Stress projections and data-driven modelling

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The Multiscale Spectrum of Constitutive Modeling in Solid Mechanics
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Take-home messages

Orthogonal stress projections are most helpful in consistently organize data to build empirical constitutive laws from experiments and simulations

The kinematic meaning of tensorial bases is key to discriminating the independent effects that concur in determining the stress response

Multiscale simulations in two equations

Balance of momentum:

$$\rho \frac{D\boldsymbol{v}}{Dt} = \mathrm{div}\,\mathbf{T} + \boldsymbol{f}$$

Constitutive law:

$$\mathbf{T}(\boldsymbol{x}, t) = \hat{\mathbf{T}}(\ldots \text{whatever kinematical quantity you like} \ldots)$$

Objectives:

- Determine the local value of the stress from microscale simulations constrained by the macroscopic generalized kinematics
- Use the balance of momentum (together with other equations) to move forward in the macroscopic dynamics

Tensorial bases and stress projections

A local tensorial basis for the linear space of stress tensors is given by six symmetric tensors

$$\big(\mathbf{B}_1, \mathbf{B}_2, \mathbf{B}_3, \mathbf{B}_4, \mathbf{B}_5, \mathbf{B}_6\big)$$

with the same covariance properties as $\mathbf{T}$ and orthonormal with respect to the scalar product defined by $\mathbf{A} \cdot \mathbf{B} = \mathrm{tr}(\mathbf{A}^\mathsf{T}\mathbf{B})$

For a given basis, we can write, in absolute generality, the local identity

$$\mathbf{T} = \beta_1\mathbf{B}_1 + \beta_2\mathbf{B}_2 + \beta_3\mathbf{B}_3 + \beta_4\mathbf{B}_4 + \beta_5\mathbf{B}_5 + \beta_6\mathbf{B}_6$$

where β_k is the k-th projection given by $\beta_k = \mathbf{T} \cdot \mathbf{B}_k$

Remark 1: *this expansion is not a constitutive law*

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An unsatisfactory example

We can take an orthonormal basis $(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ for the ambient three-dimensional space and define

$$\mathbf{X}_1 = \boldsymbol{x}_1 \otimes \boldsymbol{x}_1\,, \quad \mathbf{X}_2 = \boldsymbol{x}_2 \otimes \boldsymbol{x}_2\,, \quad \mathbf{X}_3 = \boldsymbol{x}_3 \otimes \boldsymbol{x}_3$$

$$\mathbf{X}_4 = \frac{1}{\sqrt{2}}(\boldsymbol{x}_1 \otimes \boldsymbol{x}_2 + \boldsymbol{x}_2 \otimes \boldsymbol{x}_1)$$

$$\mathbf{X}_5 = \frac{1}{\sqrt{2}}(\boldsymbol{x}_2 \otimes \boldsymbol{x}_3 + \boldsymbol{x}_3 \otimes \boldsymbol{x}_2)$$

$$\mathbf{X}_6 = \frac{1}{\sqrt{2}}(\boldsymbol{x}_3 \otimes \boldsymbol{x}_1 + \boldsymbol{x}_1 \otimes \boldsymbol{x}_3)$$

This is the most common choice for the representation of data *but* it is lacking a kinematic or material meaning of the chosen directors

A better example

We can take an orthonormal set $(\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3)$ of local material directions (in the ambient space) and set

$$\mathbf{Z}_1 = \boldsymbol{m}_1 \otimes \boldsymbol{m}_1\,, \quad \mathbf{Z}_2 = \boldsymbol{m}_2 \otimes \boldsymbol{m}_2\,, \quad \mathbf{Z}_3 = \boldsymbol{m}_3 \otimes \boldsymbol{m}_3$$

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It may look the same, but the meaning produces a deep difference
Most importantly, this basis *remains adapted to the local deformation*

Application: linear elasticities

Choose your favorite linearized measure of strain,
call it $\mathbf{E}$, and set $E_k = \mathbf{E} \cdot \mathbf{Z}_k$

