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USING DEAL.II FOR STRUCTURAL ANALYSIS OF A MEDICAL OXYGEN CYLINDER

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The undersigned certify that they have read, and recommended to the Institute of Engineering for acceptance, a project report entitled "Using deal.ii for structural analysis of a Medical Oxygen Cylinder"submitted by Himal Kumar Rana Magar, Khim Bahadur Basnet and Lilanath Ghimire in partial fulfillment of the requirements for the degree of Bachelor of Mechanical Engineering.

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ABSTRACT

Medical Oxygen Cylinders being convenient containers for transportation and storage of oxygen gas has wide range of applications in industries and hospitals. Storing oxygen at high pressure in cylinders increases the risk of structural failure. This study aims to develop a program based on open source C++ library for Finite Element Analysis (FEA) in thin-walled cylinders and to apply the program to perform structural analysis and safety assessment of medical oxygen cylinders operating below their working pressure. To achieve this goal, a literature review was conducted to identify gaps in the use of open-source software for FEA in thin-walled cylinders. Open source FEA library called deal.ii was used to construct the program. This C++ based program was verified by comparing it with the hoop stress results from theoretical calculation and ANSYS for a simple hollow cylinder. The study then proceeded to create a detailed CAD model of the medical oxygen cylinder for a parametric study for varying wall thickness and material. The model was simplified and meshed for FEA, with pressure and fixity constraints applied during simulation. The parametric simulations were run through the developed program which showed that maximum hoop stress occurs in the region around neck of the cylinder. The methodology involved verification of the program by comparing the results with that of ANSYS and theoretical calculations in case of simple hollow cylinder in which maximum error was found to be 0.875 %. Parametric analysis for variying material and thickness found that the cylinder with larger thickness i.e., 5.6 mm, and material 37MnSi5 undergoes through the smallest deformation. The development of the open-source software will provide a valuable resource for future research and development in this field, as well as contribute to the enhancement of the safety and reliability of medical oxygen cylinders.

Keywords: Open-source library, Finite Element Analysis, deal.ii, Medical Oxygen Cylinder, Structural analysis

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LIST OF SYMBOLS

σ	stress tensor,
$ec{b}$	body force vector,
\vec{t}	prescribed traction vector,
\vec{d}	prescribed displacement vector,
\vec{u}	displacement vector,
\vec{n}	normal vector to the surface,
Ω	open domain,
Γ_t	boundary surface when traction is prescribed,
Γ_d	boundary surface when displacement is prescribed,
$ar\Omega$	closed domain, i.e. $\overline{\Omega} = \Omega \cup \Gamma_t \cup \Gamma_d$
ϕ	shape function
Η	Hilbert space
λ	Lame Modulus,
μ	Modulus of Rigidity/Shear Modulus,
ν	Poisson's Ratio,
E	Young,s Modulus of Elasticity,
δ_{ij}	Kronecker delta operator

LIST OF ACRONYMS AND ABBREVIATIONS

DEAL	Differential Equation Analysis Library
FEA	Finite Element Analysis
FEM	Finite Element Method
MOC	Medical Oxygen Cylinder,
MPI	Message Passing Interface

CHAPTER ONE: INTRODUCTION

1.1 Background

Oxygen cylinders are high pressure thin-walled container used for various purposes. Mostly, these cylinders are used in medical sector. Typically, it contains oxygen at a pressure around 150 bar. Various sizes of oxygen cylinders are available in the market, ranging from 10 to 50 liters in capacity.

Since the discovery of oxygen, scientists and technicians have been continuously exploring and developing various technologies to produce and transport this essential gas. One such technology that has proved to be highly effective is the medical oxygen cylinder. The main function of this cylinder is to safely and affordably transport oxygen from manufacturing plants to hospitals and other medical facilities. In contrast to longer pipelines, oxygen cylinders provide a more convenient and practical solution for delivering oxygen where it is needed.

Oxygen cylinders have been designed to meet the specific requirements of medical facilities and other industries. They are manufactured using high-strength steel alloys or lightweight aluminum materials, which offer excellent strength and durability. Oxygen cylinders are available in various sizes and shapes, depending on the specific application, and can be filled with compressed oxygen gas up to a working pressure of 150Bar.

The initial development of the oxygen cylinder was around 1868 AD. As the use of oxygen increased in fields such as medicine and industry, modifications were proposed to increase the cylinder's capacity to carry oxygen at high pressure, while reducing production costs and allowing for mass production. Today, there are several types of oxygen cylinders available with similar physical appearances but varying in dimensions and materials depending on their purpose and use. Typically, oxygen cylinders are constructed using steel alloys or aluminum.

Oxygen cylinders have several uses, which include:

- Providing respiratory support in medical facilities
- · Assisting with breathing in high-altitude environments
- Supporting diving activities
- Administering oxygen therapy
- Facilitating industrial processes like welding, lamp-working, and gas cutting.

On another note, Finite Element Analysis (FEA) is used extensively in engineering and scientific fields to simulate and analyze the behavior of complex systems and structures

under various conditions. These software tools are used to predict how a particular design will perform under various loads, stresses, and strains, and can help engineers optimize designs, reduce costs, and improve performance.

The need for open source FEA software has become increasingly important in recent years, as the cost of proprietary software can be prohibitively high for small businesses, individual users, and academic institutions. Open source FEA software provides an alternative that is accessible to a wider range of users, regardless of their financial resources.

In addition to cost considerations, open source FEA software also provides benefits in terms of transparency and collaboration. With open source software, users can access the source code and modify it to suit their needs. This level of transparency also promotes collaboration and sharing among users, leading to a more robust and diverse community of developers and users.

Moreover, open source FEA software also allows for greater customization and integration with other software tools, which can improve productivity and workflow efficiency. Users can develop their own plugins or interfaces to integrate FEA software with other design or analysis tools, leading to a more streamlined design process.

Overall, the need for open source FEA software is driven by the desire for greater accessibility, transparency, collaboration, and customization in the engineering and scientific community. By leveraging the power of open source software, users can access powerful simulation and analysis tools that can help them optimize their designs, reduce costs, and improve performance.

The aim of this project is to perform a structural analysis of a medical oxygen pressure cylinder using open source platform called deal.ii. It is a large finite element library written in C++ that offers numerous capabilities to work in FEA. The goal is to determine the level of safety when the cylinder is used below its working pressure. Additionally, this project aims to provide suggestions for minimizing the risk of deformation and failure of the oxygen cylinder under low-pressure conditions. The study will focus on a typical D-type 46.7L oxygen cylinder with a working pressure of 150 bar. By conducting this analysis, It was expected to provide valuable insights that can be used to enhance the safety and reliability of oxygen cylinders in medical and other fields.



Figure 1.1: Typical Medical Oxygen Cylinder

Note: The Picture in figure 1.1 was taken in Sagarmatha Oxygen Pvt.Ltd during project field visit, it is of capacity 46.7L, More about shape, size and dimensions of oxygen cylinder is explained in Field Visit section of this report under chapter Methodology. Also, the terms displacement and deformation are used interchangeably throughout the report.

1.2 Problem Statement

Storing oxygen at high pressures in cylinders increases the risk of structural failure. The pressure can cause the cylinder to explode, leak or crack, and oxygen's chemical properties increase the likelihood of corrosion if the cylinder is filled without checking for the presence of water/humidity or an electrolytic environment on the internal surface of the cylinder. During a visit to an oxygen filling industry, it was learned that recently a oxygen cylinder failure resulted in the loss of two lives. Unfortunately, news of oxygen cylinder explosions resulting in death or serious injury has become increasingly common. Therefore, to ensure the safety of using oxygen cylinders at their maximum working pressure and temperature, a safety analysis is necessary. Predicting failure based on general knowledge or common prediction methods is challenging. Hence, this project aims to analyze the bursting failure of oxygen cylinders due to excessive pressure, determine the safety state of oxygen cylinders at their working pressure, and analyze the use of different materials and their resulting safety. The potential hazards of oxygen cylinders require that safety be a top priority, especially in the medical industry, where patients depend on them for life support. Understanding the safety limits of oxygen cylinders is essential to avoid accidents and fatalities. Therefore, this project aims to develop an open-source C++ code to predict the safety and risk of oxygen cylinders operating below their working pressure. By analyzing the structural integrity of the D-type 46.7L typical oxygen cylinder with a working pressure of 150 bar, this project aims to provide useful suggestions for minimizing the deformation and risk of failure of oxygen cylinders below their working pressure. Furthermore, the project seeks to explore the effectiveness of different materials in enhancing the safety of oxygen cylinders. Through this analysis, it is hoped that it contributes to the development of safer and more reliable oxygen cylinders for various applications.



Figure 1.2: Bursted Oxygen Cylinder (source:safetymattersweekly.com)

1.3 Objectives

1.3.1 Main Objective

To perform structural analysis and safety assessment of medical oxygen cylinder.

1.3.2 Specific Objectives

- To develop C++ code that can accurately predict the safety and risk of medical oxygen cylinders operating below their working pressure.
- To investigate the effectiveness of different materials and thicknesses in enhancing the safety of medical oxygen cylinders.
- To Compare and validate the simulation results with theoretical calculations to ensure the accuracy and reliability of the model.

CHAPTER TWO: LITERATURE REVIEW

2.1 Theoretical Background

Followings are the theories behind the working of the program and the model:

2.1.1 Mathematical Formulation

Strong Form

The strong form for the small displacement three-dimensional linear elasticity problem with Neumann and Dirichlet boundary conditions is,

Given $\vec{b}: \Omega \to \mathbb{R}^3$, $\vec{d}: \Gamma_d \to \mathbb{R}^3$, $\vec{t}: \Gamma_t \to \mathbb{R}^3$, find $\vec{u}: \bar{\Omega} \to \mathbb{R}^3$ such that,

$$-\operatorname{div}(\boldsymbol{\sigma}(\vec{u})) = \vec{b} \operatorname{in} \Omega$$
$$\vec{u} = \vec{d} \operatorname{on} \Gamma_d$$
$$\boldsymbol{\sigma}(\vec{u}) \cdot \vec{n} = \vec{t} \operatorname{on} \Gamma_t$$

Weak Form

Weak form of the problem in bi-linear form is, Given $\vec{b}: \Omega \to \mathbb{R}^3$, $\vec{d}: \Gamma_d \to \mathbb{R}^3$, $\vec{t}: \Gamma_t \to \mathbb{R}^3$, find $\vec{u}: \bar{\Omega} \to \mathbb{R}^3$ such that for $\vec{v} \in \mathbf{H}$,

$$a(\vec{u}, \vec{v}) = (\vec{t}, \vec{v})_{\Gamma_t} + (\vec{b}, \vec{v}) \text{ in } \Omega$$

where,

$$\begin{split} a(\vec{u}, \vec{v}) &= \int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} \\ (\vec{t}, \vec{v})_{\Gamma_t} &= \int_{\Gamma_t} \vec{t} \cdot \vec{v} \\ (\vec{b}, \vec{v}) &= \int_{\Omega} \vec{b} \cdot \vec{v} \\ \end{split}$$
Note:

Stress tensor for isotropic material is given by,

$$\boldsymbol{\sigma}(\vec{u}) = \lambda \left(\text{div } \vec{u} \right) \boldsymbol{I} + 2\mu\varepsilon(\vec{u})$$

where,

 λ and μ are the Lame parameters, I is the second rank identity tensor, and $\varepsilon(\bullet) := \{\nabla(\bullet) + \nabla(\bullet)^T\}/2.$

The meaning of each symbols are listed on LIST OF SYMBOLS chapter.

Finite Element Approximation

Applying finite element approximation, the problem can be expressed as the linear system of equations and is represented as,

AU=F

where,

A is the global stiffness matrix,

U is the global displacement vector,

F is the global force vector.

Global stiffness matrix is defined as,

$$A_{ij} = \sum_{k,l} \{ (\lambda \partial_l (\Phi_i)_l, \partial_k (\Phi_j)_k)_{\Omega} + (\mu \partial_k (\Phi_i)_l, \partial_k (\Phi_j)_l)_{\Omega} + (\mu \partial_k (\Phi_i)_l, \partial_l (\Phi_j)_k)_{\Omega} \}$$

here, *i* and *j* run over the global degrees of freedom while *k* and *l* run over the spacedimension, and Φ_i represents the vector shape function, which is defined as,

$$\Phi_i(\mathbf{x}) = \phi_i(\mathbf{x}) \ \mathbf{e}_{\operatorname{comp}(i)}$$

where, \mathbf{e} is the unit vector specified by comp(i) which in turn is defined as,

$$\operatorname{comp}(i) = \begin{cases} 0 & \text{if } i = 0, 3, 6, \cdots \\ 1 & \text{if } i = 1, 4, 7, \cdots \\ 2 & \text{if } i = 2, 5, 8, \cdots \end{cases}$$

The global stiffness matrix is obtained by assembling the local stiffness matrices, where local stiffness matrix on cell K is expressed as,

$$A_{ij}^{K} = \sum_{k,l} \{ (\lambda \partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{K} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{K} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{K} \}$$

This can be further arranged into,

$$A_{ij}^{K} = \left(\lambda \partial_{\operatorname{comp}(i)} \phi_{i}, \partial_{\operatorname{comp}(j)} \phi_{j}\right)_{K} + \left(\mu \partial_{\operatorname{comp}(j)} \phi_{i}, \partial_{\operatorname{comp}(i)} \phi_{j}\right)_{K} + \left(\mu \nabla \phi_{i}, \nabla \phi_{j}\right)_{K} \delta_{\operatorname{comp}(i), \operatorname{comp}(j)}$$

here, now i and j run over local degrees of freedom, and δ_{ij} is the Kronecker Delta operator.

Since, integration on computer is difficult to incorporate and sometimes even impossible, we use Gauss Quadrature formula. For this, we transform the cells from real(physical) space into parametric space and vice versa using **Jacobian** transformation, and then apply Gauss Quadrature formula to compute the integration.

Then, final expression becomes,

$$\begin{aligned} A_{ij}^{K} &= \sum_{q} \{ \lambda \left(\partial_{\operatorname{comp}(i)} \phi_{i}(q) \right) \left(\partial_{\operatorname{comp}(j)} \phi_{j}(q) \right) + \mu \left(\partial_{\operatorname{comp}(j)} \phi_{i}(q) \right) \left(\partial_{\operatorname{comp}(i)} \phi_{j}(q) \right) + \\ \mu \left(\nabla \phi_{i}(q) \right) \left(\nabla \phi_{j}(q) \right) \delta_{\operatorname{comp}(i),\operatorname{comp}(j)} \} \mathbf{J} \mathbf{X} \mathbf{W}(q) \end{aligned}$$

where, q's represent quadrature points in parametric space, and 'JxW(q)' represents the product of determinant of Jacobian and the weight at the quadrature point q.

Similarly, right-hand-side vector(global force vector) is obtained by assembling the contributions from the local force vectors, which are defined as,

$$F_i^K = \sum_{q_f} \left(t_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q_f) + \sum_q \left(b_{\operatorname{comp}(i)} \phi_i(q) \right) \operatorname{JxW}(q)$$

where q_f refers to the quadrature points on the face of the cell, since the first term is to be integrated on the face of the cell, that belongs to the boundary surface Γ_t . In the problem, traction is caused by the gas pressure, i.e.,

$$\vec{t} = -P \cdot \vec{n}$$

where, P is the pressure acting on the surface and \vec{n} is the normal surface vector of the surface.

Then,

$$\sum_{q_f} \left(t_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q_f) = \sum_{q_f} \left(-P \cdot n_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q_f)$$

Finally, the rhs vector on a local cell becomes,

$$F_i^K = \sum_{q_f} \left(-P \cdot n_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q_f) + \sum_{q} \left(b_{\operatorname{comp}(i)} \phi_i(q) \right) \operatorname{JxW}(q)$$

The complete derivation to these expressions is present in the Appendix A and is heavily based on the book by Ioannis Koutromanos and Roy (2018) and Chaves (2013).

