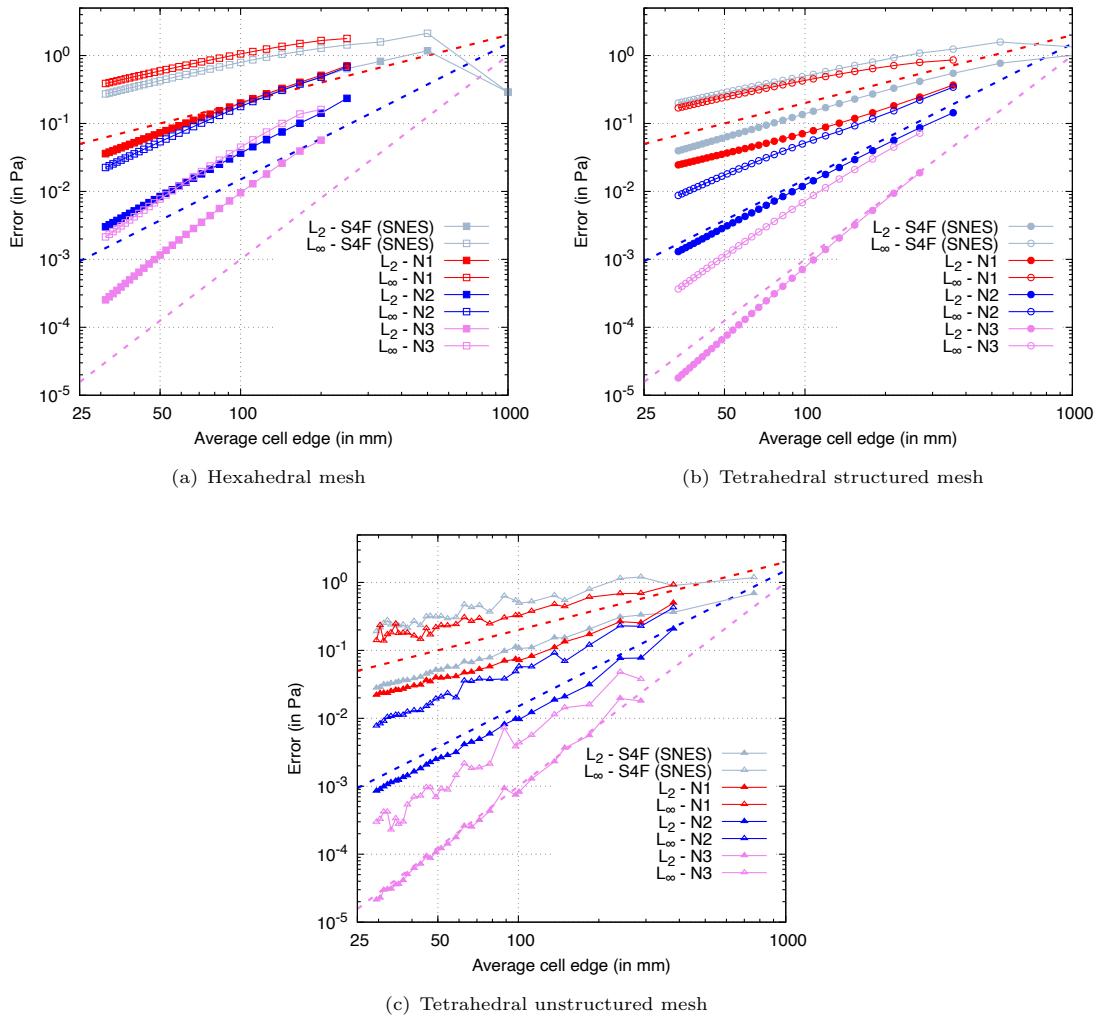
$$\mathbf{u} = \begin{pmatrix} a_x \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \\ a_y \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \\ a_z \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \end{pmatrix} \quad (9)$$

where  $a_x = 2 \mu\text{m}$ ,  $a_y = 4 \mu\text{m}$ , and  $a_z = 6 \mu\text{m}$ .

