

The stress tensor and EOM in the reference frame

1 Symmetry of Cauchy's stress tensor

In this section, we'll see why the Cauchy stress tensor must be symmetric. We'll do this in two ways: the first is intuitive and physically transparent, and the second is a bit technical and uses the machinery of continuum theories. I hope that you'll learn to appreciate both.

The first, less involved, way uses examination of an infinitesimal areal element, and the analysis of the forces acting on it. Lets do a quick warm-up using this technique, and obtain the linear momentum force balance relations $\rho \dot{\mathbf{v}} = \nabla_x \cdot \boldsymbol{\sigma}$, which is non other than the continuum analogue of $m\dot{\mathbf{v}} = \mathbf{F}$.

Lets consider forces in the x direction, acting on the 4 sides of an infinitesimal square. The traction forces in the x direction are $t_x = \sigma_{xx}n_x + \sigma_{xy}n_y$. The right side gives $t_x^R = \sigma_{xi}^R \hat{x}_i \ell$, while the left side yields $t_x^L = -\sigma_{xi}^L (-\hat{x}_i) \ell$, because the normal is outwards! Similarly, the top and bottom sides give $t_x^T = \sigma_{xi} \cdot \hat{y}_i \ell$ and $t_x^B = \sigma_{xi}^B (-\hat{y}_i) \ell$. Overall we have $t_x = \ell [(\sigma_{xx}^R - \sigma_{xx}^L) + (\sigma_{xy}^T - \sigma_{xy}^B)]$. Now we divide and multiply by ℓ , and use the derivative infinitesimal limit, we have $t_x = \ell^2 (\partial_x \sigma_{xx} + \partial_y \sigma_{xy}) = \ell^2 \nabla \cdot \boldsymbol{\sigma}$. The momentum balance equation is thus $\ell^2 \rho \dot{\mathbf{v}} = \ell^2 \nabla \cdot \boldsymbol{\sigma}$. Both sides scale with ℓ in the same way, so that ℓ does not matter at all.

Lets repeat this exercise for torque, i.e. the discrete equation $I\dot{\omega} = \tau$. We have $I\dot{\omega} = m\ell^2 \dot{\omega} = \rho \ell^4 \dot{\omega}$. Lets see what happens to the torques. $\tau = \mathbf{r} \times \mathbf{t}$. For the forces to yield torques, we must have $\mathbf{F} \perp \mathbf{r}$, so now we consider t_y on the right and left faces, and t_x on the top and bottom faces (as before).

For the left and right faces we have $\tau^R = \ell \hat{x} \times t_y^R \hat{y} = \ell^2 \hat{x} (\sigma_{yx}^R \hat{y}) = \ell^2 \sigma_{yx}^R \hat{z}$. Similarly, we have $\tau^L = (-\ell \hat{x}) \times t_y^L (-\hat{y}) = \ell^2 \sigma_{yx}^L \hat{z}$. We also have $\tau^T = \ell \hat{y} \times t_x^T \hat{x} = -\ell^2 \sigma_{xy}^T \hat{z}$. We now have the total torque as $\tau = \ell^2 (\sigma_{yx} - \sigma_{xy}) \hat{z}$. We can approximating this again with $\ell^3 \nabla \times \boldsymbol{\sigma}$.

Now, we have $\ell^4 \rho \dot{\omega} = \ell^3 \nabla \times \boldsymbol{\sigma}$ — you can see that we run into some troubles. The powers of ℓ are not identical. That is, if we consider different square sizes, $I\dot{\omega}$ scale with ℓ^4 , while τ scales with ℓ^3 only. The symmetric part of $\boldsymbol{\sigma}$ thus needs to vanish in order to prevent the torque to diverge as ℓ tends to zero.

The second method was not shown in class, but is given here for completeness. For the second way of showing angular momentum balance, we will need to use Reynold's transport theorem. In class you have proven that

$$\frac{D}{Dt} \int_{\Omega} \psi(\mathbf{x}, t) d\mathbf{x}^3 = \int_{\Omega} \left[\partial_t \psi(\mathbf{x}, t) + \nabla_x \cdot (\psi(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t)) \right] d\mathbf{x}^3 . \quad (1)$$

