Simulation of Polymer Nanocomposites Using Transformation Field Analysis (TFA)

Dr.-Ing. Imad Aldin Khattab
Technische Universität Braunschweig | Institut für Adaptronik und Funktionsintegration
i.khattab@tu-braunschweig.de | Telefon +49 (0) 531 391-8070

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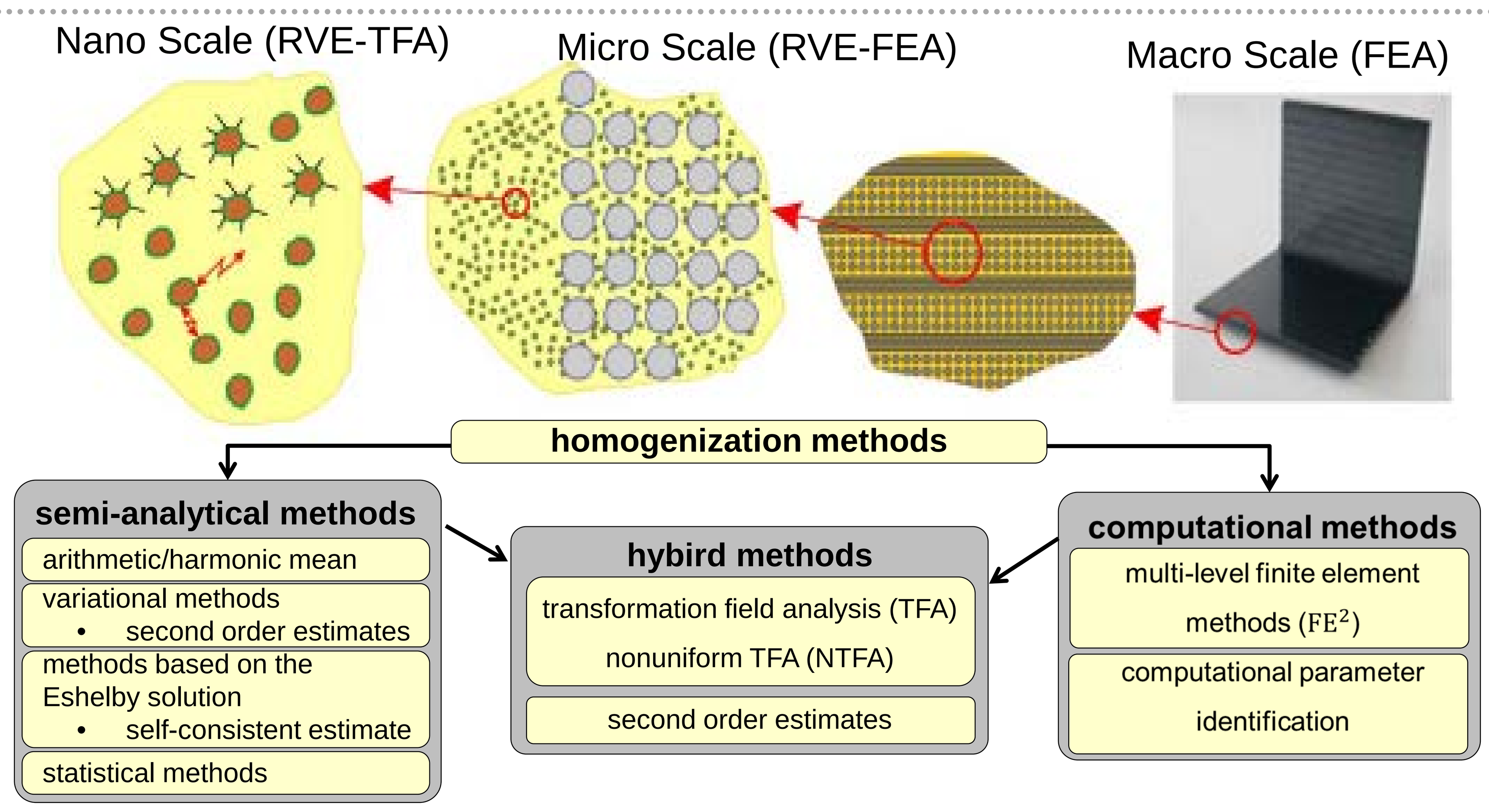
Aims of research activities

The objective of the project focuses on the development of mathematical models, i.e. analytically and/or numerically based, for an accelerated multiscale investigation of highly heterogeneous nanocomposite materials to save computational resources and time.

The Transformation Field Analysis proposed by Dvorak and co-workers can be seen as an elegant way of reducing the number of microscopic internal variables by assuming the nanoscopic fields of internal variables to be piecewise uniform.