Given a table of 36 material constants c_{ik} we can write a linear constitutive prescription as

$$\mathbf{T}(\mathbf{E}, \boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3) = \sum_{i,k=1}^{6} c_{ik} E_k \mathbf{Z}_i =: \mathbb{C}\mathbf{E}\,,$$

where the Voigt representation c_{ik} of the elasticity tensor defines

$$\mathbb{C} := \sum_{i,k=1}^{6} c_{ik} \mathbf{Z}_i \otimes \mathbf{Z}_k$$

that is a completely intrinsic expression

Starting from a meaningful tensorial quantity

A second strategy involves choosing a symmetric tensorial quantity with some specific kinematic meaning, making sure that it transforms as $\mathbf{T}$

We denote by $\mathbf{A}$ the normalized deviatoric part of such a tensor and by $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ its eigenvectors. In full generality, we can write

$$\mathbf{A} = \frac{s}{\sqrt{3/2 + 2\alpha^2}} \left[\boldsymbol{a}_1 \otimes \boldsymbol{a}_1 - (1/2 + \alpha) \boldsymbol{a}_2 \otimes \boldsymbol{a}_2 - (1/2 - \alpha) \boldsymbol{a}_3 \otimes \boldsymbol{a}_3 \right]$$

with $s = \pm 1$ and $0 \leq \alpha \leq 1/2$

With these choices, $\mathbf{A}$ is orthogonal to

$$\mathbf{J} = \frac{\mathbf{Id}}{\sqrt{3}} = \frac{1}{\sqrt{3}} \left[\boldsymbol{a}_1 \otimes \boldsymbol{a}_1 + \boldsymbol{a}_2 \otimes \boldsymbol{a}_2 + \boldsymbol{a}_3 \otimes \boldsymbol{a}_3 \right],$$

and this will allow us to isolate the spherical part of the stress

Completing the orthonormal basis

We just need to compute the vector product

$$\frac{s}{\sqrt{9/2+6\alpha^2}}\begin{pmatrix}1\\1\\1\end{pmatrix}\times\begin{pmatrix}1\\-(1/2+\alpha)\\-(1/2-\alpha)\end{pmatrix}=\frac{s}{\sqrt{9/2+6\alpha^2}}\begin{pmatrix}2\alpha\\3/2-\alpha\\-3/2-\alpha\end{pmatrix}$$

thus completing the tensorial basis with

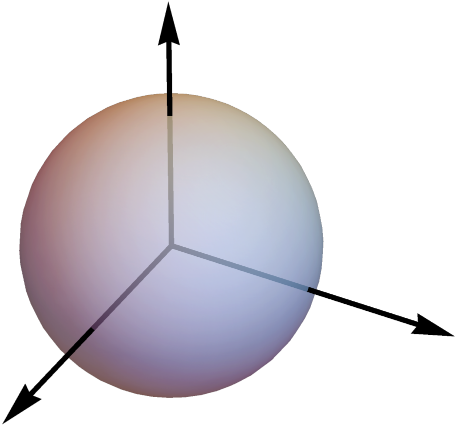
$$\mathbf{A}_0=\frac{s}{\sqrt{9/2+6\alpha^2}}\left[2\alpha\boldsymbol{a}_1\otimes\boldsymbol{a}_1+(3/2-\alpha)\boldsymbol{a}_2\otimes\boldsymbol{a}_2-(3/2+\alpha)\boldsymbol{a}_3\otimes\boldsymbol{a}_3\right]$$

$$\mathbf{A}_1=\frac{1}{\sqrt{2}}\left[\boldsymbol{a}_2\otimes\boldsymbol{a}_3+\boldsymbol{a}_3\otimes\boldsymbol{a}_2\right]$$

$$\mathbf{A}_2=\frac{1}{\sqrt{2}}\left[\boldsymbol{a}_3\otimes\boldsymbol{a}_1+\boldsymbol{a}_1\otimes\boldsymbol{a}_3\right]$$

$$\mathbf{A}_3=\frac{1}{\sqrt{2}}\left[\boldsymbol{a}_1\otimes\boldsymbol{a}_2+\boldsymbol{a}_2\otimes\boldsymbol{a}_1\right]$$

$\mathbf{T} = -p\mathbf{J} + \mu\mathbf{A} + \nu_0\mathbf{A}_0 + \nu_1\mathbf{A}_1 + \nu_2\mathbf{A}_2 + \nu_3\mathbf{A}_3$