You'll be glad to know that there is a more useful version of this theorem. Since in the theorem ψ can be any field, one can replace it by $\rho \psi$. Then, using Leibniz's rule for the divergence $\nabla \cdot (f\mathbf{g}) = f \nabla \cdot \mathbf{g} + \mathbf{g} \cdot \nabla f$, we get (I omit all the arguments of the functions for

readability. Remember that everything is a function of (\mathbf{x}, t) :

$$\begin{aligned} \frac{D}{Dt} \int_{\Omega} \rho \psi d\mathbf{x}^3 &= \int_{\Omega} [\partial_t(\rho\psi) + \nabla_{\mathbf{x}} \cdot (\rho\psi\mathbf{v})] d\mathbf{x}^3 \\ &= \int_{\Omega} \left[\rho \left(\partial_t \psi + \mathbf{v} \cdot \nabla_{\mathbf{x}} \psi \right) + \psi \left(\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho\mathbf{v}) \right) \right] d\mathbf{x}^3 . \end{aligned} \quad (2)$$

Note that the expression in the first brackets is exactly $\frac{D}{Dt}\psi$. Also, the term in the second brackets vanishes identically due to mass conservation (Eq. (4.5) in Eran's lecture notes). Thus, we conclude that Reynold's theorem can be reformulated in a more pleasant way:

$$\frac{D}{Dt} \int_{\Omega} \rho(\mathbf{x}, t) \psi(\mathbf{x}, t) d\mathbf{x}^3 = \int_{\Omega} \rho(\mathbf{x}, t) \frac{D}{Dt} \psi(\mathbf{x}, t) d\mathbf{x}^3 . \quad (3)$$

Very loosely speaking, this means that in the material coordinates, the operator $\frac{D}{Dt}(\cdot)$ commutes with the operator $\int_{\Omega} \rho(\mathbf{x}, t)(\cdot) d\mathbf{x}^3$. Remember that ψ can be a tensor of any rank.

Physically, the symmetry of Cauchy's stress tensor is the local version of the conservation of angular momentum. To see this, we first define the total angular momentum \mathbf{J} (do not confuse with the Jacobian J):

$$\mathbf{J} = \int_{\Omega} \rho(\mathbf{x}, t) \mathbf{r} \times \mathbf{v}(\mathbf{x}, t) d\mathbf{x} , \quad (4)$$

analogous to $m\mathbf{r} \times \mathbf{v}$. We apply Reynold's theorem to this definition, getting

$$\frac{D\mathbf{J}}{Dt} = \int_{\Omega} \rho (\dot{\mathbf{r}} \times \mathbf{v} + \mathbf{r} \times \dot{\mathbf{v}}) d\mathbf{x} = \int_{\Omega} \rho \mathbf{r} \times \dot{\mathbf{v}} d\mathbf{x} , \quad (5)$$

where we used the fact that $\dot{\mathbf{r}} \times \mathbf{v} = \mathbf{v} \times \mathbf{v} = 0$. Newton's second law says that

$$\frac{D\mathbf{J}}{Dt} = \int_{\Omega} (\mathbf{r} \times \mathbf{b}) d\mathbf{x} + \int_{\partial\Omega} (\mathbf{r} \times \mathbf{t}) ds , \quad (6)$$

where \mathbf{b}, \mathbf{t} are the body force and traction fields, respectively. We use the relation $\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$, and equate Eqs. (5) and Eqs. (6):

$$\int_{\Omega} \mathbf{r} \times [\rho\dot{\mathbf{v}} - \mathbf{b}] d\mathbf{x} - \int_{\partial\Omega} (\mathbf{r} \times \boldsymbol{\sigma}\mathbf{n}) ds = 0 . \quad (7)$$

Here we use a little lemma:

Lemma: Let \mathbf{u}, \mathbf{A} be vector and tensor fields defined in the region Ω . Then

$$\int_{\partial\Omega} \mathbf{u} \times \mathbf{A}\mathbf{n} ds = \int_{\Omega} [\boldsymbol{\mathcal{E}} : (\text{grad } \mathbf{u})\mathbf{A}^T + \mathbf{u} \times \text{div } \mathbf{A}] dv , \quad (8)$$

where $\boldsymbol{\mathcal{E}}$ is the Levi-Civita tensor. To see this, write in index notation

