Exact tensor closures for the three dimensional Jeffery's equation

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This paper presents an exact formula for calculating the fourth-moment tensor from the second-moment tensor for the three dimensional Jeffery's equation. Although this approach falls within the category of a moment tensor closure, it does not rely upon an approximation, either analytic or curve fit, of the fourth-moment tensor as do previous closures. This closure is orthotropic in the sense of Cintra, J. S. & Tucker (1995), or equivalently, a natural closure in the sense of Verleye, V. & Dupret (1993). The existence of these explicit formulae has been asserted previously, but as far as the authors know, the explicit forms have yet to be published. The formulae involve elliptic integrals, and are valid whenever fiber orientation was isotropic at some point in time. Finally, this paper presents the *Fast Exact Closure* (FEC), a fast and in principle exact method for solving Jeffery's equation, which does not require approximate closures, nor the elliptic integral computation.

Key Words: Jeffery's equation, moment tensors, elliptic integral, fibers, directional orientation

1. Introduction

Jeffery's equation (Jeffery, G.B. 1923) concerns the motion of the direction of an axisymmetric fiber under the influence of a Stokesian fluid whose velocity field is $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$. If $\mathbf{p}$ is the unit vector along the axis of a fiber which is following the fluid, then it obeys the equation

$$\dot{\mathbf{p}} = \tfrac{1}{2}\Omega \cdot \mathbf{p} + \tfrac{1}{2}\lambda\Gamma \cdot \mathbf{p} - \tfrac{1}{2}\lambda\Gamma : \mathbf{ppp}. \tag{1.1}$$

Here Ω is the vorticity, that is, the anti-symmetric part $\nabla\mathbf{u} - (\nabla\mathbf{u})^T$ of the Jacobian of the velocity field $\nabla\mathbf{u} = (\partial u_i/\partial x_j)_{1 \le i,j \le 3}$, and Γ is the rate of strain tensor, that is, the symmetric part $\nabla\mathbf{u} + (\nabla\mathbf{u})^T$ of the Jacobean of the velocity field.

This is commonly extended to a formula for the fiber orientation distribution $\psi = \psi(\mathbf{x}, \mathbf{p}, t)$, where $\mathbf{p}$ is an element of the 2-dimensional sphere S. Thus given a subset E of S, the proportion of fibers whose direction is in E is given by $\int_E \psi(\mathbf{x}, \mathbf{p}, t)\, d\mathbf{p}$, where $d\mathbf{p}$ represents the usual integration over S. In particular, an isotropic distribution is represented by $\psi = 1/4\pi$. Then Jeffery's equation for the fiber orientation distribution is

$$\frac{D}{Dt}\psi = -\nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}}\psi) \tag{1.2}$$

where D/Dt represents the material derivative $\partial/\partial t + \mathbf{u} \cdot \nabla$. Industrial forms of equa-

tion (1.2) often include a rotary diffusivity term to account for particle interaction, but that applied study is left for the related work in Montgomery-Smith, S.J. *et al.* (2010*b*).

Since equation (1.2) is, in effect, a partial differential equation in 5-spatial dimensions, calculating this numerically can be rather daunting. Hence Hinch, E.J. & Leal (1976) suggested to recast the equation in terms of the higher order moment tensors. For example, the second and fourth moment tensors are given by

$$A = \int_S \mathbf{pp}\psi \, d\mathbf{p}, \qquad \mathbb{A} = \int_S \mathbf{pppp}\psi \, d\mathbf{p}. \tag{1.3}$$

Then Jeffery's equation for the second order moment tensor is

$$\frac{D}{Dt}A = \tfrac{1}{2}(\Omega \cdot A - A \cdot \Omega + \lambda(\Gamma \cdot A + A \cdot \Gamma) - 2\lambda\mathbb{A} : \Gamma). \tag{1.4}$$

The difficulty with this equation is that it involves the fourth order moment tensor. To circumvent this problem, various authors (see e.g., Hinch, E.J. & Leal 1976; Altan, M.C. *et al.* 1989, 1990; Verleye, V. & Dupret 1993; Cintra, J. S. & Tucker 1995; VerWeyst, B.E. *et al.* 1999; Chung, D.H. & Kwon 2002; Han, K.-H. & Im 2002; Jack, D.A. & Smith 2005; Jack D.A. *et al.* 2008) have proposed *closures*, that is, formulae to calculate the fourth order moment tensor $\mathbb{A}$ from the second order moment tensor A. Many of the approximate closures involve coefficients obtained by fitting numerical data found by solving equation (1.2) using a finite element method (see e.g., Bay, R.S. 1991).

Verleye, V. & Dupret (1993) proposed what they called the *natural closure*. If there was an exact formula for the closure, then it must be the case that the formula is of the form

$$\mathbb{A} = \sum_{0 \le m \le n \le 2} \beta_{mn}\mathcal{S}(A^m \otimes A^n). \tag{1.5}$$

Here $\mathcal{S}$ represents the symmetrization of a rank 4 tensor, that is

$$\mathcal{S}(\mathbb{B})_{i_1 i_2 i_3 i_4} = \tfrac{1}{24}\sum_\sigma \mathbb{B}_{i_{\sigma_1} i_{\sigma_2} i_{\sigma_3} i_{\sigma_4}}, \tag{1.6}$$

where the sum is over all permutations $\sigma = (\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ of $(1, 2, 3, 4)$. Furthermore, β_{mn} are symmetric functions of the eigenvalues of A, or equivalently, functions of the three invariants of A, that is, the coefficients of the characteristic polynomial of A, which are the trace of A, the trace of the adjoint of A, and the determinant of A. That m and n need only sum up to 2 follows from the Cayley-Hamilton Theorem.

