Fiber Orientation Descriptors:

How we got here and what comes next

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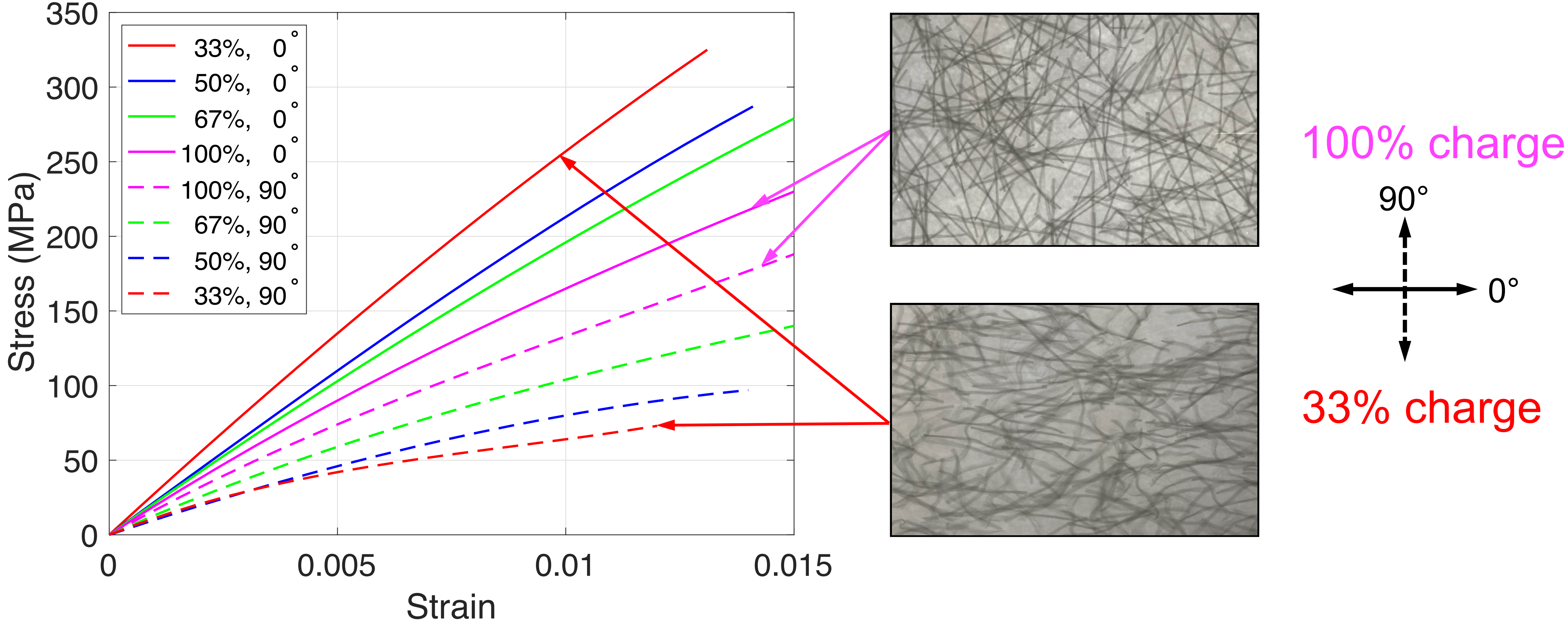
ILLINOIS

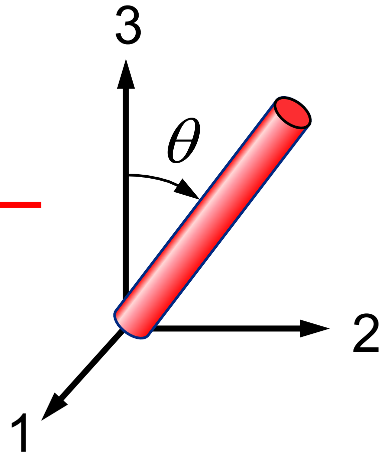
Processing affects properties
by changing the fiber orientation state



C. Y. Chen and C. L. Tucker, “Mechanical property predictions for short fiber/brittle matrix composites,” *J. Reinf. Plast. Compos., 3, 120-129, 1984.*

To connect processing, structure, and properties we need good orientation descriptors

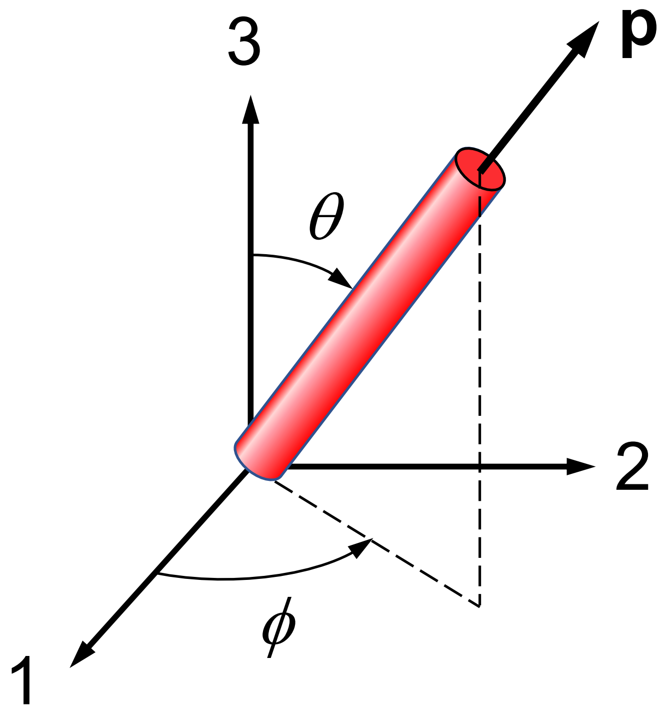
~~Hermans (1946):~~ $f_a = \frac{1}{2}\left[3\langle \cos^2\theta \rangle - 1\right]$



We want descriptors that can:

- ✗ represent any orientation state
- be measured experimentally
- ✗ be used to predict flow-induced orientation
- be used to predict properties

Describing the orientation of a single, rigid fiber is easy but real composites have a distribution of orientations



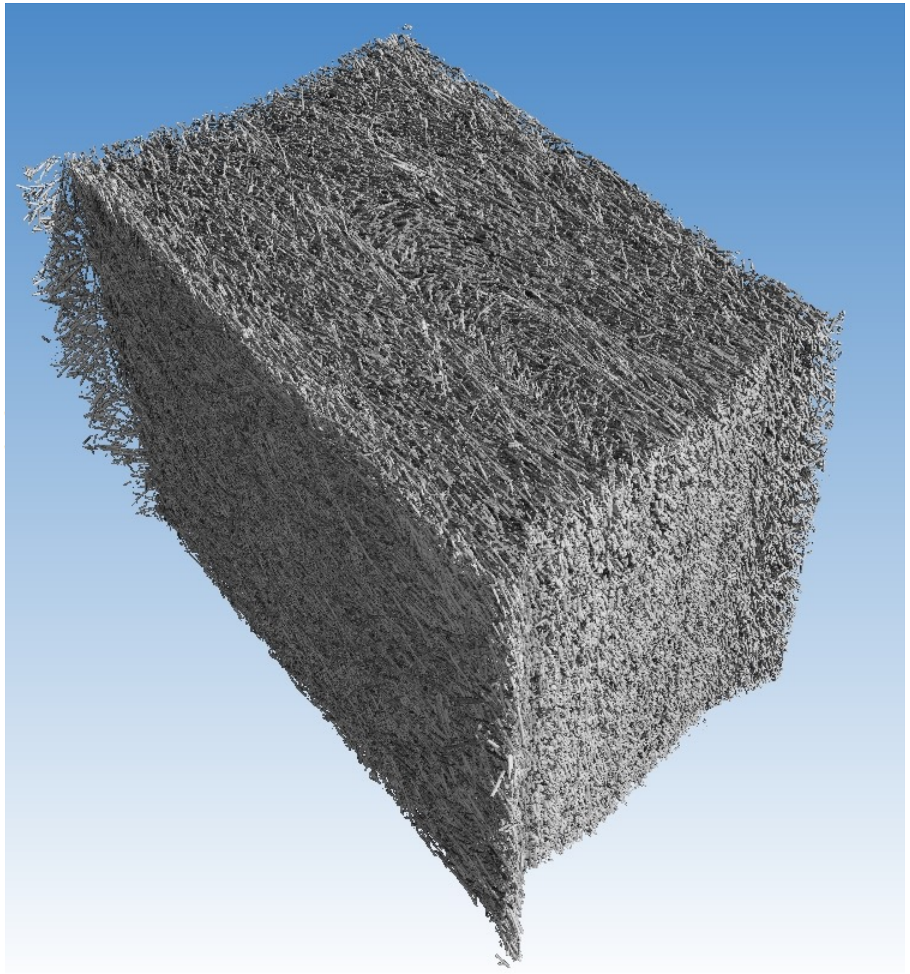
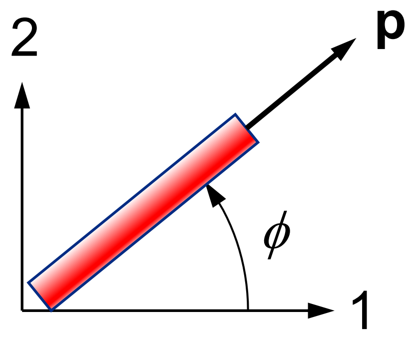


