On Implicit Constitutive Theories

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- *This is the end I aim to: to acquire knowledge of the union of mind with the whole of nature. To do this it is necessary first to understand as much of nature as suffices for acquiring such knowledge, and to form a society of the kind that permits as many as possible to acquire such knowledge ::: because it is possible to gain more free time and convenience in life, mechanics is in no way to be despised.*

– B. Spinoza

- *We come to the composition of a continuum, whose hitherto unsurmounted difficulty has sorely taxed the wits of all the learned, and everyone without exception acknowledges it to be virtually insurmountable. Most of them mask it in obscure terminology with repeated and tortuous distinctions and sub-distinctions, so that no-one may openly catch them despairing of other means of solution which might yield to the light of reason; but they must necessarily conceal it in the darkness of confusion, so that it may not be laid bare by perspicuous argument.*

  – Fransescoe de Oviedo (1602-1651)

  (translation appears in Discourse of things above reason, In **Selected Philosophical Papers of Robert Boyle**, *edited by M. A. Stewart).*

- *In the presentation of a novel outlook with wide ramifications a single line of communication from premises to conclusions is not sufficient for intelligibility. Your audience will construe whatever you say in conformity with pre-existing outlook.*

– A.N. Whitehead

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Constitutive Equations

- How a body responds to stimuli, depends on how it is constituted and its constitution is expressed by "constitutive equations".
- The coinage "constitutive equation" unfortunately does not describe how a material is constituted. It is an incorrect usage of the English word "constitutive".
- The difference between how a body is constituted and what one means by "constitutive equations" can be best understood if we think in terms of a black box responding to an input by exhibiting a certain output, the input-output relation does not reveal the contents of the black box.
- There is nothing to prevent two different black boxes having the same input-output relation, similarly there is nothing that prevents two different bodies to respond in the same manner.

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The terms “constitutive relation”, “constitutive function”, “constitutive equation” and “constitutive expression” are used interchangeably in continuum mechanics. This imprecise, careless and slipshod usage of these terms, as though they have the same signification, masks crucial differences and obscures fundamental and profound implications with regard to describing the response characteristics of bodies, and this point cannot be overemphasized. The term “constitutive function” suggests that the characterization of material is through the specification of explicit expressions for a certain variable, say the stress, in terms of kinematical quantities such as the strain, or the velocity gradient. The term “relation” (binary relation), on the other hand, implies that given two sets A and B, the member of one is related to the members of the other, usually expressed as $x\mathrm{R}y$ wherein $x \in A$ and $y \in B$.

Newton is unequivocal about the fact that force is the cause and motion is the effect as evidenced by the following sentiments:

- *The causes by which true and relative motion are distinguished, one from the other, are the forces impressed upon bodies to generate motion.*

- *The alteration of motion is ever proportional to the motive force impressed; and is made in the direction of the right line in which that force is impressed.*

– Newton Principia, 1687

- *A constitutive equation is a relation between forces and motions. In popular terms, force is applied to a body to "cause" it to undergo a motion, and the motion "caused" differs according to the nature of the body. In continuum mechanics the forces of interest are contact forces, which are specified by the stress tensor $\mathbb{T}$.*

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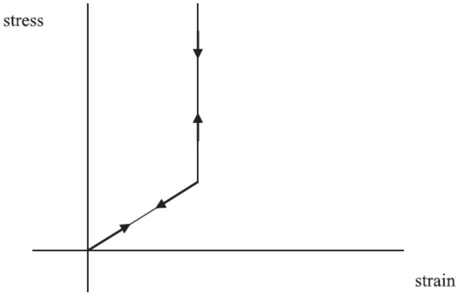

- The response is non-dissipative.
- Stored energy ψ depends on both $\mathbf{F}$ and $\mathbf{T}$.

$$\psi = \psi(\sigma, \epsilon) = \begin{cases} \hat{\psi}(\epsilon) & \forall \quad 0 \leq \sigma \leq \sigma_{cr} \\ \psi_{cr} = \text{constant} & \forall \quad \sigma > \sigma_{cr} \end{cases} \tag{1}$$

