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FAST SOLUTIONS FOR THE FIBER ORIENTATION OF CONCENTRATED SUSPENSIONS OF SHORT-FIBER COMPOSITES USING THE EXACT CLOSURE METHOD

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ABSTRACT

The kinetics of the fiber orientation during processing of short-fiber composites governs both the processing characteristics and the cured part performance. The flow kinetics of the polymer melt dictates the fiber orientation kinetics, and in turn the underlying fiber orientation dictates the bulk flow characteristics. It is beyond computational comprehension to model the equation of motion of the full fiber orientation probability distribution function. Instead, typical industrial simulations rely on the computationally efficient equation of motion of the second-order orientation tensor (also known as the second-order moment of the orientation distribution function) to model the characteristics of the fiber orientation within a polymer suspension. Unfortunately, typical implementation forms of any order orientation tensor equation of motion requires the next higher, even ordered, orientation tensor, thus necessitating a closure of the higher order expression. The recently developed Fast Exact Closure avoids the classical closure problem by solving a set of related second-order tensor equations of motion, and yields the exact solution for pure Jeffery's motion as the diffusion goes to zero. Typical closures are obtained through a fitting process, and are often obtained by fitting for orientation states obtained from solutions of the full orientation distribution function, thus tying the closure to the flows from which it was fit. With the recent understandings of the limitations of the Folgar and Tucker (1984) model of fiber interactions during processing, it has become clear the importance of developing a closure that is independent of any choice of fitting data. The Fast Exact Closure presents an alternative in that it is constructed independent of any fitting process. Results demonstrate that when diffusion exists, the solution is not only physical, but solutions for flows experiencing Folgar-Tucker diffusion are shown to exhibit an equal to or greater accuracy than solutions relying on closures developed via a curve fitting approach.

INTRODUCTION

With the increasing industrial demand for high strength, low weight, rapidly produced parts, understanding the final part performance for short fiber injection molded composites from the underlying microstructure is becoming increasingly important. The kinetics of the fiber orientation during processing of a short-fiber composite governs both the processing characteristics and the cured part performance [1]. The flow kinetics of the polymer melt dictates the fiber orientation kinetics, and in turn the underlying fiber orientation dictates the bulk flow characteristics [2,3]. The Folgar-Tucker model for fiber interactions within the suspension has been accepted industrially for several decades [4], but with recent advances in part repeatability the limitation of their model has been observed [5]. Recent models [6-9] do not follow the same form as the Folgar-Tucker model and thus orientation prediction methods that are fit to the Folgar-Tucker model results may be invalid. Industrial simulations of the Folgar-Tucker model are beyond computational comprehension and thus the equation of motion for the moments of the distribution is traditionally solved [1]. Unfortunately the equation of motion for the moments of the distribution requires knowledge of the next higher ordered moment. Thus requiring some form of a closure to approximate the higher order moment in terms of the lower order moment. Advani and Tucker's [1] hybrid closure has been used extensively in industrial simulations but has been shown to be inadequate in representing accurately the fiber orientation distribution function [10]. With the advent of the othotropic closure by Cintra and Tucker, high accuracy closures became available. Unfortunately, nearly all of the orthotropic closures were formed through a fitting process by taking information available from known flow solutions based on the Folgar and Tucker model of diffusion [12-17]. Thus it is unclear if any of these fitted closures could be, with high confidence, employed within the new diffusion models for fiber collision. It is important to point out, that the orthotropic closures of Wetzel [18] and VerWeyst [19] were constructed based on distributions formed through the elliptic integral form over various orientations encompassing the eigenspace [11], and as such are fit independent of any particular fiber orientation flow field. Dupret and Verleye [20] proposed the natural closure as an exact formula for a closure, however, their form was only suited for two dimensional flow and their three dimensional form still required a fitting process to construct the closure. Verleye and Dupret [21] noted the existence of an exact closure in the general 3D case, provided the fiber orientation distribution was at sometime isotropic.