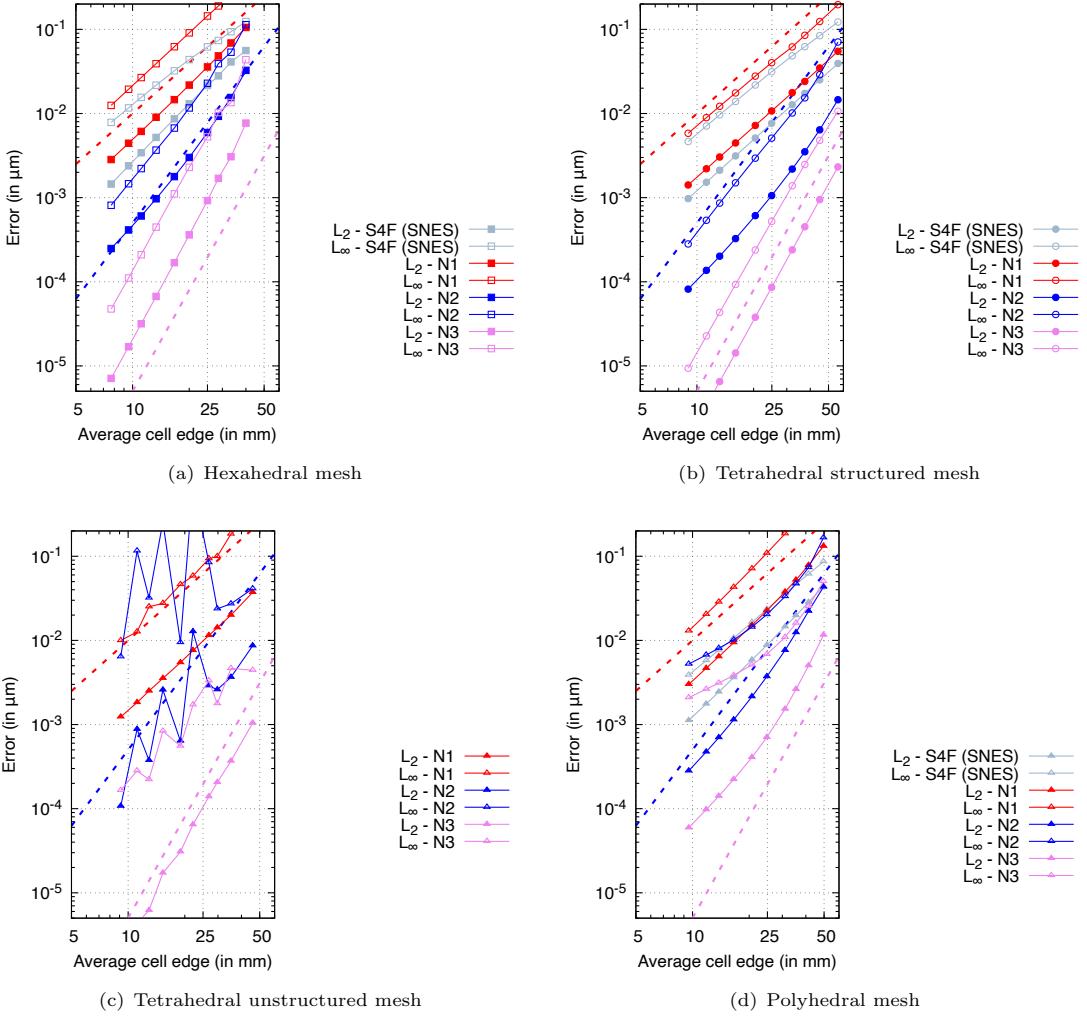
The Cartesian coordinates are given by  $x$ ,  $y$  and  $z$ . The corresponding manufactured body force term ( $\mathbf{f}_b$  in Equation 3) can be found in authors previous publication [3] or obtained by manufactured solution procedure.