Transformation field analysis (TFA) is a method for incremental solution of loading problems in **inelastic heterogeneous media** and composite materials.



TFA Method

Local fields

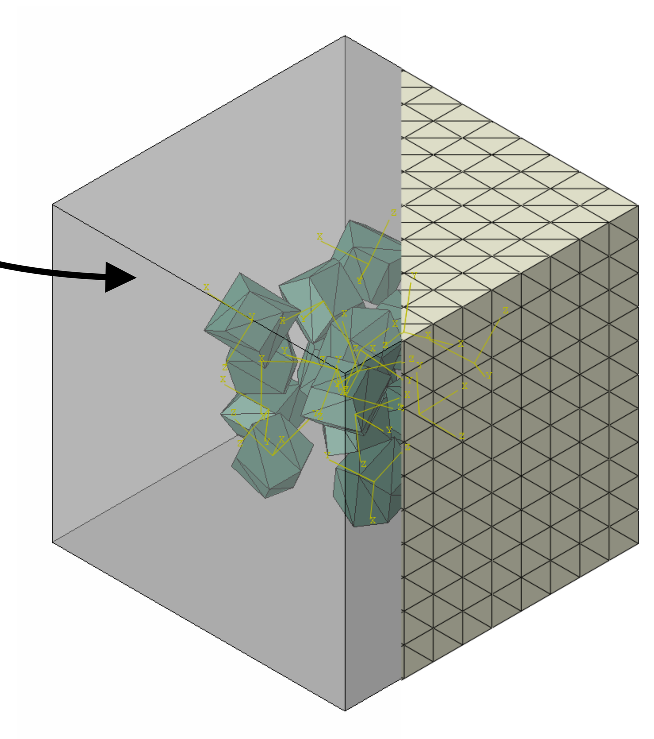
$\sigma_r = L_r \varepsilon_r + \lambda_r,$

$\varepsilon_r = M_r \sigma_r + \mu_r,$ r = 1,2, …, Q

$M_r = L_r^{-1}.$

$\lambda_r = -L_r \mu_r$ the Uniform transformation stress and strain.

λ_r and μ_r, represent local fields that are not reversed by removing the mechanical loads **(e.g., temperature changes, electrical loads or inelastic deformations).**



The overall response of the RVE

$$\bar{\sigma} = \bar{L}\bar{\varepsilon} + \bar{\lambda},$$
$$\bar{\varepsilon} = \bar{M}\bar{\sigma} + \bar{\mu},$$
$$\bar{\lambda} = \sum_{r=1}^{Q} c_r A_r^{\ T} \lambda_r$$
$$\bar{\mu} = \sum_{r=1}^{Q} c_r B_r^{\ T} \mu_r \qquad r = 1,2,\dots,Q$$

The overall elastic stiffness and compliance

$$\bar{L} = \sum_{r=1}^{Q} c_r L_r A_r$$
$$\bar{M} = \sum_{r=1}^{Q} c_r M_r B_r \qquad \bar{L} = \bar{M}^{-1}$$