Cintra, J. S. & Tucker (1995) proposed what they called the *orthotropic closure*. If there was an exact formula for the closure, then it must be the case that if A is diagonal, then $\mathbb{A}_{ijkl}$ must be zero if any index is repeated an odd number of times, and otherwise depend only on the diagonal entries of A in such a manner that

$$\mathbb{A}_{1111}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1111}(A_{11}, A_{33}, A_{22}), \tag{1.7a}$$

$$\mathbb{A}_{1122}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1122}(A_{22}, A_{11}, A_{33}), \tag{1.7b}$$

$$\mathbb{A}_{2222}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1111}(A_{22}, A_{11}, A_{33}), \tag{1.7c}$$

$$\mathbb{A}_{3333}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1111}(A_{33}, A_{11}, A_{22}), \tag{1.7d}$$

$$\mathbb{A}_{1133}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1122}(A_{11}, A_{33}, A_{22}), \tag{1.7e}$$

$$\mathbb{A}_{2233}(A_{11}, A_{22}, A_{33}) = \mathbb{A}_{1122}(A_{22}, A_{33}, A_{11}). \tag{1.7f}$$

They set

$$\mathbb{A}_{1111}(A_{11}, A_{22}, A_{33}) = f(A_{11}, A_{22}, A_{33}), \tag{1.8a}$$

$$\mathbb{A}_{2222}(A_{11}, A_{22}, A_{33}) = g(A_{11}, A_{22}, A_{33}), \tag{1.8b}$$

$$\mathbb{A}_{3333}(A_{11}, A_{22}, A_{33}) = h(A_{11}, A_{22}, A_{33}), \tag{1.8c}$$

When $A_{11} \geq A_{22} \geq A_{33}$, and then searched for the three functions $f(x, y, z)$, $g(x, y, z)$ and $h(x, y, z)$. They were then able to compute $\mathbb{A}_{1122}$, etc., using the relationship $\sum_i \mathbb{A}_{iijk} = A_{jk}$.

As noted in Cintra, J. S. & Tucker (1995), since they come from identical assumptions, the natural closure and the orthotropic closure must be theoretically identical, in that the β_{mn} must be uniquely determinable from the $\mathbb{A}_{iijj}$ and vice versa. This can be seen explicitly by assuming that A is diagonal in equation (1.5), and seeing that this creates six equations. The transformation from the natural closure to the orthotropic closure is immediate. The converse transformation is seen by solving the six equations for the six unknowns β_{mn}. Calculation shows that the resulting six by six matrix is invertible if and only if the diagonal entries of A are distinct. If any of them are repeated, then the β_{mn} can be obtained by a limiting process. This suggests that while the natural and orthotropic closures are mathematically equivalent, and that numerically the orthotropic closure will be more stable when any of the eigenvalues of A are repeated, and indeed numerical experiments seem to bare this out.

Verleye, V. & Dupret (1993) noted that indeed there is an exact closure, *in the particular case that the fiber orientation distribution is at some time isotropic.* Throughout this paper, this will be the standing assumption, unless otherwise stated.

Their exact closure followed from an exact solution to Jeffery's equation in this particular case provided by Dinh, S.M. & Armstrong (1984) and Lipscomb, G G II. *et al.* (1988). Verleye and Dupret gave explicit formulae in the two dimensional case (see also Altan & Tang 1993, who independently performed the same calculations), but cited an 'in preparation' article for the three dimensional case, merely noting that the calculations involved elliptic integrals.

Verweyst in his Ph.D. thesis (VerWeyst, B.E. 1998), indicated similar exact calculations, for which he cited a 'personal communication' from Wetzel. Wetzel in his Ph.D. thesis (Wetzel, E.D. 1999) provides calculations for a different but related problem, and gives his solution in terms of elliptic integrals. Therefore we are somewhat certain that he also obtained the formulae of Verleye and Dupret.

However, neither Dupret, Verleye, Verweyst, nor Wetzel seem to have published their calculations. The traditional approach is to perform these sorts of calculations using spherical coordinates and the Legendre form of elliptic integrals. However we prefer to use Cartesian coordinates on the sphere (which we think of as embedded in three dimensional Euclidean space) and the Carlson form of the elliptic integrals. As such, it is quite possible that our formulae are more compact than the form they may have obtained. Also, the approach taken here will easily generalize to other spacial dimensions, should the need arise.

Our analysis also yields what we shall call the *Fast Exact Closure* (FEC), a rather fast method of solving Jeffery's equation. This method calculates $\mathbb{A}$ by neither using approximate closures, nor computing elliptic integrals, but rather by computing an ancillary quantity B, which is easily computed via an ordinary differential equation.

Finally we note that earlier publications asserted these formulae exist only in the case $\lambda = 1$. However following the work of Lipscomb, G G II. *et al.* (1988), it was realized that this restriction is unnecessary.

2. The Exact Formulae

Dinh, S.M. & Armstrong (1984) (for the case $\lambda = 1$) and Lipscomb, G G II. *et al.* (1988) noted that equation (1.1) can be solved by $\mathbf{p} = \mathbf{q}/|\mathbf{q}|$, where $\mathbf{q}$ satisfies the equation (see Theorem 3.1 in §3 for the proof)

$$\dot{\mathbf{q}} = \tfrac{1}{2}(\Omega + \lambda\Gamma) \cdot \mathbf{q}. \tag{2.1}$$

From this they deduced that if the fiber orientation distribution is initially isotropic, that is, $\psi = 1/4\pi$ at $t = 0$, then the solution to equation (1.2) is (see Theorem 3.2 in §3 for the proof)

$$\psi(\mathbf{p}) = \frac{1}{4\pi(B : \mathbf{pp})^{3/2}}. \tag{2.2}$$

Here $B = C^T C$ where C satisfies the equation

$$\frac{D}{Dt}C = -\tfrac{1}{2}C \cdot (\Omega + \lambda\Gamma), \quad C = I \text{ at } t = 0, \tag{2.3}$$

or equivalently that B satisfies

$$\frac{D}{Dt}B = -\tfrac{1}{2}(B \cdot (\Omega + \lambda\Gamma) + (-\Omega + \lambda\Gamma) \cdot B), \quad B = I \text{ at } t = 0. \tag{2.4}$$

We note parenthetically that equation (2.2) generalizes as follows: if $\psi = \psi_0$ at $t = 0$, then from Theorem 3.2

$$\psi(\mathbf{p}) = \frac{\psi_0(C \cdot \mathbf{p}/|C \cdot \mathbf{p}|)}{(B : \mathbf{pp})^{3/2}}. \tag{2.5}$$

For the purposes of the exact closure, the precise nature of B is not required. All that is necessary to know is that B is a positive definite matrix with determinant one.