$$\begin{aligned} \int_{\partial\Omega} \mathbf{u} \times \mathbf{A}\mathbf{n} ds &= \int_{\partial\Omega} \mathcal{E}_{ijk} u_j (\mathbf{A}\mathbf{n})_k ds = \int_{\partial\Omega} \mathcal{E}_{ijk} u_j A_{kl} n_l ds \\ &= \int_{\partial\Omega} (\boldsymbol{\mathcal{E}} : \mathbf{u}\mathbf{A})_{il} n_l ds = \int_{\Omega} \text{div} (\boldsymbol{\mathcal{E}} : \mathbf{u}\mathbf{A}) dv \\ &= \int_{\Omega} \partial_l (\mathcal{E}_{ijk} u_j A_{kl}) dv = \int_{\Omega} \left[\underbrace{\mathcal{E}_{ijk} (\partial_l u_j) A_{kl}}_{\boldsymbol{\mathcal{E}} : (\text{grad } \mathbf{u})\mathbf{A}^T} + \underbrace{\mathcal{E}_{ijk} u_j (\partial_l A_{kl})}_{\mathbf{u} \times \text{div } \mathbf{A}} \right] dv . \end{aligned} \quad (9)$$

We now plug that into (7) to get

$$\int_{\Omega} \mathbf{r} \times [\rho \dot{\mathbf{v}} - \mathbf{b} - \operatorname{div} \boldsymbol{\sigma}] dv - \int_{\Omega} \boldsymbol{\varepsilon} : \boldsymbol{\sigma}^T dv = 0 . \quad (10)$$

The first integrand vanishes identically, as this is an equation of motion. The second one can be integrated on an arbitrary volume and so we see that $\boldsymbol{\varepsilon} : \boldsymbol{\sigma}^T = 0$, or in other words, $\boldsymbol{\sigma}$ is symmetric.

2 Properties of the stress tensor

2.1 Maximal shear/normal stress/strain

It is instructive to examine the planes on which the normal or shear stresses are maximal. As a motivation, we'll note that some materials, when stretched, tear in a plane perpendicular to the stretching direction. This is very intuitive, because the normal (dilatational) stress is highest on this plane. When compressed, however, things are not as simple. When a metal is compressed above its capability to sustain the deformation, it typically undergoes irreversible deformation in a plane at 45° to the compression, cf. Fig. 1. But why at 45° ? That's because it is much easier to perform irreversible deformation in shear than in compression (the shear strength is much smaller than the compressive hardness). Phenomena which are shear-driven occur at planes which have maximal shear.

In general, say we have a stress tensor $\boldsymbol{\sigma}$. What is the normal stress on a given plane? It is given by the normal component of the force on that plane. If the normal to the plane is $\hat{\mathbf{n}}$, the force is $\boldsymbol{\sigma} \hat{\mathbf{n}}$, and the normal component is $\sigma_n = \hat{\mathbf{n}}^T \boldsymbol{\sigma} \hat{\mathbf{n}}$. Note that if $\hat{\mathbf{t}}_1, \hat{\mathbf{t}}_2$ are vectors orthogonal to $\hat{\mathbf{n}}$ (tangent to the plane) then the stress in the coordinate system $\{\hat{\mathbf{n}}, \hat{\mathbf{t}}_1, \hat{\mathbf{t}}_2\}$ is

$$[\boldsymbol{\sigma}]' = \begin{pmatrix} - & \hat{\mathbf{n}} & - \\ - & \hat{\mathbf{t}}_1 & - \\ - & \hat{\mathbf{t}}_2 & - \end{pmatrix} [\boldsymbol{\sigma}] \begin{pmatrix} | & | & | \\ \hat{\mathbf{n}} & \hat{\mathbf{t}}_1 & \hat{\mathbf{t}}_2 \\ | & | & | \end{pmatrix} ,$$

so σ_n is simply the nn component of $\boldsymbol{\sigma}$ written in the new basis. Note that σ_n goes like $\sim \mathbf{n}^2$, and not like $\sim \mathbf{n}$ as one might think.

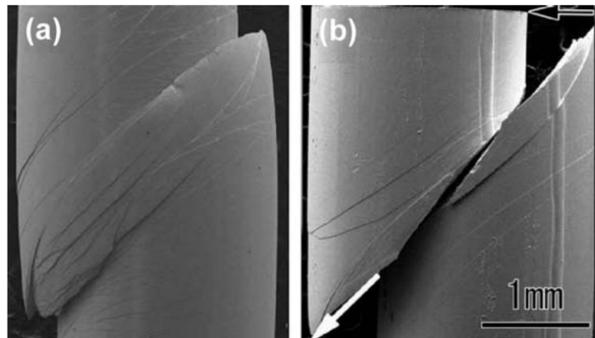


Figure 1: Compressive shear failure (shear banding) of a metallic glass. Wait, what? What does it even mean a metallic glass? can a material be both a metal and a glass? Hang on in the course to find out. From: Louzguine-Luzgin et. al., *Metals* **3** (2013).