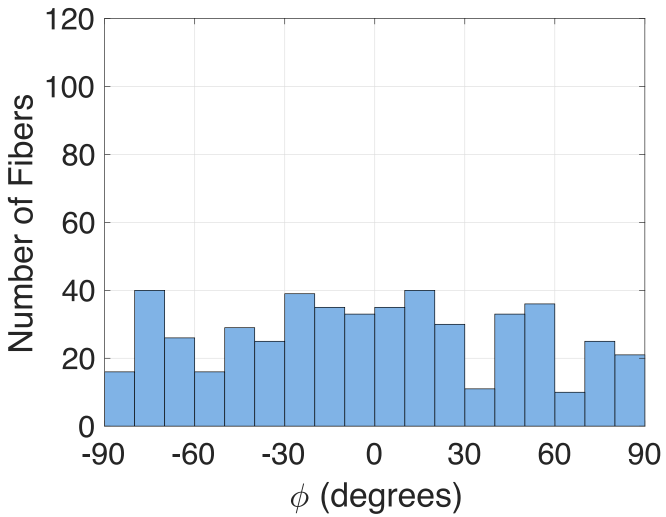
Image by Dr. Thomas Reidel

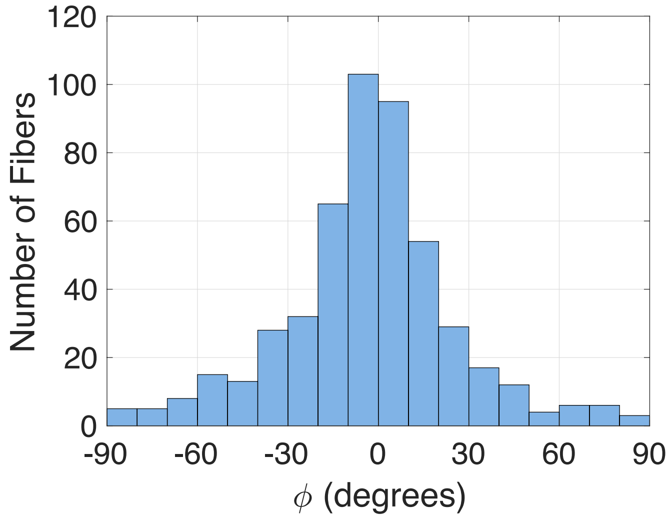
Groups of fibers can be described by the orientations of many fibers $\mathbf{p}^k, \quad k = 1 \text{ to } N$



planar orientation

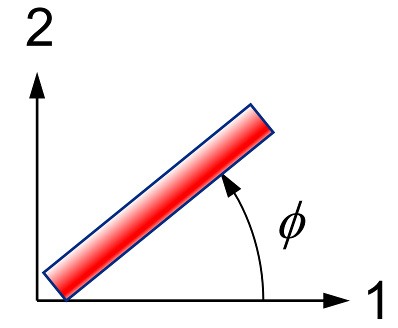
$$\mathbf{p} = \left\{ \begin{array}{c} \cos\phi \\ \sin\phi \end{array} \right\}$$



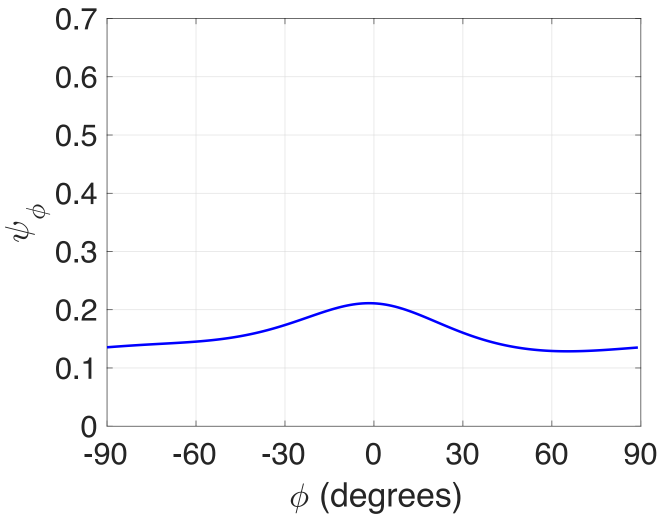


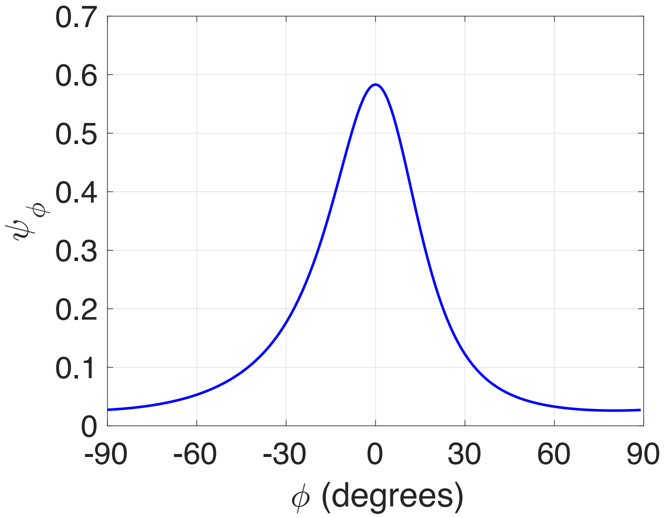
We can also use an orientation distribution function

$$P(\phi^* \leq \phi < \phi^* + \mathrm{d}\phi) = \psi_\phi(\phi^*)\,\mathrm{d}\phi$$



planar orientation

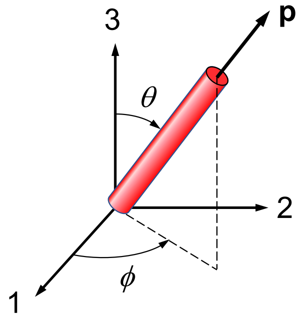




We can describe groups of fibers using orientation tensors

For each fiber, find

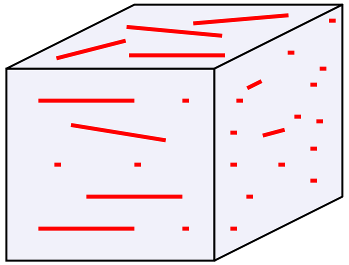
$$\mathbf{pp} = p_i p_j = \begin{bmatrix} p_1p_1 & p_1p_2 & p_1p_3 \\ p_2p_1 & p_2p_2 & p_2p_3 \\ p_3p_1 & p_3p_2 & p_3p_3 \end{bmatrix}$$



Average over all fibers

$$\mathbf{A} = \langle \mathbf{pp} \rangle$$

$$A_{ij} = \langle p_i p_j \rangle = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

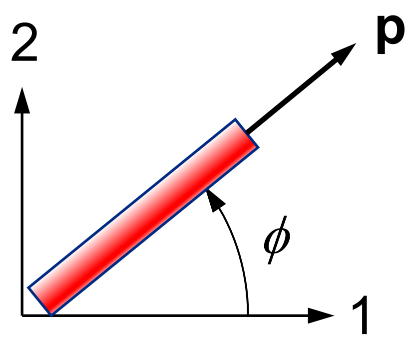


$$A_{ij} = A_{ji} \qquad A_{11} + A_{22} + A_{33} = 1$$

Fourth order tensor:

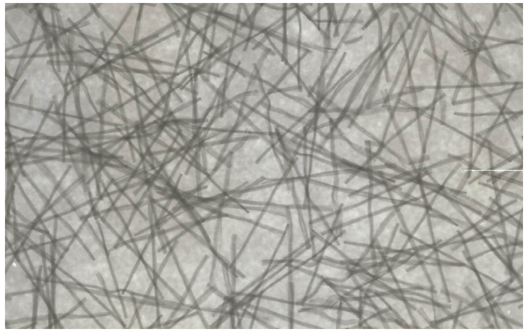
$$\mathbb{A} = \langle \mathbf{pppp} \rangle \qquad \mathbb{A}_{ijkl} = \langle p_i p_j p_k p_l \rangle$$

Orientation tensors work for planar orientation as well



planar orientation

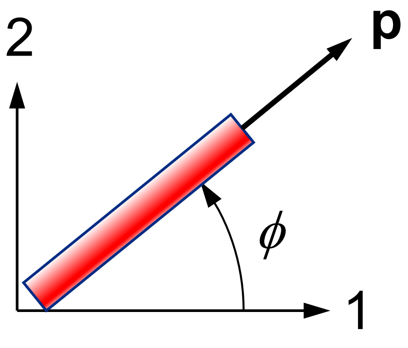
$$\mathbf{A} = \begin{bmatrix} \langle p_1 p_1 \rangle & \langle p_1 p_2 \rangle \\ \langle p_2 p_1 \rangle & \langle p_2 p_2 \rangle \end{bmatrix}$$



$$\mathbf{A} = \begin{bmatrix} 0.555 & -0.013 \\ -0.013 & 0.445 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 0.820 & -0.032 \\ -0.032 & 0.180 \end{bmatrix}$$

Orientation tensors also provide principal values and principal directions of orientation

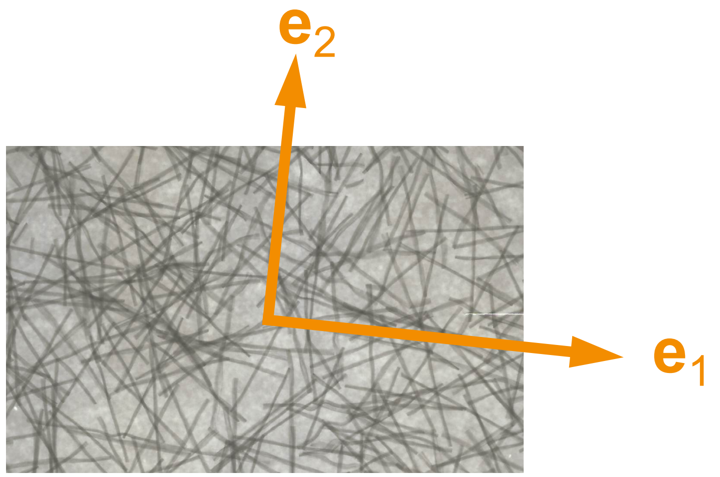


planar orientation

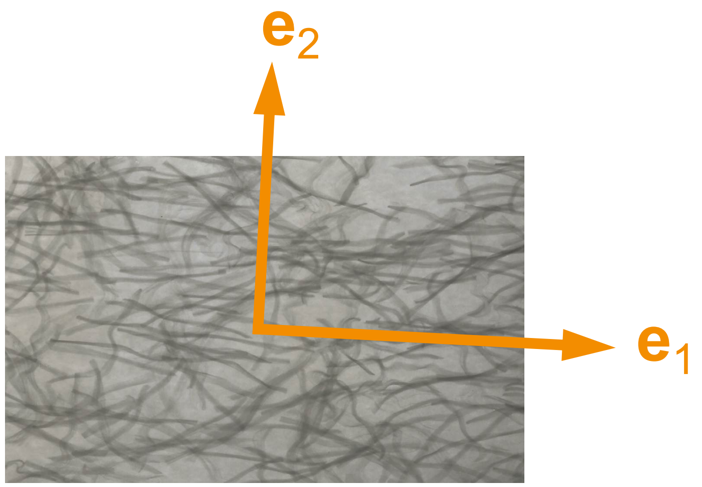
$$\mathbf{A} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \mathbf{e}_2$$