From the definition, the formula for the second order moment tensor is

$$A = \int_S \frac{\mathbf{pp}}{4\pi(B : \mathbf{pp})^{3/2}} \, d\mathbf{p}. \tag{2.6}$$

Verleye and Dupret assert, without proof but somewhat reasonably, that this provides a one-one correspondence between positive definite matrices B with determinant one, and positive definite matrices A with trace one. Thus by inverting this formula, one obtains a formula for B in terms of A.

The integral in equation (2.6) may be transformed to the formula (see Theorem 3.3 in §3)

$$A = \tfrac{1}{2} \int_0^\infty \frac{(B + sI)^{-1} \, ds}{\sqrt{\det(B + sI)}}. \tag{2.7}$$

To perform this calculation numerically, diagonalize B with an orthogonal matrix. Then A is transformed to a diagonal matrix via exactly the same similarity matrix, and equation (2.7) becomes (see Theorem 3.3 in §3)

$$A_{11} = \tfrac{1}{2} \int_0^\infty \frac{ds}{(b_1 + s)^{3/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}, \tag{2.8a}$$

$$A_{22} = \tfrac{1}{2} \int_0^\infty \frac{ds}{\sqrt{b_1 + s}(b_2 + s)^{3/2}\sqrt{b_3 + s}}, \tag{2.8b}$$

$$A_{33} = \tfrac{1}{2} \int_0^\infty \frac{ds}{\sqrt{b_1 + s}\sqrt{b_2 + s}(b_3 + s)^{3/2}}, \tag{2.8c}$$

where b_1, b_2, b_3 are the diagonal entries of B. These integrals are one third the r_D Carlson

form of the elliptic integrals (Carlson 1995). The Carlson elliptic integrals have good numerical algorithms to compute them, for example, they are part of the suite of special functions provided by the GNU Scientific Library (GNU Scientific Library 2009), and are also described in the book Press, W.H. *et al.* (2003).

The fourth order moment tensor is, by definition

$$\mathbb{A} = \int_S \frac{\mathbf{pppp}}{4\pi(B : \mathbf{pp})^{3/2}} \, d\mathbf{p}, \tag{2.9}$$

which may be transformed to

$$\mathbb{A} = \tfrac{3}{4} \int_0^\infty \frac{s \, \mathcal{S}((B + sI)^{-1} \otimes (B + sI)^{-1}) \, ds}{\sqrt{\det(B + sI)}}, \tag{2.10}$$

or in the special case that B is diagonal (or equivalently when A is diagonal) can be computed via the equations

$$\mathbb{A}_{1111} = \tfrac{3}{4} \int_0^\infty \frac{s \, ds}{(b_1 + s)^{5/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}, \tag{2.11a}$$

$$\mathbb{A}_{2222} = \tfrac{3}{4} \int_0^\infty \frac{s \, ds}{\sqrt{b_1 + s}(b_2 + s)^{5/2}\sqrt{b_3 + s}}, \tag{2.11b}$$

$$\mathbb{A}_{3333} = \tfrac{3}{4} \int_0^\infty \frac{s \, ds}{\sqrt{b_1 + s}\sqrt{b_2 + s}(b_3 + t)^{5/2}}, \tag{2.11c}$$

$$\mathbb{A}_{1122} = \tfrac{1}{4} \int_0^\infty \frac{s \, ds}{(b_1 + s)^{3/2}(b_2 + s)^{3/2}\sqrt{b_3 + s}}, \tag{2.11d}$$

$$\mathbb{A}_{1133} = \tfrac{1}{4} \int_0^\infty \frac{s \, ds}{(b_1 + s)^{3/2}\sqrt{b_2 + s}(b_3 + s)^{3/2}}, \tag{2.11e}$$

$$\mathbb{A}_{2233} = \tfrac{1}{4} \int_0^\infty \frac{s \, ds}{\sqrt{b_1 + s}(b_2 + s)^{3/2}(b_3 + s)^{3/2}}, \tag{2.11f}$$

all the other coefficients of $\mathbb{A}$ being zero. In the case that the eigenvalues of B are distinct, these can be computed by the easily derived formulae

$$\mathbb{A}_{1122} = \frac{b_1 A_{11} - b_2 A_{22}}{2(b_1 - b_2)}, \tag{2.12a}$$

$$\mathbb{A}_{1133} = \frac{b_1 A_{11} - b_3 A_{33}}{2(b_1 - b_3)}, \tag{2.12b}$$

$$\mathbb{A}_{2233} = \frac{b_2 A_{22} - b_3 A_{33}}{2(b_2 - b_3)}, \tag{2.12c}$$

$$\mathbb{A}_{1111} = A_{11} - \mathbb{A}_{1122} - \mathbb{A}_{1133}, \tag{2.12d}$$

$$\mathbb{A}_{2222} = A_{22} - \mathbb{A}_{1122} - \mathbb{A}_{2233}, \tag{2.12e}$$

$$\mathbb{A}_{3333} = A_{33} - \mathbb{A}_{1133} - \mathbb{A}_{2233}. \tag{2.12f}$$

If two of the eigenvalues are equal, for example $b_1 = b_2 \neq b_3$ and $A_{11} = A_{22} \neq A_{33}$, we see from equation (2.11) that $A_{1111} = A_{2222} = 3A_{1122}$, and hence those parts of

equation (2.12) that don't involve division by zero give the formulae

$$\mathbb{A}_{1133} = A_{2233} = \frac{b_1 A_{11} - b_3 A_{33}}{2(b_1 - b_3)}, \tag{2.13a}$$

$$\mathbb{A}_{1122} = \tfrac{1}{4}(A_{11} - \mathbb{A}_{1133}), \tag{2.13b}$$

$$\mathbb{A}_{1111} = A_{2222} = A_{11} - \mathbb{A}_{1122} - \mathbb{A}_{1133}, \tag{2.13c}$$

$$\mathbb{A}_{3333} = A_{33} - 2\mathbb{A}_{1133}, \tag{2.13d}$$

and similar expressions exist when $b_1 \neq b_2 = b_3$ and $A_{11} \neq A_{22} = A_{33}$ or when $b_1 = b_3 \neq b_2$ and $A_{11} = A_{33} \neq A_{22}$. If all three of the eigenvalues are equal, that is $b_1 = b_2 = b_3 = 1$ and $A_{11} = A_{22} = A_{33} = \frac{1}{3}$ then

$$\mathbb{A}_{1111} = \mathbb{A}_{2222} = \mathbb{A}_{3333} = \tfrac{1}{5}, \tag{2.14a}$$

$$\mathbb{A}_{1122} = \mathbb{A}_{1133} = \mathbb{A}_{2233} = \tfrac{1}{15} \tag{2.14b}$$

(that is, if $B = I$, then $A = \frac{1}{3}I$ and $\mathbb{A} = \frac{1}{5}\mathcal{S}(II)$).