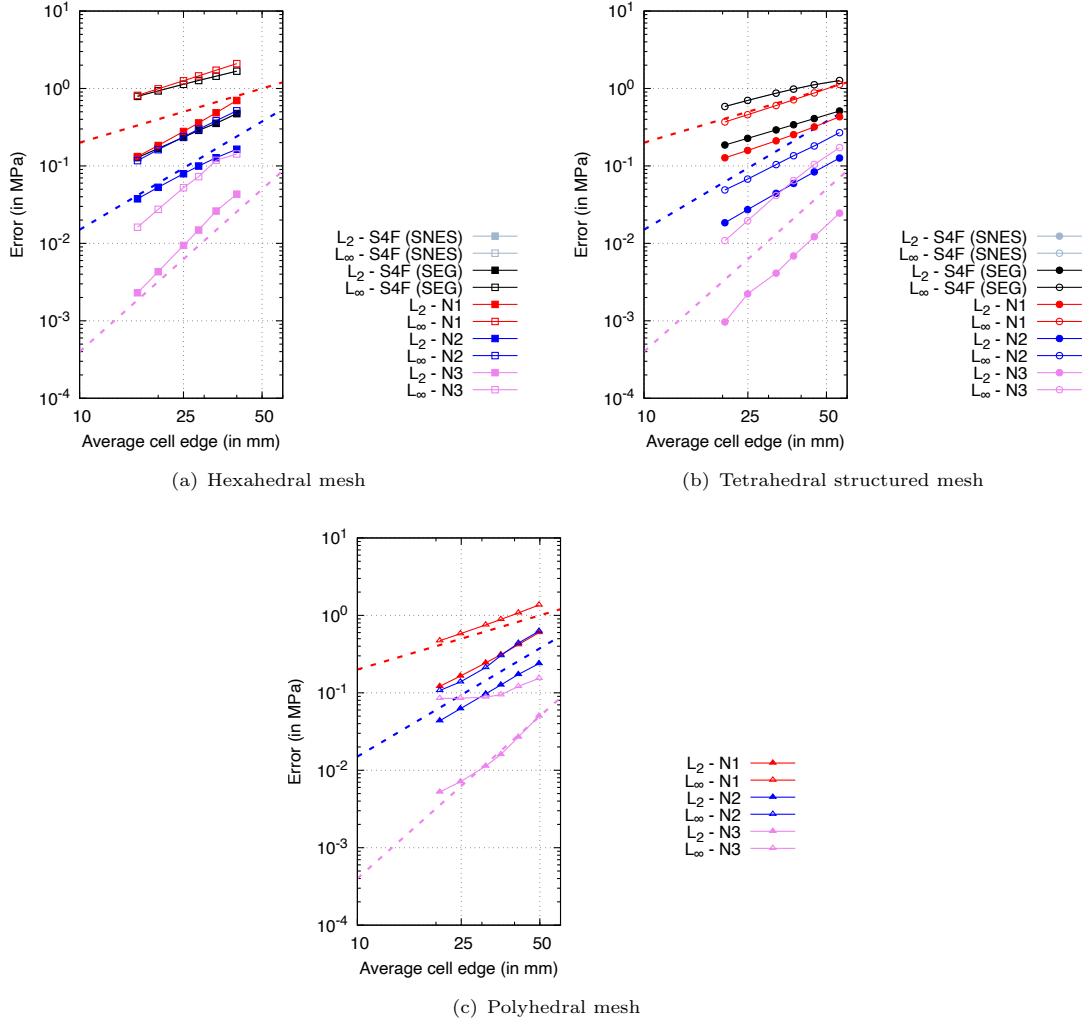
**Fig. 2** Manufactured solution cube (2D case): error convergence for displacement magnitude



**Fig. 3** Manufactured solution cube (2D case): error convergence for stress magnitude



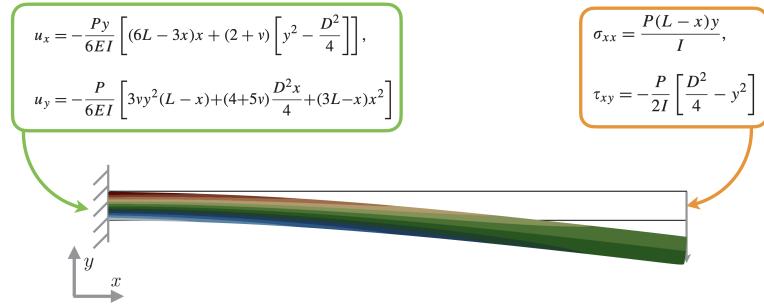
**Fig. 4** Manufactured solution cube (3D case): error convergence for displacement magnitude



