The *natural*-conformation tensor constitutive laws

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Abstract

In this work we revisit the seminal work of Renardy [M. Renardy, J. Non-Newtonian Fluid Mech., 52(1) (1994), 91-95] on the reformulation of the stress tensor in its "natural" basis, and present a generic framework for the *natural*-conformation tensor for a large class of differential constitutive models. We show that the proposed dyadic transformation can be equated as an orthogonal transformation of the conformation tensor into a streamlined orthonormal basis given by a rotation tensor expressed in terms of the unit velocity vectors. We also show that the *natural*-conformation tensor formulation is a particular sub-case of the *kernel*-conformation tensor transformation [A.M. Afonso, F.T. Pinho, M.A. Alves, J. Non-Newtonian Fluid Mech. 167-168(2012) 30-37] with the *kernel* function acting on the rotation of the eigenvectors rather than on the magnitude of the extension of the conformation tensor.

Keywords: Natural-conformation tensor transformation, "natural" basis reformulation, computational rheology

1. The natural basis tensor reformulation

More than 30 years ago, Renardy [9] proposed a stress reformulation by representing the extra-stress tensor in its "natural" basis, rather than in Cartesian or polar coordinates. It was proposed that this "natural" basis in planar flow be aligned with the streamlines. The idea was based on the key evidence that in a flow near a re-entrant corner, where the upper convected derivative dominates, the stresses are of the type $h(\psi)\mathbf{u}\mathbf{u}^T$, for an arbitrary $h(\psi)$ function of the stream function ψ and \mathbf{u} the velocity field. Hinch [7] had earlier used this exact solution to derive a local similarity solution for the Oldroyd-B model.

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Following this simple observation, Renardy proposed the extra-stress tensor in its "natural" basis, aligned with streamlines. As such, the extra stress tensor \mathbf{T} is represented relative to a basis formed with the dyadic products of \mathbf{u} and \mathbf{v} ,

$$\mathbf{T} = \lambda \mathbf{u} \mathbf{u}^T + \mu (\mathbf{u} \mathbf{v}^T + \mathbf{v} \mathbf{u}^T) + \nu \mathbf{v} \mathbf{v}^T, \tag{1}$$

where λ , μ , ν were termed the natural stress variables. The vector \mathbf{v} is taken perpendicular to the velocity \mathbf{u} such that the determinant formed from their components is unity. Explicitly, for 2D flow,

$$\mathbf{u} = (u, v), \qquad \mathbf{v} = \left(-\frac{v}{u^2 + v^2}, \frac{u}{u^2 + v^2}\right).$$
 (2)

For models such as UCM, a significant decoupling in the component equations for the natural stress variables takes place in steady flow. In fact, the equation for ν is decoupled from the rest. This is significant, as it is the term $\mathbf{v}\mathbf{v}^T$ which grows unboundedly at solid boundaries where the velocity vanishes. By keeping the equation for ν separate, it avoids the excitation of numerical discretization errors which were found to amplify at the downstream wall of re-entrant corners [12].

2. The natural stress formulation

In general flows, it is advantageous to consider the conformation tensor **A** instead of the extra-stress tensor, using the same "natural" basis alignment. This is apparent when considering High Weissenberg number boundary layers [11, 10, 15], for example. Specifically,

$$\mathbf{A} = \lambda \mathbf{u} \mathbf{u}^T + \mu (\mathbf{u} \mathbf{v}^T + \mathbf{v} \mathbf{u}^T) + \nu \mathbf{v} \mathbf{v}^T.$$
 (3)

The two representations are related through $\mathbf{T} = \frac{\eta_p}{\tau_p}(\mathbf{A} - \mathbf{I})$, where η_p is the polymer viscosity and τ_p its relaxation time. Evans and Oishi [4] proposed to term (3) the Natural Stress Formulation. The use of the conformation tensor is motivated by several reasons. Primarily it must remain positive definite, due to its representation as a variance-covariance matrix in the microstructure model. Also, for simple models such as UCM, the range of stresses are restricted due to the extra-stress being dependent on the relative strain Finger tensor. This again manifests itself in the conformation tensor having to remain positive definite. This condition is also suffice to ensure that the UCM equations never become Hadamard unstable i.e. catastrophically unstable to short waves [8]. It is also beneficial in viscoelastic models where the identity term plays a significant role in the boundary layer equations at solid surfaces. This is seen in the Giesekus model for general flows at high Weissenberg numbers [6] and specifically at re-entrant corners [3].

