SimuStruct: Simulated Structural Plate with Holes Dataset with Machine Learning Applications

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Abstract

This paper introduces the SimuStruct dataset, which consists of 2D structural parts along with their respective meshes and the outputs of numerical simulations for various properties such as linear and elastic material, boundary and loading conditions, and different levels of refinement. The dataset includes the classic case of plates with holes, which is a common and analytically resolvable 2D case found in different mechanical design applications. SimuStruct provides a diverse and realistic dataset as it includes multiple cases for different loading and boundary conditions, various material properties, and mesh refinement levels. Furthermore, it is flexible, versatile, and scalable as all algorithms and codes, where each case is solved using standard Finite Element Method (FEM) with the open-source package FEniCS. The primary aim of the SimuStruct dataset is to serve as training and evaluation data for Machine Learning (ML)-based methods in structural analysis and optimal mesh generation, thereby supporting the development of ML-based optimal mechanical design solutions. In this paper, it is also presented an application of SimuStruct to train and test a Graph Neural Network (GNN) model to predict stress-strain fields, demonstrating the dataset's potential for use in structural analysis. The SimuStruct dataset will facilitate the integration of the Mechanical Engineering and Machine Learning communities and enable faster and more efficient research in the computational design field.

1 Introduction

Computational tools have recently shown potential for automatic generative design and surrogate modeling of mechanical systems, including individual parts like seat brackets Alderton (2018), as well as complete systems car chassis Alderton (2016). The automatic design process involves a mechanical property simulator and an optimization module to find the optimal configuration while considering design restrictions such as stress, displacement, stiffness, mass, and manufacturing constraints. Traditionally, numerical simulation has been carried out using the Finite Element Method (FEM), which is accurate but computationally intensive and slow for rapid optimization cycles. This limits the feasibility of generative design for realistic mechanical systems.

To overcome FEM's limitations previous identify, Machine Learning (ML) methods have been proposed, such as Multilayer Perceptrons (MLPs) Ribeiro et al. (2021), Convolutional Neural Networks (CNNs) Nie et al. (2019), Graph Neural Network (GNNs) Maurizi et al.

(2022), and Physics-Informed Neural Networks (PINNs) Haghighat et al. (2021). These methods train a model to predict the mechanical response of a system, allowing for faster exploration in the design space. For example, ML has been used to speed up simulations related to spaceship design, reducing the run time from 200 hours to a few seconds Swischuk et al. (2020). However, challenges exist when using ML instead of traditional methods for simulations. Firstly, ML models may only solve one type of case (e.g., wheels), making it unclear how to train them for more than one mechanical family. Secondly, comparing various ML approaches is challenging due to the lack of a standard set of cases for evaluation.

In recent years, Machine Learning algorithms have revolutionized many areas of computer science, including shape datasets (traceparts; thangs) used in geometry processing tasks such as classification, segmentation, surface normal estimation, automated meshing and cleaning, and shape retrieval. However, most of the existing datasets are limited in their applicability to mechanical design tasks, with few datasets available for structural analysis. While datasets such as simJEB Whalen et al. (2021) and Mechanical MNIST Lejeune (2020) exist, they are not easily scalable for other applications or do not represent real cases of mechanical engineering. Therefore, there is a need for new datasets that can better serve the purposes of mechanical design and structural analysis.

Thin plates with holes are widely used in industries like automotive, aerospace, and maritime. However, these plates may exhibit geometric discontinuities, such as holes of varying sizes and shapes. Such discontinuities serve multiple purposes, including reducing the overall weight of the structure, establishing bolted and/or riveted joints, and enabling access to other parts of the structure. These plates are a simple 2D classic case of mechanical engineering and can be found in various applications such as airplane doors and windows Ukadgaonker et al. (2000), joints of fuselage plates by rivets Zhou & Fei (2017), bolted beam joints Wang et al. (2017), cooling holes in turbine blades Dong et al. (2017) and plate for humerus fracture Kim et al. (2021); Zhang et al. (2016). Incorporating plate examples into new datasets could be particularly valuable for advancing the field of mechanical design and structural analysis.