The exact closure can be summarized by first diagonalizing A, then computing B by inverting the formulae (2.8), then computing $\mathbb{A}$ using (2.11), and then using the inverse of the similarity matrix from the diagonalization of A to transform $\mathbb{A}$. To compute the formulae (2.11), use (2.12), (2.13), or (2.14), as appropriate.

These numerical calculations will necessarily take some time to perform (particularly the inversion process which requires a multidimensional root finding). VerWeyst, B.E. (1998) described a different process where these formulae were used to generate values which were then fitted to polynomial approximations to the functions f, g and h as in equation (1.8).

3. Proofs of the Required Theorems for the Exact Closure

THEOREM 3.1. *Equation* (2.1) *is an explicit solution of equation* (1.1)

Proof. This follows by simply substituting $\mathbf{p} = \mathbf{q}/|\mathbf{q}|$ into equation (1.1). $\square$

THEOREM 3.2. *The initially isotropic orientation distribution function from equations* (2.2) *and* (2.5) *are solutions to equation* (1.2).

Proof. If E is a subset of S, then the proportion of fibers whose direction is contained in E is

$$\int_E \psi(\mathbf{p})\, d\mathbf{p} = \frac{4}{\pi^{1/2}} \int_{r=0}^{\infty} \int_{\mathbf{p} \in E} \psi(\mathbf{p}) r^2 e^{-r^2}\, d\mathbf{p}\, dr = \frac{1}{\pi^{3/2}} \int_{\mathbf{q} \in \bar{E}} \psi\left(\frac{\mathbf{q}}{|\mathbf{q}|}\right) e^{-|\mathbf{q}|^2}\, d\mathbf{q}. \quad (3.1)$$

Here $\bar{E}$ denotes the set of elements $\mathbf{q} \in \mathbb{R}^3 - \{0\}$ such that $\mathbf{q}/|\mathbf{q}| \in E$. The first equality follows because $\int_0^\infty r^2 e^{-r^2}\, dr = \pi^{1/2}/4$. The second equality is just the conversion from spherical coordinates to Cartesian coordinates, noting that $4\pi r^2 dr d\mathbf{p} = d\mathbf{q}$.

Note that equation (2.1) is solved by setting $\mathbf{q} = C^{-1} \cdot \mathbf{p}(0)$ where C satisfies equation (2.3), because C^{-1} satisfies the equation

$$\frac{D}{Dt} C^{-1} = \tfrac{1}{2}(\Omega + \lambda \Gamma) \cdot C^{-1}, \quad C^{-1} = I \text{ at } t = 0. \tag{3.2}$$

Thus a fiber which at time t is in a direction $\mathbf{p}$ will have come from a fiber which at time $t = 0$ was in the direction $\mathbf{p}_0 = C \cdot \mathbf{p}/|C \cdot \mathbf{p}|$. The set E will have come from

the set $E_0 = \{C \cdot \mathbf{p}/|C \cdot \mathbf{p}| : \mathbf{p} \in E\}$, and the set $\bar{E}$ will have come from the set $\bar{E}_0 = C \cdot \bar{E} := \{C \cdot \mathbf{q} : \mathbf{q} \in \bar{E}\}$. Thus

$$\int_E \psi(\mathbf{p}) \, d\mathbf{p} = \int_{E_0} \psi_0(\mathbf{p}) \, d\mathbf{p}. \tag{3.3}$$

Rewriting equation (3.1) for the time $t = 0$, we obtain

$$\int_{E_0} \psi_0(\mathbf{p}) \, d\mathbf{p} = \pi^{-3/2} \int_{\mathbf{q} \in \bar{E}_0} \psi_0 \left(\frac{\mathbf{q}}{|\mathbf{q}|} \right) e^{-|\mathbf{q}|^2} \, d\mathbf{q}. \tag{3.4}$$

Performing the change of variables $\mathbf{q} \mapsto C \cdot \mathbf{q}$, and noting that $d\mathbf{q} = d(C \cdot \mathbf{q})$ (because the determinant of C is one), we obtain

$$\begin{aligned}
\int_{E_0} \psi_0(\mathbf{p}) \, d\mathbf{p} &= \pi^{-3/2} \int_{\mathbf{q} \in \bar{E}} \psi_0 \left(\frac{C \cdot \mathbf{q}}{|C \cdot \mathbf{q}|} \right) e^{-|C \cdot \mathbf{q}|^2} \, d\mathbf{q} \\
&= \pi^{-3/2} \int_{\mathbf{p} \in E} \int_{r=0}^{\infty} \psi_0 \left(\frac{C \cdot \mathbf{p}}{|C \cdot \mathbf{p}|} \right) r^2 e^{-|C \cdot \mathbf{p}|^2 r^2} \, dr d\mathbf{p},
\end{aligned} \tag{3.5}$$

where the last equality follows by converting Cartesian coordinates to spherical coordinates. Combining this with equation (3.1), and noting that these equations work for any subset E of S, we obtain

$$\psi(\mathbf{p}) = 4\pi^{-1/2} \psi_0 \left(\frac{C \cdot \mathbf{p}}{|C \cdot \mathbf{p}|} \right) \int_{r=0}^{\infty} r^2 e^{-|C \cdot \mathbf{p}|^2 r^2} \, dr = \frac{\psi_0(C \cdot \mathbf{p}/|C \cdot \mathbf{p}|)}{|C \cdot \mathbf{p}|^3} \tag{3.6}$$

as required. Equation (2.2) is an immediate corollary of equation (2.5). $\qquad\square$

THEOREM 3.3. *The transformation of the second-order orientation tensor of equations* (2.7) *and* (2.8) *from equation* (2.6) *is valid.*