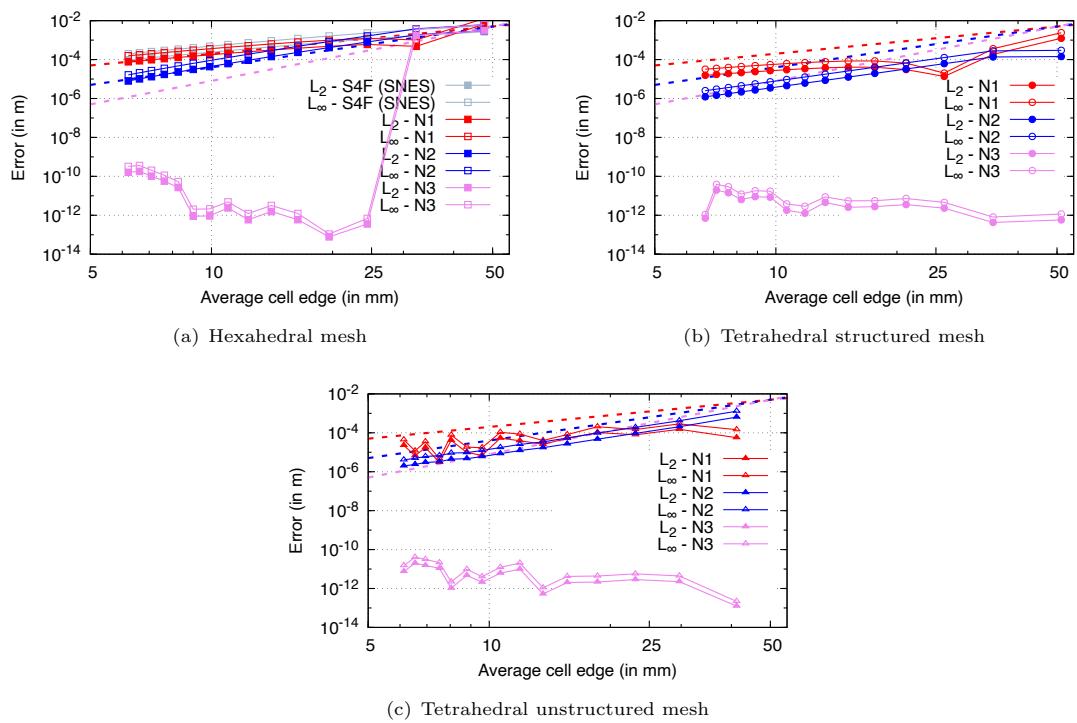
**Fig. 5** Manufactured solution cube (3D case): error convergence for stress magnitude

## 5.2 Case 2: Cantilever beam

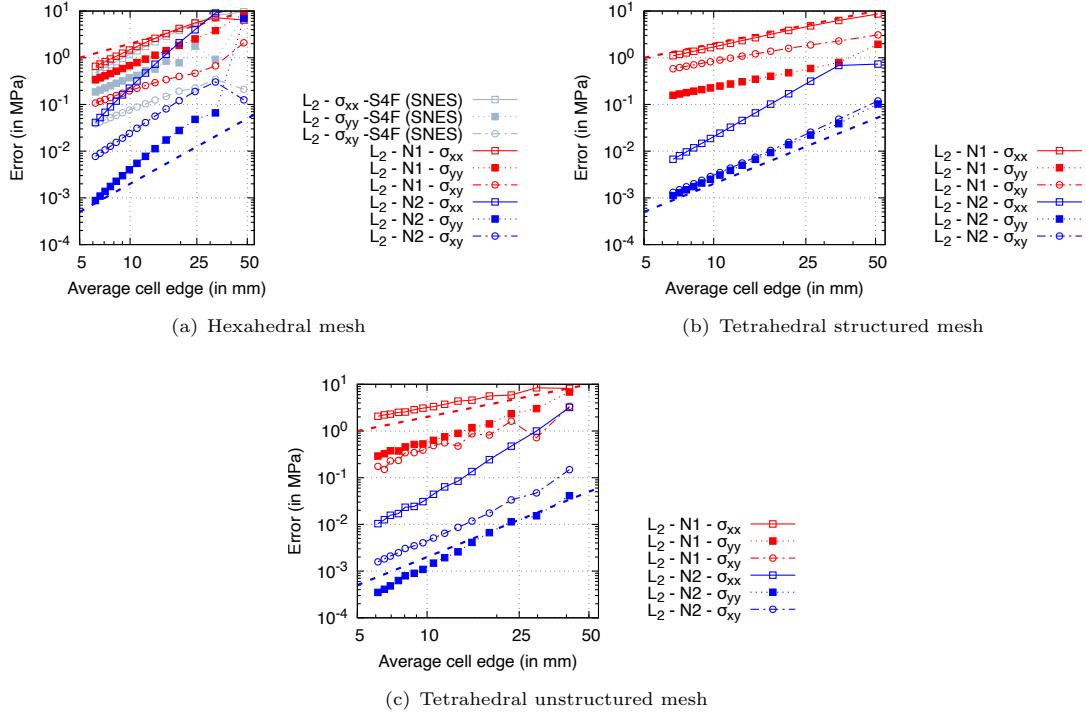
The test case geometry, shown in Fig. 6(a), is a rectangular beam with dimensions of  $2 \text{ m} \times 0.2 \text{ m}$ , a Young's modulus of  $E = 200 \text{ GPa}$ , and a Poisson's ratio of  $\nu = 0.3$ . The top and bottom boundaries of the beam are traction-free, and plane strain conditions are assumed. The left end of the beam is constrained by the analytical displacement, while the right end is subjected to the corresponding analytical traction of  $(0, 1) \text{ MPa}$ . This setup enables quantification of the difference between the predicted displacement and the analytical solution as a measure of convergence across the entire domain, rather than only at the beam end. Convergence is assessed using 15 successively refined grids.



