

## Modeling and Characterization of Continuous-Discontinuous Long Fiber-Reinforced Polymer Structures

Thomas Böhlke (KIT-ITM), Frank Henning (KIT-FAST), Luise Kärgler (KIT-FAST),  
Thomas Seelig (KIT-IFM), Kay André Weidenmann (KIT-IAM-WK)

14. Deutsches LS-DYNA Forum

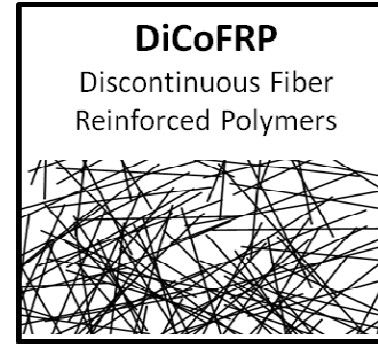
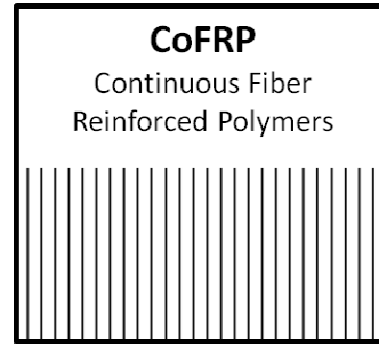


# Outline

- Introduction of GRK2078 CoDiCoFRP
  - Motivation and Objectives
  
- Research Topics
  - Preliminary Remarks on Short Fiber Reinforced Polymers
  - Microscale Characterization
  - Microscale Simulation and Homogenization
  - Macroscale Simulation and Characterization
  - Form Filling Micromechanical Modeling
  
- Conclusions and Outlook

# FRP Classes: Introduction and Application

- + High fiber volume content
- + Controlled fibers alignment
- + High stiffness and strength
- Restricted formability
- High cycle times
- High scrap rate
- Extensive trimming

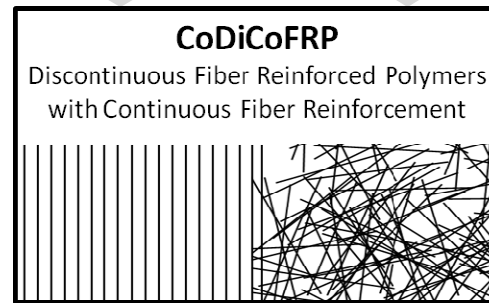


- + Good formability
- + Function integration potential
- + Low finishing demands
- + Low cycle times
- Low stiffness and strength
- Process related complex microstructure

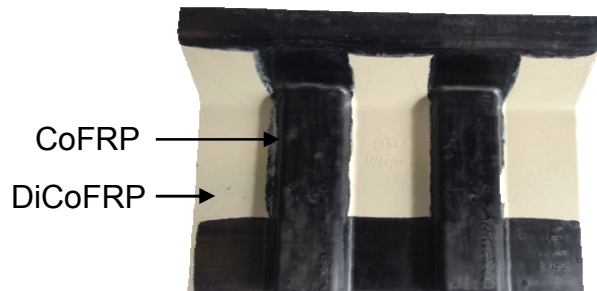


Source: BMW AG Group

Carbon cell



Frontend made of DiCoFRP



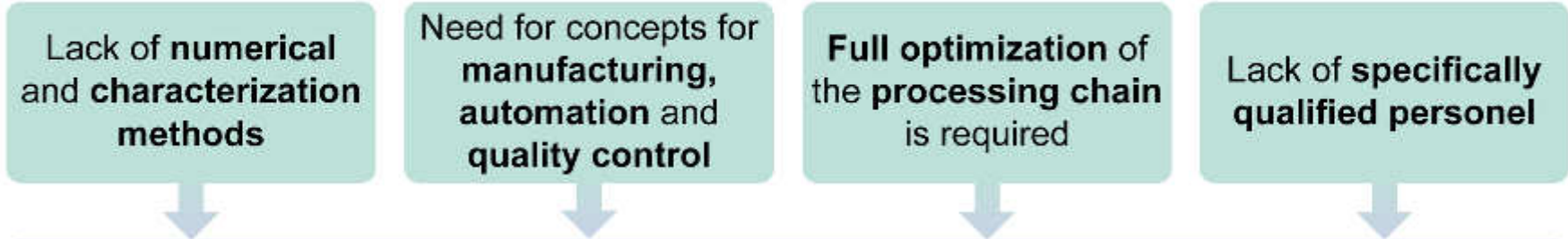
CoDiCoFRP component (front side)



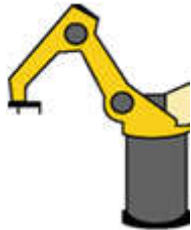
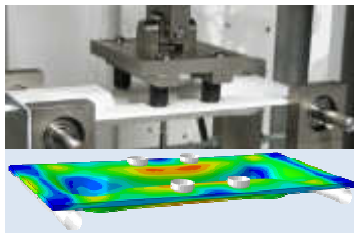
CoDiCoFRP component (back side)

# Challenges and Program Objectives

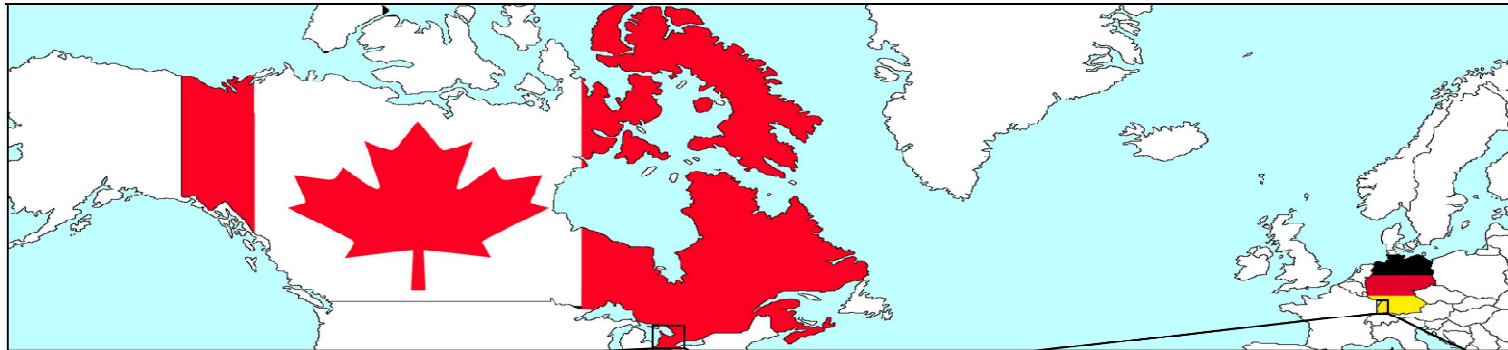
## Challenges



## IRTG Objectives



# GRK 2078 Twin Regions



# DFG GRK2078 Participating Institutes



Thomas Böhlke, Institute of Engineering Mechanics



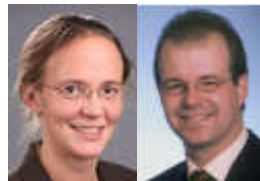
Peter Elsner, Frank Henning, Fraunhofer-ICT



Albert Albers, Institute of Product Engineering



Peter Gumbsch, Jörg Hohe, Fraunhofer-IWM



Britta Nestler, Kay Weidenmann, Institute for Applied Materials



Luise Kärger, Institute for Vehicle Science



Gisela Lanza, Jürgen Fleischer, Volker Schulze, Institute of Production Science



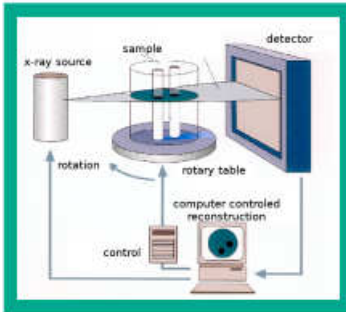
Thomas Seelig, Institute of Mechanics

# Motivation: Homogenization of Elastic Properties of Short-Fiber Reinforced Composites

Contact: Viktor Müller

# $\mu$ CT Measurement and Fiber Segmentation

Müller et al. (JCM, 2015), cooperation with Dillenberger, Glöckner, Kolling



$\mu$ CT measurement

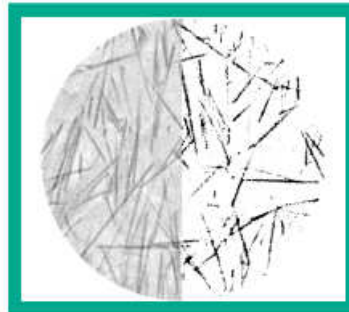
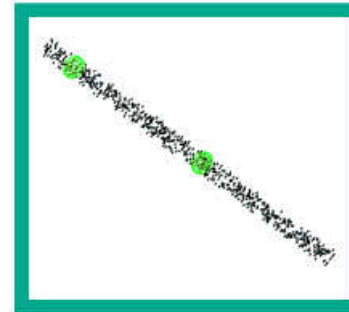
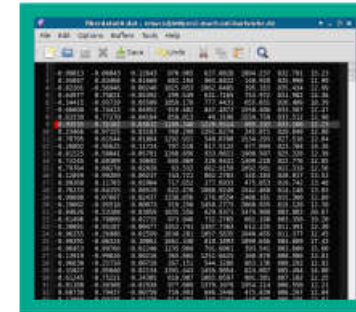


image processing



percolation algorithm



resultant data



Fraunhofer-ITWM





# IDD scheme: continuous formulation

Zheng and Du (2001), Du and Zheng (2002), Wu (1997), Müller and TB (IJSS, 2015)

$$\mathbb{C}^{\text{IDD}} = \mathbb{C}_M + \left( \mathbb{I}^s - \sum_{\beta=1}^{N_F} c_{\beta} \mathbb{M}_{\beta} \mathbb{P}_{\beta}^{\text{D}} \right)^{-1} \sum_{\alpha=1}^{N_F} c_{\alpha} \mathbb{M}_{\alpha}$$

with  $\mathbb{M}_{\gamma} = (\mathbb{C}_{\gamma} - \mathbb{C}_M) (\mathbb{I}^s + \mathbb{P}_{\gamma} (\mathbb{C}_{\gamma} - \mathbb{C}_M))^{-1}$

## Using averaged microstructure description

$$\mathbb{C}^{\text{IDD}} = \mathbb{C}_M + \left( \mathbb{I}^s - c_F \int_S f(\mathbf{n}) \mathbb{M}(\mathbf{n}) \mathbb{P}^{\text{D}}(\mathbf{n}) \, dS \right)^{-1} c_F \int_S f(\mathbf{n}) \mathbb{M}(\mathbf{n}) \, dS$$

with  $\mathbb{M}(\mathbf{n}) = (\mathbb{C}_F - \mathbb{C}_M) (\mathbb{I}^s + \mathbb{P}(\mathbf{n}) (\mathbb{C}_F - \mathbb{C}_M))^{-1}$