eigenvalues   eigenvectors

$\lambda_1 + \lambda_2 = 1$ so $\lambda_1 \in [0.5, 1]$



$\lambda_1 = 0.556$



$\lambda_1 = 0.821$

The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites

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Synopsis

The properties of a set of even-order tensors, used to describe the probability distribution function of fiber orientation in suspensions and composites containing short rigid fibers, are reviewed. These tensors are related to the coefficients of a Fourier series expansion of the probability distribution function. If an n-th-order tensor property of a composite can be found from a linear average of a transversely isotropic tensor over the distribution function, then predicting that property only requires knowledge of the n-th-order orientation tensor. Equations of change for the second- and fourth-order tensors are derived; these can be used to predict the orientation of fibers by flow during processing. A closure approximation is required in the equations of change. A hybrid closure approximation, combining previous linear and quadratic forms, performs best in the equations of change for planar orientation. The accuracy of closure approximations is also explored by calculating the mechanical properties of solid composites with three-dimensional fiber orientation. Again the hybrid closure works best over the full range of orientation states. Tensors offer considerable advantage for numerical computation because they are a compact description of the fiber orientation state.

INTRODUCTION

The orientation behavior of short fibers immersed in a viscous fluid is an important problem in the processing of composite materials. Whenever such a material is formed, the flow changes the orientation of the fibers. This fiber orientation pattern is the dominant structural feature of a short fiber composite. The composite is stiffer and stronger in the direction of greatest orientation, and weaker and more compliant in the direction of least orientation. Theories exist which can predict the mechanical properties of the composite once the fiber orientation state is known.[1–6] More recently, efforts have been made to derive quantitative relationships between processing conditions and fiber ori-

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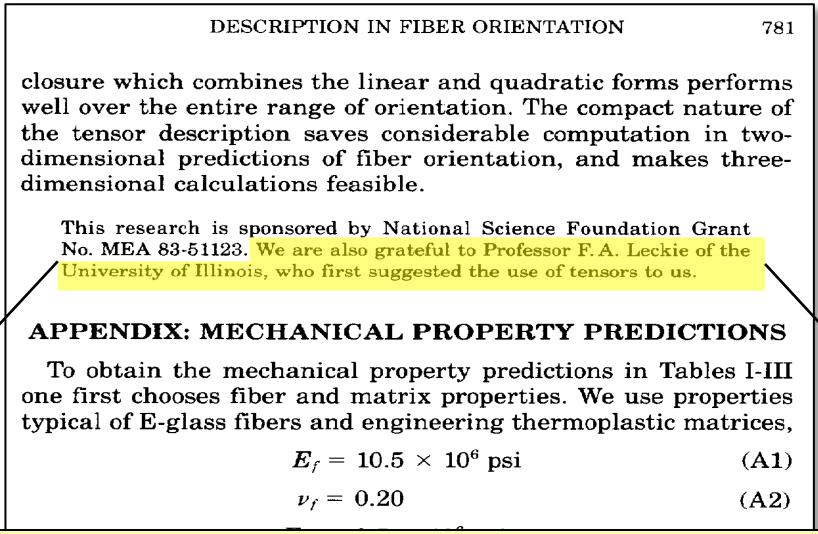
Advani and Tucker,
Journal of Rheology, 1987

Prof. Frederick A. Leckie

1929-2013



DESCRIPTION IN FIBER ORIENTATION 781

closure which combines the linear and quadratic forms performs well over the entire range of orientation. The compact nature of the tensor description saves considerable computation in two-dimensional predictions of fiber orientation, and makes three-dimensional calculations feasible.

This research is sponsored by National Science Foundation Grant No. MEA 83-51123. We are also grateful to Professor F. A. Leckie of the University of Illinois, who first suggested the use of tensors to us.

APPENDIX: MECHANICAL PROPERTY PREDICTIONS

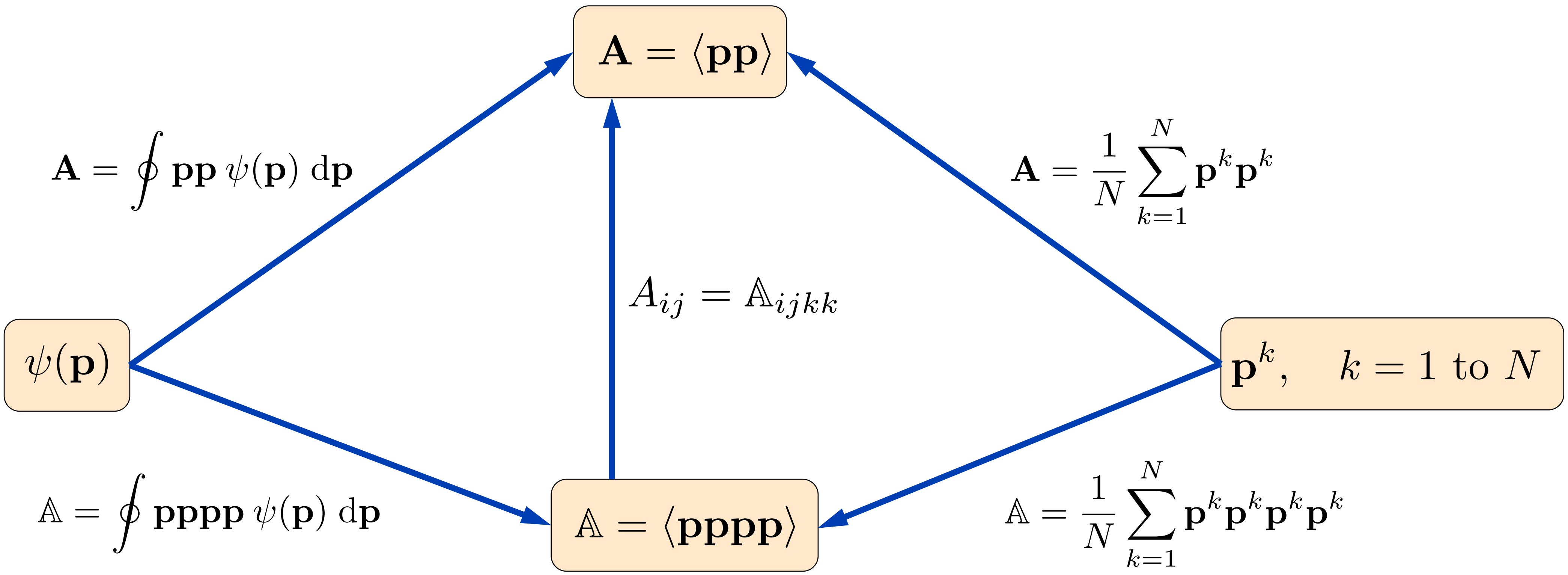
To obtain the mechanical property predictions in Tables I-III one first chooses fiber and matrix properties. We use properties typical of E-glass fibers and engineering thermoplastic matrices,

$$E_f = 10.5 \times 10^6 \text{ psi} \quad (A1)$$

$$\nu_f = 0.20 \quad (A2)$$

We are also grateful to Professor F. A. Leckie of the University of Illinois, who first suggested the use of tensors to us.

Some conversions between descriptors are easy



Some conversions between descriptors are easy;
others are difficult and require approximations

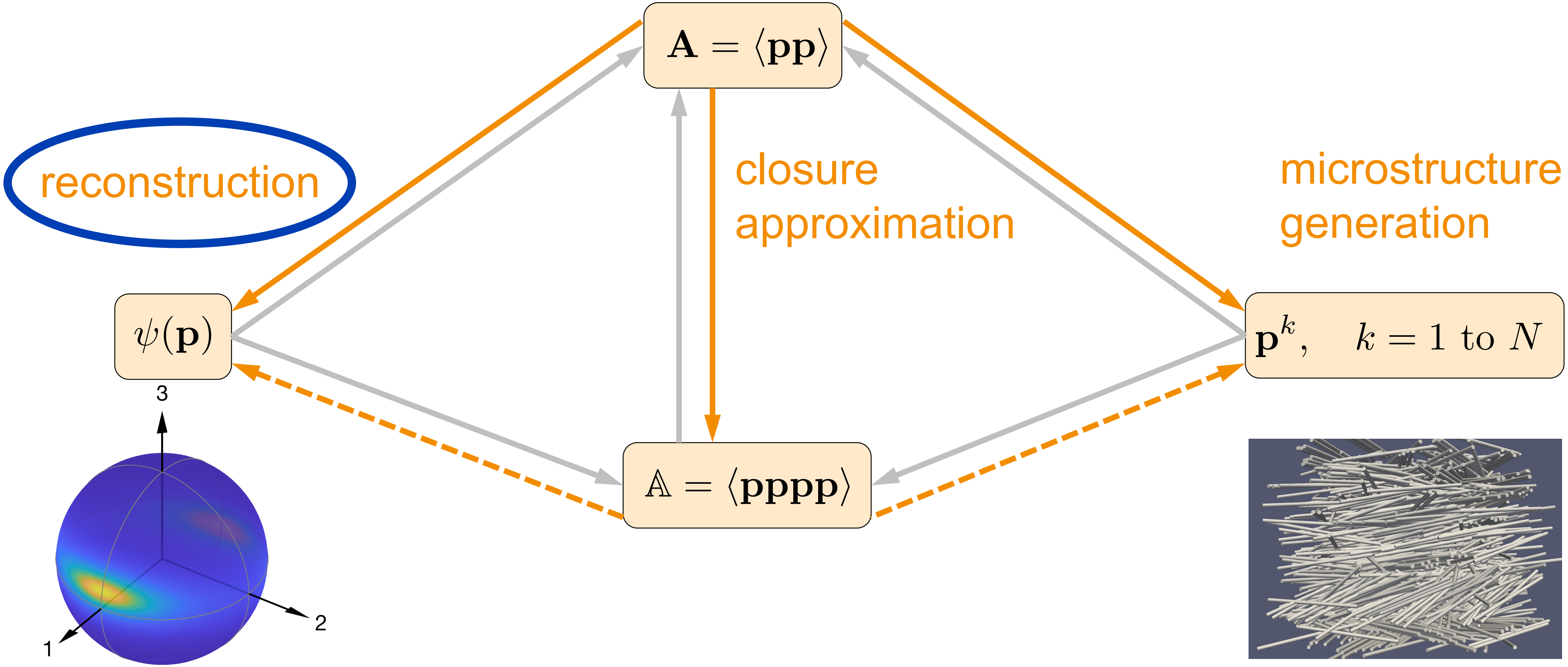
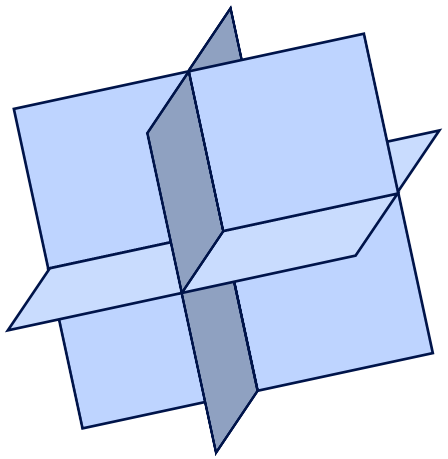