2.1.2 Thin-Walled Cylinder

In the case of thin-walled cylinders, the relationship between the wall thickness and diameter is often expressed as D/t » 1, where D/t typically exceeds 20. Due to the radially symmetric geometry and loading of cylindrical vessels, the stresses within them do not vary in the angular direction. The impact of end caps can be ignored at locations far enough from them. Additionally, as the wall thickness is insignificant, radial stress is considered absent. The two types of stress that exist in a pressure-filled thin-walled cylinder are hoop stress and longitudinal stress.



Figure 2.1: Thin-walled cylinder

The Hoop stress, σ_{θ} and axial stress, σ_z acting on the cylinder are given by,

$$\sigma_{\theta\theta} = \frac{P \cdot r}{t}$$
$$\sigma_{zz} = \frac{P \cdot r}{2t}$$

thus, hoop stress is twice the axial stress in case of thin wall cylinder in case of closed end cylinder, i.e., $\sigma_{\theta\theta} = 2\sigma_{zz}$.

2.2 FEA of Thin-Walled Cylinders

Thin-walled cylinders are widely used in various engineering applications, such as pressure vessels, storage tanks, pipelines, and aerospace structures. The structural behavior of thin-walled cylinders is complex and depends on factors such as the geometry, material properties, loading conditions, and boundary conditions. Finite Element Analysis (FEA) is a powerful tool for analyzing the stress, deformation, and failure of thin-walled cylinders. In recent years, there has been an increasing interest in the FEA of thin-walled cylinders due to its potential for improving the design, optimization, and safety of engineering structures. In this literature review, we will survey and analyze the existing research on the FEA of thin-walled cylinders, focusing on the key challenges, methodologies, and applications.

In a study done by Abdussalam (2006), FEA of the design and manufacture of aerosol cans was done. The author prefers the FEA over traditional "Design-by-test" methods because of repeatability and rapid re-analysis capacity.

Finite element analysis has also been used to investigate catastrophic failures of thinwalled cylinders. Mirzaei (2008) discussed the finite element simulations of deformation and fracture of a gas cylinder that catastrophically failed as a result of an accidental explosion. The FEA results clearly showed that the stresses caused by the assumed loading profile were indeed capable of creating local ruptures at the actual crack initiation sites.

Major of the studies involve comparison of FEA result with theoretical calculations and experimental data. A study performed Finite element analysis of specified thick wall cylinder with help of ANSYS software and compared its result with experimental result and theoretical calculation by Lame's equation (Macwan et al., 2011). They measured hoop strain and hoop stress by experimental setup for internal as well as external surface of cylinder and by numerical and theoretical method they calculated hoop and radial stress and concluded that there is about one percentage error between results of theoretical calculation and experiment result and, 4 percentage error between result of experiment and numerical solution.

Rangari (2012) performed finite element analysis of LPG cylinder to verify its burst pressure. In this research the researchers assumed an LPG cylinder of material low carbon steel and calculated maximum shear stress, equivalent shear stress at critical area of failure by FEA on ANSYS Workbench as well as by using theoretical calculation and compared results. They concluded the verification of ANSYS result with theoretical result.

Wang et al. (2017) studied the buckling behavior of tori-spherical bottom head of a residential water heater tank. Both FEA and Hydrostatic test results were correlated to find that the effect of geometric imperfection has more effect on buckling pressure than contact imperfection. P. Palanivelu (2017) performed Finite element analysis on a typical pressure vessel with ellipsoidal head to determined stress distribution and critical points of possible failure and result compared with theoretical calculation. The research found that equator of head of pressure vessel is critical point for failure.

Mohamed (2018) showed that the finite element method can give results with good agreement with the criteria of mechanics of material. Nevertheless, the model was of thinwalled cylinder and simplified geometry, it clearly shows the distribution of hoop and longitudinal stresses over the cylinder thickness.

Yin et al. (2019) conducted FEA analysis using ANSYS workbench to analyze a 40L industrial gas cylinder and found the maximum stresses are near to the allowable stresses. The authors also used equivalent linearization method to optimize the cylinder structure. It was found that these methods significantly improve the safety of the cylinder transportation process.

Das and Islam (2019) compared the deformation and stress distribution for continuous, discontinuous and material interface joint with help of FEA result for a thick wall pressure vessel and found that effect of geometry discontinuity is quite significant in von-misses and hoop stress.

Nendra Wibawa et al. (2021) did FEA for thick-walled cylinder for rocket motor case, in which they performed FE simulation for different wall thickness of thick-walled cylinder with same length and same outer diameter also for every increasing thickness they increased internal pressure for three different material Aluminum 6061, CFRP, GFRP and concluded that maximum hoop and longitudinal stress decreases for increase in wall thickness for given reference rocket motor casing.

FEA with nonlinear stabilization techniques and failure criterion can determine the burst pressures of the thin-walled cylinders accurately, while the conventional elastic-strain hardening plasticity material model may overestimate the burst pressure of a cylinder composed of plain carbon steel with a yield plateau(Wang et al., 2021).

2.3 Deal.ii

Finite Element Analysis (FEA) of thin-walled cylinders involves complex mathematical models and requires high-performance computing resources. Open-source software provides a cost-effective and customizable solution for FEA, as it enables users to access and modify the source code for their specific needs. Deal.ii (Arndt et al., 2022) is a C++ software library supporting the creation of finite element codes and an open community of users and developers. Deal.ii is a powerful open-source finite element software package that provides a wide range of tools and capabilities for FEA of various types of problems. It has strong focus on high-performance and parallel computing, which is essential for efficiently solving large-scale FEA problems.

Bangerth et al. (2007) in their paper, provide an overview of the deal.ii library, including its design principles, basic usage, and capabilities. It also discusses some of the advanced features of deal.ii, such as support for adaptive mesh refinement and parallel computing. This paper (Kronbichler & Kormann, 2012) describes the development of a generic interface for parallel computing in deal.ii. The authors demonstrate the effectiveness of their approach using a variety of test cases, including the solution of the Navier-Stokes equations.

This paper (Arndt et al., 2021a) provides an overview of the new features and improvements in deal.ii release 9.0. The authors discuss enhancements to the finite element spaces supported by deal.ii, improvements in the parallel computing capabilities, and updates to the interface for mesh generation (Arndt et al., 2021b)provides an overview of the parallel capabilities of deal.ii and its applications in solving elasticity equations. The authors discuss the parallel algorithms used in deal.ii, including domain decomposition and shared memory parallelization, and demonstrate their effectiveness in solving a range of elasticity problems.

2.4 Research gap

The literature review on Finite Element Analysis (FEA) in thin-walled cylinders reveals that the use of open source software for this application is limited. While there is existing research on FEA in thin-walled cylinders, the majority of studies have utilized commercial software. Therefore, a research gap exists regarding the application of open source software for FEA in thin-walled cylinders. Further investigation is required to explore the potential benefits and limitations of utilizing open source software for this application, and to determine the accuracy and reliability of results obtained from such software.

CHAPTER THREE: METHODOLOGY

This project involved designing and simulating a Medical oxygen cylinder to assess its safety and strength conditioning under different materials and geometric properties (thickness). The methodological flow chart of this project is shown in figure 3.1. The project began with a literature review and field visits to understand the different types and specifications of oxygen cylinders available in the local as well as global market. Using this information, a detailed CAD model of the cylinder was created in SOLIDWORKS, including multiple versions with varying wall thicknesses for the simulation and analysis. The model was later simplified and meshed for finite element analysis, with pressure and fixity constraints applied during simulation. The simulations were run through the deal.ii library based C++ code and verified using theoretical calculations and ANSYS simulations. furthermore for entire course of this project literature review was conducted on related topics .

In conclusion, the project showcases the importance of a comprehensive and data-driven approach to designing, simulating and analyzing engineering systems. By using a range of methods, including literature reviews, field visits, CAD modeling, meshing, parametrization, coding and simulations, This project work provided a sound understanding of analysis under different study parameters. This projects highlighted the value of collaboration between different engineering disciplines, as this project drew on knowledge from multiple areas, including mechanical engineering, materials science, and computational modeling. The resulting oxygen cylinder analysis results are expected to have a significant positive impact on construction of upcoming oxygen bottles, providing a reliable and safe oxygen cylinder for patients as well as for industrial purposes.



Figure 3.1: Methodology Flowchart

Each stage of the project work is explained in the respective sections.

3.1 Literature Review

Throughout the duration of the project, a comprehensive literature review was conducted to ensure that, the standard pathway were follower for project. Literature review was conducted to consult and analyze existing research and theories in order to compare the output of each step with those of established methods. This process was to ensure that the project was rigorous, thorough, and aligned with established best practices in the field. By conducting a careful and thorough literature review, to create a project upon existing knowledge that was grounded in solid research and theory.

3.2 Field Visit

During the starting of this project, field visits were conducted to two of the re-known oxygen gas manufacturing and refilling industries in Nepal to gain a better understanding of the different dimensions, capacities, and materials of oxygen cylinders that are available in the local market. These visits allowed to observe firsthand the different types of cylinders that were being used and imported from India and China. The carefully documentation of findings from these field visits were done and, which are presented in below. This information includes a summary of the different types of cylinders that were observed, their respective dimensions and capacities, and the materials used in their construction.

- 1. Sagarmatha Oxygen Pvt. Ltd (Patan Industrial State, Lalitpur)
 - Visited: 2079/04/24
 - Available Sizes (10L, 20L, 47L i.e. 46.7L & 50L)
 - Outer Diameter (OD)=232mm
 - Height(H) = 1370 mm
 - Working Pressure=150bar
 - Circumference of Neck: Upper (c') =25cm, Lower (c'') =35cm
 - Upper Neck Height $(H_1) = 20$ mm
 - Lower Neck Height $(H_2) = 45$ mm
 - Height to Head Start $(H_n) = 1235$ mm
 - Head Profile: Spherical
- 2. Kantipur Oxygen Limited (Harsiddhi, Lalitpur)
 - Visited: 2079/04/24
 - OD =232mm
 - *H*=1350mm

- Pressure =150bar
- H_1 =3cm
- *H*₂=6cm
- C'=25cm
- C"=35cm
- Hole Dia. =3mm
- Thickness (t)=5.4mm
- Weight (W)=50.7kg
- Head Profile: Spherical

The above geometrical parameters are as shown in figure:



Figure 3.2: Body And Head Profile

- 3. Model finalized for simulation
 - OD=232mm
 - *H*=1365mm
 - Thickness(t)=5.6mm/5.5mm/5.4mm
 - Material = 32CrMo4/37MnSi5/34Mn2V

Following are some of the pictures taken during our project field:



Figure 3.3: Picture of Body And Head Profile



Figure 3.4: Valve in Head



Figure 3.5: Cylinder Bottom Profile

3.3 Geometrical and material properties

Based on preliminary field study, literature review, and analysis of design standards and codes, the necessary design geometry for a Medical oxygen cylinder with a capacity of 46.7L (internal volume) was obtained. This involved carefully considering the appropriate dimensions and specifications for the cylinder, including its diameter, height, and thickness, as well as other critical design elements. With this design geometry in hand, further calculations, processing ,refinement and simulation were performed and our that ensured the design met all necessary standards and requirements. This included analyzing the strength and safety of the cylinder, as well as considering factors such as weight, portability, and ease of use. By using a rigorous and data-driven approach, we were able to design and analyse a high-quality and effective medical oxygen cylinder that met all necessary specifications and requirements and which can be used in our deal.ii based simulation.

In selecting the appropriate geometry for this study, thorough review of the literature and field visit data was conducted. After careful consideration, the geometry proposed in (Yin et al., 2019) was chosen based on its suitability for research question of this project and its demonstrated effectiveness in previous studies. The studied cylinder geometry is of the following dimensions:

Outer Diameter	Wall Thickness	Height	
	5.4 mm		
232 mm	5.5 mm	1365 mm	
	5.6 mm		

Table 3.1: Dimensions of Medical Oxygen cylinder.

On literature review, the materials used in manufacture of high pressure gas cylinder are majorly 34Mn2V (Yin et al., 2019), 34CrMO4 (Bultel & Vogt, 2010; Li et al., 2019) and 37MnSi5. The material properties are shown in the table 3.2:

Material	Modulus of Elasticity (GPa)	Poisson's ratio	density (Kg/m ³)
34Mn2V	185	0.3	7850
34CrMo4	197	0.29	7850
37MnSi5	206	0.3	7850

Table 3.2: Materials and their properties.

The formulae to calculate the Lame's parameters out of **E** and ν are:

$$\mu = G = \frac{E}{2(1+\nu)}$$
$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

The following geometrical design consideration(Yin et al., 2019) were assumed for concave bottom profile:

- $t_1 = (2.0 \sim 2.6)t = 2.3t$
- $t_2 = (1.8 \sim 2.2)t = 2t$
- $t_3 = (2.0 \sim 2.6)t = 2.3t$
- $r = (0.07 \sim 0.09)OD = 0.08OD$
- $h = (0.13 \sim 0.16)OD = 0.15OD$
- Transition = 2h

Where t is the thickness of the oxygen bottle wall and OD is the outer diameter of the oxygen bottle.



Figure 3.6: Cylinder Base Profile

The geometrical parameters of concave bottom profile, which was used for modelling are:

Η	OD	t	t1	t2	t3	r	h	Transition
1365	232	5.4	12.42	11.88	12.42	18.56	33.64	67.28
		5.5	12.65	12.1	12.65	18.56	33.64	67.28
		5.6	12.88	12.32	12.88	18.56	33.64	67.28

Table 3.3: Concave Bottom Design Parameters

Note: All dimensions in table 3.3 are in mm.

3.4 CAD Modelling

In order to incorporate the design of an oxygen cylinder into a simulation platform, computeraided design (CAD) software was employed to create a highly accurate and detailed 3D model of the cylinder. This involved the inclusion of all relevant design components and specifications. A crucial consideration in this modeling process was determining the optimal wall thickness for the cylinder. To enable an analysis of the design during simulation, multiple versions of the model were generated with varying wall thicknesses. This facilitated an evaluation of the cylinder's strength and safety under different geometrical and material conditions and uses. Utilizing the SOLIDWORKS software, a precise and comprehensive model of the oxygen cylinder was produced. A snapshot of the resulting 3D model of the full-scale oxygen cylinder created using SOLIDWORKS is displayed below.



Figure 3.7: CAD Model in SOLIDWORKS

3.5 Simplification

In order to ensure an efficient and accurate simulation process for stress and deformation analysis, the original CAD model was simplified while maintaining the overall dimensions. This simplification involved the creation of a computationally streamlined version of the model that still effectively captured the essential design features and characteristics of the cylinder. The simplification of the CAD model increased the ability to reduce its complexity and streamline the simulation process, leading to the obtainment of approximated results for stress and deformation with greater efficiency and accuracy. The geometry of the simulation was generated in Gmsh, utilizing a combination of CAD models and manual input. The geometry was then partitioned into distinct regions to define the meshing areas. The meshing process involved the definition of the element size, selection of the meshing algorithm, and specification of the boundary conditions.



Figure 3.8: Simplified geometry in Gmsh.

3.6 FEA in ANSYS

FEA Simulations were also performed using ANSYS software to verify the program based on deal.ii since it is well-established and reliable FEA software. It enabled the crossvalidation of the accuracy and reliability of the results, and to ensure that the findings were not specific to any particular software package. The same geometry and boundary conditions were applied and the corresponding hoop stress and deformations were noted for every model for each material.

3.7 Theoretical Calculation

Theoretical calculations were done to determine the hoop stress in the midsection of the cylinder using the theory from solid mechanics as mentioned in the theoretical background section. Hoop stress for each model of varying thickness was calculated and later compared with the FEA results. It may be noted that throughout the report, theoretical calculation and analytical calculation were used interchangeably.