**Fig. 6** Cantilever beam case: geometry and boundary conditions



**Fig. 7** Cantilever beam case: displacement magnitude discretisation errors



**Fig. 8** Cantilever beam case:  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{xy}$  stress discretisation errors. Results for  $N = 3$  are not shown because stress error is around  $\sim 10^{-12}$

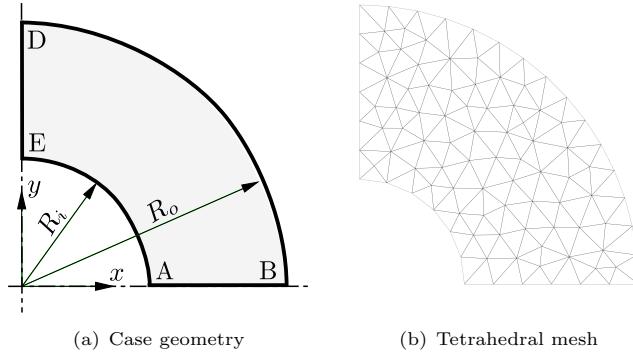
### 5.3 Case 3: Internally pressurised thick-walled cylinder

In this case, a homogeneous thick-wall cylindrical pressure vessel with an inner radius  $R_i = 7$  m, outer radius  $R_o = 18.625$  m, and loaded internally with pressure  $p = 100$  MPa is analysed. Two types of material are considered:

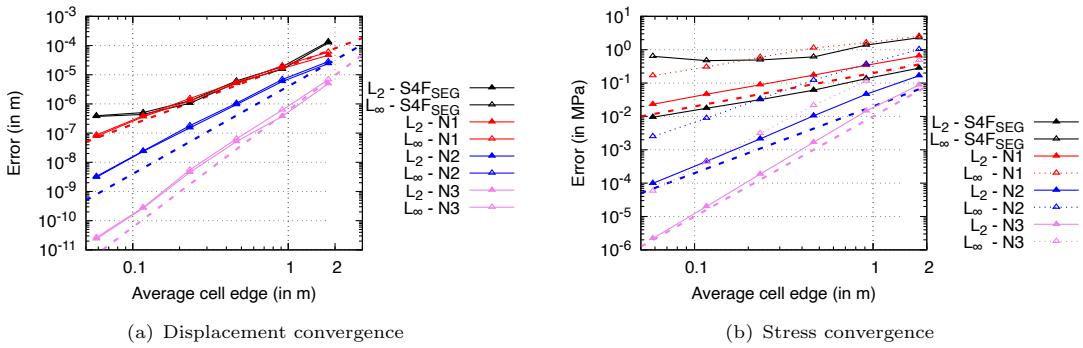
- i. Small strain, linear-elastic [4]:  $E = 10$  GPa,  $\nu = 0.3$ .
- ii. Finite strain, Mooney-Rivlin law [5]:  $c_{10} = 80$  MPa,  $c_{01} = 20$  MPa, and  $c_{11} = 0.0$  MPa and Poisson's ratio  $\nu = 0.49$

The problem is considered plane stress, with the 2-D computational domain comprising a quarter of the cylinder geometry. The cylinder is discretised with series of unstructured tetrahedral grids. Gravitational and inertial effects are neglected. Linear elastic case is solved using one loading increment while hyperelastic case is solved using 100 equal loading increments. Analytical solutions are available in [6] and [7].