The time and spatial evolution of this conformation tensor obeys an evolution equation, represented by the following generic differential constitutive model,

$$\frac{\mathrm{D}\mathbf{A}}{\mathrm{D}t} = \frac{\partial\mathbf{A}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{A} = \mathbf{A}(\nabla \mathbf{u}) + (\nabla \mathbf{u})^{T}\mathbf{A} + \frac{\mathcal{F}(\mathbf{A})}{Wi}\mathcal{H}(\mathbf{A})$$
(4)

where $\mathcal{F}(\mathbf{A})$ is a scalar and $\mathcal{H}(\mathbf{A})$ a tensor, and both of these functions allow the definition of a specific constitutive model, such as the Oldroyd-B (UCM), PTT or FENE-type models. The Weissenberg number is defined as Wi = $\tau_p U/L$, where U and L are characteristic velocity and length scales, respectively. It is a non-dimensional parameter that measures the elasticity of a fluid, indicating the degree of anisotropy or orientation generated by the deformation.

For computational purposes, Evans and Oishi [4] suggested a form of (3) using rescaled natural stress variables, namely

$$\mathbf{A} = \hat{\lambda}\hat{\mathbf{u}}\hat{\mathbf{u}}^T + \hat{\mu}(\hat{\mathbf{u}}\hat{\mathbf{v}}^T + \hat{\mathbf{v}}\hat{\mathbf{u}}^T) + \hat{\nu}\hat{\mathbf{v}}\hat{\mathbf{v}}^T, \tag{5}$$

where

$$\hat{\lambda} = |\mathbf{u}|^2 \lambda, \quad \hat{\mu} = \mu, \quad \hat{\nu} = \frac{\nu}{|\mathbf{u}|^2},$$
 (6)

and

$$\hat{\mathbf{u}} = \frac{\mathbf{u}}{|\mathbf{u}|} = \frac{1}{|\mathbf{u}|} \begin{pmatrix} u \\ v \end{pmatrix} \qquad \hat{\mathbf{v}} = |\mathbf{u}|\mathbf{v} = \frac{1}{|\mathbf{u}|} \begin{pmatrix} -v \\ u \end{pmatrix}, \tag{7}$$

are unit vectors.

3. The *natural*-conformation tensor formulation

In this short note we present a generalization for the natural-conformation tensor formulation for a family of differential constitutive equations, following the key idea that the natural-conformation tensor, \mathbf{N} , can be obtained by equating the proper relation with the conformation tensor, \mathbf{A} . Therefore, based on the original idea proposed by Renardy [9], we can define the natural-conformation tensor, \mathbf{N} , as the orthogonal transformation of the conformation tensor,

$$\mathbf{N} = \mathbf{R}^{\mathbf{T}} \mathbf{A} \mathbf{R},\tag{8}$$

where the *natural* basis rotation tensor, \mathbf{R} , is a proper rotation tensor transforming into a streamlined orthonormal basis defined by three unitary vectors, $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$, with $|\hat{\mathbf{u}}| = |\hat{\mathbf{v}}| = |\hat{\mathbf{v}}| = 1$, $\hat{\mathbf{u}} \cdot \hat{\mathbf{v}} = 0$ and $\hat{\mathbf{u}} \times \hat{\mathbf{v}} = \hat{\mathbf{w}}$. Denoting by $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ the unit vectors in fixed Cartesian x, y and z directions, we have

$$\mathbf{R} = \hat{\mathbf{u}}\hat{\mathbf{i}}^T + \hat{\mathbf{v}}\hat{\mathbf{j}}^T + \hat{\mathbf{w}}\hat{\mathbf{k}}^T. \tag{9}$$

