

A Python package for homogenization procedures in fiber reinforced polymers

Nicolas Christ ^{1,2}, Benedikt M. Scheuring ¹, John Montesano ³, and Jörg Hohe ²

1 Karlsruhe Institute of Technology, Karlsruhe, Germany 2 Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany 3 University of Waterloo, Waterloo, ON, Canada

DOI: 10.21105/joss.05295

Software

- Review C²
- Repository ¹
- Archive ^[2]

Editor: Kevin M. Moerman 🖒 💿 Reviewers:

- @likask
 - Onicoguaro
 - Olizarett

Submitted: 27 February 2023 Published: 11 July 2023

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License (CC BY 4.0).

Summary

The Python package HomoPy is a numerical software tool which provides computational methods in the field of continuum mechanics with a specific emphasize on fiber reinforced composites. Experimental research has shown that hybridization effects for multi-inclusion composites exist (Fu & Lauke, 1998a; Summerscales & Short, 1978; Swolfs et al., 2014), which raises the demand to have numerical methods at hand to predict the effective properties of such composites. With a multi-inclusion Mori-Tanaka approach and the laminate theory incorporating the shear-lag modified Halpin-Tsai approach, HomoPy provides a solution to this demand.

The key element of HomoPy is the calculation and visualization of effective elastic stiffness properties of hybrid materials, i.e. multi-inclusion composites, using homogenization procedures. The current homogenization implementations are the conventional, three-dimensional Mori-Tanaka approach (cf. Mori & Tanaka (1973)) in the formulation of Benveniste (1987) with a possible orientation averaging scheme after Advani & Tucker (1987). A comprehensive study on the effects of the orientation averaging on homogenization procedures can be found in Bauer & Böhlke (2022). To circumvent effective stiffness tensors, which are not major-symmetric and therefore violate thermodynamical principles, the algorithm in Jiménez Segura et al. (2023) was implemented and can be activated by a flag parameter to ensure symmetric stiffnesses. Alternatively, the shear-lag modified Halpin-Tsai approach (cf. Fu et al. (2019)) for purely planar information, for which the laminate theory is used to calculate effective stiffness properties, is available. The use field of these tools is academic research. An illustration of the implemented procedures is given in Figure 2.

Furthermore, HomoPy has the functionality to visualize the effective stiffness properties following Böhlke & Brüggemann (2001), which allows for an intuitive comparison of different composites. The resulting effective properties can then be used in consequent numerical simulations.



Figure 1: Logo of HomoPy.



Statement of need

Current ecological developments call for technical solutions to reduce the CO2 emissions of future innovations. Significant potential for promoting a better eco-balance lies in the development of new material systems, especially in the field of lightweight construction. Fiber-reinforced polymers (FRP) are a promising class of materials in the field of lightweight construction. The fibers used have high specific strength and stiffness properties, so that less material is required to achieve comparable properties compared with conventional materials, e.g. steel. The polymer serves to hold the fibers in place, transfer stresses between them, and increase the toughness properties of the composite. For more literature on FRP, see Christensen & Mccoy (1980) and Chawla (2019).

A general challenge in using FRP in engineering is that predictive simulations rely on robust material models. Since it is a highly inhomogeneous material, the computational cost increases dramatically if all components are modeled directly, i.e., if a full-field simulation is used. To circumvent this, homogenization methods have been developed in the last decades. The goal of a homogenization method is to calculate the material properties of a synthetic homogeneous material, which should then behave effectively like the inhomogeneous material.



Figure 2: Schematic of implemented homogenization methods, where \mathbb{C}_i is the stiffness tensor of component i, $\overline{\mathbb{C}}$ is the effective stiffness tensor, ϕ_i is the orientation angle of fiber i and a_i its aspect ratio. Illustration in reference to Fu & Lauke (1998b).

Christ et al. (2023). A Python package for homogenization procedures in fiber reinforced polymers. *Journal of Open Source Software*, 8(87), 5295. 2 https://doi.org/10.21105/joss.05295.



HomoPy was developed to contain two commonly used homogenization methods, that is, the Mori-Tanka (cf. Mori & Tanaka (1973)) for 3D stiffness predictions and a shear-lag modified Halpin-Tsai method (cf. Cox (1952) and Halpin (1969)) for planar predictions, i.e. laminate predictions, which is based on the formulations in Fu et al. (2019). The goal of HomoPy is to provide an open-source implementation of these methods with a particular focus on hybrid FRP modeling. Other modules offering similar functionalities are available, e.g. fiberpy and mechmean (cf. Bauer (2022)), but to the author's knowledge none of them provide the capability to model hybrid FRPs consisting of different fiber materials and/or geometries. A key element in HomoPy is the implementation of the graphical representation of the effective directional stiffnesses according to Böhlke & Brüggemann (2001). Comparing different material systems or FRP tape layup orientations is intuitively easier with a graphical representation than comparing up to 21 stiffness components each. The package mechkit (cf. Bauer et al. (2022)) also offers this visualization procedure, but is further capable of visualizing the generalized bulk modulus. fiberoripy (cf. Meyer et al. (2022)) uses a different general algorithm to represent second and forth order tensors, focusing on fiber orientation tensors rather than stiffness tensors. Other visualization tools can be found in the package continuum-mechanics (cf. Guarín-Zapata (2020)), though the visualization is designed to represent phase speed tensors. To the authors' knowledge, only HomoPy offers a visualization tool for elastic tensors in laminates and 2D stiffness tensors in general, respectively.

