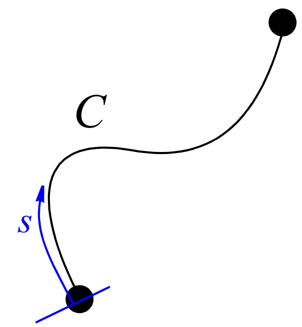
Line integrals in 3D



A line integral in space is often written in the form

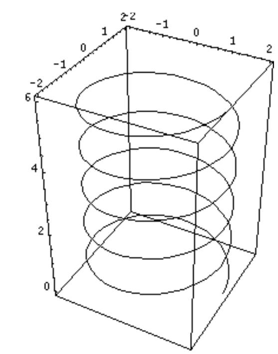
$$\int_C f(\underset{\sim}{\boldsymbol{x}})\,d\underset{\sim}{\boldsymbol{x}}$$

a path in space.

To evaluate line integrals, you *must* describe the path *parametrically* in the form

$$\underset{\sim}{\boldsymbol{x}} = \underset{\sim}{\boldsymbol{x}}(s).$$

Often, for example, s is selected to equal the arc length along the line, but *other interpretations might be more natural*.



EXAMPLE: Points on a helix may be described parametrically by

$$\underset{\sim}{\boldsymbol{x}} = \underset{\sim}{\boldsymbol{x}}(\theta) = R\cos\theta\,\underset{\sim}{\boldsymbol{e}}_1 + R\sin\theta\,\underset{\sim}{\boldsymbol{e}}_2 + k\,\theta\,\underset{\sim}{\boldsymbol{e}}_3.$$

Here, the parameter is the cylindrical θ coordinate, R (a constant) is the radius, and the constant k controls the rate of climb.

Once the path is parameterized, the integral is evaluated by $\displaystyle\int_C f(\underset{\sim}{\boldsymbol{x}})\,d\underset{\sim}{\boldsymbol{x}} = \int_{s_1}^{s_2} f(\underset{\sim}{\boldsymbol{x}})\frac{d\underset{\sim}{\boldsymbol{x}}}{ds}\,ds$.

Often, the "parameter" is "time" so that $\int_C f(\underset{\sim}{x})\,d\underset{\sim}{x} = \int_{t_1}^{t_2} f(\underset{\sim}{x})\dot{\underset{\sim}{x}}\,dt$.

Higher-order line integrals

In materials modeling, work is often written as

$$W = \int \underset{\approx}{\sigma} : d\underset{\approx}{\varepsilon}$$

This is a *line integral* in tensor space.

The strain path must be defined parametrically.

Usually, the parameter is time t, so the line integral is evaluated by

$$W = \int \underset{\approx}{\sigma} : \dot{\underset{\approx}{\varepsilon}}\,dt$$

Exact differentials in three dimensions

Under what conditions does there exist a potential $u(x_1, x_2, x_3)$ such that

$$du = f_1 dx_1 + f_2 dx_2 + f_3 dx_3$$

where the f_k are each functions of x_1, x_2, and x_3.

What does the notation $\int (f dx + g dy)$ mean ?!?

If the potential exists, then (by the chain rule) $f_i = \dfrac{\partial u}{\partial x_i}$

Mixed partials are order independent: $\dfrac{\partial^2 u}{\partial x_i \partial x_j} = \dfrac{\partial^2 u}{\partial x_j \partial x_i}$

Which implies that, if a potential exists, then $\boxed{\dfrac{\partial f_i}{\partial x_j} = \dfrac{\partial f_j}{\partial x_i}}$.

Conversely, if the functions f_k satisfy this equation, then a potential exists.

In other words, for a potential to exist, the matrix $H_{ij} = \dfrac{\partial f_i}{\partial x_j}$ must be symmetric.

An integral $\int (f_1 dx_1 + f_2 dx_2 + f_3 dx_3) = \int \underset{\sim}{\mathbf{f}} \bullet d\underset{\sim}{\mathbf{x}}$ is "path independent" only if the potential exists

and its value is $\int \underset{\sim}{\mathbf{f}} \bullet d\underset{\sim}{\mathbf{x}} = \int du = u^{\text{final}} - u^{\text{initial}}$.

Integrability

Consider a vector $\underset{\sim}{\boldsymbol{y}}$ that is a proper function of another vector $\underset{\sim}{\boldsymbol{x}}$.

Then $$dy_i = \frac{\partial y_i}{\partial x_j} dx_j$$

or $$dy_i = C_{ij} dx_j,$$ where $$C_{ij} = \frac{\partial y_i}{\partial x_j}$$

Order of second-partial derivatives may be swapped:

$$\frac{\partial^2 y_i}{\partial x_j \partial x_k} = \frac{\partial^2 y_i}{\partial x_k \partial x_j}.$$

Therefore $$\frac{\partial C_{ij}}{\partial x_k} = \frac{\partial C_{ik}}{\partial x_j}$$

Inverse question:

Given a tensor C_{ij} that varies with $\underset{\sim}{\boldsymbol{x}}$, under what conditions will a field $\underset{\sim}{\boldsymbol{y}}$ exist for which $C_{ij} = \dfrac{\partial y_i}{\partial x_j}$?

ANSWER: The field $\underset{\sim}{\boldsymbol{y}}$ will exist if and only if $\dfrac{\partial C_{ij}}{\partial x_k} = \dfrac{\partial C_{ik}}{\partial x_j}$.

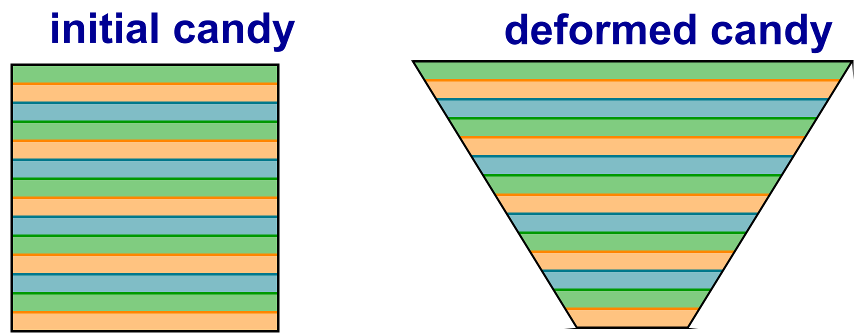
If so, $C_{ij} = \dfrac{\partial y_i}{\partial x_j}$ represents a set of nine coupled PDEs that may be solved to find the field $\underset{\sim}{\boldsymbol{y}}$.

Application: Compatibility

For large deformations, the deformation gradient tensor is defined $F_{ij} = \partial x_i / \partial X_j$.

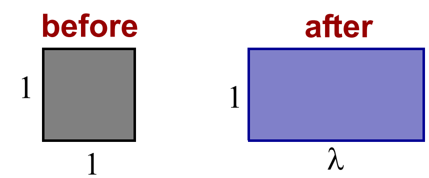
A spatially varying field F_{ij} is physically realizable if and only if $\dfrac{\partial F_{ij}}{\partial X_k} = \dfrac{\partial F_{ik}}{\partial X_j}$.

