Gauge conditions on the "square root" of the conformation tensor in rheological models

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\textbf{A B S T R A C T}

Symmetric positive-definite conformation-tensors are ubiquitous in models of viscoelasticity. In this paper, the multiplicative decomposition of the conformation tensor is revisited. The nonuniqueness in this decomposition is exploited (i) to ensure stationarity of the decomposed dynamics whenever the conformation tensor is stationary, and (ii) to impose gauge conditions (cf. symmetric square root, or Cholesky decomposition) in the dynamics, for both deterministic and stochastic settings. The general procedure developed in this paper is exemplified on the upper-convected Maxwell model, and a (typically) increased numerical accuracy of the modified dynamics is found.

1. Introduction

A large class of models for viscoelastic fluids is formulated in terms of the (dimensionless) conformation tensor $c$, with an evolution equation for $c$ and a constitutive relation for the stress tensor in terms of $c$. Examples for such models are the upper-convected Maxwell model, the FENE-P model, the Giesekus model, and the Oldroyd-A/B models. In [1–3], it has been proposed to use a multiplicative decomposition

\begin{equation}
    c = b \cdot b^T,
\end{equation}

for reformulating such rheological models in terms of the quantity $b$.

The decomposition (1) is not unique, there being two levels of nonuniqueness. The first level concerns the dimensionality of $b$. If $c$ is a $3 \times 3$-tensuror, as is assumed throughout this entire paper, $b$ is $3 \times N$ with $N \geq 3$ in general. Expressing the decomposition (1) in terms of the column vectors of $b$, $b_i$ ($i = 1, \ldots, N$), one finds,

\begin{equation}
    c = \sum_{i=1}^{N} b_i b_i^T.
\end{equation}

In this form, one recognizes the close analogy of (1) with the microscopic definition of the conformation tensor as the average of the dyadic product $r_i r_i^T$ of the, appropriately scaled, end-to-end (or segment) vector $r_i$ of a chain, by using $b_i = r_i / \sqrt{N}$. Correspondingly, $N$ is the number of vectors in the ensemble. Searching for a set $b_i$ to represent a certain conformation tensor $c$, the condition $N \geq 3$ reflects the fact that generally the rank of the conformation tensor is equal to three; $N = 3$ is sufficient if the column vectors $b_i$ are linearly independent. The second level of nonuniqueness of the decomposition (1) reflects that an arbitrary orthogonal transformation multiplied to the right of $b$ leaves $c$ unchanged. In this paper, the focus is on the case $N = 3$ and the invariance of the decomposition (1) with respect to orthogonal transformations.

Several concrete decompositions of the form (1) have been proposed in the literature. For example, Vaithianathan and Collins [1] have used the Cholesky decomposition, i.e. $b$ being lower triangular, to ensure the positive definiteness of the conformation tensor in turbulent-flow calculations. Balci et al. [2] have employed the symmetric square root, which proved to be advantageous for accuracy and stability in comparison to $c$-based formulations [2,4] and which has been used e.g. for stress-diffusion analysis in creeping viscoelastic flow [5] and studies on turbulent drag reduction [6]. Hütter et al. [3] have employed an interpretation in which the kinematics of $b$ is identical to that of the deformation gradient in solid mechanics, i.e. the column vectors of $b$ display contravariant deformation behavior; $b$ has therefore been called the "contravariant deformation". It has been shown that this formulation has increased numerical stability in contrast to the $c$-formulation, comparable to the log-$c$-formulation [7]. The existence of these three choices for $b$ (using the Cholesky decomposition, symmetry, and contravariance, respectively) is a manifestation of the second-level nonuniqueness discussed above. In other words, these choices differ in the way the nonuniqueness has been eliminated by choosing a corresponding orthogonal transformation on the right-hand side (r.h.s.) of $b$.

While the contravariant formulation [3] has a more direct relation to the microstructure as compared to the Cholesky decomposition [1] and the symmetric square root [2], it suffers from spurious rotations. Particularly, it has been observed [7] that e.g. under imposed

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shear-deformation the contravariant deformation \( b \) keeps rotating while the
conformation tensor \( c \) reaches a stationary state. This complicates
steady-state and perturbation analyses and also it could lessen the gain
in numerical stability and/or accuracy.

The goal of this paper is twofold. On the one hand, the evolution
equation for the contravariant deformation \( b \) introduced in [3] shall be
amended in such a way that the spurious \( b \)-rotations in situations of sta-
tionary \( c \)-states are eliminated. On the other hand, a general procedure
shall be presented for eliminating the nonuniqueness in the decompo-
sition (1) according to certain gauge conditions, by appropriate modifi-
cation of the \( b \)-dynamics, even in the presence of fluctuations. It will be
discussed how these two tasks are closely related.

This paper is organized as follows. In Section 2, the nonuniqueness
in the decomposition (1) is examined from the viewpoint of evolution
equations, which will highlight the importance of the infinitesimal gen-
erators of orthogonal transformations (Lie algebra) in the dynamics of
\( b \); this will be called the differential approach. Section 3 puts empha-
sis on the nonuniqueness of the decomposition (1) and the orthogonal
transformation (Lie group) on the r.h.s. of \( b \) itself; this will be called
the integral approach. The lessons learned in these two sections will be
illustrated with numerical calculations of the upper-convected Maxwell
model in Section 4. Finally, the paper ends with a discussion and con-
clusions, Section 5.

The following notation will be used in this paper, for clarity and con-
ciseness. Vectors and second-order quantities are denoted by bold-face
symbols, while fourth-order quantities are bold face with a superscript
“\( (4) \)”. The inner product is denoted by \( [A \cdot B]_{ij} = \sum A_{ij}B_{jk} \), while \( A \circ
B = \sum A_{ij}B_{ij} \) (note the order of indices), \( [A^{(4)} \circ B]_{ijkl} = \sum_{ij} A^{(4)}_{ijkl}B_{ijkl} \), and
\( [A^{(4)} \circ B^{(4)}]_{ijkl} = \sum_{ijkl} A^{(4)}_{ijmn}B^{(4)}_{ijkl} \). While a superscript “\( T \)” denotes
the regular matrix-transpose for a second-rank quantity, the transpose
of a fourth-order quantity is defined by \( [A^{(4)\cdot T}]_{ijkl} = A^{(4)_{ijkl}} \). Beyond the
inner products defined above, summations are indicated by \( \Sigma \) (i.e. no
Einstein summation convention is used), and the summation indices run
from 1 to 3, unless indicated otherwise.