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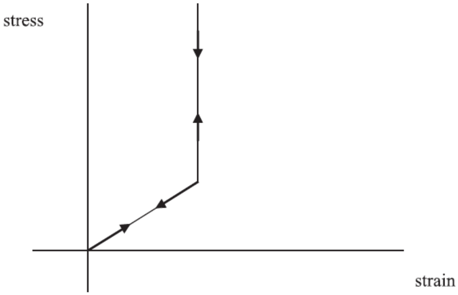

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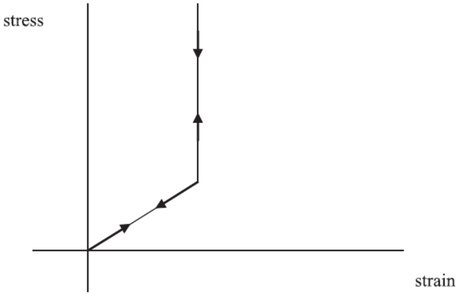

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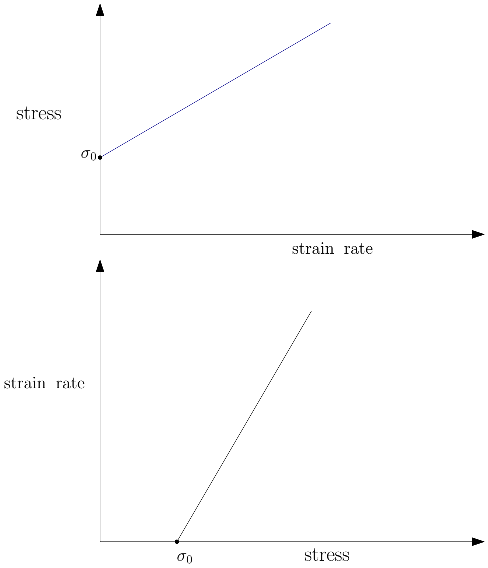
Bingham Fluid



- One should provide expressions for kinematical quantities (effects) in terms of stress (cause).
- This may not be possible, in which case one might have the more complicated situation of relations between causes and effects, which is forces and kinematical quantities.
- In classical theories like linearized elasticity it is done both ways as it is in linearized viscoelasticity.

Example

$\boldsymbol{T} = 2\mu\boldsymbol{\epsilon} + \lambda\mathrm{tr}(\boldsymbol{\epsilon})\mathbf{1}$

where λ, μ are the Lame constants.

While the Lame constant μ is the shear modulus and has clear physical underpinning and can be measured directly, the Lame constant λ cannot be measured directly, $(3\lambda + 2\mu)$ has a physical basis, it is the bulk modulus and can be measured directly.

Equivalently, $= \frac{1}{1+E}\boldsymbol{T} - \nu\mathrm{tr}(\boldsymbol{T})\mathbf{1}$, E is the Young's modulus and ν is the Poisson's ratio.

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One could also do so in the Navier-Stokes theory though it is never done so. In fact, it makes much more sense to do so especially when it comes to enforcing constraints such as incompressibility.

$$\boldsymbol{T} = -p_{\mathrm{th}}(\rho, \theta)\mathbf{1} + \lambda(\rho, \theta)\mathrm{tr}(\boldsymbol{D})\mathbf{1} + 2\mu(\rho, \theta)\boldsymbol{D} \tag{2}$$

Suppose $3\lambda + 2\mu \neq 0$. Then one can rewrite the above as (Rajagopal, 2012)

$$\boldsymbol{D} = \frac{p_{\mathrm{th}}}{3\lambda + 2\mu}\mathbf{1} - \frac{\lambda \mathrm{tr}(\boldsymbol{T})}{2\mu(3\lambda + 2\mu)}\mathbf{1} + \frac{1}{2\mu}\boldsymbol{T} \tag{3}$$

The question is whether $3\lambda + 2\mu$ can be zero. In fact Stokes makes the assumption that it is zero. One can show that this assumption is untenable. It is WRONG (As Sheharazade said "that is another story"). Books like that by Batchelor use incorrect mathematics to be in conformity with the Great Stokes.

