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Fiber orientation tensor approximations based on an implicitly defined closure approach

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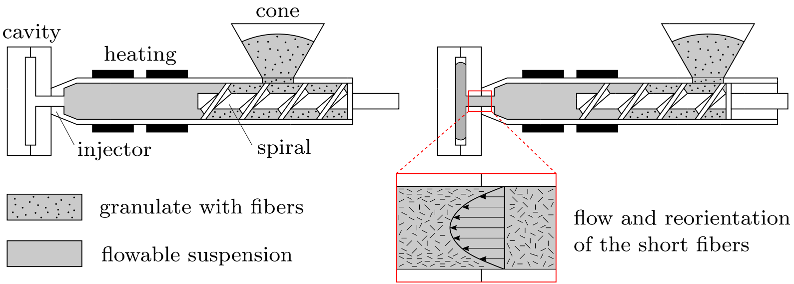
Contents

Motivation

- Application of short fiber reinforced polymers in lightweight design
- Injection molding process
- Fiber orientation evolution during mold filling
- Final effective anisotropy depends on local fiber orientation



Tucker (2022)
Figure: Karl et al. (2021)

Fiber orientation tensors

- Second- and fourth-order orientation tensors of the first kind

$$\boldsymbol{N} = \int_{\mathcal{S}} f(\boldsymbol{n})\boldsymbol{n}\otimes\boldsymbol{n}\,\mathrm{d}S$$

$$\mathbb{N} = \int_{\mathcal{S}} f(\boldsymbol{n})\boldsymbol{n}\otimes\boldsymbol{n}\otimes\boldsymbol{n}\otimes\boldsymbol{n}\,\mathrm{d}S$$

- Fiber orientation evolution equation

$$\dot{\boldsymbol{N}} = \boldsymbol{W}\boldsymbol{N} - \boldsymbol{N}\boldsymbol{W} + \frac{\alpha^2 - 1}{\alpha^2 + 1}\left(\boldsymbol{D}\boldsymbol{N} + \boldsymbol{N}\boldsymbol{D} - 2\mathbb{N}[\boldsymbol{D}]\right) + 2C_{\mathrm{I}}\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{N})$$

- Closure function $\mathbb{F}$ required for closure

$$\mathbb{N} \approx \mathbb{F}(\boldsymbol{N})$$

Kanatani (1984)
Folgar & Tucker (1984)
Advani & Tucker (1987)

Required algebraic properties of $\mathbb{F}(\boldsymbol{N})$

- Full index symmetry
- Contraction condition $\mathbb{N}[\boldsymbol{I}] = \boldsymbol{N}$ or $N_{ijkk} = N_{ij}$
- Trace condition $\mathbb{N} \cdot \mathbb{I} = N_{klkl} = 1$
- Trace-preserving property during evolution $\mathrm{tr}(\mathbb{N}[\boldsymbol{D}]) = \boldsymbol{N} \cdot \boldsymbol{D} = N_{ij} D_{ij}$

Advani & Tucker (1987)
Petty et al. (1999)

Implicit closure approach

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- Closure tensor $\boldsymbol{B}$ (unknown) is used instead of the given $\boldsymbol{N}$

$$\mathbb{N} \approx \mathbb{F}(\boldsymbol{B})$$

- Closure tensor $\boldsymbol{B}$ is implicitly defined via the contraction condition

$$\mathbb{F}(\boldsymbol{B})[\boldsymbol{I}] = \boldsymbol{N}$$

- Function $\boldsymbol{F}$ (whose roots $\boldsymbol{B}$ are sought)

$$\boldsymbol{F}(\boldsymbol{B}) = \mathbb{F}(\boldsymbol{B})[\boldsymbol{I}] - \boldsymbol{N}$$

- Newton's method

$$\boldsymbol{B}_{n+1} = \boldsymbol{B}_n - \left(\frac{\partial \boldsymbol{F}(\boldsymbol{B}_n)}{\partial \boldsymbol{B}_n} \right)^{-1} [\boldsymbol{F}(\boldsymbol{B}_n)]$$

- If $\mathbb{F}$ is modeled fully symmetric, all properties of $\mathbb{N}$ are met

Karl et al. (2023)

Implicit quadratic closure (SIQ)