The Exact Closure of Mongomery-Smith *et al.* [22] presents an alternative that provides the exact solution for pure Jeffery's motion where there is no diffusion (i.e., the dilute regime). In the present paper we present a summary of the recently developed Fast Exact Closure (FEC) and leave the full details of its derivation to the related journal paper [23]. We will show that when diffusion exists, results are not only physical, but solutions for flows experiencing Folgar-Tucker diffusion are shown to exhibit an equivalent accuracy to that of solutions from the best of the fitted closures. By numerical construction the FEC is nearly as fast as the highly efficient, but inaccurate, hybrid closure, with the same accuracy and stability as that of the best of the fitted closures. The algorithm for the FEC requires the simultaneous computation of the second order moment of the orientation distribution and a related second order tensor. Most striking is the absence of the fourth-order orientation tensor at any point in the transient solution of the second-order orientation tensor. By solving these two second-order systems simultaneously there is no need for any curve fitting in either construction or implementation. The Fast Exact Closure is unique, in that the systematic development approach can be readily applied as new diffusion models are developed, such as that of the anisotropic rotary diffusion model of Phelps and Tucker [7].

SHORT-FIBER REINFORCED POLYMER COMPOSITES FLOW MODELING

Jeffery's equation [24] has been used extensively to predict the motion of the direction of axi-symmetric fibers under the influence of low Reynold's number Newtonian fluids, whose velocity field is $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$. The directions of the fibers are represented by the fiber orientation distribution $\psi(\mathbf{x}, \mathbf{p}, t)$, where $\mathbf{p}$ is the direction vector from the origin to a point on the unit sphere S. Jeffery's equation for the fiber orientation distribution is expressed as

$$\frac{D\psi}{Dt} = -\frac{1}{2}\nabla_{\mathbf{p}} \cdot \big((\boldsymbol{\Omega} \cdot \mathbf{p} + \lambda\boldsymbol{\Gamma} \cdot \mathbf{p} - \lambda\boldsymbol{\Gamma}\colon \mathbf{ppp})\psi\big) \qquad (1)$$

where $\boldsymbol{\Omega}$ is the vorticity, that is the axi-symmetric part of the velocity gradient, $\boldsymbol{\Omega} = \boldsymbol{\nabla}\mathbf{v} - (\boldsymbol{\nabla}\mathbf{v})^{\mathrm{T}}$ and $\boldsymbol{\Gamma}$ is the rate of deformation tensor, that is the symmetric part of the velocity gradient $\boldsymbol{\Gamma} = \boldsymbol{\nabla}\mathbf{v} + (\boldsymbol{\nabla}\mathbf{v})^{\mathrm{T}}$. The parameter λ is often taken to be a function of the fiber aspect ratio. Observe that the material derivative of the orientation is expressed to recognize that the fibers move with the bulk motion of the fluid, and $\nabla_{\mathbf{p}}$ is the gradient operator restricted to the sphere.

Equation (1) is only valid for dilute suspensions, and it is typical to express semi-dilute and concentrated suspensions through the generalized Fokker-Planck or the Smoluchowski equation [29] as

$$\frac{D\psi}{Dt} = -\frac{1}{2}\nabla_{\mathbf{p}} \cdot \big((\boldsymbol{\Omega} \cdot \mathbf{p} + \lambda\boldsymbol{\Gamma} \cdot \mathbf{p} - \lambda\boldsymbol{\Gamma}\colon \mathbf{ppp})\psi\big) + \Delta_{\mathbf{p}}(D_r\psi) \qquad (2)$$

where the D_r, often called the rotary diffusion, is a function that captures the fiber interactions and is often assumed to be a function of the fiber geometry, fiber concentration, and the flow kinetics. Here $\Delta_{\mathbf{p}}$ is the Beltrami-Laplace operator on the sphere. The industrially employed Folgar and Tucker model [4] defines to rotary diffusion as $D_r = C_I\dot{\gamma}$, where $\dot{\gamma} = \left(\frac{1}{2}\boldsymbol{\Gamma}\colon \boldsymbol{\Gamma}^{\mathrm{T}}\right)^{1/2}$ and C_I is a constant that depends on the fiber geometry and fiber concentration. There are several authors who have more extensive forms for the rotary diffusion (see e.g., [6-9]), but none have experienced the industrial acceptance of the Folgar and Tucker form.