To this point, HomoPy is limited to calculating the effective elastic properties with the two methods mentioned above. Possible extensions for the future include thermal expansion properties and other homogenization methods.

Acknowledgements

The research documented in this manuscript has been funded by the German Research Foundation (DFG) within the International Research Training Group "Integrated engineering of continuous-discontinuous long fiber-reinforced polymer structures" (GRK 2078/2). The support by the German Research Foundation (DFG) is gratefully acknowledged.

In addition, N.C. acknowledges Julian Karl Bauer for valuable technical discussions.

References

- Advani, S. G., & Tucker, C. L. (1987). The use of tensors to describe and predict fiber orientation in short fiber composites. *Journal of Rheology*, 31(8), 751–784. https://doi. org/10.1122/1.549945
- Bauer, J. K. (2022). *Mechmean* (Version v0.1.0). Zenodo. https://doi.org/10.5281/zenodo. 6461940
- Bauer, J. K., & Böhlke, T. (2022). On the dependence of orientation averaging mean field homogenization on planar fourth-order fiber orientation tensors. *Mechanics of Materials*, *170*, 104307. https://doi.org/10.1016/j.mechmat.2022.104307
- Bauer, J. K., Kinon, P. L., Hund, J., Latussek, L., Meyer, N., & Böhlke, T. (2022). Mechkit: A continuum mechanics toolkit in python. *Journal of Open Source Software*, 7(78), 4389. https://doi.org/10.21105/joss.04389
- Benveniste, Y. (1987). A new approach to the application of mori-tanaka's theory in composite materials. *Mechanics of Materials*, 6(2), 147–157. https://doi.org/10.1016/0167-6636(87) 90005-6
- Böhlke, T., & Brüggemann, C. (2001). Graphical representation of the generalized hooke's law. *Technische Mechanik*, 21.



- Chawla, K. K. (2019). *Composite materials*. Springer International Publishing. https: //doi.org/10.1007/978-3-030-28983-6
- Christensen, R., & Mccoy, J. (1980). Mechanics of composite materials. Journal of Applied Mechanics, 47, 460. https://doi.org/10.1115/1.3153710
- Cox, H. L. (1952). The elasticity and strength of paper and other fibrous materials. British Journal of Applied Physics, 3(3), 72–79. https://doi.org/10.1088/0508-3443/3/3/302
- Fu, S.-Y., & Lauke, B. (1998a). Characterization of tensile behaviour of hybrid short glass fibre/calcite particle/ABS composites. *Composites Part A: Applied Science and Manufacturing*, 29(5), 575–583. https://doi.org/10.1016/S1359-835X(97)00117-6
- Fu, S.-Y., & Lauke, B. (1998b). The elastic modulus of misaligned short-fiber-reinforced polymers. Composites Science and Technology, 58(3), 389–400. https://doi.org/10.1016/ S0266-3538(97)00129-2
- Fu, S.-Y., Lauke, B., & Mai, Y. W. (2019). Science and engineering of short fibre-reinforced polymer composites (Second edition). Woodhead Publishing. ISBN: 9780081026236
- Guarín-Zapata, N. (2020). Continuum_mechanics: Continuum mechanics calculations in python (Version 0.2.1). https://doi.org/10.5281/zenodo.4029448
- Halpin, J. C. (1969). Effects of environmental factors on composite materials. https://doi. org/10.21236/ad0692481
- Jiménez Segura, N., Pichler, B. L. A., & Hellmich, C. (2023). Concentration tensors preserving elastic symmetry of multiphase composites. *Mechanics of Materials*, 178, 104555. https: //doi.org/10.1016/j.mechmat.2023.104555
- Meyer, N., kraussco, & JulianKarlBauer. (2022). *Meyer-nils/fiberoripy: v1.1.0* (Version v1.1.0). Zenodo. https://doi.org/10.5281/zenodo.7305587
- Mori, T., & Tanaka, K. (1973). Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta Metallurgica, 21(5), 571–574. https://doi.org/10.1016/ 0001-6160(73)90064-3
- Summerscales, J., & Short, D. (1978). Carbon fibre and glass fibre hybrid reinforced plastics. *Composites*, 9(3), 157–166. https://doi.org/10.1016/0010-4361(78)90341-5
- Swolfs, Y., Gorbatikh, L., & Verpoest, I. (2014). Fibre hybridisation in polymer composites: A review. Composites Part A: Applied Science and Manufacturing, 67, 181–200. https: //doi.org/10.1016/j.compositesa.2014.08.027