FRAUNHOFER-INSTITUT FÜR WERKSTOFFMECHANIK IWM

USER'S MANUAL OF PUCK ANALYSIS TOOL

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Verification of composite laminates under cryogenic thermo-mechanical loading – CCN

Final Report of CCN1

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1 Introduction

The failure analysis for structures designed from fiber reinforced polymers or fiber reinforced materials in general is commonly done by applying a failure criterion calculating the margin of safety (MoS) for the individual plies. The simplest failure criteria are the maximum strain or the maximum stress criteria and quadratic criteria like the Tsai-Wu criterion [Tsa71]. However, even though these criteria might give a good estimate of the critical loading state for multi-axial stress-states, they are formulated purely phenomenologically without any knowledge of the critical failure modes. In contrast to this, the Puck Failure Criterion [Puc98] is advantageous since it combines different individual failure criteria for different failure modes.

The Puck failure criteria differentiates between tensile and compressive fiber failure and inter fiber-failure. The latter is further divided into tensile failure, shear failure and compressive failure. For the practical application such a failure mode-based criteria has two main advantages: first of all, the fit to experimental data will be much better and thus the modeling error will be smaller. This has been demonstrated for ambient and cryogenic temperatures in [IWM18a, IWM19]. Second, the application of a failure-mode based criterion gives the designer important information not only on where the component might fail, but also on how this component (failure-mode) might fail. This in turn gives important information on how the component can be optimized with respect to its overall strength.

For the practical application of the Puck Failure Criterion for a failure analysis two things need to be done: First the material parameters for the failure criteria need to be estimated based on experimental data. Second the criteria need to be evaluated for the component under investigation using stress data obtained by the finite element method. Since the experimental data commonly shows a large amount of scatter, the first part is often the key challenge for a robust failure analysis.

The failure analysis tool "Puckfailure" helps with both, the parameter estimation, applying different numerical optimization strategies, as well as the evaluation of the structural integrity based on finite element results from Nastran.

This manual serves as a guideline to perform these three consecutive tasks, namely

1. Perform the experimental characterization at different temperatures (Chapter 5)
2. Use the Python Tool Module 1 "Puck Estimator" to determine the relevant material parameters for the Puck criterion (Chapter 4, and especially Chapter 4.2)
3. Use the Python Tool "FE Processor" to post-process results obtained by the Finite Element Code Nastran (Chapter 4, and especially Chapter 4.3)

In general Task 1 and 2 is only performed once for a certain material, while Task 3 is repeated for different components and different boundary conditions (loads, temperatures,…). Chapter 2 gives a short introduction of the Puck failure criterion for plane stress conditions and gives a short summary of the theoretical fundamentals of the applied optimization procedures. The reader familiar with the Puck failure criterion and optimization via the least-square method as well as the maximum likelihood method might want to skip this first chapter or might only want to consider the nomenclature (Section 2.4) used in this manual.

2
Puck's FRP failure criterion

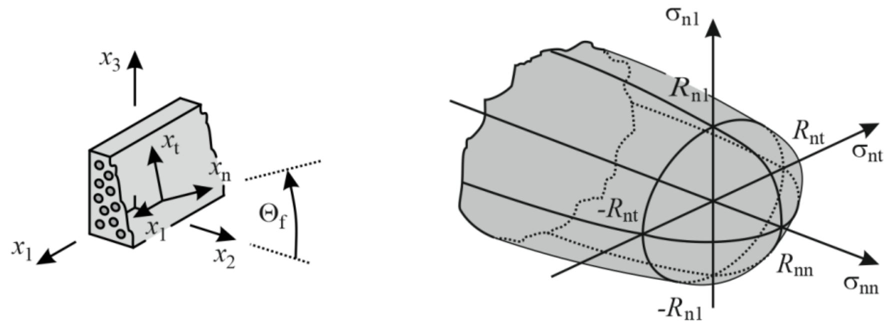
2.1
Basic ideas and general formulation

Puck and Schürmann formulated a mechanism-based failure criterion for unidirectional FRP plies [Puc98], [Puc02a], motivated by the theoretical and practical shortcomings of several earlier FRP failure criteria, which mostly use interpolations between selected failure points. For example, such failure points are the tensile and compressive strengths both longitudinal and transverse to the fiber direction, or the inter-fiber shear strength. For cases of multiaxial combined stress states, these strengths are interpolated by analytical (for example quadratic) functions. However, there is no physical background behind these functions. In contrast, Puck and Schürmann's criterion is based on failure mechanisms assuming that failure occurs either by fiber failure (due to either tension or compression), or by inter fiber failure within the matrix. The former results in a crack oriented normal to the fiber direction, whereas the latter results in an initially unknown fracture plane. Three different failure modes are distinguished at inter fiber failure, which depend on the transverse tensile stress σ_{22} as well as on the inter fiber shear stress σ_{12} and result in specific fracture modes. For the definition of the stress components σ_{ij} with $i,j \in \{1,2,3\}^2$ and $i,j \in \{1,n,t\}^2$ the reader is referred to Figure 1a.

Failure initiation within the **fiber direction** is assessed in terms of the two partial criteria

$$f_{\mathrm{ff}}(\boldsymbol{\sigma}) = \begin{cases} \frac{\sigma_{11}}{S_{11}^t} \leq 1 \text{ for } \sigma_{11} > 0, \\ \frac{|\sigma_{11}|}{S_{11}^c} \leq 1 \text{ for } \sigma_{11} < 0, \end{cases} \tag{1}$$

assuming failure in the context of the maximum stress criterion: failure is assumed when either of the partial criteria is violated, that is when the stress component σ_{11} within the fiber direction reaches the tensile or compressive strength S_{11}^t and S_{11}^c, respectively, irrespectively of the other stress components. Although S_{11}^t and S_{11}^c are associated with tensile and compressive stress, both are assumed to be positive here by definition.



(a) fracture plane (b) master failure surface

Figure 1: Puck failure criterion: The idea of the fracture plane and the master failure surface.

Perpendicular to the fiber direction, failure is assumed to occur in a "fracture plane" rotated by an *a priori* unknown angle Θ_f around the x_1-axis out of the x_1-x_2-plane (see Figure 1(a)). Using the standard formulae for coordinate transformation, the normal and shear stresses on the fracture plane are given by:

Puck's FRP failure criterion

$$\begin{pmatrix}\sigma_{nn}\\ \sigma_{nt}\\ \sigma_{n1}\end{pmatrix} = \begin{pmatrix} cos^2\Theta_f & sin^2\Theta_f & 2sin\Theta_f cos\Theta_f & 0 & 0\\ -sin\Theta_f cos\Theta_f & sin\Theta_f cos\Theta_f & cos^2\Theta_f - sin^2\Theta_f & 0 & 0\\ 0 & 0 & 0 & sin\Theta_f & cos\Theta_f \end{pmatrix} \begin{pmatrix}\sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{pmatrix} \tag{2}$$

For the stress vector (2) on the fracture plane, Puck and Schürmann [Puc98], [Puc02a] postulate a "master failure surface" according to

$$\begin{aligned} & c_2\left(\frac{\sigma_{nn}}{R_\perp^{tA}}\right)^2 + c_1\frac{\sigma_{nn}}{R_\perp^{tA}} + \left(\frac{\sigma_{nt}}{R_{\perp\perp}^{sA}}\right)^2 + \left(\frac{\sigma_{n1}}{R_{\perp||}^{sA}}\right)^2 \le 1 \qquad \text{for } \sigma_{nn} > 0\\ & \left(\frac{\sigma_{nt}}{R_{\perp\perp}^{sA}}\right)^2 + \left(\frac{\sigma_{n1}}{R_{\perp||}^{sA}}\right)^2 + 2p_{\perp\perp}^{(-)}\frac{\sigma_{nn}}{R_{\perp\perp}^{sA}} \le 1 \qquad \text{for } \sigma_{nn} < 0 \end{aligned} \tag{3}$$

where R_{nn}, R_{nt} and R_{n1} are the normal and shear strengths in the fracture plane coordinate system according to Figure 1(b). The inclination angle Θ_f for the fracture plane needs to be determined such that the most critical stress state develops, i.e. it is assumed that always such a failure mode develops that failure occurs at the earliest possible instant. Usually, the determination of the failure plane inclination angle Θ_f requires an iterative procedure (e.g. Wiegand et al. [Wie08]). Within this procedure, the angle is chosen such that the state point $(\sigma_{nn},\ \sigma_{nt},\ \sigma_{n1})$ is found at the closest possible position to the master failure surface (3) according to Figure 1 (b).

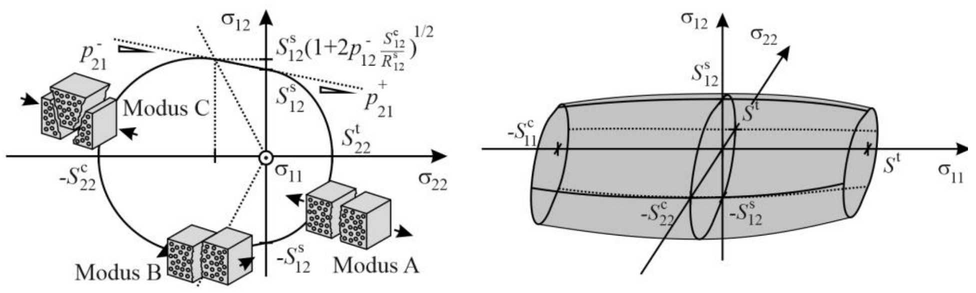
2.2
Failure envelope for plane stress states