The *natural* basis rotation tensor, \mathbf{R} , is a real, orthogonal matrix, with columns represented by unit vectors, it belongs to the special orthogonal group with dimensions three, such as $\mathbf{R^T} = \mathbf{R^{-1}}$, $\mathbf{R^TR} = \mathbf{RR^T} = \mathbf{I}$ and $\det \mathbf{R} = +1$. We can use this property and perform the material derivative on both sides of $\mathbf{R^TR} = \mathbf{I}$, obtaining $\frac{D\mathbf{R^T}}{Dt}\mathbf{R} + \mathbf{R^T}\frac{D\mathbf{R}}{Dt} = \mathbf{0}$, which indicates that $\mathbf{\Omega} = \frac{D\mathbf{R^T}}{Dt}\mathbf{R}$ is a skew-symmetric tensor satisfying $\mathbf{\Omega} + \mathbf{\Omega}^T = \mathbf{0}$.

The *natural* conformation tensor differential constitutive model can be derived by equating the material derivative on relation (8) and using the generic differential constitutive model for the conformation tensor of Equation (4), to obtain:

$$\frac{D\mathbf{N}}{Dt} = \mathbf{N}\widetilde{\nabla \mathbf{u}} + \widetilde{\nabla \mathbf{u}}^{\mathbf{T}} \mathbf{N} + \frac{\mathcal{F}(\mathbf{N})}{Wi} \mathcal{H}(\mathbf{N}), \qquad (10)$$

where the *natural* velocity gradient tensor is defined by $\widetilde{\nabla \mathbf{u}} = \mathbf{R}^T \nabla \mathbf{u} \mathbf{R} - \Omega$.

The natural velocity gradient tensor can be related to a symmetric natural rate of strain tensor, $\widetilde{\mathbf{D}} = \frac{1}{2} \left[\widetilde{\nabla \mathbf{u}} + \widetilde{\nabla \mathbf{u}}^{\mathbf{T}} \right] = \mathbf{R}^{\mathbf{T}} \mathbf{D} \mathbf{R}$, and an anti-symmetric natural vorticity tensor $\widetilde{\mathbf{W}} = \frac{1}{2} \left[\widetilde{\nabla \mathbf{u}} - \widetilde{\nabla \mathbf{u}}^{\mathbf{T}} \right] = \mathbf{R}^{\mathbf{T}} \mathbf{W} \mathbf{R} - \mathbf{\Omega}$. This natural vorticity tensor can be also described as a form of the relative-rate-of-rotation tensor proposed by Astarita [2], measuring the rate of rotation of the material as measured by an observer who is fixed, not into the principal directions of the rate of strain as proposed by Astarita [2], but rather into the principal streamline direction.

As final remark, if we use other orthogonal basis in Equation (8), for instance, the set of eigenvectors of the conformation tensor it self, meaning that $\mathbf{R}|\Omega \to \mathbf{O}|\mathcal{O}$, we obtain, by Equation (10), the *eigendecomposed* version of Vaithianathan and Collins [14], for the diagonal tensor, $\mathbf{\Lambda} = \mathbf{O}^{\mathbf{T}}\mathbf{A}\mathbf{O}$,

$$\frac{D\mathbf{\Lambda}}{Dt} = \mathbf{\Lambda} \overline{\nabla \mathbf{u}} + \overline{\nabla \mathbf{u}}^{\mathbf{T}} \mathbf{\Lambda} + \frac{\mathcal{F}(\mathbf{\Lambda})}{Wi} \mathcal{H}(\mathbf{\Lambda})$$
(11)

where $\overline{\nabla \mathbf{u}} = \mathbf{O^T} \nabla \mathbf{uO} - \mathbf{\mathcal{O}}$, and $\mathbf{\mathcal{O}} = \frac{D\mathbf{O^T}}{Dt}\mathbf{O}$ is the corresponding spin tensor. This means that the *natural*-conformation tensor reformulation is an orthogonal operation on the eigenvectors of the conformation tensor, and therefore can be devised as a particular case of the *kernel*-conformation tensor transformation [1]. In the *natural* conformation tensor differential constitutive model the *kernel* operation acts directly in the orientation of the principal directions of the eigenvectors rather than on the magnitude of the extension of the conformation tensor.