Unfortunately, the form of Equation (2) does not lend itself easily to industrial computations. Either the solution approach requires a computationally expensive finite element/difference approach, such as that of the commonly employed algorithm of Bay [25], or the computationally efficient and numerically accurate Spherical Harmonic approach of Montgomery-Smith *et al.* [26]. Unfortunately, neither approach lends itself readily to the fully coupled problem between the fiber orientation and the flow kinetics. Instead, the moment tensor popularized by Advani and Tucker [1] is often employed. For example, the second- and fourth-order moment tensors (also called orientation tensors) are expressed, respectively, as

$$\mathbf{A} = \oint_S \mathbf{pp}\psi(\theta, \phi)d\mathbf{p} \qquad (3)$$

$$\mathbb{A} = \oint_S \mathbf{pppp}\psi(\theta, \phi)d\mathbf{p} \qquad (4)$$

The Jeffery's Equation with diffusion from Equation (2) can be expressed in terms of the orientation tensors as

$$\frac{D\mathbf{A}}{Dt} = \frac{1}{2}(\boldsymbol{\Omega} \cdot \mathbf{A} - \mathbf{A} \cdot \boldsymbol{\Omega} + \lambda(\boldsymbol{\Gamma} \cdot \mathbf{A} + \mathbf{A} \cdot \boldsymbol{\Gamma}) - 2\lambda\mathbb{A}\colon \boldsymbol{\Gamma}) + \mathcal{D}[\mathbf{A}] \qquad (5)$$

where for the Folgar and Tucker model of diffusion $\mathcal{D}[\mathbf{A}]$, is expressed as

$$\mathcal{D}[\mathbf{A}] = D_r(2\mathbf{I} - 6\mathbf{A}) \qquad (6)$$

with $D_r = C_I\dot{\gamma}$, and for Phelps and Tucker's ARD model the diffusion term $\mathcal{D}[\mathbf{A}]$ is expressed as

$$\mathcal{D}[\mathbf{A}] = 2\mathbf{D_r} - 2(\mathrm{Tr}\mathbf{D_r})\mathbf{A} - 5(\mathbf{A} \cdot \mathbf{D_r} + \mathbf{D_r} \cdot \mathbf{A}) + 10\mathbb{A}\colon \mathbf{D_r} \qquad (7)$$

where the second-order tensor $\mathbf{D_r}$ (an anisotropic form of the rotary diffusion) is obtained from experimental observations. Notice in Equation (5), that both of the diffusion forms from Equation (6) and (7) requires the fourth-order orientation tensor. The Koch [8] model for diffusion requires the sixth-order orientation tensor as well, and the anisotropic diffusion form of Jack *et al.* [9] requires the tenth-order orientation tensor. Regardless, the computation of the second-order orientation tensor equation of motion of Equation (5) requires information that is not directly available from the second-order orientation tensor. There are a wide range of authors who have provided closures that approximate the fourth-order orientation tensor from the second-order orientation tensor, and for the sixth-order orientation tensor required for the Koch model there is one known closure that approximates the sixth-order orientation tensor directly from the second-order orientation tensor [27].

THE FAST EXACT CLOSURE

Verleye and Dupret [21] noted the existence of an exact closure for Jeffery's equation in the absence of the diffusion terms, and this explicit form, called the Exact Closure, was derived in Montgomery-Smith *et al.* [22]. The Exact Closure was enhanced further by Montgomery-Smith *et al.* [23] by presenting a systematic approach to represent the equations of motion for the orientation tensor for models with diffusion (i.e., semi-dilute and concentrated suspensions). This enhancement to include diffusive terms, called the Fast Exact Closure (FEC), can be applied to a wide variety of diffusion models[1]. The FEC seeks to solve an alternative form of Equation (5) by solving, simultaneously, the coupled ODEs for the symmetric second-order tensors **A** and **B**, whose equations of motion for the Folgar-Tucker diffusion model are expressed as

$$\frac{D\mathbf{A}}{Dt} = \tfrac{1}{2}\mathbb{C}\colon[\mathbf{B}\cdot(\mathbf{\Omega}+\lambda\mathbf{\Gamma}) + (-\mathbf{\Omega}+\lambda\mathbf{\Gamma})\cdot\mathbf{B}] + D_r(2\mathbf{I}-6\mathbf{A}) \qquad (8)$$

$$\frac{D\mathbf{B}}{Dt} = -\tfrac{1}{2}(\mathbf{B}\cdot(\mathbf{\Omega}+\lambda\mathbf{\Gamma}) + (-\mathbf{\Omega}+\lambda\mathbf{\Gamma})\cdot\mathbf{B}) - D_r\mathbb{D}\colon(2\mathbf{I}-6\mathbf{A}) \qquad (9)$$