2. Differential approach

Typical single-mode conformation tensor models can be written in the
form
\[
\dot{c} = \kappa \cdot c + c \cdot \kappa^T + \Gamma(c),
\]  
(3)
where \( \kappa \) denotes the material (substantial) time-derivative, \( \kappa = (\text{Vr}))^T \)
the transpose of the gradient of the velocity field \( \text{Vr} \) and \( \Gamma(c) \) is the
conformation-dependent relaxation. For the Maxwell model, \( \Gamma = -(c-1)/\tau \)
with relaxation time \( \tau \). The form (3) represents upper-convected,
also known as contravariant converted, behavior for an unconstrained
tensor. However, the procedure described in this paper transvers
easily to a much wider class of models, knowing that the inverse of an
upper-convected tensor is lower-convected, and that an unconstrained
tensor can be used as an auxiliary quantity for deriving the dynamics of
constrained tensors, e.g. constraints on the trace (via \( c^t = c/\text{tr}(c) \) or the
determinant (via \( c^t = c/\sqrt{\text{det}(c)} \)).

For a reformulation of \( c \)-based models in terms of \( b \), one searches for
a dynamics of \( b \) which, by way of the chain rule,
\[
\dot{c} = b \cdot b^T + b \cdot b^\cdot T,
\]  
(4)
reproduces the dynamics of \( c \) (3).

Inspired by the kinematics of affine deformation and the analogy to
solid mechanics, it has been proposed [3] to choose \( \kappa \cdot b \) for the effect
of imposed deformation on the dynamics of \( b \), i.e.
\[
b = \kappa \cdot b + X,
\]  
(5)
with a yet unknown quantity \( X \). Compatibility of (5) with (3) requires
\[
X \cdot b^T + b \cdot X^T = \Gamma(c),
\]  
(6)
where relation (1) has been used. This condition can be simplified by
writing
\[
X = \frac{1}{2} \Gamma(c) \cdot b^T - 1 + Y,
\]  
(7)
which casts the compatibility between (3) and (5) into the requirement
that \( Y \cdot b^T \) must be anti-symmetric. In other words, the evolution equa-
tion for \( b \) can be written in the form
\[
b = b^T + b^T \cdot b \cdot A,
\]  
(8)
with \( A \) being anti-symmetric, and where the abbreviations
\[
b^T = \kappa \cdot c,
\]  
(9)
\[
b^T = \frac{1}{2} \Gamma(c) \cdot b^T - 1,
\]  
(10)
have been introduced for later convenience, in order to denote the con-
tributions to the dynamics associated to imposed deformation (d) and
relaxation (r), respectively. The quantity \( A \) has been put to the right of \( b \),
representative of generating an orthogonal transformation on the r.h.s.
of \( b \), in line with the discussion in Section 1. The possibility to include
terms as the third contribution to the r.h.s. of (8) in the dynamics of \( b \) is
the basis not only of this paper, but also of the work of Balci et al. [2].

With a suitable choice of \( A \) one can try to avoid the spurious oscill-
lations of \( b \) for situations in which \( c \) is stationary. Multiplying (8) from the
right with \( b^T \) for stationary \( b \), one obtains
\[
0 = \kappa \cdot c + \frac{1}{2} \Gamma(c) + b \cdot A \cdot b^T.
\]  
(11)
Notably, the symmetric contribution to (11) is equal to the stationarity
condition for \( c \), see (3). In contrast, the anti-symmetric contribution to
(11) gives rise to
\[
b \cdot A \cdot b^T = \frac{1}{2} (\kappa \cdot c - c \cdot \kappa^T).
\]  
(12)
This relation can be interpreted in two distinct ways. On the one hand,
one can interpret it as a definition for \( A \) to make \( b \) stationary if \( c \) is sta-
tionary; since \( c \) is positive definite, the inverse of \( b \) exists, and (12)
can be used to determine \( A \). On the other hand, (12) can be interpreted as
a condition which must be fulfilled in stationary states by a more gen-
eral expression \( A = A(b) \). Beyond stationary states, \( A = A(b) \) might not
fulfill (12), but that is also not necessarily a problem, if the goal is to
specifically cancel the non-stationarity in \( b \) if \( c \) is stationary. It is note-
worthy that, in stationary states, the structure of (11), (12) is such that
for any solution \( b \) also \( b \cdot Q = 0 \) is a solution, with an arbitrary orthogonal
transformation \( Q \). In other words, there is an entire family of solutions
\( b \) to (11) and (12), specific choices for which will be discussed in the
following section.

3. Integral approach

3.1. Some specific gauges

In this section, the starting point for discussing the non-uniqueness
in the multiplicative decomposition (1) is the properties of the quantity
\( b \) itself, rather than its dynamics as was considered in Section 2. Since
the conformation tensor \( c \) is symmetric and positive definite, it can al-
ways be diagonalized in a proper coordinate system. If \( R \) denotes an
appropriate orthogonal transformation, one can write
\[
c = R \cdot c_{\text{diag}} \cdot R^T,
\]  
(13)
with
\[
c_{\text{diag}} = \sum \lambda_i \vec{b}_i^T \vec{b}_i^T,
\]  
(14)
\[
c_{\text{diag}} = \sum \lambda_i \vec{X}_i \vec{X}_i^T.
\]  
(15)
where \( \lambda_i \) denote the eigenvalues of \( \mathbf{c} \), and \( \hat{e}_i \) and \( \hat{x}_i \) are the (right-handed) sets of eigenvectors and orthonormal basis vectors in Cartesian space, respectively. It is noted for later convenience, that \( \hat{e}_i \) are the column vectors of \( \mathbf{R} \), since \( \hat{e}_i = \mathbf{R} \cdot \hat{x}_i \). Departing from the form (13) of the conformation tensor \( \mathbf{c} \), the most general form of \( \mathbf{b} \) can be written as

\[
\mathbf{b} = \mathbf{R} \cdot \sqrt{\mathbf{c}_{\text{diag}}} \cdot \mathbf{Q},
\]

where the specific choice for the orthogonal transformation \( \mathbf{Q} \) fixes the gauge, i.e. determines the specific properties of \( \mathbf{b} \). Particular choices are the following:

- **Require \( \mathbf{b} \) to be symmetric:**
  \[
  \mathbf{Q} = \mathbf{R}^T.
  \]

- **Orthogonal column-vectors:** Using
  \[
  \mathbf{Q} = \mathbf{I},
  \]

in (16), the column vectors of \( \mathbf{b} \) are equal to \( \sqrt{\mathbf{c}} \hat{e}_i \). This means that the eigenvalues and eigenvectors can be obtained readily, without the need for diagonalization of \( \mathbf{c} \). Since the column vectors of \( \mathbf{b} \) are orthogonal to each other but not normalized, this will be called the orthogonal gauge.

- **Cholesky decomposition:**
  \[
  \mathbf{c} = \mathbf{L} \cdot \mathbf{L}^T,
  \]

with \( \mathbf{L} \) a lower-triangular matrix.

It is noted that all three gauges (17)–(19) eliminate the spurious rotations in \( \mathbf{b} \) for stationary \( \mathbf{c} \), which can be seen as follows. While \( \mathbf{b} \) is in the most general case nine degrees of freedom, imposing one of the gauges (17)–(19) reduces the number of degrees of freedom to six, which is in line with the conformation tensor itself. Therefore, if \( \mathbf{c} \) is stationary, also \( \mathbf{b} \) must be stationary when using one of the above three gauges (17)–(19).