In many cases in the integrity analysis of composite laminates, the consideration of plane stress states with $\sigma_{33} = \sigma_{23} = \sigma_{13} = 0$ is sufficient since for plane structures, no pronounced stresses acting transversely to the laminate plane develop. In this case, an analytical solution to the optimization problem for the determination of the failure plane angle Θ_f can be derived (Puck and Schürmann [Puc98], [Puc02a]). In this case, the inter fiber failure criteria are obtained for the three inter fiber failure modes A, B and C. In this context, mode A describes a tensile failure mode with a complete separation of the specimen. Mode B describes a shear failure mode without or with limited friction of the failure surfaces due to a possible compressive normal load. Mode C describes a failure of the laminate ply under compression, occurring locally by means of a wedge-like shearing mode. The Failure modes are also illustrated in Figure 2(a). The individual failure criteria are assembled to a continuous, but not necessarily smooth, joint failure surface as follows:

$$f_{\mathrm{iff}}(\boldsymbol{\sigma}) = \begin{cases} \left(\left(\frac{\sigma_{12}}{S_{21}^s}\right)^2 + \left(1 - p_{21}^+\frac{S_{22}^t}{S_{21}^s}\right)^2\left(\frac{\sigma_{22}}{S_{22}^t}\right)^2\right)^{\frac{1}{2}} + p_{21}^+\frac{\sigma_{22}}{S_{21}^s} \le 1, & \text{if } \sigma_{22} > 0 \ \text{(Mode A)}\\ \left(\left(\frac{\sigma_{12}}{S_{21}^s}\right)^2 + \left(p_{21}^-\frac{\sigma_{22}}{S_{21}^s}\right)^2\right)^{\frac{1}{2}} + p_{21}^-\frac{\sigma_{22}}{S_{21}^s} \le 1, & \text{if } 0 \le \left|\frac{\sigma_{22}}{\sigma_{21}}\right| \le \frac{\sigma_{22}^A}{|\sigma_{21}^C|} \ \text{(Mode B)}\\ \left(\left(\frac{\sigma_{12}}{2(1+p_{22}^-)R_{21}^s}\right)^2 + \left(\frac{\sigma_{22}}{S_{22}^c}\right)^2\right)\frac{S_{22}^c}{-\sigma_{22}} \le 1, & \text{if } 0 \le \frac{\sigma_{21}}{\sigma_{22}} \le \frac{|\sigma_{21}^C|}{\sigma_{22}^A} \ \text{(Mode C)} \end{cases} \tag{4}$$

$$\text{with } R_{22}^A = \frac{S_{22}^C}{2(1+p_{22}^-)} \quad \text{and} \quad \sigma_{21}^c = S_{21}\sqrt{1+2p_{22}^-}. \tag{5}$$

The corresponding joint failure envelope for the inter fiber modes is Illustrated in Figure 2(a) and the full three-dimensional failure envelope, including the fiber failure modes is Illustrated in Figure Figure 2(b).



(a) inter fiber failure envelope

(b) complete failure envelope

Figure 2: Puck criterion, failure envelope for plane stress states.

In Equation (4) the material strength R_{nn}, R_{nt} and R_{n1} related to the fracture plane (Equation (3)) have been replaced by the inter fiber tensile S_{22}^t, compressive S_{22}^c and shear strength S_{12}^s, respectively. Whereas the latter is related to the stress state of the local material coordinate axis. The parameters p_{21}^+, p_{21}^- are additional material parameters describing the slope of the inter fiber failure envelope towards the positive and negative side of the σ_{12}-axis and p_{22}^- implicitly describes the position of the intersection between modes B and C (Figure Figure 2(a)). This parameter is related to the other parameters by

$$p_{22}^- = \frac{1}{2}\left(\left(1 + 2p_{21}^- \frac{S_{22}^c}{S_{21}^s}\right)^{\frac{1}{2}} - 1\right) \qquad (6)$$

and does not provide an independent material parameter.

So far no interaction between the inter fiber failure mode (Equation (1)) and the fiber failure mode (Equation (4)) have been considered. From a physical point of view, such a coupling might occur since single fibers are breaking long before the material globally fails at $S_{11}^{t,c}$, causing microcracks in the matrix and fiber-matrix interface failure in the vicinity of the fiber breaks. These in turn will reduce the strength of the material transverse to the fiber direction compared to the undamaged material. These interactions can be easily introduced into the Puck model in a phenomenological way by scaling the Puck function for the intra fiber failure modes (Equation (4)) with a weakening factor f_w as

$$\tilde{f}_{\mathrm{iff}}(\boldsymbol{\sigma}) = \frac{f_{\mathrm{iff}}(\boldsymbol{\sigma})}{f_{\mathrm{w}}(\boldsymbol{\sigma})} \quad \text{with} \quad f_w(\boldsymbol{\sigma}) = 1 - \left(0.9 f_{\mathrm{ff}}(\boldsymbol{\sigma})\right)^n \quad \text{and} \quad n > 0. \qquad (7)$$

The parameter n describes the narrowing of the failure envelope along the x_1-axis towards the tensile and compressive strengths S_{11}^t and S_{11}^c (see Figure 2(b)). This means that the size of the inter fiber failure envelope – which is illustrated in Figure 2(a) for $\sigma_{11} = 0$ – is decreased if high longitudinal stresses σ_{11} occur.

The value of the parameter n is not further described by Puck and Schürmann [Puc98, Puc02a] and in general it must be determined from experimental data. While explicitly stating that this might not be fully justified, Puck and Schürmann apply the same degradation for tensile and compressive stresses.

Compared to the classical more phenomenological failure criteria like the Tsai-Hill or Tsai-Wu criteria [Tsa71], [Tsa80], Puck's criterion has the advantage of a strictly mechanistic foundation. Furthermore - due to its mechanistic foundation - Puck's criterion, if violated, allows to decide about the active failure mode and thus the underlying mechanism (tensile or compressive fiber failure or inter fiber failure in either of the modes A, B or C). By this means, strategies for an appropriate improvement of the structure under consideration can be derived directly from the results of the integrity analysis.

2.3 The Reserve Factor and Margin of Safety

For the practical application of a structural integrity analysis the reserve factor and the margin of safety have been adopted as the main measures of interest. The reserve factor R is defined as the ratio between the actual load (stress) and the failure load (stress), i.e.

$$R f_{\max}(\boldsymbol{\sigma}) = 1 \quad \text{with} \quad f_{\max}(\boldsymbol{\sigma}) = \max\{f_{IFF}, f_{FF}\}. \tag{8}$$

Assuming a linear behavior, a reserve factor $R > 1$ means the load can be increased by a factor R until failure occurs, a value of $R = 1$ means that failure occurs at the considered load and a value of $R < 1$ means that the Load must be reduced by a factor of R to prevent failure. The margin of safety is defined as

$$MoS = R - 1 = \frac{1 - f_{\max}(\boldsymbol{\sigma})}{f_{\max}(\sigma)} \tag{9}$$

And similar, a value of $mos > 0$ means the load can be increased before failure occurs and a value of $mos \leq 0$ means that failure occurs without further reducing the external load or increasing the material strength.

2.4 Material Parameters

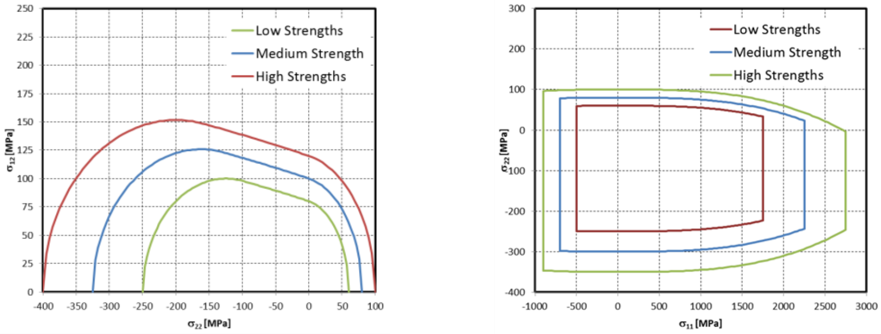
The independent material parameters of the Puck failure criterion for plane stress states are summarized in the following Table

Parameter	Description
S_{11}^{c}	Compressive strength in fiber direction
S_{11}^{t}	Tensile strength in fiber direction
S_{22}^{c}	Compressive strength perpendicular to the fiber direction
S_{22}^{t}	Tensile strength perpendicular to the fiber direction
S_{12}^{s}	In-Plane shear strength
p_{12}^{+}	Slope of Mode A failure
p_{12}^{-}	Slope of Mode B failure
n	Weakening factor for fiber failure – inter fiber failure interaction

The way the parameters define the Puck's inter fiber failure envelope and Puck's biaxial failure envelope is illustrated in the following. The procedure to determine these parameters by the FE-Puck evaluation tool is described later in Chapter 4 and 4.2.

In Figure 3 the effects of the leading strengths values – namely the longitudinal tensile and compressive strengths values S_{11}^{t} and S_{11}^{c}, the transverse tensile and compressive strengths values S_{22}^{t} and S_{22}^{c}, and the inter fiber shear strength R_{21}^{s} – are illustrated by means of a stepwise increase of these values. Increasing strength values results in an overall widened inter fiber failure envelope without any effect on the envelope's shape.

Regarding the biaxial failure envelope, however, increasing the strength values widen the envelope, but also increase the dependence of the transverse strength on the longitudinal stress component σ_{11} as long as the parameters n in Equation (7) is kept constant.



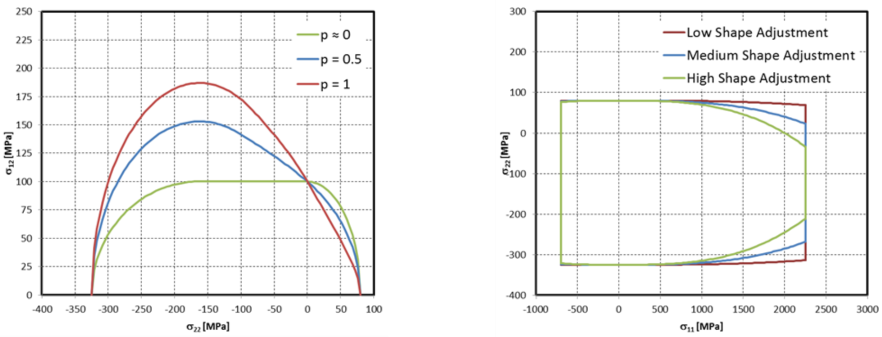
(a) inter fiber failure envelope, i.e. cross section of Figure 2a

(b) biaxial failure envelope, i.e. cross section of Figure 2b

Figure 3: Effects of the strength parameters on the failure envelopes.

Figure 4 shows the influence of the shape parameters on the inter fiber failure envelope as well as on the biaxial failure envelope, based on constant strength values. Regarding the inter fiber failure envelope in Figure 4(a), the shape parameter p_{21}^{-} describes the envelope’s slope in the mode B section ($\sigma_{22} < 0$). Since there is a smooth transition from the mode C section to the mode B section, p_{21}^{-} also describes the envelope’s shape in the mode C section. The shape parameter p_{21}^{+} describes the envelope’s initial slope in the mode A section ($\sigma_{22} \geq 0$) at $\sigma_{22} = 0$. A smooth transition from the mode B to the mode A section is usually desired, *i.e.* the two parameters are equal $p_{21}^{+} = p_{21}^{-}$.

Figure 4 (b) shows the influence of the transverse strength degradation in the biaxial failure envelope. Here, the least pronounced degradation curve (Low Shape Adjustment, very high exponent n in (7)) results in a shape near a corresponding maximum stress criterion.



(a) inter fiber failure envelope

(b) biaxial failure envelope

Figure 4: Effects of the shape parameters on the failure envelopes.