Example: every layer in the following picture appears to stretch horizontally:



A horizontal stretch *for a homogeneous deformation* has a deformation gradient of the form

$$[\underset{\approx}{\mathbf{F}}] = \begin{bmatrix} \lambda & 0 \\ 0 & 1 \end{bmatrix}$$



You might be (wrongly) tempted to say that the “candy” problem must have the same $\underset{\approx}{\mathbf{F}}$ of a similar form:

$$[\underset{\approx}{\mathbf{F}}] = \begin{bmatrix} \alpha X_2 + \beta & 0 \\ 0 & 1 \end{bmatrix}$$ (this is WRONG)

This must be wrong, however, because $\dfrac{\partial F_{11}}{\partial X_2} \neq \dfrac{\partial F_{12}}{\partial X_1}$ (Compatibility is violated!)

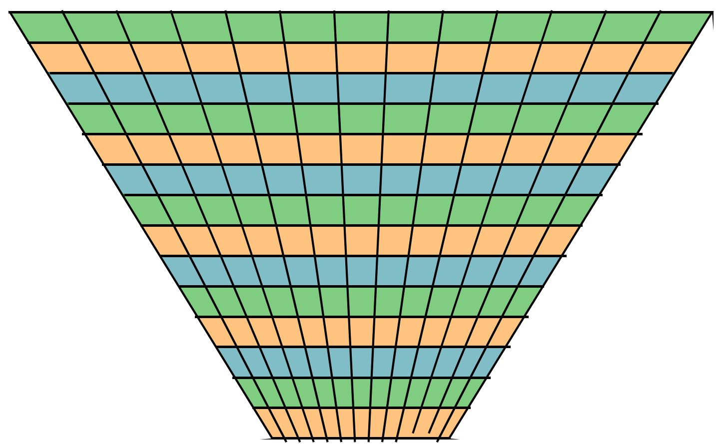
An *allowable* answer is

$$[\underset{\sim}{\boldsymbol{F}}] = \begin{bmatrix} \alpha X_2 + \beta & \alpha X_1 \\ 0 & 1 \end{bmatrix}$$

The “bad” solution presumed that squares deformed to *rectangles*.

This “good” solution lets squares deform to *parallelograms*.

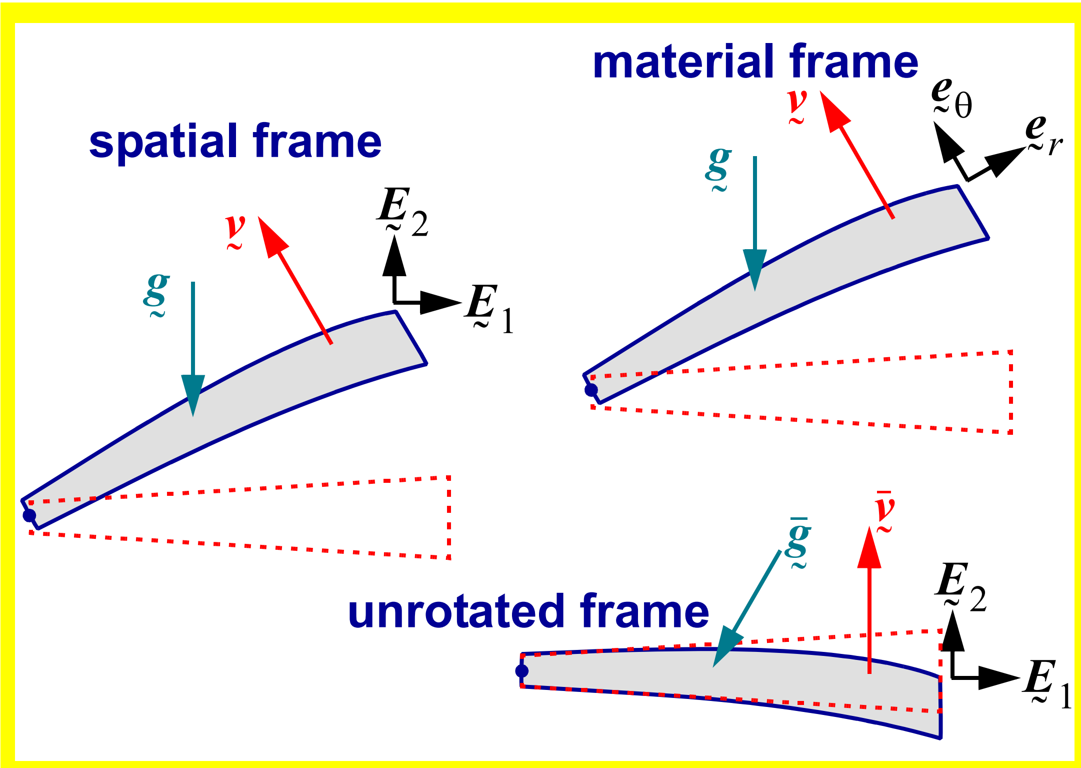
deformed candy



Frame Indifference

Preliminaries

Multiple ways to analyze stresses on a windmill blade:

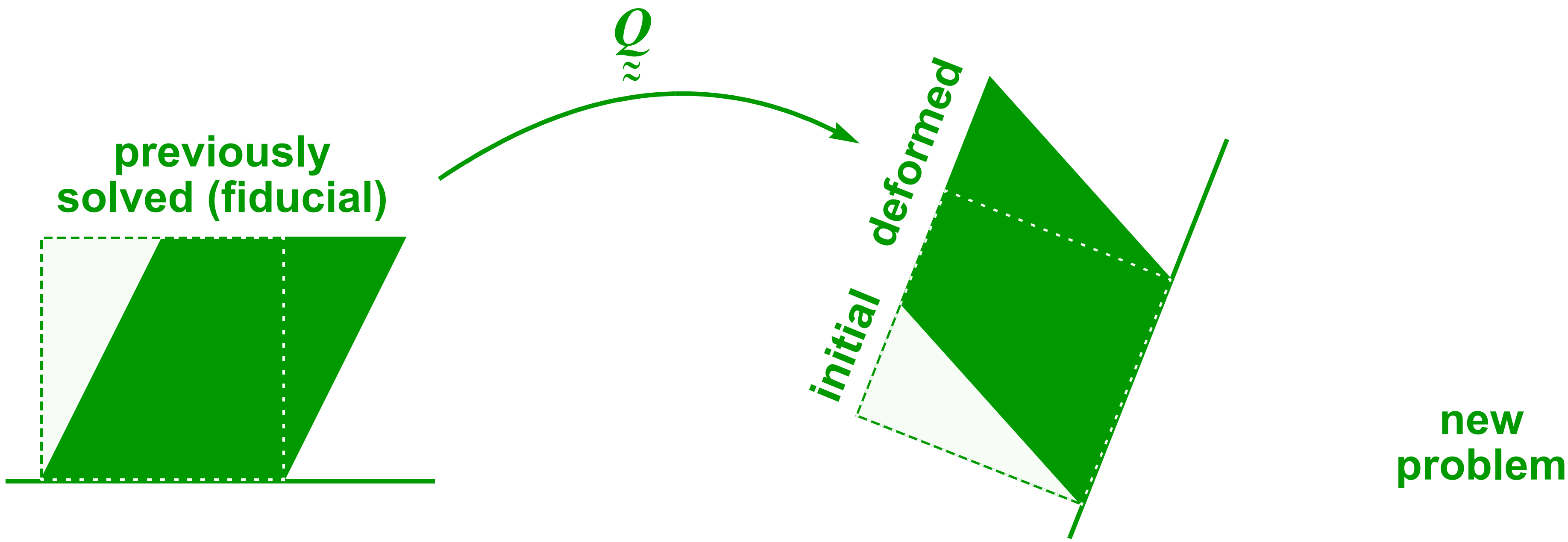


Suppose a deformation field is identical to one that you have analyzed in the past, except it is rigidly rotated and/or translated.