Example for 3D case

Here we present the demonstration for a 3D case for the generalization for the natural conformation tensor formulation. There are infinite possibilities to define the *natural* basis rotation tensor, \mathbf{R} , in a 3D flow. One possibility to define the *natural* basis rotation tensor is to use a Frenet-Seret type of representation [13] for the streamlined orthonormal basis defined by three unitary vectors, $\left\{\hat{\mathbf{u}} = \frac{\mathbf{u}}{|\mathbf{u}|}, \hat{\mathbf{v}} = \frac{d\hat{\mathbf{u}}/ds}{|d\hat{\mathbf{u}}/ds|}, \hat{\mathbf{w}} = \hat{\mathbf{u}} \times \hat{\mathbf{v}}\right\}$, defined as the unit tangent vector, the normal vector, and the binormal vector, respectively. Here, we propose a different streamlined orthonormal basis in which the plane of rotation is formed by $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}} = \frac{-v}{\sqrt{u^2+v^2}}\hat{\mathbf{i}} + \frac{u}{\sqrt{u^2+v^2}}\hat{\mathbf{j}} + 0\hat{\mathbf{k}}$, meaning that the axis of rotation is along a unit vector $\hat{\mathbf{w}} = \frac{\hat{\mathbf{u}} \times \hat{\mathbf{v}}}{|\hat{\mathbf{u}} \times \hat{\mathbf{v}}|}$, forming the orthonormal basis: $\left\{\hat{\mathbf{u}} = \frac{\mathbf{u}}{|\mathbf{u}|}, \hat{\mathbf{v}}, \hat{\mathbf{w}} = \frac{\hat{\mathbf{u}} \times \hat{\mathbf{v}}}{|\hat{\mathbf{u}} \times \hat{\mathbf{v}}|}\right\}$. This representation preserves the original idea from Renardy [9], preserving the same definition for both the angle and axis

of rotation, $\cos \theta = \frac{u}{|\mathbf{u}|}$ and $\hat{\mathbf{w}}$ (or $\hat{\mathbf{k}}$ in a 2D case), respectively. Using this representation in dyadic products (9), \mathbf{R} takes the form of,

$$\mathbf{R} = \begin{bmatrix} \frac{u}{|\mathbf{u}|} & \frac{-v}{\sqrt{u^2 + v^2}} & \frac{-uw}{\sqrt{(uw)^2 + (vw)^2 + (u^2 + v^2)^2}} \\ \frac{v}{|\mathbf{u}|} & \frac{u}{\sqrt{u^2 + v^2}} & \frac{-vw}{\sqrt{(uw)^2 + (vw)^2 + (u^2 + v^2)^2}} \\ \frac{w}{|\mathbf{u}|} & 0 & \frac{u^2 + v^2}{\sqrt{(uw)^2 + (vw)^2 + (u^2 + v^2)^2}} \end{bmatrix}.$$
 (12)

The conformation tensor can be defined in the dyadic decomposition, as:

$$\mathbf{A} = \mathbf{R} \mathbf{N} \mathbf{R}^{\mathsf{T}} = \mathbf{R} \begin{bmatrix} n_{11} & n_{12} & n_{13} \\ n_{12} & n_{22} & n_{23} \\ n_{13} & n_{23} & n_{33} \end{bmatrix} \mathbf{R}^{\mathsf{T}}$$

$$= \begin{bmatrix} \frac{u}{|\mathbf{u}|} & \frac{-v}{\sqrt{u^{2}+v^{2}}} & \frac{-uw}{\sqrt{(uw)^{2}+(vw)^{2}+(u^{2}+v^{2})^{2}}} \\ \frac{v}{|\mathbf{u}|} & \frac{u}{\sqrt{u^{2}+v^{2}}} & \frac{-vw}{\sqrt{(uw)^{2}+(vw)^{2}+(u^{2}+v^{2})^{2}}} \\ \frac{w}{|\mathbf{u}|} & 0 & \frac{u^{2}+v^{2}}{\sqrt{(uw)^{2}+(vw)^{2}+(u^{2}+v^{2})^{2}}} \end{bmatrix} \begin{bmatrix} n_{11} & n_{12} & n_{13} \\ n_{12} & n_{22} & n_{23} \\ n_{13} & n_{23} & n_{33} \end{bmatrix} \begin{bmatrix} \frac{u}{|\mathbf{u}|} \\ \frac{-v}{\sqrt{u^{2}+v^{2}}} \\ \frac{-uw}{\sqrt{(uw)^{2}+(vw)^{2}+(u^{2}+v^{2})^{2}}} \end{bmatrix} (13)$$

