- Material Prediction Fitting Tool Manual -

J. Plagge, 31.10.2020 (v. 1.0)

Foreword

The presented tool was designed to allow easy and fast platform-independent fitting of finite-strain material models, primarily for technical rubbers. It includes “easy standard” models like Neo-Hooke and Ogden as well as more sophisticated models, which include viscoelasticity and damage.

The probably most powerful model is labeled “DIK” and was recently published by me and coworkers (Plagge, J., et al., *International Journal of Engineering Science* 151 (2020): 103291), most notably A. Ricker who did the major part of numerical implementation into ABAQUS. It describes the whole phenomenology of filled rubber and is, given its complexity, extremely fast and stable.

Moreover, the tool allows you to enter your own hyperelastic free energy density to play around a little bit or to add missing models.

The tool is free to use, but will not display the fit parameters of the more complex models by default. If you are interested to see them please contact me (j.plagge@materialprediction.de) or N.H. Kröger (n.kroeger@materialprediction.de). Moreover, all material models are available for purchase for use in ABAQUS, MSC Mark, COMSOL Multiphysics and ANSYS.

For those interested in the technical details:

- The program runs on a python/bokeh server who remotely performs all the calculations. Fitting will not be run on your local computer. **So please do not just do 50 parameter variations of complex models using huge data sets for fun, as this will consume most of the servers’ computational power!**
- The program was developed for 1080p (“Full-HD”) and Google Chrome or Mozilla Firefox. If it isn’t displayed (blank page) please check for browser updates. In case this doesn’t help disable all JavaScript or Ad-blockers, or contact your IT.
- Unless you do not hit the “Make Excel” button no data will be stored on the server (all operations are performed in working memory). Hitting the button will generate an Excel-file with all the input data and results on the hard drive of the server for technical reasons.

In case of questions regarding the program feel free to contact me. Feature requests are highly welcome as well.

Fit – Tool Overview: Main Controls

Using the **default key** allows you to try out all main features of the fitting tool. **Full-feature keys** are available for **purchase** for export of the model parameters.

Click to see an **example data set**:
- Example 1 is the famous **Treloar data set**.
- Example 2 is a dataset with **complex deformation** protocol and **relaxation**.
- Example 3 is a **multi-hysteresis experiment** (uniaxial and biaxial).

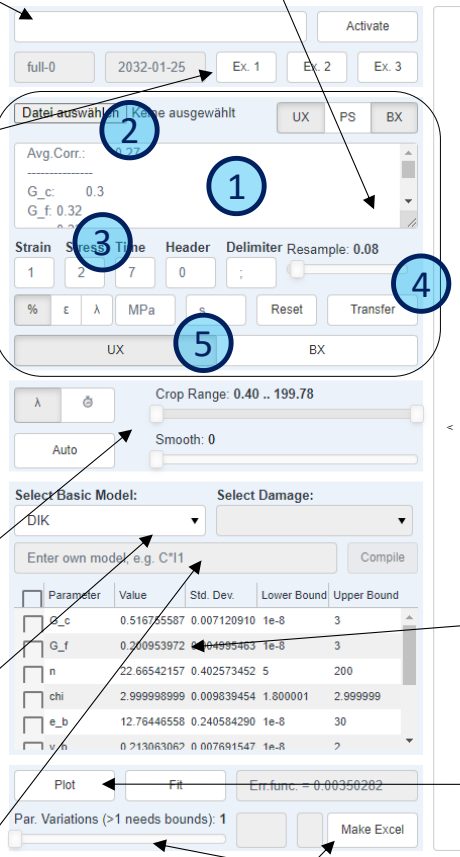
Copy-paste **your experimental data** into the textbox (1), or load it via the file input dialogue (2).
Then, specify the columns for strain, stress and time (3) (enter "/" if not available), the amount of header lines and the delimiter. Below you may select the units of the data.
Hitting the "**Transfer**" (4) button transfers the data to the plot window corresponding to the deformation mode selected below (5) .