where **A** shares the same physical meaning as the second-order orientation tensor defined in Equation (3), $\mathbf{\Omega}$ is the vorticity tensor, $\mathbf{\Gamma}$ is the rate of deformation tensor, λ is the shape parameter defined in Jeffery's equation, and **I** is the identity tensor. The second-order tensors **A** and **B** mathematically share the same principal frame, with the eigenvalues of **A** labeled as a_1, a_2, and a_3 and the eigenvalues of **B** labeled as b_1, b_2, and b_3. When the fiber orientation is isotropic, $\mathbf{A} = \frac{1}{3}\mathbf{I}$ and $\mathbf{B} = \mathbf{I}$. Throughout the entire flow history, the matrices **A** and **B** remain positive definite, simultaneously diagonalizable, and satisfy $\mathrm{tr}\mathbf{A} = \det\mathbf{B} = 1$. Observe that both sets of ODEs for **A** and **B** have either the fourth-order tensors $\mathbb{C}$ or $\mathbb{D}$, where $\mathbb{D}$ is the tensor inverse of $\mathbb{C}$. In [23] the tensor $\mathbb{C}$ in the principal frame of **B** (which is the same as saying in the principal frame of **A**) is shown to be a series of straight forward functions of the eigenvalues of **A** and **B** expressed simply as (where we assume $a_1 \geq a_2 \geq a_3$ and $b_1 \geq b_2 \geq b_3$)

$$\begin{aligned} \mathbb{C}_{1122} &= \frac{a_1 - a_2}{2(b_2 - b_1)} \\ \mathbb{C}_{1133} &= \frac{a_1 - a_3}{2(b_3 - b_1)} \\ \mathbb{C}_{2233} &= \frac{a_2 - a_3}{2(b_3 - b_2)} \end{aligned} \qquad (10)$$

$$\begin{aligned} \mathbb{C}_{1111} &= \tfrac{1}{2}b_1^{-1} - \mathbb{C}_{1122} - \mathbb{C}_{1133} \\ \mathbb{C}_{2222} &= \tfrac{1}{2}b_2^{-1} - \mathbb{C}_{1122} - \mathbb{C}_{2233} \\ \mathbb{C}_{3333} &= \tfrac{1}{2}b_3^{-1} - \mathbb{C}_{1133} - \mathbb{C}_{2233} \\ \mathbb{C}_{ijkl} &= 0 \ \text{ if } \ i \neq j \neq k \end{aligned} \qquad (11)$$

where in the principal frame of **B**, the fourth-order tensor $\mathbb{D}$ relates to the fourth-order tensor $\mathbb{C}$ as

$$\begin{aligned} \begin{bmatrix} \mathbb{D}_{1111} & \mathbb{D}_{1122} & \mathbb{D}_{1133} \\ \mathbb{D}_{2211} & \mathbb{D}_{2222} & \mathbb{D}_{2233} \\ \mathbb{D}_{3311} & \mathbb{D}_{3322} & \mathbb{D}_{3333} \end{bmatrix} &= \begin{bmatrix} \mathbb{C}_{1111} & \mathbb{C}_{1122} & \mathbb{C}_{1133} \\ \mathbb{C}_{2211} & \mathbb{C}_{2222} & \mathbb{C}_{2233} \\ \mathbb{C}_{3311} & \mathbb{C}_{3322} & \mathbb{C}_{3333} \end{bmatrix}^{-1} \\ \mathbb{D}_{ijij} = \mathbb{D}_{ijji} &= \frac{1}{4\mathbb{C}_{ijij}} \ \text{ if } \ i \neq j \\ \mathbb{D}_{ijkk} &= 0 \ \text{ if } \ i \neq j \neq k \end{aligned} \qquad (12)$$

If two or more eigenvalues are close to each other, the expressions in Equation (10) give rise to large numerical errors and divide by zero exceptions. In [23] methods are discussed for computing $\mathbb{C}$ from a series expansion about these apparent singularities, and the approach is readily programmed and quite robust.

Algorithm Summary

The basic procedure for solving the equation of motion for the second-order orientation tensor **A** is given as follows:

- Define the initial conditions for **A** and **B** as well as the physical constants such as λ and any constants needed for the diffusion model $\mathcal{D}[\mathbf{A}]$.
- For a given moment in time, t_i, rotate the tensors **A** and **B** into their principal reference frame to obtain their eigenvalues.
- If the eigenvalues are distinct, use Equations (10) and (11) to compute $\mathbb{C}$. If any eigenvalues are close to each other see [23] for the appropriate procedure to compute $\mathbb{C}$.
- Compute $\mathbb{D}$ with Equation (12) then compute $\frac{D\mathbf{A}}{Dt}$ and $\frac{D\mathbf{B}}{Dt}$ using Equations (8) and (9), both given in the principal frame of **A** and **B**.
- Rotate $\frac{D\mathbf{A}}{Dt}$ and $\frac{D\mathbf{B}}{Dt}$ into the original coordinate reference frame, and using a Runge-Kutta approach extrapolate from time t_i to obtain **A** and **B** at t_{i+1}.

