Thermo-mechanics & constitutive relations
some rough notes

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Indices and bold notation used for tensor - sorry for the confusion - should be clear enough hopefully

1 Preliminaries

Under the small perturbation hypothesis, strain are small and given by

$$\epsilon_{ij} = \frac{1}{2} \left(u_{i,j} + u_{j,i} \right) \tag{1}$$

where u_i is the displacement vector. The material and time derivatives merges. The strain rate is simply the time-derivative of the strain. The change of solid mass density are also negligible. We write time-derivative with a dot.

I refer you to [4, 2] to a much more details description. I also recommend [3] as a general plasticity textbook.

1.1 Conservation of energy

$$\rho \dot{e} = \sigma_{ij} \dot{\epsilon}_{ij} - Q_{i,i} + r \tag{2}$$

where Q_i is the heat flux, r any possible hear sources, and e the internal energy per unit of mass.

1.2 2nd principle and Clausius-Duhem inequality

Introducing the conservation of energy in the second principle of thermodynamics $\dot{s} \geq -\frac{Q_{i,i}}{T} + r/T$, denoting $\Psi = e - Ts$ the specific free energy (per unit of mass), s being the entropy per unit of mass. We obtain the Clausius-Duhem inequality:

$$\sigma_{ij} \dot{\epsilon}_{ij} - \rho \left(\dot{\Psi} + \dot{T}s \right) - \frac{Q_i T_{,i}}{T} \geq 0 \tag{3}$$

The state variables are: T, ϵ_{ij} and some hidden states variables α_k.

1.3 Using Clausius Duhem

We suppose that the infinitesimal strain ϵ_{ij} partition in an "elastic" (recoverable) part and an "inelastic" (plastic in what follows) parts:

$$\epsilon_{ij} = \epsilon_{ij}^e + \epsilon_{ij}^p \tag{4}$$

Generally, we write the specific free energy of the solid as a function of:

- temperature T

- elastic strains ϵ_{ij}^e

- internal variables α_k (the latter can be tensorial, scalar or vectorial)

in other words:
$$\Psi(T, \epsilon_{ij}^e, \alpha_k) \tag{5}$$

Introducing in the Clausius Duhem equation, we obtain:

$$\left(\sigma_{ij} - \rho\frac{\partial\Psi}{\partial\epsilon_{ij}^e}\right)\dot{\epsilon}_{ij}^e + \sigma_{ij}\dot{\epsilon}_{ij}^p - \rho\left(s + \frac{\partial\Psi}{\partial T}\right)\dot{T} - \rho\frac{\partial\Psi}{\partial\alpha_k}\dot{\alpha}_k - \frac{Q_i T_{,i}}{T} \geq 0 \tag{6}$$

In addition, to model all possible viscous effect, we postulate that the stress tensor is the sum of an elastic and a viscous part:
$$\sigma_{ij} = \sigma_{ij}^e + \sigma_{ij}^v \tag{7}$$

and assume that the elastic part of the stress tensor is equal to the derivative of the specific free energy w.r to the elastic strain
$$\sigma_{ij}^e = \rho\frac{\partial\Psi}{\partial\epsilon_{ij}^e} \tag{8}$$

In the absence of viscous stress, for a transformation under constant uniform temperature, no plastic deformation and variation of internal variables, Clausius-Duhem inequality is indeed satisfied. Then further more, for any elastic strain, it follows that the entropy is the derivative of the specific energy w.r. to the temperature:
$$s = -\rho\frac{\partial\Psi}{\partial T} \tag{9}$$

Denoting by A_k the conjugate thermodynamics forces of the internal variable α_k:

$$A_k = \rho\frac{\partial\Psi}{\partial\alpha_k} \tag{10}$$

We can thus re-write the Clausius-Duhem inequality as:

$$\sigma_{ij}^v\dot{\epsilon}_{ij}^e + \sigma_{ij}\dot{\epsilon}_{ij}^p - A_k\dot{\alpha}_k - \frac{Q_i T_{,i}}{T} \geq 0 \tag{11}$$