### 3.2. Gauges in deterministic dynamics

The gauge freedom is eliminated by imposing certain conditions on \( \mathbf{b} \), e.g. conditions related to (17)–(19). In the sequel, it is assumed that in general the conditions on \( \mathbf{b} \) are of the form

\[
\mathbf{g}_n(\mathbf{b}) = 0, \quad n = 1, 2, 3.
\]

Notably, in the case of a three-dimensional formulation, three conditions are needed to determine the orthogonal transformation \( \mathbf{Q} \) in (16) and the antisymmetric \( \mathbf{A} \) in the equation Eq. (8) uniquely. If the initial condition for \( \mathbf{b} \) is compatible with the gauge of interest, the conditions for respecting the gauge conditions (20) in the course of time are

\[
\mathbf{g}_n = \frac{\partial \mathbf{g}_n}{\partial \mathbf{b}} \circ \mathbf{b} = 0,
\]

where it has been assumed that the constraints \( \mathbf{g}_n \) do not depend on time explicitly.

The two contributions to the evolution equation of \( \mathbf{b} \), imposed deformation (d) and relaxation (r), enter both the evolution of \( \mathbf{c} \) (4) and the gauge conditions (21) additively. Therefore, they are discussed separately in the sequel. Following Section 2, adding a term of the form \( \mathbf{b} \cdot \mathbf{A} \) to the dynamics of \( \mathbf{b} \), see (8), leaves the dynamics of \( \mathbf{c} \) invariant. For each of the two contributions to the dynamics, \( \mathbf{c} \in \{d, r\} \), the corresponding contribution to \( \mathbf{A} \) in the transformation

\[
\dot{\mathbf{b}}^c = \mathbf{b}^c + \mathbf{A}^c, \quad c \in \{d, r\},
\]

is determined by making use of the gauge conditions (21),

\[
\frac{\partial \mathbf{g}_n}{\partial \mathbf{b}} \circ \left( \mathbf{b}^n + \mathbf{A}^c \right) = 0, \quad n = 1, 2, 3, \ c \in \{d, r\}.
\]

Due to the differential formulation, the quantity \( \mathbf{A}^c \) must be a homogeneous function of degree unity in \( \mathbf{b}^c \).

\[
\mathbf{A}^c = \mathbf{A}^{(d)}(\mathbf{b})^c
\]

where \( \mathbf{A}^{(d)} \) does not depend on the specific contribution (c) considered. Inserting (24) into the gauge condition (23), and requiring that the latter is valid for any \( \mathbf{b}^c \), the gauge conditions become

\[
\frac{\partial \mathbf{g}_n}{\partial \mathbf{b}} \circ \left( \mathbf{b}^n + \mathbf{A}^{(d)} \right) = 0, \quad n = 1, 2, 3,
\]

with \( \mathbf{1}^{(d)}_{ij} = \delta_{ij} \). Due to the anti-symmetry of \( \mathbf{A}^c \), it can be represented as a linear combination of the three generators of orthogonal transformations,

\[
\mathbf{A}_i = -\sum_{jk} \epsilon_{ijk} \hat{\mathbf{x}}_j \hat{\mathbf{x}}_k^T, \quad i = 1, 2, 3,
\]

which satisfy \( \mathbf{A} \circ \mathbf{A} = 2 \delta_{ij} \), as well as \( [\mathbf{A}_i, \mathbf{A}_j] = \sum_{k} \epsilon_{ijk} \mathbf{A}_k \). Therefore, \( \mathbf{A}^c \) can be represented uniquely as \( \mathbf{A}^c = \sum c_i^2 \mathbf{A}_i \), with coefficients \( c_i^2 \) determined uniquely by \( \mathbf{A}^r \). According to (24), the coefficients \( c_i^2 \) must be homogeneous functions of degree unity in \( \mathbf{b}^c \), which implies the form

\[
\mathbf{A}^{(d)} = \sum_i c_i \mathbf{A}_i.
\]

The matrices \( a_i \) need to be determined on the basis of the gauge conditions (25), whereby the gauge conditions get encoded in the evolution equations for \( \mathbf{b} \), (8), in terms of this gauge-specific choice of \( \mathbf{A} \).

### 3.3. Gauges in stochastic dynamics

If the number of polymer chains (or chain segments) \( N \) contained in a certain control volume is small (\( N \leq \mathcal{O}(10^3) \)), the conformation tensor (2) will display statistical fluctuations. Particularly, it can be shown that, if each of the \( N \) chain vectors \( \mathbf{r}_1 \) fluctuates with a characteristic magnitude, the resulting fluctuations in \( \mathbf{b} \) can be expressed in a form that uses only three (representative, i.e. linearly independent) chain vectors, with their fluctuations being scaled by the factor \( 1/\sqrt{N} \). In other words, one can choose \( \mathbf{b} \) in the decomposition (1) to be a \( 3 \times 3 \)-matrix, where the fluctuations on its column vectors are the fluctuations of typical chain vectors multiplied by \( 1/\sqrt{N} \).

In contrast to ordinary differential equations discussed in Section 3.3, stochastic differential equations (SDE) have been employed to include the effects of thermal fluctuations [3]. The SDE describing the evolution of \( \mathbf{b} \) is of incremental form \( \text{d} \mathbf{b} = \ldots \) with four contributions corresponding to imposed deformation (\( \text{d}^d \mathbf{b} \)), relaxation (\( \text{d}^r \mathbf{b} \)), thermal drift (\( \text{d}^\theta \mathbf{b} \)) related to the fluctuations, and fluctuations (\( \text{d}^f \mathbf{b} \)). An example of an SDE for \( \mathbf{b} \) is the upper-convedted Maxwell model with thermal fluctuations [3], for which the material (substantial) increment [3] is, using the Itô interpretation of stochastic calculus [8,9] (here and throughout the entire paper),

\[
\text{d} \mathbf{b} = \mathbf{x} \cdot \text{d} \mathbf{B} - \frac{1}{2\tau} (\mathbf{b} - \mathbf{b}^{-1,T}) \text{d}t + \frac{\Theta}{2\tau} (\mathbf{b}^{-1,T} \text{d}t + \sqrt{\frac{2\tau}{\tau}} \text{dW}_t),
\]

with \( \Theta \) the strength of the thermal fluctuations, and \( \text{dW}_t \) the increments of uncorrelated Wiener processes representative of white noise,

\[
\langle \text{dW}_t \rangle = 0,
\]

\[
\langle \text{dW}_t, dW_r \rangle = \delta(t-t') \text{d}t \text{d}t' \mathbf{1}^{(d)}.
\]

Specifically for the Maxwell model, the strength of thermal fluctuations can be written as \( \Theta = 1/N \), where \( N \) denotes the number of end-to-end (or segment) vectors in the control volume [3]. Therefore, the last term on the r.h.s. of (28) reflects what has been discussed in the beginning of
this section. It is mentioned that also the deformation-related contribution to \(28\), \(\delta^2 b\), and the corresponding term in (5), can be explained directly based on the kinematics of vectors [3].

