On the Modeling of Entropy Producing Processes

K. R. Rajagopal

Texas A&M University

August 2007



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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."

E. Mach



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 "Everything of importance has been said by somebody who did not discover it."

A. N. Whitehead



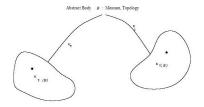


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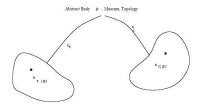


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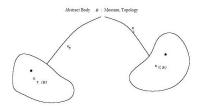


• κ_{τ} , $\kappa_{\rm t}$ - Placers



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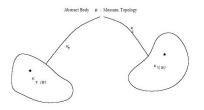
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- κ_{τ} , $\kappa_{\rm t}$ Placers
- $\kappa_{\tau}(\mathcal{B}), \kappa_{t}(\mathcal{B})$ -Configurations

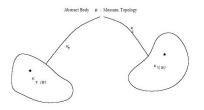


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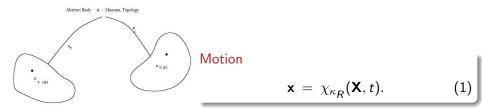
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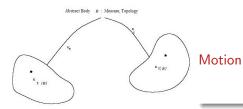




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$$\mathbf{x} = \chi_{\kappa_R}(\mathbf{X}, t). \tag{1}$$

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- Motion is a one-parameter family of placers.

Relative Motion

$$\xi = \chi_{\kappa_R} \left(\chi_{\kappa_R}^{-1}(\mathbf{x}, t), \tau \right) = \chi_t(\mathbf{x}, \tau).$$
 (2)

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Deformation Gradient

$$\mathbf{F}_{\kappa_{R}} \equiv rac{\partial \chi_{\kappa_{R}}}{\partial \mathbf{X}}.$$



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Deformation Gradient

$$\mathbf{F}_{\kappa_{R}} \equiv \frac{\partial \chi_{\kappa_{R}}}{\partial \mathbf{X}}.$$

• \mathbf{F}_{κ_R} is a linear transformation from the tangent space at \mathbf{X} to the tangent space at \mathbf{x} .



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Relative Deformation Gradient

$$\mathbf{F}_{\kappa_{\rm t}} \equiv \frac{\partial \chi_t}{\partial \mathbf{x}}.$$
 (4)



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Lagrangian

$$\phi = \hat{\phi}(\mathbf{X}, t); \quad \nabla \phi := \frac{\partial \hat{\phi}}{\partial \mathbf{X}}; \quad \frac{d\phi}{dt} := \frac{\partial \hat{\phi}}{\partial t}$$
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Eulerian

$$\phi = \tilde{\phi}(\mathbf{x}, t); \quad \text{grad}\phi := \frac{\partial \tilde{\phi}}{\partial \mathbf{x}}; \quad \frac{\partial \phi}{\partial t} := \frac{\partial \tilde{\phi}}{\partial t}$$
(6)



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Classical Constitutive Relations

Classical Elasticity

$$\mathbf{T} = \mathbf{f}_{\kappa_{\mathrm{R}}}(\mathbf{F}_{\kappa_{\mathrm{R}}})$$



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$$\mathbf{T} = \mathbf{f}_{\kappa_{\mathrm{R}}}(\mathbf{F}_{\kappa_{\mathrm{R}}})$$

Navier Stokes Fluid

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D}; \quad \mathbf{D} := \frac{1}{2} \left[\operatorname{grad} \mathbf{V} + (\operatorname{grad} \mathbf{V})^{\mathrm{T}} \right]$$
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Stokesian Fluid

$$\textbf{T}=\textbf{f}(\textbf{D})$$

(9)

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- The stress is completely known from a kinematical measurement from a single configuration.



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$$\mathbf{T} = \begin{cases} -p_1 \mathbf{I} + 2\mu_1 \mathbf{D}_{\kappa_{(t)}} & \forall t \le t', \\ -p_2 \mathbf{I} + \hat{\mu}_1 \mathbf{D}_{\kappa_{(t)}} + \hat{\mu}_2 (\mathbf{D}_{\kappa_{(t)}})^2 & \forall t > t' \end{cases}$$
(12)

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• Most bodies have more than one stress-free configuration (modulo rigid motion) ... Eckart (1940s)



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- To define a "Body" it is necessary to know the natural configurations that a body is capable of existing in. In any process, we need to know which natural configurations are accessed.
- Natural configuration \approx Equivalence class of configurations.