QUESTION: Can you use the already-solved problem to help you solve the new problem?

ANSWER: Yes, but you need to decide: "space rotation" or "superimposed rotation" ?

SPACE ROTATION PROBLEM (easy)



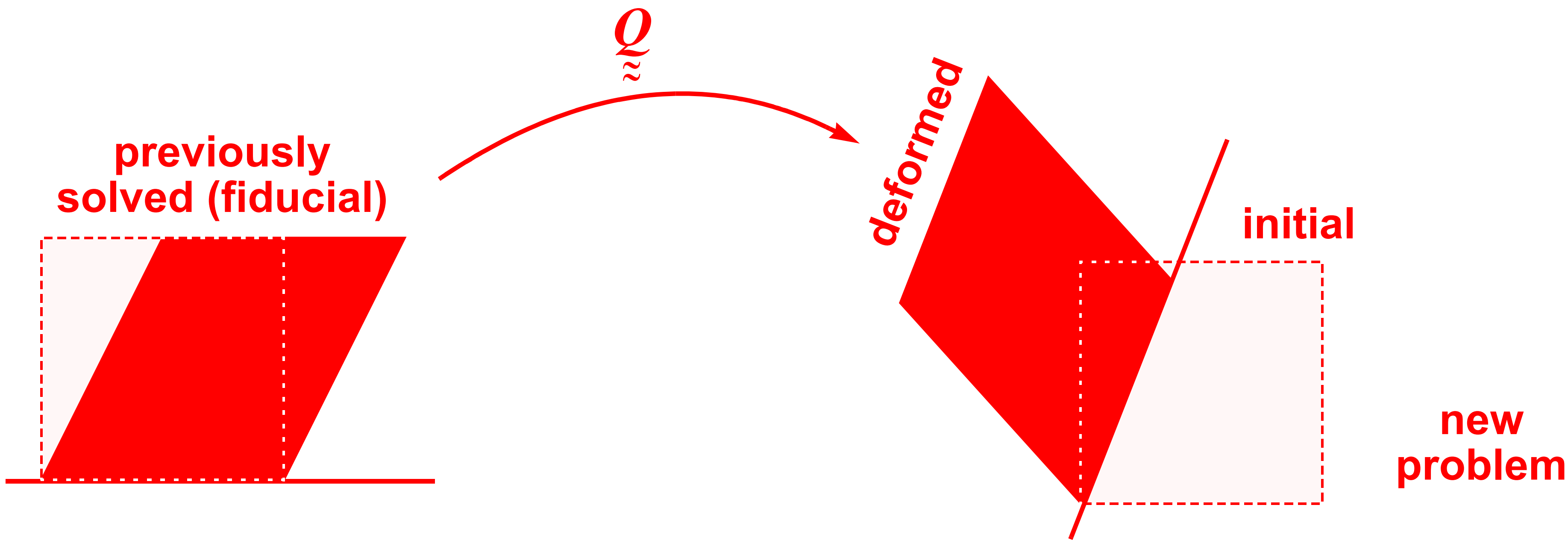
all scalars: $s^{\text{new}} = s^{\text{old}}$ $\qquad$ $s^{\text{new}} = s^{\text{old}}$

all free vectors: $\underset{\sim}{v}^{\text{new}} = \underset{\approx}{Q} \bullet \underset{\sim}{v}^{\text{old}}$ $\qquad$ $v_i^{\text{new}} = Q_{ip} v_p^{\text{old}}$

all second-order tensors: $\underset{\approx}{T}^{\text{new}} = \underset{\approx}{Q} \bullet \underset{\approx}{T}^{\text{old}} \bullet \underset{\approx}{Q}^T$ $\qquad$ $T_{ij}^{\text{new}} = Q_{ip} Q_{jq} T_{pq}^{\text{old}}$

all third-order tensors: $\qquad$ $\zeta_{ijk}^{\text{new}} = Q_{ip} Q_{iq} Q_{ir} \zeta_{pqr}^{\text{old}}$

SUPERIMPOSED ROTATION PROBLEM (harder)



spatial (objective) **scalars:** $s^{\text{new}} = s^{\text{old}}$

spatial (objective) **vectors:** $\underset{\sim}{v}^{\text{new}} = \underset{\approx}{Q} \bullet \underset{\sim}{v}^{\text{old}}$

spatial (objective) **tensors:** $\underset{\approx}{T}^{\text{new}} = \underset{\approx}{Q} \bullet \underset{\approx}{T}^{\text{old}} \bullet \underset{\approx}{Q}^{T}$

reference scalars: $s^{\text{new}} = s^{\text{old}}$

reference vectors: $\underset{\sim}{v}^{\text{new}} = \underset{\sim}{v}^{\text{old}}$

reference tensors: $\underset{\approx}{T}^{\text{new}} = \underset{\approx}{T}^{\text{old}}$

multi-point quantities: transform like neither spatial nor reference quantities.

TERMINOLOGY

fiducial = previously solved problem.

star = new problem with *same* initial state, and deformed state identical to the fiducial problem but with superimposed rotation.

spatial (objective): a quantity that transforms like the *space rotation* problem.

reference: a quantity that is unaffected by superimposed rotation

multi-point: a quantity that is neither objective nor reference

The superimposed rotation problem

A "**material fiber**" $\underset{\sim}{\mu}$ is a vector connecting two points in a body.

Any *initial* material fiber $\underset{\sim}{\mu}_0$ is a reference quantity ($\underset{\sim}{\mu}_0^* = \underset{\sim}{\mu}_0$).

The *deformed* material fiber is a spatial quantity ($\underset{\sim}{\mu}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\sim}{\mu}$).

The deformation gradient is a **two-point tensor**.

Let $\underset{\approx}{\boldsymbol{F}}$ = deformation gradient for the fiducial problem.

Let $\underset{\approx}{\boldsymbol{F}}^*$ = deformation gradient for the "star" problem

$$\underset{\approx}{\boldsymbol{F}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{F}} \qquad \text{(two-point)}$$

Likewise, the polar rotation tensor becomes, after superimposed rotation,

$$\underset{\approx}{\boldsymbol{R}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{R}} \qquad \text{(two-point)}$$

Cauchy stress is force per *current* area, not force per initial area.

Its definition requires no knowledge of the initial configuration.

$$\underset{\approx}{\sigma}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\sigma} \bullet \underset{\approx}{\boldsymbol{Q}}^T \qquad \text{(spatial, objective)}$$

The right polar stretch tensor $\underset{\approx}{\boldsymbol{U}}$ is defined as material stretch that occurs *before* rotation. It is therefore unaffected by superimposed rotation:

$$\underset{\approx}{\boldsymbol{U}}^* = \underset{\approx}{\boldsymbol{U}} \qquad \text{(reference)}$$

The left polar stretch tensor $\underset{\approx}{\boldsymbol{V}}$ is the stretch *after* material rotation.