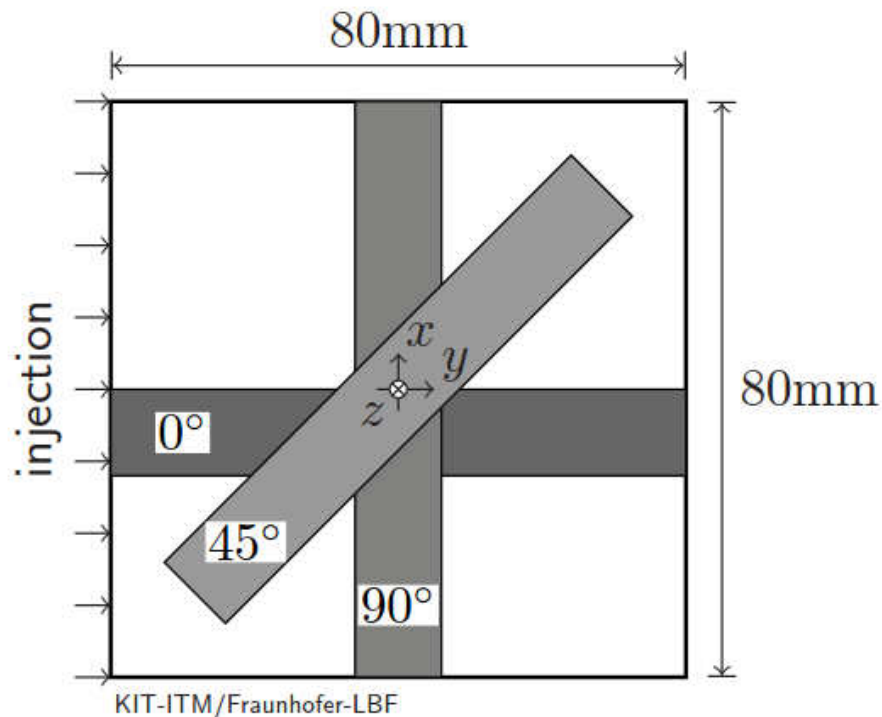
$c_F, f(\mathbf{n})$ : total vol. frac. of fibers, FODF

$\mathbb{P}(\mathbf{n}) = \mathbb{P}(\mathbb{C}_M, \mathbb{C}_F, \mathbf{n}, \omega)$ : Hill's pol. tensor of fiber with const. aspect ratio

$\mathbb{P}^{\text{D}}(\mathbf{n}) = \mathbb{P}^{\text{D}}(\mathbb{C}_M, \mathbb{C}_F, \mathbf{n}, \omega^{\text{D}})$ : Hill's pol. tensor of cell with const. aspect ratio

# Preparation of specimen

Müller et al. (JCM, 2015)

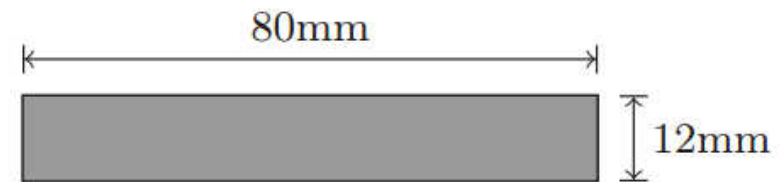


## $\mu$ CT specimen

Diameter:  $d = 2 \text{ mm}$  Height:  $h = 2.5 \text{ mm}$

Position:  $P(0, 0)$

## Geometry of specimen



Depth:  $t = 2.5 \text{ mm}$

## Glass fibers

$E_F = 73.0 \text{ GPa}$ ,  $\nu_F = 0.22$

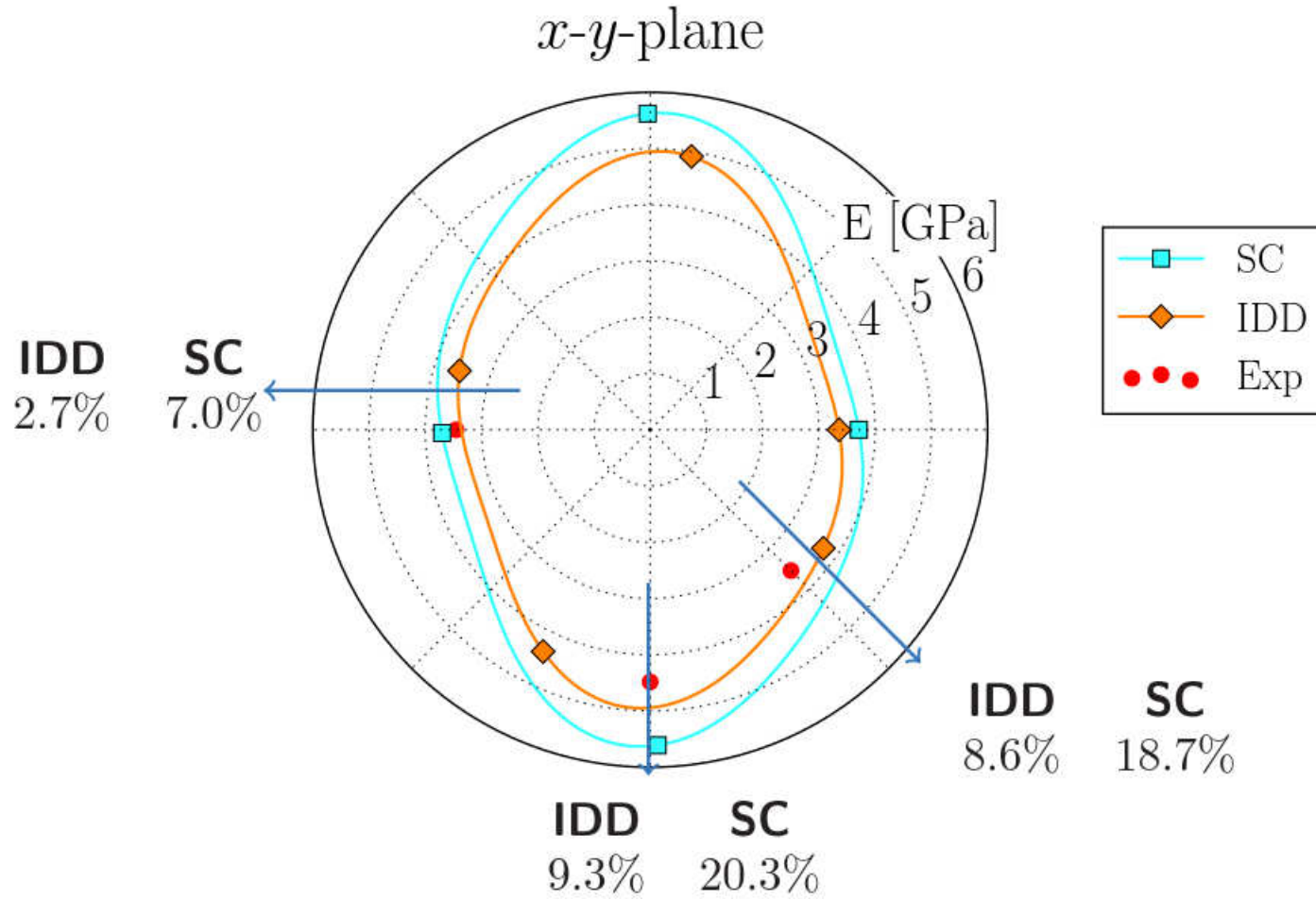
$c_F = 30 \text{ wt.-%}$

## Polypropylene matrix

$E_M = 1.705 \text{ GPa}$ ,  $\nu_M = 0.355$

# Numerical vs experimental results

Müller et al. (JCM, 2015)



# Maximum entropy principle (MEP)

Wu (1997), TB (2005), Müller and TB (CSTE, 2015)

## First moment problem

$$\begin{aligned}\bar{S} &:= - \int_S \bar{f}(\mathbf{n}) \ln(\bar{f}(\mathbf{n})) \, dS \rightarrow \max \\ \mathcal{C}_{\langle 0 \rangle} &:= \int_S \bar{f}(\mathbf{n}) \, dS - 1 \stackrel{!}{=} 0 \\ \mathcal{C}_{\langle 2 \rangle} &:= \int_S \bar{f}(\mathbf{n}) (\mathbf{n} \otimes \mathbf{n})' \, dS - (\mathbf{N})' \stackrel{!}{=} 0 \\ \mathcal{C}_{\langle 4 \rangle} &:= \int_S \bar{f}(\mathbf{n}) (\mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n})' \, dS - (\mathbf{N})' \stackrel{!}{=} 0\end{aligned}$$

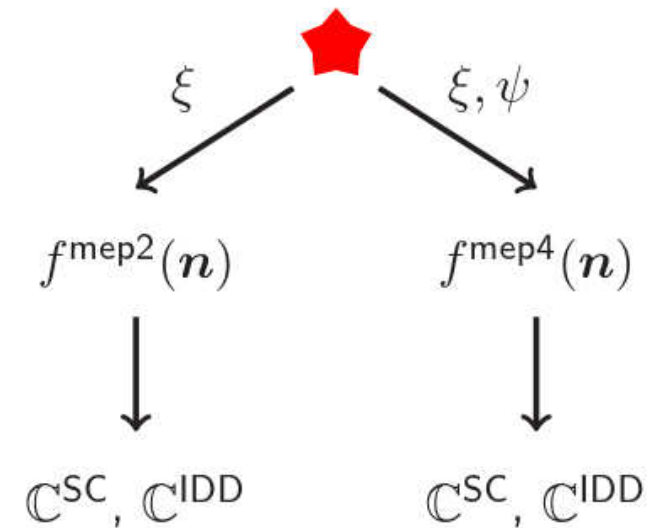
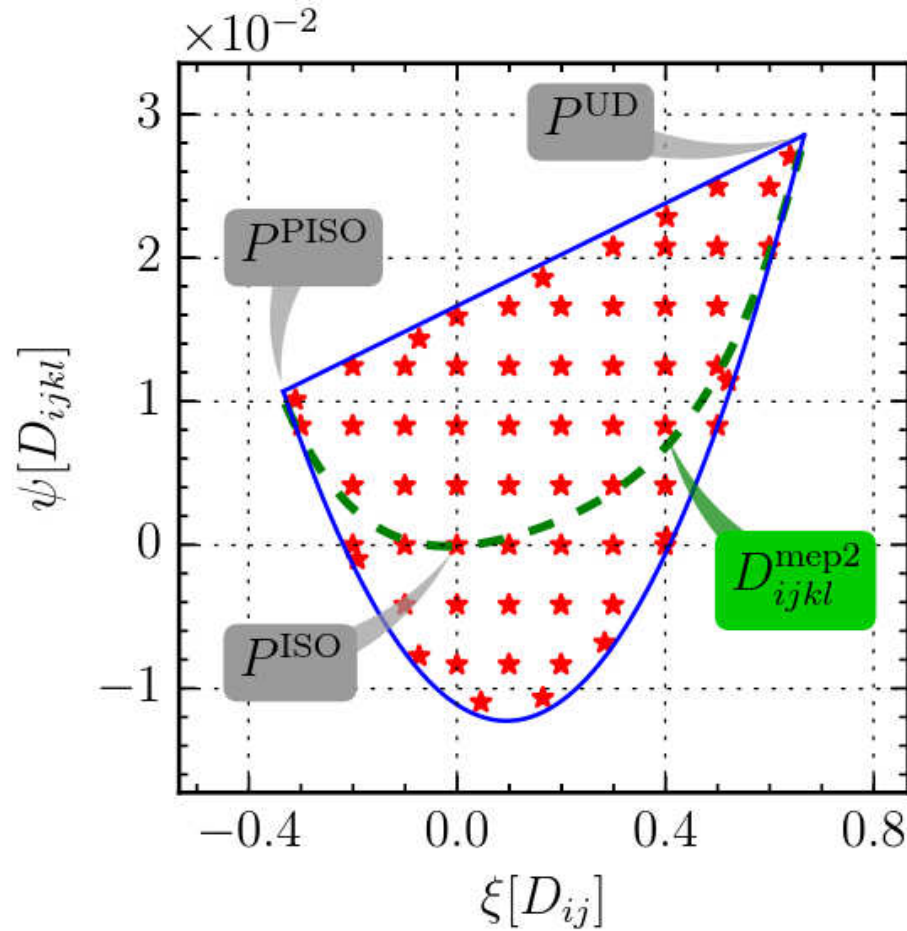
## Second moment problem

Optimization with Lagrange multipliers  $G, G, \mathbb{G}$

$$\mathcal{F} = \bar{S} - G \cdot \mathcal{C}_{\langle 0 \rangle} - G \cdot \mathcal{C}_{\langle 2 \rangle} - \mathbb{G} \cdot \mathcal{C}_{\langle 4 \rangle}$$