Proof. Note that if B is diagonal with diagonal entries b_1, b_2, b_3, then from equation (3.6)

$$\psi(\mathbf{p}) = \frac{1}{\pi^{3/2}} \int_0^{\infty} r^2 \exp(-r^2(b_1 p_1^2 + b_2 p_2^2 + b_3 p_3^2)) \, dr. \tag{3.7}$$

By symmetry we can see that the off diagonal entries of A are zero, and that the diagonal entries are computed, for example, by

$$\begin{aligned}
A_{11} &= \frac{1}{\pi^{3/2}} \int_S \int_{r=0}^{\infty} r^2 p_1^2 \exp(-r^2(b_1 p_1^2 + b_2 p_2^2 + b_3 p_3^2)) \, dr d\mathbf{p} \\
&= \frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} \frac{q_1^2}{|\mathbf{q}|^2} \exp(-(b_1 q_1^2 + b_2 q_2^2 + b_3 q_3^2)) \, d\mathbf{q}.
\end{aligned} \tag{3.8}$$

Now, if we set

$$f(s) = \frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} \frac{q_1^2}{|\mathbf{q}|^2} \exp(-((b_1 + s)q_1^2 + (b_2 + s)q_2^2 + (b_3 + s)q_3^2)) \, d\mathbf{q}, \tag{3.9}$$

then we see that

$$f'(s) = -\frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} q_1^2 \exp(-((b_1 + s)q_1^2 + (b_2 + s)q_2^2 + (b_3 + s)q_3^2)) \, d\mathbf{q}$$

$$= -\frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} q_1^2 e^{-(b_1+s)q_1^2} \, dq_1 \int_{-\infty}^{\infty} e^{-(b_2+s)q_2^2} \, dq_2 \int_{-\infty}^{\infty} e^{-(b_3+s)q_3^2} \, dq_3 \qquad (3.10)$$

$$= -\frac{1}{2(b_1 + s)^{3/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}.$$

Since it is evident that $f(s) \to 0$ as $s \to \infty$, we obtain

$$A_{11} = \tfrac{1}{2} \int_0^{\infty} \frac{ds}{(b_1 + s)^{3/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}. \qquad (3.11)$$

To show equation (2.7), it is only necessary to consider the case when B is diagonal, and in this case the formula follows immediately from (2.8). $\qquad\square$

THEOREM 3.4. *The transformation of the fourth-order orientation tensor of equations (2.10) and (2.11) from equation (2.9) is valid.*

Proof. We illustrate the proof of equation (2.11) with the example

$$\mathbb{A}_{1111} = \frac{1}{\pi^{3/2}} \int_S \int_{r=0}^{\infty} r^2 p_1^4 \exp(-r^2(b_1 p_1^2 + b_2 p_2^2 + b_3 p_3^2)) \, dr d\mathbf{p}$$

$$= \frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} \frac{q_1^4}{|\mathbf{q}|^4} \exp(-(b_1 q_1^2 + b_2 q_2^2 + b_3 q_3^2)) \, d\mathbf{q}. \qquad (3.12)$$

We set

$$g(s) = \frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} \frac{q_1^4}{|\mathbf{q}|^4} \exp(-((b_1 + s)q_1^2 + (b_2 + s)q_2^2 + (b_3 + s)q_3^2)) \, d\mathbf{q}, \qquad (3.13)$$

and we see that

$$g''(s) = \frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} q_1^4 \exp(-((b_1 + s)q_1^2 + (b_2 + s)q_2^2 + (b_3 + s)q_3^2)) \, d\mathbf{q}$$

$$= \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} q_1^4 e^{-(b_1+s)q_1^2} \, dq_1 \int_{-\infty}^{\infty} e^{-(b_2+s)q_2^2} \, dq_2 \int_{-\infty}^{\infty} e^{-(b_3+s)q_3^2} \, dq_3 \qquad (3.14)$$

$$= \frac{3}{4(b_1 + s)^{5/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}$$

Since

$$g(s) = \int g'(s) \, ds = sg'(s) - \int sg''(s) \, ds, \qquad (3.15)$$

it follows that

$$\mathbb{A}_{1111} = \tfrac{3}{4} \int_0^{\infty} \frac{s \, ds}{(b_1 + s)^{5/2}\sqrt{b_2 + s}\sqrt{b_3 + s}}. \qquad (3.16)$$

To show equation (2.10), again it is only necessary to prove this in the case when B is diagonal. The following identities are useful. If U and V are diagonal matrices, then

$$\mathcal{S}(UV)_{iiii} = U_{ii}V_{ii}$$

$$\mathcal{S}(UV)_{iijj} = \tfrac{1}{6}(U_{ii}V_{jj} + U_{jj}V_{ii}) \quad \text{if } i \neq j \qquad (3.17)$$

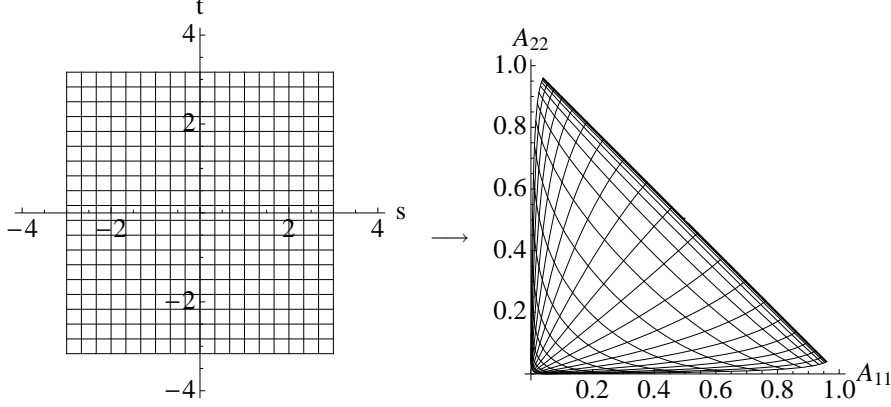$$\mathcal{S}(UV)_{iijk} = 0 \quad \text{if } i \neq j \text{ and } j \neq k,$$

FIGURE 1. Diagram illustrating how γ maps a grid in the s-t plane to the A_{11}-A_{22} plane.

where no summation is implied for repeated indices. □

THEOREM 3.5. *The mapping from B to A defined by equation* (2.7) *is one-one and onto.*

Proof. This is equivalent to showing that the map from $\{(b_1, b_2, b_3) : b_1, b_2, b_3 > 0, b_1 b_2 b_3 = 1\}$ to $\{(A_{11}, A_{22}, A_{33}) : A_{11}, A_{22}, A_{33} > 0, A_{11} + A_{22} + A_{33} = 1\}$ defined by equation (2.8) is one-one and onto. To this end, consider the map γ that takes (s, t) to the values of (A_{11}, A_{22}) when $(b_1, b_2, b_3) = (e^{s+t}, e^{s-t}, e^{-2s})$. In Figure 1, we show how γ maps a grid in the s-t plane to the A_{11}-A_{22} plane, providing a 'picture proof' that the map is one-one and onto.