Superposed rigid rotation will re-orient the eigenvectors without changing the eigenvalues.

$$\underset{\approx}{\boldsymbol{V}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{V}} \bullet \underset{\approx}{\boldsymbol{Q}}^T \qquad \text{(spatial, objective)}$$

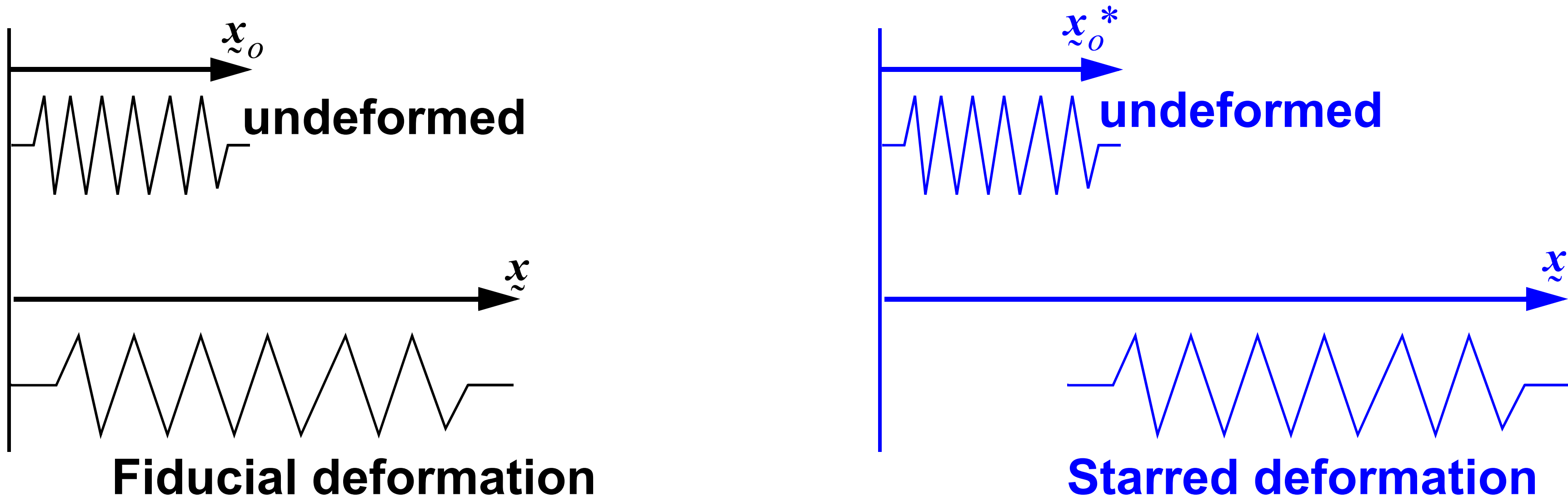
The **principle of material frame indifference** (PMFI) is the very intuitive requirement that superimposed rigid motion of a material will require the applied forces and stresses to co-rotate and co-translate in a manner consistent with their definition. Regardless of whether you apply a material model for the fiducial problem or for the star problem, the results must be consistent with these “objectivity” relations.

Mathematics of frame indifference (introduction)

Spring Example: Translational frame indifference

spring constant
change in length

Force in spring: $f = k\delta$.



Let $\underset{\sim}{x}$ = current location of the tip of the spring.
Let $\underset{\sim}{x}_o$ = original (unstressed) location of the tip of the spring.

First (BAD) attempt at a *vector* spring equation:

$\underset{\sim}{f} = k(\underset{\sim}{x} - \underset{\sim}{x}_o)$ ← (violates translational PMFI)

Consider

Fiducial deformation: stretch the spring by some known amount.

Starred deformation: stretch the spring by the same amount and also translate it by an amount $\underset{\sim}{c}$.

Both scenarios involve the same *starting* tip location, so

$$\underset{\sim}{x}_o^* = \underset{\sim}{x}_o . \tag{1}$$

The star deformation has the same final tip location *plus extra translation* $\underset{\sim}{c}$*:*

$$\underset{\sim}{x}^* = \underset{\sim}{x} + \underset{\sim}{c} . \tag{2}$$

The problems differ only by translation, so they both involve the same spring elongation. They *should* therefore involve the same spring force.

$$\underset{\sim}{f}^*_{\text{desired}} = \underset{\sim}{f} .$$

Does the model $\underset{\sim}{f} = k(\underset{\sim}{x} - \underset{\sim}{x}_o)$ give this desired result?

For starred deformation, this (bad) spring model predicts

$$\underset{\sim}{f}^*_{\text{predicted}} = k(\underset{\sim}{x}^* - \underset{\sim}{x}_o^*) \tag{3}$$

Substitute (1) and (2) into (3) to obtain

$$\underset{\sim}{f}^*_{\text{predicted}} = k(\underset{\sim}{x} + \underset{\sim}{c} - \underset{\sim}{x}_o) = \underset{\sim}{f}^*_{\text{desired}} + k\underset{\sim}{c} .$$

$\underset{\sim}{f}^*_{\text{predicted}} \neq \underset{\sim}{f}^*_{\text{desired}}$ **(NOT translationally invariant!)**

Spring Example: Rotational frame indifference.

To satisfy *translation* invariance, consider a revised spring equation

$$\underset{\sim}{f} = k(\underset{\sim}{L} - \underset{\sim}{L}_o) \qquad \leftarrow \text{better, but still bad.} \qquad (\text{here, } \underset{\sim}{L} = \underset{\sim}{x}^{\text{tip}} - \underset{\sim}{x}^{\text{tail}})$$

Because $\underset{\sim}{L}$ represents the difference between two points on the spring, it will be invariant under a superimposed translation.

Under *translation*, $\underset{\sim}{L}^* = \underset{\sim}{L}$

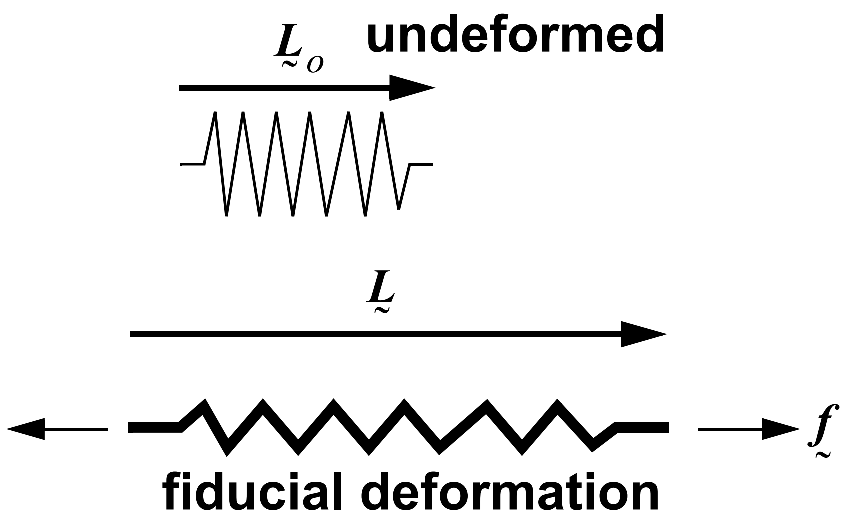
As before, $\underset{\sim}{L}_o^* = \underset{\sim}{L}_o$. Therefore, $\underset{\sim}{f}^* = \underset{\sim}{f}$ under translation, as desired.