We can separate the thermal and the intrinsic dissipation:

$$\phi = \phi_{th} + \phi_{intr} \tag{12}$$

with

$$\phi_{th} = -\frac{Q_i T_{,i}}{T} \tag{13}$$

$$\phi_{intr} = \underbrace{\sigma_{ij}^v\dot{\epsilon}_{ij}^e}_{\phi_v} + \underbrace{\sigma_{ij}\dot{\epsilon}_{ij}^p - A_k\dot{\alpha}_k}_{\phi_p} \tag{14}$$

Decoupling of thermal and intrinsic dissipation It is usual to enforce that both ϕ_{th} and ϕ_{intr} must be greater or equal than zero. This is always warranted (pending some peculiar cases associated with shock waves where temperature and entropy may be locally discontinuous across the shock).

The positivity of the thermal dissipation, is ensured by Fourier's law, which states that heat flow from high to low temperature:
$$Q_i = -\lambda T_{,i} \tag{15}$$

such that we have

$$\phi_{th} = \frac{Q_i Q_i}{T\lambda} \geq 0 \tag{16}$$

as the thermal conductivity λ is positive.

2   Heat equation

We have

$$\dot{e} = \dot{\Psi} + T\dot{s} + s\dot{T} \tag{17}$$

expressing $\dot{\Psi}$ as function of its depending variables, we obtain

$$\rho\dot{e} = \sigma_{ij}^e \dot{\epsilon}_{ij}^e + A_k \dot{\alpha}_k + \rho T \dot{s} \tag{18}$$

such that the conservation of energy becomes:

$$\sigma_{ij}^e \dot{\epsilon}_{ij}^e + A_k \dot{\alpha}_k + \rho T \dot{s} = \sigma_{ij} \dot{\epsilon}_{ij} - Q_{i,i} + r \tag{19}$$

now we also have $s = -\partial\Psi/\partial T$, such that:

$$\dot{s} = -\frac{\partial^2 \Psi}{\partial T^2}\dot{T} - \frac{\partial^2 \Psi}{\partial T \partial \epsilon_{ij}^e}\dot{\epsilon}_{ij}^e - \frac{\partial^2 \Psi}{\partial T \partial \alpha_k}\dot{\alpha}_k \tag{20}$$

$$= \frac{\partial s}{\partial T}\dot{T} - \frac{1}{\rho}\frac{\partial \sigma_{ij}^e}{\partial T}\dot{\epsilon}_{ij}^e - \frac{1}{\rho}\frac{\partial A_k}{\partial T}\dot{\alpha}_k \tag{21}$$

Introducing the heat capacity $C = T\partial s/\partial T$, and Fourier's law, we obtain:

$$\rho C \dot{T} - T\left(\frac{\partial \sigma_{ij}^e}{\partial T}\dot{\epsilon}_{ij}^e + \frac{\partial A_k}{\partial T}\dot{\alpha}_k\right) = \underbrace{\sigma_{ij}^v \dot{\epsilon}_{ij}^e + \sigma_{ij}\dot{\epsilon}_{ij}^p - A_k\dot{\alpha}_k}_{\phi_{intr}} + (\lambda T_{,i})_{,i} + r \tag{22}$$

Usually, the terms associated with thermo-mechanical coupling on the RHS are negligible compared to the heat capacity: $T\left(\frac{\partial \sigma_{ij}^e}{\partial T}\dot{\epsilon}_{ij}^e + \frac{\partial A_k}{\partial T}\dot{\alpha}_k\right) \ll \rho C \dot{T}$.

Plastic deformation and the evolution of internal variables result in heat production (remember $\phi_{intr} \geq 0$).

3   Examples of material behavior

3.1   Viscoelasticity

3.1.1   Kelvin-voigt

We set the following ansatz for the behavior:

$$\epsilon_{ij}^p = 0 \quad \alpha_k = 0 \quad \sigma_{ij}^v = \eta\dot{\epsilon}_{ij}, \tag{23}$$

thus taking a viscous stress similar to a Newtonian fluid.

In 1D, we therefore have the following ODE

$$E\epsilon + \eta\dot{\epsilon} = \sigma \tag{24}$$

Such a rheological model consists of a spring in parallel with a dashpot.