This work introduces the Simulated Structural Parts Dataset (SimuStruct), a dataset of 2D structural parts containing numerical solutions: displacement, stress and strain fields and von Misses stress, and meshes and geometry to plates with holes case studies, to help overcome the previous limitations. SimuStruct aims to serve as training and evaluation data for ML-based methods for computing stress-strain fields and optimal mesh definition and therefore support the development of ML-based optimal mechanical design solutions. In addition, the dataset is intended to be used in academia and industry, contributing to the connection of the Mechanical Engineering and ML community, which will accelerate the research in computational mechanical design.

2 SimuStruct

2.1 Definition

SimuStruct, or the Simulated Structural Parts Dataset, provides numerical solutions for displacement, stress and strain fields, and von Mises stress, as well as meshes and geometries for 2D structural parts, specifically plates with holes. It includes multiple geometric cases of plates with holes, different loading and boundary conditions, and various mesh refinements, enabling quick analyses and optimization procedures in mechanical design tasks. To gain a better grasp of the fundamental concepts of structural material behaviour, it is suggested referring to Appendix A.

The dataset is generated using standard FEM with scripted automation of model generation through FEniCSx Alnæs et al. (2015), a python open-source library for FEM analysis. SimuStruct serves as both training and evaluation data for ML-based methods for computing stress-strain fields and optimal mesh definition, facilitating the development of ML-based mechanical design solutions.

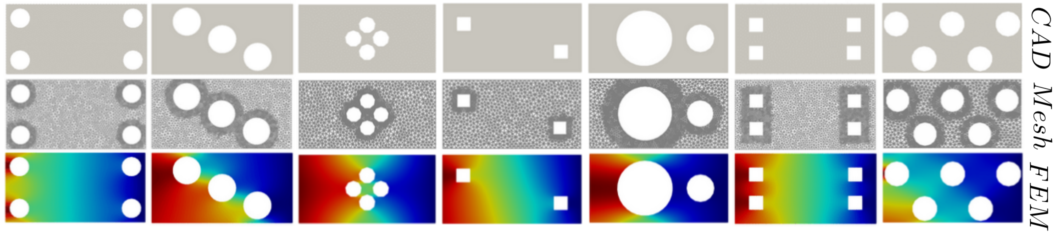


Figure 1: SimuStruct: a collection of geometry, meshes, and FEM simulations for plate with holes under different conditions of mesh refinement, linear and elastic material properties, and boundary and loading conditions.

2.2 Comparison with Other Structural Datasets

SimuStruct is a versatile dataset for structural analysis that has several advantages over similar datasets such as simJEB and Mechanical MNIST. While simJEB focuses on 3D geometries, specifically jet engine brackets, and Mechanical MNIST on 2D geometries, both datasets lack control over the geometry generation. In contrast, SimuStruct offers a set of 2D parametric geometries that were previously created by the developers, providing full control over the construction process. This feature makes SimuStruct highly adaptable and expandable for various types of mechanics problems. SimuStruct also features shapes that are more realistic than handwritten digits used in Mechanical MNIST and is not restricted to a single component geometry like simJEB.

Regarding the loading and boundary conditions cases, simJEB contains only four cases, Mechanical MNIST also studies only four cases. However, SimuStruct presents a meaningful improvement since it performs 9 cases. SimuStruct differs from simJEB and Mechanical MNIST in terms of mesh generation. While simJEB used automated meshing without studying mesh refinement, and Mechanical MNIST studied mesh refinement but only performed simulations with the optimal mesh, SimuStruct conducted a study on mesh refinement by performing six types of refinement for each model. This aspect of SimuStruct is noteworthy as it facilitates studies on the trade-off between runtime and accuracy.

Regarding the FEM software, Mechanical MNIST simulations use open-source software, FEniCSx, and simJEB uses commercial software, Altair, SimuStruct follows the Mechanical MNIST methodology, using FEniCSx, making the simulation process more flexible. In contrast to Mechanical MNIST, which only outputs displacements, and simJEB, which displays both displacements and Von Mises stress, SimuStruct outputs a wider range of results, including displacements, stress components, strain components, Von Mises stress. Moreover, SimuStruct stands out for its use of multiple materials that have isotropic and elastic linear behavior, with variations in their mechanical properties such as Young's modulus and Poisson's ratio.