The stress and strain local fields in the subvolumes

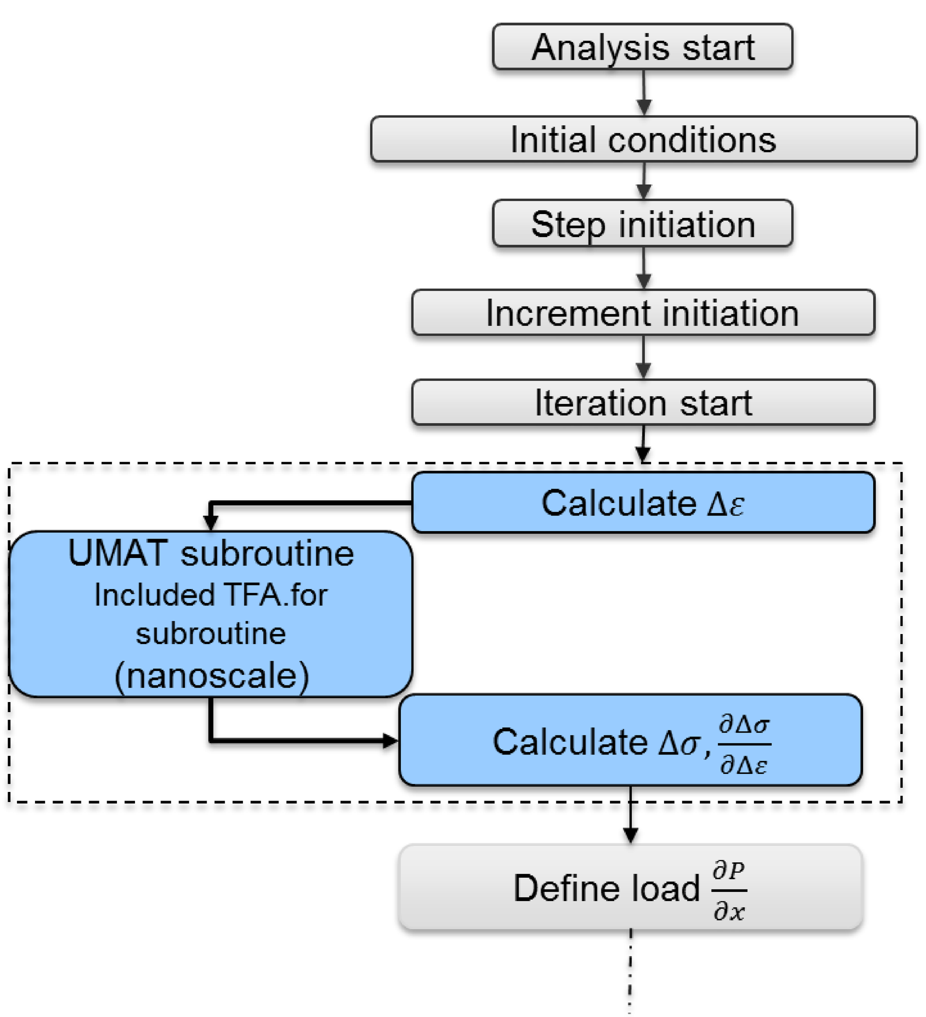
$$\varepsilon_r = A_r \bar{\varepsilon} + \sum_{s=1}^{Q} D_{rs}\mu_s, \quad \sigma_r = B_r \bar{\sigma} + \sum_{s=1}^{Q} F_{rs}\lambda_s, \quad s, r = 1,2,\dots,Q$$

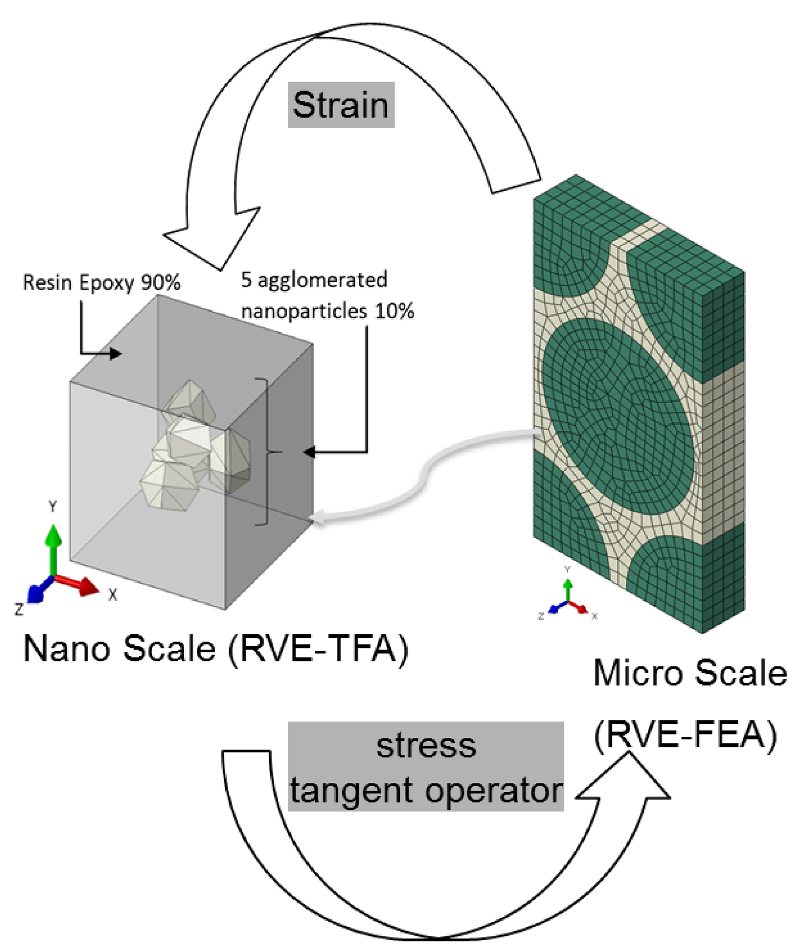
$\boldsymbol{A_r}$ **and** $\boldsymbol{B_r}$ are strain and stress concentration factors for subvolume V_r

$\boldsymbol{D_{rs}}$ **and** $\boldsymbol{F_{rs}}$ are transformation influence functions.