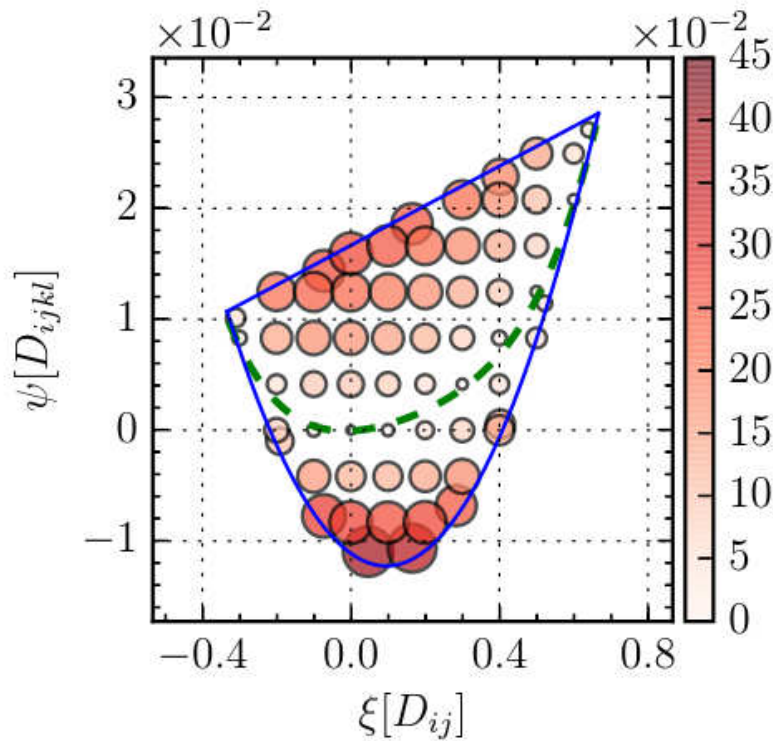
# Parameter space for irreducible parameters

Müller and TB (IJSS, 2015)

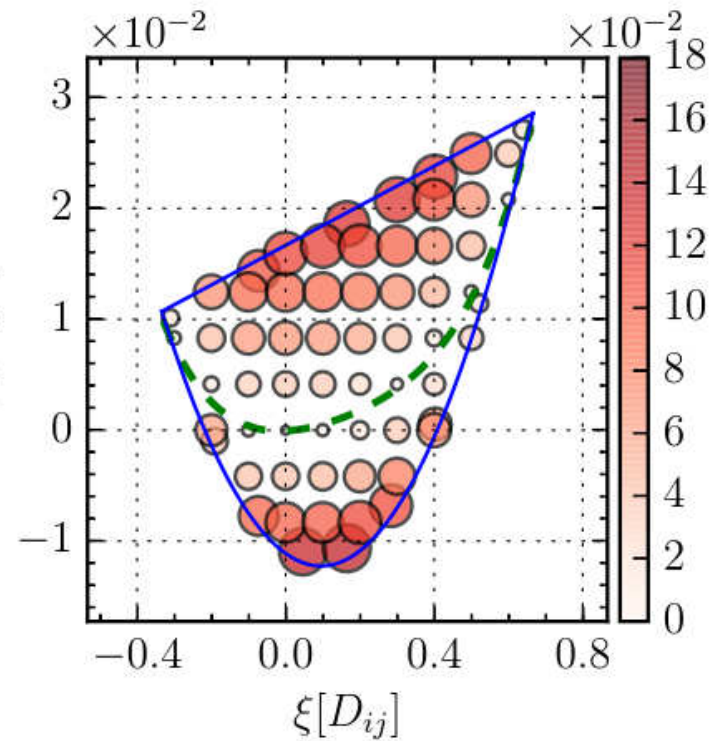


# Deviation of Young's modulus (IDD)

Müller and TB (IJSS, 2015)



$$\frac{\|E_0^{\text{mep4}} - E_0^{\text{mep2}}\|}{\|E_0^{\text{mep4}}\|}$$



$$\frac{\|E_{90}^{\text{mep4}} - E_{90}^{\text{mep2}}\|}{\|E_{90}^{\text{mep4}}\|}$$

# Mean Field vs Full-Field Modeling

## Material and microstructure parameter

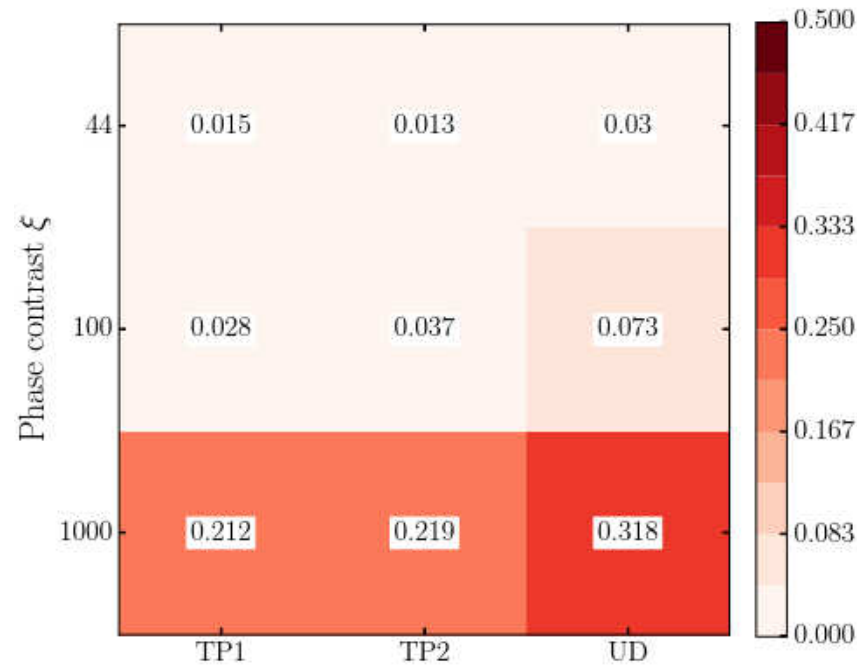
Microstructure	Fiber vol. fraction		Material combination			
TP1	TP1/TP2	UD	$E_F$ [GPa]	$\eta = 44$	$\eta = 100$	$\eta = 1000$
TP2	13%	13%	$\nu_F$	1.665	1	1
UD		17%	$E_M$ [GPa]	0.36	0.36	0.36
		12%	$\nu_M$	73	100	1000
				0.36	0.36	0.36

$$N^{TP1} = \begin{bmatrix} 0.61 & & \\ & 0.36 & \\ & & 0.03 \end{bmatrix} \quad N^{TP2} = \begin{bmatrix} 0.80 & & \\ & 0.18 & \\ & & 0.02 \end{bmatrix} \quad N^{UD} = \begin{bmatrix} 1.0 & & \\ & 0.0 & \\ & & 0.0 \end{bmatrix}$$

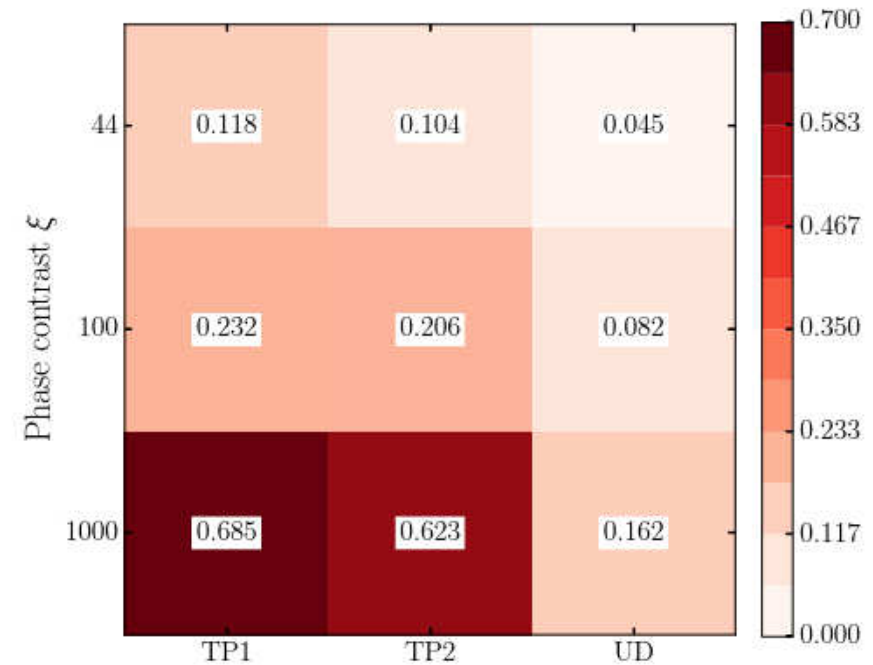
# Influence of Phase Contrast and Microstructure

Müller et al. (2015)

**MF-IDD vs FFT-BS for  $c_F = 13\%$**



**MF-SC vs FFT-BS for  $c_F = 13\%$**



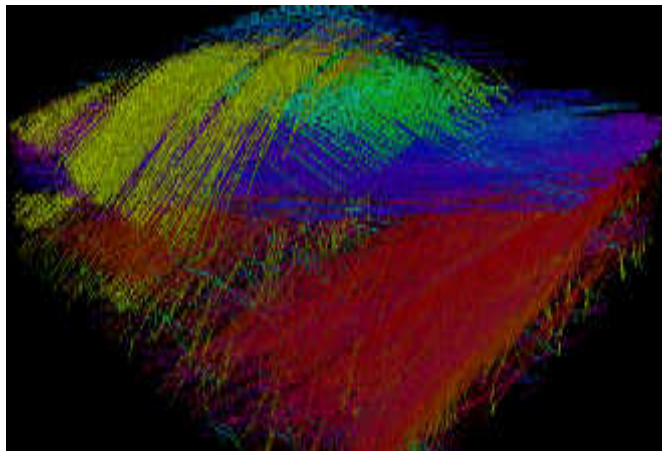


# Microscale Characterization

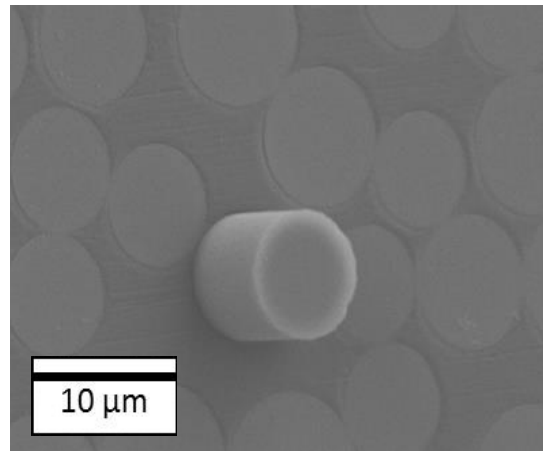
Contact: Pascal Pinter, [pascal.pinter@kit.edu](mailto:pascal.pinter@kit.edu), KIT IAM-WK

# Microscale Characterization

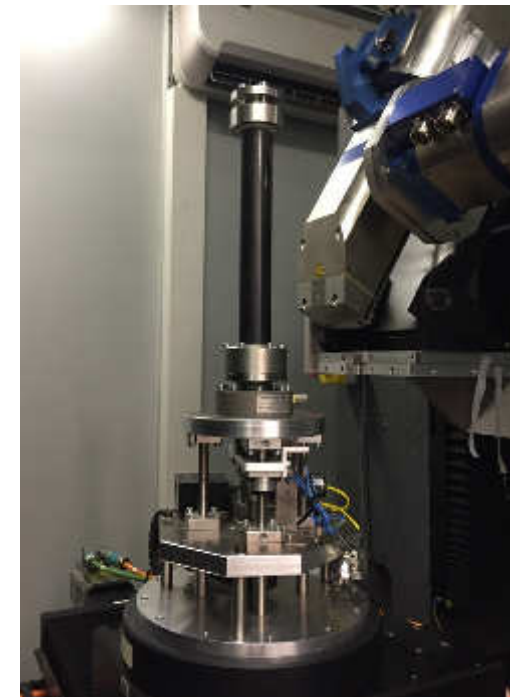
- Development and application of destructive and non-destructive testing methods:
  - Determination of 4<sup>th</sup> order orientation tensors directly from  $\mu$ CT-scans via in-house software “Composight”
  - Fiber length distributions from  $\mu$ CT-scans
  - Mechanical properties of fibers
  - Interfacial shear strength
  - In-Situ tensile tests for validation of models