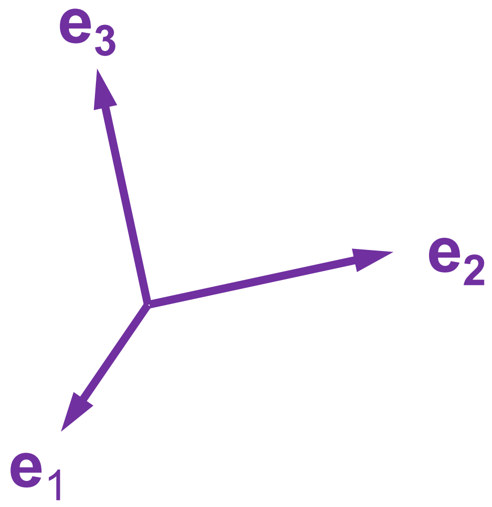
Image by Drs. Armin Kech and Susanne Kugler

Any symmetric second-order tensor is orthotropic . . .

Orthotropic: three perpendicular planes of mirror symmetry



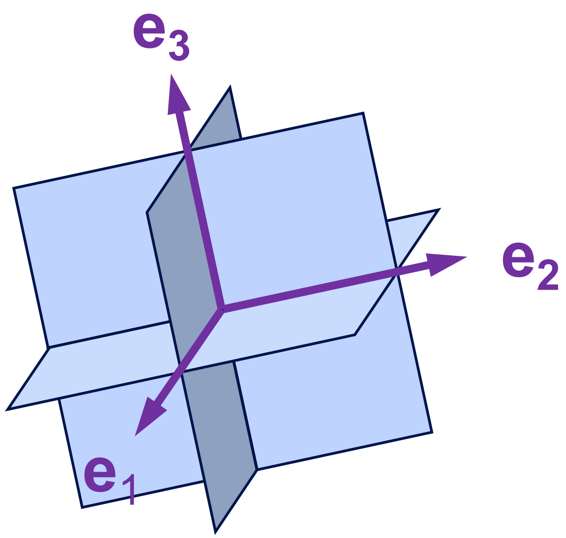
$$\mathbf{A} = \lambda_1 \mathbf{e}_1\mathbf{e}_1 + \lambda_2 \mathbf{e}_2\mathbf{e}_2 + \lambda_3 \mathbf{e}_3\mathbf{e}_3$$



Any symmetric second-order tensor is orthotropic . . .

Orthotropic: three perpendicular planes of material symmetry

$$\mathbf{A} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \mathbf{e}_3$$



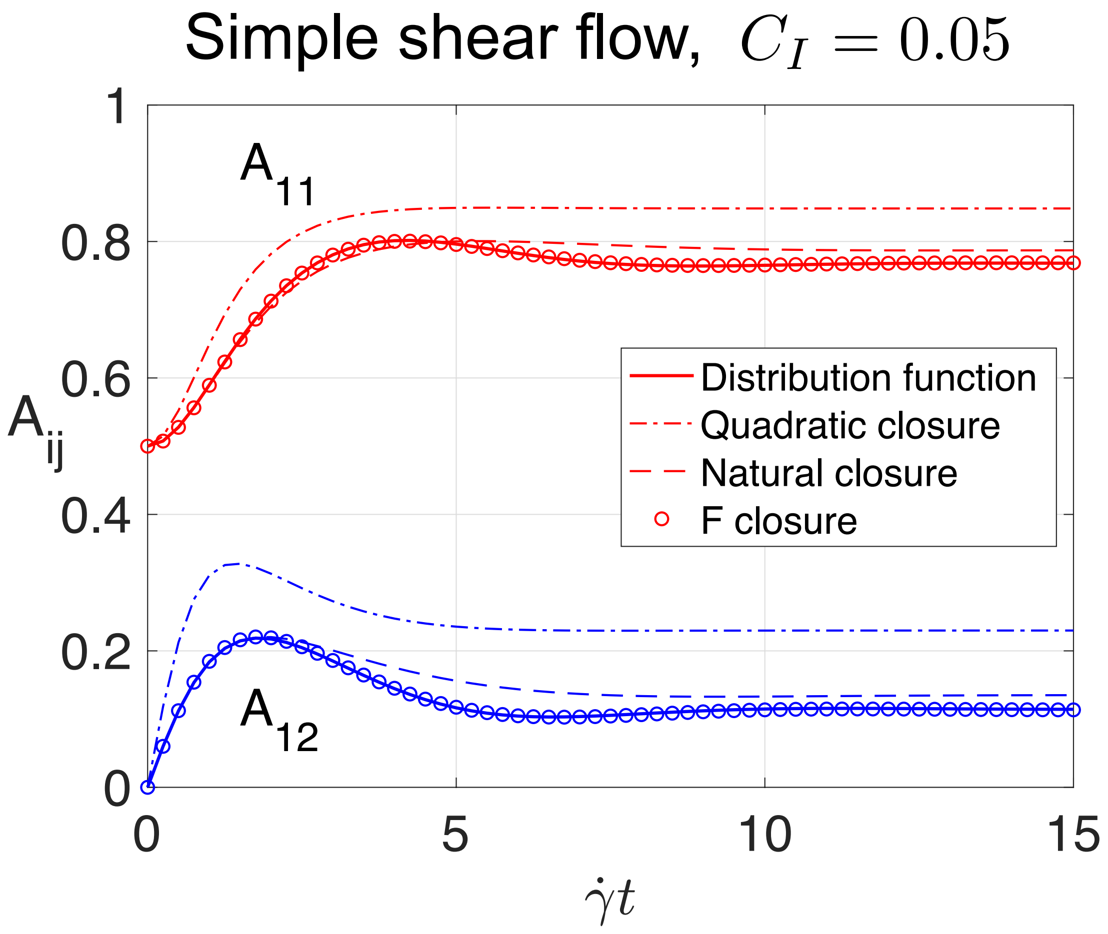
so any ψ_ϕ or $\mathbb{A}$ reconstructed from $\mathbf{A}$ must be orthotropic

Can create non-orthotropic closures using information from the rate-of-deformation tensor*

Planar F closure (non-orthotropic):

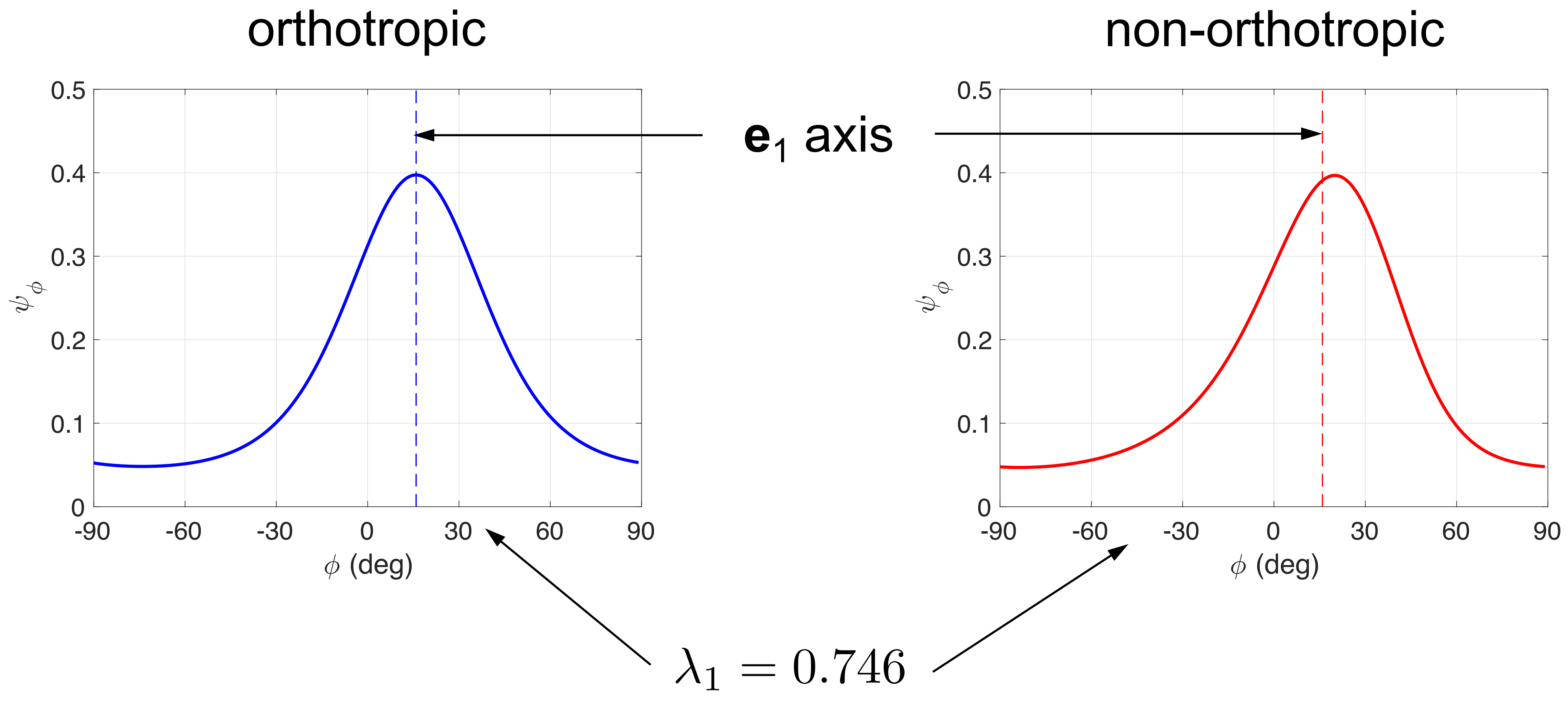
$$\mathbb{A} = f(\mathbf{A},\ \mathbf{D}/\dot{\gamma},\ C_I)$$

$$D_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$$



* C. L. Tucker, *JNNFM*, *310*, 104939 (2023)