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- We need to define "states", "processes", and "process classes": Isothermal, Adiabatic, Isentropic, Isenthalpic, Isobaric, Isotonic, Non-Dissipative, etc.
- Different natural configurations are accessed during different processes. The natural configuration is a part of the specification of the "state" of the body.



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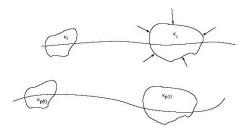


Figure: $\kappa_{p(\tau)}$ Natural configuration corresponding to κ_{τ} and $\kappa_{p(t)}$ natural configuration corresponding to κ_t

• We are used to drawing the ubiquitous potato.



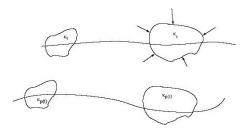


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- The notion of configuration is a local notion.



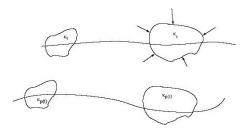


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- We are used to drawing the ubiquitous potato.
- The notion of configuration is a local notion.
- If one inhomogeneously deforms a body and then removes the traction, it is possible that the unloaded body will not fit together compatably and be simultaneously stress free in an Euclidean space.

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• However, it can be unloaded in a non-Euclidean space in which it fits together and is stress free (Eckart 1940s).



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- However, a "sufficiently small" neighborhood of a material point can be unloaded to a stress free state in Euclidean space, i.e., if the deformation is reasonably smooth, we can pick sufficiently small neighborhoods wherein the deformation is homogeneous. The notion of a configuration really applies to an appropriately small neighborhood of a point.



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- Henceforth, for the sake of illustration, let us assume homogeneous deformations.





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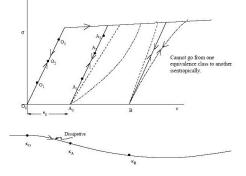


Figure: Traditional Plasticity



Twinning

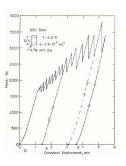


Figure: Modulo variants, we have two natural configurations, that corresponding to O and F, and these two natural configurations have different material symmetries.



Twinning

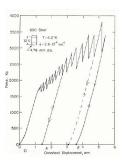


Figure: Modulo variants, we have two natural configurations, that corresponding to O and F, and these two natural configurations have different material symmetries.

 In twinning there are a finite number. As many as the number of variants.



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Viscoelasticity



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- Viscoelasticity
- Superplasticity



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- Viscoelasticity
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 - In classical elasticity the natural configuration does not evolve.



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- Viscoelasticity
- Superplasticity
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- Classical theories are trivial examples:
 - In classical elasticity the natural configuration does not evolve.
 - In classical fluids the current configuration is the natural configuration.





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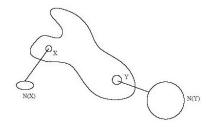


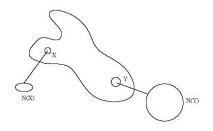
Figure: Configuration as a local notion



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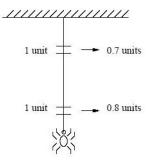


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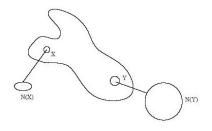
Figure: Spider spinning a web

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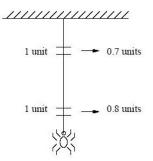


Figure: Configuration as a local notion

Figure: Spider spinning a web

 New material is laid in a stressed state. It can have a different natural configuration than the material laid down previously.



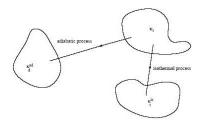


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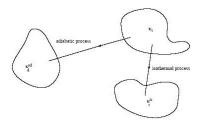
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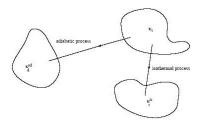


• Think in terms of Global configurations.



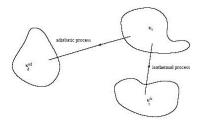


• Think in terms of Global configurations.





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 More than one Natural Configuration can be associated with the current deformed configuration.