3 Optimization Procedures for Parameter Estimation

For the estimation of the Puck parameters two methods are available. The first one is a very simple estimation using the well-known method of least square optimization. The second method uses the so called maximum likelihood estimation. Within this second approach it is also possible to calculate a confidence Interval as well as to consider additional boundary conditions resulting in a conservative estimation. The theoretical details of the Maximum Likelihood estimation procedure is described in the following.

3.1 Maximum Likelihood Estimation

The principle of the maximum likelihood estimation is as follows [Aldrich1997]: By assuming a probability density function $\rho(\boldsymbol{\sigma}_i, \boldsymbol{\theta})$ for the scatter of the experimental data $\boldsymbol{\sigma}_i, i = 1, \dots, n$, the maximum likelihood method calculates the Puck parameters $\boldsymbol{\theta}$ that most likely will result in the given experimental data.

For this, the probability is measured by the so-called likelihood function

$$L(\boldsymbol{\theta}; \boldsymbol{\sigma}) = \prod_{i=1}^{n} \rho_i(\boldsymbol{\theta}; \boldsymbol{\sigma}_i) \tag{10}$$

which is the joint probability of the n independent measurements $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}$ is the array collecting all experimental data points. Note that in contrast to the probability density function itself, the Puck material parameters act here as the variable, whereas the measurements are seen as the (fixed) parameters of the likelihood functions. Thus, the likelihood function measures how likely the given experimental data will result from a probability density with statistical parameters $\boldsymbol{\theta}$.

An estimation for the Puck parameters is then simply obtained by maximizing the logarithm of the likelihood function

$$\boldsymbol{\theta} = \arg\max_{\boldsymbol{\theta}\in\mathcal{G}}(\ln\big(L(\boldsymbol{\theta}; \boldsymbol{\sigma})\big) = \arg\min_{\boldsymbol{\theta}\in\mathcal{G}}(-\ln\big(L(\boldsymbol{\theta}; \boldsymbol{\sigma})\big). \tag{11}$$

In here $\mathcal{G}$ is the space of (physically) admissible material parameters, and the logarithm is chosen for computational reasons since the product in Equation (10) becomes a summation which is computationally more stable. As a general boundary condition to the optimization problem (11) it is required, that the slope of both, the Mode A and the Mode B failure condition is negative at $\sigma_{22} = 0$, which is equivalent to

$$p_{21}^{-} > 0 \text{ and } p_{21}^{+} > 0. \tag{12}$$

Finally, to solve this optimization problem an additional assumption on the probability density function $\rho(\boldsymbol{\sigma}_i, \boldsymbol{\theta})$ is required. In general, the user of this tool will have access to insufficient data to perform a statistic hypothesis test. But since the experimental data $x_i, i = 1, \dots, n$ represent the measurements from uniaxial tensile tests and these are found to follow a normal distribution [Liang2018], the assumption that the test data follows a normal distribution is adopted here.

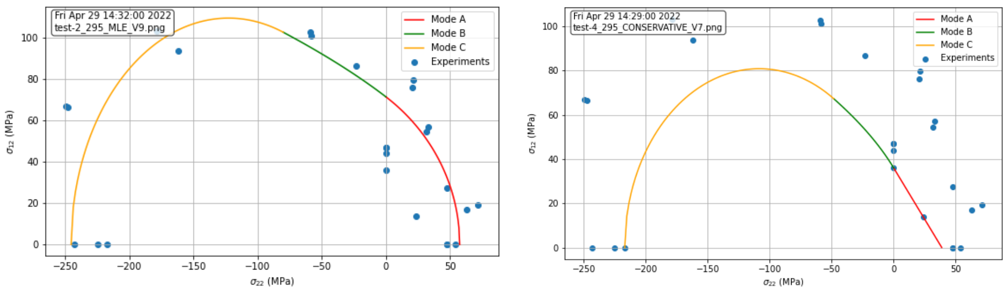
To solve the optimization problem a sequential least squares programming method complemented with a basin-hopping approach, as provided by the "basinhopping" method together with the SLSQP method from the python scipy library, is used. Details of the implementation can be found in the scipy documentation. This optimization algorithm is chosen since it allows to find the global minima of constrained optimization problems considering the boundary conditions given in Equation (12) and (13).

Figure 5 shows an example of the Puck failure envelope obtained by the maximum likelihood for the standard approach and the conservative approach described in the next section.

3.1.1 Conservative Estimation

As an additional variant of the previously described parameter estimation using the maximum likelihood approach, a conservative estimation procedure is applicable. This conservative procedure results in Puck material parameters that represent a strict lower bound of the experimental data. This is realized by further restricting the admissible parameter space $\mathcal{G}$ by the constraint that the Puck criterion is larger or equal to 1 for all given experimental data points:

$$f(\boldsymbol{\sigma}_i) \geq 1 \quad \forall \mathrm{i} = 1, \dots, \mathrm{n}. \tag{13}$$



(a) Puck failure envelope using the maximum likelihood method

(b) Puck failure envelope using the maximum likelihood method together with the conservative boundary condition

Figure 5: Comparison of the standard maximum likelihood method and the conservative approach

3.1.2 Confidence Interval Calculation

In addition to the estimation of the Puck parameter themselves, the likelihood approach is also applied to estimate the confidence interval of the estimated parameters. For this an α-confidence interval $CI_i = [\theta_L^i, \theta_U^i]$ is calculated for every parameter θ^i such that this parameter lays within this interval with a probability of α:

$$P\left(\theta_L^i \leq \theta^i \leq \theta_U^i\right) = \alpha. \tag{14}$$

In this tool, the interval is calculated by applying the so-called Profile-Likelihood method [Ven88] which calculates upper and lower bounds θ_U^i and θ_L^i for every parameter θ^i individually such that

$$CI_i = \left[\theta_L^i, \theta_U^i\right] = \{\theta^i : L_{PL}(\Theta_i) - L(\widehat{\boldsymbol{\Theta}}) \leq q_k(\alpha)\} \tag{15}$$

In here, $\widehat{\boldsymbol{\Theta}}$ is the solution (11), $q_k(\alpha)$ is the (α)th quantile of the χ^2 distribution for k degrees of freedoms and $L_{PL}(\Theta_i)$ is the profile likelihood function for the parameter of interest θ_i:

$$L_{PL}(\Theta_i) = \max_{\boldsymbol{\Theta} \in \Psi(\Theta_i)} L(\boldsymbol{\Theta}). \tag{16}$$

The latter is nothing else then the maximum likelihood problem where the parameter Θ_i is held constant. In the implementation Θ_i according to (15) is found by incrementally increasing (decreasing) by $\Theta_i = \Theta_i \pm h$ for the lower (upper) bound until a Θ_i is found that fulfills

$$L_{PL}(\Theta_i) - L(\widehat{\boldsymbol{\Theta}}) \leq q_k(\alpha). \tag{17}$$

As a default value the tool tries to determine the 95% confidence interval ($\alpha = 0.95$), however if the scatter of the experimental data is large, this can result in unphysical (negative) Puck material parameters, that are violating (12) or Puck material parameters that are resulting in failure envelopes that are crossing each other. In such a case α is automatically reduced (until α = 0.3) until upper and lower limits are found that result in physically admissible upper and lower limits.

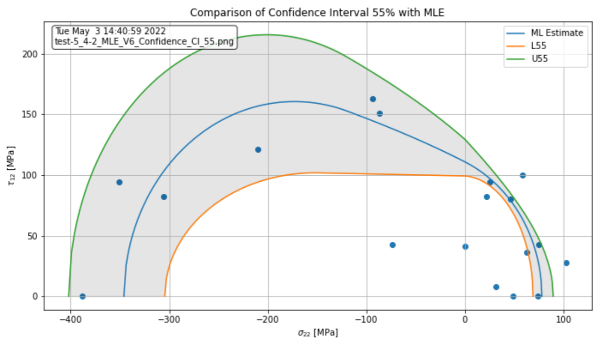


Figure 6: Maximum Likelihood estimation of Pucks failure envelope together with the 55% confidence interval.

4 FE-Puck Evaluation Tool

4.1 Getting Started

4.1.1 Overview

The FE-Puck evaluation tool consists of two individual modules. The first module, the Puck Estimator, is used to determine the Puck material parameters as a best fit to given experimental data. The second module, the FE-Processor, is used to run a structural integrity analysis using stress field data from the FE Solver MSC Nastran in the hdf5-file format (https://www.hdfgroup.org/solutions/hdf5/). For this, the Puck Failure criterion is evaluated for all elements (or certain subsets with user specified materials ids) and the resulting margin of safety is stored in an amended version of the h5 FE Results File given from MSC Nastran. This file can then be used to further post-process the margin of safety using the post-processor Patran or by Python using the h5py package. Additionally, a csv output file (the Margin of Safety File) is generated summarizing the Margin of Safety as well as the most critical failure mode according to Chapter 2.2.

Both modules, the Puck-Estimator and the FE-Processor, can be executed individually or sequentially whereas in the latter case the output from the Puck estimator, namely the estimated Puck material parameters, are automatically used to run the structural failure analysis. The dataflow for both, the full analysis using both modules and the individual use of one of the tools is illustrated in Figure 7. If temperature dependency needs to be considered, either the experimental data (as an input for the Puck-Estimator) or the Puck material parameters (as an Input for the FE-Processor) needs to be given for several temperatures. If either of these datas is given for (at least) 2 temperatures, the Puck-Estimator interpolates (or extrapolates) the data for the required temperatures during the calculation of the margin of safety considering the Temperature field data from the FE Result.

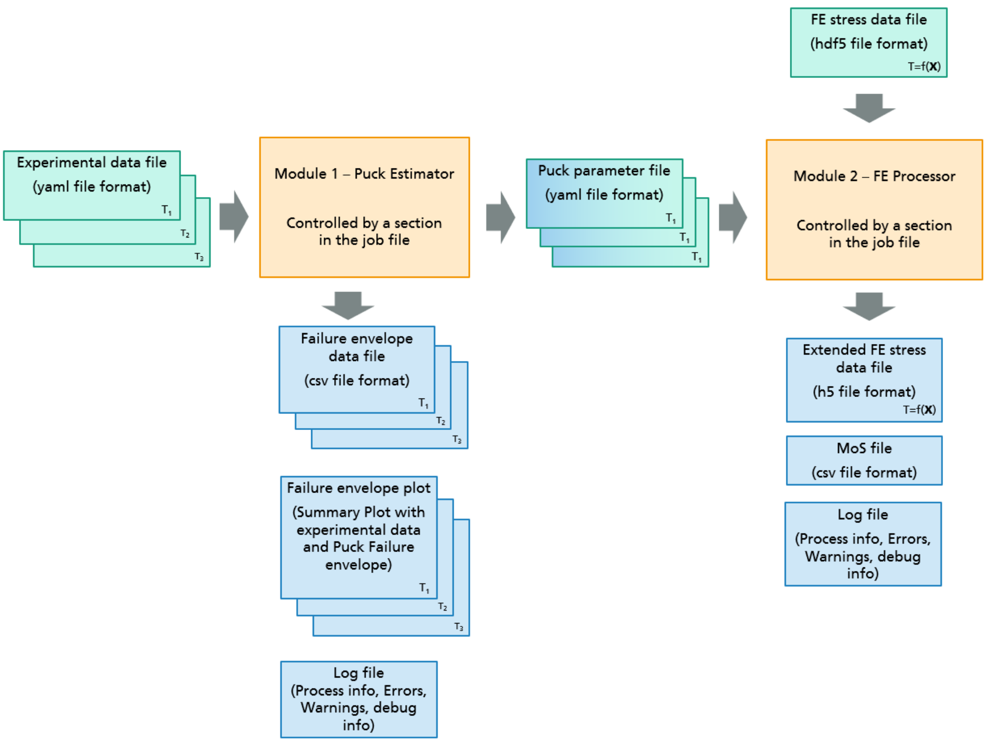


Figure 7: Data flow FE Puck evaluation tool, the colors refer to Input (green), processing (yellow) and output (blue).