Under creep conditions, the strain thus evolves as

$$\epsilon = \frac{\sigma}{E}\left(1 - e^{-Et/\eta}\right) \tag{25}$$

Note that such a model can not simulate stress relaxation after a fixed imposed strain step ! The stress is constant when the strain rate is zero. It is therefore quite unrealistic for most applications.

3.1.2 Maxwell

Maxwell viscoelastic model corresponds to the following ansatz:

$$\sigma_{ij}^v = 0, \quad \dot{\epsilon}_{ij}^p \neq 0, \alpha_k = 0 \tag{26}$$

Here viscous effects are accounted for via inelastic deformation.

More specifically, assuming that the viscoelasticity only acts in shear, the inelastic part of the strain (the viscous part) is taken akin to a fluid

$$\dot{\epsilon}_{ij}^p = \dot{\epsilon}_{ij}^v = \frac{1}{\eta} \left((1 + \nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij} \right) \tag{27}$$

In addition, the elastic part of the constitutive relation holds. For an isotropic material

$$\sigma_{ij} = \frac{E}{1 + \nu} \left(\epsilon_{ij} - \epsilon_{ij}^p \right) + \frac{E\nu}{(1 + \nu)(1 - 2\nu)} \left(\epsilon_{kk} - \epsilon_{kk}^p \right) \delta_{ij} \tag{28}$$

In uni-axial condition, taking the time-derivative of the elastic relation, we obtain the following ode:

$$\dot{\sigma}/E + \frac{1}{\eta}\sigma = \dot{\epsilon} \tag{29}$$

Under creep condition (constant stress), the material "flow" indifinetely like a fluid. Under imposed fixed strain ϵ_o, the stress "relaxes" as follow

$$\sigma(t) = E\epsilon_o e^{-t\eta/E} \tag{30}$$

Such a Maxwell rheology consists of a spring and a dashpot in series.

3.1.3 Generalized Maxwell

It consists of combining N Maxwell elements in parallel, with usually one strictly elastic element.

Writing tensors in bold, we have

$$\boldsymbol{\sigma} = E_\infty \boldsymbol{c} : \boldsymbol{\epsilon} + \sum_{k=1,n} \eta_k \dot{\boldsymbol{\epsilon}}_k^v \tag{31}$$

$$\dot{\boldsymbol{\epsilon}}_k^v = \frac{E_k}{\eta_k} \boldsymbol{c} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_k^v) \tag{32}$$

with $\boldsymbol{c}$ the elastic stiffness tensor divided by Young modulus (thus only function of Poisson's ratio):

$$c_{ijkl} = \frac{1}{2(1 + \nu)}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{\nu}{(1 + \nu)(1 - 2\nu)} \tag{33}$$

Many others viscoelastic models exist. Anisotropy can be accounted for, similarly a volumetric viscosity can be introduced etc.

3.2 Viscoplasticity

Somehow, very related to viscoelasticity, pending the introduction of a "yield limit" below which the behavior is strictly elastic. However, the stresses can exceed such a limit and drives inelastic deformation.

3.2.1 Bingham: simplest rigid-viscoplastic model

In many materials, at ordinary temperatures, rate-dependent inelastic deformation is insignificant below a yield stress. The simplest model is the so-called Bingham model, which states that the material is rigid below the yield stress and flow like a Newtonian fluid if the yield is reached.

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\boldsymbol{\epsilon}} = 0 \qquad \sqrt{J_2(\boldsymbol{s})} \leq \sigma_Y \tag{34}$$

$$\dot{\boldsymbol{\epsilon}}^p = \frac{\sqrt{J_2(\boldsymbol{\sigma})} - \sigma_Y}{\eta} \frac{\boldsymbol{s}}{\|\boldsymbol{s}\|} \tag{35}$$

where J_2 is the second invariant of the deviatoric part of the stress tensor $\boldsymbol{s} = \boldsymbol{\sigma} - \frac{1}{3}Tr(\boldsymbol{\sigma})\boldsymbol{I}$: $J_2 = \frac{\boldsymbol{s}:\boldsymbol{s}}{2}$, and $\|\boldsymbol{s}\| = \sqrt{J_2}$. Note that under simple (pure) shear, $\sqrt{J_2(\boldsymbol{\sigma})} = \tau$. Such a model is popular to model some complex fluids - such as toothpaste. We see that the volumetric part of the inelastic strain is zero in such a model.