To show that the map is one-one, it is sufficient to show that $\gamma(s, t)$ gives a family of curves with negative slope if s is fixed, and t is allowed to range freely, and that $\gamma(s, t)$ gives a family of curves with positive slope if the roles of s and t are reversed.

For example, let us prove that $\partial A_{11}/\partial t < 0$. We have that $\partial B/\partial t = G \cdot B$ with $G = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, that is, B satisfies equation (2.4) with $\Gamma = -G$, $\Omega = 0$, $\lambda = 1$ and $\mathbf{u} = 0$. (Since B is diagonal, we have $B \cdot G = G \cdot B$.) Hence A satisfies equation (1.4) with the same parameters, and so $\partial A_{11}/\partial t = -A_{11} + \mathbb{A}_{1111} - \mathbb{A}_{1122} = -2\mathbb{A}_{1122} - \mathbb{A}_{1133} < 0$. Similarly, $\partial A_{22}/\partial t > 0$, and hence $\gamma(s, t)$ gives a family of curves with negative slope if s is fixed and t is allowed to range freely.

To show that the map is onto, it is sufficient to see that the map γ 'stakes out' the appropriate region, which follows because $\gamma(s, t) \to (0, 0)$ as $s \to \infty$, $\gamma(s, t)$ converges to a point on the line $A_{11} + A_{22} = 1$ as $s \to -\infty$, $A_{11} \to 0$ as $t \to \infty$, and $A_{22} \to 0$ as $t \to -\infty$.

For example, as $s \to -\infty$, we see from equation (2.2) that the fiber orientation distribution concentrates on the equator $p_3 = 0$. Hence $A_{33} \to 0$, and so $A_{11} + A_{22} = 1 - A_{33} \to 1$. Since A_{11} and A_{22} increase as s decreases, they must also individually converge to limits. □

4. The Fast Exact Closure (FEC)

Our analysis yields another method for solving Jeffery's equation, with the proviso that the probability distribution was isotropic at some time in its history where the goal is to solve equation (1.4). The difficulty of finding B can be solved by simultaneously solving

equation (2.4) along with equation (1.4). During this process, $\mathbb{A}$ can be calculated using (2.12)-(2.14). In this way, an exact solution is obtained, without the need to compute the elliptic integrals.

The only difficulty will be with the initial data. If it is isotropic, one simply sets $A = \frac{1}{3}I$ and $B = I$ at $t = 0$. Conversely, if the initial data is not isotropic, then the initial data for B can be calculated by inverting equation (2.7). This can be performed by diagonalizing A, computing B by inverting equation (2.8), and then reversing the change of basis that was used to diagonalize A. While this calculation could conceivably be quite slow, as the inversion of equation (2.8) will require a three-dimensional root finding method as well as computing the elliptic integrals, this needs to be performed only for the initial step.

This method should run at about the same speed as computing the orthotropic closure algorithms of Cintra, J. S. & Tucker (1995), or VerWeyst, B.E. *et al.* (1999). The work load of this algorithm involves solving an ordinary differential equation in about eleven variables, where the main computational effort will be the diagonalization of the matrices, and performing the basis change for the rank two and rank four tensors. (Note that A and B will be simultaneously diagonalizable, that is, the orthogonal matrix used to diagonalize one of the second-order tensors can and should be used to diagonalize the other.)

A downside to this algorithm is that the computation (2.12) will become numerically problematic if any of the eigenvalues of B are close to each other. The solution is to use formulae similar to (2.13) or (2.14) if any of the eigenvalues are close to each other. If two of the eigenvalues are close to each other, for example $b_1 = b_2 + \epsilon$, we see from equation (2.11) that $A_{1111} + A_{2222} = 6A_{1122} + O(\epsilon^2)$, and hence

$$\mathbb{A}_{1133} = \frac{b_1 A_{11} - b_3 A_{33}}{2(b_1 - b_3)}, \tag{4.1a}$$

$$\mathbb{A}_{2233} = \frac{b_2 A_{22} - b_3 A_{33}}{2(b_2 - b_3)}, \tag{4.1b}$$

$$\mathbb{A}_{1122} = \tfrac{1}{8}(A_{11} + A_{22} - \mathbb{A}_{1133} - \mathbb{A}_{2233}) + O(\epsilon^2), \tag{4.1c}$$

$$\mathbb{A}_{1111} = A_{11} - \mathbb{A}_{1122} - \mathbb{A}_{1133}, \tag{4.1d}$$

$$\mathbb{A}_{2222} = A_{22} - \mathbb{A}_{1122} - \mathbb{A}_{2233}, \tag{4.1e}$$

$$\mathbb{A}_{3333} = A_{33} - \mathbb{A}_{1133} - \mathbb{A}_{2233}, \tag{4.1f}$$

where similar forms exist when $b_1 = b_3 + \epsilon$ or $b_2 = b_3 + \epsilon$. If all three of the eigenvalues are almost equal, that is $b_1 = 1 + c_1$, $b_2 = 1 + c_2$, $b_3 = 1 + c_3$ with $c_1, c_2, c_3 = O(\epsilon)$ (so necessarily $c_1 + c_2 + c_3 = O(\epsilon^2)$)

$$\mathbb{A}_{1111} = \tfrac{1}{5} - \tfrac{3}{14}c_1 - \tfrac{3}{70}c_2 - \tfrac{3}{70}c_3 + O(\epsilon^2), \tag{4.2a}$$

$$\mathbb{A}_{2222} = \tfrac{1}{5} - \tfrac{3}{70}c_1 - \tfrac{3}{14}c_2 - \tfrac{3}{70}c_3 + O(\epsilon^2), \tag{4.2b}$$