4.1.2 Installation for users

Unpack the zip folder to your preferred folder. The tool itself can be found in the subfolder **`\bin`** subfolder (see next section). Since the tool is started from the command window you might want to add the folder to your PATH variable of your system to easy access the tool from every folder.

4.1.3 Running the Tool from the Command Line

The tool is started from the command line by running **`PuckFailure.exe`** from the folder **`\bin`**, or if you added this folder to the PATH variable by simply running **`PuckFailure.exe`**. The Job-File with the defined job parameters is referred to by the **`--job`** argument:

```
your_installation_path\bin\PuckFailure --job=your_job_file.job
```

Additional (optional) parameters are:

`--work:` Predefines the working directory where all results are stored, default is current-directory/results

`--estimator` or **`--e:`** executes only the Puck Estimator tasks

`--feproc` or **`--f`**: executes only the FE Processor tasks

4.1.4 The Job-File

The tasks that need to be executed from the Puck tool are defined in a **`*.job`** file. The general structure of such a job file is shown in **Fehler! Verweisquelle konnte nicht gefunden werden.**. In here, different, consecutive or non-consecutive, tasks can be defined. Every task, always starts with a task name in square brackets **`[task-name]`**, followed by the definition of the task by the keyword **`task`**. Two tasks are implemented in the tool, which can be activated by assigning the task value **`puck-estimator`** or **`fe-processor`** to the **`task`** keyword.

For the Puck Estimator the input needs to be supplemented with a link to a **`*.yaml`** file by the keyword **`exp_data`** containing the relevant experimental data (see Section 4.2.2).

For the **`fe_processor`** task, the Puck parameter file parameters (see section 4.2.3 and 4.3.2) in the yaml-format and the FE results file in hdf5-format (.h5) are used as input. The Puck Parameter File is referenced via the **`puck`** keyword of the task. This file can be created by a previous performed puck-estimator task or by hand. The FE Results File is generated by MSC Nastran by a static analysis with a model containing composite laminate elements of which the properties are defined with PCOMP property cards. The FE Results File is referenced through the **`fe_data`** keyword of the fe-processor task.

The example in shown in **Fehler! Verweisquelle konnte nicht gefunden werden.** is a minimal working example, further (optional) keywords are available to control the execution and the output of the Puck Tool. These are detailed in Section 4.2.1 for the Puck Estimator and in Section 4.3.1 for the FE Processor.

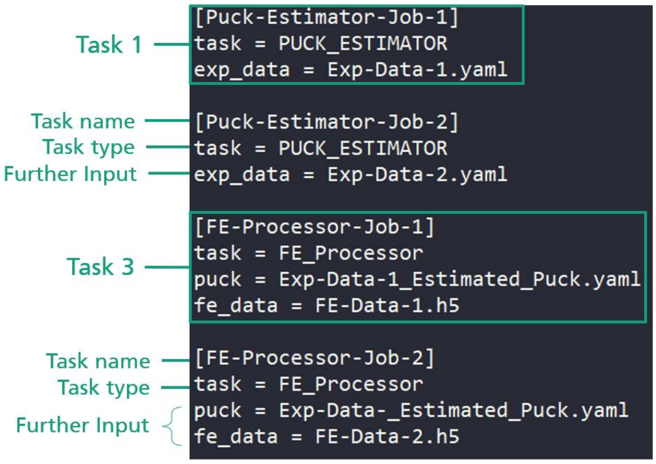


Figure 8: Structure of the Job File defining the different tasks that should be executed from the Puck Tool. Here four tasks (two Puck Estimators and two FE-Processors) with different input data are defined.

4.1.5 The Log file

All diagnostics during the execution of the tool are logged in the log-file. The log file contains an echo of the provided job-file and any warning of error messages. The developers tried to complement the error message as good as possible with instructions on how to solve the problem. The log-file gets the name of the job file in which the file name extension of the job-file is replaced with ".log".

4.1.6 Output Storage and Naming Convention

By default, all output data generated by the Puck Tool is stored in a (possible new generated) subfolder `'/Results'` stored in the current working directory. In here the results are further sorted according to the task names specified in square brackets (See Section 4.1.4). As an alternative a non-default result folder can be specified by the keyword **`results`** (See Section 4.2.1.9 and 4.3.1.8).

The files themselves are either named according to the task name (with additional information as a suffix) for the Puck estimator or according to the given h5 FE Stress Data File used for the failure analysis with the FE Processor (with the suffix _puck). In the latter case a copy of the FE Stress Data File is generated to ensure that existing FE results are not affected in case the program evaluation is interrupted or fails (which of course should never happen).

If any result file already exists in the specified (or default) result folder, for example from a previous run, the existing file is renamed with an appending `'_V1'`. If this also exists, the file is renamed with `'_V2'` and so forth. By this, the newest result file never has an appending `'_Vx'` whereas the older files are sorted with increasing version numbers.

4.2 The Puck Estimator

The purpose of the Puck estimator is to determine the Puck failure envelope material properties based on given experimental data. The following sub-sections describe the keywords to control the execution of the Puck Estimator task. The Puck Estimator task can be activated by assigning the value **`puck_estimator`** to the keyword "task".

4.2.1 Input - Job-File

4.2.1.1 Keyword task

Keyword	**task (mandatory)**
Description	Defines the task to be executed from the Puck Tool
Restrictions	Requires experimental data, either referred by the exp_data keyword
Allowed values	
puck_estimator	Estimates the Puck material parameter based on the given experimental data. Data must be provided by the exp_data keyword

4.2.1.2 Keyword exp_data

Keyword	**exp_data (mandatory)**
Description	Specifies the Experimental Data File with the experimental data used to estimate the Puck material parameters. See Section 4.2.2 for details on the Experimental Data File format
Restrictions	-
Allowed Values	
Filename	The filename of the Experimental Data File. This file is expected to be in the current directory
Relative Path	A relative path to the Experimental Data File, for example: `'inputdata/dataset1/expData_t1.yaml'`
Absolute Path	An absolute path to the Experimental Data File, for example: `'D:/inputdata/dataset1/expData_t1.yaml'`

4.2.1.3 Keyword excl_data

Keyword	**excl_data (optional)**
Description	This keyword specifies the experimental data to be excluded for the parameter estimation procedure
Restrictions	-
Allowed Values	
List	A list of experimental data points to be excluded in the format **`Temperature:{ID1,ID2,…}`** Example 1: The experimental data points at temperature 4.2K with IDs 10,17,55 are excluded by **`excl_data = 4.2:{10,17,55}`** Example 2: The experimental data points at temperature 4.2K with IDs 10,17,55 and the experimental data points at temperature 295K with IDs 4,17,22 are excluded by **`excl_data = 4.2:{10,17,55},295:{4,17,22}`**
Range	If the data to be excluded is a consecutive list, the IDs can also be defined in a numpy.arange() style. The format is

	`Temperature:{first-ID (inclusive), last-ID (exclusive): increment (default=1)}` Example: The experimental data points at 4.2K with IDs 5,6,7,8,9,10 can be excluded by **`excl_data = 4.2K:{5,11}`**

4.2.1.4 Keyword add

Keyword	**add (optional)**
Description	The **`add`** keyword specifies an existing Puck Failure Envelope File of which the data will be added to the Puck failure envelope data that is going to be generated in the current run. The Experimental Data File may contain test data for a certain temperature and at the same time the referenced Puck Parameter File also contains a failure envelope for the same temperature. If these two Puck failure envelopes have the same estimation type (see keyword **`est_type`**), the Puck failure envelope will be regenerated and the existing Puck failure envelope from the reference Puck Parameter File will not be used.
Restrictions	-
Allowed Values	
filename	The Experimental Data File, this file is expected to be in the current directory
relative path	A relative path to the Experimental Data File, for example: `'inputdata/dataset1/expData_t1.yaml'`
absolute path	An absolute path to the Experimental Data File, for example: `'D:/inputdata/dataset1/expData_t1.yaml'`

4.2.1.5 Keyword est_type

Keyword	**est_type (optional)**
Description	Selects the algorithm to be used for the Puck parameter estimation.
Restrictions	The chosen algorithm is only applied for the estimation of the intra-fiber failure material parameters (see Equation (4)). The parameters for the fiber failure mode (S_{11}^t and S_{11}^c) are simply calculated as the mean value (**`MLE`**, **`LSE`**) or as the minimum value (**`conservative`**) of the corresponding tensile and compression test data. The same holds irrespective of the chosen failure type (keyword failure_type). The interaction parameter n is not estimated by any of the implemented algorithms, if needed, n can be added by hand using a text editor.
Allowed Values	
`MLE` (default)	Use the maximum-likelihood estimation procedure
`LSE`	Use the least-square estimation procedure

`conservative`	Use the maximum-likelihood estimation procedure with the additional constraint that the resulting Puck value for all provided data points must be greater than one, i.e. all experimental data points must lay outside of the resulting Puck failure envelope.

4.2.1.6 Keyword failure_type

Keyword	**Failure_type (optional)**
Description	Specifies for which type of failure(s) (i.e. Intra-fiber failure, fiber failure or both together) the Puck parameters should be estimated.
Restrictions	A routine to determine both, the intra fiber failure and the fiber failure together with the interaction parameter n (see Equation (7)) is not available. Thus the parameter value **`iff_weak`** is only available for the FE Processor and not for the Puck Processor (see Section 4.3.1.5).
Allowed Values	
`FF_only`	Only the parameters (S_{11}^t and S_{11}^c) for the fiber failure mode are estimated (see Equation (1)).
`IFF_only` (default)	Only the parameters for the intra fiber failure mode ($S_{22}^c, S_{22}^t, S_{12}^s, p_{12}^+$, and p_{12}^-) are estimated (see Equation (4)).
`IFF_FF`	Both the parameters (S_{11}^t and S_{11}^c) for the fiber failure mode and the parameters for the intra fiber failure modes ($S_{22}^c, S_{22}^t, S_{12}^s, p_{12}^+$, and p_{12}^-) are estimated (see Equation (1) and (4)).