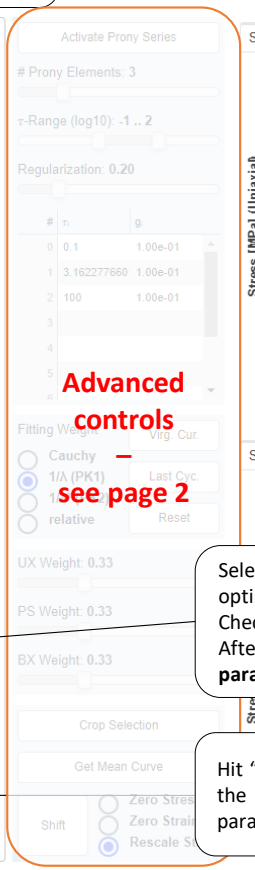
The selected data (5) may be **cropped** respective strain or time, or **smoothed**.

Select the **model to fit**. For some models you may select a damage implementation. All models are available for purchase for ABAQUS, also for MSC Marc, COMSOL Multiphysics and ANSYS.

If model "Custom" was selected, you may **construct your own free energy density** here. Use L1, L2, L3 for the principal stretches, or I1 and I2 for the well-known invariants. Then, hit "Make Model" to compile it.
Example (Mooney Rivlin): A*I1 + B*I2, or A*(L1^2+L2^2+L3^2) + B*I2, ….

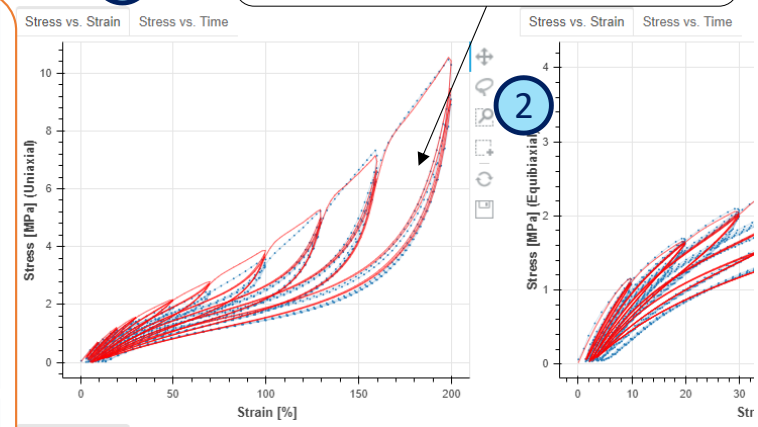
Select which **deformation modes** you would like to fit: Uniaxial (UX), Planar Strain / Pure Shear (PS) and equibiaxial stretch (BX).



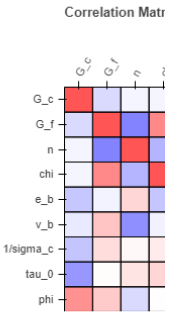


Advanced controls – see page 2

The **plot window** shows the data and the corresponding fit. It also allows to view stress vs. time (1) and to select specific regions of the data for fitting via the lasso or box-select tool (2).



Select **start parameters and boundaries** for optimization before starting the fitting procedure. Checking the box fixes the parameter during fitting. After fitting it shows the **result including the parameters' uncertainties**.



Hit "Plot" to **plot the model** using the parameters in the table, or "Fit" to **start fitting** using the parameters in the table as initial guess.

This slider allows **start parameter variations**: For each variation the algorithm generates random start parameters within their given boundaries. This may help to find the global minimum.

Finally, you might want to download the fitting results as **Excel – file**.

Fit – Tool Overview: Advanced Controls

Toggle this button to **add a Prony series** to the model chosen in the main control (previous slide). The Prony series is defined in accordance to the Abaqus manual.