A planar distribution function that is non-orthotropic is asymmetric about the principal axes of A



Reconstruction of planar distribution functions

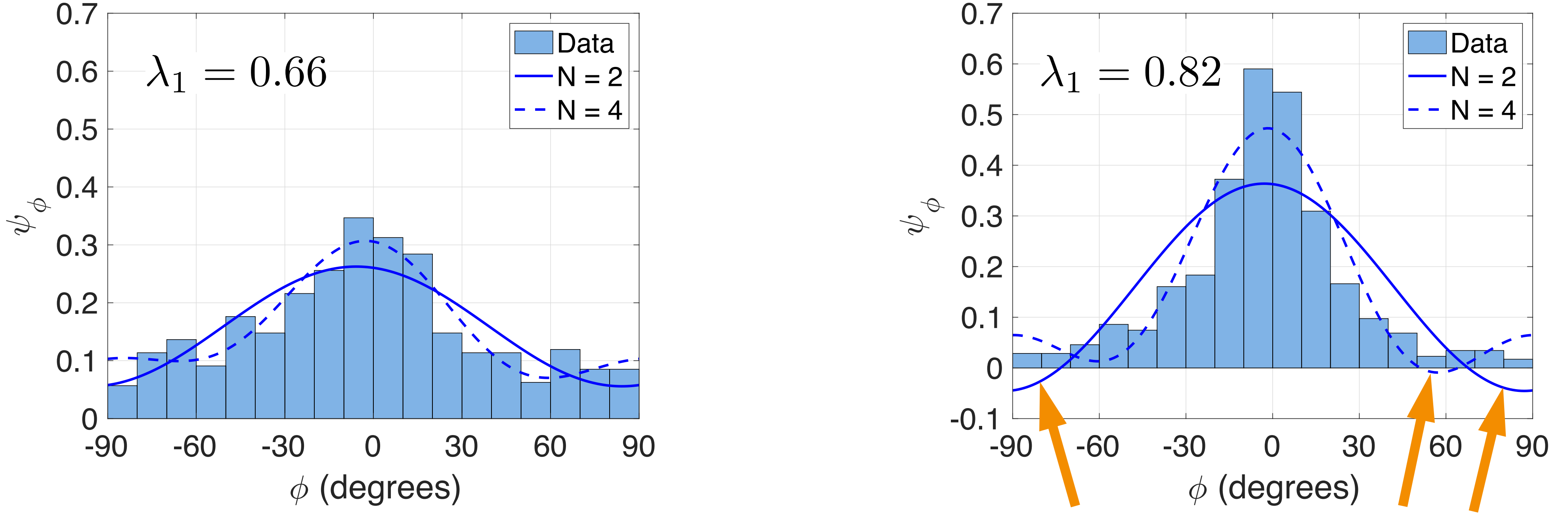
Fourier series reconstructions are non-physical for common orientation states

$$\tilde{\psi}_\phi(\mathbf{p}) = \frac{1}{2\pi}\left[1 + \mathbf{p}\cdot\mathbf{A}'\cdot\mathbf{p} + \mathbf{pp} : \mathbb{A}' : \mathbf{pp} + \ldots\right]$$

$\mathbf{A}'$, $\mathbb{A}'$ = deviatoric parts

2nd order (up to $\mathbf{p}\cdot\mathbf{A}'\cdot\mathbf{p}$)

4th order (up to $\mathbf{pp} : \mathbb{A}' : \mathbf{pp}$)



A better approach is to start with a function that guarantees feasible results

2nd order: $$\tilde{\psi}_\phi(\mathbf{p}) = f(\mathbf{p}\cdot\mathbf{T}\cdot\mathbf{p})$$

non-negative function

adjust to match $\mathbf{A}$

4th order: $$\tilde{\psi}_\phi(\mathbf{p}) = f(\mathbf{pp} : \mathbb{T} : \mathbf{pp})$$

adjust to match $\mathbb{A}$

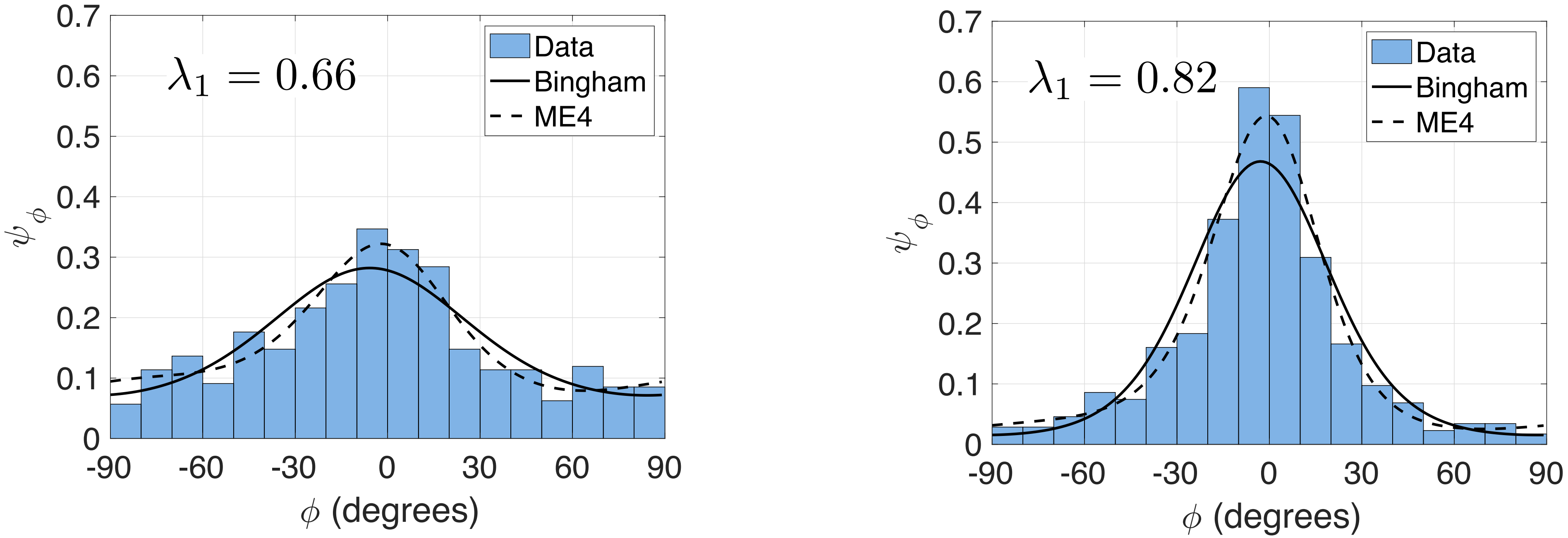
Example 1: Maximum entropy distributions

0[th] order $\tilde{\psi}_\phi(\mathbf{p}) = \frac{1}{2\pi}$

maximize $S = -\int_0^{2\pi} \tilde{\psi}_\phi \ln(\tilde{\psi}_\phi)\, d\phi$

2[nd] order (Bingham, 1975) $\tilde{\psi}_\phi(\mathbf{p}) = \exp(\mathbf{p} \cdot \mathbf{T} \cdot \mathbf{p})$

4[th] order (ME4) $\tilde{\psi}_\phi(\mathbf{p}) = \exp(\mathbf{pp} : \mathbb{T} : \mathbf{pp})$



Example 2: Power law distributions

Elliptical radius (ER)

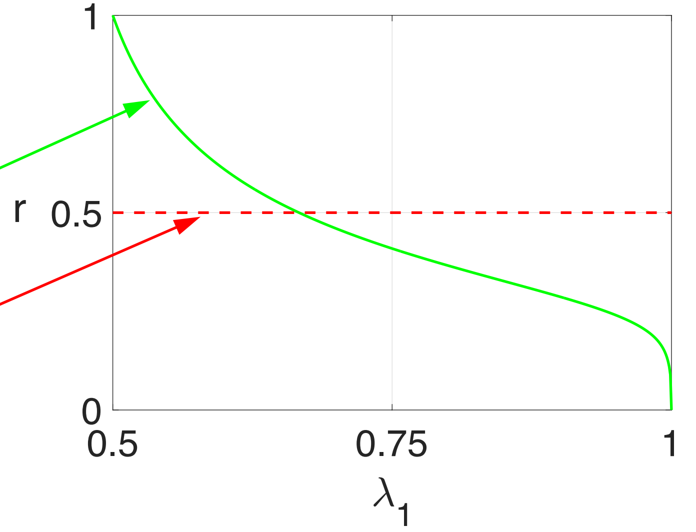
Nabergoj et al. (2022)