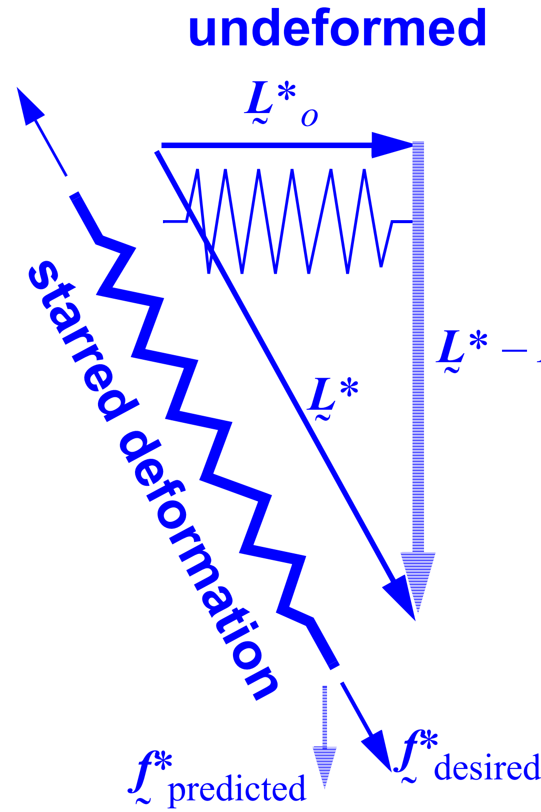
This model permits force to *co-translate* with the spring. That's good. However . . .

Another requirement of PMFI:

Force must *co-rotate* with the spring.

This model FAILS in this respect.





MODEL PREDICTION

$$\underset{\sim}{f}^* = k(\underset{\sim}{L}^* - \underset{\sim}{L}^*{}_o)$$

PROPOSED MODEL

$$\underset{\sim}{f} = k(\underset{\sim}{L} - \underset{\sim}{L}_o)$$

fiducial: stretch the spring without rotation

starred: same deformation as fiducial, but also rigidly rotate the spring.

$$\underset{\sim}{L}_o^* = \underset{\sim}{L}_o \qquad \underset{\sim}{L}^* = \underset{\approx}{Q} \bullet \underset{\sim}{L} \qquad \underset{\sim}{f}^*{}_{\text{desired}} = \underset{\approx}{Q} \bullet \underset{\sim}{f}.$$

From the sketch, it's clear that $\underset{\sim}{f}^*{}_{\text{predicted}} \neq \underset{\sim}{f}^*{}_{\text{desired}}$ **(NOT rotationally invariant!)**

In fact, $\underset{\sim}{f}^*_{\text{predicted}} - \underset{\sim}{f}^*_{\text{desired}} = k(\underset{\approx}{Q} \bullet \underset{\sim}{L}_o - \underset{\sim}{L}_o)$. PMFI requires this to be $\underset{\sim}{0}$, which happens only if $\underset{\approx}{Q} = \underset{\approx}{I}$.

At last. . . a spring model that satisfies PMFI.

To satisfy both translational and rotational frame indifference, consider

$$\underset{\sim}{f} = k\delta\underset{\sim}{n} \qquad \text{where } \delta \equiv \|\underset{\sim}{L}\| - \|\underset{\sim}{L}_o\| \text{, and } \underset{\sim}{n} = \frac{\underset{\sim}{L}}{\|\underset{\sim}{L}\|}$$

← This one satisfies PMFI **!**

The only difference between the fiducial and starred deformations is a rigid motion.

Therefore, deformed lengths are the same in both cases. Hence, $\|\underset{\sim}{L}^*\| = \|\underset{\sim}{L}\|$.

As before, the initial state is the same for both cases, so $\|\underset{\sim}{L}_o^*\| = \|\underset{\sim}{L}_o\|$.

Consequently,

$$\delta^* = \delta$$

Under a superimposed rigid motion, $\underset{\sim}{L}^* = \underset{\approx}{Q} \bullet \underset{\sim}{L}$. Therefore,

$$\underset{\sim}{n}^* = \underset{\approx}{Q} \bullet \underset{\sim}{n}.$$

Thus,

$$\underset{\sim}{f}^*_{\text{predicted}} = k\delta^*\underset{\sim}{n}^* = k\delta\underset{\approx}{Q} \bullet \underset{\sim}{n} = \underset{\approx}{Q} \bullet (k\delta\underset{\sim}{n}) = \underset{\approx}{Q} \bullet \underset{\sim}{f} = \underset{\sim}{f}^*_{\text{desired}}$$

YAHOO! **Success at last!**.

PMFI in material constitutive models

Any material model must be invariant under a basis change (space rotation problem).
This requirement is *necessary,* but unrelated to PMFI.

PMFI requires *consistency* of predictions when comparing deformations that differ by superimpose rotation. You can work out *in advance* how variables *should* transform under superimposed rotation.

Input (independent variables) sent to your constitutive model must convey sufficient information to allow model predictions (output dependent variables) to transform correctly under superimposed rotation.

- If you apply your model to a fiducial problem, then you obtain a certain fiducial prediction.
- If you apply the model to a "star" problem that is identical to the fiducial problem except that the input corresponds to a superimposed rotation, then the output needs correspond to the superimposed rotation.

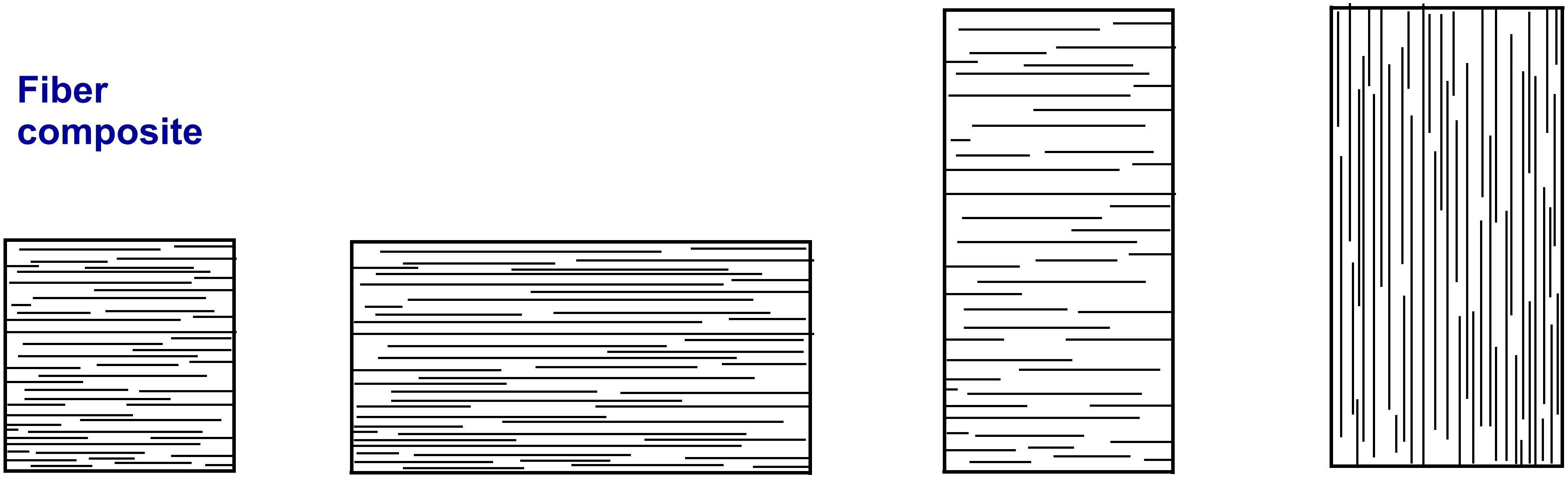
Suppose the model takes the stretch $\underset{\approx}{\boldsymbol{V}}$ as its <u>only</u> input, and returns the Cauchy stress $\underset{\approx}{\sigma}$ as output.