popraviti slova na slici 8



**Fig. 9** Plate hole case geometry and mesh

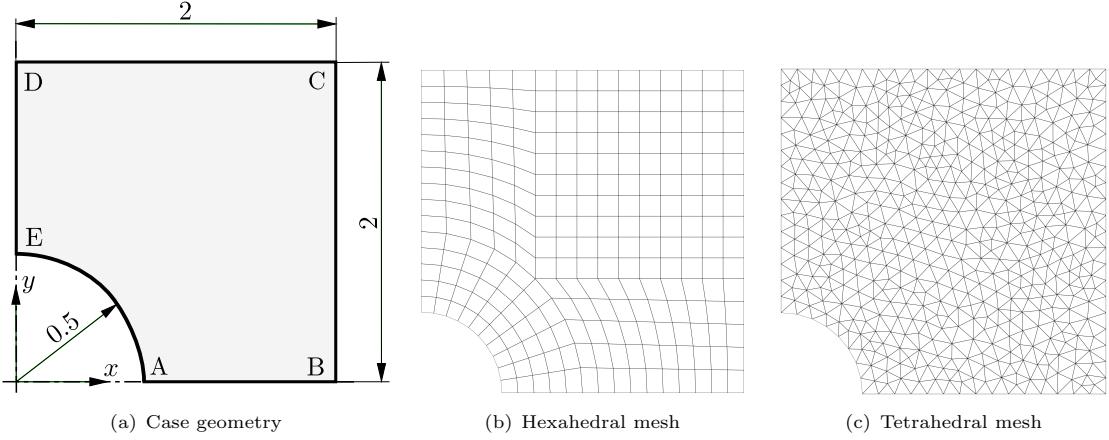


**Fig. 10** Pressurised cylinder case: displacement and stress magnitude discretisation errors for linear elastic material

#### 5.4 Case 4: Cooks membrane

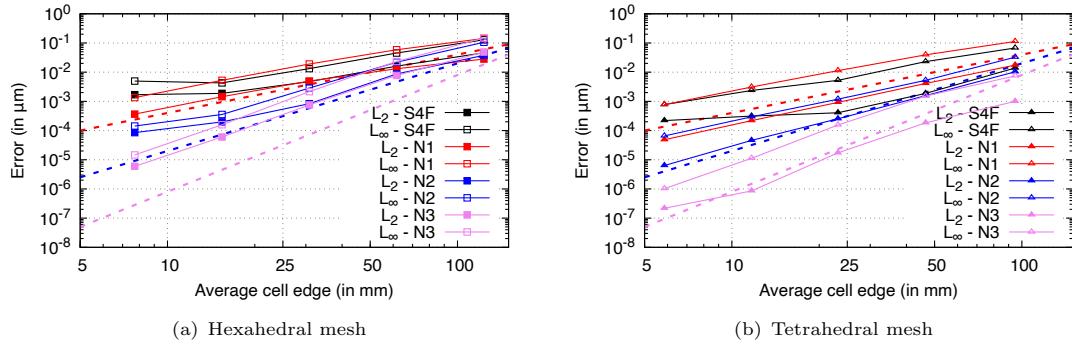
#### 5.5 Case 4: Plate hole

This benchmark problem consists of a thin, infinitely large plate with a circular hole, subjected to uniaxial tension. Owing to the symmetry of the geometry and loading, only one quarter of the plate is modeled as a finite domain. To minimize the influence of the finite computational boundaries, the exact tractions obtained from the analytical solution [8] are prescribed on the outer edges BC and CD. Symmetry boundary conditions are applied on boundaries AB and DE, while zero traction is specified on the hole boundary. The material properties are defined by a Young's modulus of  $E = 200$  GPa and a Poisson's ratio of  $\nu = 0.3$ .