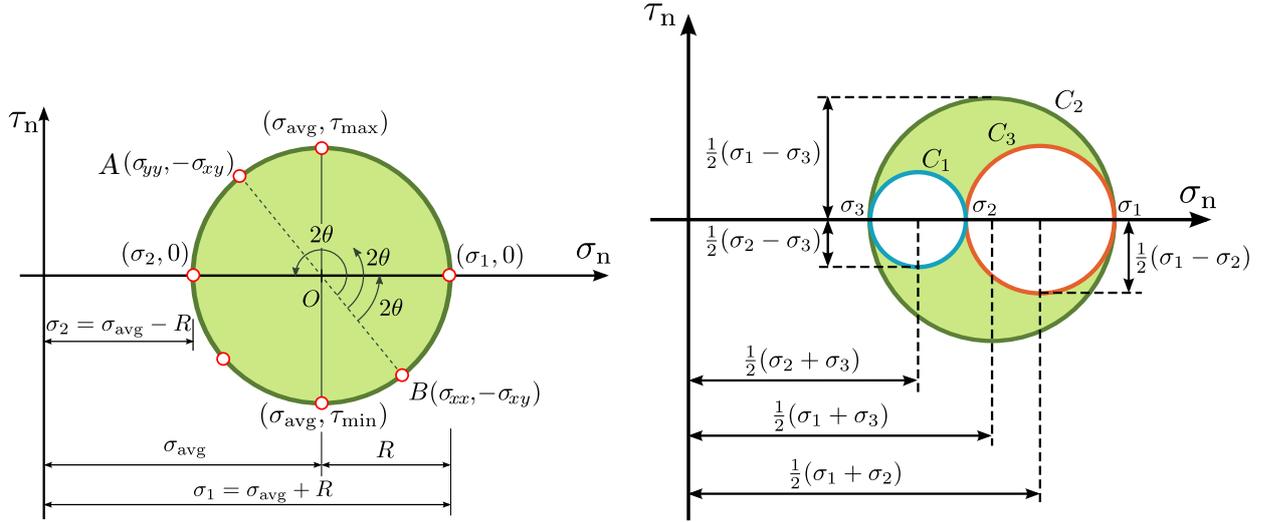


Figure 2: Illustration of Mohr's circle in 2D (left) and 3D (right), adapted from Wikipedia.

So say we apply uniaxial stress, so that the stress tensor is of the form (forget for the moment about the 3rd dimension):

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (11)$$

Rotating by an angle α we get

$$\boldsymbol{\sigma} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} = \sigma_1 \begin{pmatrix} \cos^2 \alpha & -\cos \alpha \sin \alpha \\ -\cos \alpha \sin \alpha & \sin^2 \alpha \end{pmatrix}$$

So you see that the maximal shear stress occurs for $\alpha = 45^\circ$.

2.2 Mohr's circle

2.2.1 2D case

We saw that different planes are subject to different shear and normal (compressive) stresses. Mohr's circle is a simple geometrical way to see all possible shear and normal stresses of a given stress state. Here we'll only consider a 2D system (later in the course we'll see exactly what we mean when we say 2D), but this concept can be generalized also to 3D.

Let's consider a general stress state,

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix}, \quad (12)$$

and ask what is the normal and shear stresses, which we'll denote by σ_n and τ_n , on a plane in an angle θ to the x axis. This means we need to rotate the stress by α , and look at the 11 and 12 components of the resulting matrix. Performing the matrix multiplication,

we get

$$\sigma_n = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) + \frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \cos 2\theta + \sigma_{xy} \sin 2\theta \quad (13)$$

$$\tau_n = -\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \sin 2\theta + \sigma_{xy} \cos 2\theta \quad (14)$$

If we look in the $\sigma_n - \tau_n$ plane, what geometrical form do these equations describe? It is easy to see that the answer is a circle:

$$\begin{aligned} \tau_n^2 + \left(\sigma_n - \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) \right)^2 &= \\ \left(\sigma_{xy} \cos 2\theta - \frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \sin 2\theta \right)^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \cos 2\theta + \sigma_{xy} \sin 2\theta \right)^2 &= \\ = \sigma_{xy}^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \right)^2 & \end{aligned}$$

This is a circle of radius $\sqrt{\sigma_{xy}^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy})\right)^2}$, centered around $\sigma_n = \frac{1}{2}(\sigma_{xx} + \sigma_{yy})$ and $\tau_n = 0$. This circle is called Mohr's circle, and is shown in Fig. 2.