$$\mathbb{A}_{3333} = \tfrac{1}{5} - \tfrac{3}{70}c_1 - \tfrac{3}{70}c_2 - \tfrac{3}{14}c_3 + O(\epsilon^2), \tag{4.2c}$$

$$\mathbb{A}_{1122} = \tfrac{1}{15} - \tfrac{3}{70}c_1 - \tfrac{3}{70}c_2 - \tfrac{1}{70}c_3 + O(\epsilon^2), \tag{4.2d}$$

$$\mathbb{A}_{1133} = \tfrac{1}{15} - \tfrac{3}{70}c_1 - \tfrac{1}{70}c_2 - \tfrac{3}{70}c_3 + O(\epsilon^2), \tag{4.2e}$$

$$\mathbb{A}_{2233} = \tfrac{1}{15} - \tfrac{1}{70}c_1 - \tfrac{3}{70}c_2 - \tfrac{3}{70}c_3 + O(\epsilon^2). \tag{4.2f}$$

For example, if you believe that your ODE solver is accurate to n digits, it is appropriate to use (4.1) or (4.2) if any of the eigenvalues of B have a relative difference bounded by about $10^{-n/3}$. The resulting $\mathbb{A}$ should then be accurate to about $2n/3$ digits. The hope is this loss of precision is unlikely to have a large effect on the final solution, because the

event that B has eigenvalues close to each other should happen somewhat rarely, and these events will largely be integrated out by equation (2.4).

5. Behavior of the Fast Exact Closure (FEC)

Direct solutions of the tensor C of equation (2.3) will serve as the basis upon which to compare the effectiveness of the FEC. The transient solution of C in equation (2.3), assuming constant velocity gradients, is given by

$$C = \exp\left(-\frac{t}{2}\left(\Omega + \lambda\Gamma\right)\right), \tag{5.1}$$

where exp denotes the matrix exponential. The solution for B readily follows from the definition $B = C^T C$ from the solution of C in equation (2.3), and the second-order orientation tensor A is obtained from equation (2.6). This solution approach, which we term the analytic solution, is only effective for flows originating from an isotropic initial condition with constant velocity gradients, but will serve as the basis upon which to compare results from various closures which numerically solve the equation of motion for the orientation tensor A of equation (1.4).

To demonstrate the effectiveness of the FEC, solutions are compared to results from several popular closures, the quadratic (Doi, M. 1981), the hybrid (Advani, S.G. & Tucker 1987) and the ORT (VerWeyst, B.E. 1998; VerWeyst, B.E. & III 2002), and all results will be compared to the analytic solutions from equation (5.1). The three comparison closures are selected based on their common employment in industrial simulations of fiber orientation (e.g., the quadratic and the hybrid) and their known accuracy (e.g., the ORT). It is expected the ORT closure's accuracy will be quite high considering it is based off of similar 'exact' calculations (VerWeyst, B.E. 1998) to the FEC. The ORT is known to give similar results to the IBOF closure of Chung, D.H. & Kwon (2002) which is an extension of the natural closure discussed by Verleye, V. & Dupret (1993). Solutions for the existing closures (quadratic, hybrid, or ORT) are performed by solving equation (1.4) and using the respective closure to approximate $\mathbb{A}$ in terms of A.

The simple shear flow considered ($\mathbf{v} = [Gx_3, 0, 0]^T$ where G is the scalar magnitude of the rate of deformation $G = ||\Gamma||$) begins from an initial isotropic orientation (i.e., $\psi = \frac{1}{4\pi}$). The primary reason for choosing a pure shearing flow is twofold. The first, and primary, reason is due to the prevalence of shearing dominated flows in industrial injection molding processes. An alternative, yet more constraining, motivation for choosing a pure shearing flow is to demonstrate the FEC's ability to capture the correct period for the Jeffery orbit. It is this oscillatory nature of the orientation in pure Jeffery's motion that causes significant numerical difficulties for classical approaches that rely on alternative methods such as finite differences (Bay, R.S. & Tucker 1991; Bay, R.S. 1991) or the Spherical Harmonic Expansion approach (see e.g., Bird, R. B. *et al.* 1987; Montgomery-Smith, S.J. *et al.* 2010a). It is worthwhile to note that the interior of the eigenspace triangle containing all possible orientations (see e.g., Cintra, J. S. & Tucker 1995, for a full discussion) with an initial isotropic orientation state can only be populated by shearing flows, whereas orientations occurring on the boundaries are caused by pure elongational flows and will have two repeated eigenvalues of A and B.

Solutions of pure shear flow are run for the orientation parameter $\lambda = 0.98$, which corresponds to a fiber aspect ratio of $a_r = L/d \simeq 9.95$. The results for the second-order orientation tensor A from each solution approach is given in Figure 2 and compared to direct computations of the analytic solution of equation (5.1) for the tensor C and then using the elliptic integral relationship of equation (2.8) to obtain A. As observed in the

figure, the periodic nature of the orientation solution of A_{ij} is captured reasonably will by each of the solution approaches. An ellipsoid experiencing Jeffery motion in a pure shearing flow will rotate with a period, τ, of (Jeffery, G.B. 1923)

$$\tau = \frac{2\pi}{||\Gamma||\sqrt{(1-\lambda^2)}},\tag{5.2}$$

where the solution of equation (5.2) may be obtained by analyzing the eigenvalues of $\Omega + \lambda\Gamma$ from equation (2.1). In our example $\lambda = 0.98$ and $||\Gamma|| = G$ and thus $\tau = 31.574/G$. This period can be observed by noting a particular orientation condition, and tabulating the time it takes to return to the same orientation state. Since there are numerical errors introduced by the numerical solution of a system of ODEs with a periodic solution, returning to the numerically identical orientation state may never occur. Thus, we compare the initial isotropic orientation to that of the orientation occurring near where the three eigenvalues are nearest to each other and can approximate the period of the numerical solution for pure show flow through the expression

$$\tau_{\text{Closure}} = t \text{ such that } |a_1 - a_3| \text{ is minimized over } Gt \in [30, 33],\tag{5.3}$$