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Early implicit rate type theories for fluids are due to Burgers and Oldroyd. Implicit theories have been discussed in great generality including implicit theories wherein the material moduli depend on both the invariants of the stress and the velocity gradient has been carried out by Rajagopal (2003), (2006), (2007). A reasonably general implicit model (Prusa and Rajagopal (2012)):

$$\mathfrak{F}_{s=0}^{\infty}\{\rho(t-s), \theta(t-s), \boldsymbol{T}(t-s), \boldsymbol{F}(t-s)\} = \boldsymbol{0} \tag{4}$$

A special sub-class (Rajagopal 2012): $\overset{\overset{(n)}{\nabla}}{\boldsymbol{T}}$

$$\mathfrak{R}\{\rho, \theta, \boldsymbol{T}, \boldsymbol{D}, \overset{\nabla}{\boldsymbol{T}}, \overset{\nabla}{\boldsymbol{D}}, \cdots \overset{\overset{(n)}{\nabla}}{\boldsymbol{T}}, \overset{\overset{(n)}{\nabla}}{\boldsymbol{D}}\} = \boldsymbol{0} \tag{5}$$

where ∇ denotes a frame indifferent material time derivative and $\overset{(n)}{\nabla}$ denotes the frame indifferent n^{th} time derivative. The Navier-Stokes, Maxwell, Oldroyd and Burgers models are special sub-classes of the above model.

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Why consider such implicit models

Consider the following generalization of the Navier-Stokes fluid:

$$\boldsymbol{T} = -p\mathbf{1} + 2\mu(p, \operatorname{tr}(\boldsymbol{D}^2))\boldsymbol{D}, \tag{6}$$

$$\operatorname{tr}(\boldsymbol{D}) = 0 \tag{7}$$

Since $p = -\frac{1}{3}\operatorname{tr}(\boldsymbol{T})$, it belongs to the class of implicit fluid models

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Fluids with pressure dependent viscosity have been studied by several persons: Bulicek, Gazzola, Hron, Kannan, Malek, Prusa, Rajagopal, Renardy, Saccomandi, Srinivasan, and others.
Consider the more general model:

$$\boldsymbol{h}(\rho, \boldsymbol{T}, \boldsymbol{D}) = \boldsymbol{0} \tag{9}$$

Since the fluid is isotropic,
$\boldsymbol{Q}\boldsymbol{h}(\rho, \boldsymbol{T}, \boldsymbol{D})\boldsymbol{Q}^T = \boldsymbol{h}(\rho, \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^T, \boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^T) \quad \forall\, \boldsymbol{Q} \in \mathcal{O}$
Thus,

$$\begin{gathered}\alpha_0\mathbf{1} + \alpha_1\boldsymbol{T} + \alpha_2\boldsymbol{D} + \alpha_3\boldsymbol{T}^2 + \alpha_4\boldsymbol{D}^2 + \alpha_5(\boldsymbol{T}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{T}) \\ +\alpha_6(\boldsymbol{T}^2\boldsymbol{D} + \boldsymbol{D}^2\boldsymbol{T}) + \alpha_7(\boldsymbol{T}\boldsymbol{D}^2 + \boldsymbol{D}\boldsymbol{T}^2) + \alpha_8(\boldsymbol{T}^2\boldsymbol{D}^2 + \boldsymbol{D}^2\boldsymbol{T}^2) = \boldsymbol{0}\end{gathered} \tag{10}$$

The material functions $\alpha_i, i = 0 \ldots 8$ depend on the density and the invariants.