There are several numerical steps that that can be performed to drastically reduce the computational overhead. Such as performing all operations in the principal reference frame of **B**. This will avoid the costly rotation of the fourth-order tensors $\mathbb{C}$ and $\mathbb{D}$, which requires 4×81 multiplication operations for each independent component of $\mathbb{C}$ and $\mathbb{D}$, whereas the rotation of $\frac{D\mathbf{A}}{Dt}$ and $\frac{D\mathbf{B}}{Dt}$ only requires 2×9 multiplication operations of the independent components of **A** and the independent components of **B**. It is worthwhile to note, that this numerically efficient procedure could be similarly

[1] The full and complete derivation of the Fast Exact Closure (FEC) is provided in Montgomery-Smith *et al.* [23].

performed for many of the orthotropic closures, and as will be shown in the following results, the computational efforts for the orthotropic closures can be rapidly diminished using this approach.

Numerical and Implementation Issues

There are several issues in the implementation of the FEC closure that should be noted. There exists a choice to either compute the basis of the orthonormal eigenvalues from either **A** and **B**, where in principal these should be identical. But due to numerical imprecision, the basis of the two systems will tend to drift from each other, thus we chose to compute the basis from **B** and compute the approximate eigenvalues of **A** in this basis forcing the remaining off diagonal terms to be zero. These off-diagonal terms are numerically zero, but the setting of them to zero prevents numerical drift. This assumption of selecting the basis to correspond with **B** somewhat arbitrarily assumes that the quantity of **B** is somehow more fundamental and **A**, but this is reasonable as **A** is the derived quantity (which continues to hold even in the case when there is no diffusion). Although it is mathematically sound to compute all nine components of **A** and all nine components of **B**, it is best to use the symmetric nature of both second-order tensors. It was also observed that numerical drift is avoided in the computations when the property $\mathrm{tr}\mathbf{A} = \det\mathbf{B} = 1$ is used to compute one of the diagonal components, such as A_{33} and B_{33}, instead of using their corresponding ODEs.

COMPUTED RESULTS

Results are presented to demonstrate the accuracy of the FEC closure for the fiber orientation in a system governed by the Folgar and Tucker [4] model of diffusion. To quantify the accuracy in representing the fiber orientation, all results are compared to those from the Spherical Harmonic approach [26]. The Spherical Harmonic approach expands the orientation distribution function, $\psi(\theta,\phi)$, using the complex spherical harmonics Y_l^m [28] to any desired order as [26]

$$\psi(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \hat{\psi}_l^m Y_l^m \qquad (13)$$

where $\hat{\psi}_l^m$ are the complex spherical harmonic coefficients that contain information pertaining to the orientation. The equation of motion for $\psi(\theta,\phi)$ of Equation (2) is expanded using (13) and transient solutions of $\frac{\mathrm{D}\psi}{\mathrm{Dt}}$ using the Spherical Harmonic expansion approach are obtained. These solutions have been shown to be accurate to the eighth-decimal place (see e.g., [26]), and thus will be considered to be the exact.

Simulations of the FEC closure are performed using an in-house developed single-threaded code using Intel's FORTRAN 90 compiler, version 11.1 and all computations are solved on a standard desktop with Intel's I7, 2.93 GHz with 8 GB of Ram. All flows begin from an initial isotropic orientation defined by $\mathbf{A} = \frac{1}{3}\mathbf{I}$ and $\mathbf{B} = \mathbf{I}$. Results are compared to two commonly employed industrial closures to solve Equation (5), the Hybrid [1] and the ORT [19]. The Hybrid is known for its rapid computational speeds and ability to remain within the physical orientation space. The ORT is known to be one of the most accurate closures, but carries with it excessive computational overheads beyond that of the Hybrid.