When a "star" stretch $\underset{\approx}{\boldsymbol{V}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{V}} \bullet \underset{\approx}{\boldsymbol{Q}}^T$ is sent as input,

PMFI demands that the model must return $\underset{\approx}{\sigma}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\sigma} \bullet \underset{\approx}{\boldsymbol{Q}}^T$ as output.

Here's why a model that takes only left stretch V is deficient.

Fiber composite



$$[F] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [F] = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \qquad [F] = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \qquad [F] = \begin{bmatrix} 0 & -1 \\ 2 & 0 \end{bmatrix}$$

$$[R] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [R] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [R] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [R] = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$[V] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [V] = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \qquad [V] = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \qquad [V] = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

PMFI in general materials modeling

When testing for frame indifference, you must first note what variables are involved.

You must use physical reasoning along with rigorous mathematical consistency analysis to assert how those quantities are *supposed to* change upon a superimposed rigid motion.

PMFI analysis for <u>linear</u> elasticity. Consider a constitutive model in which Cauchy stress $\underset{\approx}{\sigma}$ is regarded to depend linearly on some *spatial* strain $\underset{\approx}{\varepsilon}$.

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}, \qquad \text{or} \qquad \underset{\approx}{\sigma} = \underset{\approx\approx}{E} : \underset{\approx}{\varepsilon} \tag{1}$$

Since Cauchy stress is spatial, this constitutive model satisfies PMFI only if

$$\underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\sigma} \bullet \underset{\approx}{\boldsymbol{Q}}^T = \underset{\approx\approx}{E} : (\underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\varepsilon} \bullet \underset{\approx}{\boldsymbol{Q}}^T) \qquad \text{for all orthogonal } \underset{\approx}{\boldsymbol{Q}}$$

Indicial form, recalling Eq. (1),

$$Q_{pi}(E_{ijkl}\varepsilon_{kl})Q_{qj} = E_{pqmn}(Q_{mk}\varepsilon_{kl}Q_{nl})$$

This must hold for all strains, and therefore, PMFI requires that

$$Q_{pi}(E_{ijkl})Q_{qj} = E_{pqmn}(Q_{mk}Q_{nl})$$

which may be rearranged to give

$$E_{ijkl} = E_{pqmn}(Q_{pi}Q_{qj}Q_{mk}Q_{nl})$$

This says that $\underset{\approx\approx}{E}$ must be isotropic.

If your material is *anisotropic*, then you *must* receive more than just spatial strain as input to satisfy PMFI.

Satisfying PMFI does not per se make your model valid for large deformations.

A model that satisfies PMFI is merely self-consistent for arbitrarily large rotations. PMFI says *nothing* about whether your model is any good for large material *distortions* (i.e., problems where material fibers significantly rotate and stretch *relative to other fibers*).

Alternative configurations and alternative stress/strain measures are often used to get better results under large distortions. Finding appropriate representations for distortion of material symmetry directions is primarily the subject of *physics*, not PMFI.

Stress Rates

PMFI in rate forms of constitutive equations

Consider a constitutive law

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}, \qquad \text{or} \qquad \underset{\sim}{\sigma} = \underset{\approx}{\underset{\sim}{E}} : \underset{\sim}{\varepsilon}$$

in which the stiffness tensor is constant and the stress and strain are both spatial.

To satisfy PMFI, let's presume that the stiffness tensor is also isotropic.

Taking the time rate of both sides gives

$$\dot{\sigma}_{ij} = E_{ijkl}\dot{\varepsilon}_{kl}, \qquad \text{or} \qquad \dot{\underset{\sim}{\sigma}} = \underset{\approx}{\underset{\sim}{E}} : \dot{\underset{\sim}{\varepsilon}}$$

This rate constitutive equation satisfies PMFI because it was obtained by differentiating a frame indifferent equation. Here's why . . .

For for isotropic linear elasticity, the stress deviator S_{ij} is related to the strain deviator γ_{ij} by

$$\underset{\approx}{\mathbf{S}} = 2G\underset{\approx}{\gamma},$$

where G is the shear modulus (a constant). Under superimposed rotation, this becomes

$$\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\mathbf{S}} \bullet \underset{\approx}{\mathbf{Q}}^T = 2G\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\gamma} \bullet \underset{\approx}{\mathbf{Q}}^T.$$

In rate form,

$$\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\dot{\mathbf{S}}} \bullet \underset{\approx}{\mathbf{Q}}^T + \underset{\approx}{\dot{\mathbf{Q}}} \bullet \underset{\approx}{\mathbf{S}} \bullet \underset{\approx}{\mathbf{Q}}^T + \underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\mathbf{S}} \bullet \underset{\approx}{\dot{\mathbf{Q}}}^T = 2G[\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\dot{\gamma}} \bullet \underset{\approx}{\mathbf{Q}}^T + \underset{\approx}{\dot{\mathbf{Q}}} \bullet \underset{\approx}{\gamma} \bullet \underset{\approx}{\mathbf{Q}}^T + \underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\gamma} \bullet \underset{\approx}{\dot{\mathbf{Q}}}^T].$$

Recalling that $\underset{\approx}{\mathbf{S}} = 2G\underset{\approx}{\gamma}$, the **RED** terms involving $\underset{\approx}{\dot{\mathbf{Q}}}$ all cancel, leaving only

$$\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\dot{\mathbf{S}}} \bullet \underset{\approx}{\mathbf{Q}}^T = 2G[\underset{\approx}{\mathbf{Q}} \bullet \underset{\approx}{\dot{\gamma}} \bullet \underset{\approx}{\mathbf{Q}}^T]$$

which is self consistent with

$$\underset{\approx}{\dot{\mathbf{S}}} = 2G\underset{\approx}{\dot{\gamma}}$$

PMFI is satisfied for the rate equation.

In general, whenever a *non-rate* constitutive relation satisfies PMFI, then its rate form will also satisfy PMFI.

REPLACING A GENUINE STRAIN RATE WITH SOME "APPROXIMATION" TO STRAIN RATE HAS *DISTRESSING* PMFI RAMIFICATIONS!