4.2.1.7 Keyword confidence

Keyword	**confidence (optional)**
Description	Specifies if a confidence interval should be calculated. The upper and lower limits of the confidence interval is added as a new section (**`CONFIDENCE_LOWER-BOUND`** and **`CONFIDENCE_UPPER-BOUND`**) to the Puck Parameter File. Furthermore the limits are added to the resulting failure envelope plots.
Restrictions	The confidence interval calculation is only available for the maximum likelihood estimation procedure (**`est_type=MLE`**). By default, the tool aims at calculating the $\alpha = 95\%$ confidence interval. If the scatter of the given experimental data is large this might fail and result in unphysical bounds (see Section 3.1.2 for details). In that case the tool automatically reduces α and restarts the confidence interval estimation. If α becomes smaller then 50% this iterative procedure is stopped and the confidence interval calculation is terminated.
Allowed Values	
`true`	Confidence interval is calculated
`false` (default)	Confidence interval is not calculated

4.2.1.8 Keyword plot_info

Keyword	**plot_info (optional)**

Description	Selects the additional information to be added to the resulting Puck failure envelope plots
Restrictions	-
Allowed Values	
`ID`	The ID, as provided by the Experimental Data File, is printed next to the plotted experimental data points. This helps to identify experimental data points to exclude from the estimation by the keyword excl_data
`Puck`	The resulting Puck values are printed next to the experimental data points
`false` (default)	No additional information is added to the plot

4.2.1.9 Keyword results

Keyword	**results (optional)**
Description	Specifies a path to the result directory where the output data is stored. If no path is provided a new directory "Results" is created where a subfolder, labelled with the taskname specified in the Job File, is created for every task of the current job.
Restrictions	-
Allowed Values	
relative path	A relative path to the result directory, for example: `'output-data/myResults'`. Use `'./'` to save the results in the current directory
absolute path	An absolute path to the result directory, for example: `'D:/failure-analysis/outputdata/myResults'`

4.2.2 Input - the Experimental Data File

The experimental data for the Puck estimation tool is given by a hierarchic yaml file which is structured as shown in Figure 9. It consists of 3 levels, whereas each sub-level needs to be indented by two preceding spaces.

The first level specifies the temperature in Kelvin, this block can be repeated several times. In case there exists more than one temperature block the parameter estimation is executed for every temperature individually.

The second level specifies the experiment type. Here a number between 0 and 90 (degrees) can be given specifying the fiber orientation with respect to the loading axis. Alternatively, one can specify experimental data from a shear experiment by the keyword Shear.

The third level specifies an experiment ID together with the corresponding experimental value (failure stress). The given experimental IDs within a temperature block must be unique but not necessary consecutively numbered.

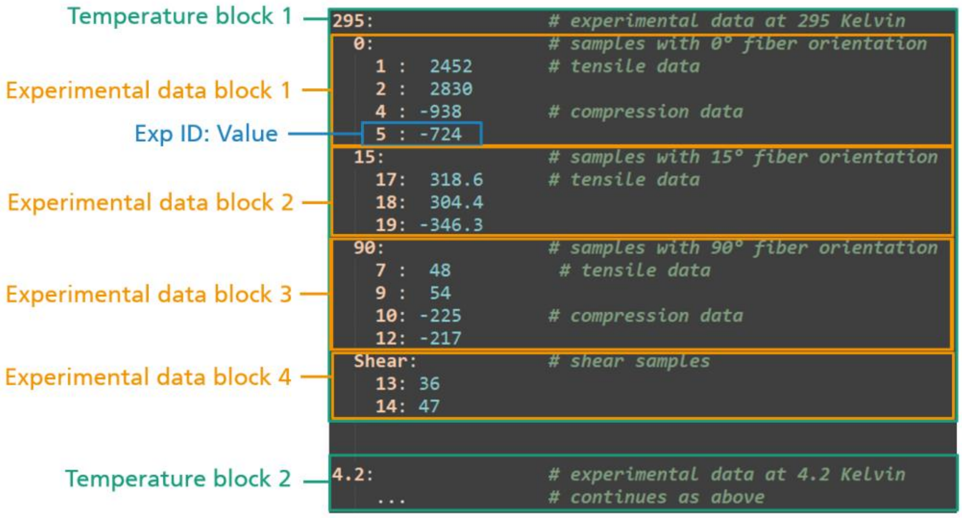


Figure 9: Structure of the Experiment Data File specifying the experimental input for the Puck estimation procedure

4.2.3 Output – the Puck Parameter File

The output is stored in the same yaml file format as the experimental data is given as an input (Section 4.2.2). Again, the result is organized in three levels whereas each sub-level needs to be indented by two preceding spaces (Figure 10). The first level specifies the temperature, the second level specifies the applied estimation type (MLE, LSE, CONSERVATIVE or CONFIDENCE_LOWER-BOUND and CONFIDENCE_UPPER-BOUND for the confidence intervals). The parameter declaration is as summarized in Section 2.4.

This Puck Parameter File, as generated by the Puck Estimation tool can be directly used as an input for the FE-Evaluation Tool (see Section 4.3 and 4.3.2) without any additional changes.

```
295:
  CONFIDENCE_LOWER-BOUND:
    P12NEG: 0.0172
    P12POS: 0.0773
    S12SHEAR: 99.2394
    S22C: 304.456
    S22T: 68.8894
  CONFIDENCE_UPPER-BOUND:
    P12NEG: 0.7172
    P12POS: 0.8773
    S12SHEAR: 129.2394
    S22C: 401.956
    S22T: 89.3894
  MLE:
    P12NEG: 0.4171954319
    P12POS: 0.4172954319
    S12SHEAR: 110.7393818019
    S22C: 345.9560129798
    S22T: 77.8894402011

4.2:
...  # continues as above
```

Figure 10: Structure of the Puck Parameter File containing the estimated Puck parameters

4.2.4 Output – the Puck Failure Envelope plot and the Puck envelope data file

Beside the Puck parameters written to the Puck Parameter File explained in Section 4.2.3, a plot of the resulting failure envelope in the σ_{22}, σ_{12}-space in generated for every estimated Puck parameter set. Additionally the underlying experimental data is added to the plot and, if requested by the keyword **`plot_info`**, the corresponding Puck value (Equation (4)) or the experiment id from Experimental Data File is plotted next to the data point.

In addition to the Puck failure envelope plot, the failure envelope data is written to the Failure Envelope Data File as discrete data point in the σ_{22}, σ_{12}-space.

4.3 The FE Processor

The purpose of the FE Processor is to post-process numerical results from the FE tool MSC Nastran. For this the FE Stress Data File with the file name extension ".h5" is read by the tool and the margin of safety is calculated for laminate composite elements of which the properties are defined with PCOMP cards, or only for specified parts (see keyword **`mat_id`** in Section 4.3.1.4). The margin of safety is then stored in a copy of the FE Stress Data File under the variable "failure_index". Additionally the csv Margin of Safety File , giving the margin of safety for every element together with additional information on the failure mode (mode A,B,C from Equation (4)), is generated.

4.3.1 Input - Job-File

4.3.1.1 Keyword task

Keyword	**task (mandatory)**
Description	Specifies the task to be executed from the Puck Tool
Restrictions	FE results must be provided by the keyword **`fe_data`** and Puck parameters by the keyword **`puck`**
Allowed values	
FE-Processor	Evaluates the margin of safety for given finite element results and Puck parameters.

4.3.1.2 Keyword fe_data

Keyword	**fe_data (mandatory)**
Description	Specifies the FE Stress Result File containing the finite element results to be post-processed
Restrictions	The provided FE Stress Result File must contain finite element results created by the MSC Nastran solver. In addition, the FE Stress Result File must contain stress data calculated by one of the following composite elements: cquad4, cquad8, ctria3, ctria6 The tool has been tested with results generated by the MSC Nastran Solver version 2021. Other Versions (newer and older) might work as well but were not tested.
Allowed values	
filename	The filename of hdf5 FE Stress Result File, this file is expected to be in the current directory
relative path	A relative path to the FE Stress Result File, for example: `'inputdata/dataset1/myFE-Results.h5'`
absolute path	An absolute path to the FE Stress Result File, for example: `'D:/inputdata/dataset1/myFE-Results.h5'`

4.3.1.3 Keyword puck

Keyword	**puck (mandatory)**
Description	Specifies one or more Puck Failure Envelope files containing the required parameters to describe the failure envelopes to be applied. For each material used by the plies of which the integrity has to be verified a Puck Failure Envelope file has to be provided. These input files can be generated by hand or can be obtained as an output from the Puck estimator (see Section 4.2.3). Note: if the Puck Parameter File is generated from a previous task in the same job file, the location where the Puck Parameter File is stored from this previous job needs to be specified a priori. This can be either the default path (generated in the current directory as `'/results/<<taskidenitifier>>'`) or the path specified by the **`result`** keyword (see Section 4.2.1.9).
Restrictions	If multiple Puck Parameter Files are given (see the List option below) these should be in the same order as the material ids specified via the **`mat_ids`** keyword. For material ids used in composite laminates in the FE model, but not referenced by the keyword **`mat_ids`**, a warning will be printed and the margin of safety for elements with the missing material ids are evaluated to NaN.
Allowed values	
filename	The filename of the Puck Parameter file, this file is expected to be in the current directory
relative path	A relative path to the Puck Parameter File, for example: `'puck = inputdata/dataset1/myPuckData.yaml'`
absolute path	An absolute path to the Puck Parameter File, for example: `'puck = D:/inputdata/dataset1/myPuckData.yaml'`

List	If different Puck datasets should be used for different materials (see above) a list of Puck Parameter Files can be provided, for example:
	`'puck = inputdata/myPuckData-mat1.yaml,`
	`        inputdata/myPuckData-mat2.yaml,`
	`        inputdata/myPuckData-mat3.yaml'`
	
	the items in the list do not necessarily need to be unique (can contain repeated datasets) if different material ids need to be evaluated based on the same Puck parameters.