Upon including stochastic dynamics as described just above, the treatment for the deterministic case discussed earlier in this paper requires two main modifications. Namely, the compatibility of dynamics (4) and the gauge conditions (21) are replaced by, using Itô’s calculus [8,9],

\[
dc = \langle db \cdot d\bar{T} + b \cdot db \\ d db \rangle + \left( \langle d b \cdot d b \rangle \right)_{\text{Itô}},
\]

(31)

\[
dgab = \frac{\partial g_{ab}}{\partial b} \otimes db + \frac{1}{2} \left( \partial^2 g_{ab} \otimes db \otimes db \right)_{\text{Itô}} = 0,
\]

(32)

where \([\ldots]_{\text{Itô}}\) implies that in \(db\) only terms involving the Wiener increments, \(\delta b\), are kept and subsequently reduced to zero (see Table 3.1 in [9]).

\[
dW_r/dW_r \rightarrow d1^{(4)}. \]

(33)

In contrast, the first two terms on the r.h.s. of (31) and the first term on the r.h.s. of (32) contain all four contributions (\(d, r, t, f\)) to the dynamics.

The three deterministic contributions, imposed deformation (\(d\)), relaxation (\(r\)), and thermal drift (\(t\)), do not enter the second-order Itô contributions in the dynamics of \(c\) (31) and in the gauge conditions (32). Therefore, they can be treated analogously to the deterministic case in Section 3.2, by replacing (22) by the corresponding transformation of the increments,

\[
d'c = d^2 c + b \cdot dA^c; \quad c \in \{d, r, t, r\}. \tag{34}
\]

The relation (24) for the deterministic case must be replaced by \(dA^c = \bar{A}^{(4)} \otimes d^2 b\), where \(\bar{A}^{(4)}\) is again given by the gauge conditions (25).

For the fluctuating contribution to the \(b\)-dynamics, \(d^2 b\), the situation is a little more involved, because a transformation analogous to (34) enters also the second-order Itô contributions in the dynamics of \(c\) (31) and in the gauge conditions (32). A procedure simply analogous to the one described above for the three deterministic contributions will thus not work. Instead, the adaptation of (34) to fluctuations is

\[
d'c = (d^2 b \cdot b \cdot dA^c) + (dC^{(4)} + b \cdot dA^{(4)}), \tag{35}
\]

where the anti-symmetric \(dA^{(4)}\) is a fluctuating term to ensure compatibility of the fluctuations with the gauge of interest, while \(dC^{(4)}\) and \(dA^{(4)}\) are deterministic. The contributions to the \(c\)-evolution arising from \(dA^{(4)}\) by way of the third term on the r.h.s. of (31) are to be compensated by \(dC^{(4)}\) in order to leave the \(c\)-dynamics invariant, while the anti-symmetric \(dA^{(4)}\) must be chosen in such a way that the \(dC^{(4)}\) contribution is compatible with the gauge of interest. The details of determining \(dA^{(4)}\), \(dC^{(4)}\), and \(dA^{(4)}\) are described in Appendix A.

Similar to the deterministic case, also in the stochastic case the quantities \(\tilde{a}\) play the key role for encoding the gauge conditions in the evolution equation for \(b\), as will be discussed on the bases of the examples in Section 3.4.

### 3.4. Examples

In the sequel, the three gauges (17)–(19) are discussed. According to Section 3.2.3, and Appendix A, the main ingredients are the first- and second-order derivatives of the gauge conditions \(g_{ab}\) and the explicit expressions for the quantities \(\tilde{a}\). Note that the second-order derivative of \(g_{ab}\) is only required when dealing with fluctuations, i.e., in the context of SDEs, see Section 3.3 and Appendix A.

**Example 1** Symmetric gauge, (17). The requirement for symmetry of \(b\) is represented by the conditions

\[
g_{ab}(b) = A_{ab} \otimes b = 0, \quad n = 1, 2, 3, \tag{36}
\]

with first- and second-order partial derivatives

\[
\frac{\partial g_{ab}}{\partial b} = A_{a}, \tag{37}
\]

\[
\frac{\partial^2 g_{ab}}{\partial b \partial b} = 0. \tag{38}
\]

The fact that the second-order derivative vanishes implies that (see Appendix A, (A.5)) \(\partial A^{(4)}\) can be determined along the same lines as all other anti-symmetric contributions, i.e., \(dA^{(4)} = A^{(4)} \otimes dC^{(4)}, \) with \(A^{(4)}\) given by (27).

Inserting the derivative (37) and the form (27) for \(A^{(4)}\) into the gauge condition (25), and using the identity \(A_{ij} \cdot A_{i} = \hat{x}_{ij} \hat{x}_{ij} - \delta_{ij} I\), the gauge conditions become

\[
A_{a} - \sum_{j}[b^{(j)} - tr(b)1]_{a_{j}} \tilde{a}_{j} = 0, \tag{39}
\]

where \(b^{(j)}\) will be used in the sequel, in view of the gauge condition. The inverse of the matrix \(b - tr(b)1\) exists\(^1\) and can be calculated analytically.\(^2\) Based on (39), the expressions for \(\tilde{a}_{j}\) are thus given by

\[
\tilde{a}_{j} = \sum_{j}([b - tr(b)1]^{-1})_{a_{j}j}. \tag{40}
\]

The bracket-expression in (40) plays the key role also in the treatment of Balci et al.[2], where the symmetric gauge has been derived for the first time, in the absence of fluctuations.

For all models studied in [3], the relaxation \((r)\) and thermal drift \((t)\) contributions to the dynamics are linear combinations of terms of the form \(c^{(e)} \cdot b^{(1-T)}\). This latter expression is obviously symmetric, if \(b\) itself is symmetric. Since \(\tilde{a}\) are linear combinations of the anti-symmetric generators of orthogonal transformations \(A_{a}\), one finds that these two contributions to the dynamics automatically preserve the gauge (17).

**Example 2** Orthogonal gauge, (18). Orthogonality of the column vectors of \(b, b_{i} = \hat{x}_{ij} \cdot \hat{x}_{ji} \) \((i = 1, 2, 3)\), is expressed by the gauge conditions

\[
g_{ab}(b) = b_{i} \cdot b_{j} = \delta_{ij}, \quad n \notin \{i, j\} \text{ and } i < j. \tag{41}
\]

i.e., \(b^{T} \cdot b = e_{\text{diag}}\). The first- and second-order partial derivatives of the conditions (41) are given by

\[
\frac{\partial g_{ab}}{\partial b} = b_{i} \hat{x}_{ijn} + b_{j} \hat{x}_{ijn}, \tag{42}
\]

\[
\frac{\partial^2 g_{ab}}{\partial b \partial b} = [\hat{x}_{ij} \hat{x}_{jn} + \hat{x}_{in} \hat{x}_{jn}]_{\text{1=2}}, \tag{43}
\]

where the subscript \(1=2\) indicates that the first and second indices must be interchanged.