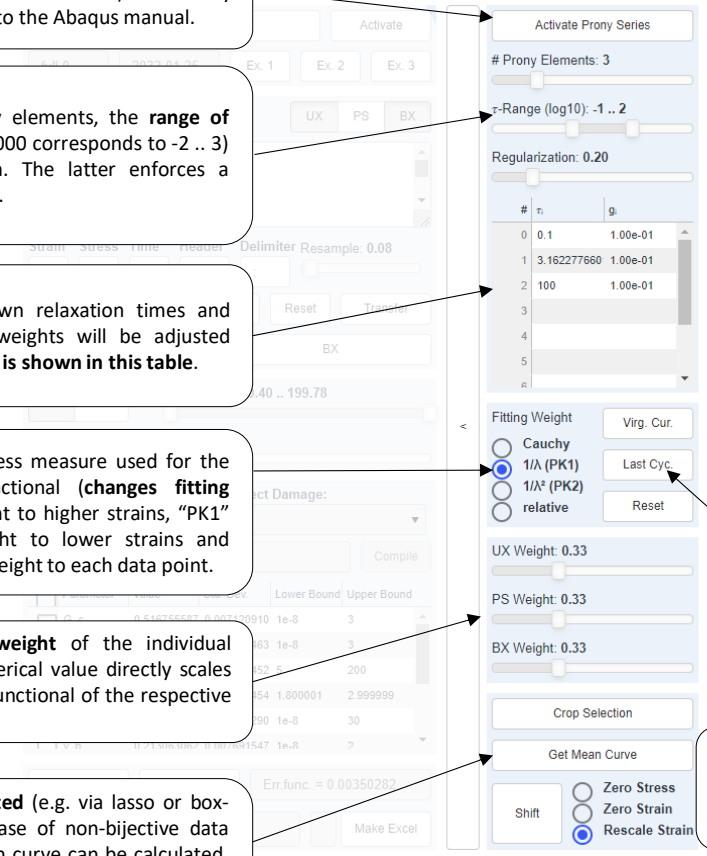
Choose the **number** of Prony elements, the **range of relaxation times** (e.g. 0.01 .. 1000 corresponds to -2 .. 3) and degree of **regularization**. The latter enforces a smooth weight (g_i) distribution.

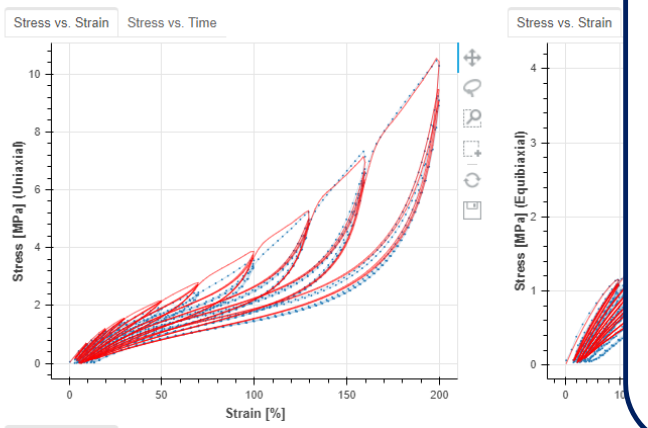
Here you may enter your own relaxation times and corresponding weights. The weights will be adjusted during fitting. **The fitting result is shown in this table**.

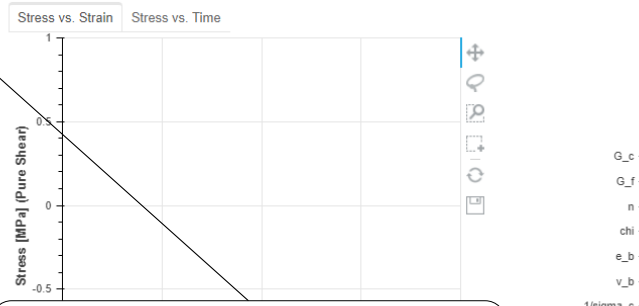
Here you may choose the stress measure used for the calculation of the error-functional (**changes fitting weight**): "Cauchy" shifts weight to higher strains, "PK1" is default, "PK2" shifts weight to lower strains and "relative" puts equal relative weight to each data point.