4.3.1.4 Keyword mat_ids

Keyword	**mat_ids (mandatory)**
Description	Is used to relate the given Puck Parameter Files sets (keyword **`puck`**) to material ids used in the Nastran FE Model
Restrictions	For material ids used in composite laminates in the FE model, but not referenced by the keyword **`mat_ids`**, a warning will be printed and the margin of safety for elements with the missing material ids are evaluated to NaN. A reason for not including a material id in the list can be that this corresponding material is not UD fiber composite.
Allowed values	

Number	If only a single Puck Parameter File is given by the `puck` keyword, a single material id is expected.
List	If multiply Puck Parameter Files are given, the same number of material ids need to be given in the order corresponding to the order of the Puck Failure Envelope files specified via the `puck` keyword. The nth material id is considered to correspond to the nth Puck Failure Envelope file.

4.3.1.5 Keyword failure_type

Keyword	**failure_type (optional)**
Description	Specifies which failure type will be used for the integrity evaluation.
Restrictions	Depending on the chosen failure type different Puck material parameters are required in the Puck Parameter File (Section 4.3.2), these are specified below. If a parameter is missing an error will occur, if additional parameters are given that are not required by the chosen failure type a warning will be printed to the log file.
Allowed values	
`FF_only`	The margin of safety is calculated with respect to the fiber failure mode only (see Equation (1)). Required parameters are S11T and S11C (S_{11}^{t} and S_{11}^{c})
`IFF_only` (default)	The margin of safety is calculated with respect to the intra fiber failure mode only (See Equation (4)). Required parameters are ($S_{22}^{c}, S_{22}^{t}, S_{12}^{s}, p_{12}^{+}$, and p_{12}^{-}).
`IFF_FF`	The margin of safety is calculated for both, the fiber failure see (Equation (1)) and the intra fiber failure mode (Equation (4)) and the most critical of these is given as an output. Required parameters are ($S_{11}^{t}, S_{11}^{c}, S_{22}^{c}, S_{22}^{t}, S_{12}^{s}, p_{12}^{+}$, and p_{12}^{-})
`IFF_weak`	The margin of safety is calculated for both, the fiber failure and the intra fiber failure mode whereas for the intra fiber failure mode the interaction (weakening) with the fiber failure mode is activated (Equation (7)). Again the margin of safety of the most critical mode is given as an output. Required parameters are $S_{11}^{t}, S_{11}^{c}, S_{22}^{c}, S_{22}^{t}, S_{12}^{s}, p_{12}^{+}$ and n whereas if the Puck parameters are obtained from the Puck estimation tool, the interaction exponent n is not estimated and need to be added by hand using a text editior.

4.3.1.6 Keyword est_type

Keyword	**est_type (optional)**
Description	Specifies which Puck parameters should be used from the Puck Parameter File (see Section 4.3.2) based on the algorithm that was used to estimate the parameters
Restrictions	If this keyword is not provided the tool tries to load the Puck parameters according to the following order: MLE, LSE, conservative,

	confidence_lower-bound, confidence_upper-bound
Allowed Values	
`MLE` (default 1)	Use the Parameter obtained by the maximum-likelihood estimation procedure
`LSE` (default 2)	Use the Parameter obtained by the least-square estimation procedure
`Conservative` (default 3)	Use the Parameter obtained by the maximum-likelihood estimation procedure with the additional constraint that the resulting Puck value for all provided data points must be greater than one, i.e. all experimental data points must lay outside of the resulting Puck failure envelope.
`confidence_lower-bound` (default 4)	Use the parameter obtained as a lower confidence bound if the confidence interval calculation was activated (and successful) by the keyword confidence (see Section 4.2.1.7)
`confidence_upper-bound` (default)	Use the parameter obtained as a upper confidence bound if the confidence interval calculation was activated (and successful) by the keyword confidence (see Section 4.2.1.7)

4.3.1.7 Keyword def_temp

Keyword	**def_temp (optional)**
Description	By this keyword a temperature (in Kelvin) can be specified for the whole provided FE Model in case the temperature is not specified in the FE Stress Data File. This temperature is used to choose the related material properties from the provided Puck material properties.
Restrictions	If no dataset exists for the specified temperature the tool tries to interpolate (or extrapolate) the material properties from the given data. This requires that at least two Puck datasets are provided in each of the Puck Parameter files from which an interpolation is possible. If the temperature is neither specified in the FE Stress Data File nor specified by this keyword, a warning is printed to both the log file and the screen and room temperature (296.15K) is assumed for the whole model. If in turn, the temperature is provided by the **`def_temp`** keyword and defined in the FE Stress Data File, the temperature in the FE Stress Data File is preferred and the temperature provided by the **`def_temp`** keyword is ignored. Note that when temperature fields are provided in the FE Stress Data File for each subcase for which stress values for each element are included as well, then the element temperature is computed by averaging the temperatures at the connected FE nodes. This average temperature is used to interpolate the Puck failure envelope parameters.
Allowed Values	
temperature value	

4.3.1.8 Keyword results

Keyword	**results (optional)**
Description	Specifies a path where the output data is stored. If no path is provided a new directory "Results" is created where a subfolder, labelled with the taskname specified in the Job File, is created for every task of the current job.
Restrictions	
Allowed Values	
relative path	A relative path, for example: `'outputdata/myResults'`. Use `'./'` to save the results in the current directory
absolute path	An absolute path, for example: `'D:/failure-analysis/outputdata/myResults'`

4.3.2 Input – the Puck Parameter File

The Puck material parameters as provided by the **`puck`** keyword for the FE evaluation tool are given in the same way as the estimated Puck material parameters are generated as an output from the Puck estimation tool, see Section 4.2.3 for a detailed description of the Puck Parameter File.

4.3.3 Input – the FE Stress Data File

The FE Results to be post-processed by the FE evaluation tool need to be provided (by the keyword **`fe_data`**) as an hdf5 file generated from MSC Nastran 2021 or newer.

4.3.4 Output – the Extended FE Results file

A copy of the provided FE Stress Data File is generated. This copy is extended with the variable "failure_index" which contains the margin of safety for all elements with the requested material ids. This file is generated such that it can be visualized by the Nastran post-processor in the same way as the original (input) file.

If necessary this file can also be manually inspected for example by the hdfViewer ([HDF® View - The HDF Group]) or the Python h5py package.

Figure 11 shows the data structure of the margin of safety data in the "failure_index" variable which can be found in the Extended Fe Stress Data File under ['NASTRAN']['RESULT']['ELEMENTAL']['FAILURE_INDEX']. In here the margin of safety is given as "FP" for every domain "DOMAIN_ID' every element "EID" and every laminate layer "LAMID". The minimum Margin of Safety over all layers in one element is given by the "FMAX" variable in the corresponding laminate layer. The remaining variables "FM", "FB" and "FFLAG" do not have any meaning.

	0								
	EID	THEORY	LAMID	FP	FM	FB	FMAX	FFLAG	DOMAIN_ID
0	3	PUCK	1	-0.12070...	0.0	-1.0	NaN		1
1	3		2	5.16448...	0.0	-1.0	NaN		1
2	3		3	-0.44406...	0.0	-1.0	NaN		1
3	3		4	4.13557...	0.0	-1.0	NaN		1
4	3		5	21.2026...	0.0	-1.0	NaN		1
5	3		6	-0.55505...	0.0	-1.0	-0.55505...		1
6	3		7	2.07087...	0.0	-1.0	NaN		1
7	3	PUCK	1	-0.24594...	0.0	-1.0	NaN		2
8	3		2	0.63959...	0.0	-1.0	NaN		2
9	3		3	4.60955...	0.0	-1.0	NaN		2
10	3		4	-0.09062...	0.0	-1.0	NaN		2
11	3		5	-0.34316...	0.0	-1.0	-0.34316...		2
12	3		6	0.29219...	0.0	-1.0	NaN		2
13	3		7	-0.31612...	0.0	-1.0	NaN		2

Figure 11: The margin of safety data as stored in the hdf5 result file as variable "failure_index"

4.3.5 Output – the Margin of Safety File

In addition to the Extended Result File, the margin of safety is written to the csv Margin of Safety File (Figure 12), whereas the structure is basically the same as in the hdf5-file with the only difference that here also the leading (critical) failure mode (IFF_A,IFF_B, IFF_C or FF_compr and FF_tensile) is given.

EID,	PLY,	MOS,	DOMAIN ID,	maxValue,	MODE
3.0,	1.0,	-0.12070690851549318,	1.0,	nan,	IFF_A
3.0,	2.0,	5.164485689242316,	1.0,	nan,	IFF_C
3.0,	3.0,	-0.44406831942370134,	1.0,	nan,	IFF_A
3.0,	4.0,	4.135571135562704,	1.0,	nan,	IFF_C
3.0,	5.0,	21.202670883210192,	1.0,	nan,	IFF_C
3.0,	6.0,	-0.5550573034918528,	1.0,	-0.5550573034918528,	IFF_A
3.0,	7.0,	2.0708729600773026,	1.0,	nan,	IFF_C
3.0,	1.0,	-0.24594699801736103,	2.0,	nan,	IFF_A
3.0,	2.0,	0.6395975062362121,	2.0,	nan,	IFF_B
3.0,	3.0,	4.609553790149584,	2.0,	nan,	IFF_B
3.0,	4.0,	-0.09062927898419101,	2.0,	nan,	IFF_B
3.0,	5.0,	-0.34316299637359765,	2.0,	-0.34316299637359765,	IFF_A
3.0,	6.0,	0.29219218385636325,	2.0,	nan,	IFF_B
3.0,	7.0,	-0.3161245112372014,	2.0,	nan,	IFF_A

Figure 12: Alternative csv output of the margin of safety with the additional information on the failure mode

4.4 Examples

In the following some examples are described and further discussed to illustrate the possible ways to use the Puck Evaluation tool. The corresponding example files can be found in the subfolder '/examples'.