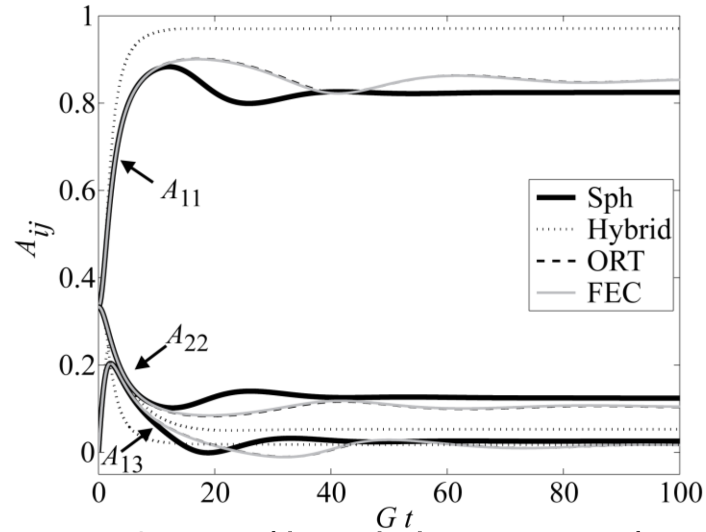

Figure 1: Comparison of the second-order orientation tensors for simple shear flow, $\boldsymbol{C_I} = \mathbf{10^{-3}}$, $\boldsymbol{\lambda} = \mathbf{0.9}$.

Simple Shear Flow

The first example is that of simple shear flow defined by a velocity vector $\mathbf{v} = (Gx_3, 0, 0)$. In this flow, fibers will tend to orient along the x_1 direction. In the absence of diffusion, a fiber will periodically rotate about the x_2 axis in a well defined Jeffery orbit (see e.g. [22]), but with increasing diffusion the oscillatory effects will be smoothed out on the bulk fiber orientation. Simple shear flow commonly occurs in industrial applications, and is of particular interest due to the propensity of many closures to perform poorly in a shearing flow due to the oscillatory nature of solutions for low levels of diffusion (see e.g., [11,16,26]). Two examples of a low diffusion shearing flow are presented, the first in Figure 1 for $C_I = 10^{-3}$, $\lambda = 0.99$ and the second in Figure 2 for $C_I = 10^{-3}$, $\lambda = 1$. As observed in the figures, both the FEC and the ORT closures yield nearly identical results, whereas the Hybrid has a considerable error. It is worthwhile to note, that the results from the ORT and the FEC closures are both quite accurate, and perform better than many of the existing closures (see the related IMCEC'2010 paper [35] for comparisons with several of the commonly employed industrial closures). The initial oscillations of the solution in the shearing flow for $\lambda = 0.99$ are quite expected due to the periodic nature of the fiber motion, whereas the flow with $\lambda = 1$ there should be no periodic nature as this case corresponds to infinite aspect ratio fibers. Since there is diffusion in this example, the oscillations become damped rather quickly. When the diffusion goes to zero, the oscillations become quite difficult to follow for many of the existing closures, whereas the FEC captures these oscillations quite well (see e.g. [22]).

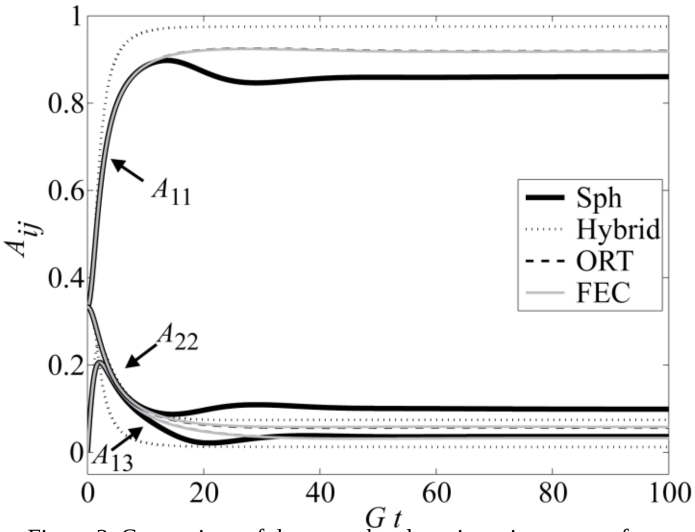

Figure 2: Comparison of the second-order orientation tensors for simple shear flow, $\boldsymbol{C_I = 10^{-3}}$, $\boldsymbol{\lambda = 1}$.