where a_1, a_2 and a_3 are the eigenvalues of the second-order orientation tensor A in descending order, $a_1 \geq a_2 \geq a_3 \geq 0$. Therefore, the orientation from the numerical solutions employing closures will be closest to isotropic ($a_1 = a_2 = a_3 = 1/3$) when $a_1 \simeq a_3$. The FEC, ORT, Hybrid and Quadratic closures have observed periods of, respectively, $G\tau_{\text{FEC}} = 31.572$, $G\tau_{\text{ORT}} = 31.708$, $G\tau_{\text{Hybrid}} = 31.081$, and $G\tau_{\text{Quadratic}} = 31.575$. Each of the closures are reasonably accurate, whereas the FEC and Quadratic closures are the most effective in representing the actual period. But by observing the orientation path taken by each of the closures, the quadratic and the hybrid are clearly ineffective at predicting the orientation state during most of the flow history. The FEC and ORT closures follow the analytic solution quite well. To aid in comparing between closures, the error is plotted in Figure 2 where the error is defined as the difference in the eigenvalues from the analytic solution and the numeric solution from the closures as

$$Err^2 = \sum_{i=1}^{2} \left(a_i^{\text{Analytic}} - a_i^{\text{Closure}} \right)^2.\tag{5.4}$$

The value of Err shows the effectiveness of a closure in conjunction with the solution of the ODEs in equations (1.4) and (2.4) and where it has the greatest deviation in the orientation solution. It is interesting to note that the FEC performs quite well throughout much of the flow history. This characteristic is true, except when the orientation approaches isotropic. This is not unexpected due to the nature of the closure since this is where the eigenvalues of A all approach the same value of $1/3$ and the approximation of equation (4.2) must be accepted due to the aforementioned numerical limitations of repeated eigenvalues. It is worthwhile to note that both the ORT and the FEC yield solutions that are a considerable improvement over the commonly employed Quadratic and Hybrid closures, which for the ORT is not surprising and this characteristic has been widely discussed in the literature. It is not intended that the reader should infer that the FEC is proposed as an improvement over the quite sufficient ORT closure, where the accuracy to the third decimal place observed by the ORT closure is considered quite acceptable in injection molding predictions (see e.g., Chung, D.H. & Kwon (2002)), but the FEC serves as a starting point for the development of a new class of closures for fiber systems with colliding particles which add a diffusion term to equation (1.2) (see e.g., Montgomery-Smith, S.J. *et al.* 2010a, for a listing of existing diffusion models). For
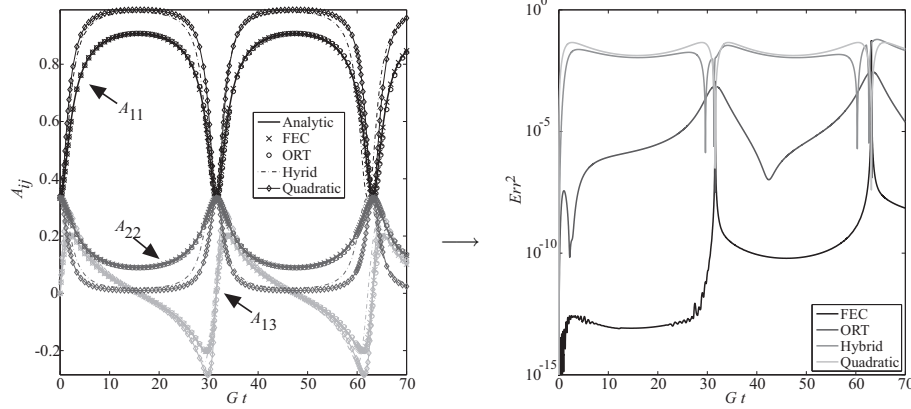
FIGURE 2. Plot of A_{11} for Simple Shear flow with $\lambda = 0.98$ from various closures along with the associated error Err.

the industrially applicable case of concentrated suspensions of fibers, extensions to the FEC have been performed by the authors in Montgomery-Smith, S.J. *et al.* (2010*b*) for Jeffery's equation with rotary diffusion.

The authors have performed similar studies for flows beyond pure shear, and the results and conclusions for virtually all flows are identical to those from simple shear. It is expected that flows with repeated eigenvalues (i.e., orientations occurring on the boundaries of the eigenspace triangle containing all physically possible orientations discussed in Cintra, J. S. & Tucker (1995)) would cause problems due to the numerical approximation that must be made in equations (4.1) or (4.2). But for flows that have some non-zero shear coupled with elongation, as would be expected in virtually all industrial flows, the FEC and the ORT closure both perform quite well and the aforementioned conclusions for the accuracy and stability for pure shear were equivalent for all flows investigated with mixed shearing and uniaxial elongation. The primary difference between the pure shear flow and the shear-elongation flows is the absence of any periodic behavior due to the elongation, and thus the numerical issues in the ODE solution are greatly diminished as $t \to \infty$. It is noted that coupled flows with shearing and biaxial elongation were also performed, and for cases when biaxial elongation dominated the flow, numerical instabilities were observed in the FEC since $a_1 \simeq a_2$ remains true throughout the entire flow history. This case is worthwhile to recognize, but is not of a significant concern as this orientation state will rarely, if ever, occur in actual industrial processes.

6. Conclusion

In this paper, we have presented an exact closure, which was at least in part, understood by previous authors. We have found that an analysis of the formulae gives rise to the Fast Exact Closure (FEC), which exactly solves Jeffery's equation in a fast manner for any orientation that at one point in time was isotropic. This work demonstrates that the observations by previous authors were correct that solutions of the Jeffery equation must exist. The FEC closure presents a systematic approach to solve the Jeffery's equation while simultaneously solving a related differential equation, thus avoiding both the cumbersome elliptic integral evaluation and the necessity for a closure of a higher order moment tensor. It is noted that industrial simulations often add in a term like $C_I \|\Gamma\|(2I - 6A)$ to equation (1.4), and then presume that the closure that creates $\mathbb{A}$ from A is still valid. However, to add diffusion terms to the FEC method will require

adding a similar term to equation (2.4), or perhaps some other approach. For the work which explores industrial approximations to versions of Jeffery's equation with diffusion terms added, for example, the Folgar-Tucker equation Folgar, F.P. & Tucker (1984), the interested reader is directed toward Montgomery-Smith, S.J. *et al.* (2010*b*).

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