A point on the circle corresponds to an admissible pair (σ_n, τ_n) , and rotating the axes by θ corresponds to traversing an angle 2θ along the circle. This means that rotating by 180° puts you back where you started, which is not surprising. The intersections of the circle with the σ_n axis are the eigenvalues of $\boldsymbol{\sigma}$ – the principal stresses.

2.2.2 3D case

In 3D things are less simple because we have 2 angles of rotation. We denote the he principal stresses (i.e. the eigenvalues of $\boldsymbol{\sigma}$ by $\sigma_1 > \sigma_2 > \sigma_3$, and start with coordinates in which $\boldsymbol{\sigma}$ is diagonal. If we choose a plane whose normal is \vec{n} , then the force (per unit area) on this plane is $\vec{T} = \boldsymbol{\sigma}\vec{n}$. As in 2D, we denote the normal pressure $\vec{T} \cdot \vec{n} = (\boldsymbol{\sigma}\vec{n}) \cdot \vec{n}$ by σ_n and the shear force by τ_n . We thus have

$$T^2 = (\boldsymbol{\sigma}\vec{n})^2 = \sigma_{ij}\sigma_{ik}n_jn_k = \sigma_n^2 + \tau_n^2 = \sigma_1^2n_1^2 + \sigma_2^2n_2^2 + \sigma_3^2n_3^2 \quad (15)$$

$$\sigma_n = \sigma_1n_1^2 + \sigma_2n_2^2 + \sigma_3n_3^2 \quad (16)$$

$$n_in_i = n_1^2 + n_2^2 + n_3^2 = 1 \quad (17)$$

These are three equations, which we can solve for the three variables n_i^2 to get

$$n_1^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_2)(\sigma_n - \sigma_3)}{(\sigma_1 - \sigma_2)(\sigma_1 - \sigma_3)} \geq 0 \quad (18)$$

$$n_2^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_3)(\sigma_n - \sigma_1)}{(\sigma_2 - \sigma_3)(\sigma_2 - \sigma_1)} \geq 0 \quad (19)$$

$$n_3^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_1)(\sigma_n - \sigma_2)}{(\sigma_3 - \sigma_1)(\sigma_3 - \sigma_2)} \geq 0 \quad (20)$$

The 1st and 3rd denominators are positive, and the 2nd is negative, so we have

$$\tau_n^2 + (\sigma_n - \sigma_2)(\sigma_n - \sigma_3) \geq 0 \quad (21)$$

$$\tau_n^2 + (\sigma_n - \sigma_3)(\sigma_n - \sigma_1) \leq 0 \quad (22)$$

$$\tau_n^2 + (\sigma_n - \sigma_1)(\sigma_n - \sigma_2) \geq 0 \quad (23)$$

After some trivial algebraic manipulations, these can be re-written as

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_2 + \sigma_3)\right]^2 \geq \left(\frac{1}{2}(\sigma_2 - \sigma_3)\right)^2 \quad (24)$$

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_1 + \sigma_3)\right]^2 \leq \left(\frac{1}{2}(\sigma_1 - \sigma_3)\right)^2 \quad (25)$$

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_1 + \sigma_2)\right]^2 \geq \left(\frac{1}{2}(\sigma_1 - \sigma_2)\right)^2 \quad (26)$$

These are equations of three circles, which are shown in Fig. 2.

3 Equations of motion in the reference configuration

As Eran stressed in class, this step is crucial because in a generic problem we do not know in advance what is the deformed configuration and therefore it is very useful to describe the motion in the undeformed coordinates. We remark again that in standard linear elasticity the two sets of coordinates are the same to linear order, so this distinction is not emphasized in this kind of treatments.