3.8 FEA using Deal.ii

To conduct FEA in deal.ii, following steps were incorporated:



Figure 3.9: Algorithm for FEA in deal.ii

3.8.1 Meshing

The meshing stage of our project involved the process of discretizing the CAD model of the D-Type Medical oxygen cylinder into a finite number elements. In this study, Gmsh software was used to generate the mesh for the simulation. Gmsh is an open-source 3-D finite element grid generator with a build-in CAD engine and post-processor (Geuzaine & Remacle, 2009). It supports a variety of mesh types, including 1D, 2D, and 3D meshes, as well as structured and unstructured meshes. The *.geo* script used to create and mesh the geometry is provided in APPENDIX C.


Figure 3.10: Simplified geometry after meshing in Gmsh.



Figure 3.11: Actual geometry after meshing in Gmsh.

3.8.2 Boundary Id Assignation

The boundary id section involved assigning the appropriate boundary id to the solid model, to apply pressure and fixity constraints to the model during subsequent stages of the study. Boundary ids were to be applied in the form of physical ids in Gmsh. But the assignment of physical ids to the model in itself was not successful in this study as it assigned only geometric ids to the geometrical entities. So, the physical ids needed to be assigned manually. The meshed model being collection of large number of nodes and elements, it was not possible to do manually. So, a custom python script was made which assigns element with physical id which is unique for each geometric ids. Later on, Boundary conditions were applied specifically selecting those physical id's then taken as boundary id. The python script used in this step is provided in APPENDIX D.

3.8.3 Mesh Ordering

During the meshing process, the generated mesh was unstructured mesh of smaller elements that accurately represented the behavior of the geometry under different loads and conditions. However, to effectively perform the calculations using C++ code, it was necessary to rearrange these elements in a specific order generally called structured mesh. So, a C++ script, tethex (martemyev, 2013) was used to rearrange the mesh and convert tetrahedral elements to hexahedral elements that allowed our C++ code to efficiently perform the necessary calculations for stress and deformation analysis.

3.8.4 Simulation

To obtain displacement and stress, simulations of each CAD model of the Medical oxygen cylinder was run on C++ code, which was based on the deal.ii library. For simple geometries, simple program utilizing the shared memory system was successful. However, for actual cylinder CAD model, this program failed to converge due to the lack of enough memory. To this end,the distributed memory system using MPI into the program was incorporated. Nevertheless, stress calculation part could not be included into this code. Thus, only displacement in case of real cylinder was computed. The simulation part was done for three levels of geometry: Actual cylinder, Simplified cylinder and Hollow cylinder. For hollow cylinder (only cylindrical section), number of elements being comparatively small, both stresses and displacements were calculated. But for simplified and actual cylinder only displacements were calculated. We simulated our code for following material properties:

- 34Mn2V ($\lambda = 106.3 \ GPa, \ \mu = 71.154 \ GPa$)
- 34CrMo₄ ($\lambda = 105.44 \ GPa, \ \mu = 76.356 \ GPa$)
- 37MnSi5 ($\lambda = 118.84 \ GPa, \ \mu = 79 \ GPa$)

The boundary conditions applied in the simulation model included a fixed bottom surface and a pressure of 150 bar on the internal surfaces. The fixed bottom surface was implemented to prevent any movement or displacement of the system, while the 150 bar (15MPa) pressure on the internal surfaces provided a realistic representation of the operating conditions.

In this way, a number of simulations were conducted in our program. For deflection, C++ codes incorporating both shared memory system and distributed memory were able to be developed. However, for stress calculation, only shared memory system was used on a simple code. These simulations allowed to accurately model the behavior of the cylinder under different loads and conditions, and provided detailed information on its structural integrity and performance. The code developed for simulation are provided in APPENDIX B. First section of appendix gives code for stress and deformation calculation using shared

memory only and second section of appendix is about calculation of deformation by MPI.

3.8.5 Visualization

In order to visualize the simulation results, an open-source data visualization software, ParaView was used

3.9 Parametrization

The geometry of model was varied by adjusting the thickness of the cylinder, as well as testing the impact of different material properties on maximum hoop stress and maximum deformation. By simulating the model with these varying parameters, ability to better understanding of how changes in geometry and materials impacted the overall performance and safety of the Medical oxygen cylinder. These simulations allowed to optimize the design of the cylinder and ensure that it met all necessary performance and safety standards.

3.10 Verification and Validation

In the verification and validation section, results from the program simulation and theoretical calculations were compared and contrasted. In order to compare the results, the deformation and stress in the mid-section of the cylinder were taken into consideration. To further ensure the correctness of program, ANSYS simulation was conducted side-byside. After a number of iterations and update, the results and the program were verified and validated.

3.11 Conclusion

After the careful examination of simulation results, conclusions were drawn about the strength and safety of the MOC for different materials and thicknesses. With this, documentation of the project was proceeded.

CHAPTER FOUR: RESULTS AND DISCUSSION

4.1 Hollow Cylinder

Hollow cylinder of different thickness i.e., 5.4, 5.5 and 5.6mm are assigned different materials and simulated in code as well as in ANSYS Mechanical, and following results were obtained. Further error on Hoop stress was calculated for deal.ii simulation with comparison to analytical calculation.

		Theoritical	Ansys		Deal.ii		% Error
Thickness	Material	Hoop Stress (MPa)	Hoop Stress (MPa)	Max Disp. (mm)	Hoop Stress (MPa)	Max Disp. (mm)	Hoop Stress
5.4	34Mn2V	322.2222	326.2764	0.6049	320.01	0.604	0.6859
5.4	34CrMo4	322.2222	325.6583	0.5511	320.15	0.550	0.6431
5.4	37MnSi5	322.2222	325.4323	0.5496	320.15	0.544	0.6440
5.5	34Mn2V	316.3636	318.4060	0.5932	313.90	0.592	0.7787
5.5	34CrMo4	316.3636	318.7604	0.5403	314.03	0.539	0.7376
5.5	37MnSi5	316.3636	318.3780	0.5388	314.03	0.534	0.7364
5.6	34Mn2V	310.7143	313.2900	0.5817	308.00	0.581	0.8749
5.6	34CrMo4	310.7143	313.3700	0.5299	308.11	0.529	0.8382
5.6	37MnSi5	310.7143	313.2500	0.2837	308.13	0.523	0.8327

Table 4.1: Comparison of simulation results for Hollow Cylinder

From the above table, error in Hoop stress is calculated by deal.ii simulation is under one percent (average error is 0.75 %) in comparison with theoretical calculation. Also the results from the deal.ii program has a close match with the result obtained with ANSYS simulations. The analysis revealed that our calculations were within a small margin of error compared to the commercial software, indicating the reliability of our methodology. This comparison of results of deal.ii based simulation to analytical calculation and AN-SYS further provided a rigid belief that the algorithm used in this project work produces accurate results. It is also expected that the code works for all similar kind of geometrical interfaces as well as the code can be manipulated to work for different geometries.

Also. the deal.ii based code provided can be accessed and simulated for thin cylindrical geometries for various materials to understand further about the influence of materials to the deformation and stress so that a step toward optimization of material can be initiated. To better understand the relationship between material as well as geometric properties, it was plotted in figures 4.1 and 4.2.



Figure 4.1: Hoop stress vs thickness for hollow cylinder



Figure 4.2: Deformation vs thickness for hollow cylinder

From the plot of thickness and hoop stress, it is clear that the stress is independent of choice of material and decreases with increase in thickness which perfectly aligned with theory that the stresses in thin wall cylinder is irrespective of material but is inversely proportional to thickness of section. Similarly, when the deformation vs thickness plot is analyzed it was found that the deformation also decreases with increase in thickness of the wall. When both of plots are generalized explicitly, a idea of relationship between hoop stress and deformation can be pictured mentally. Simply the relation of stress seems linearly proportional with deformation, this fact can be used when we have deformation to compare but no stresses values are provided. From the deformation vs thickness plot 4.2, the material 34Mn2V suffer from largest deformation whilst 37MnSi5 undergoes through the smallest deformation for the same thickness, and loading conditions, so the material 37MnSi5 could be more reliable to use for production of thin wall cylinders whose functionality are to provide a high pressure resistant work.

4.2 Simplified Cylinder

For the computational ease, simplified oxygen cylinder was simulated under different material and geometrical properties. The comparison of maximum deformations obtained from deal.ii and ANSYS simulation is shown in table 4.2 below:

Thicknose	Matorial	deal.ii	ANSYS	% difference	
THICKNESS	Wateria	Maximum Disp.	Maximum Disp.	∞ unrerence	
5.4	34Mn2V	0.5415	0.5641	4.007	
5.4	34CrMo4	0.5276	0.5488	3.868	
5.4	37Mn\$i5	0.4869	0.4996	2.542	
5.5	34Mn2V	0.5282	0.5184	1.890	
5.5	34CrMo4	0.5147	0.5053	1.855	
5.5	37MnSi5	0.4750	0.4589	3.518	
5.6	34Mn2V	0.5152	0.5362	3.907	
5.6	34CrMo4	0.5022	0.5219	3.775	
5.6	37MnSi5	0.4633	0.4749	2.429	

Table 4.2: Comparison of max. deformation (in mm) for simplified cylinder

It is to be noted that the % difference is obtained from dividing the difference by the ANSYS result in the table 4.2. It is evident that the results by open source simulation and ANSYS simulation are in close proximity. Moreover, they also agree on the distribution of deformation and location of maximum deformation on cylinder body which is inferred from the figures 4.3 and 4.4. Maximum deformation appears on the region of top head near the neck section. Thus, it can be concluded that the consideration of neck and head region is very crucial in designing a oxygen or pressurized gas cylinder.



Figure 4.3: Displacement result from ANSYS(34Mn2V, 5.5mm)



Figure 4.4: Displacement result from deal.ii (34Mn2V, 5.5mm)



Figure 4.5: Deformation vs thickness for simplified cylinder

The maximum deformation vs thickness plot for different materials as shown in figure 4.5 suggest that the maximum deformation decreases for increasing thickness for all materials, also the correlation between maximum deformation and thickness seems linear as in the case of hollow cylinder. In sum up, it is found that cylinder made up of material 34Mn04 with thickness 5.6 mm is most safe with least deformation while that of 37MnSi5 with thickness 5.4 mm is relatively least safe.

4.3 Actual Cylinder

Actual model of oxygen cylinder was simulated under different material conditions for a nominal thickness of 6mm.The comparison for maximum deformation obtained from deal.ii and ANSYS Simulation is shown in Table below:

Material	ANSYS	deal.ii	% difference	
34Mn2V	0.42601	0.44395	4.211	
34CrMo4	0.41752	0.43151	3.351	
37MnSi5	0.37625	0.39868	5.961	

Table 4.3: Comparison of deformation (in mm) of actual cylinder

From the table, it is again found that the maximum deformation by deal.ii simulation and ANSYS simulation are quiet similar(within 6% difference range) as well as also the distribution of deformation and location of maximum deformation on cylinder body are similar for both which are shown in figures 4.6 and 4.7.



Figure 4.6: Displacement result from ANSYS (37MnSi5)



Figure 4.7: Displacement result from deal.ii (37MnSi5)

The results for other materials are placed in APPENDIX F. In all of the results the maximum deformation obtained was about 0.5mm which is very insignificant as compared to overall body dimension. This indicated that MOC is safe in 150 bar pressure . Nevertheless, in order to predict further about failure or safety we need to analyse the maximum and Von-misses stresses. But for actual real model, stress could not be calculated so, this remains as a part of shortcoming of this project. This was due to limit of computational power and time available. It also hampered the computation for actual oxygen cylinder model for different thicknesses. So, simulation was done for only one thickness for deformation whilst assigning different material properties.

Although the stress was not calculated in actual MOC model and simplified Model, it was done for hollow cylinder model which is a section of oxygen cylinder itself i.e., dimensions of cylinder are similar and just head and bottom profile are removed. From the comparison of simulation results in case of hollow cylinder, the program was verified. It was evident that the deformation was quiet similar for simplified and hollow cylinder and a little bit less in actual MOC. Also, hoop stress for all of them were found to be almost identical whilst the axial stress is very less in hollow cylinder as compared with that of actual and simplified MOC. In sum up, hoop stress was in the range of 300-350 Mpa and the axial stress was in the range of 130-180 Mpa manifesting that for thin-wall cylinder axial stress is half of the hoop stress. From these analyses, it was concluded that none of the geometry suffer maximum stress greater than 400 Mpa. Since, all the materials have Yield Stress of about 450 Mpa, this assured the safety of the vessel. From the results, it was inferred that MOCs are safe under working pressure of 150 bar.

CHAPTER FIVE: CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusion

In conclusion, this project successfully demonstrated the use of a deal.ii based program for analyzing stress and deformation on an oxygen cylinder. The methodology involved verification of the program by comparing the results with that of ANSYS and theoretical calculations in case of simple hollow cylinder in which maximum error was found to be 0.875 %. After that, the program was used to simulate the actual cylinder in which maximum deformation in the cylinder was found to be 0.44395 mm in case of 34Mn2V material with thickness 5.6 mm. For different materials, the simulation was repeated.

The findings of this project have important implications for the field of engineering and materials science, particularly for the design of safer and more efficient oxygen cylinders. The ability to accurately predict the stress and deformation on the cylinder can help engineers better understand the behavior of these cylinders under different conditions, such as changes in pressure or temperature, and design them accordingly. Additionally, the use of a deal.ii-based code for such simulations can be a valuable tool for researchers and engineers in various industries.

However, it is important to note that this project is not without its limitations. The simulations were conducted under certain assumptions and simplifications, and it is possible that more complex real-world scenarios may yield different results. Furthermore, the use of different simulation tools and software may also yield different results, and further studies can be conducted to compare the performance of different simulation tools for this application.

In conclusion, this project successfully demonstrated the use of a deal.ii-based code for analyzing stress and deformation on an oxygen cylinder. The results showed that the code was a reliable tool for simulating stress and deformation on the cylinder, and the findings have important implications for the field of engineering and materials science. Future studies can build upon these findings and further investigate the performance of different simulation tools and software for this application.

5.2 Recommendation

From the perspective of entire project work, concluding remarks and literature review, some recommendations were put forward to researchers, students or those who are interested in Finite analysis, Oxygen Cylinder, Open Source Implementation. These recommendation can encourage readers to further investigate and build upon the findings of this study, ultimately contributing to a better understanding of the behavior of oxygen cylinders and their optimization for use in various industries. The recommendations are:

1. Use of alternative simulation tools:

While the deal.ii-based code was found to be a reliable tool for simulating stress and deformation on an oxygen cylinder, it may be worthwhile to investigate the use of other simulation tools and software for this application. This can help validate the results obtained from the current simulation and provide a more comprehensive understanding of the behavior of oxygen cylinders under different conditions.

2. Conducting experimental studies:

While simulations can provide valuable insights into the behavior of oxygen cylinders, they may not always accurately represent real-world scenarios. Therefore, it may be worthwhile to conduct experimental studies to validate the findings obtained from the simulations and provide more accurate data for future analysis.

3. Optimization of cylinder design:

The insights obtained from this study can be used to optimize the design of oxygen cylinders, making them safer and more efficient. Future studies can focus on incorporating different design features to enhance the performance of these cylinders under different conditions.

4. Investigation of other cylinder materials:

This study focused on analyzing stress and deformation on an oxygen cylinder made from a specific set materials. However, it may be worthwhile to investigate the behavior of cylinders made from other materials like aluminium alloy, as the findings may differ depending on the material properties.

5. Further investigation into the effect of environmental conditions:

The simulations conducted in this study assumed certain environmental conditions (Standard normal temperature and pressure). Future studies can investigate the effect of changes in environmental conditions such as temperature, humidity, and pressure on the stress and deformation of oxygen cylinders.