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- Chosen closure function

$$\begin{aligned}\mathbb{N} \approx \mathbb{F}(\boldsymbol{B}) &= \operatorname{sym}(\boldsymbol{B} \otimes \boldsymbol{B}) \\ &= \frac{1}{3}\left(\boldsymbol{B} \otimes \boldsymbol{B} + \boldsymbol{B} \square \boldsymbol{B} + (\boldsymbol{B} \square \boldsymbol{B})^{\mathsf{T}_\mathsf{R}}\right) \\ N_{ijkl} &= \frac{1}{3}\left(B_{ij}B_{kl} + B_{ik}B_{lj} + B_{il}B_{kj}\right)\end{aligned}$$

- Contraction condition

$$\begin{aligned}\boldsymbol{F}(\boldsymbol{B}) &= \mathbb{F}(\boldsymbol{B})[\boldsymbol{I}] - \boldsymbol{N} \\ &= \frac{1}{3}\left(\operatorname{tr}(\boldsymbol{B})\boldsymbol{B} + 2\boldsymbol{B}^2\right) - \boldsymbol{N}\end{aligned}$$

Karl et al. (2023)

- Exact for UD, ISO and PI orientation states
- 1D formulation possible

Implicit hybrid closure (SIHYB)

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- Chosen closure function

$$\mathbb{F}(\boldsymbol{B}) = (1-k)\left(-\frac{3}{35}\operatorname{sym}(\boldsymbol{I}\otimes\boldsymbol{I}) + \frac{6}{7}\operatorname{sym}(\boldsymbol{I}\otimes\boldsymbol{B})\right) + k\operatorname{sym}(\boldsymbol{B}\otimes\boldsymbol{B})$$
$$k = 1 - 27\det(\boldsymbol{N})$$

- Contraction condition

$$\boldsymbol{F}(\boldsymbol{B}) = \frac{1-k}{7}\Big(\operatorname{tr}(\boldsymbol{B}) - 1\Big)\boldsymbol{I} + \Big(1 - k + \frac{k}{3}\operatorname{tr}(\boldsymbol{B})\Big)\boldsymbol{B} + \frac{2k}{3}\boldsymbol{B}^2 - \boldsymbol{N},$$

- Exact for UD, ISO and PI orientation states
- 1D formulation possible

Karl et al. (2023)

Estimation of effective properties

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- Fiber orientation state

$$N_{ij} = \begin{pmatrix} 0.392 & 0.111 & -0.006 \\ 0.111 & 0.584 & -0.005 \\ -0.006 & -0.005 & 0.024 \end{pmatrix}$$

- Mori-Tanaka model with orientation average $\langle \cdot \rangle_\mathrm{F}$

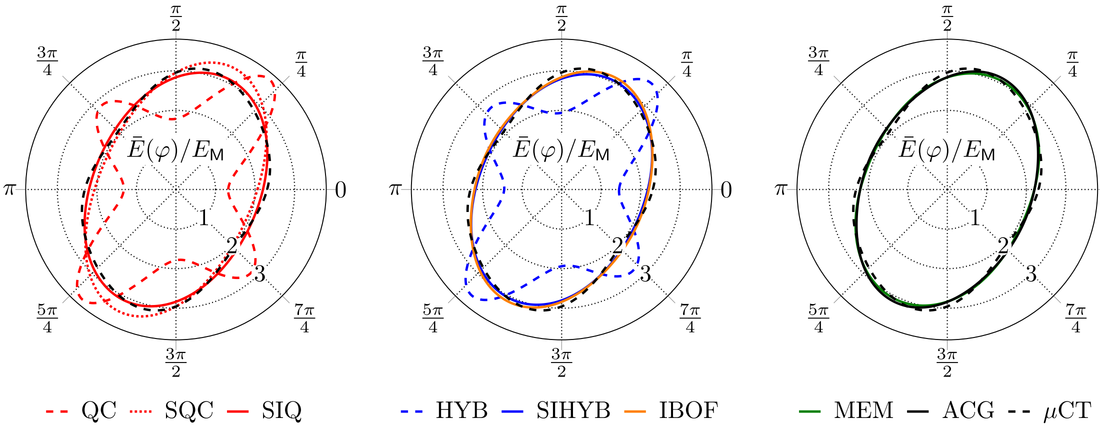
$$\bar{\mathbb{C}} = \mathbb{C}_\mathrm{M} + c_\mathrm{F} \left(c_\mathrm{F} \delta \mathbb{C}^{-1} + c_\mathrm{M} \left\langle \left(\delta \mathbb{C}^{-1} + \mathbb{P}_0 \right)^{-1} \right\rangle_\mathrm{F}^{-1} \right)^{-1}$$