The Piola-Kirchoff stress tensor was defined in class by the relation

$$\mathbf{T} = \mathbf{P}d\mathbf{S} = \boldsymbol{\sigma}d\mathbf{s} = \mathbf{t} , \quad (27)$$

where \mathbf{t} is the infinitesimal forces in the spatial coordinate and \mathbf{T} is its (fictitious) correspondent in the material coordinates. How does $d\mathbf{S}$ relate to $d\mathbf{s}$? Consider an arbitrary line element $d\mathbf{X}$ going through $d\mathbf{S}$. The spanned volume is $dV = d\mathbf{S} \cdot d\mathbf{X}$. Correspondingly, in the deformed coordinates we have $dv = d\mathbf{s} \cdot d\mathbf{x}$. By definition of the Jacobian, we know that the ratio of the volumes is $dv = JdV$. Since $d\mathbf{x} = \mathbf{F}d\mathbf{X}$ we have

$$dX_i F_{ji} ds_j = dx_j ds_j = dv = JdV = JdX_i dS_i . \quad (28)$$

Since $d\mathbf{X}$ was arbitrary, we get $ds_j F_{ji} = JdS_i$ or in more convenient notation

$$\mathbf{F}^T d\mathbf{s} = Jd\mathbf{S} , \quad d\mathbf{s} = J\mathbf{F}^{-T}d\mathbf{S} . \quad (29)$$

Plugging that into (27) we have

$$\mathbf{P} = J\boldsymbol{\sigma}\mathbf{F}^{-T} . \quad (30)$$

So now we know how \mathbf{P} relates to $\boldsymbol{\sigma}$. But what are its equations of motion? For this we need 3 lemmas:

1. Piola's identity: $\nabla_{\mathbf{X}} \cdot (J\mathbf{F}^{-T}) = 0$.
2. For every two tensors \mathbf{A}, \mathbf{B} , we have $\text{div}(\mathbf{AB}) = (\text{grad } \mathbf{A}) : \mathbf{B} + \mathbf{A} \text{div } \mathbf{B}$.
3. For every tensor \mathbf{A} we have $\text{div}_{\mathbf{x}} \mathbf{A} = (\text{grad}_{\mathbf{X}} \mathbf{A}) : \mathbf{F}^{-T}$.

The proofs of these lemmas are trivial:

1. Integrate $\nabla_{\mathbf{X}} \cdot (J\mathbf{F}^{-T})$ over an arbitrary volume Ω_0 :

$$\begin{aligned} \int_{\Omega_0} \nabla_{\mathbf{X}} \cdot (J\mathbf{F}^{-T}) d^3\mathbf{X} &= \int_{\partial\Omega_0} J\mathbf{F}^{-T} d\mathbf{S} = \int_{\partial\Omega} d\mathbf{s} \\ &= \int_{\partial\Omega} \mathbf{I} d\mathbf{s} = \int_{\Omega} (\nabla_{\mathbf{x}} \cdot \mathbf{I}) d^3\mathbf{x} = 0 . \end{aligned} \quad (31)$$

2. $\partial_j(A_{ik}B_{kj}) = \partial_j A_{ik}B_{kj} + A_{ik}\partial_j B_{kj}$.

3. $\frac{\partial A_{ij}}{\partial x_j} = \frac{\partial X_k}{\partial x_j} \frac{\partial A_{ij}}{\partial X_k}$.

Using these lemmas, and defining the *reference body force* by $\mathbf{B}(\mathbf{X}, t) \equiv J(\mathbf{X}, t)\mathbf{b}(\mathbf{x}, t)$, we get

$$\begin{aligned} \nabla_{\mathbf{X}} \cdot \mathbf{P} &= \nabla_{\mathbf{X}} \cdot (\boldsymbol{\sigma} J\mathbf{F}^{-T}) = \nabla_{\mathbf{X}} \boldsymbol{\sigma} : (J\mathbf{F}^{-T}) + \underbrace{\boldsymbol{\sigma} \nabla_{\mathbf{X}} \cdot (J\mathbf{F}^{-T})}_{=0} \\ &= J\nabla_{\mathbf{X}} \boldsymbol{\sigma} : \mathbf{F}^{-T} = J\nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = J(\rho\dot{\mathbf{v}} - \mathbf{b}) \\ &\Rightarrow \boxed{\rho_0 \dot{\mathbf{V}} = \nabla_{\mathbf{X}} \cdot \mathbf{P} + \mathbf{B}} \end{aligned} \quad (32)$$

Note the resemblance to the equation of motion in the deformed coordinates:

$$\rho\dot{\mathbf{v}} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} + \mathbf{b} . \quad (33)$$

One more point: having Eq. (32) is not enough in order to formulate a problem in the \mathbf{X} coordinates. We also need to transform the boundary conditions to the material coordinates in order to fully define the problem. If the boundary conditions are forces, then they have to be transformed to the fictitious material coordinates forces. In the case of free boundary conditions (i.e. zero tractions) it is easy - they remain free.