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APPENDIX A: MATHEMATICAL DERIVATION

Strong Form

Suppose we have a three-dimensional solid elastic body. The body is subjected to body forces \vec{b} acting in the domain denoted by Ω and traction \vec{t} on the boundary denoted by Γ_t with displacements \vec{d} assigned on the boundary denoted by Γ_d as shown in figure A.1 below.



Figure A.1: Solid Body

To derive the governing equation, we consider a small cuboid element inside the domain. The stresses and body forces on the cuboid are acting as shown in figure A.2.



Figure A.2: Cuboid element

We can obtain three equilibrium equations for the element,

$$\{ (\sigma_{xx} + \Delta \sigma_{xx}) - \sigma_{xx} \} \cdot \Delta y \Delta z + \{ (\sigma_{xy} + \Delta \sigma_{xy}) - \sigma_{xy} \} \cdot \Delta x \Delta z + \\ \{ (\sigma_{xz} + \Delta \sigma_{xz}) - \sigma_{xz} \} \cdot \Delta x \Delta y + b_x \cdot \Delta x \Delta y \Delta z = 0 \\ \{ (\sigma_{yx} + \Delta \sigma_{yx}) - \sigma_{yx} \} \cdot \Delta y \Delta z + \{ (\sigma_{yy} + \Delta \sigma_{yy}) - \sigma_{yy} \} \cdot \Delta x \Delta z + \\ \{ (\sigma_{yz} + \Delta \sigma_{yz}) - \sigma_{yz} \} \cdot \Delta x \Delta y + b_y \cdot \Delta x \Delta y \Delta z = 0 \\ \{ (\sigma_{zx} + \Delta \sigma_{zx}) - \sigma_{zx} \} \cdot \Delta y \Delta z + \{ (\sigma_{zy} + \Delta \sigma_{zy}) - \sigma_{zy} \} \cdot \Delta x \Delta z + \\ \{ (\sigma_{zz} + \Delta \sigma_{zz}) - \sigma_{zz} \} \cdot \Delta x \Delta y + b_z \cdot \Delta x \Delta y \Delta z = 0 \\$$

Expanding and then dividing each equation by the volume of the element, i.e. $\Delta x \Delta y \Delta z$,

$$\frac{\Delta\sigma_{xx}}{\Delta x} + \frac{\Delta\sigma_{xy}}{\Delta y} + \frac{\Delta\sigma_{xz}}{\Delta z} + b_x = 0$$
$$\frac{\Delta\sigma_{yx}}{\Delta x} + \frac{\Delta\sigma_{yy}}{\Delta y} + \frac{\Delta\sigma_{yz}}{\Delta z} + b_y = 0$$
$$\frac{\Delta\sigma_{zx}}{\Delta x} + \frac{\Delta\sigma_{zy}}{\Delta y} + \frac{\Delta\sigma_{zz}}{\Delta z} + b_z = 0$$

Now, if we take the limit i.e. $\lim_{\Delta x\to 0}$, $\lim_{\Delta y\to 0}$, and $\lim_{\Delta z\to 0}$, we get,

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + b_x = 0$$
$$\frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + b_y = 0$$
$$\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + b_z = 0$$

In vector notation,

$$\vec{\nabla} \cdot \vec{\sigma}_x + b_x = 0$$
$$\vec{\nabla} \cdot \vec{\sigma}_y + b_y = 0$$
$$\vec{\nabla} \cdot \vec{\sigma}_z + b_z = 0$$

which can be written as,

$$\operatorname{div}(\boldsymbol{\sigma}(\vec{u})) + \vec{b} = 0$$

This is the governing equation for the domain. We need to get the governing equation for entire closed domain, i.e. $\bar{\Omega} = \Omega \cup \Gamma$.

For the boundary with traction, consider a tetrahedral element with the diagonal face aligning with the boundary surface Γ_t . The stresses and prescribed traction are acting on the element as shown in figure A.3. Before proceeding with derivation, we consider the vector surface on which traction acts, is $\Delta \vec{S}$ with direction cosines n_x, n_y , and n_z such that,

$$\Delta S_x = \Delta S \cdot n_x$$

$$\Delta S_y = \Delta S \cdot n_y$$

$$\Delta S_z = \Delta S \cdot n_z, \text{ where, } \Delta S = |\Delta \vec{S}|$$



Figure A.3: Tetrahedral element

Now, for tetrahedral element, three equilibrium equations are as follows,

$$-\sigma_{xx} \cdot \Delta S_x - \sigma_{xy} \cdot \Delta S_y - \sigma_{xz} \cdot \Delta S_z + t_x \cdot \Delta S = 0$$

$$-\sigma_{yx} \cdot \Delta S_x - \sigma_{yy} \cdot \Delta S_y - \sigma_{yz} \cdot \Delta S_z + t_y \cdot \Delta S = 0$$

$$-\sigma_{zx} \cdot \Delta S_x - \sigma_{zy} \cdot \Delta S_y - \sigma_{zz} \cdot \Delta S_z + t_z \cdot \Delta S = 0$$

Dividing each term by ΔS , we get,

$$-\sigma_{xx} \cdot \frac{\Delta S_x}{\Delta S} - \sigma_{xy} \cdot \frac{\Delta S_y}{\Delta S} - \sigma_{xz} \cdot \frac{\Delta S_z}{\Delta S} + t_x \cdot = 0$$

$$-\sigma_{yx} \cdot \frac{\Delta S_x}{\Delta S} - \sigma_{yy} \cdot \frac{\Delta S_y}{\Delta S} - \sigma_{yz} \cdot \frac{\Delta S_z}{\Delta S} + t_y \cdot = 0$$

$$-\sigma_{zx} \cdot \frac{\Delta S_x}{\Delta S} - \sigma_{zy} \cdot \frac{\Delta S_y}{\Delta S} - \sigma_{zz} \cdot \frac{\Delta S_z}{\Delta S} + t_z \cdot = 0$$

Substituting the expressions of direction cosines, we get,

$$-\sigma_{xx} \cdot n_x - \sigma_{xy} \cdot n_y - \sigma_{xz} \cdot n_z + t_x = 0$$

$$-\sigma_{yx} \cdot n_x - \sigma_{yy} \cdot n_y - \sigma_{yz} \cdot n_z + t_y = 0$$

$$-\sigma_{zx} \cdot n_x - \sigma_{zy} \cdot n_y - \sigma_{zz} \cdot n_z + t_z = 0$$

Now, rearranging and writing each equation in vector notation,

$$ec{\sigma}_x \cdot ec{n} = t_x$$
 $ec{\sigma}_y \cdot ec{n} = t_y$
 $ec{\sigma}_z \cdot ec{n} = t_z$

In more compact form,

$$\boldsymbol{\sigma}(\vec{u})\boldsymbol{\cdot}\vec{n}=\vec{t}$$

Finally, for boundary Γ_d , where displacements are specified, following relation can be written,

$$u_x = d_x$$
$$u_y = d_y$$
$$u_z = d_z$$

In vector notation,

 $\vec{u}=\vec{d}$

Finally, the strong form for the small displacement three-dimensional linear elasticity problem with Neumann and Dirichlet boundary conditions is,

Given $\vec{b}: \Omega \to \mathbb{R}^3$, $\vec{d}: \Gamma_d \to \mathbb{R}^3$, $\vec{t}: \Gamma_t \to \mathbb{R}^3$, find $\vec{u}: \bar{\Omega} \to \mathbb{R}^3$ such that,

$$-\operatorname{div}(\boldsymbol{\sigma}(\vec{u})) = \vec{b} \text{ in } \Omega$$
$$\vec{u} = \vec{d} \text{ on } \Gamma_d$$
$$\boldsymbol{\sigma}(\vec{u}) \cdot \vec{n} = \vec{t} \text{ on } \Gamma_t$$

Weak Form

In order to be able to work with Finite Element Method, we need to obtain the weak form of the governing equations derived. We take the vector product of strong form with the test function vector \vec{v} belonging to the Hilbert Space **H** and integrate the equation for entire domain, we get,

$$-\int_{\Omega} \operatorname{div}(\boldsymbol{\sigma}(\vec{u})) \cdot \vec{v} = \int_{\Omega} \vec{b} \cdot \vec{v}$$
$$\int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} - \int_{\Gamma} (\boldsymbol{\sigma}(\vec{u}) \cdot \vec{n}) \cdot \vec{v} = \int_{\Omega} \vec{b} \cdot \vec{v}$$
$$\int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} - \int_{\Gamma_d} (\boldsymbol{\sigma}(\vec{u}) \cdot \vec{n}) \cdot \vec{v} - \int_{\Gamma_t} (\boldsymbol{\sigma}(\vec{u}) \cdot \vec{n}) \cdot \vec{v} = \int_{\Omega} \vec{b} \cdot \vec{v}$$
$$\int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} - \int_{\Gamma_t} \vec{t} \cdot \vec{v} = \int_{\Omega} \vec{b} \cdot \vec{v}$$
$$\int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} = \int_{\Gamma_t} \vec{t} \cdot \vec{v} + \int_{\Omega} \vec{b} \cdot \vec{v}$$

In bi-linear form,

$$a(\vec{u}, \vec{v}) = (\vec{t}, \vec{v})_{\Gamma_t} + (\vec{b}, \vec{v})$$

In this way, weak form of the problem is,

Given $\vec{b}: \Omega \to \mathbb{R}^3$, $\vec{d}: \Gamma_d \to \mathbb{R}^3$, $\vec{t}: \Gamma_t \to \mathbb{R}^3$, find $\vec{u}: \bar{\Omega} \to \mathbb{R}^3$ such that for $\vec{v} \in \mathbf{H}$,

$$a(\vec{u}, \vec{v}) = (\vec{t}, \vec{v})_{\Gamma_t} + (\vec{b}, \vec{v}) \text{ in } \Omega$$

Note:

$$\begin{aligned} a(\vec{u}, \vec{v}) &= \int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \nabla \vec{v} \\ &= \int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \varepsilon(\vec{v}) \\ &= \int_{\Omega} (\lambda (\operatorname{div} \vec{u}) \mathbf{I} + 2\mu\varepsilon(\vec{u})) : \varepsilon(\vec{v}) \\ &= \int_{\Omega} \lambda (\operatorname{div} \vec{u}) \mathbf{I} : \varepsilon(\vec{v}) + 2\mu\varepsilon(\vec{u}) : \varepsilon(\vec{v}) \\ &= \int_{\Omega} \lambda (\operatorname{div} \vec{u}) (\operatorname{div} \vec{v}) + 2\mu\varepsilon(\vec{u}) : \varepsilon(\vec{v}) \end{aligned}$$
(Cinatl, 2018)

Finite Element Approximation

Since, working with infinite-dimensional solution is difficult and not feasible and so on, we take the subset of the infinite-dimensional Hilbert space, i.e., we consider finite numbers of nodes. The domain is discretized into small finite numbers of elements. This discretized domain is called mesh. Thus, considering N nodes, vector-valued approximated solution and test function (global) are re-written as,

$$\vec{u} \approx \vec{u^{h}} = \begin{cases} u_{x}^{h} = \sum_{i=0}^{N} U_{ix}\phi_{i}(\mathbf{x}) \\ u_{y}^{h} = \sum_{j=0}^{N} U_{jy}\phi_{j}(\mathbf{y}) \\ u_{z}^{h} = \sum_{k=0}^{N} U_{ky}\phi_{k}(\mathbf{z}) \end{cases} \text{ and } \vec{v} \approx \vec{v^{h}} = \begin{cases} v_{x}^{h} = \sum_{i=0}^{N} V_{ix}\phi_{i}(\mathbf{x}) \\ v_{y}^{h} = \sum_{j=0}^{N} V_{jy}\phi_{j}(\mathbf{y}) \\ v_{z}^{h} = \sum_{k=0}^{N} V_{kz}\phi_{k}(\mathbf{z}) \end{cases}$$

In deal.ii, this is achieved in following manner,, We express vector-valued basis function as,

$$\Phi_i(\mathbf{x}) = \phi_i(\mathbf{x}) \ \mathbf{e}_{\operatorname{comp}(i)}$$

Thus, vector-valued test function can be represented as,

$$\vec{v^h} = \begin{bmatrix} \phi_0 & 0 & 0 & \phi_3 & 0 & 0 & \phi_6 & 0 & \cdots & 0 \\ 0 & \phi_1 & 0 & 0 & \phi_4 & 0 & 0 & \phi_7 & \cdots & 0 \\ 0 & 0 & \phi_2 & 0 & 0 & \phi_5 & 0 & 0 & \cdots & \phi_{3N-1} \end{bmatrix} * \begin{cases} V_0 \\ V_1 \\ V_2 \\ \vdots \\ V_{3N-3} \\ V_{3N-2} \\ V_{3N-1} \end{cases}$$

Similarly, solution vector can be represented as,

$$\vec{u^{h}} = \begin{bmatrix} \phi_{0} & 0 & 0 & \phi_{3} & 0 & 0 & \phi_{6} & 0 & \cdots & 0\\ 0 & \phi_{1} & 0 & 0 & \phi_{4} & 0 & 0 & \phi_{7} & \cdots & 0\\ 0 & 0 & \phi_{2} & 0 & 0 & \phi_{5} & 0 & 0 & \cdots & \phi_{3N-1} \end{bmatrix} * \begin{cases} U_{0} \\ U_{1} \\ U_{2} \\ \vdots \\ U_{3N-3} \\ U_{3N-2} \\ U_{3N-1} \end{cases}$$

where, N is the number of nodes. It is to be noted that each consecutive set of three values

in the coefficient column vector represents vector displacement at the corresponding node. For example, the set (U_0, U_1, U_2) represents vector displacement at node 0. In sum up, the solution in deal.ii is approximated as ,

$$\vec{u}(\mathbf{x}) \approx \vec{u^h}(\mathbf{x}) = \sum_j \Phi_j(\mathbf{x}) U_j$$

Also, the test function is approximated as,

$$\vec{v}(\mathbf{x}) \approx \vec{v^h}(\mathbf{x}) = \sum_i \Phi_i(\mathbf{x}) \ V_i$$

Substituting these expressions, we get,

$$\begin{aligned} a(\vec{u}, \vec{v}) &\approx a(\vec{u^h}, \vec{v^h}) \\ &= \int_{\Omega} \lambda \left(\operatorname{div} \vec{u^h} \right) \left(\operatorname{div} \vec{v^h} \right) + 2\mu \varepsilon (\vec{u^h}) : \varepsilon (\vec{v^h}) \\ &= \lambda \int_{\Omega} \operatorname{div} \left(\sum_j \Phi_j U_j \right) \operatorname{div} \left(\sum_i \Phi_i V_i \right) + 2\mu \int_{\Omega} \varepsilon \left(\sum_j \Phi_j U_j \right) \varepsilon \left(\sum_i \Phi_i V_i \right) \\ &= \sum_i \sum_j \left[\lambda \int_{\Omega} (\operatorname{div} \Phi_i) (\operatorname{div} \Phi_j) + 2\mu \int_{\Omega} \varepsilon \left(\Phi_i \right) : \varepsilon \left(\Phi_j \right) \right] U_j V_i \end{aligned}$$

And,

$$\begin{aligned} (\vec{t}, \vec{v})_{\Gamma_t} &\approx (\vec{t}, \vec{v^h})_{\Gamma_t} \\ &= \int_{\Gamma_t} \vec{t} \cdot \sum_i \Phi_i V_i \\ &= \sum_i \left[\int_{\Gamma_t} \vec{t} \cdot \Phi_i \right] V_i \end{aligned}$$

Also,

$$\begin{array}{lll} (\vec{b}, \vec{v}) &\approx & (\vec{b}, \vec{v^h}) \\ &= & \int_{\Omega} \vec{b} \cdot \sum_i \Phi_i V_i \\ &= & \sum_i \left[\int_{\Omega} \vec{b} \cdot \Phi_i \right] V_i \end{array}$$