Here you can **choose the weight** of the individual deformation modes. The numerical value directly scales the contribution to the error-functional of the respective mode

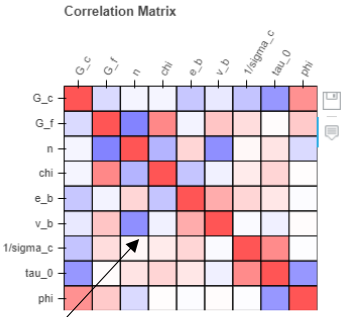
Here you may **crop the selected** (e.g. via lasso or box-select tool) **data points**. In case of non-bijective data (e.g. a cropped loop) the mean curve can be calculated. The remaining data can then be **shifted to the strain- or stress-origin**, or the strain axis can be recalculated such that the offset is set as reference length.







These buttons allow you to **auto-select** the data points corresponding to the "**virgin**" curve (primary loading) or the **last cycles** of a multi-hysteresis experiment.



After fitting, the **parameter correlation** matrix is displayed here. Generally, a matrix with off-diagonal elements close to 0 (white) indicates a well-parameterized model.

material prediction

The program is in a relatively early stage, so if it crashes just refresh the page (F5) and start over. Optimized for Google Chrome and 1080p.

Please report any bugs, criticism, compliments or needs to

Dr. Jan Plagge
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If you are interested in purchasing a key or a subroutine, please do not hesitate to contact us.

Dr. Nils Hendrik Kröger
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Uploading Raw Data

Experimental data can be uploaded in text-format (ASCII, Unicode, …) only, currently no Excel or related is supported.

Before uploading data you should checkmark the boxes right to the file-input button (Button 2 as indicated on the overview slide), determining which deformation modes you would like to fit (in parallel).

To upload a file just hit Button 2 and select your file. Alternatively, you may just copy-paste your data into the window below the button.

Then, specify the columns for strain, stress and time (if this is not available just enter "/"). Moreover, you have to select the input format of strain (% = engineering strain x 100, ε = engineering strain, λ = stretch ratio). The units of stress and strain just change the labels of the plots and do not influence the fitting.

Usually, the program should figure out the number of header lines ("Skip") and the column-separating delimiter automatically during file upload. If it fails, or you pasted your data into the window, you can manually change them in the respective text input fields.

Afterwards, select the deformation mode this data belongs to (UX = uniaxial, PS = planar strain / pure shear, BX = equibiaxial).

The "resample" slider allows you to control how much data points are put into the program. A value of 1 deactivates resampling such that all data points are taken over. A value of 0.1 means that data is resampled such that 10% of the original data points remain. Note that resampling ignores the spacing of the original points – the resampling will always result in equidistant points in the time-domain. Generally, it is advisable to keep the amount of points low (e.g. < 1000) to speed up fitting and the overall usability of the program, even though there is no upper bound.

Clicking the transfer button (button 4) transfers the data into the plot window reserved for the chosen deformation mode.

Additional notes:

- The program doesn't care about the decimal separator (e.g. 3.142 or 3,142). If the separator is "," the comma is automatically forbidden as delimiter for obvious reasons.

Uploading data including commands

In many cases it is more convenient to bundle the data on the local computer and to upload all data at once, including the input commands. To do this just place all your data (text documents) together with a "load_files.txt"-file in a .zip container and upload it via the file-input dialogue. The structure of the "load_files.txt" document has to be as below:

```
key = Uix/3Lhiffx0L(…)

model = James
start_par_variations = 2
fit_directly = yes

mode = UX
filename = Example_09_UX.txt
col_time = 6
col_strain = 1
col_stress = 2
skip_header = 5
delimiter = ;
unit_strain = %
resample = auto
crop_strain = 0..165

mode = PS
filename = Example_09_PS.txt
col_time = 3
col_strain = 1
col_stress = 2
skip_header = auto
delimiter = auto
unit_strain = %
resample = 1
crop_time = 0..565

mode = BX
filename = Example_09_BX.txt
col_time = 7
…
```

(optional) If available, enter your key here

(optional) Here you may specify which model from the list shall be selected after loading the file, how many start-parameter variations shall be performed and if the fitting shall start directly after loading the file. If a "damage concept" shall be used append it using a "_", e.g. "James_DorfmannOgden".