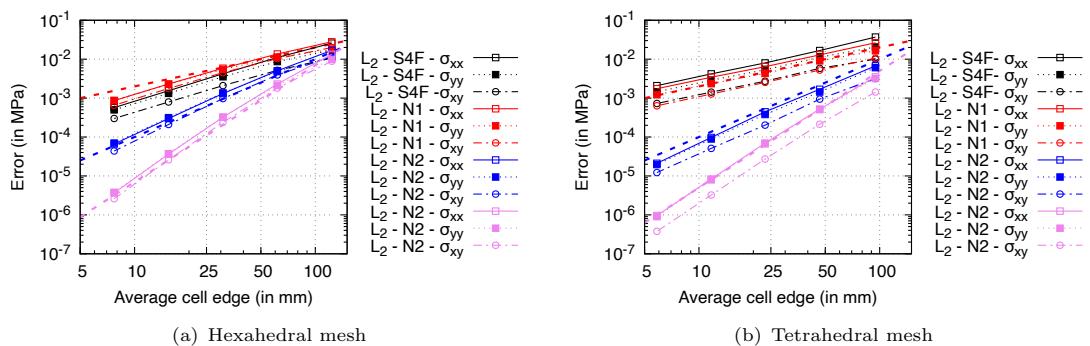


**Fig. 11** Plate hole case geometry and mesh

Hexahedral mesh with N3 needs 20 neighbours to avoid ill conditioning. This results in lower slope for displacement but not affecting the stresses. I'm not sure why S4F results flatten on finer meshes.



**Fig. 12** Plate hole case: displacement magnitude discretisation errors



**Fig. 13** Plate hole case:  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{xy}$  stress discretisation errors.

## 5.6 Case 5: Elliptic plate

## 5.7 Case 6: Spherical cavity

## 5.8 Case 7: Idealised ventricle

## 5.9 Error-cost relationship

## 5.10 Stabilisation scheme

## 5.11 Effects of poor interpolation conditioning

Plate hole sa hex mrezom tu staviti i objasniti sto se desava u 2D-u sa kondicijskim brojem interpolacije

## 5.12 Code parallelisation

# 6 Conclusions

**Data Availability.** To be updated The codes presented are publicly available at <https://github.com/solids4foam/solids4foam> on the `feature-petsc-sn3s` branch, and the cases and plotting scripts are available at <https://github.com/solids4foam/solid-benchmarks>.

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## Appendix A Mechanical Laws

### A.1 Linear Elasticity

The definition of engineering stress  $\sigma_s$  for linear elasticity can be given as

$$\begin{aligned}\sigma_s &= 2\mu\varepsilon + \lambda \operatorname{tr}(\varepsilon) \mathbf{I} \\ &= \mu\nabla\mathbf{u} + \mu(\nabla\mathbf{u})^T + \lambda(\nabla \cdot \mathbf{u}) \mathbf{I}\end{aligned}\quad (\text{A1})$$

where  $\lambda$  is the first Lamé parameter, and  $\mu$  is the second Lamé parameter, synonymous with the shear modulus. The Lamé parameters can be expressed in term of the Young's modulus ( $E$ ) and Poisson's ratio  $\nu$  as

$$\mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad (\text{A2})$$

### A.2 St. Venant-Kirchoff Hyperelasticity

The St. Venant-Kirchoff model defines the second Piola–Kirchhoff stress  $\mathbf{S}$  as

$$\mathbf{S} = 2\mu\mathbf{E} + \lambda \operatorname{tr}(\mathbf{E}) \mathbf{I} \quad (\text{A3})$$

where, as before,  $\lambda$  is the first Lamé parameter, and  $\mu$  is the second Lamé parameter. The Lagrangian Green strain  $\mathbf{E}$  is defined as

$$\mathbf{E} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T + \nabla\mathbf{u} \cdot \nabla\mathbf{u}^T) \quad (\text{A4})$$

The true stress can be calculated from the second Piola–Kirchhoff stress as

$$\boldsymbol{\sigma} = \frac{1}{J} \mathbf{F} \cdot \mathbf{S} \cdot \mathbf{F}^T \quad (\text{A5})$$

### A.3 Neo-Hookean Hyperelasticity

The definition of true (Cauchy) stress  $\boldsymbol{\sigma}$  for neo-Hookean hyperelasticity can be given as

$$\boldsymbol{\sigma} = \frac{\mu}{J} \operatorname{dev}(\bar{\mathbf{b}}) + \frac{\kappa}{2} \frac{J^2 - 1}{J} \mathbf{I} \quad (\text{A6})$$

where, once again,  $\mu$  is the shear modulus, and  $\kappa$  is the bulk modulus. The bulk modulus can be expressed in terms of the Young's modulus ( $E$ ) and Poisson's ratio  $\nu$  as

$$\kappa = \frac{E}{3(1-2\nu)} \quad (\text{A7})$$

The volume-preserving component of the elastic left Cauchy–Green deformation tensor is  $\bar{\mathbf{b}}$  is given as

$$\bar{\mathbf{b}} = J^{-2/3} \mathbf{b} = J^{-2/3} \mathbf{F} \cdot \mathbf{F}^T \quad (\text{A8})$$

In the limit of small deformations  $\|\nabla \mathbf{u}\| \ll 1$ , neo-Hookean hyperelasticity (Equation A6) reduces to linear elasticity (Equation A1).