Inserting the derivative (42) and the form (27) for \(A^{(4)}\) into the gauge condition (25), and using the explicit form (26) for \(A_{a}\), as well as (41), one obtains

\[
\tilde{a}_{j} = \frac{1}{\lambda_{kj}} \frac{1}{\lambda_{kj} - \lambda_{ij}} b_{i} \hat{x}_{ijn} + b_{j} \hat{x}_{ijn}, \quad i \notin \{k, l\} \text{ and } k < l. \tag{44}
\]

As mentioned earlier, the typical building blocks of the relaxation and thermal drift contributions to the dynamics are \(c^{(e)} \cdot b^{(1-T)}\) [3], which can be written as \(b^{(1-T)} \cdot c_{\text{diag}}^{(e)}\) by virtue of the decomposition (3) and with

\(^{1}\) With \(b = R \cdot e_{\text{diag}} \cdot R^{T}\), one finds \(b - tr(b)1 = R \cdot [\sqrt{e_{\text{diag}}} - tr(\sqrt{e_{\text{diag}}})]1 \cdot R^{T}\), where the matrix in the bracket is diagonal and has as its ii-element \(-\sum_{i} \sqrt{e_{i}}\), which is negative definite for positive \(c\).

\(^{2}\) For example, using the Cayley–Hoffman theorem [10], \(b^{2} - I, b^{2} + I, b - I, 1 = 0 \) with \(I = tr(b), I_{2} = I/(I_{2} - tr(b^{2})), \) and \(I_{3} = det b, \) one finds: \((b - I, 1)^{T} = (b^{2} + I_{2} 1)/(I_{2} - I_{1} I_{2}).\)
The gauge having Appendix references correction Fig. end, Fig. 1. Maxwell model (28) without fluctuations (θ = 0) and without corrections: \(b_{xy} (\square, \text{black}), b_{yx} (\blacklozenge, \text{red}), b_{yy} (\blacklozenge, \text{green}), b_{yx} (\bullet, \text{blue})\). Time step: \(\Delta t/\tau = 10^{-3}\). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

\[
\mathbf{b}^T \cdot \mathbf{c} = c_{\text{diag}}. \quad \text{This implies, using (24) with (27) and (44), that these two contributions to the dynamics automatically preserve the gauge (18).}
\]

In view of the expressions (44), the practical implementation of the orthogonal gauge requires care in situations where some of the eigenvalues of \(\mathbf{c}\) become nearly equal. A corresponding example is studied in Appendix B.

**Example 3** Cholesky-decomposition gauge, (19). The conditions for having \(\mathbf{b}\) in lower-triangular form are

\[
g_n(\mathbf{b}) = \mathbf{x}_j^T \cdot \mathbf{b} \cdot \mathbf{x}_j = 0, \quad n \notin \{i, j\} \text{ and } i < j, \quad (45)
\]

with first- and second-order partial derivatives

\[
\frac{\partial g_n}{\partial \mathbf{b}} = \mathbf{x}_j, \quad \frac{\partial^2 g_n}{\partial \mathbf{b} \partial \mathbf{b}} = \mathbf{0}. \quad (46)
\]

The fact that the second-order derivative vanishes implies \(d \mathcal{A}^{(\ell)} = \mathcal{A}^{(\ell)} \odot d \mathcal{C}^{(\ell)}\), in analogy to the case of gauge (17).

Fig. 2. Maxwell model without fluctuations (θ = 0) and with the differential correction defined by using (12) as a definition: \(b_{xy} (\square, \text{black}), b_{yx} (\blacklozenge, \text{red}), b_{yy} (\blacklozenge, \text{green}), b_{yx} (\bullet, \text{blue})\). Time step: \(\Delta t/\tau = 10^{-3}\). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Inserting the derivative (46) and the form (27) for \(\mathcal{A}^{(\ell)}\) into the gauge condition (25), and making use of the lower triangularity of \(\mathbf{b}\), the solution for \(\mathbf{a}\) can be written in the form

\[
\mathbf{a}_1 = -\frac{b_{11} b_{22}^{-1}}{b_{11} b_{22} \mathbf{x}_j} \tilde{x}_j^2 + \frac{\mathbf{1} b_{22}^{-1}}{b_{22} \mathbf{x}_j} \tilde{x}_j^2, \quad (48)
\]

\[
\mathbf{a}_2 = -\frac{1}{b_{11}} \mathbf{x}_j \tilde{x}_j^2, \quad (49)
\]

\[
\mathbf{a}_3 = \frac{1}{b_{11}} \mathbf{x}_j \tilde{x}_j^2. \quad (50)
\]

Contrary to the other two gauges (17) and (18), the gauge (19) for the lower triangularity of \(\mathbf{b}\) is not automatically respected by the relaxation and thermal drift contributions to the dynamics. Particularly, as an example consider a contribution to the \(\mathbf{b}\)-dynamics of the form \(b_{11}^{-1} \mathbf{x}_j \tilde{x}_j^2\) (e.g. see (28)), for which \(\mathbf{a}_1 \odot b_{11}^{-1} \mathbf{x}_j \tilde{x}_j^2 \neq 0\) in general.

4. **Numerical calculations for the upper-convected Maxwell model**

For illustration purposes, the three gauges (17)–(19) discussed above are applied to the \(\mathbf{b}\)-formulation of the upper-convected Maxwell model (28) with relaxation time \(\tau\), for start-up simple-shear flow, \(\mathbf{s} = \mathbf{i} \mathbf{x}_j \mathbf{x}_j^2\).
with constant shear-rate $\dot{\gamma}$ for $t \geq 0$. If fluctuations are included in the Maxwell model, $\Theta > 0$, one finds $2k_B\mathbf{M}^{(\Theta)} = (\Theta/\tau)\mathbf{I}^{(\Theta)}$ (see [3] for details). For the numerical calculations, explicit expressions for the fluctuation-related contributions in terms of $\Delta t$ are given in Appendix A.

For all simulations except gauge (18), the initial condition is

$$b(t = 0) = \sqrt{c_{eq}}\mathbf{1}. \quad (51)$$

with $c_{eq} = 1 + 4\Theta$. In contrast, for gauge (18) the initial condition used is given by the solution derived in Appendix B, i.e. (B.3) with (B.6), for $\gamma = 10^{-2}$ and $\phi = (\gamma + \pi)/4$, multiplied by $\sqrt{c_{eq}}$. For this initial condition, the cosine of the angles between the column vectors of $\mathbf{b}$ is smaller than $10^{-9}$, thus respecting the condition for the gauge (18) quite accurately. The time steps are used in the respective figure captions. For the simulations of gauge (18), an adaptive time step has been used of the form $\Delta t/\tau = \xi[\Delta t/\tau]_0$ with constant $[\Delta t/\tau]_0$ and a scaling factor $\xi$ that depends on the actual state of the system,

$$\xi = \min(1,|\lambda_4 - \lambda_5|,|\lambda_4 - \lambda_6|,|\lambda_2 - \lambda_3|)^{n/4}. \quad (52)$$

with $n = 1$ for $\Theta = 0$, and $n = 3$ for $\Theta > 0$. For solving the evolution equation for $\mathbf{b}$ numerically, the Euler scheme is used.