3 Methodology

The process of generating and processing the dataset is fully described in Figure 2. First, the geometries are defined (Step 1), drawing inspiration from Peterson's stress intensity factor compendium Pilkey et al. (2020), which is a widely recognized reference in the mechanical engineering community. The dataset includes various geometric cases, such as rectangular plates with holes of different shapes, including circular, rectangular, and elliptical holes. Different types of hole orientations, such as random, row of holes, and patterns like D diamond, rectangular, and circular, are also implemented in the dataset. Geometry properties are saved in a JSON file.

The next step is to define the loading and boundary conditions (Steps 2 and 3). Two types of loading conditions are considered: uniaxial and biaxial tension. The boundary conditions may be free, simply supported, or clamped. Considering the different loading and boundary conditions, there are a total of nine combinations, which are saved in JSON files.

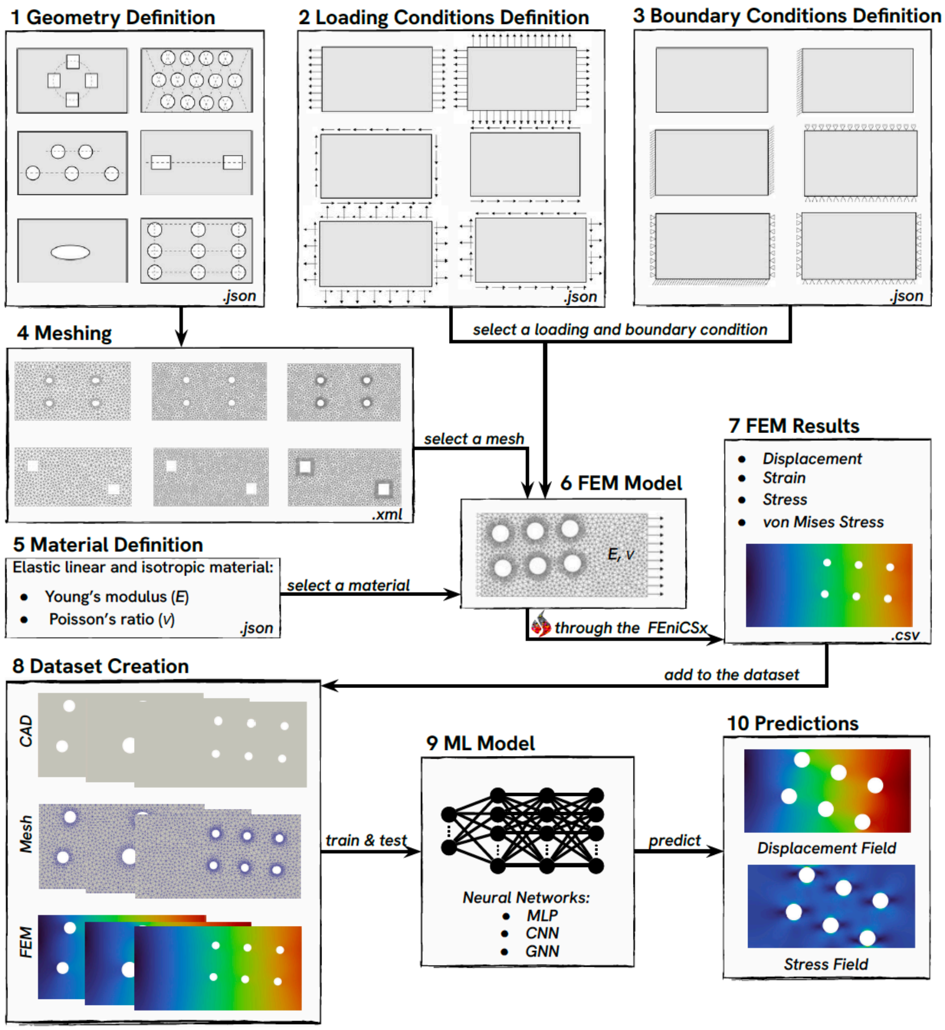


Figure 2: The SimuStruct generation process involves the following steps: (1) geometry definition, (2) loading condition definition, (3) boundary condition definition, (4) meshing, and (5) material definition. These inputs are used to create a (6) FEM model. The FEM results (7) are obtained using FEniCSx to build the dataset (8). This dataset can then be used to train and test machine learning models (9) to make predictions for the problem being analyzed (10).