Finally, the approximated weak form becomes,

$$\begin{aligned} a(\vec{u^h}, \vec{v^h}) &= (\vec{t}, \vec{v^h})_{\Gamma_t} + (\vec{b}, \vec{v^h}) \\ \sum_i \sum_j \left[\lambda \int_{\Omega} (\operatorname{div} \Phi_i) (\operatorname{div} \Phi_j) + 2\mu \int_{\Omega} \varepsilon \left(\Phi_i \right) : \varepsilon \left(\Phi_j \right) \right] U_j V_i = \sum_i \left[\int_{\Gamma_t} \vec{t} \cdot \Phi_i \right] V_i + \sum_i \left[\int_{\Omega} \vec{b} \cdot \Phi_i \right] V_i \\ \sum_i \left[\sum_j \left[\lambda \int_{\Omega} (\operatorname{div} \Phi_i) (\operatorname{div} \Phi_j) + 2\mu \int_{\Omega} \varepsilon \left(\Phi_i \right) : \varepsilon \left(\Phi_j \right) \right] U_j \right] V_i = \sum_i \left[\left[\int_{\Gamma_t} \vec{t} \cdot \Phi_i \right] + \left[\int_{\Omega} \vec{b} \cdot \Phi_i \right] \right] V_i \\ \sum_i \left[\sum_j \left[\lambda \int_{\Omega} (\operatorname{div} \Phi_i) (\operatorname{div} \Phi_j) + 2\mu \int_{\Omega} \varepsilon \left(\Phi_i \right) : \varepsilon \left(\Phi_j \right) \right] U_j = \left[\int_{\Gamma_t} \vec{t} \cdot \Phi_i \right] + \left[\int_{\Omega} \vec{b} \cdot \Phi_i \right] \right] V_i \end{aligned}$$

By definition, V_i cannot be zero for all j from 0 to 3N-1, thus column vector $\{V\}$ cannot be zero. Therefore, for i = 0 to 3N - 1, the expression inside the big brackets must be valid, i.e.,

for i = 0 to 3N - 1,

$$\sum_{j} A_{ij} U_j = F_i$$

In matrix form,

AU = F

Where,

$$\begin{split} A_{ij} &= \lambda \int_{\Omega} (\operatorname{div} \Phi_{i}) (\operatorname{div} \Phi_{j}) + 2\mu \int_{\Omega} \varepsilon (\Phi_{i}) : \varepsilon (\Phi_{j}) \\ &= \lambda \sum_{k,l} (\partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{\Omega} + 2\mu * \left(\frac{1}{2} \left(\sum_{k,l} (\partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{\Omega} + \sum_{k,l} (\partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{\Omega} \right) \right) \\ &= \lambda \sum_{k,l} (\partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{\Omega} + \mu \left(\sum_{k,l} (\partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{\Omega} + \sum_{k,l} (\partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{\Omega} \right) \\ &= \sum_{k,l} (\lambda \partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{\Omega} + \sum_{k,l} (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{\Omega} + \sum_{k,l} (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{\Omega} \\ &= \sum_{k,l} \{ (\lambda \partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{\Omega} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{\Omega} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{\Omega} \} \end{split}$$

here, l and k run through 0 to dim-1. Similarly,

$$F_{i} = \int_{\Gamma_{t}} \vec{t} \cdot \Phi_{i} + \int_{\Omega} \vec{b} \cdot \Phi_{i}$$

$$= \sum_{l} (t_{l}, (\Phi_{i})_{l})_{\Gamma_{t}} + \sum_{l} (b_{l}, (\Phi_{i})_{l})_{\Omega}$$

$$= \sum_{l} \{ (t_{l}, (\Phi_{i})_{l})_{\Gamma_{t}} + (b_{l}, (\Phi_{i})_{l})_{\Omega} \}$$

Now, for each cell $K \in T \approx \Omega$ and the cell face $X \in T_b \approx \Gamma_t$, local cell matrix and right hand side vectors are given by,

$$\begin{aligned} A_{ij}^{K} &= \sum_{k,l} \{ (\lambda \partial_{l}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{k})_{K} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{k}(\Phi_{j})_{l})_{K} + (\mu \partial_{k}(\Phi_{i})_{l}, \partial_{l}(\Phi_{j})_{k})_{K} \} \\ &= (\lambda \partial_{\text{comp}(i)} \phi_{i}, \partial_{\text{comp}(j)} \phi_{j})_{K} + \sum_{l} (\mu \partial_{l} \phi_{i}, \partial_{l} \phi_{j})_{K} \ \delta_{\text{comp}(i),\text{comp}(j)} + (\mu \partial_{\text{comp}(j)} \phi_{i}, \partial_{\text{comp}(i)} \phi_{j})_{K} \\ &= (\lambda \partial_{\text{comp}(i)} \phi_{i}, \partial_{\text{comp}(j)} \phi_{j})_{K} + (\mu \nabla \phi_{i}, \nabla \phi_{j})_{K} \ \delta_{\text{comp}(i),\text{comp}(j)} + (\mu \partial_{\text{comp}(j)} \phi_{i}, \partial_{\text{comp}(i)} \phi_{j})_{K} \\ &= (\lambda \partial_{\text{comp}(i)} \phi_{i}, \partial_{\text{comp}(j)} \phi_{j})_{K} + (\mu \partial_{\text{comp}(j)} \phi_{i}, \partial_{\text{comp}(i)} \phi_{j})_{K} \ \delta_{\text{comp}(i),\text{comp}(j)} \\ &= (\lambda \partial_{\text{comp}(i)} \phi_{i}, \partial_{\text{comp}(j)} \phi_{j})_{K} + (\mu \partial_{\text{comp}(j)} \phi_{i}, \partial_{\text{comp}(i)} \phi_{j})_{K} \ \delta_{\text{comp}(i),\text{comp}(j)} \end{aligned}$$

It should be noted that for local cell matrix, i and j run through 0 to $3 \cdot n - 1$ where n is the no. of nodes on the cell.

And,

$$F_{i}^{K} = \sum_{l} \{ (t_{l}, (\Phi_{i})_{l})_{X} + (b_{l}, (\Phi_{i})_{l})_{K} \}$$

$$= \sum_{l} (t_{l}, (\Phi_{i})_{l})_{X} + \sum_{l} (b_{l}, \phi_{i}\delta_{l, \text{comp}(i)})_{K}$$

$$= (t_{\text{comp}(i)}, \phi_{i})_{X} + (b_{\text{comp}(i)}, \phi_{i})_{K}$$

Quadrature

Since integration on real cell is difficult, we use mapping to compute the integration. In this, we map the real cell to the reference cell using **Jacobian**,

Reference (parent) cell is just tri-unit cube. Since, the integral limits are from -1 to 1, now we can use Gauss Quadrature formula to calculate the integration numerically.

$$\begin{aligned} \left(\lambda\partial_{\mathrm{comp}(i)}\phi_{i},\partial_{\mathrm{comp}(j)}\phi_{j}\right)_{K} &\approx \sum_{q}\lambda\left(\partial_{\mathrm{comp}(i)}\phi_{i}(q)\right)\left(\partial_{\mathrm{comp}(j)}\phi_{j}(q)\right)\mathrm{JxW}(q) \\ &\mu\left(\partial_{\mathrm{comp}(j)}\phi_{i},\partial_{\mathrm{comp}(i)}\phi_{j}\right)_{K} &\approx \sum_{q}\mu\left(\partial_{\mathrm{comp}(j)}\phi_{i}(q)\right)\left(\partial_{\mathrm{comp}(i)}\phi_{j}(q)\right)\mathrm{JxW}(q) \\ &\left(\mu\nabla\phi_{i},\nabla\phi_{j}\right)_{K}\delta_{\mathrm{comp}(i),\mathrm{comp}(j)} &\approx \sum_{q}\mu\left(\nabla\phi_{i}(q)\nabla\phi_{j}(q)\right)_{K}\delta_{\mathrm{comp}(i),\mathrm{comp}(j)}\mathrm{JxW}(q) \\ &\left(t_{\mathrm{comp}(i)},\phi_{i}\right)_{K} &\approx \sum_{q}\left(t_{\mathrm{comp}(i)}\phi_{i}(q_{f})\right)\mathrm{JxW}(qf) \\ &\left(b_{\mathrm{comp}(i)},\phi_{i}\right)_{K} &\approx \sum_{q}\left(b_{\mathrm{comp}(i)}\phi_{i}(q)\right)\mathrm{JxW}(q) \end{aligned}$$

where, JxW(q) is the product of determinant of Jacobian and the weights corresponding to the quadrature point q.

In the problem, traction is that of pressure, i.e.,

$$\vec{t} = -P \cdot \vec{n}$$

where, P is the pressure acting on the surface and \vec{n} is the normal surface vector of the surface. Thus, traction is the pressure acting on the surface normally. Then,

$$\sum_{q_f} \left(t_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q) = \sum_{q_f} \left(-P \cdot n_{\operatorname{comp}(i)} \phi_i(q_f) \right) \operatorname{JxW}(q)$$

Substituting the expressions,

$$\begin{aligned} A_{ij}^{K} &= \sum_{q} \{ \lambda \left(\partial_{\operatorname{comp}(i)} \phi_{i}(q) \right) \left(\partial_{\operatorname{comp}(j)} \phi_{j}(q) \right) + \mu \left(\partial_{\operatorname{comp}(j)} \phi_{i}(q) \right) \left(\partial_{\operatorname{comp}(i)} \phi_{j}(q) \right) + \\ \mu \left(\nabla \phi_{i}(q) \right) \left(\nabla \phi_{j}(q) \right) \delta_{\operatorname{comp}(i),\operatorname{comp}(j)} \} \mathbf{J} \mathbf{x} \mathbf{W}(q) \end{aligned}$$

Also,

$$F_i^K = \sum_{q_f} \left(-P \cdot n_{\mathsf{comp}(i)} \phi_i(q_f) \right) \mathsf{JxW}(q_f) + \sum_{q} \left(b_{\mathsf{comp}(i)} \phi_i(q) \right) \mathsf{JxW}(q)$$

where q_f refers to the quadrature points on the face of the cell.

Stress Calculation

The constitutive relation between the stress and strain is,

$$\boldsymbol{\sigma}(\vec{u}) = \mathcal{C} : \varepsilon(\vec{u})$$

where, C is rank-4 coefficient(stress-strain) tensor, and $\varepsilon(\vec{u})$ is strain. For isotropic material, elements of coefficient tensor are given by,

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$$

where, δ_{ij} 's are Kronecker delta functions. And the strain is given by,

$$\epsilon(\vec{u})_{kl} = \frac{1}{2}(\partial_k \vec{u}_l + \partial_l \vec{u}_k)$$

In tensorial notation:

$$\varepsilon(\vec{u}) = \frac{1}{2} \left(\nabla \vec{u} + \left(\nabla \vec{u} \right)^T \right)$$

Stress transformation

Since, the formulation is worked on cartesian coordinate system, we need to transform the stress into polar coordinate system to obtain hoop and radial stresses.

For this, a transformation matrix is constructed,

$$\mathbf{P} = \begin{bmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{bmatrix}$$

where, $\theta = \arctan \frac{y}{x}$.

Therefore, if the stress in cartesian coordinate system is,

$$oldsymbol{\sigma}_{C} = egin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}$$

and stress in polar coordinate system is,

$$oldsymbol{\sigma}_P = egin{bmatrix} \sigma_{rr} & \sigma_{r heta} & \sigma_{rz} \ \sigma_{ heta r} & \sigma_{ heta heta} & \sigma_{ heta z} \ \sigma_{zr} & \sigma_{z heta} & \sigma_{zz} \end{bmatrix}$$

then, the transformation relation is given by,

$$\boldsymbol{\sigma}_P = [\mathbf{P}][\boldsymbol{\sigma}_C][\mathbf{P}]^T$$

Accessing the diagonal elements of σ_P gives the radial stress, hoop stress and axial stress respectively.

APPENDIX B: CODE FOR SIMULATION

Code For Deformation and Stress

```
#include <deal.II/base/symmetric tensor.h>
2 #include <deal.II/base/tensor.h>
3 #include<deal.II/base/timer.h>
4 #include <deal.II/base/quadrature_lib.h>
5 #include <deal.II/base/function.h>
6 #include <deal.II/base/tensor.h>
7 #include<deal.II/physics/transformations.h>
8 #include <deal.II/lac/vector.h>
9 #include <deal.II/lac/full matrix.h>
10 #include <deal.II/lac/sparse_matrix.h>
#include <deal.II/lac/dynamic_sparsity_pattern.h>
12 #include <deal.II/lac/solver cg.h>
13 #include <deal.II/lac/precondition.h>
14 #include <deal.II/lac/affine_constraints.h>
15 #include <deal.II/grid/tria.h>
16 #include <deal.II/grid/grid_generator.h>
17 #include <deal.II/grid/grid_refinement.h>
18 #include <deal.II/dofs/dof handler.h>
19 #include <deal.II/dofs/dof_tools.h>
20 #include <deal.II/fe/fe_values.h>
21 #include <deal.II/numerics/vector tools.h>
22 #include <deal.II/numerics/matrix_tools.h>
23 #include <deal.II/numerics/data_out.h>
24 #include <deal.II/numerics/error_estimator.h>
25 #include <deal.II/fe/fe_system.h>
26 #include <deal.II/fe/fe_q.h>
27 #include <fstream>
28 #include <iostream>
  #include <vector>
29
  #include <algorithm>
30
31
  namespace Program
32
  {
33
    using namespace dealii;
34
35
      template <int dim>
36
    SymmetricTensor<4, dim> get_stress_strain_tensor(const double lambda,
37
                                                const double mu)
38
    {
39
      SymmetricTensor<4, dim> tmp;
40
      for (unsigned int i = 0; i < dim; ++i)</pre>
41
        for (unsigned int j = 0; j < dim; ++j)</pre>
42
```

```
for (unsigned int k = 0; k < dim; ++k)</pre>
43
            for (unsigned int l = 0; l < dim; ++1)</pre>
44
               tmp[i][j][k][l] = (((i == k) && (j == 1) ? mu : 0.0) +
45
                                 ((i == 1) && (j == k) ? mu : 0.0) +
46
                                 ((i == j) && (k == 1) ? lambda : 0.0));
47
       return tmp;
48
     }
49
50
     template <int dim>
51
     inline SymmetricTensor<2, dim>
52
     get_strain(const std::vector<Tensor<1, dim>> &grad)
53
     {
54
       Assert(grad.size() == dim, ExcInternalError());
55
56
       SymmetricTensor<2, dim> strain;
57
       for (unsigned int i = 0; i < dim; ++i)</pre>
58
         strain[i][i] = grad[i][i];
59
60
       for (unsigned int i = 0; i < dim; ++i)</pre>
61
         for (unsigned int j = i + 1; j < dim; ++j)</pre>
62
           strain[i][j] = (grad[i][j] + grad[j][i]) / 2;
63
64
       return strain;
65
     }
66
     \ensuremath{//} to transform stress from cartesian to polar coordinate system
67
     template <int dim>
68
     inline SymmetricTensor<2,dim>
69
     cart_to_polar(const Point<dim> &point,
70
                                const SymmetricTensor<2,dim> &stressC)
71
     {
72
       const double theta = atan(point[1]/point[0]);
73
       const double sintheta = sin(theta);
74
       const double costheta = cos(theta);
75
76
       Tensor<2,dim> lambda({{ costheta, sintheta, 0},
77
                            { -sintheta, costheta, 0},
78
                            \{0, 0, 1\}\});
79
       SymmetricTensor<2,dim> stressP;
80
       for (unsigned int i = 0; i < 3; ++i) {</pre>
81
               for (unsigned int k = 0; k < 3; ++k) {</pre>
82
                double tmp2=0;
83
                for (unsigned int j = 0; j < 3; ++j) {</pre>
84
                  double tmp = 0;
85
                  for (unsigned int 1 = 0; 1 <3; ++1)</pre>
86
                    tmp += stressC[j][l]*lambda[k][l];
87
                  tmp2 += lambda[i][j]*tmp;
88
                }
89
```

```
stressP[i][k] = tmp2;
90
               }
91
     }
92
       return stressP;
93
     }
94
95
     template <int dim>
96
     class ElasticProblem
97
     {
98
     public:
99
       ElasticProblem();
100
       void run();
101
102
     private:
103
104
       void setup_system();
       void assemble_system();
105
       void solve();
106
       void stressCalc();
107
       void refine_grid();
108
       void output_results(const unsigned int cycle) const;
109
110
       Triangulation<dim> triangulation;
111
       DoFHandler<dim> dof_handler;
112
113
       FESystem<dim> fe;
114
115
       AffineConstraints<double> constraints;
116
117
       SparsityPattern sparsity_pattern;
118
       SparseMatrix<double> system_matrix;
119
120
       Vector<double> solution;
121
       Vector<double> system_rhs;
122
       std::vector<SymmetricTensor<2,dim>> stress;
123
       Vector<double> norm_of_stress;
124
125
       Vector<double> radial_stress;
126
       Vector<double> hoop_stress;
127
       Vector<double> axial_stress;
128
129
       Vector<double> residual;
130
       static const SymmetricTensor<4, dim> stress_strain_tensor;
131
       const QGauss<dim> quadrature_formula;
132
     };
133
134
     template <int dim>
135
     const SymmetricTensor<4, dim> ElasticProblem<dim>::stress_strain_tensor =
136
```

```
get_stress_strain_tensor<dim>(/*lambda = */ 12.232e10,
137
                                   /*mu = */ 7.e10);
138
     template <int dim>
139
     class BOdyForceValues : public Function<dim>
140
     {
141
     public:
142
       BOdyForceValues();
143
144
       virtual void vector_value(const Point<dim> &p,
145
                                Vector<double> & values) const override;
146
147
       virtual void
148
       vector_value_list(const std::vector<Point<dim>> &points,
149
                        std::vector<Vector<double>> & value_list) const override;
150
151
     };
152
153
     template <int dim>
154
     BOdyForceValues<dim>::BOdyForceValues()
155
       : Function<dim>(dim)
156
     {}
157
158
159
     template <int dim>
160
     inline void BOdyForceValues<dim>::vector_value(const Point<dim> & /*p*/,
161
                                            Vector<double> &values) const
162
     {
163
       Assert(values.size() == dim, ExcDimensionMismatch(values.size(), dim));
164
165
       const double g = 9.81;
166
       const double rho = 7850;
167
168
       values = 0;
169
       values(dim - 1) = -rho * g;
170
     }
171
172
173
174
     template <int dim>
175
     void BOdyForceValues<dim>::vector_value_list(
176
       const std::vector<Point<dim>> &points,
177
       std::vector<Vector<double>> & value_list) const
178
     {
179
       const unsigned int n_points = points.size();
180
181
       Assert(value_list.size() == n_points,
182
              ExcDimensionMismatch(value_list.size(), n_points));
183
```