Orientation analysis (SMC)



Push-Out-Test

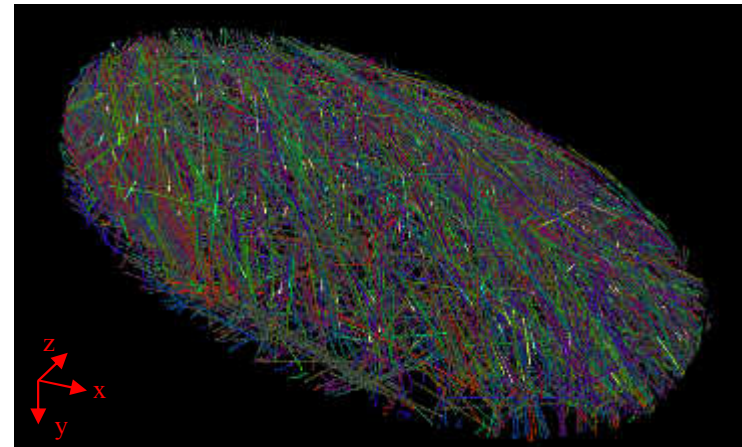


In-Situ-Stage

[Contact: Pascal Pinter, [pascal.pinter@kit.edu](mailto:pascal.pinter@kit.edu), KIT IAM-WK]

# Microscale Characterization

- Developed methods during IRTG:
  - Fiber orientation distributions:  
Calculation of 4<sup>th</sup> order orientation tensors from  $\mu$ CT-Images
  - Fiber length distribution (FLD):  
Possible specimen size of  $D=4$  mm with 81% correctly traced fibers



LFT20  $\varnothing$  4 mm specimen - independent fibers are illustrated in different colors

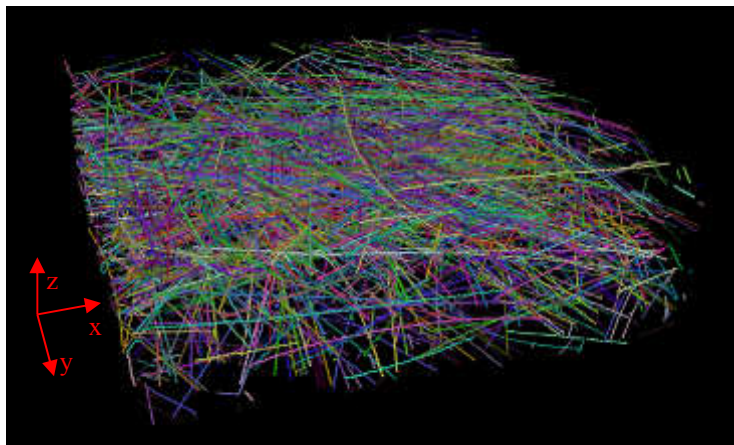
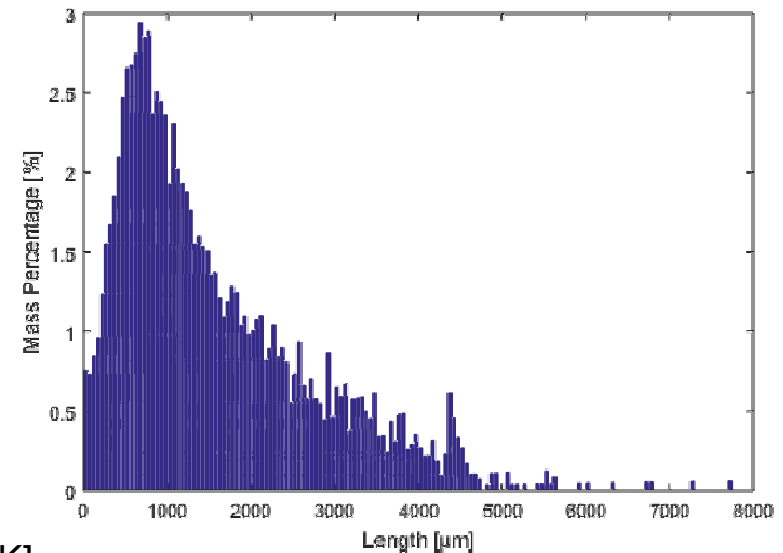


Image detail of same specimen  $1.8 \times 1.8 \times 0.5$  mm<sup>3</sup>



Fiber Length Distribution

[Contact: Pascal Pinter, [pascal.pinter@kit.edu](mailto:pascal.pinter@kit.edu), KIT IAM-WK]

# Microscale Simulation and Homogenization

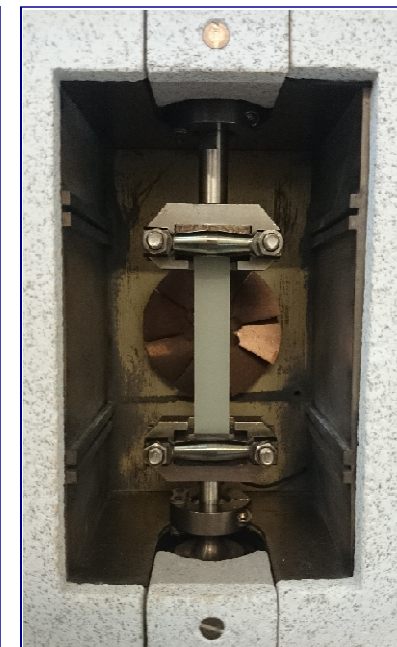
Contact: Loredana Kehrner, [loredana.Kehrner@kit.edu](mailto:loredana.Kehrner@kit.edu), KIT ITM

# Characterization of mechanical properties by DMA

- Dynamic mechanical analysis (DMA) with GABO Eplexor 500 N
- Analysis of thermal and viscoelastic material properties
- Measured quantities  $E^* = E' + iE''$
- Specifications:

$E^*$ : dynamic modulus,  
 $E'$ : storage modulus,  
 $E''$ : loss modulus

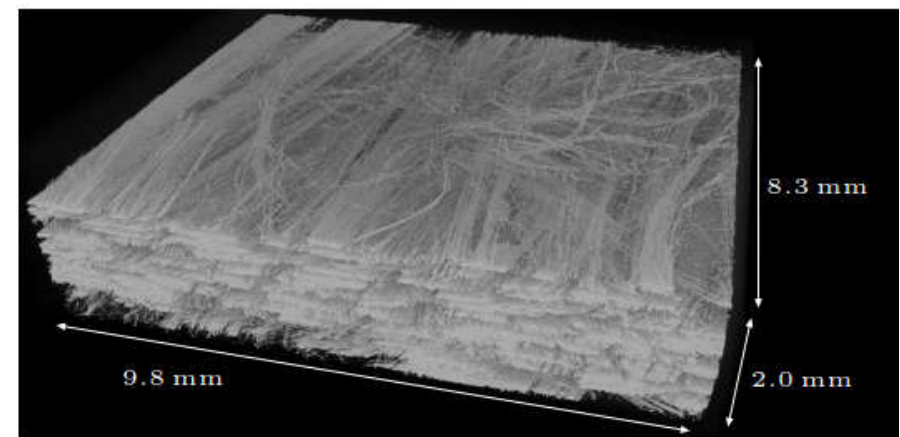
Static force	1500 N
Dynamic force	± 500 N
Temperature range	-150°C to 500°C
Frequency range	0.01 Hz to 100 Hz



# Experimental results for tension mode under thermal load by DMA

- GF DiCoFRTS

Resin system	VE resin
Fiber type	Glass
Fiber length	25 mm
Fiber content	41 wt.-%, 23 vol.-%

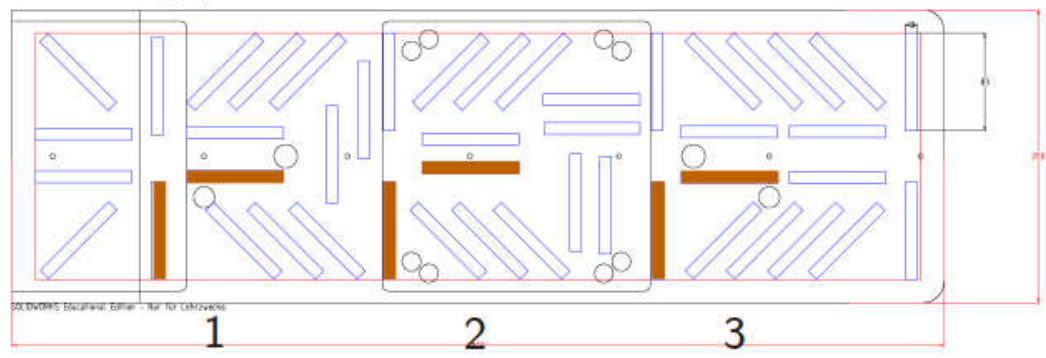


Source: P. Pinter (IAM-WK, KIT)

- Plate specifications:  
800 mm × 250 mm × 2 mm

- Filling of plate with resin at 33%, 50% and 100%

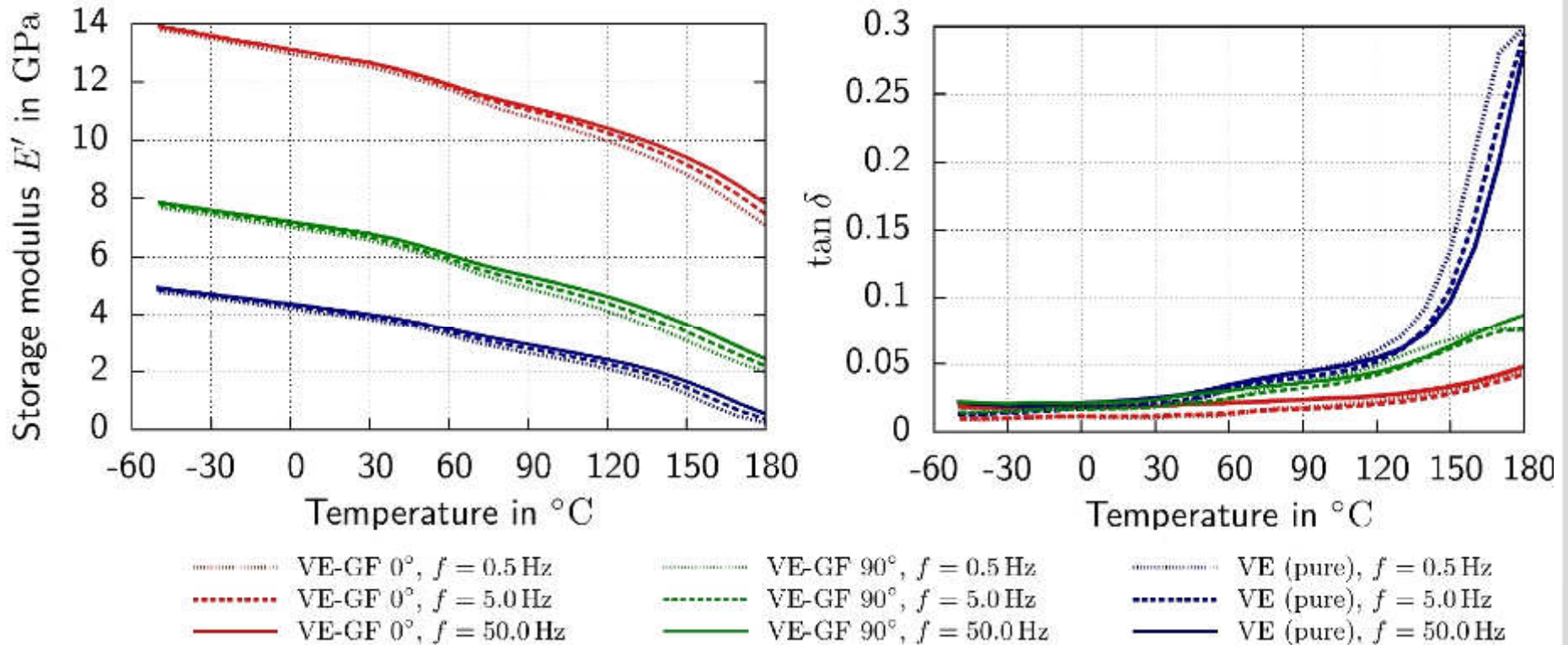
- Cutting plan



Mould charged with approx. 60% of semi-finished product

# Experimental results for tension mode under thermal load by DMA

- Comparison of storage modulus for different temperature and frequency loads on VE-GF and pure VE