An extension, is to account for a non-linearity of the strain rate with the applied stress above the yield stress. For a rigid-viscoplastic material, it is refereed to as the Herschel-Bulkley model:

$$\dot{\boldsymbol{\epsilon}}^p = \left\langle \frac{\sqrt{J_2(\boldsymbol{\sigma})} - \sigma_Y}{k} \right\rangle^{1/n} \frac{\boldsymbol{s}}{\|\boldsymbol{s}\|} \tag{36}$$

with $n > 0$. $n < 1$ testifiy of a shear thinning behavior, while $n > 1$ indicates shear-thickennning. We have introduced the Macauley bracket (the ramp function: $< x >= x$ if $x > 0$, zero otherwise). Explore that we can invert and express the deviatoric stress tensor directly as function of the strain rate (recall that a fluid is incompressible - zero volumetric strain). Obtain the expression of the tangent viscosity (at a given level of imposed strain rate).

Uniaxial strain Under uniaxial strain σ, $J_2 = 2\sigma^2/6$, such that the yield criteria is in that case $\sigma \leq \sqrt{3}\sigma_Y$. Denoting $Y = \sqrt{3}\sigma_Y$, the yield for general stress is often rewritten as $\sigma_{eq} = \sqrt{3J_2} \leq Y$.

3.2.2 Elasto-viscoplasticity

A simple and popular model for elasto-viscoplasticity is the so-called Norton-Hoff model. It is nothing else that a Herschel-Bulkley model including an elastic behavior. The Norton model for creep of metal is the limit where the yield limit is negligible.

Mathematically, it is practical to introduce a yield function f (e.g. function of J_2):

$$f(\boldsymbol{s}) = \sqrt{3J_2} - Y \tag{37}$$

such that the elasto-viscoplastic relations is simply

$$\boldsymbol{\sigma} = \boldsymbol{C} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^p) \tag{38}$$

(which can be similarly expressed in terms of rate). and the plastic strain rate is given by the following associated flow rule:

$$\dot{\boldsymbol{\epsilon}}^p = 0 \qquad f < 0 \tag{39}$$

$$\dot{\boldsymbol{\epsilon}}^p = \left(\frac{\sqrt{3J_2} - Y}{k} \right)^N \frac{3}{2} \frac{\boldsymbol{s}}{\sqrt{3J_2}} = \frac{\partial \Omega}{\partial \boldsymbol{s}} \tag{40}$$

with $\Omega = \frac{k}{N+1} \left(\frac{\sqrt{3J_2}-Y}{k} \right)^{N+1}$ a flow potential. Note the usual notation $\sigma_{eq} = \sqrt{3J_2} = \sqrt{\frac{3}{2}\boldsymbol{s} : \boldsymbol{s}}$.

Remark : many more complicated models can be developed, notably incorporating internal variables such as the accumulated inelastic strain (via its invariants), or/and plastic work.

3.2.3 Effect of temperature

Temperature has of course an important effet on viscosity (viscosity usually decreases exponentially with temperature). Similarly the stress exponents of the Norton-Hoff model varies with temperature etc.

3.3 Rate-independent elasto-plasticity

3.3.1 Perfect plasticity - no internal variables

Notion of yield and plastic flow rule. In general term, the yield function is a scalar function defined in terms of the stress tensor (usually via its invariant) , and some parameters defining the yield limit.

Associated plastic flow is written as:

$$\dot{\boldsymbol{\epsilon}}^p = 0 \qquad f < 0 \tag{41}$$

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\lambda}\frac{\partial f}{\partial \boldsymbol{\sigma}} \quad f = 0 \tag{42}$$

where $\dot{\lambda} > 0$ is the plastic multiplier. Such an associated flow rule indicates that plastic flow occurs along the gradient of the yield function (i.e. normal to the yield function) There is of course the complementary condition: $\dot{\lambda}f = 0$, as $f < 0$ implies $\dot{\lambda} = 0$ and $f = 0$ when $\dot{\lambda} > 0$.