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$\boldsymbol{Q}\boldsymbol{h}(\rho, \boldsymbol{T}, \boldsymbol{D})\boldsymbol{Q}^T = \boldsymbol{h}(\rho, \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^T, \boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^T) \quad \forall\, \boldsymbol{Q} \in \mathcal{O}$
Thus,

$$\begin{aligned} &\alpha_0 \mathbf{1} + \alpha_1 \boldsymbol{T} + \alpha_2 \boldsymbol{D} + \alpha_3 \boldsymbol{T}^2 + \alpha_4 \boldsymbol{D}^2 + \alpha_5(\boldsymbol{T}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{T}) \\ &+\alpha_6(\boldsymbol{T}^2\boldsymbol{D} + \boldsymbol{D}^2\boldsymbol{T}) + \alpha_7(\boldsymbol{T}\boldsymbol{D}^2 + \boldsymbol{D}\boldsymbol{T}^2) + \alpha_8(\boldsymbol{T}^2\boldsymbol{D}^2 + \boldsymbol{D}^2\boldsymbol{T}^2) = \mathbf{0} \end{aligned} \tag{10}$$

The material functions $\alpha_i, i = 0 \ldots 8$ depend on the density and the invariants.

- Unknowns:
  - Stress - six scalars since it is symmetric
  - Velocity - three three scalars
  - Density - one scalar
- Total of 10 unknowns
- Constitutive relations: six scalar equations
- Balance of mass: one scalar equation
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The insidious effect of mathematics on physics

- When one has a constitutive expression for the stress in terms of either the density and the displacement (solids) or velocity(fluids), and substitutes this expression into the balance of linear momentum, one has just the balance of linear momentum and the balance of mass (four equations) for the density and either displacement or velocity (four equations).
- However, one increased the order of the equation!
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Consider how an incompressible Navier-Stokes fluid is expressed:

$$\boldsymbol{T} = -p\boldsymbol{I} + 2\mu\boldsymbol{D}, \tag{11}$$

$$\operatorname{tr}(\boldsymbol{D}) = 0 \tag{12}$$

We have introduced a "Lagrange multiplier" (constraint reaction) "p" which we know nothing about. We do not know the space which it belongs to, etc.

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Suppose we start with (Srinivasa and Rajagopal (2012))

$$\boldsymbol{L} := \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} = \boldsymbol{f}(\rho, \theta, \boldsymbol{T}). \tag{13}$$

Balance of angular momentum (symmetry of stress) and Galilean Invariance leads to

$$\boldsymbol{D} = \boldsymbol{f}(\rho, \theta, \boldsymbol{T}). \tag{14}$$

Isotropy of the fluid leads to

$$\boldsymbol{f}(\rho, \theta, \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^T) = \boldsymbol{Q}\boldsymbol{f}(\rho, \theta, \boldsymbol{T})\boldsymbol{Q}^T \ \forall \ \boldsymbol{Q} \ \in \ \mathcal{O} \tag{15}$$

and representation theorems lead to

$$\boldsymbol{D} = \gamma_1 \mathbf{1} + \gamma_2 \boldsymbol{T} + \gamma_3 \boldsymbol{T}^2, \tag{16}$$

where the $\gamma_i, i = 1, 2, 3$ depend on $\rho, \theta, \mathrm{tr}\boldsymbol{T}, \mathrm{tr}\boldsymbol{T}^2$ and $\mathrm{tr}\boldsymbol{T}^3$

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Starting with this model one can show that the Stokes assumption is incorrect.

To describe an incompressible fluid within the above context, the constitutive relation would be

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Leads to exceedingly interesting models for solid behavior. We will only consider elastic response.

Classical Cauchy elastic body:

$$\boldsymbol{T} = \delta_1 \mathbf{1} + \delta_2 \boldsymbol{B} + \delta_3 \boldsymbol{B}^2 \tag{20}$$

where the δ_i, $i = 1, 2, 3$ depends on ρ, θ, $\mathrm{tr}\boldsymbol{B}$, $\mathrm{tr}\boldsymbol{B}^2$, $\mathrm{tr}\boldsymbol{B}^3$.
Let us consider an implicit constitutive relation of the form

$$\boldsymbol{f}(\boldsymbol{T}, \boldsymbol{B}) = \mathbf{0}. \tag{21}$$

Standard arguments in the case of isotropic bodies leads to

$$\begin{aligned} &\alpha_0 \mathbf{1} + \alpha_1 \boldsymbol{T} + \alpha_2 \boldsymbol{B} + \alpha_3 \boldsymbol{T}^2 + \alpha_4 \boldsymbol{B}^2 \\ &+\alpha_5 \boldsymbol{TB} + \boldsymbol{BT} + \alpha_6 \boldsymbol{T^2 B} + \boldsymbol{B T^2} \\ &+\alpha_7 \boldsymbol{B^2 T} + \boldsymbol{B^2} + \alpha_8 \boldsymbol{T^2 B^2} + \boldsymbol{B^2 T^2} \end{aligned} \tag{22}$$