Using the geometry properties, meshes were generated (Step 4). Those meshes consist of regular triangular elements, where the element size is parametrically controlled. Several meshes were created for each geometric case, with different levels of refinement, to study the mesh resolution and sensitivity to the output results. The meshes are divided into two groups: those with and without refinement around the holes. For each group, three levels of refinement were created, and these meshes are written in XML files. The next step is to define the material properties (Step 5). It is considered a material with linear-elastic and isotropic behavior. The material is characterized by the Young's modulus and Poisson's ratio. Different materials are defined by varying the material properties, and they are stored in JSON files.

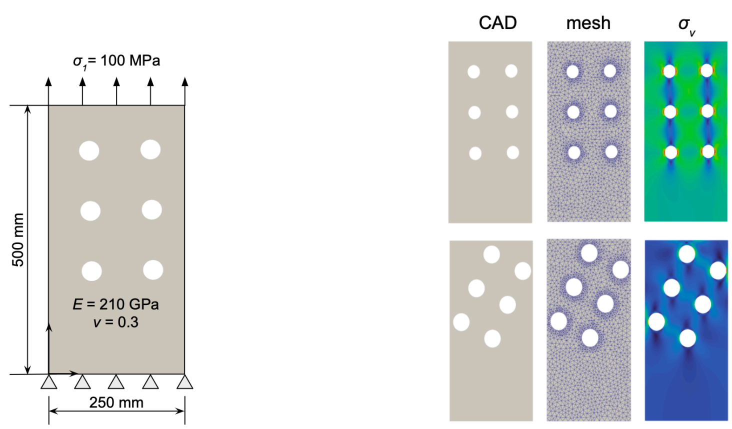
Using the mesh, material, loading, and boundary conditions, a numerical model is created (Step 6). Once the model is created, it is solved using FEniCSx. The FEM results include displacement, stress, strain fields, and von Mises stress (Step 7). This information is saved in CSV files. By repeating this process for different configurations, the dataset with geometry, meshes, and numerical results is obtained (Step 8). Finally, this dataset is used to train-test machine learning models, such as MLPs, CNNs, and GNNs (Step 9), to make predictions for the problem under analysis (Step 10) and to evaluate possible approaches for structural analysis based on ML.

4 Application

In order to showcase the potential and practicality of SimuStruct, it is presented an application that employs a GNN model for predicting the instantaneous von Mises stress field. The model is trained and tested using the Simustrdat dataset.

The study focuses on a plate with six circular holes arranged in a rectangular pattern under uniaxial loading. The plate is subjected to loading on the top, σ_1, and is simply supported on the bottom side. The material behavior considered in the analysis is linear elastic, with a Young's modulus of 210 GPa and a Poisson ratio of 0.3, consistent with the linear behavior of a typical steel alloy. Fig. 3a illustrates the properties of the plate.

To address this problem, it is generated a dataset of 1000 cases using SimuStruct. Fig. 3b displays several samples of this dataset.



(a) (b)

Figure 3: Case study of von Mises stress prediction using the SimuStruct dataset: (a) Schematic representation of a rectangular plate with circular holes under uniaxial loading at the top and simply supported at the bottom; (b) Representative samples from the SimuStruct dataset, where each row displays a sample consisting of a CAD model (Column 1), mesh (Column 2), and von Mises stress field (σ_v) (Column 3).

In Fig. 4, the results are presented. It is observed a lower absolute difference and a higher R^2 value of 0.94, which is closer to 1. This indicates that the predicted results from the GNN model are more accurate and closely aligned with the FEM results.

Based on the last results, it can be concluded that the SimuStruct dataset has great potential for use in structural analysis and expanded to a diverse geometrical cases.

5 Conclusion

In this paper, it is presented the SimuStruct dataset, which provides a comprehensive set of 2D part simulations with varying boundary and loading conditions, material properties, and mesh refinement levels. The achieved results showed that ML models trained on the SimuStruct dataset have high accuracy in predicting mechanical behavior, demonstrating the dataset's high potential in the field of structural analysis.