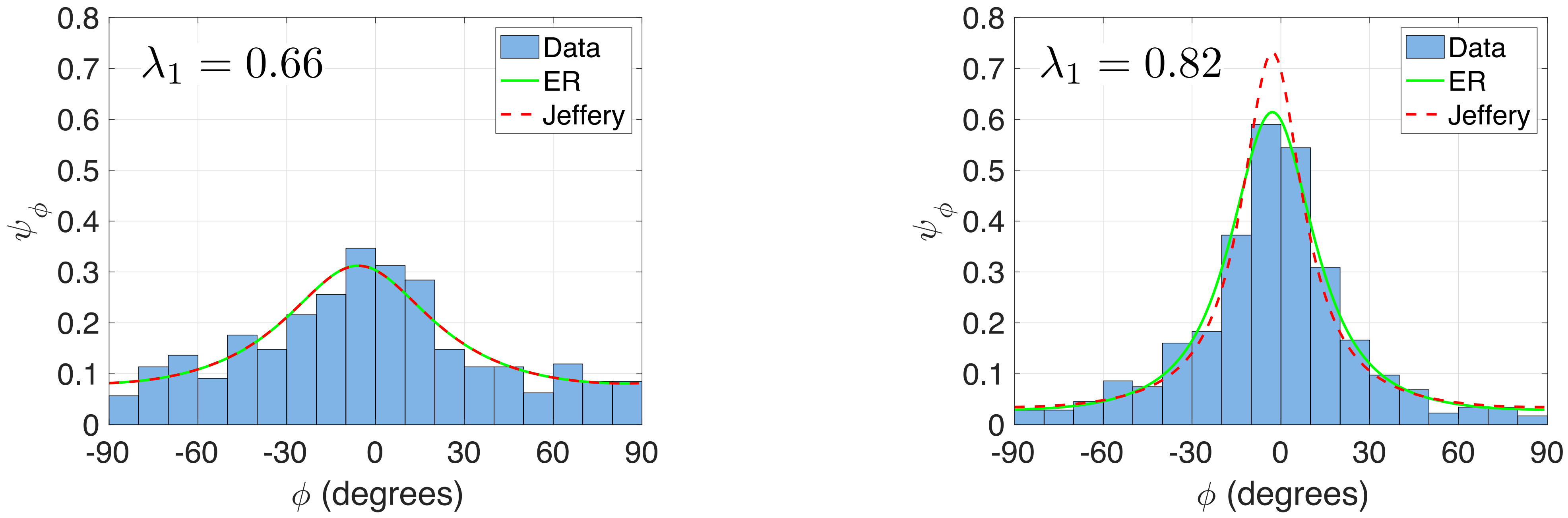
$$\tilde{\psi}_\phi(\mathbf{p}) = (\mathbf{p}\cdot\mathbf{T}\cdot\mathbf{p})^{-1/2r}$$

Jeffery distribution

Verleye and Dupret, 1993

$$\tilde{\psi}_\phi(\mathbf{p}) = (\mathbf{p}\cdot\mathbf{T}\cdot\mathbf{p})^{-1}$$





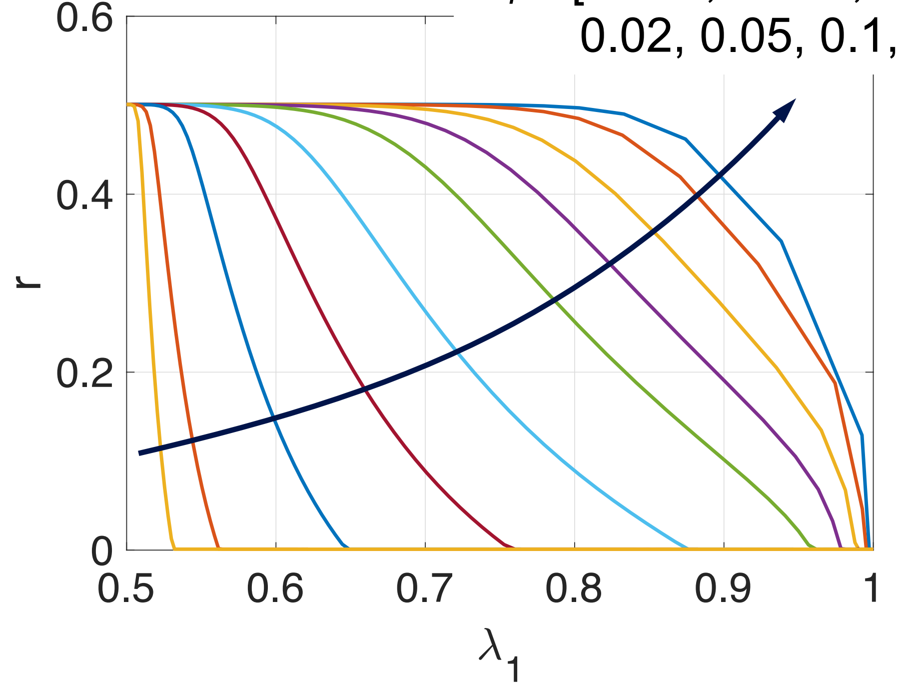
We can improve accuracy by using a 4th order power law and by optimizing *r*

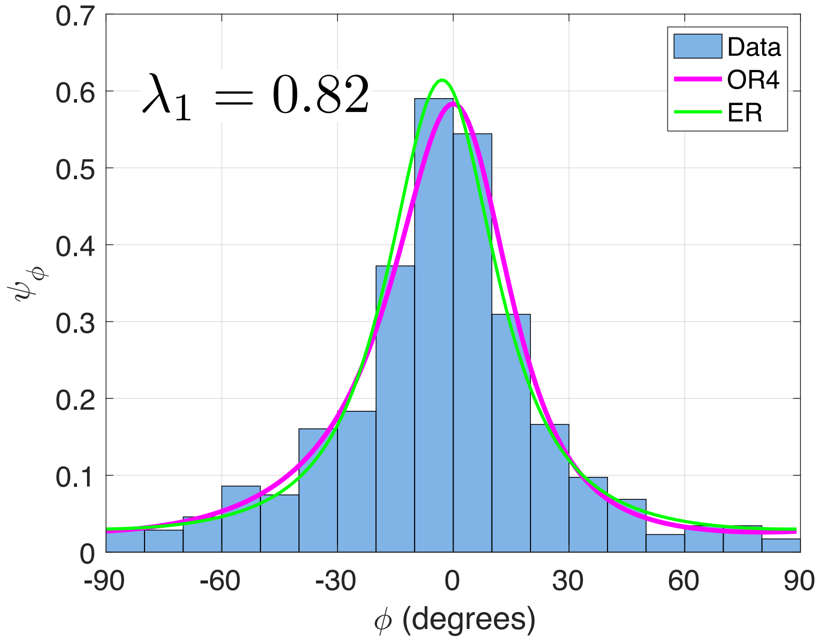
Optimized *r* (OR4): $$\tilde{\psi}_\phi(\mathbf{p}) = (\mathbf{pp} : \mathbb{T} : \mathbf{pp})^{-1/2r}$$

$$r = f(\lambda_1, C_I)$$

interaction coefficient

C_I = [0.001, 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1]



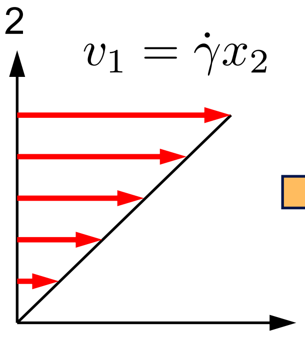


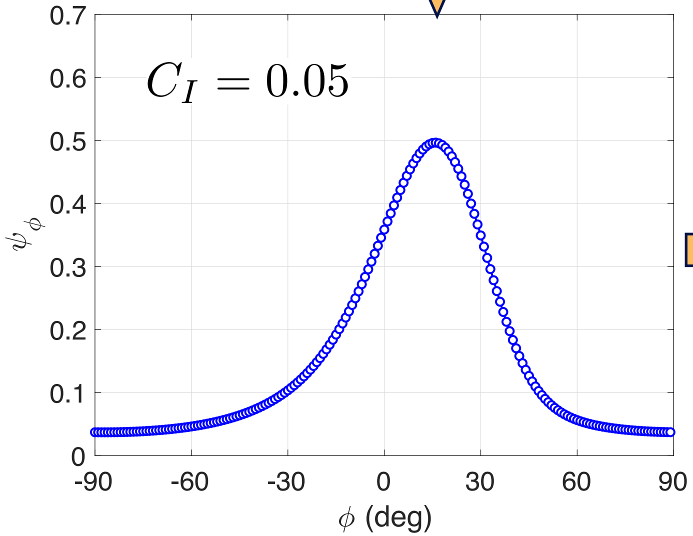
For a precise test, reconstruct distributions from the planar Folgar-Tucker model

Jeffery fiber motion: aligns fibers

interaction coefficient: randomizes fibers

$$\frac{\mathrm{D}\psi_\phi}{\mathrm{D}t} = -\frac{\partial}{\partial \phi}\left(\psi_\phi \dot{\phi}\right) + C_I \dot{\gamma} \frac{\partial^2 \psi_\phi}{\partial \phi^2}$$