$$= n_{11} \hat{\mathbf{u}} \hat{\mathbf{u}}^{T} + n_{22} \hat{\mathbf{v}} \hat{\mathbf{v}}^{T} + n_{33} \hat{\mathbf{w}} \hat{\mathbf{w}}^{T} + n_{12} (\hat{\mathbf{u}} \hat{\mathbf{v}}^{T} + \hat{\mathbf{v}} \hat{\mathbf{u}}^{T}) + n_{13} (\hat{\mathbf{u}} \hat{\mathbf{w}}^{T} + \hat{\mathbf{w}} \hat{\mathbf{u}}^{T}) + n_{23} (\hat{\mathbf{w}} \hat{\mathbf{v}}^{T} + \hat{\mathbf{v}} \hat{\mathbf{w}}^{T}).$$

For the 2D case, the natural basis rotation tensor obtained from Equation (12), takes the form

$$\mathbf{R} = \frac{1}{|\mathbf{u}|} \begin{bmatrix} u & -v & 0 \\ v & u & 0 \\ 0 & 0 & |\mathbf{u}| \end{bmatrix},\tag{14}$$

and the conformation tensor can be expressed by,

$$\mathbf{A} = \mathbf{R} \begin{bmatrix} n_{11} & n_{12} & 0 \\ n_{12} & n_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{R}^{\mathbf{T}} = \mathbf{R} \begin{bmatrix} \hat{\lambda} & \hat{\mu} & 0 \\ \hat{\mu} & \hat{\nu} & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{R}^{\mathbf{T}} \\
= \frac{1}{|\mathbf{u}|^{2}} \begin{bmatrix} u & -v & 0 \\ v & u & 0 \\ 0 & 0 & |\mathbf{u}| \end{bmatrix} \begin{bmatrix} \hat{\lambda} & \hat{\mu} & 0 \\ \hat{\mu} & \hat{\nu} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u & v & 0 \\ -v & u & 0 \\ 0 & 0 & |\mathbf{u}| \end{bmatrix} \\
= \frac{1}{|\mathbf{u}|^{2}} \begin{bmatrix} \hat{\lambda} u^{2} - 2\hat{\mu} uv + \hat{\nu} v^{2} & \hat{\lambda} uv + \hat{\mu} (u^{2} - v^{2}) - \hat{\nu} uv & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
= \frac{\hat{\lambda}}{|\mathbf{u}|^{2}} \begin{bmatrix} u^{2} & uv & 0 \\ uv & v^{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{\hat{\mu}}{|\mathbf{u}|^{2}} (\begin{bmatrix} -uv & u^{2} & 0 \\ -v^{2} & uv & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} -uv & -v^{2} & 0 \\ u^{2} & uv & 0 \\ 0 & 0 & 0 \end{bmatrix}) + \frac{\hat{\nu}}{|\mathbf{u}|^{2}} \begin{bmatrix} v^{2} & -uv & 0 \\ -uv & u^{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
= \hat{\lambda} \hat{\mathbf{u}} \hat{\mathbf{u}}^{T} + \hat{\mu} (\hat{\mathbf{u}} \hat{\mathbf{v}}^{T} + \hat{\mathbf{v}} \hat{\mathbf{v}}^{T}) + \hat{\nu} \hat{\mathbf{v}} \hat{\mathbf{v}}^{T} \end{aligned}$$
(16)

which recovers the relations proposed by Evans and Oishi [4] in (5). We can also observe that $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are eigenvectors of both the first a fourth dyadic products in (5), whilst separately $\hat{\mathbf{u}}$ the third dyadic term. Consequently we have the following diagonalisations

$$\hat{\mathbf{u}}\hat{\mathbf{u}}^T = \mathbf{R} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \mathbf{R}^T, \quad \hat{\mathbf{v}}\hat{\mathbf{v}}^T = \mathbf{R} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{R}^T, \tag{17}$$

and further

$$\hat{\mathbf{u}}\hat{\mathbf{v}}^T = \mathbf{R} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mathbf{R}^T, \ \hat{\mathbf{v}}\hat{\mathbf{u}}^T = \mathbf{R} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \mathbf{R}^T.$$
 (18)

so that expression (5) can be written succinctly in the matrix form **RNR**^T.