$$\bar{\mathbb{V}} = \mathbb{C}_\mathrm{M} + \frac{c_\mathrm{F}}{c_\mathrm{M}} \left\langle \mathbb{P}_0^{-1} \right\rangle_\mathrm{F}$$

- Aspect ratio $\alpha = 26$
- Fiber volume fraction $c_\mathrm{F} = 0.13$
- PP matrix ($E = 1.6\ \mathrm{GPa}, \nu = 0.4$) and glass fibers ($E = 73\ \mathrm{GPa}, \nu = 0.22$)

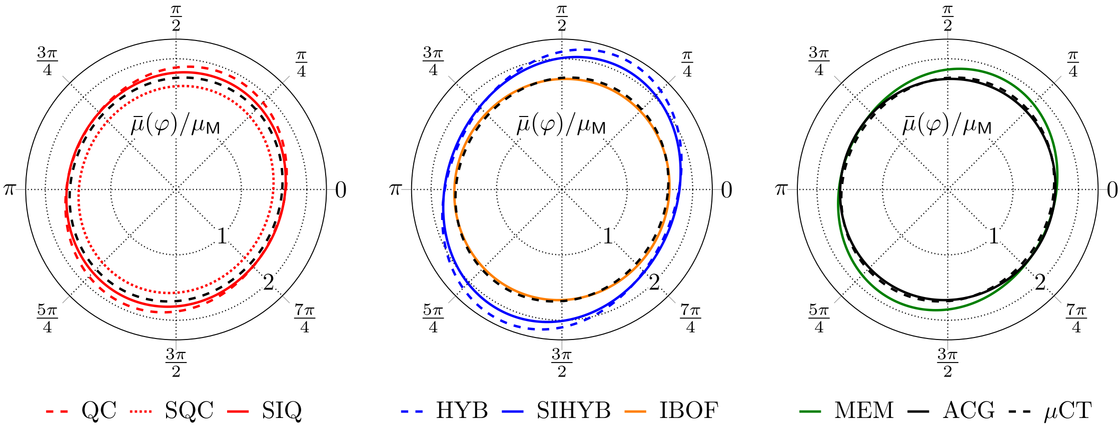
Müller et al. (2016)
Mori & Tanaka (1973)
Benveniste (1987)
Schürmann (2007)
Bertóti & Böhlke (2017)

Effective stiffness



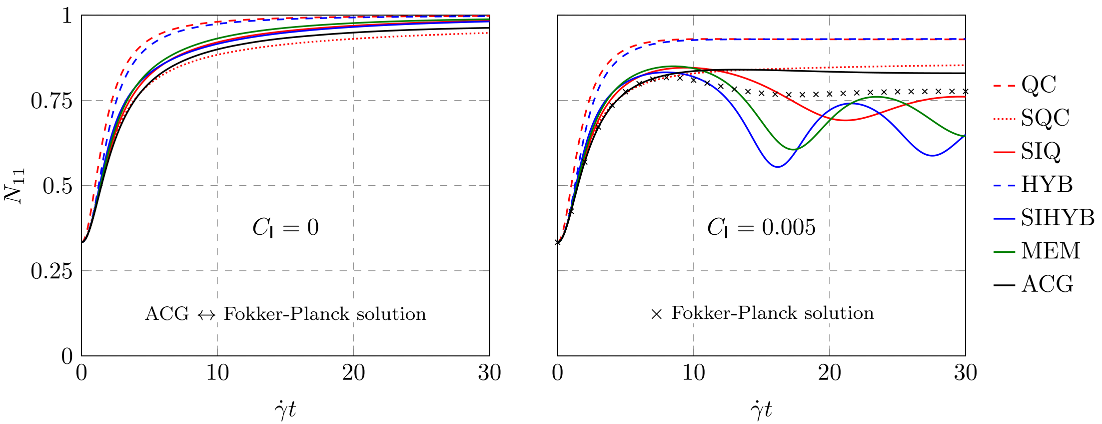
Karl et al. (2023)