In order to assess how well the gauge conditions are respected in the actual numerical simulations, the following quantities are introduced:

- Symmetric gauge, (17): Defining $b_\Lambda = (\mathbf{b} - \mathbf{b}^T)/2$,

$$\epsilon_s = \frac{\text{tr}(b_\Lambda \cdot b_\Lambda^T)}{\text{tr}(\mathbf{b} \cdot \mathbf{b}^T)}. \quad (53)$$

- Orthogonal gauge, (18): Defining $\cos \theta_{ij} = b_{ij}^T \cdot b_i / (\|b_i\|\|b_j\|)$,

$$\epsilon_\perp = \sqrt{\frac{1}{3}\left(\cos \theta_{12}\right)^2 + \left(\cos \theta_{13}\right)^2 + \left(\cos \theta_{23}\right)^2}. \quad (54)$$

- Cholesky-decomposition gauge, (19):

$$\epsilon_L = \frac{\sum_{i,j,k} b_{ij}^2}{\text{tr}(\mathbf{b} \cdot \mathbf{b}^T)}. \quad (55)$$

The quantities (53)–(55) are defined in such a way that they equal zero if the respective gauge-condition is satisfied exactly, and in the numerical calculations they should be orders of magnitude smaller than unity.

For the deformation considered in this numerical case study, the analytical solution for the conformation tensor in the absence of thermal
fluctuations \((\Theta = 0)\) is known,
\[
c_e = 1 + \text{Wi} \left( 1 - e^{-\tau} \right) \left( \dot{x}_1 \dot{x}_2 \tau + \ddot{x}_1 \right) \\
+ 2 \text{Wi}^2 \left( 1 - e^{-\tau} - \tau e^{-\tau} \right) \dot{x}_1 \dot{x}_2 \tau,
\]
with dimensionless time \(\tilde{t} = t/\tau\). This result is used to quantify the relative error of the numerical solution with respect to the analytical solution in terms of
\[
\varepsilon_{\text{rel}} = \sqrt{\frac{\sum_c \left[ \varepsilon(t_i) - c_e(t_i) \right] \otimes \left[ \varepsilon(t_i) - c_e(t_i) \right]}{\sum_c c_e(t_i) \otimes c_e(t_i)}},
\]
where the summations run over a thousand moments in time \(t_i\), distributed equidistantly over the simulated time-interval. Furthermore, \(c\) stands for the conformation tensor determined via (1) from the numerical solution \(\hat{b}\).

Finally, it is also examined how rapidly the gauge conditions [(17)–(19)] become compatible with the steady-state condition (12) as the steady state is approached in the course of time. In the absence of fluctuations \((\Theta = 0)\), this compatibility is quantified, at every moment in time, in terms of
\[
\varepsilon_{\text{sec}} = \sqrt{\frac{\Delta \otimes \Delta}{(\kappa \cdot c) \otimes (\kappa \cdot c)}},
\]
with
\[
\Delta = b \cdot A \cdot b^\top + \frac{1}{2} (\kappa \cdot c - c \cdot \kappa^\top),
\]
where \(A = A^4 + A^1\), and \(c\) is given by (1).

Fig. 6. Maxwell model without fluctuations \((\Theta = 0)\). Check of steady-state compatibility (12) for gauges (17) (a), (18) (b), (19) (c). Symbols: \(\Delta t/\tau = 10^{-1} (\bullet\text{, red}), \Delta t/\tau = 10^{-2} (\triangle, \text{green}), \Delta t/\tau = 10^{-3} (\blacksquare, \text{blue})\). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

In Figs. 1–6, the results of the dynamic simulations for the Maxwell model in start-up simple-shear flow with Weissenberg number \(\text{Wi} = \rho \tau = 1\) are shown for the deterministic case \((\Theta = 0)\) without corrections, (28), and when corrections according to (12) and (17)–(19) are included. The spurious oscillations present in the uncorrected dynamics (28) (Fig. 1) (see also [7]) vanish upon including the differential correction (12) (Fig. 2) or any of the gauges (17)–(19) (Figs. 3–5). For the symmetric gauge (17) and the Cholesky-decomposition gauge (19), the relative error in respecting the corresponding gauge condition is of the order of the numerical precision of the calculation (see Figs. 3 and 5). This is because, for these gauges, the gauge conditions \(g_a\) are linear in \(b\), and therefore their expansion to first order is analytically exact, making the gauge correction for every finite time-step analytically exact. In contrast, for the orthogonal gauge (18), the relative error in respecting the gauge condition is many orders of magnitude larger than the numerical precision of the calculation (see Fig. 4) with a significant time-step dependence. All these findings related to Figs. 1 and 3–5 for deterministic dynamics \((\Theta = 0)\) apply also to the case when thermal fluctuations are included \((\Theta > 0)\), see Appendix C for details. Finally, Fig. 6 shows the steady-state compatibility, i.e., fulfillment of (12), for the gauges (17)–(19). As required, the closer one gets to the true stationary state, the better the condition (12) is fulfilled.

The effects of time-step size and modification of the dynamics on the accuracy of the numerical solution in the absence of fluctuations \((\Theta = 0)\) are examined in Table 1. One observes that for all cases, except for the orthogonal gauge (18), the relative error of the numerical solution compared to the analytical solution decreases proportionally with the size of the time step. The differential, symmetric and...
Cholesky-decomposition modifications to the dynamics increase the accuracy by a factor of approx. 3 – 5 as compared to the unmodified dynamics. In contrast, the relative error of the orthogonal gauge (18) shows a rather weak dependence on the size of the time step, performing better than the other gauges at the largest time-step examined, but worse at the smaller ones.

5. Discussion and conclusions

This paper has been concerned with the multiplicative decomposition of the, symmetric and positive definite, conformation tensor. In particular, the nonuniqueness in this decomposition has been exploited to serve two goals. For the first goal, spurious rotations in the dynamics of \( b \) when \( c \) is stationary can be eliminated. The key ingredient in this part was Eq. (12), which can be interpreted either as a definition of the anti-symmetric quantity \( A \) or as a condition on \( A \) which must be satisfied in stationary situations by a more general expression \( A = A(b) \). This relates directly to the second goal served by the exploitation of the nonuniqueness in the decomposition, namely, gauge conditions can be imposed on \( b \) directly by appropriate choice of \( A = A(b) \). The specific cases examined are the symmetric gauge (resulting in what is called the “symmetric square root” in the literature), the orthogonal gauge (keeping the column vectors of \( b \) perpendicular to each other), and the Cholesky-decomposition gauge (\( b \) being lower-triangular).