4.4.1 Example 1 – Minimal working example Puck Estimator

The Job File of the first example is shown in Figure 1, besides the task and the experimental data no further keywords are used. As experimental input datasets for two temperatures (4.2K and 295K) are specified. Both contains several datapoints for tensile and compression experiments for different fiber orientations (0°,15°,30°,60°,75° and 90°) as well as some datapoints from shear experiments.

```
[example-1]
task = PUCK_ESTIMATOR
exp_data = example-1-testdata.yaml
```

(a)

```
[example-2]
task = FE_PROCESSOR
puck = Results/example-1/example-1_Estimated_Puck.yaml
fe_data = example-2.h5
```

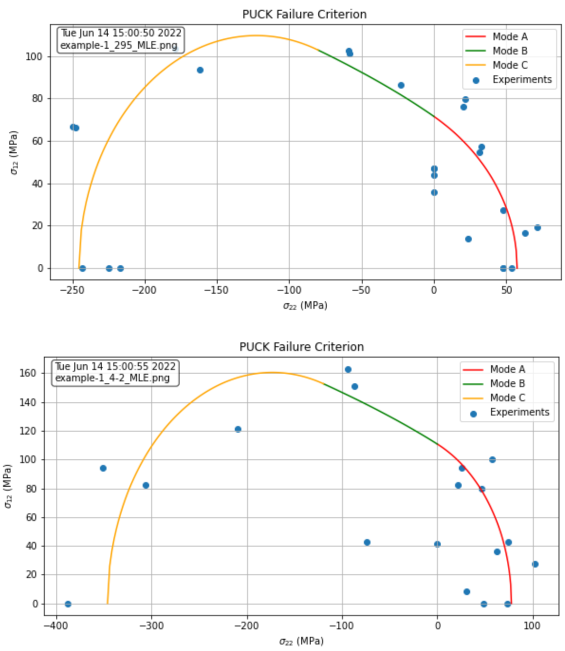
(b)

Figure 13: Job File of Example 1 (a) and example 2 (b)

As a result the Puck Material parameters for the inter-fiber failure modes (Mode A,B and C) are obtained applying the default maximum likelihood estimation (mle) method. The parameters are stored according to the temperature in the corresponding Puck Parameter File that can be found under `'./Results/example-1/example-1_Estimated_Puck.yaml'`. As a further output, plots are generated showing the resulting failure envelope together with the experimental data points (see Figure 14).

```
4.2:
  MLE:
    P12NEG: 0.4170476749
    P12POS: 0.4171476749
    S12SHEAR: 110.7461763598
    S22C: 345.9902463798
    S22T: 77.8909034898
295:
  MLE:
    P12NEG: 0.4760425224
    P12POS: 0.4761425224
    S12SHEAR: 71.5071093475
    S22C: 245.4113898757
    S22T: 57.583781848
```

(a)



(b)

Figure 14: Example 1 - The resulting Puck Parameter File giving the Puck material parameters for two temperatures (a) and the failure envelope Plots together with the experimental data points (b)

4.4.2 Example 2 – Minimal working example FE Processor

In the second example (Job File shown in Figure 13) the previously generated Puck material parameters are used for an integrity analysis using FE results provided by the keyword **`fe_data`**. The temperature used for this evaluation is defined in the FE Stress Data file as 20°C, the Puck failure envelope data are therefore interpolated by the FE Processor using the provided temperature sets for 4.2K and 295K. The Extended FE Stress Data File is found in '/Results/example-2/example-2_Puck.h5' containing a new data block **`'failure_Index'`** giving the margin of safety as the variable 'FP'. The minimum Margin of Safety over all plies for every element is provided in the 'FMAX' variable. Almost the exact same information is written to the csv Margin of Safety File for direct access or further (simplified) post-processing. However, the Margin of Safety File also provides the respective critical failure mode.

	EID	THEORY	LAMID	FP	FM	FB	FMAX	FFLAG	DOMAIN_ID
0	1	PUCK	1	14.713429210311666	0.0	-1.0	14.71342...		1
1	1		2	15.015077038300419	0.0	-1.0	NaN		1
2	1		3	14.94888017482436	0.0	-1.0	NaN		1
3	1		4	15.076108237575411	0.0	-1.0	NaN		1
4	1		5	14.94888017482436	0.0	-1.0	NaN		1
5	1		6	15.015077038300419	0.0	-1.0	NaN		1
6	1		7	14.713429210311666	0.0	-1.0	NaN		1
7	2	PUCK	1	14.749044733565102	0.0	-1.0	14.74904...		1
8	2		2	15.045943633832875	0.0	-1.0	NaN		1
9	2		3	15.00034741242568	0.0	-1.0	NaN		1
10	2		4	15.11943112878081	0.0	-1.0	NaN		1
11	2		5	15.00034741242568	0.0	-1.0	NaN		1
12	2		6	15.045943633832875	0.0	-1.0	NaN		1
13	2		7	14.749044733565102	0.0	-1.0	NaN		1

(a)

```
EID,    PLY,    MOS,                 SUBCASE ID, MAX,                 FAILURE MODE
1.0,    1.0,    14.713429210311666, 1.0,        14.713429210311666, IFF_A
1.0,    2.0,    15.015077038300419, 1.0,        nan,                IFF_A
1.0,    3.0,    14.94888017482436,  1.0,        nan,                IFF_A
1.0,    4.0,    15.076108237575411, 1.0,        nan,                IFF_A
1.0,    5.0,    14.94888017482436,  1.0,        nan,                IFF_A
1.0,    6.0,    15.015077038300419, 1.0,        nan,                IFF_A
1.0,    7.0,    14.713429210311666, 1.0,        nan,                IFF_A
2.0,    1.0,    14.749044733565102, 1.0,        14.749044733565102, IFF_A
2.0,    2.0,    15.045943633832875, 1.0,        nan,                IFF_A
2.0,    3.0,    15.00034741242568,  1.0,        nan,                IFF_A
2.0,    4.0,    15.11943112878081,  1.0,        nan,                IFF_A
2.0,    5.0,    15.00034741242568,  1.0,        nan,                IFF_A
2.0,    6.0,    15.045943633832875, 1.0,        nan,                IFF_A
2.0,    7.0,    14.749044733565102, 1.0,        nan,                IFF_A
```

(b)

Figure 15: Example 2 – Results as given in dataset 'failure_index' in the Extended Fe Stress Data File (a) and results given in the csv Margin of Safety File (b). Both are here shown only for element 1 and 2.

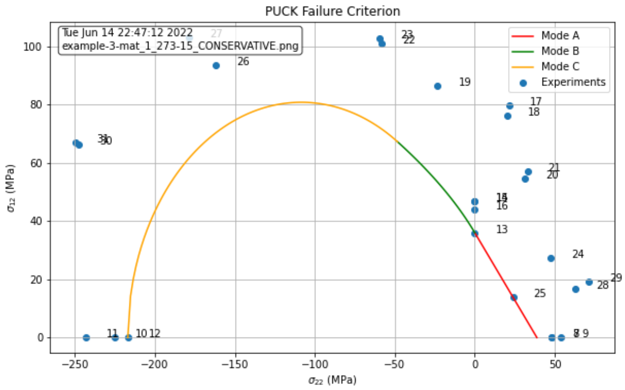
4.4.3 Example 3 – More sophisticated example

In the third example the Puck Estimator task is combined with a corresponding consecutive integrity analysis using the FE Processor. For this, in the first step the Puck material parameters including both fiber failure and inter-fiber failure (keyword **`failure_type = IFF_FF`**) are estimated for two different materials using two different material datasets (mat-1 and mat-2). Here the conservative approach (keyword **`est_type=conservative`**) is chosen which results in a Puck failure envelope not including any experimental datapoints (see Figure Figure 17).

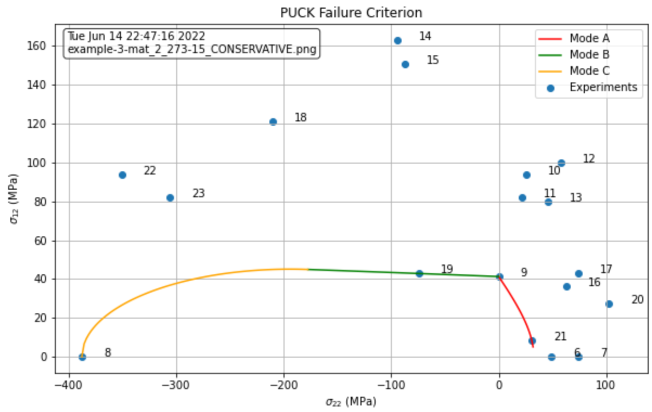
In a third task `[example-3-fe-eval]` the estimated Puck parameters are then used as an input for a failure analysis. Using the keywords **`puck`** and **`mat_ids`** the first material (mat-1) is associated with the material id 20 used in the Nastran FE analysis and the second material (mat-2) is associated with the material id 30 used in the Nastran FE analysis. For material ids 10 and 110 (also specified in the FE analysis) no Puck material datasets are provided, thus elements with these material ids are ignored in the analysis and the margin of safety is set to `NaN`.

```
[example-3-mat_1]
task = PUCK_ESTIMATOR
exp_data = example-3-testdata-mat-1.yaml
plot_info = ID
est_type = conservative
failure_type = IFF_FF

[example-3-mat_2]
task = PUCK_ESTIMATOR
exp_data = example-3-testdata-mat-2.yaml
plot_info = ID
est_type = conservative
failure_type = IFF_FF

[example-3-fe-eval]
task = FE_PROCESSOR
puck = Results/example-3-mat_1/example-3-mat_1_Estimated_Puck.yaml,
       Results/example-3-mat_2/example-3-mat_2_Estimated_Puck.yaml
mat_ids = 20,30
fe_data = example-3-fe-data.h5
def_temp = 273.15
```

Figure 16: Example 3 – Job-file containing different consecutive tasks



(a)



(b)

Figure 17: Example 3 – Resulting failure envelope for material 1 (a) and 2 (b)

5 Experimental Material Characterization

5.1 Characterization procedure

Material testing under quasi-static conditions using coupon type specimens under tension, compression and shear conditions is the most basic means of material characterization. When considering cryogenic conditions, the specimens are usually tested in a liquid nitrogen environment (77 K) or in liquid helium (4 K). In rare cases, also gaseous cryogenic helium environments have been used in order to achieve temperatures between 4 K and 77 K [Riz06].

Testing of specimens in liquid nitrogen and helium environments requires the design and availability of properly insulated vessels covering the entire test set-up. In order to keep the volume to be kept at cryogenic temperatures as small as possible for insulation purposes and in order to use as few cooling medium as possible, small scale specimens are used in most cases, rather than standard ISO type specimens for fiber reinforced plastic materials with dimensions in the range of up to 250 mm x 25 mm for tensile experiments. Nevertheless, similar strip or dog-bone like specimen geometries are used in general (e.g. [Kum05]). In order to achieve more complex local loading situations, notched tensile specimens with otherwise unchanged external geometries are used in most cases [Mor83].

The material characterization of FRP materials in the cryogenic regime in principle follows similar rules as they are established for material characterization at ambient temperatures. Nevertheless, the exposure of specimens and test rigs to cryogenic temperatures implies distinct challenges in the design of the experiments.

Considering the available space in the cryogenic test rig, experiments are often performed on specimens with reduced dimension compared to the standard test specimen sizes such as e.g. ISO 527-5 [ISO527-5] for tensile, ISO 14126 [ISO14126] for compressive or ASTM D5379/D5379M [ASTMD5379] for shear testing. Nevertheless, the test and evaluation procedures described in the standards should be followed as far as possible. The overall dimensions are mostly limited by the available material. Here some recommendations are given that yield good mechanical results to be implemented as input parameter. The dimensions given in this case are related to a 3 mm thick plate.