- Test parameters:

Static load  $\epsilon_{\text{stat}} = 0.1\%$

Contact force  $F_c = 5 \text{ N}$

Dynamic load  $\epsilon_{\text{dyn}} = 0.05\%$

Load cell capacity 500 N

# Hashin-Shtrikman related two-step method

Walpole (1969), Willis (1977), Willis(1981), Müller (2015)

- Based on generalized formulation with eigenstrains

- First step

$$\bar{\mathbb{C}}_{\alpha}^{\text{UD}+} = \mathbb{C}_{\alpha} + c_M(\mathbb{C}_M - \mathbb{C}_{\alpha}) \left( \mathbb{I}^S + c_{\alpha} \mathbb{P}_{\alpha}^{\text{UD}}(\mathbb{C}_M - \mathbb{C}_{\alpha}) \right)^{-1}$$

$$\bar{\mathbb{C}}_{\alpha}^{\text{UD}-} = \mathbb{C}_M + c_{\alpha}(\mathbb{C}_{\alpha} - \mathbb{C}_M) \left( \mathbb{I}^S + c_M \mathbb{P}_{\alpha}^{\text{UD}}(\mathbb{C}_{\alpha} - \mathbb{C}_M) \right)^{-1}$$

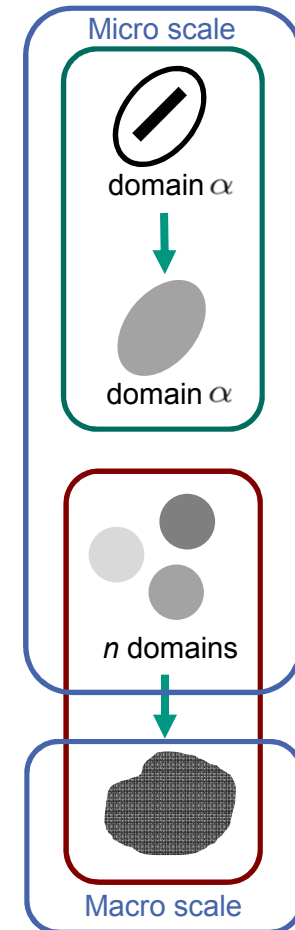
- Second step

$$\bar{\mathbb{C}}^{\text{HS}\pm} = \sum_{\alpha=1}^n \frac{c_{\alpha}}{c_F} \bar{\mathbb{C}}_{\alpha}^{\text{UD}\pm} \mathbb{A}_{\alpha}^{\text{HS}} = \sum_{\alpha=1}^n \frac{c_{\alpha}}{c_F} \bar{\mathbb{C}}_{\alpha}^{\text{UD}\pm} \mathbb{M}_{\alpha} \langle \mathbb{M} \rangle^{-1}$$

$$\mathbb{M}_{\alpha} = \left( \mathbb{I}^S + \mathbb{P}_0(\bar{\mathbb{C}}_{\alpha}^{\text{UD}\pm} - \mathbb{C}_0) \right)^{-1} \quad \text{and} \quad \langle \mathbb{M} \rangle = \sum_{\alpha=1}^n \frac{c_{\alpha}}{c_F} \mathbb{M}_{\alpha}$$

- Two-step method for formulation with variable reference stiffness  $\mathbb{C}_0$

$$\mathbb{C}_0 = (1 - a)\mathbb{C}_M + a\mathbb{C}_F \quad a \in [0, 1]$$



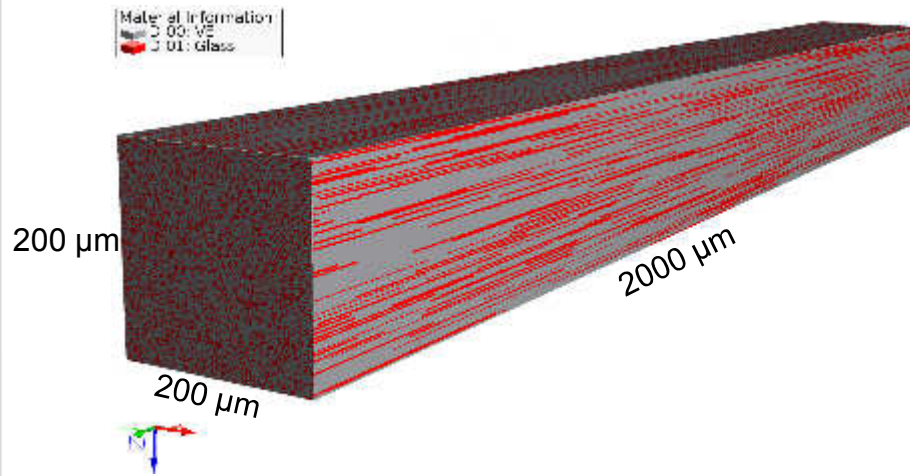


# Mean field and full field simulation

- Virtual microstructure generated with GeoDict®

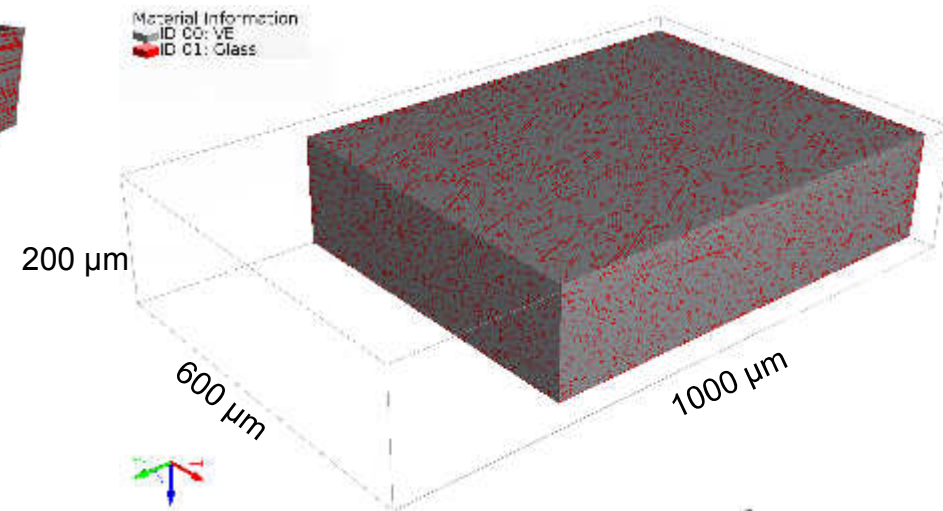
- Unidirectional long fibers

- Randomly non-uniform distributed long fibers



$l_F = 1500 \mu\text{m}$

$d_F = 10 \mu\text{m}$



$l_F = 1000 \mu\text{m}$

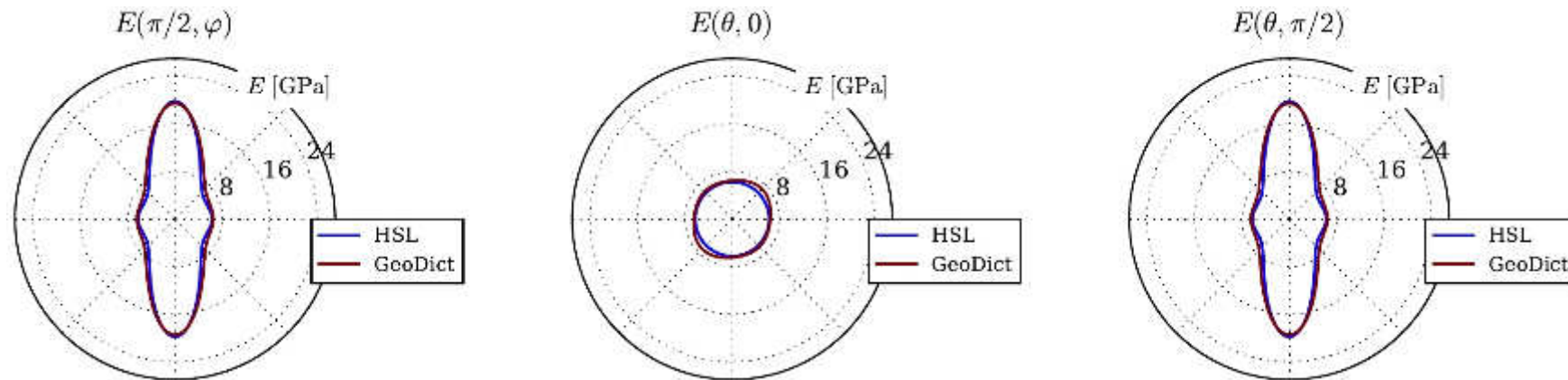
$d_F = 10 \mu\text{m}$

- Material parameters:

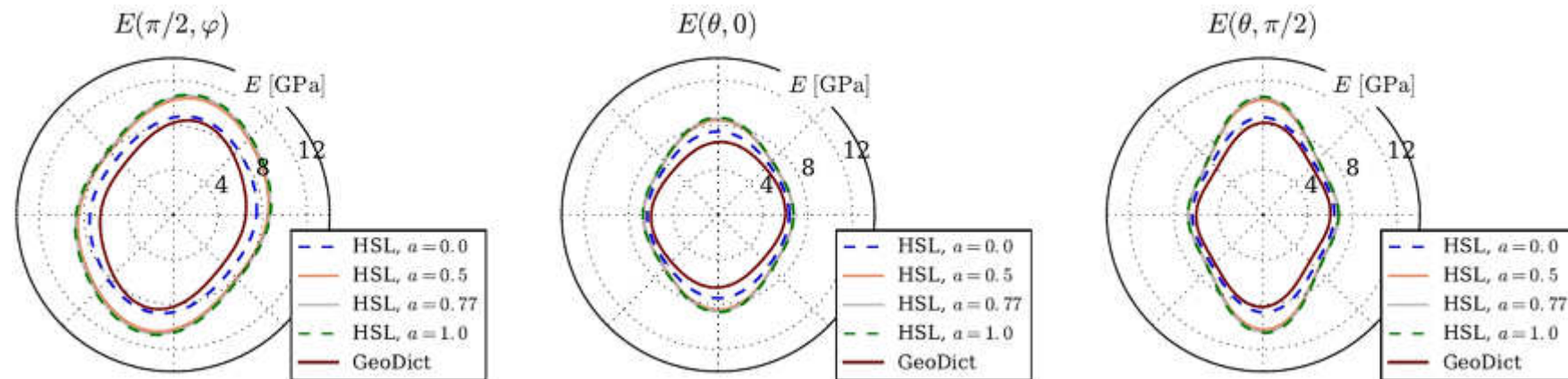
Matrix	Young's modulus $E_M$	4.0 MPa
	Poisson's ratio $\nu_M$	0.35
Fiber	Young's modulus $E_F$	73.0 MPa
	Poisson's ratio $\nu_F$	0.22
	Fiber volume fraction $c_F$	0.23