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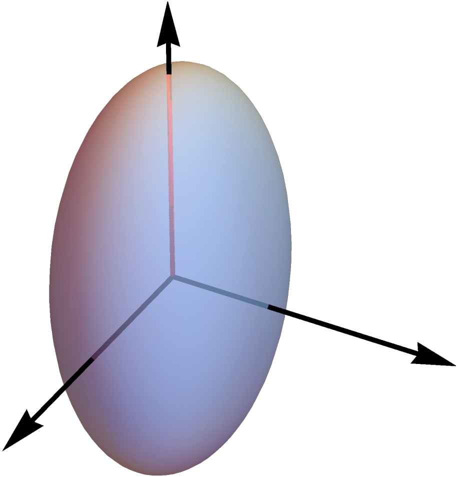

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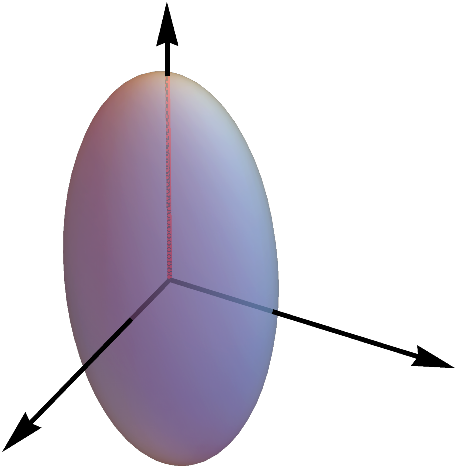

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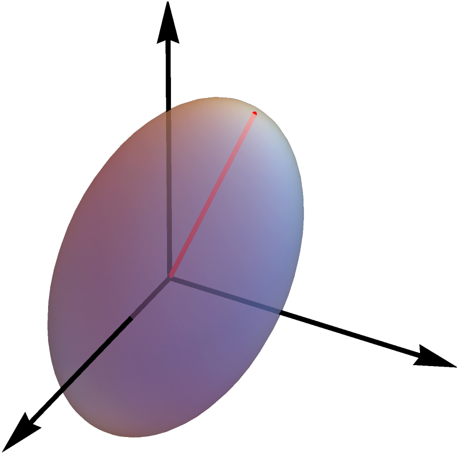

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Examples

Incompressible non-Newtonian fluids

We take $\mathbf{A} = \mathbf{D}/\|\mathbf{D}\|$, the symmetric part of the velocity gradient

The projection $\mu = \mathbf{T} \cdot \mathbf{D}$ is proportional to the rate at which the kinetic energy is transferred to other forms of energy, it leads to a generalization of the viscosity parameter for any local flow condition

The other coefficients are generalizations of the normal stress differences defined for simple shear flows

Details in: Giusteri G.G., Seto R., *J. Rheol.* 62(3), 713–723, 2018

Nonlinear elasticity

Among several possible choices, we consider $\mathbf{A}$ proportional to the deviatoric part of $\mathbf{B} = \mathbf{F}\mathbf{F}^{\mathsf{T}}$

The projections p, μ, and ν_0 correspond to stress contributions that are aligned to $\mathbf{B}$, the remaining ones are responsible for misalignments

Application: isotropic incompressible elastic materials

In this case it is natural to assume that the stress tensor must remain aligned with $\mathbf{B}$, so that $\nu_1 = \nu_2 = \nu_3 \equiv 0$ under any conditions, and p can be regarded as the multiplier of the incompressibility constraint

Denoting by λ_1^2, λ_2^2, and $(\lambda_1\lambda_2)^{-2}$ the three eigenvalues of $\mathbf{B}$, the parameter α in the definition of $\mathbf{A}$ is an explicit function of λ_1 and λ_2

If the stress projections depend solely on λ_1 and λ_2, the stress reads

$$\mathbf{T} = -p(\lambda_1, \lambda_2)\mathbf{J} + \mu(\lambda_1, \lambda_2)\mathbf{A}(\lambda_1, \lambda_2) + \nu_0(\lambda_1, \lambda_2)\mathbf{A}_0(\lambda_1, \lambda_2)$$

An empirical knowledge of the dependence of the stress projections on λ_1 and λ_2, that can be reached computationally (or experimentally) by investigating biaxial deformations, is sufficient to characterize the material and solve macroscopic continuum equations

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Thank you!