Shear/Planar Flow

The second flow considered is that of a shearing/planar flow defined by $\mathbf{v} = (-Gx_1 + Gx_3, Gx_2, 0)$. In this flow, fibers will rapidly orient along the x_2 axis with a small amount of shearing occurring along the x_1 direction in the direction of x_3. The results in Figure 3 are for $C_I = 10^{-2}$ and $\lambda = 1$, and further demonstrates, qualitatively, the stability of the FEC closure in capturing the orientation results obtained by the numerically exact Spherical Harmonic solution. Both the FEC and the ORT are much closer to the true solution, whereas the Hybrid closure tends to overpredict the alignment state.

Error Quantification

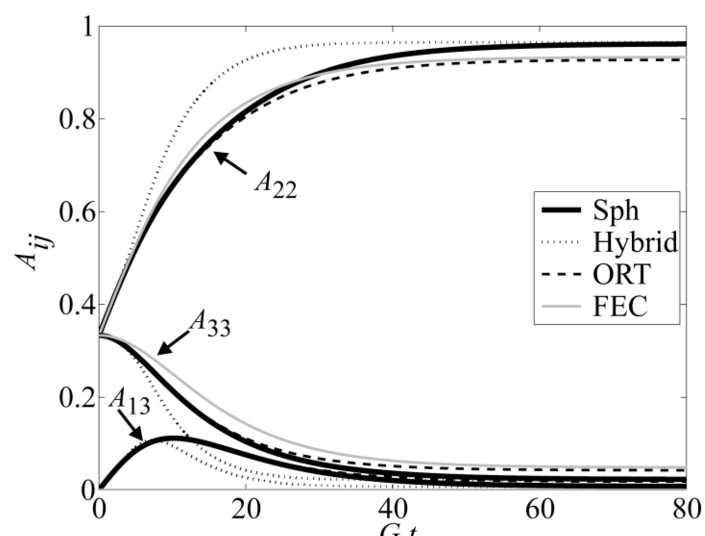

Figure 3: Comparison of the second-order orientation tensors for Shear/Planar flow, $\boldsymbol{C_I = 10^{-2}}$, $\boldsymbol{\lambda = 1}$.

Before one can confidently implement the FEC closure in industrial simulations, it is important to consider the closure's characteristics over a wide variety of flow fields that might be experienced in the industrial setting. To quantify the accuracy, the error in representing the fiber orientation state is computed

Table 1: Error in computing the second-order orientation tensor from the three closures over select flows

Flow	$\overline{Err}_{Hyb}$	$\overline{Err}_{ORT}$	$\overline{Err}_{FEC}$	$\widetilde{Err}_{Hyb}$	$\widetilde{Err}_{ORT}$	$\widetilde{Err}_{FEC}$
#1	1.4e-4	4.1e-6	2.1e-6	69	1.99	1
#2	4.4e-4	1.8e-3	1.8e-3	25	1.02	1
#3	1.8e-3	4.8e-4	4.7e-4	3.80	1.02	1
#4	1.5e-3	6.4e-4	6.3e-4	2.44	1.02	1
#5	1.5e-3	6.2e-4	6.1e-4	2.44	1.02	1
#6	3.9e-4	1.2e-4	1.2e-4	3.32	1.01	1
#7	5.5e-4	2.8e-4	2.8e-4	1.96	1.00	1
#8	3.5e-4	2.3e-4	3.4e-4	1.52	1	1.67
#9	2.0e-3	4.9e-4	4.9e-4	4.18	1	1.00
#10	2.0e-3	5.2e-4	5.2e-4	3.87	1.00	1

for 10 select flows. These 10 flows encompass much of the orientation eigenspace (see e.g. [11,36]) and are given as

1) Biaxial Elongation: $C_I = 10^{-3}$, $\lambda = 1$, $\mathbf{v} = (Gx_1, Gx_2, -2Gx_3)$
2) Uniaxial Elongation: $C_I = 10^{-3}$, $\lambda = 1$, $\mathbf{v} = (2Gx_1, -Gx_2, -Gx_3)$
3) Simple Shear: $C_I = 10^{-3}$, $\lambda = 0.99$, $\mathbf{v} = (Gx_3, 0{,}0)$
4) Simple Shear: $C_I = 10^{-3}$, $\lambda = 0.999$, $\mathbf{v} = (Gx_3, 0{,}0)$
5) Simple Shear: $C_I = 10^{-3}$, $\lambda = 1$, $\mathbf{v} = (Gx_3, 0{,}0)$
6) Shear/Biaxial: $C_I = 10^{-2}$, $\lambda = 1$, $\mathbf{v} = (Gx_1 + 2Gx_3, Gx_2, -2Gx_3)$
7) Shear/Uniaxial: $C_I = 10^{-2}$, $\lambda = 1$, $\mathbf{v} = (2Gx_1 + 3Gx_3, -Gx_2, -Gx_3)$
8) Shear/Stretch: $C_I = 10^{-2}$, $\lambda = 1$, $\mathbf{v} = (-Gx_1 + 1.5Gx_2, -Gx_2, 2Gx_3)$
9) Simple Shear: $C_I = 10^{-2}$, $\lambda = 0.99$, $\mathbf{v} = (Gx_3, 0{,}0)$
10) Simple Shear: $C_I = 10^{-2}$, $\lambda = 1$, $\mathbf{v} = (Gx_3, 0{,}0)$