184

```
for (unsigned int p = 0; p < n_points; ++p)</pre>
185
         BOdyForceValues<dim>::vector_value(points[p], value_list[p]);
186
      }
187
188
      template<int dim>
189
      class PressureBoundaryValues : public Function<dim>
190
      ſ
191
       public:
192
       PressureBoundaryValues(): Function<dim>(1)
193
       {}
194
195
        virtual double value(const Point<dim> & p,const unsigned int component = 0)
196
                                                                 const override;
197
198
      };
199
200
      template <int dim>
201
      double PressureBoundaryValues<dim>::value(const Point<dim> & /*p*/,
202
                                      const unsigned int /*component*/) const
203
      {
204
       return -1.5e07;
205
      }
206
207
208
      template <int dim>
209
      ElasticProblem<dim>::ElasticProblem()
210
        : dof_handler(triangulation)
211
        , fe(FE_Q<dim>(1), dim),quadrature_formula(fe.degree + 1)
212
      {}
213
214
215
216
      template <int dim>
217
      void ElasticProblem<dim>::setup_system()
218
      {
219
       dof_handler.distribute_dofs(fe);
220
        solution.reinit(dof_handler.n_dofs());
221
        system_rhs.reinit(dof_handler.n_dofs());
222
223
        constraints.clear();
224
       DoFTools::make_hanging_node_constraints(dof_handler, constraints);
225
       VectorTools::interpolate_boundary_values(dof_handler,
226
                                              Ο,
227
                                              Functions::ZeroFunction<dim>(dim),
228
                                               constraints);
229
        constraints.close();
230
```

231 DynamicSparsityPattern dsp(dof_handler.n_dofs(), dof_handler.n_dofs()); 232 DoFTools::make_sparsity_pattern(dof_handler, 233 dsp, 234 constraints, 235 /*keep_constrained_dofs = */ false); 236 sparsity_pattern.copy_from(dsp); 237 238 system_matrix.reinit(sparsity_pattern); 239 } 240 241 242 243 template <int dim> 244 void ElasticProblem<dim>::assemble_system() 245 { 246 QGauss<dim> quadrature_formula(fe.degree + 1); 247 248 QGauss<dim-1> face_quadrature_formula(fe.degree +1); 249 250 FEFaceValues<dim> fe_face_values(fe, 251 face_quadrature_formula, 252 update_values | update_normal_vectors| 253 update_quadrature_points | update_JxW_values); 254 255 const unsigned int n_face_q_points = face_quadrature_formula.size(); 256 257 FEValues<dim> fe_values(fe, 258 quadrature_formula, 259 update_values | update_gradients | 260 update_quadrature_points | update_JxW_values); 261 262 const unsigned int dofs_per_cell = fe.n_dofs_per_cell(); 263 const unsigned int n_q_points = quadrature_formula.size(); 264 265 FullMatrix<double> cell_matrix(dofs_per_cell, dofs_per_cell); 266 Vector<double> cell_rhs(dofs_per_cell); 267 268 std::vector<types::global_dof_index> local_dof_indices(dofs_per_cell); 269 270 std::vector<double> lambda_values(n_q_points); 271 std::vector<double> mu_values(n_q_points); 272 std::vector<double> pressure_values(n_face_q_points); 273 274 Functions::ConstantFunction<dim> lambda(12.232e10), mu(7.9e10); 275 276 BOdyForceValues<dim> gravity; 277

```
PressureBoundaryValues<dim> pressure_boundary;
278
279
        std::vector<Vector<double>> rhs_values(n_q_points,Vector<double>(dim));
280
281
        for (const auto &cell : dof_handler.active_cell_iterators())
282
          {
283
           cell_matrix = 0;
284
           cell_rhs = 0;
285
286
           fe_values.reinit(cell);
287
288
           lambda.value_list(fe_values.get_quadrature_points(), lambda_values);
289
           mu.value_list(fe_values.get_quadrature_points(), mu_values);
290
291
292
           gravity.vector_value_list(fe_values.get_quadrature_points(), rhs_values);
293
           for (const unsigned int i : fe_values.dof_indices())
294
             {
295
               const unsigned int component_i =
296
                 fe.system_to_component_index(i).first;
297
298
           for (const unsigned int j : fe_values.dof_indices())
299
                 {
300
                   const unsigned int component_j =
301
                     fe.system_to_component_index(j).first;
302
303
            for (const unsigned int q_point :
304
                        fe_values.quadrature_point_indices())
305
               {
306
               cell_matrix(i, j) +=
307
                   (
308
                   (fe_values.shape_grad(i, q_point)[component_i] * //d_comp(i)(phi_i(
309
                       \rightarrow q))
                   fe_values.shape_grad(j, q_point)[component_j] * //d_comp(j)(phi_j(q
310
                       \rightarrow ))
                   lambda_values[q_point]) //lambda
311
                   +
312
                   (fe_values.shape_grad(i, q_point)[component_j] * //d_comp(i)(phi_j(
313
                       \hookrightarrow q))
                   fe_values.shape_grad(j, q_point)[component_i] * //d_comp(j)(phi_i(q
314
                       \rightarrow ))
                   mu_values[q_point]) //mu
315
                   + //
316
                   ((component_i == component_j) ? //for Kronecker delta
317
                   (fe_values.shape_grad(i, q_point) * //grad(phi_i(q))
318
                   fe_values.shape_grad(j, q_point) * //grad(phi_i(q))
319
                   mu_values[q_point]) : //mu
320
```

```
0)
321
                           ) *
322
                   fe_values.JxW(q_point); //JxW(q)
323
                     }
324
                 }
325
             }
326
327
           for (const unsigned int i : fe_values.dof_indices())
328
             {
329
               const unsigned int component_i =
330
                 fe.system_to_component_index(i).first;
331
332
               for (const unsigned int q_point :
333
                    fe_values.quadrature_point_indices())
334
                 cell_rhs(i) += rhs_values[q_point][component_i]* //b_comp(i)
335
                               fe_values.shape_value(i, q_point)* //phi_i(q)
336
                               fe_values.JxW(q_point); //JxW(q)
337
             }
338
339
        for(unsigned int face_number =0;
340
                             face_number < GeometryInfo<dim> :: faces_per_cell;
341
                           ++face_number)
342
             {
343
        if((cell->face(face_number)->at_boundary()) &&
344
                           (cell->face(face_number)->boundary_id()== 2))
345
               {
346
                 fe_face_values.reinit(cell,face_number);
347
                 pressure_boundary.value_list(fe_face_values.get_quadrature_points(),
348
                                                                pressure_values);
349
350
            for(unsigned int i=0; i<dofs_per_cell; ++i)</pre>
351
               {
352
                const unsigned int component_i =
353
                      fe.system_to_component_index(i).first;
354
            for(const unsigned int q_index : fe_face_values.quadrature_point_indices
355
                 \rightarrow ())
               {
356
             cell_rhs(i) += (pressure_values[q_index] *
357
                          fe_face_values.normal_vector(q_index)[component_i]) * //p*
358
                               → vec(n)
                           fe_face_values.shape_value(i,q_index) * //phi_i(q)
359
                           fe_face_values.JxW(q_index); //JxW(q)
360
                   }
361
                  }
362
               }
363
             }
364
365
```

```
cell->get_dof_indices(local_dof_indices);
366
           constraints.distribute_local_to_global(
367
             cell_matrix, cell_rhs, local_dof_indices, system_matrix, system_rhs);
368
         }
369
     }
370
371
372
373
374
     template <int dim>
375
     void ElasticProblem<dim>::solve()
376
     {
377
       SolverControl solver_control(3e3, 1e-2);
378
        SolverCG<Vector<double>> cg(solver_control);
379
380
        PreconditionJacobi<SparseMatrix<double>> preconditioner;
381
       preconditioner.initialize(system_matrix);
382
383
        cg.solve(system_matrix, solution, system_rhs, preconditioner);
384
        stressCalc();
385
386
       residual.reinit(dof_handler.n_dofs());
387
        system_matrix.vmult(residual, solution);
388
        residual -= system_rhs;
389
        std::cout << "Iterations required : "</pre>
390
                 << solver_control.last_step() << '\n'
391
                 << "Max norm of residual: "
392
                 << residual.linfty norm() << '\n';
393
        constraints.distribute(solution);
394
     }
395
396
     template<int dim>
397
     void ElasticProblem<dim>::stressCalc()
398
     {
399
     FEValues<dim> fe_values(fe,
400
                            quadrature_formula,
401
                            update_values|update_gradients);
402
     std::vector<std::vector<Tensor<1,dim>>> solution_grads(
403
                                        quadrature_formula.size(),
404
                                        std::vector<Tensor<1,dim>>(dim));
405
406
     radial_stress.reinit(triangulation.n_active_cells());
407
     hoop_stress.reinit(triangulation.n_active_cells());
408
     axial_stress.reinit(triangulation.n_active_cells());
409
410
411
```

```
std::vector<SymmetricTensor<2,dim>> stress_local(triangulation.n_active_cells()
412
          \rightarrow);
     std::vector<SymmetricTensor<2,dim>> stress local polar(triangulation.
413
          \hookrightarrow n_active_cells());
     Vector<double> norm_of_stress_local(triangulation.n_active_cells());
414
     {
415
       for(auto &cell : dof_handler.active_cell_iterators())
416
       {
417
         fe_values.reinit(cell);
418
         fe_values.get_function_gradients(solution, solution_grads);
419
420
         const unsigned int cell_index = cell->active_cell_index();
421
         const Point<dim> cell_center = cell->center();
422
         SymmetricTensor<2,dim> accumulated_stress ;
423
         accumulated_stress = 0;
424
         for(unsigned int q = 0; q < quadrature_formula.size(); ++q)</pre>
425
         {
426
           const SymmetricTensor<2,dim> quad_stress = (stress_strain_tensor *
427
                                                    get_strain(solution_grads[q]));
428
           accumulated_stress += quad_stress;
429
         }
430
         stress_local[cell_index] = accumulated_stress/quadrature_formula.size();
431
         norm_of_stress_local(cell_index)= accumulated_stress.norm();
432
433
         const SymmetricTensor<2,dim> tmp = stress_local[cell_index];
434
435
         stress_local_polar[cell_index] = cart_to_polar<dim>(cell_center,tmp);
436
437
         radial_stress[cell_index] = stress_local_polar[cell_index][0][0];
438
         hoop_stress[cell_index] = stress_local_polar[cell_index][1][1];
439
         axial_stress[cell_index] = stress_local_polar[cell_index][2][2];
440
       }
441
     }
442
     stress = stress_local;
443
     norm_of_stress = norm_of_stress_local;
444
    }
445
446
447
     template <int dim>
448
     void ElasticProblem<dim>::refine_grid()
449
     {
450
       Vector<float> estimated_error_per_cell(triangulation.n_active_cells());
451
452
       KellyErrorEstimator<dim>::estimate(dof_handler,
453
                                        QGauss<dim - 1>(fe.degree + 1),
454
                                        {},
455
                                        solution,
456
```