When comparing the numerical accuracy of the different modifications of the dynamics, it is evident that all but the orthogonal gauge have increased performance as compared to the unmodified dynamics, and they also scale favorably with the size of the time step. In contrast, the orthogonal gauge is numerically subtle to implement whenever some of the eigenvalues become nearly equal, which necessitates time-step adaptation, at the cost of numerical efficiency. Therefore, while the direct availability of the eigenvectors and eigenvalues without diagonalization in the orthogonal gauge is conceptually intriguing, it might well be that in practical applications one of the other gauges combined with an eigenvector-eigenvalue analysis whenever needed is more favorable.

If thermal fluctuations are included, two different strategies can be followed. On the one hand, one can modify the deterministic contributions to the dynamics with the quantity \( A \) as defined by either (12) or one of the gauges, (17)–(19). This will eliminate the spurious rotations in the \( b \)-dynamics when \( c \) is stationary. The presence of the uncorrected fluctuations will not change this picture – the systematic spurious rotations will remain eliminated. On the other hand, one can choose to systematically eliminate degrees of freedom in \( b \) by imposing gauge conditions, e.g. (17)–(19), in the form \( g_{\alpha} = 0 \). This paper has demonstrated how to achieve this goal properly, i.e. how both deterministic and fluctuating contributions to the stochastic differential equation for \( b \) need to be treated. By respecting a certain gauge in this way, only six of the nine components of \( b \) are independent, whereby uniqueness and a one-to-one relation to the conformation tensor \( c \) are established. Which of these two strategies are followed when dealing with fluctuations depends on the final goal one has in mind.

### Appendix A. Derivation of \( dA^T, dc^T, \) and \( dA^B \) for stochastic dynamics

#### A1. General

In Section 3.3, a procedure has been outlined for imposing gauge conditions on \( b \) for the case of stochastic dynamics. In this Appendix, the corresponding quantities \( dA^T, dc^T, \) and \( dA^B \) are determined step-by-step.

It can be shown that the SDE of \( c, (31) \), is unaffected by the transformation (35) if the following conditions hold,

\[
\begin{align*}
    dA^T &= -dA^F, \\
    dc^T &= -dA^F, \\
    dA^B &= \left[ \left( \frac{1}{2} b \cdot dA^T \right) \cdot dA^T \right]_{\text{Itô}}.
\end{align*}
\]

The quantities \( dA^T \) and \( dA^F \) can be determined by making use of the gauge conditions (32). Inserting the transformation (35) into the gauge conditions (32), these conditions \( (n = 1, 2, 3) \) each contain both deterministic and fluctuating contributions, both of which must equate to zero in order to satisfy the respective gauge conditions on the level of stochastic processes, i.e. for each realization of the Wiener process increments. The gauge conditions (32) thus translate into the two conditions

\[
\begin{align*}
    \frac{d\delta g}{db} \odot \left( d^f b + b \cdot dA^T \right) &= 0, \\
    \frac{d\delta g}{db} \odot \left( dC^T + b \cdot dA^T \right) + \frac{1}{2} \left[ \frac{\partial^2 \delta g}{\partial b \partial b} \odot dD^{(4,ff)} \right]_{[1,3],[1,2],4} &= 0,
\end{align*}
\]

with

\[
dD^{(4,ff)} = \left[ \left( d^f b + b \cdot dA^T \right) \left( d^f b + b \cdot dA^T \right) \right]_{\text{Itô}}.
\]

and the subscripts \( (k, l) \) in (A.5) indicate contraction over the respective pair of indices.

The quantity \( dA^T \) can be determined on the basis of the condition (A.4), analogously to the deterministic contributions, leading to

\[
dA^T = \hat{A}^{(4)} \circ d^f b,
\]

with \( \hat{A}^{(4)} \) determined by (25). Thereafter, the quantity \( dA^B \) can be determined from the condition (A.5). It is mentioned that, if the second-order derivatives of the gauge conditions \( g_{\alpha} \) vanish, \( dA^B \) can be determined in a way analogous to (A.7). In all other cases, solution of (A.5) is slightly more involved.

In view of numerical applications, it is useful to write the Itô expressions (A.3) and (A.6) in more explicit form. To that end, consider the following general form of the fluctuating contribution to the dynamics,

\[
d^f b = B^{(4)} \odot dW^T,
\]

based on which the generalized mobility tensor \( M^{(4)} \) can be introduced through

\[
2k_B M^{(4)} = B^{(4)} \odot B^{(4),T},
\]

for later convenience, with \( k_B \) the Boltzmann constant. Using (A.7) for \( dA^T \), the Itô expressions for \( dC^T \) (A.3) and \( dD^{(4),ff} \) (A.6) can be written as

\[
\begin{align*}
    dC^T &= 2k_B \left[ \left( 1^4 + \frac{1}{2} b \cdot \hat{A}^{(4)} \right) \odot M^{(4)} \odot \hat{A}^{(4),T} \right]_{[1,2],3} dt, \\
    dD^{(4),ff} &= 2k_B \left[ \left( 1^4 + b \cdot \hat{A}^{(4)} \right) \odot M^{(4)} \odot \left( 1^4 + b \cdot \hat{A}^{(4)} \right) \right] T dt.
\end{align*}
\]

Making use of the general expression (27) for \( \hat{A}^{(4)} \) highlights the key role played by the quantities \( q_{\alpha} \) in the determination of all three quantities \( dA^T, dc^T, \) and \( dA^B \) in the transformation (35) of the fluctuations.
A2. Maxwell model

Inserting the form (27) for $\lambda^{(k)}$ and using $2\kappa_0M^{(k)} = (\Theta/\tau)I^{(k)}$ (see [3] for details) for the Maxwell model, the expressions for $dC^{(k)}$ (A.10) and $dB^{(k)}$ (A.11) become

$$dC^{(k)} = \Theta \left( \sum \dot{a}_i \cdot A_i + \frac{1}{2} \sum_{i,j} (\dot{a}_i \cdot \dot{a}_j) \cdot b \cdot A_i \cdot A_j \right) dt, \quad (A.12)$$

$$dB^{(k)} = \Theta \left( i^{(k)} + \sum \dot{a}_i b \cdot A_i + \sum b \cdot A_i \cdot \dot{a}_i + \sum_{i,j} (\dot{a}_i \cdot \dot{a}_j) \cdot b \cdot A_i \cdot A_j \right) dt. \quad (A.13)$$

For the numerical implementation, the following expressions needed in (A.5) for gauge (18) are also provided,

$$\frac{\partial e_{\mu\nu}}{\partial b} \otimes (b \cdot dA^{(k)}) = -dA^{(k)} e_{\mu\nu}(\lambda_i - \dot{\lambda}_i), \quad n \notin \{i, j\} \text{ and } i \neq j, \quad (A.14)$$

$$\frac{\partial^2 e_{\mu\nu}}{\partial b \partial b} \otimes dA^{(k)} = \frac{\Theta}{\tau} \left( \sum_k (\dot{a}_k \cdot X_{ij}) \otimes (b \cdot A_k) + \sum_k (b \cdot A_k \cdot X_{ij}) \otimes \dot{a}_k + \sum_{i,j} (\dot{a}_k \cdot \dot{a}_j) \cdot (b \cdot A_k \cdot X_{ij}) \otimes (b \cdot A_j) \right) dt, \quad (A.15)$$

with

$$X_{ij} = \dot{x}_i \dot{x}_j^T + \dot{x}_j \dot{x}_i^T. \quad (A.16)$$

and where $dA^{(k)} = \sum dA^{(k)} A_i$ and $b^T \cdot b = \epsilon_{axx}$ have been employed in (A.14).