The so-called "rate" of deformation tensor $\underset{\approx}{\boldsymbol{D}}$ is just the symmetric part of the velocity gradient:

$$\underset{\approx}{\boldsymbol{D}} = \tfrac{1}{2}(\underset{\approx}{\boldsymbol{L}} + \underset{\approx}{\boldsymbol{L}}^T), \text{ where } L_{ij} = \frac{\partial v_i}{\partial x_j}.$$

If the principal directions of stretch never change, it equals the rate of the logarithmic strain. Otherwise, it is not a true rate.

The rate of logarithmic strain, $\underset{\approx}{\dot{\varepsilon}}$, is very difficult to compute, whereas $\underset{\approx}{\boldsymbol{D}}$ is very easy to compute.

For this reason, many people take a perfectly valid (PMFI-conforming) constitutive model in rate form

$$\underset{\approx}{\dot{\sigma}} = g(\underset{\approx}{\dot{\varepsilon}})$$ [satisfies PMFI if the material is isotropic]

and **mess it up** by replacing it with

$$\underset{\approx}{\dot{\sigma}} = g(\underset{\approx}{\boldsymbol{D}}).$$ [violates PMFI]

The original material model $\dot{\underset{\approx}{\sigma}} = g(\dot{\underset{\approx}{\varepsilon}})$ satisfied PMFI because

$$\underset{\approx}{\boldsymbol{Q}} \bullet \dot{\underset{\approx}{\boldsymbol{S}}} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underbrace{\dot{\underset{\approx}{\boldsymbol{Q}}} \bullet \underset{\approx}{\boldsymbol{S}} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{S}} \bullet \dot{\underset{\approx}{\boldsymbol{Q}}}^T}_{\text{These terms cancel with those on right-hand side}} = 2G[\underset{\approx}{\boldsymbol{Q}} \bullet \dot{\underset{\approx}{\gamma}} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underbrace{\dot{\underset{\approx}{\boldsymbol{Q}}} \bullet \underset{\approx}{\gamma} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\gamma} \bullet \dot{\underset{\approx}{\boldsymbol{Q}}}^T}]$$

The new (bad) material model $\dot{\underset{\approx}{\sigma}} = g(\underset{\approx}{\boldsymbol{D}})$ violates PMFI.

The tensor $\underset{\approx}{\boldsymbol{D}}$ is spatial, so the PMFI requirement is

$$\underset{\approx}{\boldsymbol{Q}} \bullet \dot{\underset{\approx}{\boldsymbol{S}}} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underbrace{\dot{\underset{\approx}{\boldsymbol{Q}}} \bullet \underset{\approx}{\boldsymbol{S}} \bullet \underset{\approx}{\boldsymbol{Q}}^T + \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{S}} \bullet \dot{\underset{\approx}{\boldsymbol{Q}}}^T}_{\text{These terms no longer “go away”}} = 2G[\underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{D}}^{\text{dev}} \bullet \underset{\approx}{\boldsymbol{Q}}^T]$$

Replacement of a *genuine* strain rate with $\underset{\approx}{\boldsymbol{D}}$ is going to require replacing $\dot{\underset{\approx}{\sigma}}$ with a “**pseudo stress rate**” (often more graciously called an **objective stress rate**) that subtracts away the offending terms.

The violation of PMFI can be "repaired" by replacing the "bad" constitutive model with

$$\overset{\circ}{\underset{\approx}{\sigma}} = g(\underset{\approx}{\boldsymbol{D}}),$$

where $\overset{\circ}{\underset{\approx}{\sigma}}$ denotes a special "co-rotational" rate that *effectively eliminates the part of the stress rate caused by rotation rates*.

The co-rotational rate $\overset{\circ}{\underset{\approx}{\sigma}}$ is (*must be*) a spatial tensor to satisfy PMFI for isotropic materials.

Objective co-rotational rates (Convected, Jaumann, Polar)

Co-rotational stress rates are often defined in the form

$$\overset{\circ}{\underset{\approx}{\sigma}} = \dot{\underset{\approx}{\sigma}} - \underset{\approx}{\Lambda} \bullet \underset{\approx}{\sigma} - \underset{\approx}{\sigma} \bullet \underset{\approx}{\Lambda}^T$$

The tensor $\underset{\approx}{\Lambda}$ is required only to transform under superimposed rotation so that

$$\underset{\approx}{\Lambda}^* = \underset{\approx}{\Upsilon} + \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\Lambda} \bullet \underset{\approx}{\boldsymbol{Q}}^T, \qquad \text{where} \qquad \underset{\approx}{\Upsilon} = \dot{\underset{\approx}{\boldsymbol{Q}}} \bullet \underset{\approx}{\boldsymbol{Q}}^T$$

This will ensure that the pseudo (co-rotational) stress rate is spatial (as needed by PMFI):

$$\overset{\circ}{\underset{\approx}{\sigma}}{}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \overset{\circ}{\underset{\approx}{\sigma}} \bullet \underset{\approx}{\boldsymbol{Q}}^T$$

Possible choices for the "nebulous" spin-like tensor $\underset{\approx}{\Lambda}$

Velocity gradient ($L_{ij} = \partial v_i / \partial x_j$)

Convected rate

If $\underset{\approx}{\Lambda} = \underset{\approx}{L}$ then $\overset{\circ}{\underset{\approx}{\sigma}} = \dot{\underset{\approx}{\sigma}} - \underset{\approx}{L} \bullet \underset{\approx}{\sigma} - \underset{\approx}{\sigma} \bullet \underset{\approx}{L}^T$

Vorticity tensor ($\underset{\approx}{W} = \mathrm{skw}\underset{\approx}{L}$). Being skew symmetric, $\underset{\approx}{W}^T = -\underset{\approx}{W}$.

Jaumann rate

If $\underset{\approx}{\Lambda} = \underset{\approx}{W} = \frac{1}{2}(\underset{\approx}{L} - \underset{\approx}{L}^T)$ then $\overset{\circ}{\underset{\approx}{\sigma}} = \dot{\underset{\approx}{\sigma}} - \underset{\approx}{W} \bullet \underset{\approx}{\sigma} + \underset{\approx}{\sigma} \bullet \underset{\approx}{W}$

The the nebulous tensor $\underset{\approx}{\Lambda}$ can be taken as the polar spin tensor

Polar rate

If $\underset{\approx}{\Lambda} = \underset{\approx}{\Omega} = \dot{\underset{\approx}{R}} \bullet \underset{\approx}{R}^T$ then $\overset{\circ}{\underset{\approx}{\sigma}} = \dot{\underset{\approx}{\sigma}} - \underset{\approx}{\Omega} \bullet \underset{\approx}{\sigma} + \underset{\approx}{\sigma} \bullet \underset{\approx}{\Omega}$

All of these choices ensure that

$$\overset{\circ}{\underset{\approx}{\sigma}}{}^* = \underset{\approx}{Q} \bullet \overset{\circ}{\underset{\approx}{\sigma}} \bullet \underset{\approx}{Q}^T$$

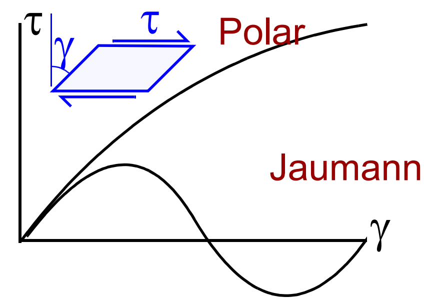
In other words, the co-rotational rate is a spatial tensor! Consequently, the "repaired" constitutive model $\overset{\circ}{\underset{\approx}{\sigma}} = g(\underset{\approx}{D})$ satisfies PMFI so long as the constitutive function g is isotropic.