Application

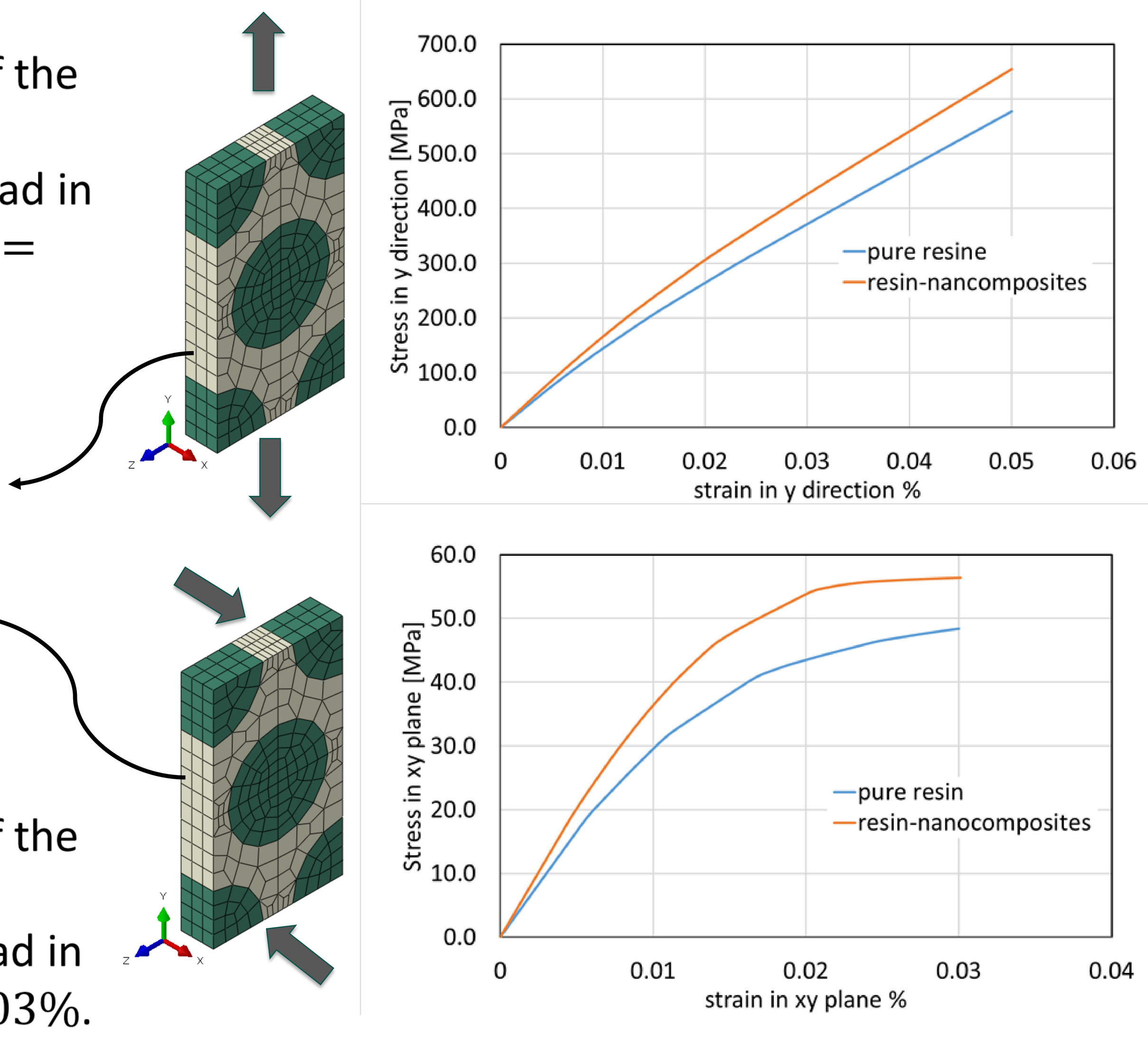
- **Connect the mathematical model (TFA) to a higher FE scale by multiscale approach (UMAT) i.e.,(TFA/FEA) Nano/Micro scale**





- **Predict the elastoplastic behaviour under various mechanical loads**

1. The Response of the RVE under displacement load in y direction $\varepsilon_x = 0.05\%$.
2. The Response of the RVE under displacement load in xy plane $\varepsilon_x = 0.03\%$.



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