4. Numerical results

In this section, we present numerical results for the 4:1 contraction benchmark flow using the Oldroyd-B viscoelastic model. For this, we set $\mathcal{F}(\mathbf{A}) = 1$ and $\mathcal{H}(\mathbf{A}) = (\mathbf{A} - \mathbf{I})$ in Eq. (4). The same substitutions are applied to Eq. (10), but using \mathbf{N} instead of \mathbf{A} . The natural-conformation tensor formulation was implemented in an in-house code using a finite difference scheme. For more details about the code, refer to [5]. The simulations were conducted with the following parameters: Reynolds number Re = 0.01, Weissenberg number Wi = 1, and solvent viscosity ratio $\beta = 0.5$. A non-uniform Cartesian mesh, with a minimum element size of $\Delta x_{min} = \Delta y_{min} = 4 \times 10^{-3}$, was employed to discretize the domain, with a finer mesh near the corners.

Figure 1 illustrates the slope of the u-velocity component and pressure obtained with both the natural-conformation and the Cartesian formulation, compared to the expected asymptotic results. The u-velocity component aligns reasonably well with the inclination line, and the natural-conformation formulation shows better convergence behavior. Although the pressure results do not fully capture the expected theoretical behavior, a slight improvement is observed with the use of the natural-conformation formulation.

Finally, Figure 2 displays the results for the stress and natural components, comparing both the Cartesian and *natural*-conformation formulations. Once again, the *natural*-conformation formulation accurately captures the expected asymptotic behavior. However, the Cartesian stress results are less satisfactory, indicating a lack of resolution.

5. Discussion

In this work, we have a generic framework for the *natural*-conformation tensor for a large class of differential constitutive models. We show that the proposed dyadic transformation proposed by Renardy [9] can be equated as a proper rotation of the conformation tensor into a streamlined orthonormal basis given by a rotation tensor expressed in terms of the unit velocity vectors. We also show that the *natural*-conformation tensor formulation is a particular sub-case of the *kernel*-conformation tensor transformation [1] with the *kernel*

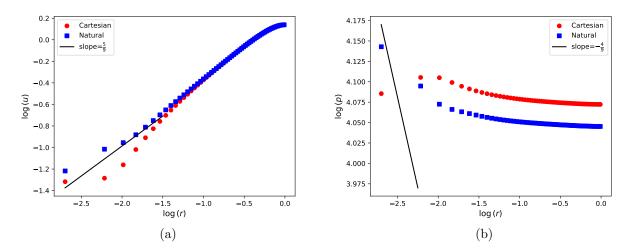


Figure 1: Numerical verification of the asymptotic behavior for the u-velocity component and pressure p using both Cartesian and natural-conformation formulations.

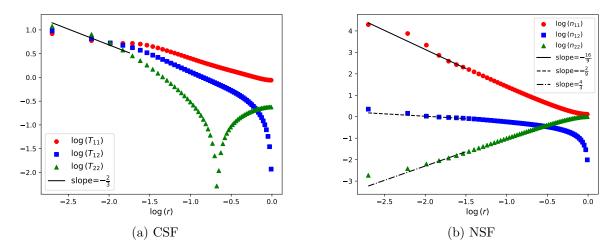


Figure 2: Numerical verification of the asymptotic behavior for the polymer and natural stress components using Cartesian and *natural*-conformation formulations, respectively.

function acting on the rotation of the eigenvalues rather than on the magnitude of the eigenvalues.

The main contributions of this short communication can be summarized as follows:

- A simple relation between the *natural* basis tensor reformulation proposed by Renardy [9] and the *natural*-conformation tensor was presented;
- The *natural*-conformation tensor formulation for a family of differential constitutive laws for two and three dimensional unsteady flows have been presented.

In the extension of this work, further details regarding the stabilization methods for the numerical method for the *natural*-conformation tensor in 3D and different strategies for the transient term in the *natural* velocity gradient tensor.

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