Anisotropy can be accommodated by introducing additional "material orientation" input variables that transform spatially.

Oscillatory stresses under simple shear. **REMEMBER!** satisfying PMFI will not ensure the model will give accurate or even reasonable results.

To demonstrate that satisfying PMFI is merely a *consistency* condition that is *necessary but not sufficient* to obtain sensible constitutive model predictions, Dienes[1] considered simple shear with isotropic linear-elasticity in the form

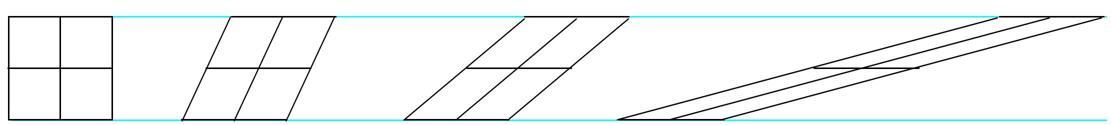
$$\overset{\circ}{\underset{\approx}{\sigma}} = \underset{\approx\approx}{\boldsymbol{E}}:\underset{\approx}{\boldsymbol{D}}$$



Dienes demonstrated that the *Jaumann* rate predicts anomalous oscillatory shear stresses whereas the polar rate predicts intuitively more appealing monotonically increasing shear stress.

The Jaumann rate performs so poorly because it uses vorticity $\underset{\approx}{\boldsymbol{W}}$ as the "material spin" used to "subtract away" the rotational part of the stress rate.

However, for simple shear, vorticity $\underset{\approx}{\boldsymbol{W}}$ is constant throughout time. The Jaumann objective rate effectively presumes that a material element tumbles *unceasingly*. Drawing a single material element as it deforms demonstrates that such thinking is flawed.



1. DIENES, J.K. (1979) *Acta Mechanica* **32**, pp. 217-232.
Incidentally, this effect was reported in the rheology literature earlier than Dienes' paper. Dienes influenced the *solid mechanics* community.

Lie derivatives and reference configurations

Lie derivatives justify the concept of *reference* constitutive models by making the connection with co-rotational (objective) rates clear.

Let $\underset{\approx}{\boldsymbol{G}}$ denote any tensor that transforms under a rigid superimposed rotation $\underset{\approx}{\boldsymbol{Q}}$ according to

$$\underset{\approx}{\boldsymbol{G}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{G}} \qquad \text{(two point tensor)}$$

Some choices . . .

- **co-convected:** $\underset{\approx}{\boldsymbol{G}} = \underset{\approx}{\boldsymbol{F}}$, where $\underset{\approx}{\boldsymbol{F}}$ is the deformation gradient tensor.
- **contra-convected:** $\underset{\approx}{\boldsymbol{G}} = J\underset{\approx}{\boldsymbol{F}}^{-T}$, where $J = \det\underset{\approx}{\boldsymbol{F}}$.
- **polar:** $\underset{\approx}{\boldsymbol{G}} = \underset{\approx}{\boldsymbol{R}}$, where $\underset{\approx}{\boldsymbol{R}}$ is the polar rotation tensor.

Consider any spatial tensor $\underset{\approx}{\boldsymbol{A}}$. Define a generalized "overbar" operation as

$$\overline{\underset{\approx}{\boldsymbol{A}}} \equiv \underset{\approx}{\boldsymbol{G}}^{-1} \bullet \underset{\approx}{\boldsymbol{A}} \bullet \underset{\approx}{\boldsymbol{G}}^{-T}$$

The basis expansion of $\overline{\underset{\approx}{\boldsymbol{A}}}$ is

$$\overline{\underset{\approx}{\boldsymbol{A}}} = A_{ij}(\underset{\approx}{\boldsymbol{G}}^{-1} \bullet \underset{\sim}{\boldsymbol{e}}_i)(\underset{\sim}{\boldsymbol{e}}_j \bullet \underset{\approx}{\boldsymbol{G}}^{-T}) = A_{ij}(\underset{\approx}{\boldsymbol{G}}^{-1} \bullet \underset{\sim}{\boldsymbol{e}}_i)(\underset{\approx}{\boldsymbol{G}}^{-1} \bullet \underset{\sim}{\boldsymbol{e}}_j),$$

If a tensor $\underset{\approx}{\boldsymbol{A}}$ is a spatial, then $\underset{\approx}{\boldsymbol{A}}^* = \underset{\approx}{\boldsymbol{Q}} \bullet \underset{\approx}{\boldsymbol{A}} \bullet \underset{\approx}{\boldsymbol{Q}}^T$, and therefore $\overline{\underset{\approx}{\boldsymbol{A}}}$ is a *reference* tensor $\overline{\underset{\approx}{\boldsymbol{A}}}^* = \overline{\underset{\approx}{\boldsymbol{A}}}$

To take rates of $\overline{\mathbf{A}} \equiv \mathbf{G}^{-1} \bullet \mathbf{A} \bullet \mathbf{G}^{-T}$, you need the following helper identity for the rate of an inverse:

$$\frac{d}{dt}\mathbf{G}^{-1} = -\mathbf{G}^{-1} \bullet \dot{\mathbf{G}} \bullet \mathbf{G}^{-1} = -\mathbf{G}^{-1} \bullet \mathbf{\Lambda}, \qquad \text{where} \qquad \mathbf{\Lambda} \equiv \dot{\mathbf{G}} \bullet \mathbf{G}^{-1}.$$

Using this, you can show that

$$\dot{\overline{\mathbf{A}}} = \mathbf{G}^{-1} \bullet \mathring{\mathbf{A}} \bullet \mathbf{G}^{-T}, \qquad \text{where } \mathring{\mathbf{A}} = \dot{\mathbf{A}} - \mathbf{\Lambda} \bullet \mathbf{A} - \mathbf{A} \bullet \mathbf{\Lambda}^T.$$

which may be written

$$\dot{\overline{\mathbf{A}}} = \overline{\mathring{\mathbf{A}}}$$

The *ordinary* rate of the bared tensor is the same as the bar operation acting on the co-rotational rate.

Most textbooks write this "Lie derivative" in an equivalent (but more confusing) way:

$$\mathring{\mathbf{A}} = \mathbf{G} \bullet \frac{d}{dt}(\mathbf{G}^{-1} \bullet \mathbf{A} \bullet \mathbf{G}^{-T}) \bullet \mathbf{G}^T.$$

WHY ARE LIE DERIVATIVES USEFUL?

Lie derivatives let you apply a constitutive model in a *reference* configuration where rates are *genuine true rates*, not pseudo rates, and you can prove that the result will be identical to a more complicated model that uses pseudo (co-rotational) rates in a spatial formulation.

You can write a material model that presumes no rotation (which is often the case for available experimental data). Once you match non-rotational data adequately, you can "upgrade" your non-rotational computer model to satisfy PMFI by merely adding a pre-conditioning wrapper that "un-transforms" all spatial inputs to the reference state prior to calling the model. Results are then transformed in this wrapper back to the spatial frame and sent back to the host finite element code.