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$$\boldsymbol{B} = \bar{\alpha}_0 \mathbf{1} + \bar{\alpha}_1 \boldsymbol{T} + \bar{\alpha}_2 \boldsymbol{T}^2, \tag{23}$$

is also a subclass of the above implicit equation.
Suppose we require that

$$\max_{\boldsymbol{X} \in \kappa(B), t \in \mathbb{R}} \|\nabla_{\boldsymbol{x}} \boldsymbol{u}\| = O(\delta), \qquad \delta << 1, \tag{24}$$

where $\|.\|$ stands for the trace norm, induced through the scalar product.
It follows that

$$\boldsymbol{B} = \mathbf{1} + 2\boldsymbol{\epsilon} + \boldsymbol{O}(\delta)^2 \tag{25}$$

In the case of a Cauchy elastic body we are inexorably led to

$$\boldsymbol{T} = \lambda(\mathrm{tr}\boldsymbol{\epsilon})\mathbf{1} + 2\mu\boldsymbol{\epsilon} \tag{26}$$

We have a linear relationship between the stress and the strain.

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Linearization of the implicit model leads to

$$\boldsymbol{\epsilon}+\hat{\alpha}_1\mathbf{1}+\hat{\alpha}_2\boldsymbol{T}+\hat{\alpha}_3\boldsymbol{T}^2+\hat{\alpha}_4\left[\boldsymbol{T}\boldsymbol{\epsilon}+\boldsymbol{\epsilon}\boldsymbol{T}\right]+\hat{\alpha}_5\left[\boldsymbol{T}^2\boldsymbol{\epsilon}+\boldsymbol{\epsilon}\boldsymbol{T}^2\right]=0. \quad (27)$$

- We have a non-linear relationship between the linearized strain and the stress!!
- Has tremendous applications in Fracture Mechanics.
- Even when we linearize (27) we obtain

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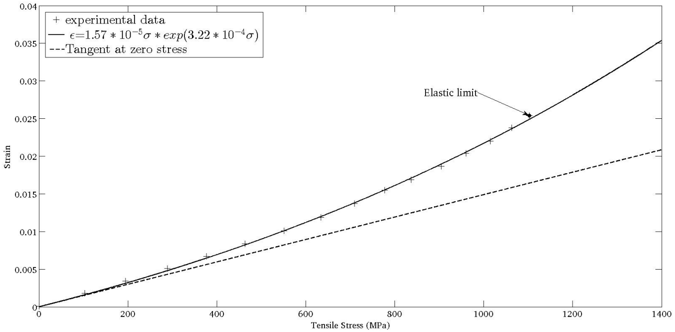

+ experimental data
$\epsilon=1.57*10^{-5}\sigma*exp(3.22*10^{-4}\sigma)$
---Tangent at zero stress
Elastic limit
Strain
Tensile Stress (MPa)
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
200
400
600
800
1000
1200
1400

- Can show that strains can be bounded at crack tip for the anti-plane stress problem (Rajagopal and Walton (2011)).
- Can show the strain is bounded at the tip of a V-notch (Kulvait, Malek and Rajagopal (2012)).