# Comparison between full field and mean field homogenization

## ■ Young's modulus for UD fibers in matrix material



## ■ Young's modulus for randomly non-uniform distributed fibers in matrix material

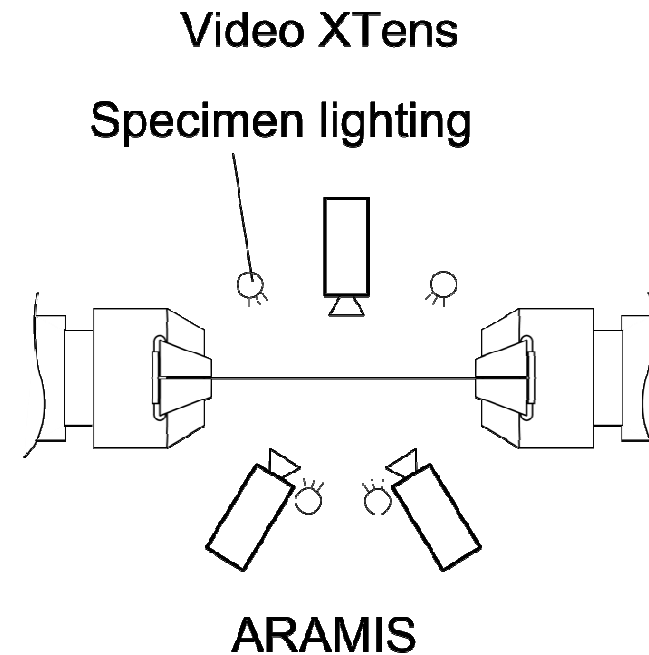


# Macroscale Simulation and Characterization

Contact:

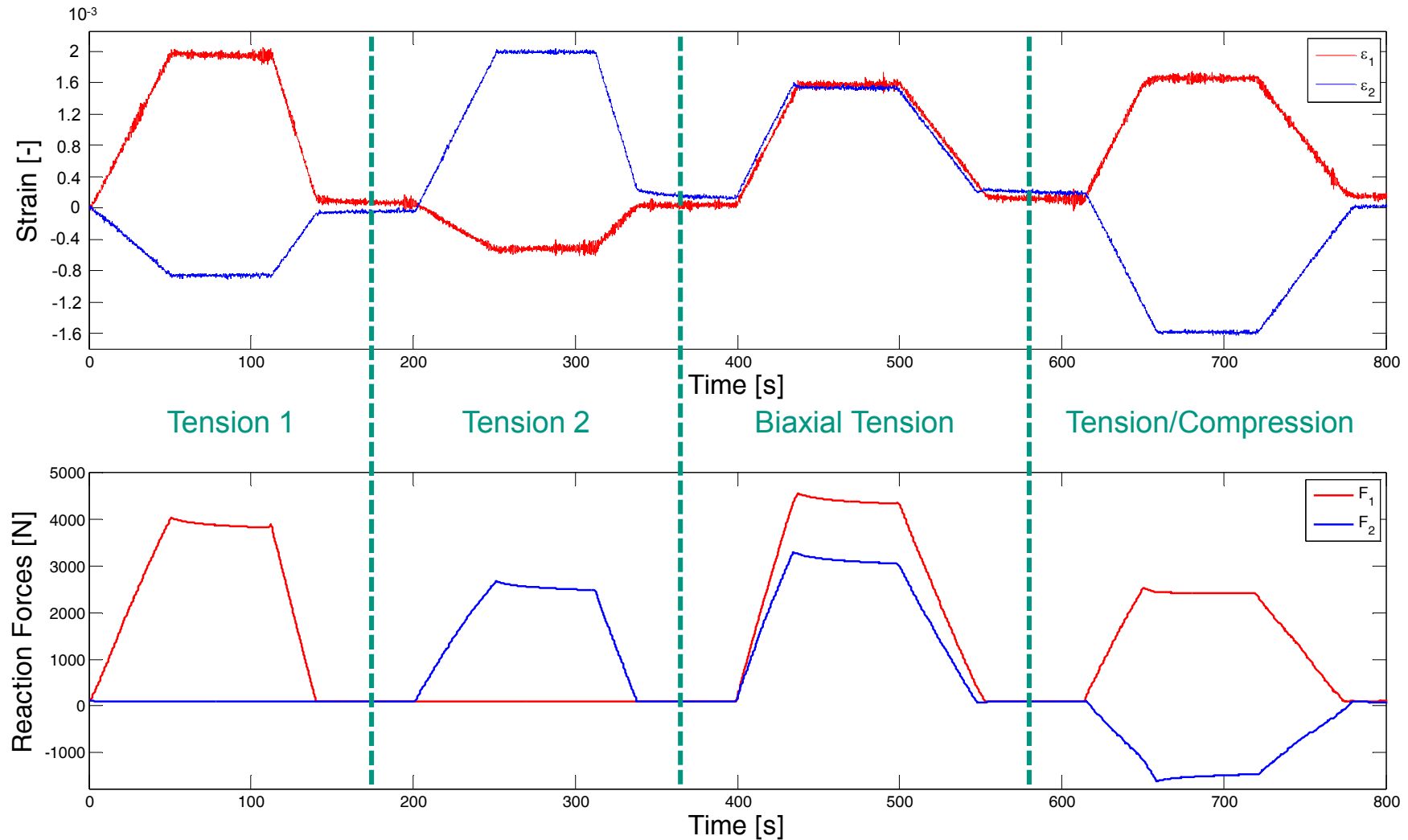
Malte Schemmann, [malte.schemmann@kit.edu](mailto:malte.schemmann@kit.edu), KIT ITM

# Biaxial Tensile Machine (ITM)

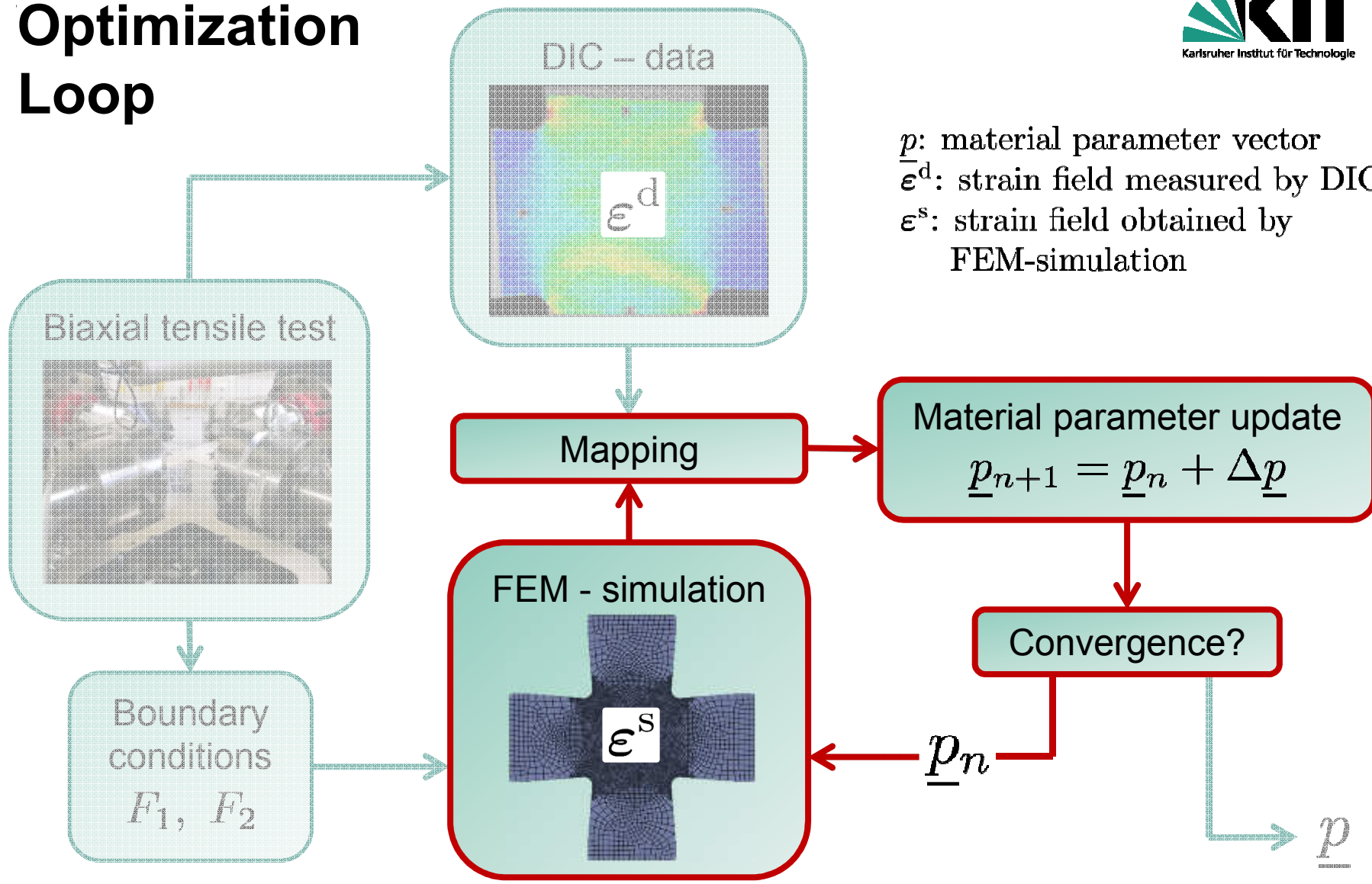


- Actors: four independent axes (maximum load: 150kN)
- Sensors:
  - Force measurement (on all four axes)
  - Integrated strain (Video XTens)
  - Full strain field via digital image correlation (GOM ARAMIS 4M)
- Active midpoint control

# Viscoelastic Biaxial Tensile Tests: Prescribed Strain / Force Paths



# Optimization Loop



# Inverse Parameter Identification

- Problem: Find parameter  $\underline{p}$  that minimizes the error Function  $f(\underline{p})$

$$\underline{r}(\underline{p}) = \sum_{i=1}^K \sum_{j=1}^N \begin{pmatrix} |\varepsilon_{11,i,j}^{\text{sim}}(\underline{p}) - \varepsilon_{11,i,j}^{\text{exp}}| \\ |\varepsilon_{22,i,j}^{\text{sim}}(\underline{p}) - \varepsilon_{22,i,j}^{\text{exp}}| \\ |\gamma_{12,i,j}^{\text{sim}}(\underline{p}) - \gamma_{12,i,j}^{\text{exp}}| \end{pmatrix}$$