The SimuStruct dataset provides a valuable resource for developing ML-based methods for optimal mechanical design solutions, enabling faster and more accurate predictions. This

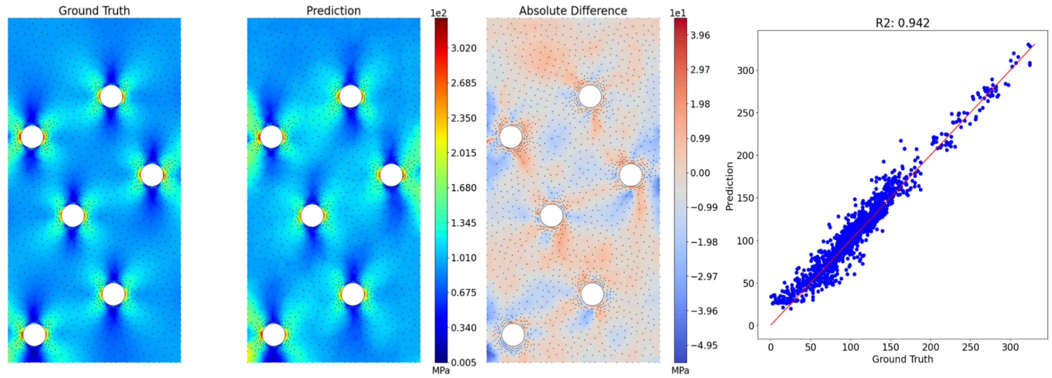


Figure 4: Comparison of ground truth (FEM results) and prediction (GNN results) for von Mises stress using the SimuStruct dataset. The results are shown through ground truth, prediction, and absolute difference fields, as well as a ground truth *vs.* prediction plot, with an R2 value provided.

dataset can also drive digital transformation in manufacturing and digital twin applications, where the ability to simulate and predict mechanical behavior accurately is essential.

Additionally, the SimuStruct dataset can bridge the gap between mechanical engineering and machine learning communities, enabling collaboration and facilitating knowledge sharing. This dataset has the potential to revolutionize the common approaches adopted on mechanical design, enabling faster and more efficient product development.

In conclusion, the SimuStruct dataset is a significant contribution to the field of mechanical engineering and machine learning, providing a valuable resource for developing design tools and driving digital transformation in manufacturing.

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A Mechanical Engineering Concepts

This appendix introduces the basic mechanical engineering concepts about FEM, Solid Mechanic and the Theory of Elasticity.

A.1 FEM

When a problem is too complex to be solved by analytical methods, it is often resort to numerical discretization methods like FEM. The idea of FEM is to replace the complex problem for a simpler one, as this numerical method allows for finding approximate solutions to the PDEs that define the problem Liu & Quek (2014). In FEM, it is possible to improve or refine the approximate solution with an increasing computational cost Rao (2018). This simulation and modelling method is used to solve different types of problems in science and engineering, such as mechanics for solids and structures (problem under study), heat transfer, acoustic, fluid mechanics and combination of those described above Liu & Quek (2014).

Finite Element Analysis (FEA) is the practical application of FEM, which uses a set of computational procedures to solve a given problem. This analysis is divided into three main steps, see image 6 Alisibramulisi et al. (2019):

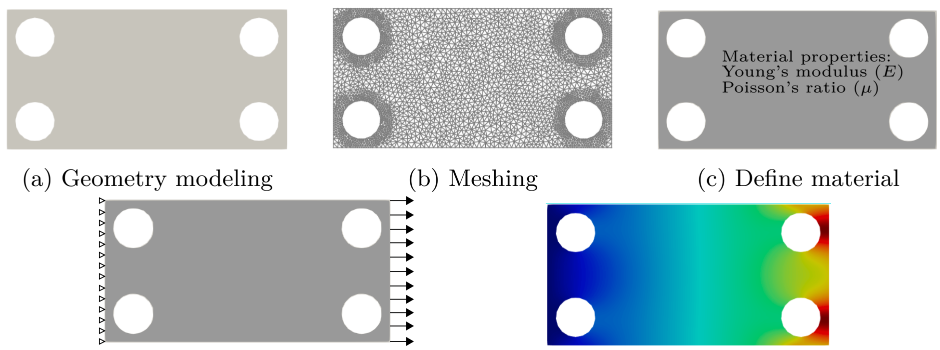
- Pre-processing: The approximate model of the problem under study is defined: geometry definition, material constitutive law, mesh elements generation, defining the boundary conditions and loading conditions.
- Processing: Once the model is defined, a computer's software/hardware capabilities are used to solve the previously discretized equations and obtain the numerical solution.
- Post-processing: The results obtained are exported and analyzed. Considering the results obtained may be necessary to make some modifications and repeat the simulation process.