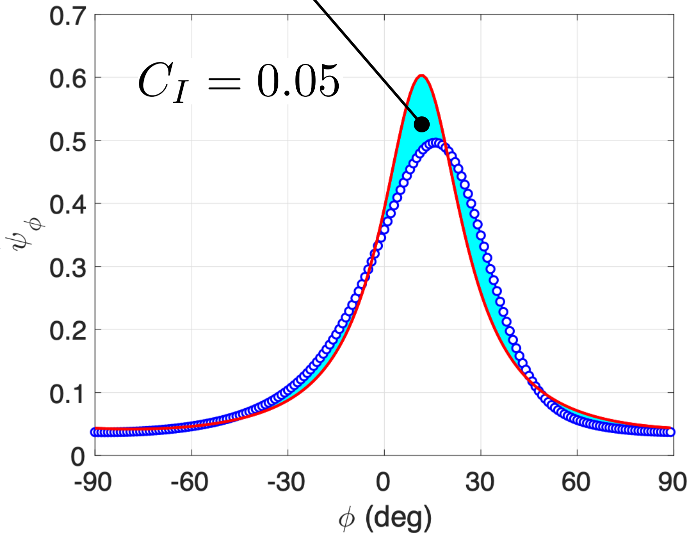




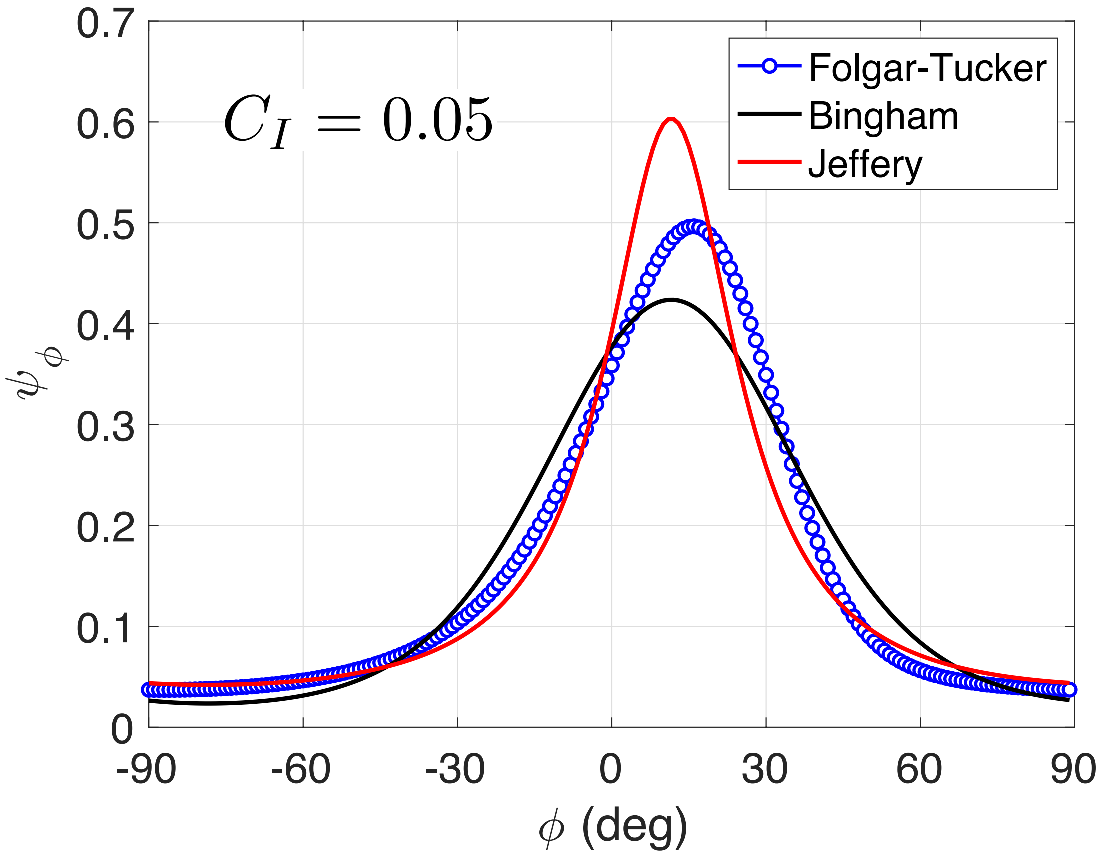
$\mathbf{A}, \mathbb{A}$

closure approx.

RMS error in ψ_ϕ

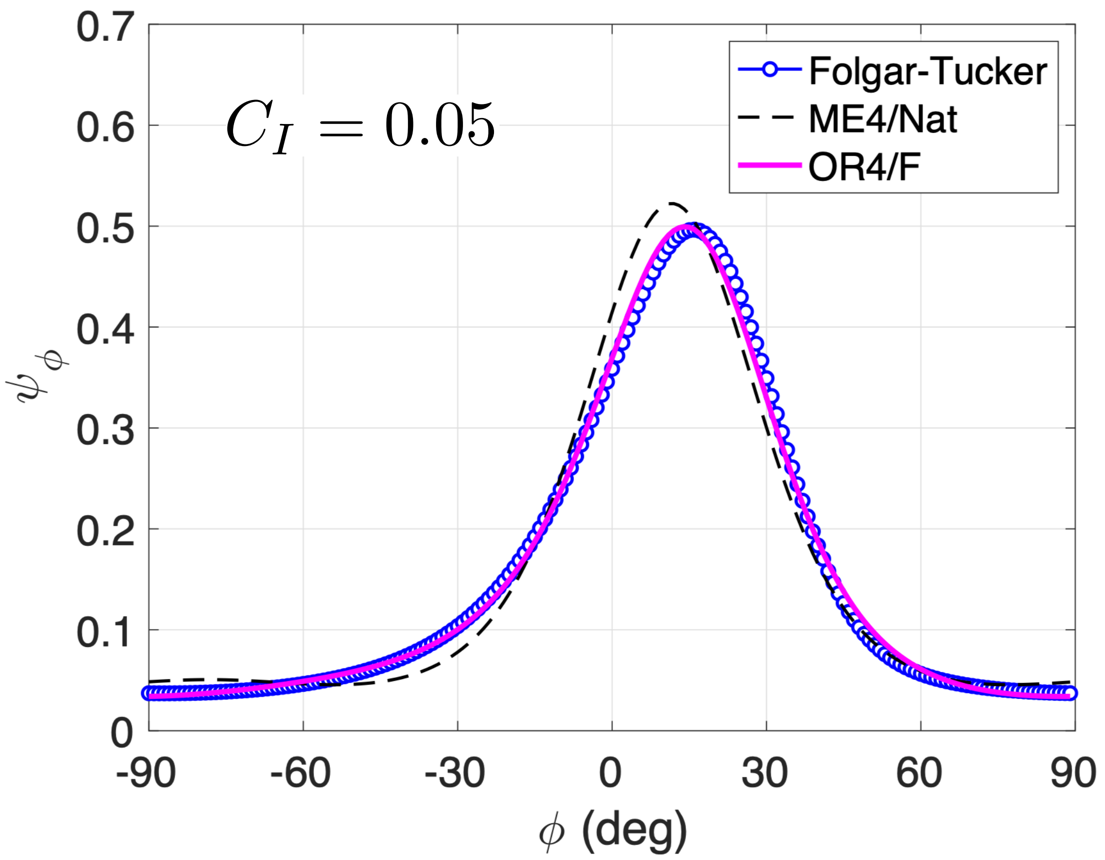


The Jeffery distribution is too sharp and the Bingham distribution is too smooth



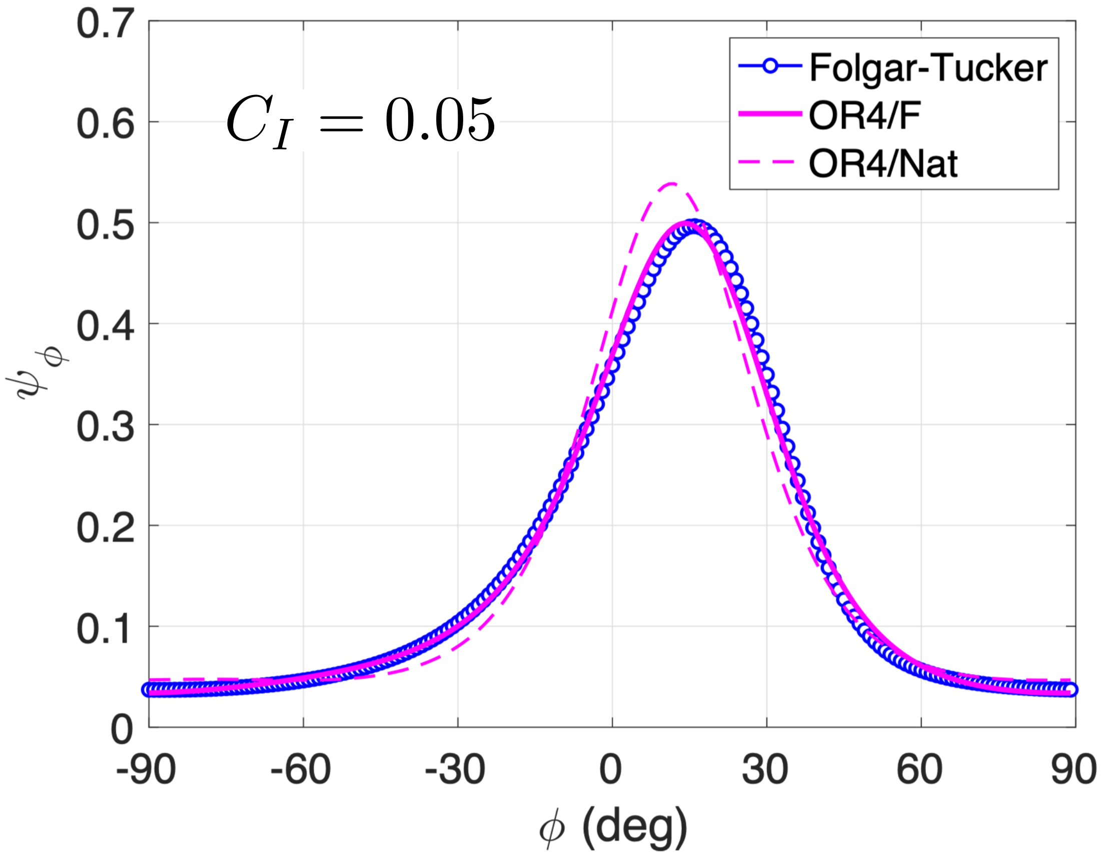
Steady state,
simple shear flow

Max Entropy 4 w/ natural closure is good, but OR4 w/ non-orthotropic F closure is better