Moreover, if plastic flow occurs ($\dot{\lambda} > 0$), the state of stress must remain on the yield function: in other words $\dot{\lambda} > 0)\dot{f} = 0$, i.e. $\dot{f} = 0$ when $\dot{\lambda} > 0$. This is called the consistency condition in elasto-plasticity.

3.3.2 J2-plasticity

Its yield function is written as:

$$f(\boldsymbol{s}) = \sqrt{3J_2} - Y = \sigma_{eq} - Y \tag{43}$$

The flow rule is taken as associated. Good model for lots of materials (metals, ...).

3.3.3 Isotropic and kinematic hardening

Isotropic hardening relates to the increase of the yield limit as plastic strain accumulates (without any effect associated to the direction of plastic strain). Also the "shape" of the yield function (the elastic domain) remains the same. It is typically "tracked" with a scalar measure of the plastic strain, i.e.:

$$\alpha = \bar{\epsilon}^p = \int_0^t \sqrt{\frac{2}{3}\dot{\epsilon}^p_{ij}\dot{\epsilon}^p_{ij}} \; \mathrm{d}t' \tag{44}$$

(Note that sometimes the accumulated plastic work $w = \int \sigma_{ij}\dot{\epsilon}^p_{ij}dt$ is also used).

The yield limit Y appears as the dual thermodynamics force (corresponding A_k) of the accumulated plastic strain measure. The simplest evolution is linear, e.g. such that

$$\dot{Y} = H\dot{\bar{\epsilon}}^p \tag{45}$$

with H a hardening modulus. Note that softening can be observed in some materials (negative H)... and is prone to the appearance of material instability.

Kinematic hardening allows to reproduce the so-called Bauschinger effect. The fact that a material plastified under tension (which exhibit hardening), then exhibits a lower yield limit. Kinematic hardening model such effects, by "translating" the yield function in the stress space. Note that the "shape" of yield function is again not modified. The total plastic strain is taken as the internal variable, and the dual thermodynamic forces is denoted as $\boldsymbol{X}$

In the context of J2-plasticity, the yield function is written as:

$$f(\boldsymbol{\sigma}, \boldsymbol{\epsilon}^p) = \sqrt{3J_2(\boldsymbol{\sigma} - \boldsymbol{X})} - Y \tag{46}$$

The flow rule is

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\lambda}\frac{\partial f}{\partial \boldsymbol{\sigma}} \tag{47}$$

$$\dot{\boldsymbol{\alpha}} = -\dot{\lambda}\frac{\partial f}{\partial \boldsymbol{X}} = \dot{\lambda}\frac{\partial f}{\partial \boldsymbol{\sigma}} = \dot{\boldsymbol{\epsilon}}^p \tag{48}$$

The simplest evolution for the thermodynamic forces $\boldsymbol{X}$ dual of the plastic strain is

$$\dot{\boldsymbol{X}} = C_o\dot{\boldsymbol{\epsilon}}^p \tag{49}$$

Isotropic and kinematic hardening can of course be combined.

3.3.4 Pressure dependent plasticity

A large number of materials exhibit a strong effect of the mean-stress on the shear resistance (rocks, some metals...).

The yield function is therefore expressed as function of the first two invariants of the stress tensor:

$$p = -\sigma_{kk}/3 \quad q = \sqrt{3J_2} \tag{50}$$

with the previous definition of J2 (as the second invariant of the deviatoric part of the stress tensor).

For example, the Drucker-Prager criteria reads

$$f(p,q) = q - 3\sin\phi p - 2c_o\cos\phi \tag{51}$$

(note - this is not exactly the correspondence to mohr-coulomb - see e.g. [1] for the correspondence of the outer and inner with MC).

Such a model has infinite yield at infinite compressive stress. As a result, a"compression" cap is often added. Such an effect is very important for soils and soft-rocks. For such material a popular function is the so-called Cam-Clay model (in its modified form):

$$f(p,q) = q^2 - M^2 p(2p_c - p) \tag{52}$$

which is a "elliptical" yield surface in the q-p plane. Note that a hardening law for the consolidation pressure p_c allows to reproduce the evolution of such pressure-dependent material toward a "critical" state where no more volumetric plastic deformation occurs [5].

The Gurson model in metal plasticity shares some similarities.

References

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