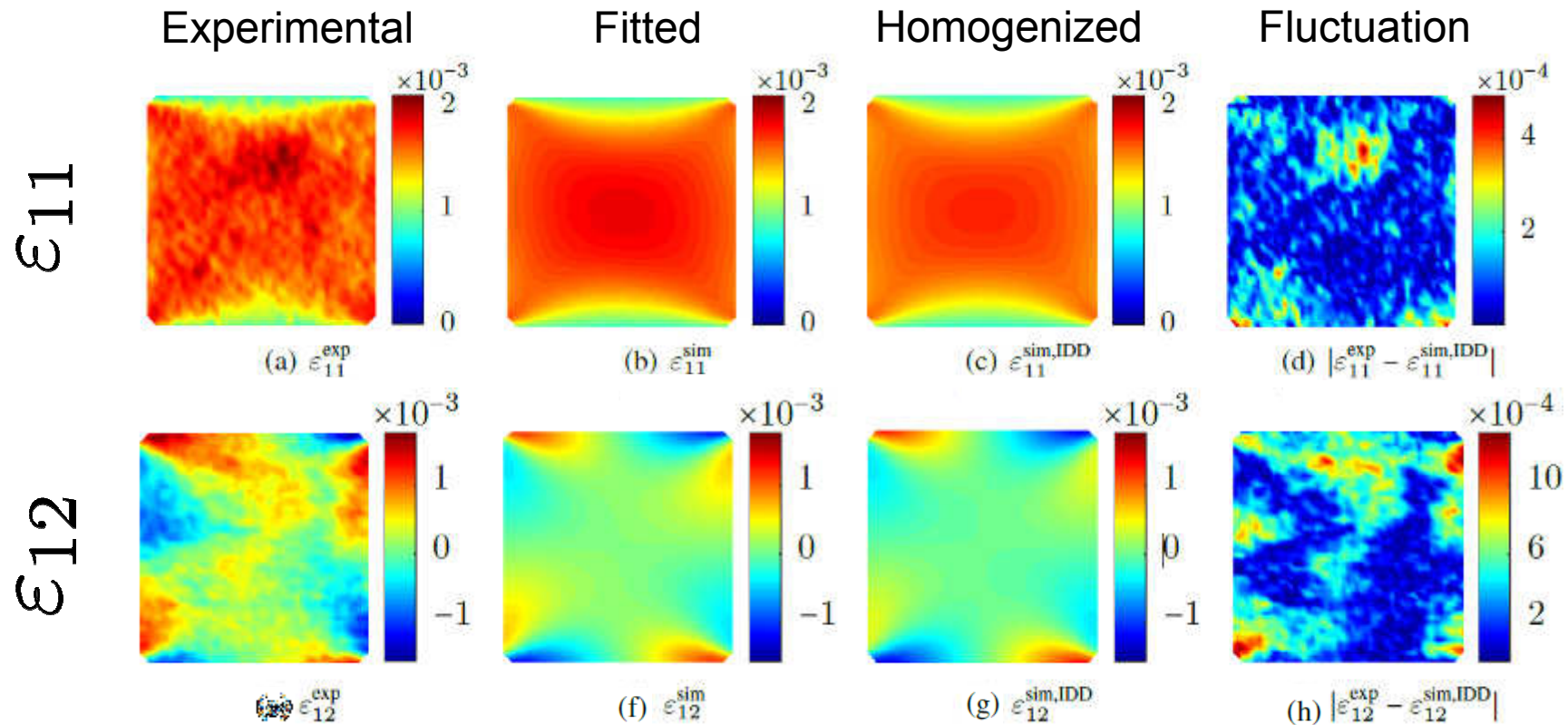
Louis (1989)  
Mahnken et al. (1996)  
Cooreman et al. (2007)

- Gauss-Newton procedure

$$f(\underline{p}) = \|\underline{r}(\underline{p})\|_2^2 = \underline{r}(\underline{p})^\top \underline{r}(\underline{p}) \rightarrow \min_{\underline{p} \in \mathcal{P}}$$

$$\underline{p}^{k+1} = \underline{p}^k - \left[ \underline{\underline{J}}(\underline{p}^k)^\top \underline{\underline{J}}(\underline{p}^k) \right]^{-1} \underline{\underline{J}}(\underline{p}^k)^\top \underline{r}(\underline{p}^k) \quad J_{ij}(\underline{p}) = \frac{\partial \varepsilon_i^s(\underline{p})}{\partial p_j}$$

# Validation Tension-Compression Loading



- The experimentally measured, fitted and homogenized strain field show a comparably good agreement
- SMC shows heterogeneities, possibly induced by varying fiber orientation or volume fraction

[Contact: Malte Schemmann, malte.schemmann@kit.edu, Loredana Kehrer, loredana.kehrer@kit.edu, KIT ITM]

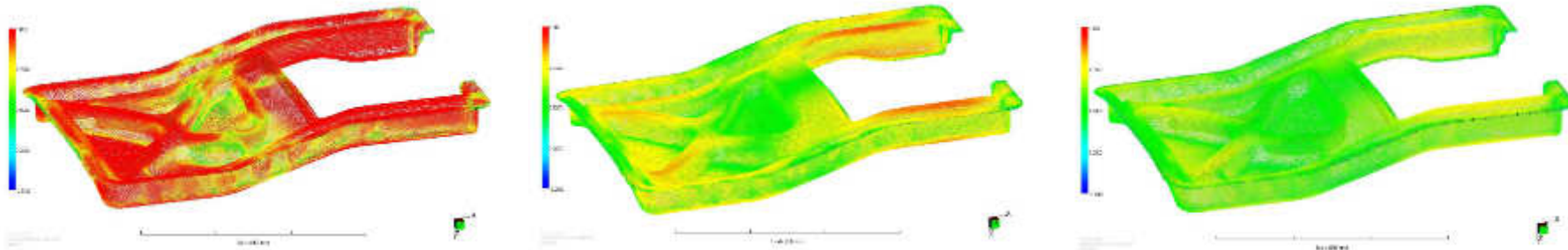


# Form Filling: Micromechanical Modeling

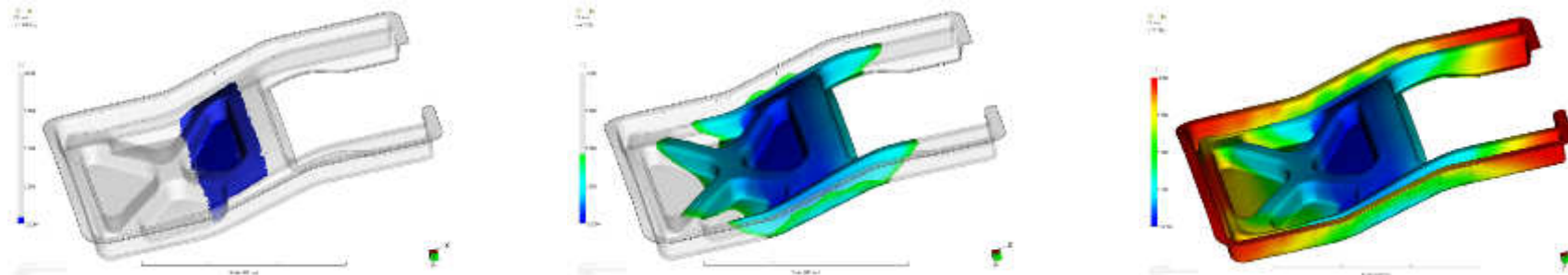
Contact: Robert Bertoti, [robert.bertoti@kit.edu](mailto:robert.bertoti@kit.edu), KIT ITM

# Form Filling Simulations – Motivation

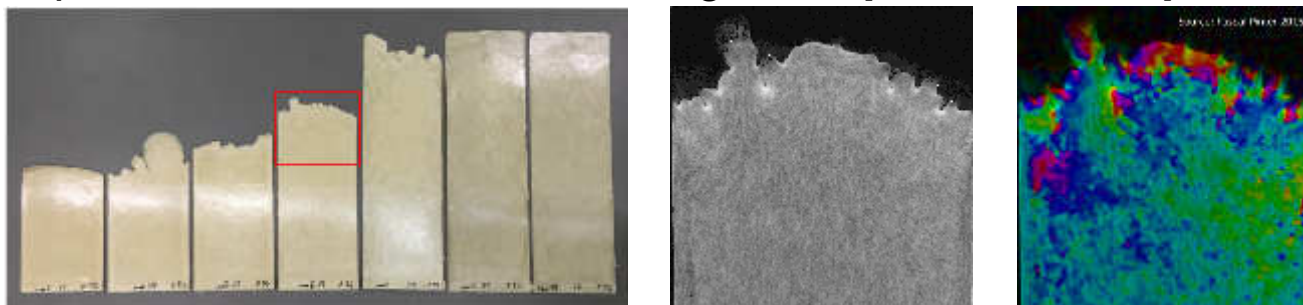
- Prediction of the **fiber orientation** of compression molded DiCoFRP (Buck2014)



- Prediction of the **flow front** evolution during compression molding (Buck2014)



- Development of the simulations through **comparison to experiments**

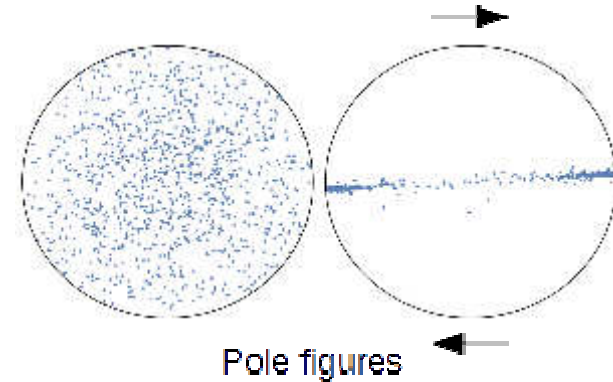


# Evolution equations of Single Fiber and FOTs

- Change of single rigid-fiber orientation (Jeffery1922)

$$\dot{n}_\alpha = \bar{W}[n_\alpha] + \bar{\xi}(\bar{D}[n_\alpha] - (n_\alpha \otimes n_\alpha \otimes n_\alpha)[\bar{D}])$$

where:  $\bar{L} = \text{grad}(\bar{v}) = \bar{D} + \bar{W}$      $\bar{D} = \frac{1}{2}(\bar{L} + \bar{L}^T)$   
 $\bar{W} = \frac{1}{2}(\bar{L} - \bar{L}^T)$      $\bar{\xi} = \frac{\bar{a}^2 - 1}{\bar{a}^2 + 1}$      $\bar{a} = \bar{l}/\bar{d}$



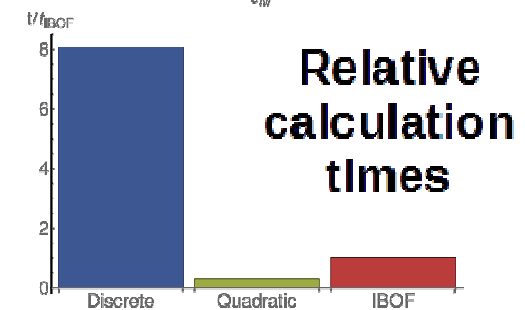
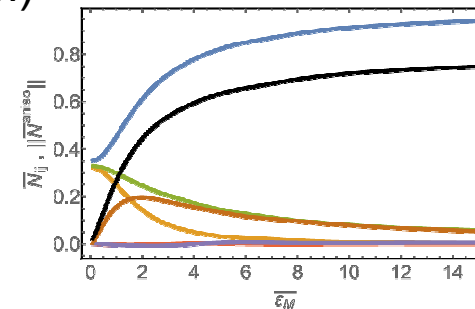
- Jeffery's equation for FOTs (including closure problem)

$$\dot{\bar{N}} = \bar{W}\bar{N} - \bar{N}\bar{W} + \bar{\xi}(\bar{D}\bar{N} + \bar{N}\bar{D} - 2\bar{N}^*[\bar{D}])$$

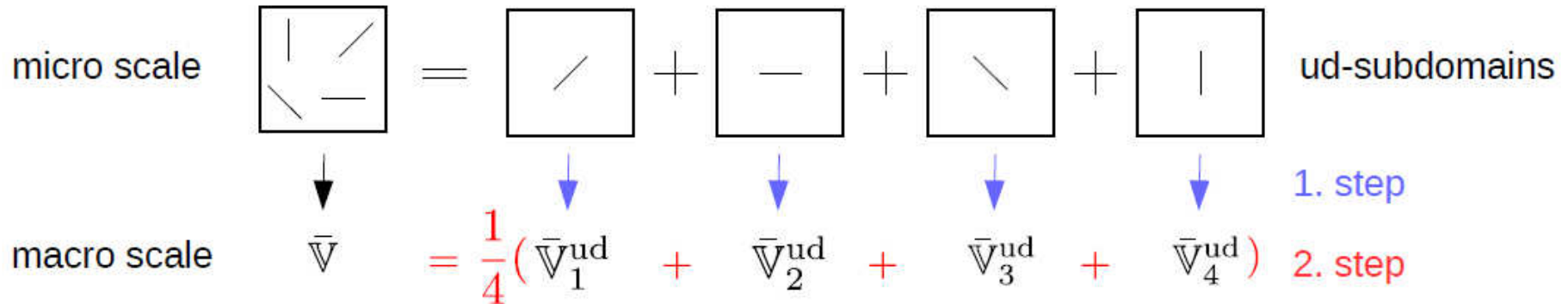
where:  $\bar{N}^{\text{Quad}} = \bar{N} \otimes \bar{N}$  (Doi1981)