The pre-processing includes four major steps Liu & Quek (2014); Rao (2018):

1. Geometry modeling: There are many ways to create the geometry, from providing points by Cartesian coordinates, lines, arcs, ..., to the use of Computer Aided Design (CAD) software packages. See image 5a.
2. Meshing: The mesh generation process, where the problem domain is divided into several small pieces, called elements. This step is also known in the literature by discretization, because the domain of the problem is divided into discrete elements. Elements usually have simple geometries, such as triangles and quadrilaterals. The vertices of elements are called nodes. See image 5b.

   In this step it is necessary to choose the type, number, size and arrangement of the elements. Note that the element size is an important parameter, as the smaller the elements, the more accurate the results. However, the associated computational costs will be higher due to the increased the number of elements, increasing the simulation time.
3. Constitutive law: In this step, it is establish the law that defines the material behavior and the respective material constants. For example, for a thermal analysis, it is necessary to provide the thermal conductivity coefficient and the relation between stress and strain. On the other hand, if the analysis is structural (case study in the article), it is necessary to indicate the Young's modulus and shear modulus, and the relation between stress and strain. See image 5c.

4. Define boundary conditions: Boundary conditions (BC) are presented in the form of mathematical equations that provide the problem with a set of additional restrictions in certain boundaries. This boundaries can be geometric identities: points, lines or curves, surfaces, and solids or mesh identities: nodes, elements, element edges and element surfaces. For structure analysis problems (problem under study), the boundary conditions are displacements and loading conditions. For heat transfer problems, the conditions are temperature, heat flux, and convection boundary conditions. See image 5d.



(a) Geometry modeling (b) Meshing (c) Define material

(d) Define BC (e) Processing and Post-processing

Figure 5: FEA steps. Pre-processing: (a), (b), (c) and (d), and Processing and Post-processing: (e).

A.2 Solid Mechanics

Solid Mechanics studies the relationships between stresses and strains, displacements and forces, and stresses/strains and forces, for certain boundary conditions. In order to make the relationships easier to understand, the following definitions are presented:

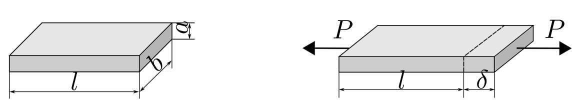
- Stress: Force per unit area. SI units: Pascal (Pa). It is equivalent to N/m² (SI). Considering the example of the axially loaded structure, Figure 6, the stress is equal to:

$$\sigma = \frac{P}{A} = \frac{P}{a \cdot b} \tag{1}$$

- Strain: Ratio between the deformation and the initial length. Deformation is the difference between the final and initial length. SI units: unitless. For the previous example, the strain is equal to:

$$\epsilon = \frac{\delta}{l} \tag{2}$$

- Displacement: Distance moved by a body in a given direction. SI units: Meter (m). Considering the same example, the displacement of the structure in the loading direction is equal to δ.



(a) Initial state (b) Final state

Figure 6: Uniaxially loaded structure.

A.3 Theory of Elasticity

Elastic materials are materials that deform when a force is applied and return to their initial position after the force is removed. In small deformation problems (strains are small compared to unity), where the deformation and load has a linear relationship, the case under study presents linear elasticity.

A.3.1 Constitutive relations

Materials can be anisotropic or isotropic. In the anisotropic materials the material property varies with the direction, while in the isotropic materials, this does not happen, the material property is not direction-dependent. To set the materials properties of the anisotropic materials several material constants are used, while an isotropic linear elastic material is characterized by only two independent elastic constants:

- Young's modulus (E): The Young's modulus is the elastic modulus in tension or compression. Measures the tensile or compressive stiffness of a solid material when the force is applied lengthwise. Is defined as the ratio of tensile/compressive stress (σ) to axial strain (ε). SI units: Pascal (Pa), It is equivalent to N/m^2 (SI);
- Poisson's ratio (ν): Poisson's ratio is the absolute value of the ratio of transverse strain to the corresponding axial strain resulting from uniformly distributed axial stress below the proportional limit of the material (the highest stress where the stress and strain are directly proportional). SI untis: unitless.