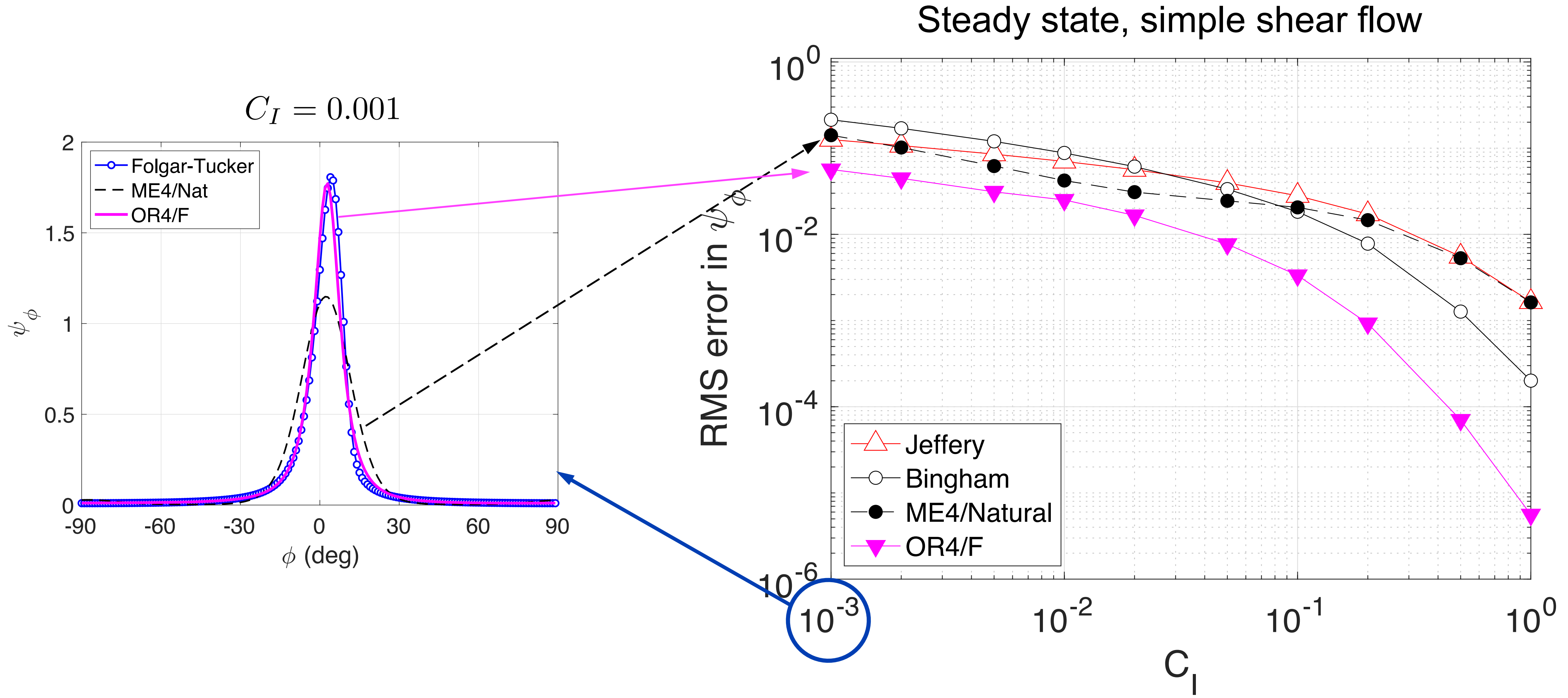
Steady state,
simple shear flow

The closure must be accurate to get a highly accurate reconstruction



Steady state,
simple shear flow

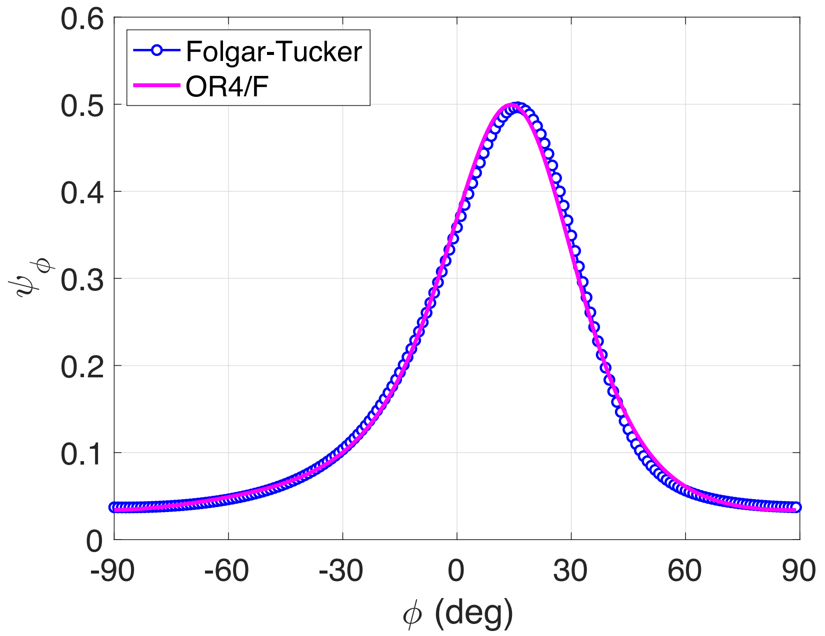
The new OR4/F approach works well across all C_I values, and is a major improvement for high alignment



Key ideas

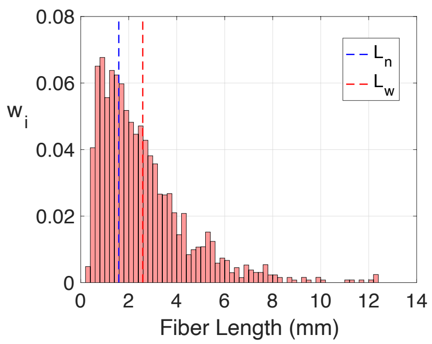
- We can improve planar reconstructions by combining
  - function based on $(\mathbf{pp} : \mathbb{T} : \mathbf{pp})^{1/2r}$
  - tuned exponent $r = f(\lambda_1, C_I)$
  - non-orthotropic closure for $\mathbb{A}$

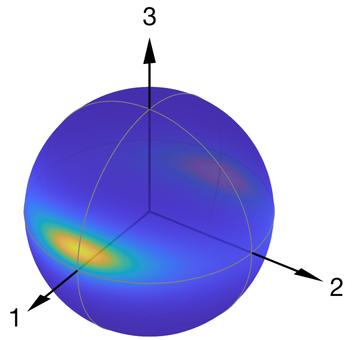
- This could be extended to 3-D



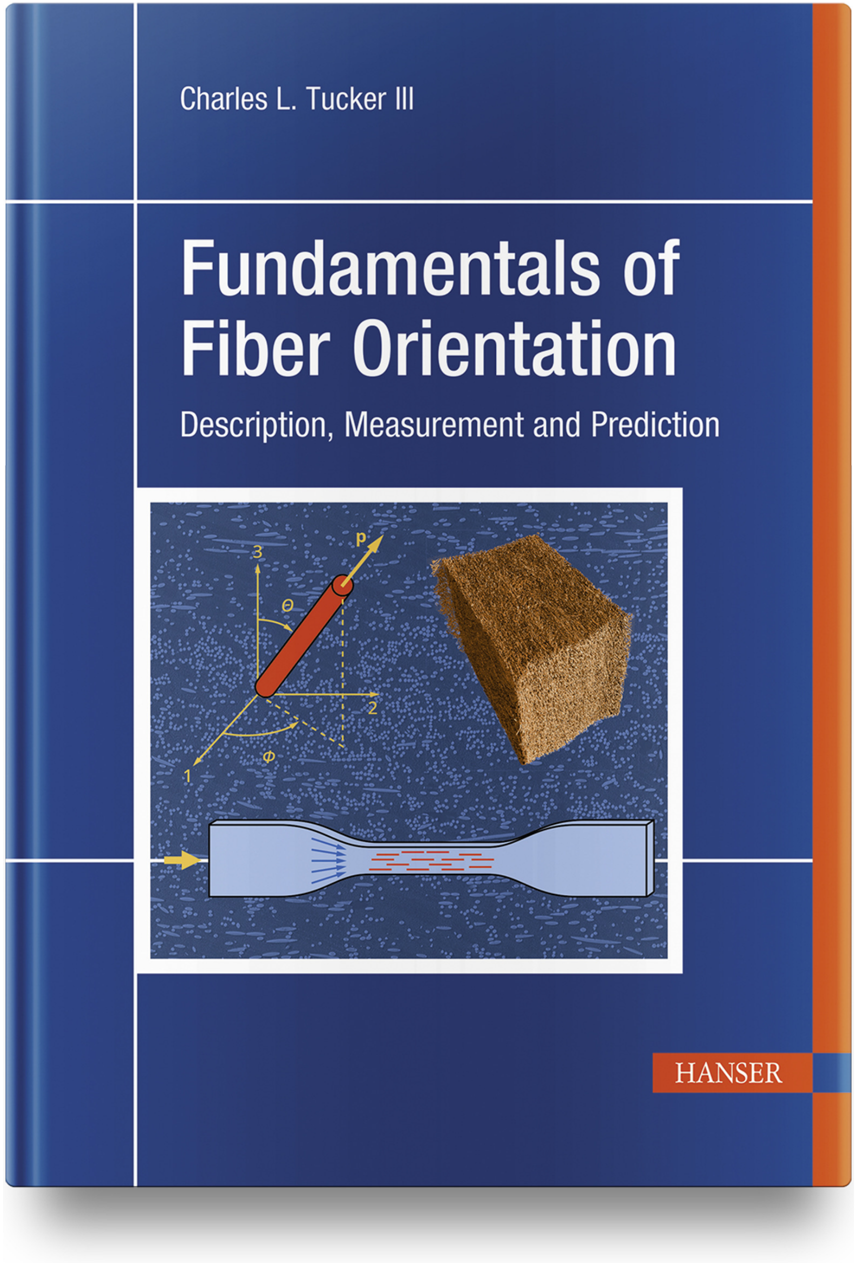
Going further will require new orientation descriptors

- Joint distributions for orientation and fiber length





- Flexible fibers
- The “fabric” of fiber-fiber contacts
- . . .



Fiber Orientation Tools

MATLAB functions for fiber orientation and mechanical property prediction

http://github.com/charlestucker3/Fiber-Orientation-Tools