The mode = ("UX", "PS" or "BX") statement starts a new block of commands. Here you have to enter:

- filename = (filename as included in the .zip, including ending)
- col_time, col_strain and col_stress = (column number of the respective quantity).
- skip_header = (number or "auto", number of header lines which can also be determined automatically)
- delimiter = (character or "auto", the column – separating character)
- unit_strain = ("%", "epsilon", "lambda")
- (optional) resample = (0..1 or "auto", determines the degree of resampling. A value of 1 indicates no resampling, a value of 0.1 samples down to 10% of the original number of datapoints.
- (optional) crop_strain = (number..number, crop data to the specified strain range given in units of "%")
- (optional) crop_time = (number..number, crop data to the specified time range given in units of the dataset)

An exemplary .zip file is available for download.

Setting Up the Fit - Basics

Before fitting the data can be manipulated in several ways.

- Data can be cropped respective strain or time. This will not delete any data but just adjust the range "seen" by the fitting algorithm. The cropping is always applied to the deformation mode selected above (Switch 5).
- Data can be smoothed using a Savitzky-Golay filter in the time-strain and time-stress domain. The "Auto" button sets the smoothing parameters such that the curve is smooth by eye but keeps its original shape.

Afterward, the model to be fitted has to be selected from the list. An overview over some of the available models is given in the Appendix.

If "Custom" is selected you can enter your own incompressible hyperelastic free energy. The algorithm automatically detects the invariants $I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$ (= `I1`) and $I_1 = \lambda_1^2\lambda_2^2 + \lambda_2^2\lambda_3^2 + \lambda_1^2\lambda_3^2$ (=`I2`) of the deformation tensor as well as the principal stretches λ_i (`L1`, `L2` or `L3`). For example, the Mooney-Rivlin model can be entered as "`A*I1+B*I2`" or "`A*(L1^2+L2^2+L3^2)+B*I2`". Clicking the "Compile" button automatically detects all variables and compiles the model to be ready for fitting.

The detected variables, or the variables corresponding to the selected model, are listed in the table below. There you may enter starting values for fitting (Column "Value") and the upper and lower bounds. Checking the boxes on the left will fix the corresponding parameter and exclude it from fitting.

By clicking the "Plot" button the program will display the model's output with the given parameters.

Optionally, you may add up to 50 start parameter variations using the slider below. During each variation the program generates a random start parameter set between the given bounds and fits again. After all variations have been carried out it selects the best fit and displays it. Note that this procedure naturally needs given bounds (especially if you choose your "own" model you have to enter them).

The fitting procedure is started by clicking the "Fit" button. Depending on the amount of data points, the complexity of the model and the amount of start parameter variations this may take a while. When the program is finished it will display the result in the plot window as well as the fitted parameters, including their standard deviation, in the table.

Finally, the "Download Excel" triggers a download – dialogue to get the data on your PC.

Setting Up the Fit – Advanced Controls and Correlation Matrix

Advanced controls can be added by clicking the high vertical button on the right side of the control pane. It allows you to …

- Add a Prony series (see Appendix for specification) in accordance with the symbol definition in the Abaqus manual. Clicking the "Activate Prony Series" button will toggle the algorithm on, which means that the series is added to the model specified in the main control pane. The number of Prony elements (up to 10), their relaxation timescale and degree of regularization may be changed below. A higher degree of regularization enforces a smooth weight (g_i) distribution. The g_i and relaxation timescales can be changed in the table below. If the "Activate Prony Series" button is set before initiating a fit the weights will be fitted as well. The result is then presented in the table. Note that adding a Prony series to the fit will significantly increase computation time.