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Inelastic Response

Consider (Rajagopal and Srinivasa (2014))

$$h(\sigma, \epsilon, \theta) = 0. \tag{29}$$

- A process is "elastic " if

$$A\dot{\epsilon} + B\dot{\sigma} + \alpha\dot{\theta} = 0 \tag{30}$$

where $A := \frac{\partial h}{\partial \epsilon}$, $B := \frac{\partial h}{\partial \sigma}$, $\alpha := \frac{\partial h}{\partial \theta}$.
- -$\left(\frac{B}{A}\right)$ is the isothermal tangent modulus when $\dot{\theta} = 0$.
- $\left(\frac{\alpha}{A}\right)$ is the coefficient of expansion.

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$$A\dot{\epsilon} + B\dot{\sigma} + \alpha\dot{\theta} = 0 \tag{30}$$

  where $A := \frac{\partial h}{\partial \epsilon}$, $B := \frac{\partial h}{\partial \sigma}$, $\alpha := \frac{\partial h}{\partial \theta}$.
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Inelastic Response

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- Let $\mathbf{X}=\{\epsilon, \sigma, \theta\}$ and $\mathbf{A_0} = \frac{\partial h}{\partial \mathbf{X}}$.
- We say that a material is "inelastic" if

$$\mathbf{A_0} \cdot \dot{\mathbf{X}} = \xi(\mathbf{X}, \dot{\mathbf{X}}). \tag{31}$$

- If $\xi \equiv 0$, we have an "elastic" body.

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- Suppose

$$\xi(\mathbf{X}, \dot{\mathbf{X}}) = w(\mathbf{X}) < \boldsymbol{\mu} \cdot \dot{\mathbf{X}} >= w(\mathbf{X})(\boldsymbol{\mu} \cdot \dot{\mathbf{X}})(\boldsymbol{\mu} \cdot \dot{\mathbf{X}}), \quad (32)$$

where $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathbf{X})$.

$$\mathbf{A_0} \cdot \dot{\mathbf{X}} = \begin{cases} w(\mathbf{X})(\boldsymbol{\mu} \cdot \dot{\mathbf{X}}) & \text{if} \boldsymbol{\mu} \cdot \dot{\mathbf{X}} \geq 0 \\ 0 & \text{otherwise.} \end{cases} \quad (33)$$

Examples (Classical Plasticity)

$$\dot{\sigma} - E\dot{\epsilon} = -H(\sigma \cdot \dot{\epsilon})H(|\sigma| - \sigma_y)\dot{\epsilon} \tag{34}$$

If $|\sigma| = \sigma_y$ and $\sigma\dot{\epsilon} > 0$, then $\dot{\sigma} = 0$

- - -perfect plastic response

$\dot{\sigma} - E\dot{\epsilon} = 0$ otherwise.

The above corresponds to $\mathbf{A_0} = (1, -E)$, $\boldsymbol{\mu} = (0, \sigma)$ and $w = \frac{E}{\sigma_y H(|\sigma| - \sigma_y)}$.

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We have a sharp transition to yield

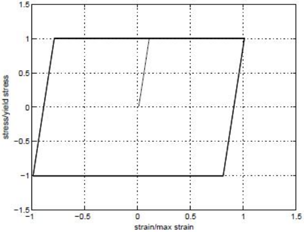

Figure : Elastic perfectly plastic response with a sharp yield point obtained by using the model (34)

Suppose

$$\dot{\sigma} - E\dot{\epsilon} = -EH(\sigma\dot{\epsilon})[1 + tanh(\alpha|\sigma| - \sigma_y)]\dot{\epsilon} \tag{35}$$

Leads to a smooth transition to yield

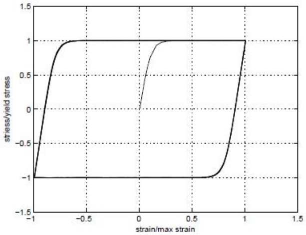

Figure : Elimination of the sharp yield point by replacing the step function with a smooth transition as shown in equation 35

Non-Classical Inelasticity

Intermettalic Alloys (Ti-Ta-Nb-Va-Zr-O)
Suppose

$$-a(\sigma+b\sigma^3)\dot{\sigma}+\dot{\epsilon}=f(\sigma)<\sigma\dot{\epsilon}>, f(\sigma)=\left[1+tanhb\left(\frac{\sigma-\sigma_y}{2\sigma}\right)\right]. \tag{36}$$