To quantify the error for each of these flows, the Frobenius Norm of the difference between the true solution $A_{ij}^{Sph}(t)$ and the approximate solution obtained from a closure $A_{ij}^{Clo}(t)$ and is computed as

$$\|Err(t)\|_{Clo} \equiv \sqrt{\sum_{i=1}^{3}\sum_{j=1}^{3}\left|A_{ij}^{Sph}(t) - A_{ij}^{Clo}(t)\right|^2} \tag{14}$$

The Frobenius Norm is then integrated over all time to obtain the average error as

$$\overline{Err}_{Clo} = \frac{1}{t_{end} - t_{start}} \int_{t_{start}}^{t_{end}} \|Err(t)\|_{Clo} dt \tag{15}$$

where t_{start} is the initial time where the fiber orientation is isotropic and t_{end} is the time when steady state is attained which in this example is defined as the moment in time when the magnitude of the largest derivative of the eigenvalues of $\mathbf{A}$ is less than $G \times 10^{-4}$. The error from each of the ten flows is given in the first three columns of Table 1 for each of the three closures. Notice that the FEC and the ORT both yield similar errors, whereas the Hybrid consistently has a considerably larger error. To aid in the comparison between the various closures, the final three columns of Table 1 error is normalized by the smallest error for a given flow as

$$\widetilde{Err}_{Clo} = \frac{\overline{Err}_{Clo}}{min\{\overline{Err}_{Hyb}, \overline{Err}_{ORT}, \overline{Err}_{FEC}\}} \quad (16)$$

In this way, the most accurate closure will have a value $\widetilde{Err}_{Clo} = 1$, and the other closures will have $\widetilde{Err}_{Clo} > 1$. As can be observed in Table 1 the FEC closure consistently performs better than the two comparison closures.

Computational Time Enhancement

A goal for any new closure, and in particular the Feast Exact Closure, is advances in computational speeds to evaluate the orientation equations of motion. Taking into account the algorithm addressed in the previous section along with the symmetries discussed, a highly efficient code was developed. The solution of the ORT and the Hybrid is also programmed using the algorithms discussed in their respective papers. As can be observed in Table 2, the CPU time of the FEC is nearly as fast as that of the original Hybrid closure, and is significantly faster than that of the ORT closure. As the Hybrid closure is considered the standard by which closures are compared to for speed, results are also normalized to that of the Hybrid's computational time. In the essence of fairness, the FEC's algorithm reduces many of the repeated computations and where appropriate performs all operations in the principal reference frame. Thus similar steps were performed for the ORT and the Hybrid closures in an attempt to reduce their computational overheads. By reducing the number of operations, the 'optimized' solution for the Hybrid and the ORT yielded results significantly faster than those for the original algorithms. Thus, the FEC closure performs as fast as the industrially employed form of the Hybrid closure and much faster than the ORT closure, but using the efficiencies of the above algorithm for the FEC, the FEC is no longer the fastest closure.

Table 2: Normalized Computational Times

Closure	CPU Time	Normalized Time
Hybrid – Original	25	1
Hybrid – Optimized	6.9	0.3
ORT – Original	770	31
ORT – Optimized	21	0.8
FEC	26	1.0

CONCLUSIONS

The Fast Exact Closure of Montgomery-Smith *et al.* [23] is a robust approach to solve the fiber orientation tensors independent of the fourth-order orientation tensor. This approach is unique in that typical methods require some form of fitting the fourth-order orientation tensor as a function of the second-order orientation tensor. Results demonstrate that the FEC is as accurate and robust as the industrially accepted orthotropic closures, while attaining computational speeds similar to the industrial form of the hybrid closure. These computational gains will lend themselves to rapid employment in industrial codes for full part simulations of the spatially varying fiber orientation.

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