- Change the fitting weight. You can choose to calculate the error functional based on Cauchy Stress (high weight on high strains), first Piola-Kirchhoff stress (=engineering stress, PK1), second Piola-Kirchhoff stress (PK2, high weight on low strains), or to calculate the error-functional based on relative deviations.

- Automatically select the data points corresponding to the virgin curve ("Virg. Cur.", primary loading curve) or the last cycles of a multi-hysteresis experiment ("Last Cyc."). Note that the non-selected points are still calculated but do not enter the error-functional anymore. This is important for time-dependent models which always require the whole material's history. Points can also be selected using the "Lasso"-tool (element 2). Multi-selections can be done using "Shift", just try it.

- The three sliders on the bottom allow you to push the weight of the error-functional towards your preferred deformation mode. The numerical values directly scale the weight of the respective error-functional.

- Moreover, the selected data (e.g. selected via the box-select or lasso tool) may be cropped. Note that this will delete the original data. The remaining data points can then be treated such that a bijection between strain and stress is achieved ("Get Mean Curve"). A typical example might be a hysteresis loop where the central line shall be extracted. Afterwards, the data can be shifted to the strain- or stress origin. Alternatively the program can search for the strain at which stress crosses zero and use this strain to calculated a new reference length ("Rescale Strain").

After fitting a correlation matrix is displayed. This is a very handy tool to judge if the model is well parameterized, even though only strictly valid for linear models. A correlation of 1.0 (deep red) between two variables A and B means that both variables have a perfect positive correlation: To achieve the same quality of fit (as quantified by the error-functional), a positive (or negative) change in variable A has to be followed by an equal positive (or negative) change in variable B. In contrast, a perfectly negative correlation of -1.0 implies that a positive (or negative) change in variable A has to be followed by an equal negative (or positive) change in variable B. A correlation of 0.0 means that both are independent which is the desired outcome.

Simple example of a "pathological" free energy density (try it using the "own" model): `A*I1+B*I1`

This will generate a correlation between A and B of -1.0: If you choose $A = 1.0$ and $B = 0.0$ or $A = 0.5$ and $B = 0.5$ or $A = -0.63$ and $B = 1.63$ will always give the same result. This model obviously has too many parameters.

Appendix

Available Models

In this section some of the available models are discussed. The list will be continuously updated.

(Simplified) Extended Non-affine tube model

Physically based, hyperelastic, predictive, 3 parameters, subroutine available

The extended non-affine tube [1] considers the combined effect of finite chain extensibility and topological constraints (packing effects and entanglements) in densely packed, non-swollen polymer networks. It was shown to deliver the best compromise between fitting quality and number of parameters [2, 3]. Moreover, it performs relatively well in predicting deformation modes, e.g. predicting the equibiaxial response from uniaxially obtained parameters.

In its original form the calculation of the strain tensor's eigenvalues is required. In [4] the model was simplified such that this is not necessary anymore, improving overall stability and speed. Both versions are available as subroutines for purchase.

DIK Model

Physically motivated, damage, viscoelasticity, predictive, 9 parameters, subroutine available

The „DIK Model" is based on physical ideas and plausible assumptions about the material's microstructure, while being designed for high efficiency and robustness in finite element applications. It was constructed using know-how about filled rubbers' microstructure, i.e. involving the non-affine tube model [1], the dynamic flocculation model [5] and its derivatives [6]. It was shown by fits to extensive experimental data that it reproduces almost the full phenomenology of filled rubbers, both at low and high strains, for different deformation states and rates, holding times, and at different temperatures. The main modeling paradigm is the stress-induced breakdown and reorganization of microscopic structures which defines the time-dependent behavior of the material and allows to reproduce logarithmic relaxation effects. The implemented set of equations is written down in [4], an earlier version can be found in [7].