Appendix B. Initial condition for start-up shear deformation with orthogonal gauge (18)

The expressions (44) for $a_\parallel$ for the orthogonal gauge (18) are well defined whenever the eigenvalues are distinct. In the following, we briefly discuss a case when eigenvalues are nearly equal, in the absence of fluctuations. As discussed in Section 3.4, the relaxation does not necessitate gauge corrections, i.e. $A^\parallel = 0$. To illustrate the subtleties involved with (44), we focus on start-up shear flow,

$$\kappa = \dot{\gamma} \dot{x}_1 \dot{x}_2^T, \quad (B.1)$$

with constant shear rate $\dot{\gamma}$ for $t \geq 0$, starting from a (nearly) isotropic state. In order to concentrate on the essence, relaxation is neglected, i.e. we consider the dynamics

$$b = \kappa \cdot b + b \cdot A^\parallel. \quad (B.2)$$

Knowing the solution to (B.2) for $A^\parallel = 0$ and since $A^\parallel$ generates an orthogonal transformation on the r.h.s. of $b$, one can make the ansatz

$$b = (1 + \gamma \dot{x}_1 \dot{x}_2^T) \cdot Q', \quad (B.3)$$

with $\gamma = \dot{\gamma} t$ and $Q'$ an orthogonal transformation. The latter is determined by

$$Q' = Q^* \cdot A^\parallel, \quad (B.4)$$

which has been obtained by inserting the ansatz (B.3) into the dynamics (B.2). Since the imposed deformation (B.1) leaves the 3-direction untouched, it is reasonable to assume that the correcting orthogonal transformation $Q'$ as well as its generator $A^\parallel$ also should not affect the 3-direction. According to the definitions (26), this implies that only $A_3$ contributes to the dynamics, i.e.

$$A^\parallel = A_3 (a_\parallel \cdot (b \cdot \kappa)). \quad (B.5)$$

In order to get an even more explicit expression for $A^\parallel$, we make the ansatz

$$Q = \cos \phi (\dot{x}_1 \dot{x}_1^T + \dot{x}_2 \dot{x}_2^T) + \sin \phi (\dot{x}_2 \dot{x}_1^T - \dot{x}_1 \dot{x}_2^T), \quad (B.6)$$

with the help of which one obtains the rotational frequency for the gauge correction,

$$\omega_A \equiv \dot{a}_3 \cdot (b \cdot \kappa) = \frac{\cos(2\phi) + \sin(2\phi)}{2 \sin(2\phi) - \cos(2\phi))}. \quad (B.7)$$

In order for $\omega_A$ to be finite in the earliest states of deformation ($\gamma \to 0$), one must have $\cos(2\phi) \to 0$, which implies that $\phi = 0$ at $t = 0$ is not a suitable initial condition. Rather, we must look for solutions of the form $\phi = q\tau \pm \pi/4$. Inserting this ansatz, the rotational frequency in the early states is finite, namely $\omega_A = \gamma (1 - q + \Theta(\gamma^2))$. The orthogonal-transformation dynamics (B.4), which reduces to $\phi = \omega_A$ upon inserting (B.5)–(B.7), requires $q = 1/4$. This proves that the expression (44) results in well-defined dynamics even in the vicinity of equilibrium where the eigenvalues of $\epsilon$ are nearly equal.

The fact that the dynamics removes the degeneracy that is present at equilibrium is paramount in the above argument. What has been shown above is that the dynamics departing from equilibrium is well behaved if one chooses the proper eigenvectors at equilibrium in anticipation of the imposed deformation. This corresponds in a more general context to approaches in perturbation theory, where at higher orders the degeneracy is removed. We expect that other subtle cases for gauge (18) can be treated in a similar manner.

Appendix C. Numerical calculations including fluctuations

In this appendix, the results of the numerical calculations of the Maxwell model (28) in start-up simple-shear flow with fluctuations are shown, with the details of the simulations being described in Section 4. In analogy to Figs. 1 and 3–5 in the absence of thermal fluctuations ($\Theta = 0$), Figs. C.7–C.10 in this Appendix present the results when thermal fluctuations are included, with $\Theta = 0.01$. 

Fig. C.7. Maxwell model (28) with fluctuations ($\Theta = 0.01$) and without corrections: $b_{\parallel x}$ (●, black), $b_{\parallel y}$ (●, red), $b_{\parallel z}$ (●, green), $b_{\parallel y}$ (●, blue). Time step: $\Delta t/\tau = 10^{-3}$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Fig. C.8. Maxwell model with fluctuations ($\Theta = 0.01$) with symmetric gauge (17). Subfigure (a): $b_{xx}$ (■, black), $b_{xy}$ (▲, red), $b_{yx}$ (▼, green), $b_{yy}$ (●, blue), with time step $\Delta t/\tau = 10^{-3}$. Subfigure (b): relative error $\varepsilon_S$ for different time steps, namely, $\Delta t/\tau = 10^{-3}$ (●, red), $\Delta t/\tau = 10^{-2}$ (▲, green), $\Delta t/\tau = 10^{-3}$ (▼, blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. C.9. Maxwell model with fluctuations ($\Theta = 0.01$) with orthogonal gauge (18). Subfigure (a): $b_{xx}$ (■, black), $b_{xy}$ (▲, red), $b_{yx}$ (▼, green), $b_{yy}$ (●, blue), with time-step parameter $[\Delta t/\tau]_0 = 10^{-3}$. Subfigure (b): relative error $\varepsilon_\perp$ for different time-step parameters, namely, $[\Delta t/\tau]_0 = 10^{-3}$ (●, red), $[\Delta t/\tau]_0 = 10^{-2}$ (▲, green), $[\Delta t/\tau]_0 = 10^{-1}$ (▼, blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Fig. C.10. Maxwell model with fluctuations ($\Theta = 0.01$) with Cholesky-decomposition gauge (19). Subfigure (a): $b_{xx}$ ( ■, black), $b_{xy}$ ( ▲, red), $b_{yx}$ ( ▼, green), with time step $\Delta \tau = 10^{-3}$. Subfigure (b): relative error $\varepsilon_L$ for different time steps, namely, $\Delta \tau = 10^{-3}$ ( ●, blue), $\Delta \tau = 10^{-2}$ ( ●, green), $\Delta \tau = 10^{-1}$ ( ▼, blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

References