(Chung2002)

$$\bar{N}^{\text{IBOF}} = \beta_1 \text{sym}(\mathbf{1} \otimes \mathbf{1}) + \beta_2 \text{sym}(\mathbf{1} \otimes \bar{N}) + \beta_3 \text{sym}(\bar{N} \otimes \bar{N}) + \beta_4 \text{sym}(\mathbf{1} \otimes \bar{N}\bar{N}) + \beta_5 \text{sym}(\bar{N} \otimes \bar{N}\bar{N}) + \beta_6 \text{sym}(\bar{N}\bar{N} \otimes \bar{N}\bar{N})$$



# Homogenization of the viscosity



- 1. step: calculating the unidirectional effective viscosity(s) (Hasin-Strikman lower bound) (Walpole1969, Castaneda1998)
- 2. step: calculating the overall effective linear viscosity (orientation averaging, Voigt average, upper bound) (Advani1987)
- It is sufficient to calculate the unidirectional effective viscosity only once, and calculate the overall effective viscosity with the help of FOTs

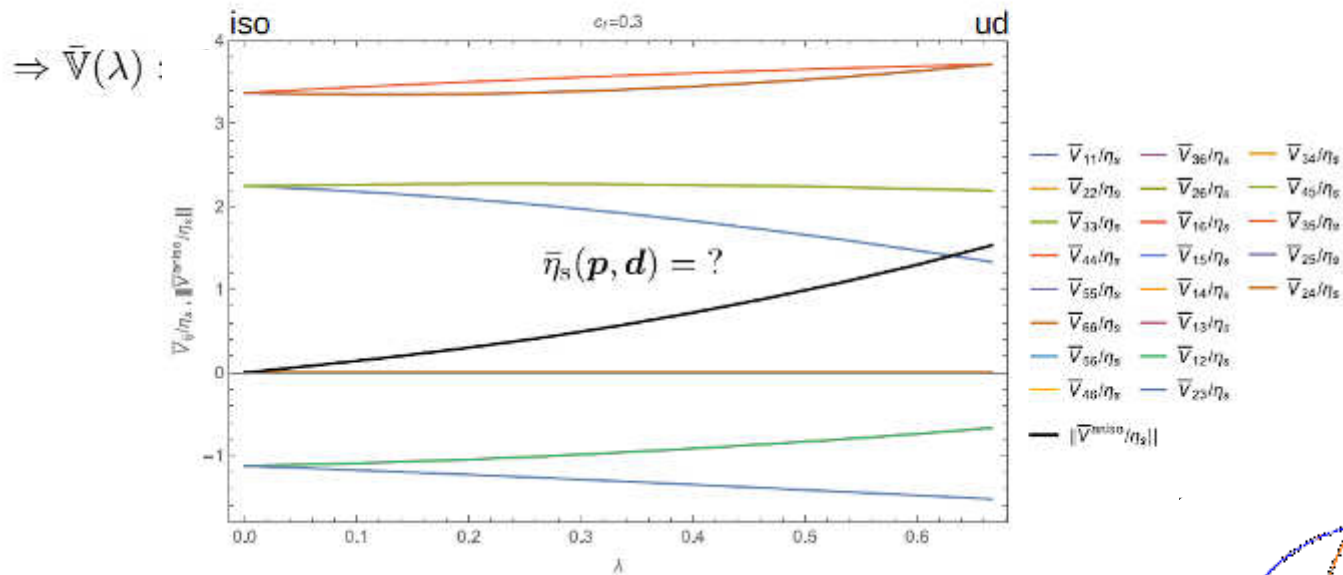
$$\bar{V}_\alpha^{ud} = V^m + \frac{c_f}{c_m} P_\alpha^{-1}$$

$$\bar{V} = \frac{1}{N} \sum_{\alpha=1}^N \bar{V}_\alpha^{ud}$$

$$\bar{V} = f(\bar{V}_x^{ud}, \bar{N}, \bar{N})$$

# Homogenization of the viscosity

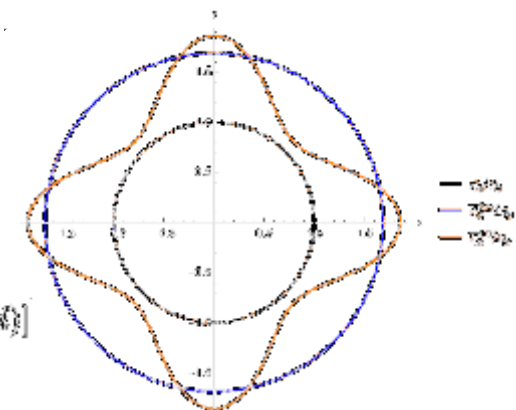
$$\bar{N}^{\text{iso}}(\lambda=0) = \begin{pmatrix} \frac{1}{3} & & \\ & \frac{1}{3} & \\ & & \frac{1}{3} \end{pmatrix} \quad \bar{N}(\lambda) = \begin{pmatrix} \frac{1}{3} + \lambda & & \\ & \frac{1}{3} + \frac{\lambda}{2} & \\ & & \frac{1}{3} + \frac{\lambda}{2} \end{pmatrix} \quad \bar{N}^{\text{ud}}(\lambda = \frac{2}{3}) = \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix}$$



## ■ Sensitivity of the effective tensorial viscosity

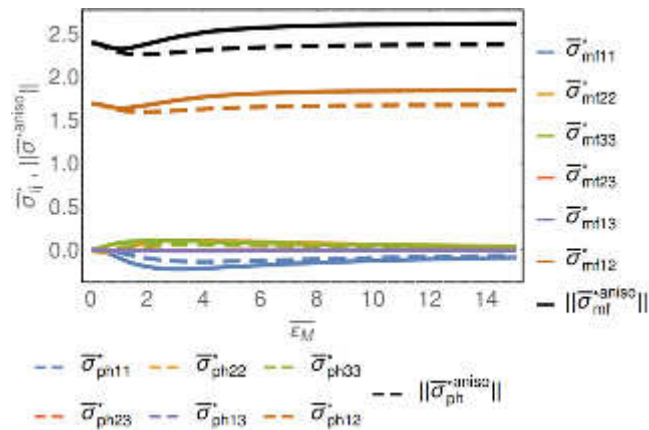
$$\bar{\Sigma}(p, d) = \frac{1}{2M(p, d)} \cdot \bar{V}^{-1} [M(p, d)]$$

$$M(p, d) = \sqrt{3} (p \otimes d + d \otimes p) / -$$

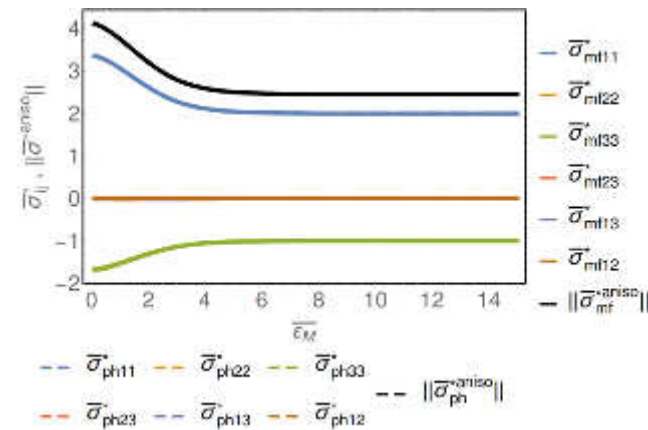


# Test Cases – Stress tensor

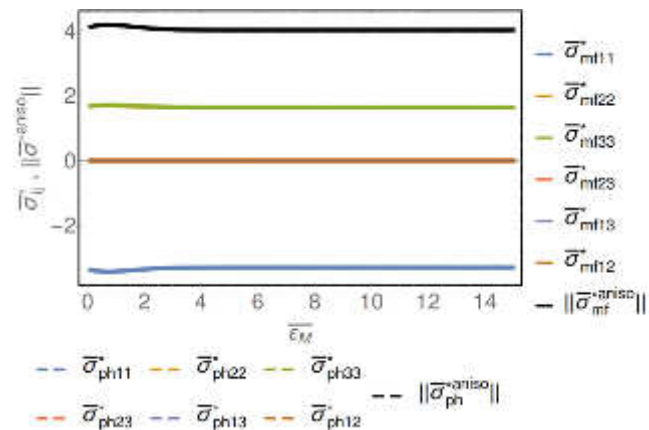
### Simple shear flow



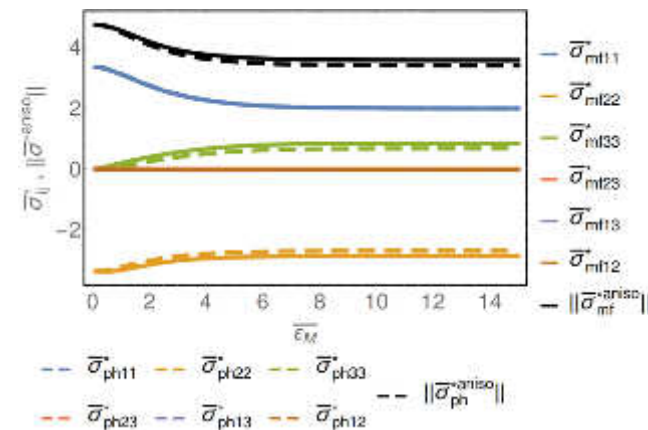
### Isochoric elongation flow



### Isochoric compression flow



### Plain strain flow



# Conclusions and Outlook

- An **interdisciplinary and integrated engineering** approach is necessary for the application of CoDiCoFRP
- A virtual process chain is required for taking the highly process-dependent material properties into account
- Adaption and validation of a complex virtual process chain is only feasible with a **standardization data formats**
- Future work will extend the material range the thermoplastics
- A reference structure will be established by GRK 2078 in 2017 :
  - Incorporation of all technology projects within the process chain
  - Geometry is obtained by fully coupled design optimization, thereby considering modfilling and structural analysis including damage

# Thank you for your attention.

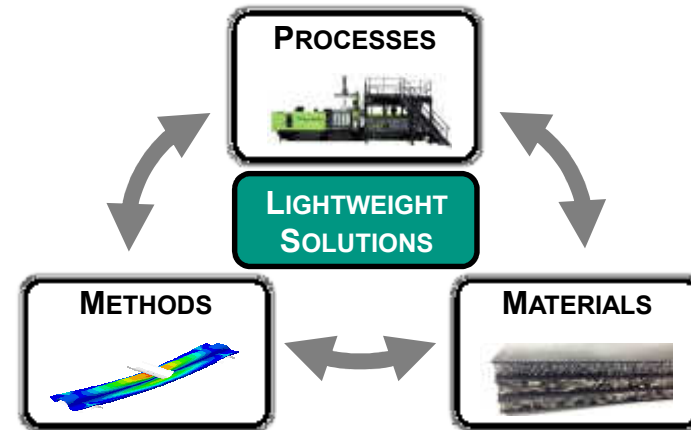


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## KIT - LIGHTWEIGHT DESIGN NETWORK



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### GRK 2078 CoDiCoFRP

[www.grk2078.kit.edu](http://www.grk2078.kit.edu)

### Contact

thomas.boehlke@kit.edu  
Karlsruhe Institute of Technology (KIT)  
Institute of Engineering Mechanics (ITM)  
Chair for Continuum Mechanics