#### A.4 Guccione Hyperelasticity

The ? ] hyperelastic law defines the second Piola-Kirchhoff stress as

$$\mathbf{S} = \frac{\partial Q}{\partial \mathbf{E}} \left( \frac{C}{2} \right) e^Q + \frac{\kappa}{2} \frac{J^2 - 1}{J} \mathbf{I} \quad (\text{A9})$$

where

$$Q(I_1, I_2, I_4, I_5) = c_t I_1^2 - 2c_t I_2 + (c_f - 2c_{fs} + c_t) I_4^2 + 2(c_{fs} - c_t) I_5 \quad (\text{A10})$$

$$\begin{aligned} \frac{\partial Q}{\partial \mathbf{E}} &= 2c_t \mathbf{E} + 2(c_f - 2c_{fs} + c_t) I_4 (\mathbf{f}_0 \otimes \mathbf{f}_0) \\ &\quad + 2(c_{fs} - c_t) [\mathbf{E} \cdot (\mathbf{f}_0 \otimes \mathbf{f}_0) + (\mathbf{f}_0 \otimes \mathbf{f}_0) \cdot \mathbf{E}] \end{aligned} \quad (\text{A11})$$

The scalars  $C$ ,  $c_f$ ,  $c_{fs}$ , and  $c_t$  are material parameters and invariants of the Green strain,  $\mathbf{E} = \mathbf{F}^T \cdot \mathbf{F}$ , are defined as

$$\begin{aligned} I_1 &= \text{tr}(\mathbf{E}), \quad I_2 = \frac{1}{2} [\text{tr}^2(\mathbf{E}) - \text{tr}(\mathbf{E} \cdot \mathbf{E})], \\ I_4 &= \mathbf{E} : (\mathbf{f}_0 \otimes \mathbf{f}_0), \quad I_5 = (\mathbf{E} \cdot \mathbf{E}) : (\mathbf{f}_0 \otimes \mathbf{f}_0) \end{aligned} \quad (\text{A12})$$

with  $\mathbf{f}_0$  representing the unit fibre directions in the initial configuration.

Equation A5 is used to convert the second Piola-Kirchhoff stress to the true stress.

## A.5 Mon-Rivlin - add here if used

## Appendix B Body Force for the Method of Manufactured Solutions Case

The body force for the manufactured solution case is [1]:

$$\mathbf{f}_b = \left( \begin{array}{l} \lambda [8a_y\pi^2 \cos(4\pi x) \cos(2\pi y) \sin(\pi z) \\ + 4a_z\pi^2 \cos(4\pi x) \cos(\pi z) \sin(2\pi y) \\ - 16a_x\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ + \mu [8a_y\pi^2 \cos(4\pi x) \cos(2\pi y) \sin(\pi z) \\ + 4a_z\pi^2 \cos(4\pi x) \cos(\pi z) \sin(2\pi y) \\ - 5a_x\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ - 32a_x\mu_\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \\ \\ \lambda [8a_x\pi^2 \cos(4\pi x) \cos(2\pi y) \sin(\pi z) \\ + 2a_z\pi^2 \cos(2\pi y) \cos(\pi z) \sin(4\pi x) \\ - 4a_y\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ + \mu [8a_x\pi^2 \cos(4\pi x) \cos(2\pi y) \sin(\pi z) \\ + 2a_z\pi^2 \cos(2\pi y) \cos(\pi z) \sin(4\pi x) \\ - 17a_y\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ - 8a_y\mu_\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \\ \\ \lambda [4a_x\pi^2 \cos(4\pi x) \cos(\pi z) \sin(2\pi y) \\ + 2a_y\pi^2 \cos(2\pi y) \cos(\pi z) \sin(4\pi x) \\ - a_z\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ + \mu [4a_x\pi^2 \cos(4\pi x) \cos(\pi z) \sin(2\pi y) \\ + 2a_y\pi^2 \cos(2\pi y) \cos(\pi z) \sin(4\pi x) \\ - 20a_z\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z)] \\ - 2a_z\mu_\pi^2 \sin(4\pi x) \sin(2\pi y) \sin(\pi z) \end{array} \right) \quad (B13)$$

## Appendix C Meshes Used with the Method of Manufactured Solutions

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