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estimated_error_per_cell); 457 458 GridRefinement::refine_and_coarsen_fixed_number(triangulation, 459 estimated_error_per_cell, 460 0.3, 461 0.03); 462 463 triangulation.execute_coarsening_and_refinement(); 464 } 465 466 467 468 template <int dim> 469 void ElasticProblem<dim>::output_results(const unsigned int cycle) const 470 471 { std::vector<std::string> solution_names(dim, "Displacement"); 472 473 std::vector<DataComponentInterpretation::DataComponentInterpretation> 474 solution_component_interpretation(475 dim, DataComponentInterpretation::component_is_part_of_vector); 476 DataOut<dim> data_out; 477 data_out.attach_dof_handler(dof_handler); 478 data_out.add_data_vector(solution, 479 solution_names, 480 DataOut<dim>::type_dof_data, 481 solution_component_interpretation); 482 // printing component stresses 483 data_out.add_data_vector(radial_stress,"radial_stress",DataOut<dim>:: 484 \hookrightarrow type_cell_data); data_out.add_data_vector(hoop_stress,"hoop_stress", DataOut<dim>:: 485 \hookrightarrow type_cell_data); data_out.add_data_vector(axial_stress,"axial_stress", DataOut<dim>:: 486 \hookrightarrow type cell data); //printing norm of stresses 487 data_out.add_data_vector(norm_of_stress,"norm_of_stress",DataOut<dim>:: 488 \hookrightarrow type_cell_data); 489 data_out.build_patches(); 490 491 std::ofstream output("37MnSi5 5.4mm simple hollow-" + std::to_string(cycle) + 492 \hookrightarrow ".vtk"); data_out.write_vtk(output); 493 } 494 495 496 497 498

```
template <int dim>
499
      void ElasticProblem<dim>::run()
500
      ł
501
       Timer timer;
502
        for (unsigned int cycle = 0; cycle < 1; ++cycle)</pre>
503
          {
504
            std::cout << "Cycle "<< cycle << ':' << std::endl;</pre>
505
506
            if (cycle == 0)
507
             {
508
               // mesh generation for simple hollow cylinder
509
               const double OD =232, THK = 5.4, Height = 1200, scale =1;
510
               const double outer_radius = scale *OD/2,
511
                            inner_radius = (outer_radius - scale * THK);
512
               GridGenerator::cylinder_shell(triangulation,
513
                                             scale*Height,
514
                                             inner_radius,
515
                                             outer_radius);
516
               for(const auto &cell : triangulation.active_cell_iterators())
517
               for (const auto &face : cell->face_iterators())
518
               if(face->at_boundary())
519
               {
520
                 const Point<dim> face_center = face->center();
521
                 if(std::fabs(face_center[2]) <1e-12)</pre>
522
                 face->set_boundary_id(0);
523
                 else if (std:: fabs(face_center[2] - (scale * Height)) <1e-12 )</pre>
524
                 face-> set_boundary_id(1);
525
                 else if (std::sqrt(face_center[0] * face_center[0] +
526
                                    face_center[1]*face_center[1]) <</pre>
527
                                    (inner_radius + outer_radius)/2)
528
                 face->set_boundary_id(2);
529
                 else
530
                 face->set_boundary_id(3);
531
               }
532
             }
533
            else
534
           {
535
            std::cout << "Refining.... "<< std::endl;</pre>
536
             refine_grid();
537
            std::cout << "...complete! "<< std::endl;</pre>
538
            }
539
           std::cout<< "time Elapsed: "<< timer.cpu_time() << "sec." << std:: endl;</pre>
540
541
            std::cout << "Number of active cells: "</pre>
542
                     << triangulation.n_active_cells() << std::endl;
543
544
           std::cout << "Setting up.... "<< std::endl;</pre>
545
```
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```
setup_system();
546
           std::cout << "...complete! "<< std::endl;</pre>
547
           std::cout<< "time Elapsed: "<< timer.cpu_time() << "sec." << std:: endl;</pre>
548
549
550
           std::cout << "Number of degrees of freedom: "<< dof_handler.n_dofs()</pre>
551
                    << std::endl;
552
           std::cout << "Assembling.... "<< std::endl;</pre>
553
           assemble_system();
554
           std::cout << "...complete! "<< std::endl;</pre>
555
           std::cout<< "time Elapsed: "<< timer.cpu_time() << "sec." << std:: endl;</pre>
556
557
           std::cout << "Solving.... "<< std::endl;</pre>
558
           solve();
559
560
           std::cout << "...complete! "<< std::endl;</pre>
           std::cout<< "time Elapsed: "<< timer.cpu_time() << "sec." << std:: endl;</pre>
561
562
           std::cout << "Outputting.... "<< std::endl;</pre>
563
           output_results(cycle);
564
           std::cout << "...complete! "<< std::endl;</pre>
565
566
567
           std::cout<< "Total time: "<< timer.cpu_time() << "sec." << std:: endl;</pre>
568
     }
569
   }
570
   } // namespace Program
571
572
573
   int main()
574
    {
575
     try
576
       {
577
         Program::ElasticProblem<3> elastic_problem_3d;
578
         elastic_problem_3d.run();
579
       }
580
     catch (std::exception &exc)
581
       {
582
         std::cerr << std::endl</pre>
583
                   << std::endl
584
                   << "-----"
585
                   << std::endl;
586
         std::cerr << "Exception on processing: "<< std::endl</pre>
587
                   << exc.what() << std::endl
588
                   << "Aborting!" << std::endl
589
                   << "-----"
590
                   << std::endl;
591
592
```

```
return 1;
593
      }
594
    catch (...)
595
      {
596
       std::cerr << std::endl</pre>
597
               << std::endl
598
               << "-----"
599
               << std::endl;
600
       std::cerr << "Unknown exception!" << std::endl</pre>
601
               << "Aborting!" << std::endl
602
               << "-----"
603
               << std::endl;
604
605
       return 1;
      }
606
607
    return 0;
608
   }
609
610
   }
611
```

Code For Deformation using MPI

```
#include <deal.II/base/timer.h>
1
  #include <deal.II/base/quadrature_lib.h>
2
  #include <deal.II/base/function.h>
3
4 #include <deal.II/base/logstream.h>
  #include <deal.II/base/multithread_info.h>
5
  #include <deal.II/lac/vector.h>
   #include <deal.II/lac/full matrix.h>
8 #include <deal.II/lac/affine_constraints.h>
  #include <deal.II/lac/dynamic_sparsity_pattern.h>
9
  #include <deal.II/lac/sparsity_tools.h>
10
  #include <deal.II/grid/grid_in.h>
11
  #include <deal.II/grid/grid_out.h>
12
  #include <deal.II/grid/tria.h>
13
  #include <deal.II/grid/grid_generator.h>
14
  #include <deal.II/grid/grid_refinement.h>
15
  #include <deal.II/dofs/dof_handler.h>
16
  #include <deal.II/dofs/dof_tools.h>
17
  #include <deal.II/fe/fe_values.h>
18
  #include <deal.II/fe/fe_system.h>
19
  #include <deal.II/fe/fe_q.h>
20
  #include <deal.II/numerics/vector tools.h>
21
22 #include <deal.II/numerics/matrix_tools.h>
23 #include <deal.II/numerics/data_out.h>
  #include <deal.II/numerics/error_estimator.h>
24
25 #include <deal.II/base/conditional_ostream.h>
26 #include <deal.II/base/mpi.h>
  #include <deal.II/lac/petsc_vector.h>
27
  #include <deal.II/lac/petsc_sparse_matrix.h>
28
  #include <deal.II/lac/petsc_solver.h>
29
  #include <deal.II/lac/petsc_precondition.h>
30
  #include <deal.II/grid/grid_tools.h>
31
  #include <deal.II/dofs/dof renumbering.h>
32
  #include <fstream>
33
   #include <iostream>
34
35
  namespace ProgramMPI
36
   {
37
    using namespace dealii;
38
39
    template <int dim>
40
    class ElasticProblem
41
    {
42
    public:
43
      ElasticProblem();
44
      void run();
45
```

```
46
     private:
47
       void setup_system();
48
       void assemble_system();
49
       unsigned int solve();
50
       void calculate_stress();
51
       void refine_grid();
52
       void output_results(const unsigned int cycle) const;
53
54
       MPI_Comm mpi_communicator;
55
56
       const unsigned int n_mpi_processes;
57
       const unsigned int this_mpi_process;
58
59
60
       ConditionalOStream pcout;
61
       GridIn<dim> gridin;
62
       Triangulation<dim> triangulation;
63
       FESystem<dim> fe;
64
       DoFHandler<dim> dof_handler;
65
66
       AffineConstraints<double> hanging_node_constraints;
67
68
       PETScWrappers::MPI::SparseMatrix system_matrix;
69
70
       PETScWrappers::MPI::Vector solution;
71
       PETScWrappers::MPI::Vector system_rhs;
72
73
       const QGauss<dim> quadrature_formula;
74
     };
75
76
     template <int dim>
77
     const SymmetricTensor<4, dim> ElasticProblem<dim>::stress_strain_tensor =
78
       get_stress_strain_tensor<dim>(/*lambda = */ 10.54448e10,
79
                                   /*mu = */ 7.6356e10);
80
81
     template <int dim>
82
     class BodyForceValues : public Function<dim>
83
     {
84
     public:
85
       BodyForceValues();
86
87
       virtual void vector_value(const Point<dim> &p,
88
                               Vector<double> & values) const override;
89
90
       virtual void
91
       vector_value_list(const std::vector<Point<dim>> &points,
92
```

```
std::vector<Vector<double>> & value_list) const override;
93
     };
94
95
96
     template <int dim>
97
     BodyForceValues<dim>::BodyForceValues()
98
       : Function<dim>(dim)
99
     {}
100
101
102
     template <int dim>
103
     inline void BodyForceValues<dim>::vector_value(const Point<dim> & /*p*/,
104
                                            Vector<double> &values) const
105
     {
106
       Assert(values.size() == dim, ExcDimensionMismatch(values.size(), dim));
107
108
       const double g = 9.81;
109
       const double rho = 7850;
110
111
       values = 0;
112
       values(dim - 2) = -rho * g;
113
     }
114
115
116
117
     template <int dim>
118
     void BodyForceValues<dim>::vector_value_list(
119
       const std::vector<Point<dim>> &points,
120
       std::vector<Vector<double>> & value_list) const
121
     {
122
       const unsigned int n_points = points.size();
123
124
       Assert(value_list.size() == n_points,
125
              ExcDimensionMismatch(value_list.size(), n_points));
126
127
       for (unsigned int p = 0; p < n_points; ++p)</pre>
128
         BodyForceValues<dim>::vector_value(points[p], value_list[p]);
129
     }
130
131
     template<int dim>
132
     class PressureBoundaryValues : public Function<dim>
133
     ſ
134
       public:
135
       PressureBoundaryValues(): Function<dim>(1)
136
       {}
137
138
```

```
virtual double value(const Point<dim> & p,const unsigned int component = 0)
139
           \hookrightarrow const override;
140
     };
141
142
     template <int dim>
143
     double PressureBoundaryValues<dim>::value(const Point<dim> & /*p*/, const
144
          → unsigned int /*component*/) const
     {
145
       return -1.5e07;//pressure value here
146
     }
147
148
     template <int dim>
149
     ElasticProblem<dim>::ElasticProblem()
150
        : mpi_communicator(MPI_COMM_WORLD)
151
        , n_mpi_processes(Utilities::MPI::n_mpi_processes(mpi_communicator))
152
        , this_mpi_process(Utilities::MPI::this_mpi_process(mpi_communicator))
153
        , pcout(std::cout, (this_mpi_process == 0))
154
        , fe(FE_Q<dim>(1), dim)
155
        , dof_handler(triangulation)
156
        , quadrature_formula(fe.degree + 1)
157
     {}
158
159
     template <int dim>
160
     void ElasticProblem<dim>::setup_system()
161
     {
162
163
       pcout << "setting up... ";</pre>
164
       GridTools::partition_triangulation(n_mpi_processes, triangulation);
165
166
       dof_handler.distribute_dofs(fe);
167
       DoFRenumbering::subdomain_wise(dof_handler);
168
169
       hanging_node_constraints.clear();
170
       DoFTools::make_hanging_node_constraints(dof_handler,
171
                                             hanging_node_constraints);
172
       hanging_node_constraints.close();
173
174
       DynamicSparsityPattern dsp(dof_handler.n_dofs(), dof_handler.n_dofs());
175
       DoFTools::make_sparsity_pattern(dof_handler,
176
177
                                     dsp,
                                     hanging_node_constraints,
178
                                     false);
179
180
       const std::vector<IndexSet> locally_owned_dofs_per_proc =
181
         DoFTools::locally_owned_dofs_per_subdomain(dof_handler);
182
       const IndexSet locally_owned_dofs =
183
```

```
locally_owned_dofs_per_proc[this_mpi_process];
184
185
       system_matrix.reinit(locally_owned_dofs,
186
                          locally_owned_dofs,
187
                          dsp,
188
                          mpi_communicator);
189
190
       solution.reinit(locally_owned_dofs, mpi_communicator);
191
       system_rhs.reinit(locally_owned_dofs, mpi_communicator);
192
     }
193
194
     template <int dim>
195
     void ElasticProblem<dim>::assemble_system()
196
     {
197
       QGauss<dim> quadrature_formula(fe.degree + 1);
198
       FEValues<dim> fe_values(fe,
199
                             quadrature formula,
200
                             update_values | update_gradients |
201
                               update_quadrature_points | update_JxW_values);
202
       QGauss<dim-1> face_quadrature_formula(fe.degree +1);
203
       FEFaceValues<dim> fe_face_values(fe,
204
                             face_quadrature_formula,
205
                             update_values | update_normal_vectors|
206
                             update_quadrature_points | update_JxW_values);
207
208
209
       const unsigned int dofs_per_cell = fe.n_dofs_per_cell();
210
       const unsigned int n_q_points = quadrature_formula.size();
211
       const unsigned int n_face_q_points = face_quadrature_formula.size();
212
213
       FullMatrix<double> cell matrix(dofs per cell, dofs per cell);
214
       Vector<double> cell_rhs(dofs_per_cell);
215
216
       std::vector<types::global_dof_index> local_dof_indices(dofs_per_cell);
217
218
       std::vector<double> lambda_values(n_q_points);
219
       std::vector<double> mu_values(n_q_points);
220
       std::vector<double> pressure_values(n_face_q_points);
221
       std::vector<Vector<double>> rhs_values(n_q_points, Vector<double>(dim));
222
223
       Functions::ConstantFunction<dim> lambda(7.923e10), mu(11.885e10);
224
225
       BodyForceValues<dim> gravity;
226
       PressureBoundaryValues<dim> pressure_boundary;
227
228
       // store the boundary ids of the surfaces where pressure to be applied
229
```

```
std::vector<int> pressure_boundary_ids =
230
            \hookrightarrow {1,3,4,20,21,22,23,24,25,26,27,28,46,47};
       // value to be added after physical tag assignation
231
       const int add_value = 100;
232
       std::transform(pressure_boundary_ids.begin(), pressure_boundary_ids.end(),
233
            pressure_boundary_ids.begin(), [add_value](int i) { return i + add_value;
234
                \rightarrow });
235
       for (const auto &cell : dof_handler.active_cell_iterators())
236
         if (cell->subdomain_id() == this_mpi_process)
237
           {
238
             cell_matrix = 0;
239
             cell_rhs = 0;
240
241
242
             fe_values.reinit(cell);
243
             lambda.value_list(fe_values.get_quadrature_points(), lambda_values);
244
             mu.value_list(fe_values.get_quadrature_points(), mu_values);
245
246
       for (unsigned int i = 0; i < dofs_per_cell; ++i)</pre>
247
               {
248
                 const unsigned int component_i =
249
                   fe.system_to_component_index(i).first;
250
251
        for (unsigned int j = 0; j < dofs_per_cell; ++j)</pre>
252
            {
253
               const unsigned int component_j =
254
                   fe.system_to_component_index(j).first;
255
256
            for (unsigned int q_point = 0; q_point < n_q_points;</pre>
257
                         ++q_point)
258
                {
259
                   cell_matrix(i, j) +=
260
                           ((fe_values.shape_grad(i, q_point)[component_i] *
261
                            fe_values.shape_grad(j, q_point)[component_j] *
262
                            lambda_values[q_point]) +
263
                            (fe_values.shape_grad(i, q_point)[component_j] *
264
                            fe_values.shape_grad(j, q_point)[component_i] *
265
                            mu_values[q_point]) +
266
                            ((component_i == component_j) ?
267
                               (fe_values.shape_grad(i, q_point) *
268
                               fe_values.shape_grad(j, q_point) *
269
                               mu_values[q_point]) :
270
                              0)) *
271
                          fe_values.JxW(q_point);
272
                       }
273
                   }
274
```