It is best fitted to data involving complex deformations, e.g. multiple cycles at different strain levels, different speeds and holding times. The model is extremely successful in predicting deformation states based on uniaxial data.

A fully working subroutine is available for purchase. It was tested for stability using a simplified bushing as shown in [4].

Prony Series Implementation

The Prony Series is implemented according to the definitions found in the ABAQUS user manual ("finite-strain viscoelasticity"). The line of reasoning shown there shall be reviewed here in a simplified version.

In linear viscoelasticity a convenient definition of the relaxation modulus in the time-domain is

$$G(t) = G_0 \left(g_\infty + \sum_{i=1}^{N} g_i \exp\left(-\frac{t}{\tau_i}\right) \right) \tag{A.1}$$

where we define $g_\infty + \sum_{i=1}^{N} g_i = 1$. The g_i are the relative weights of the individual Prony elements. N is the total number of Prony elements. With this definition it becomes clear that G_0 represents the modulus at "infinitely fast" deformations, while $G_\infty = G_0\, g_\infty$ is the modulus at "infinitely slow" deformations.

Stress is then calculated via the so-called hereditary integral

$$\sigma(t) = 2G_0\varepsilon(t) + \int_0^t 2\,\dot{G}(t')\varepsilon(t-t')\mathrm{d}t' \tag{A.2}$$

This expression is heuristically translated to the non-linear ("finite") regime by assuming that strain can be calculated via $\varepsilon(t) = \sigma_0(t)/2G_0$, where $\sigma_0(t)$ is a hyperelastic material model. Plugging this into eq. (A.2) gives

$$\sigma(t) = \sigma_0(t) - \sum_{i=1}^{N} \frac{g_i}{\tau_i} \int_0^t \sigma_0(t-t')\, \exp\left(-\frac{t'}{\tau_i}\right) \mathrm{d}t' \tag{A.3}$$

The tensorial form is obtained by replacing all σ in eq. (A.3) by the corresponding deviatoric Cauchy stress. The resulting equation is solved by a discretization of the integral, avoiding its total evaluation in each time-step.

Using this definition the hyperelastic model $\sigma_0(t)$ defines the instantaneous response ("super-fast deformation").

The tool provides also an option to fit a Prony Series with the hyperelastic material model defined as the fully relaxed state.

References

[1] M. Klüppel and G. Heinrich, "Network structure and mechanical properties of sulfur-cured rubbers," *Macromolecules,* vol. 27, p. 3596–3603, 1994.

[2] G. Marckmann and E. Verron, "Comparison of Hyperelastic Models for Rubber-Like Materials," *Rubber Chemistry and Technology,* vol. 79, pp. 835-858, 2006.

[3] H. Dal, Y. Badienia, K. Açıkgöz and F. A. Denli, "A comparative study on hyperelastic constitutive models on rubber: State of the art after 2006," in *Constitutive Models for Rubber XI*, 2019.

[4] J. Plagge, A. Ricker, N. H. Kröger, P. Wriggers and M. Klüppel, "Efficient modeling of filled rubber assuming stress-induced microscopic restructurization," *International Journal of Engineering Science,* vol. 151, p. 103291, 2020.

[5] H. Lorenz, M. Klüppel and G. Heinrich, "Microstructure-based modelling and FE implementation of filler-induced stress softening and hysteresis of reinforced rubbers," *ZAMM,* vol. 92, pp. 608-631, 2012.

[6] J. Plagge and M. Klüppel, "A physically based model of stress softening and hysteresis of filled rubber including rate-and temperature dependency," *International Journal of Plasticity,* vol. 89, p. 173–196, 2017.

[7] J. Plagge, A. Ricker and M. Klüppel, "Efficient Modeling of Inelastic Effects in Filled Rubber using LoadDependent Relaxation Times," in *Constitutive Models for Rubber XI*, 2019.