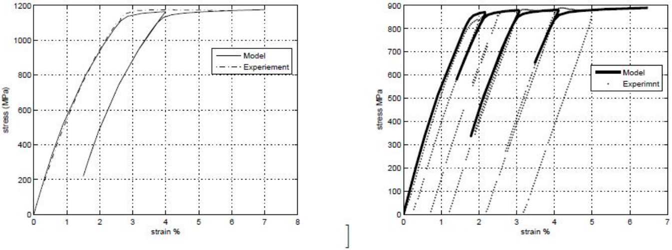

Figure : (a) Comparison of the prediction of the model 15 for gum metal with experiments by Saito et al (b) Predictions of unloading and reloading of gum metal with experiments of Besse et al

Loss of cohesion(Soils, Rocks)

$$\epsilon\dot{\sigma} - \sigma\dot{\epsilon} = H(\sigma + K\epsilon - \sigma y)(-\sigma + K\dot{\epsilon})\epsilon H(\sigma\dot{\epsilon}). \qquad (37)$$

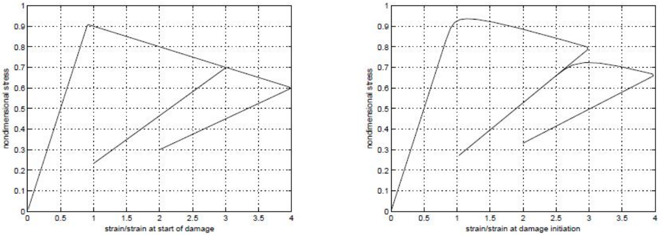

Figure : (a) A model for a degrading material with loss of stiffness and with a sharp point of degradation (b) A model with a more gradual onset of degradation. Notice how the subsequent loading causes a nonlinear response due to gradual onset of degradation compared to the sudden onset shown in figure (a). The response replicates, in an idealized way, the decrease in the moduli of rocks during compressive loading

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- For instance if one wants to model a fluid that is incompressible to mechanical stimuli but is expansible or compressible to thermal stimuli, it can be represented, in the case of the Navier-Stokes Fourier fluid, very simply as (Rajagopal (2012)).

$$\boldsymbol{D} = \beta^f(\theta)\left(\boldsymbol{T} - \frac{1}{3}\mathrm{tr}(\boldsymbol{T})\mathbf{1}\right) + \frac{1}{3}\alpha^f(\theta)\dot{\theta}\mathbf{1} \tag{38}$$

The celebrated Oberbeck-Boussinesq approximation follows very cleanly from the above representation. Practically all the justifications using the classical approach are either wrong or most convoluted.

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- Relation between the stress, the symmetric part of the velocity gradient and temperature, if one is interested in describing the possibility of a fluid that is mechanically incompressible but can undergo volume changes with regard to temperature, one would use the constraint:

$$det\boldsymbol{F} = f(p, \theta), \tag{39}$$

where $p = -\frac{1}{3}tr\boldsymbol{T}$.

- The above constraint (39) can be applied to the class of models defined through

$$\boldsymbol{T} = -p\boldsymbol{I} + 2\mu(p, \theta)\left[\boldsymbol{D} - \frac{1}{3}\left(tr\boldsymbol{D}\right)\boldsymbol{I}\right]. \tag{40}$$

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- The above approach can be extended to solids. In the case of an elastic solid that is incompressible with regard to mechanical stimuli but can expand or contract due to thermal stimuli, and which can undergo only small displacement gradients, the model becomes once again simple and elegant: $\boldsymbol{\epsilon} = \gamma_1^s(\rho, \theta, I_1, I_2, I_3)\boldsymbol{T}_d + \gamma_2^s(\rho, \theta, I_1, I_2, I_3){\boldsymbol{T}_d}^2$
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- *Aristotle has said that the sweetest of all things is knowledge. And he is right. But if you were to suppose that the publication of a new view were productive of unbounded sweetness, you would be highly mistaken. No one disturbs his fellow man with a new view unpunished.*

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