Effective viscosity



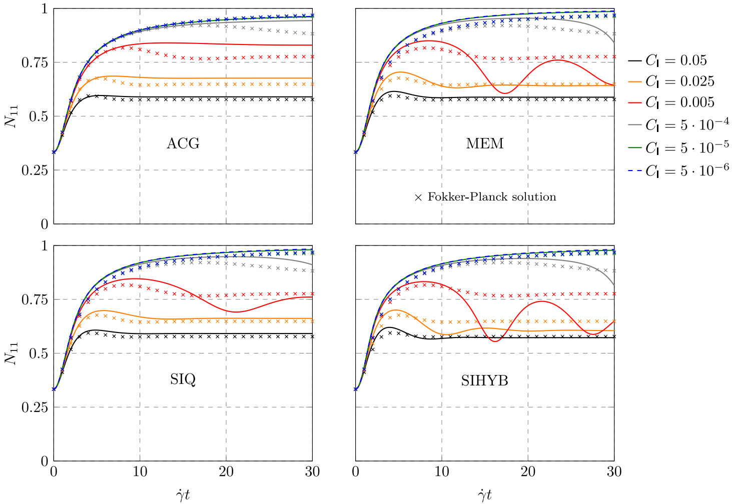
Karl et al. (2023)

Fiber orientation evolution (shear flow, $\alpha \to \infty$)



Karl et al. (2023)

Fiber orientation evolution (shear flow, $\alpha \to \infty$)



Karl et al. (2023)

Summary and conclusion

- Implicit closure approach based on contraction condition
- Fully symmetric implicit closure meets all algebraic requirements
- 1D formulation for both quadratic and hybrid approach
- Reliable estimation of anisotropic properties
- Fiber orientation evolution shows oscillations in simple shear flow
- Low-cost MEM approximation

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Appendix: Computational effort

Absolute computation time t_c and approximate relative computation time t_{rel} for all considered closure approximations.

Closure	t_c in s	t_{rel} in %
MEM	0.31688170	486024
ACG	0.11489970	176230
SIHYB	0.00011718	180
SIQ	0.00007490	115
IBOF	0.00006520	100
HYB	0.00001681	26
SQC	0.00000697	11
QC	0.00000186	3

Karl et al. (2023)

Appendix: 1D formulation of SIQ

- $\boldsymbol{F}(\boldsymbol{B}) = \boldsymbol{0}$ can be written as follows with $s = \operatorname{tr}(\boldsymbol{B})/4$

$$\boldsymbol{B}^2 + 2s\boldsymbol{B} = \frac{3}{2}\boldsymbol{N}$$

- Completing the square

$$(\boldsymbol{B} + s\boldsymbol{I})^2 = \frac{3}{2}\boldsymbol{N} + s^2\boldsymbol{I} \quad \Longleftrightarrow \quad \boldsymbol{B} = \sqrt{\frac{3}{2}\boldsymbol{N} + s^2\boldsymbol{I}} - s\boldsymbol{I}$$

- Trace of both sides ($\boldsymbol{B}$ and $\boldsymbol{N}$ share the same eigensystem)

$$(d + 4)s = \sum_{i=1}^{d} \sqrt{\frac{3\lambda_i}{2} + s^2}$$

Karl et al. (2023)

Appendix: 1D formulation of SIQ

- Newton's method for s (fixed λ_i and d)

$$f(s) = (d+4)s - \sum_{i=1}^{d} \sqrt{\frac{3\lambda_i}{2} + s^2}$$

$$f'(s) = 4 + \sum_{i=1}^{d} \underbrace{\left(1 - \frac{s}{\sqrt{\frac{3\lambda_i}{2} + s^2}}\right)}_{\geq 0} \geq 4$$

- Eigenvalues of $\boldsymbol{B}$

$$\mu_i = \sqrt{\frac{3\lambda_i}{2} + s^2} - s$$

Karl et al. (2023)

Appendix: References

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