```
}
275
             gravity.vector_value_list(fe_values.get_quadrature_points(), rhs_values)
276
                  \hookrightarrow;
277
             for (unsigned int i = 0; i < dofs_per_cell; ++i)</pre>
278
               {
279
                  const unsigned int component_i =
280
                   fe.system_to_component_index(i).first;
281
282
                 for (unsigned int q_point = 0; q_point < n_q_points; ++q_point)</pre>
283
                   cell_rhs(i) += fe_values.shape_value(i, q_point) *
284
                                  rhs_values[q_point](component_i) *
285
                                  fe_values.JxW(q_point);
286
               }
287
288
289
290
291
         for(unsigned int face_number =0; face_number < GeometryInfo<dim> ::
292
             \hookrightarrow faces_per_cell;
                                                                          ++face_number)
293
             {
294
                if (cell->face(face_number)->at_boundary() &&
295
                std::find(pressure_boundary_ids.begin(), pressure_boundary_ids.end(),
296
                     cell->face(face_number)->boundary_id()) != pressure_boundary_ids.
297
                          \hookrightarrow end())
               {
298
                 fe_face_values.reinit(cell,face_number);
299
                 pressure_boundary.value_list(fe_face_values.get_quadrature_points(),
300
                                               pressure_values);
301
           for(unsigned int i=0; i<dofs_per_cell; ++i)</pre>
302
                {
303
                   const unsigned int component_i =
304
                      fe.system_to_component_index(i).first;
305
               for(const unsigned int q_index : fe_face_values.
306

→ quadrature_point_indices())

                   {
307
                     cell_rhs(i) += (pressure_values[q_index] *
308
                                     fe_face_values.normal_vector(q_index)[component_i])
309
                                         \hookrightarrow *
                                     fe_face_values.shape_value(i,q_index) *
310
                                     fe_face_values.JxW(q_index);
311
                   }
312
                  }
313
314
               }
315
             }
316
```

```
cell->get_dof_indices(local_dof_indices);
317
             hanging_node_constraints.distribute_local_to_global(cell_matrix,
318
                                                             cell rhs,
319
                                                             local_dof_indices,
320
                                                             system_matrix,
321
                                                             system_rhs);
322
           }
323
324
       system_matrix.compress(VectorOperation::add);
325
       system_rhs.compress(VectorOperation::add);
326
       FEValuesExtractors::Scalar z_component(dim - 1);
327
       std::map<types::global_dof_index, double> boundary_values;
328
329
       // store boundary ids of surfaces which are fixed
330
       std::vector<int> fixed_boundary_ids = {18,31};
331
       // to add this value
332
       std::transform(fixed_boundary_ids.begin(), fixed_boundary_ids.end(),
333
                fixed_boundary_ids.begin(), [add_value](int i) { return i + add_value;
334
                    \rightarrow });
335
       const auto zero_function = Functions::ZeroFunction<dim>(dim);
336
337
       for (const auto& boundary_id : fixed_boundary_ids) {
338
           VectorTools::interpolate_boundary_values(dof_handler,
339
                                                boundary_id, zero_function,
340
                                                boundary_values);
341
       }
342
       MatrixTools::apply_boundary_values(
343
         boundary_values, system_matrix, solution, system_rhs, false);
344
     }
345
346
     template <int dim>
347
     unsigned int ElasticProblem<dim>::solve()
348
     {
349
       SolverControl solver_control(2e3, 1e-2);
350
       PETScWrappers::SolverCG cg(solver_control, mpi_communicator);
351
352
       PETScWrappers::PreconditionBlockJacobi preconditioner(system_matrix);
353
354
       cg.solve(system_matrix, solution, system_rhs, preconditioner);
355
             Vector<double> localized_solution(solution);
356
357
       hanging_node_constraints.distribute(localized_solution);
358
       return solver_control.last_step();
359
     }
360
361
     template <int dim>
362
```

```
void ElasticProblem<dim>::refine_grid()
363
     {
364
       const Vector<double> localized solution(solution);
365
366
       Vector<float> local_error_per_cell(triangulation.n_active_cells());
367
       KellyErrorEstimator<dim>::estimate(dof_handler,
368
                                        QGauss<dim - 1>(fe.degree + 1),
369
                                        {},
370
                                        localized_solution,
371
                                        local_error_per_cell,
372
                                        ComponentMask(),
373
                                        nullptr,
374
                                        MultithreadInfo::n_threads(),
375
                                        this_mpi_process);
376
377
       const unsigned int n_local_cells =
378
         GridTools::count_cells_with_subdomain_association(triangulation,
379
                                                        this_mpi_process);
380
       PETScWrappers::MPI::Vector distributed_all_errors(
381
         mpi_communicator, triangulation.n_active_cells(), n_local_cells);
382
383
       for (unsigned int i = 0; i < local_error_per_cell.size(); ++i)</pre>
384
         if (local_error_per_cell(i) != 0)
385
           distributed_all_errors(i) = local_error_per_cell(i);
386
       distributed_all_errors.compress(VectorOperation::insert);
387
388
389
       const Vector<float> localized_all_errors(distributed_all_errors);
390
391
       GridRefinement::refine_and_coarsen_fixed_number(triangulation,
392
                                                    localized all errors,
393
                                                    0.3,
394
                                                    0.03):
395
       triangulation.execute_coarsening_and_refinement();
396
     }
397
398
399
    template <int dim>
400
    void ElasticProblem<dim>::output_results(const unsigned int cycle) const
401
     {
402
       const Vector<double> localized_solution(solution);
403
404
       if (this_mpi_process == 0)
405
         {
406
           std::ofstream output("37MnSi7 yo ho -" + std::to_string(cycle) + ".vtk");
407
           std::vector<DataComponentInterpretation::DataComponentInterpretation>
408
             data_component_interpretation(
409
```

```
dim, DataComponentInterpretation::component_is_part_of_vector);
410
           DataOut<dim> data_out;
411
           data_out.attach_dof_handler(dof_handler);
412
413
           std::vector<std::string> solution_names(dim, "Displacement");
414
           data_out.add_data_vector(localized_solution,
415
                               solution_names,
416
                               DataOut<dim>::type_dof_data,
417
                               data_component_interpretation);
418
419
           std::vector<unsigned int> partition_int(triangulation.n_active_cells());
420
           GridTools::get_subdomain_association(triangulation, partition_int);
421
422
           const Vector<double> partitioning(partition_int.begin(),
423
424
                                            partition_int.end());
425
           data_out.add_data_vector(partitioning, "partitioning");
426
           data_out.build_patches();
427
           data_out.write_vtk(output);
428
         }
429
     }
430
431
    template <int dim>
432
     void ElasticProblem<dim>::run()
433
     ł
434
       Timer timer;
435
        for (unsigned int cycle = 0; cycle < 1; ++cycle)</pre>
436
         ł
437
           pcout << "Cycle "<< cycle << ':' << std::endl;</pre>
438
439
           if (cycle == 0)
440
             {
441
               // import the mesh file generated by Gmesh
442
               gridin.attach_triangulation(triangulation);
443
               std::ifstream f("Mesh.msh");
444
               gridin.read_msh(f);
445
             }
446
           else
447
             refine_grid();
448
449
           pcout << "Number of active cells: "</pre>
450
                 << triangulation.n_active_cells() << std::endl;
451
452
           setup_system();
453
454
           pcout << "Number of degrees of freedom:" << dof_handler.n_dofs()</pre>
455
                 << "(by_partition:";
456
```

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```
for (unsigned int p = 0; p < n_mpi_processes; ++p)</pre>
457
            pcout << (p == 0 ? '': '+')
458
                  << (DoFTools::count_dofs_with_subdomain_association(dof_handler,
459
                                                                 p));
460
           pcout << ')' << std::endl;</pre>
461
462
           assemble_system();
463
           const unsigned int n_iterations = solve();
464
465
           pcout << "Solver converged in "<< n_iterations << "iterations."</pre>
466
                << std::endl;
467
468
           output_results(cycle);
469
           pcout<< "Time:" << timer.cpu_time() << "sec." << std:: endl;</pre>
470
         }
471
     }
472
   } // namespace ProgramMPI
473
474
475
476
   int main(int argc, char **argv)
477
   {
478
     try
479
       {
480
         using namespace dealii;
481
         using namespace ProgramMPI;
482
483
         Utilities::MPI::MPI_InitFinalize mpi_initialization(argc, argv, 1);
484
485
         ElasticProblem<3> elastic_problem;
486
         elastic_problem.run();
487
       }
488
     catch (std::exception &exc)
489
       {
490
         std::cerr << std::endl</pre>
491
                  << std::endl
492
                  << "-----"
493
                  << std::endl;
494
         std::cerr << "Exception on processing: "<< std::endl</pre>
495
                  << exc.what() << std::endl
496
                  << "Aborting!" << std::endl
497
                  << "-----"
498
                  << std::endl;
499
500
         return 1;
501
       }
502
     catch (...)
503
```

```
{
504
       std::cerr << std::endl</pre>
505
              << std::endl
506
              << "-----"
507
              << std::endl;
508
       std::cerr << "Unknown exception!" << std::endl</pre>
509
              << "Aborting!" << std::endl
510
              << "-----"
511
              << std::endl;
512
513
       return 1;
     }
514
515
    return 0;
516
517 }
```

APPENDIX C: SCRIPT FOR GEOMETRY SIMPLIFICATION AND MESHING

```
1 // This script creates simplified cylinder model and mesh it.
  //lc means target mesh size
  lc = 1e-2;
3
4
   //defining points
5
6
   Point(20) = \{0, 0, 0, 1c\};
7
8 Point(2) = {0, 5.6, 0, lc};
9 Point(3) = {86, 0, 0, 1c};
10 Point(4) = {86, 5.6, 0, 1c};
11 Point(5) = {86, 30, 0, 1c};
12 Point(6) = {110.4, 30, 0, lc};
13 Point(7) = {116, 30, 0, lc};
14 Point(8) = {110.4, 1220, 0, lc};
15 Point(9) = {116, 1220, 0, lc};
16 Point(10) = { 0, 1220, 0, lc};
Point(11) = \{15, 1329.38, 0, 1c\};
   Point(12) = {15, 1335.03, 0, 1c};
18
   Point(13) = {65.05, 1309.2, 0, 1c};
19
20
   //lines
21
22
23 Line(1) = {2, 20};
24 Line(2) = {3, 20};
25 Line(3) = {2, 4};
_{26} Line(4) = {6, 8};
  Line(5) = \{7, 9\};
27
  Line(6) = \{11, 12\};
28
29
   //Circles
30
31
32 //+
33 Circle(8) = {11, 10, 8};
  //+
34
  Circle(9) = {12, 10, 9};
35
   //+
36
  Circle(10) = \{4, 5, 6\};
37
   //+
38
   Circle(11) = \{3, 5, 7\};
39
40
   //curve loop
41
42
  Physical Curve("1", 12) = {1, 3, 10, 4, 8, 6, 9, 5, 11, 2};
43
44 Curve Loop(1) = {4, -8, 6, 9, -5, -11, 2, -1, 3, 10};
```

```
Plane Surface(1) = {1};
45
46
   //Transfinite Surface {1};
47
   //Recombine Surface {1};
48
49
   Extrude {{0, 1, 0}, {0, 5.6,0}, 0.5*Pi} {
50
   Surface{1}; Layers{6};
51
   Recombine;
52
   }
53
54
  //+
55
   Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
56
     Surface{59}; Layers{8}; Recombine;
57
   }
58
  //+
59
   Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
60
     Surface{106}; Layers{8}; Recombine;
61
62 }
  //+
63
   Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
64
     Surface{153}; Layers{8}; Recombine;
65
   }
66
67
68
   Mesh.Algorithm = 6;
69
   Mesh.ElementOrder = 1;
70
   Mesh 3;
71
  Coherence Mesh;
72
```

```
//This code take step file as input and takes
1
      its cross section first and revolve that
2
      cros section with extruding mesh
       SetFactory("OpenCASCADE");
4
   v() = ShapeFromFile("file.STEP");
5
   // Get the bounding box of the volume:
   bbox() = BoundingBox Volume{v()};
   xmin = bbox(0);
8
   ymin = bbox(1);
9
   zmin = bbox(2);
10
  xmax = bbox(3);
11
   ymax = bbox(4);
12
   zmax = bbox(5);
13
14
  //Defining Necessary Parameter
15
  dx = (xmax - xmin);
16
   dy = (ymax - ymin);
17
   dz = (zmax - zmin);
18
  L = dz/2;
19
  H = dy;
20
21
  //Define Cutting Surface
22
  s() = {news};
23
24 Rectangle(s(0)) = {xmin, ymin, zmin, L, H};
  Rotate{ {0, 1, 0}, {xmin, ymin, zmin}, -Pi/2 }
25
  { Surface{s(0)}; }
26
  tx = dx / 2;
27
  ty =0;
28
   tz=0;
29
   Translate{tx, ty, tz} { Surface{s(0)}; }
30
31
32
   //Delete Everything of surface out of object
33
   i.e keeping cutting surface inside material domain only
34
   BooleanFragments{ Volume{v()}; Delete; }
35
   { Surface{s()}; Delete; }
36
   Recursive Delete { Surface{:}; }
37
38
   //Deleting everything except the surface of cut
39
     eps = 1e-4;
40
     s() = \{\};
41
      xx = xmin;
42
      yy = ymax;
43
       zz = zmax;
44
       s() += Surface In BoundingBox
45
       {xmin - eps + tx, ymin - eps +ty, zmin - eps + tz,
46
```

```
xx + eps + tx, yy + eps + ty, zz + eps +tz};
47
    dels = Surface{:};
48
    dels -= s();
49
    Delete { Volume{:}; Surface{dels()};
50
    Curve{:}; Point{:}; }
51
52
53
  //+
   Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
54
     Surface{2}; Layers{8}; Recombine;
55
   }
56
57 //+
58 Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
    Surface{12}; Layers{8}; Recombine;
59
  }
60
  //+
61
  Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
62
     Surface{22}; Layers{8}; Recombine;
63
64 }
  //+
65
66
  Extrude {{0, 1, 0}, {0, 0, 0}, Pi/2} {
67
    Surface{32}; Layers{8}; Recombine;
68
  }
69
70 Coherence;
71 Coherence Mesh;
72 //+
  //+
73
```

APPENDIX D: SCRIPT FOR BOUNDARY ID ASSIGNING

```
with open('inputmesh.txt','r') as infile,
1
       open('outputmesh.txt','w') as outfile:
2
       switch = 0
3
      turn = 0
Δ
      for line in infile:
          # Code to modify line
6
          columns = line.split(' ')
7
          # store the data in columns as strings
          if columns[0] == '$Elements\n':
0
          # when elements are found
10
              switch = 1 # turn on this switch
11
              print(columns)
12
          if switch == 1:
13
       # start reading the lines after Elements are found
14
           if len(columns)>1 and columns[1] != '15':
15
       # when the line starts containing other than 15
16
               turn = 1
17
            switch = 0
18
       # no need of this section after assigning turn is 1
19
          if turn == 1 and columns[0] != '$EndElements\n':
20
       # before reaching the endelement section
21
              tmp = int(columns[4]) + 100
22
              # assign the physical ids
23
              columns[3] = str(tmp)
24
              new_line = (' ').join(columns)
25
              # create new line after the manipulation
26
          else:
27
              new_line = line
28
          outfile.write(new_line)
29
          #write the line in new file
30
          # print(columns)
31
```

APPENDIX E: ADDITIONAL FEM RESULTS

Simulation results for hollow cylinder from deal.ii

Material : 37MnSi5



(a) Displacement, Thickness=5.4



(b) Hoop stress, Thickness=5.4



(c) Displacement, Thickness=5.5



(d) Hoop stress, Thickness=5.5



(e) Displacement, Thickness=5.6



(f) Hoop stress, Thickness=5.6

Figure E.1: Displacement and Hoop stress with different thickness (37MnSi5)

Material: 34Mn2V



(b) Hoop stress, Thickness=5.4



(c) Displacement, Thickness=5.5



(d) Hoop stress, Thickness=5.5

(f) Hoop stress, Thickness=5.6



(e) Displacement, Thickness=5.6



Material: 32CrMo4



(b) Hoop stress, Thickness=5.4



(c) Displacement, Thickness=5.5



(d) Hoop stress, Thickness=5.5

(f) Hoop stress, Thickness=5.6



(e) Displacement, Thickness=5.6

Figure E.3: Displacement and Hoop stress with different thickness (32CrM04)