The tensile experiments within the fiber direction can be performed on strip-like specimens, e.g. with a nominal cross section of 8 mm × 1 mm and a length of 150 mm (see Figure 18b). For the tensile experiments perpendicular to the fiber direction as well as all off-axis tensile experiments, a dog bone specimen geometry with a nominal cross section of 8 mm × 1 mm according to Figure 18a is possible. Care should be taken to avoid cap strip failures under test.

Experiments in compression can be performed on short rectangular specimens 7 mm in width and 10 mm in length, compere to Figure 18c. This geometry, to be tested between two parallel compression plates, was chosen in order to avoid the necessity to cool a massive alignment device (Celanese device or similar) down to cryogenic temperature and thus to avoid possible problems with friction in the sliding parts of the test rig. The specimens need to be chosen as small as possible to avoid any buckling, but large enough that the thermal stresses can fully develop. Moreover, the specimen needs to be large enough to allow stress concentrations in the boundary regions to decay in a way that they do not predominate the mechanical response. Such stress concentrations are expected to occur in the contact region between the specimen and the fixture due to friction.

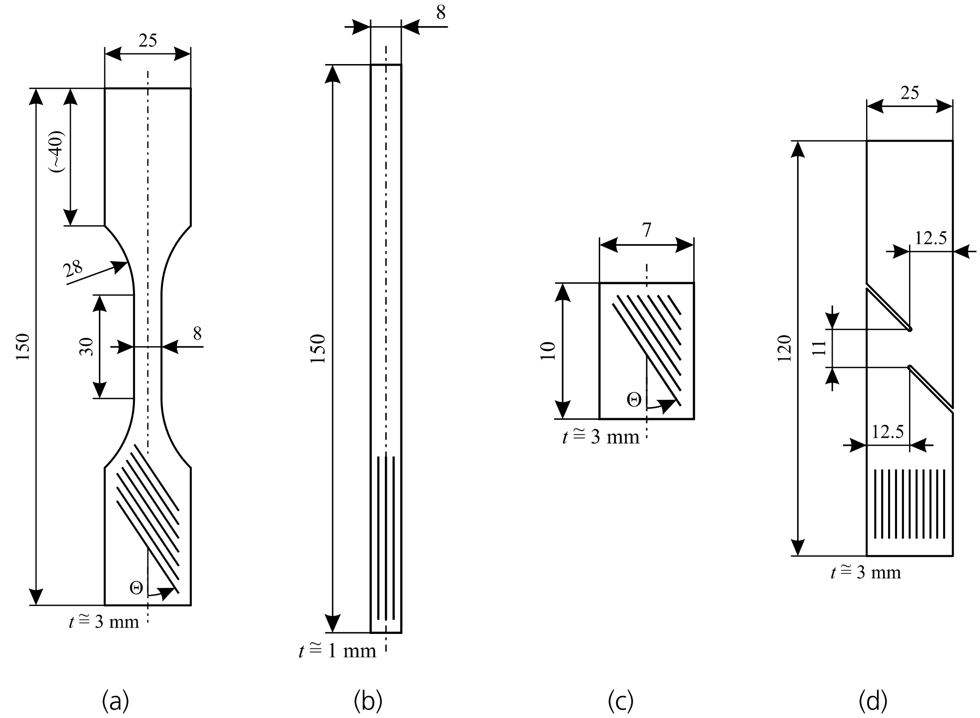


Figure 18: Specimen geometries to determine relevant stress values:
a) tensile (dog-bone) or b) tensile strip sample; c) compression; d) shear.

Shear experiments were performed by using the double slitted tensile specimen geometry according to Figure 18d with a test section of 11 mm × 3 mm. This has also the advantage that the same facility can be used as for the tensile tests. Further the limitations imposed by cryogenic testing for standard Iopescu, shear rail or picture frame tests can be avoided. Since the specimen geometry might be rather sensitive to damage during specimen preparation and test set-up, a geometry with a longer test section is recommended, e.g. 11 mm up to 20 mm. Furthermore, the test section should be protected by a clamping system during test set-up, to avoid pre-damage.

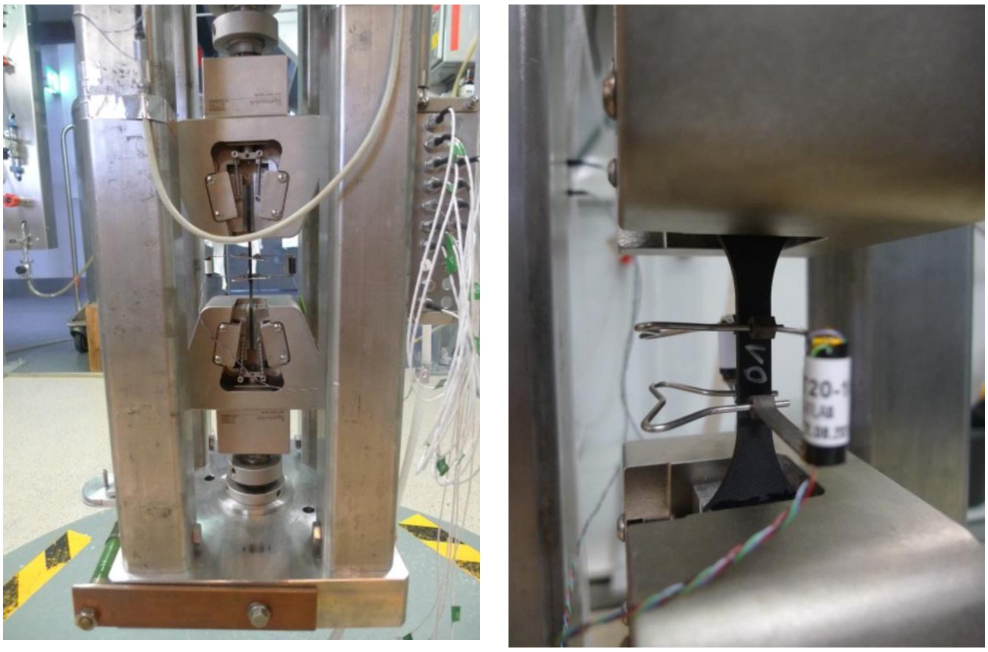
Manufacturing of specimens from available plates can be done by water jet cutting. The specimens should be supplied with cap-strips where applicable to avoid any damage of the material resulting from the clamping. All specimens loaded in tension can be fixed to the test rig by a mechanical clamping system. The specimens loaded in compression can be attached between two parallel compression plates without further fixtures or guiding devices. To obtain a comprehensive set of input parameters mechanical tests should be performed at ambient temperature as well as in the cryogenic regime, e.g. at 4.2 K using a liquid Helium environment. Other temperature levels like 77 K with liquid Nitrogen can be used if applicable. The choice of the environment derives from the advantage that liquid environments at their boiling point provide an inherently constant temperature during the test. Compared to other cryogenic liquids, liquid Helium has the advantage of providing a test temperature close to the absolute zero temperature and of safe handling.

It is recommended to investigate the effect of thermal preloads independently from the mechanical loading by selected specimens that are cooled down to 4.2 K and re-heated to ambient temperature without any mechanical load and subsequently tested at ambient temperature.

Due to the encapsulated test device and the cryogenic temperature, strain measurements with standard tactile strain gauges or optical systems are at least problematic. For this purpose, customized strain measurement systems are required, an example is shown in Fig. 2b [Nyi05].

Using a mechanical wedge clamping system compatible with cryogenic temperatures, specimens are tested under quasi-static conditions under cross-head displacement control in an electromechanical testing machine till failure. The applied cross-head velocity is recommended to be 1 mm/min. During the tensile and compressive experiments, the applied cross head displacement, resulting force and resulting strain as acquired by means of a clip-on extensometer can be continuously recorded. In the shear experiments, only the cross-head displacement and the resulting force is sufficient.

To avoid pre-damage due to the cooling, the cool down of the specimen to cryogenic temperature should be done at a moderate rate of about 1.2 K/min with a holding phase for about 30 min at 4.2 K prior to mechanical loading.



(a) (b)

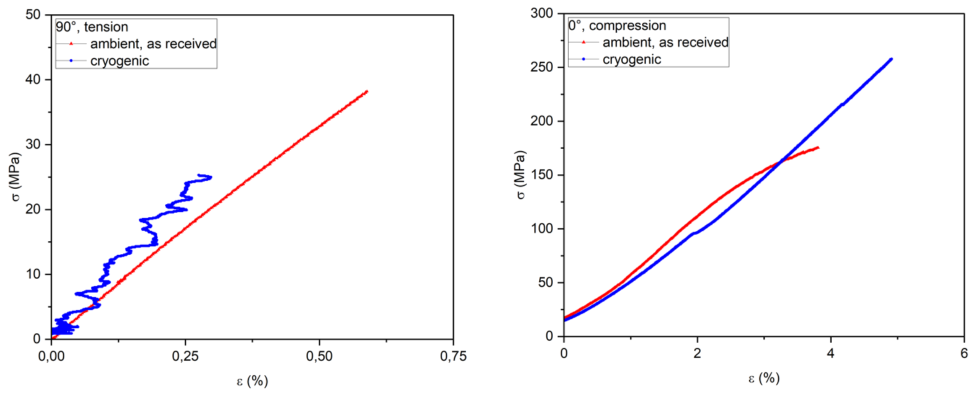
Figure 19:. On the left a test configuration also suitable for cryogenic use, showing a mounted tensile specimen. On the right side the detailed view of a mounted specimen with an attached clip-on extensometer to measure the strain during loading

5.2 Stress-strain response

The experiments should be evaluated following standard procedures in terms of the engineering stress σ obtained from the resulting force and the original cross section as well as the engineering strain ε computed from the extensometer elongation and the initial gauge length, where applicable. In all cases, the strength R_m is defined as the maximum stress achieved during the loading history. Several numbers of repetitions should be performed during the experimental investigation to minimize the uncertainty of results.

In some cases of specimens to be tested in the cryogenic regime, no valid strain results might occur due to cap strip failures or other invalid failure modes. Under these circumstances, the maximum stress attained in the respective experiment provides a lower bound on the strength of the material.

An example for possible results from the stress-strain measurements is given in Figure 20 a for tensile and b for compressive loading. Here, the loading is applied perpendicular to the unidirectional fibers in 90° direction. The maximum reached value is recorded and used for further assessment and is summarized in Table 1.



(a) (b)

Figure 20: Example of stress-strain curves, a) tensile and b) compressive, to determine maximum stress at ambient and cryogenic temperature.

Fiber - orientation	**Temperature [K]**	**Tensile [MPa]**	**Compression [MPa]**
UD-90°	292	38.2	175.4
UD-90°	4.2	25.8	257.9

Table 1

6 References

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