Balance Equations

Balance of Mass

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = \mathbf{0}$$
(13)



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Balance of Linear Momentum

$$\operatorname{div} \mathbf{T} + \rho \mathbf{b} = \rho \frac{d\mathbf{v}}{dt}.$$
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Balance of Angular Momentum

$$\mathbf{T} = \mathbf{T}^{\mathrm{T}}$$

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Balance of Energy

$$\rho \frac{d\epsilon}{dt} + \operatorname{div} \mathbf{q} - \mathbf{T} \cdot \mathbf{L} - \rho r = 0$$
 (17)



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Balance of Energy

$$\rho \frac{d\epsilon}{dt} + \operatorname{div} \mathbf{q} - \mathbf{T} \cdot \mathbf{L} - \rho r = 0$$
 (17)

Second Law

$$\rho \frac{d\eta}{dt} + \operatorname{div} \frac{\mathbf{q}}{\theta} - \frac{\rho r}{\theta} := \rho \xi \ge 0$$
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Here T = Stress, η= Specific entropy, θ= Temperature, q= Heat flux vector, r= Radiant heating

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- Ziegler suggested the use of maximization of dissipation, but not within this context.
- The maximization of entropy production makes choices amongst possible response functions. For instance, it will pick a rate of dissipation (or entropy production) from amongst a class of candidates.



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- For a class of materials, such a choice leads to a Liapunov function that decreases with time to a minimum value (Onsager/Prigogine-Minimum entropy production criterion). Rajagopal and Srinivasa(2003), Proc. Royal Society.
- There is no contradiction between these two criteria:
 - Maximization of entropy production to pick constitutive equations and the minimization of entropy production with time once a choice has been made. (Rajagopal and Srinivasa (2002)).



• During the process entropy is produced in a variety of ways:



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- During the process entropy is produced in a variety of ways:
 - Due to conduction

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 - Growth



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• Part of the energy that is supplied to the body is stored in the body in a variety of ways.



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- Part of the energy that is supplied to the body is stored in the body in a variety of ways.
- The energy supplied



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- Part of the energy that is supplied to the body is stored in the body in a variety of ways.
- The energy supplied
 - Can change the kinetic energy.



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- Part of the energy changes the "Latent Energy".



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- Part of the energy due to mechanical working is transferred as energy in its thermal form (Heat).
- Part of the energy changes the "Latent Energy".
- Part goes towards "Latent Heat".

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• The symmetry of the natural configuration associated with the material that is laid down could change as the process progresses.



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- The symmetry of the natural configuration associated with the material that is laid down could change as the process progresses.
- Consider crystallization of a polymer melt. The symmetry of the material that crystallizes could be determined by the deformation.



- The symmetry of the natural configuration associated with the material that is laid down could change as the process progresses.
- Consider crystallization of a polymer melt. The symmetry of the material that crystallizes could be determined by the deformation.
- For example one could have the crystalline material being orthotropic with the axis of othotropy being determined by the eigen-vectors of the stretch tensor or the symmetric part of the velocity gradient.



Symmetry Issues





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Entropy producing processes

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$$\mathcal{G}_{\kappa} := \{ \mathbf{H} \in \mathcal{U} | \mathbf{f}_{\kappa}(\mathbf{F}\mathbf{H}) = \mathbf{f}_{\kappa}(\mathbf{F}) \},$$
(19)
$$\mathbf{P} = \nabla \lambda$$
(20)



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• \mathcal{G}_{κ} is a group. If $\mathcal{G}_{\kappa} \supseteq \theta$, we say that the body is isotropic.



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• \mathcal{G}_{κ} is a group. If $\mathcal{G}_{\kappa} \supseteq \theta$, we say that the body is isotropic. Noll's Rule

$$\mathcal{G}_{\hat{\kappa}} := \mathbf{P} \mathcal{G}_{\kappa} \mathbf{P},$$

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(21





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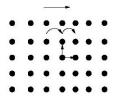
$$\mathcal{G}_{\hat{\kappa}} := \mathbf{P} \mathcal{G}_{\kappa} \mathbf{P},$$

The symmetry group for a simple fluid is the unimodular group, U (Noll).

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Entropy producing processes

Symmetry Issues





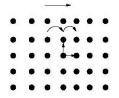
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Symmetry Issues



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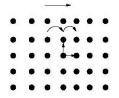


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Symmetry Issues



- After shearing the lattice structure remains the same.
- Contradicts Nolls rule.



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Image: A matrix

Solidification and Melting

• "The properties of normal liquids are strictly isotropic; they possess no crystalline structure which singles out any one direction as different from another, while true solids (excluding glasses and amorphous phases) possess non-spherical symmetries which are characteristic of the regular arrangement of their molecules in a crystalline lattice. In order to go from a liquid to a crystalline phase, therefore, it is necessary to make a change of symmetry".

Pippard (1957)



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Pippard (1957)

 "Every transition from a crystal to a liquid and a liquid to a crystal, or a crystal to another with different symmetry is associated with the appearance or disappearance of some element of symmetry, ... it can appear or disappear only as a whole, and not gradually".

Landau (19

Image: A matrix

$$\mathbf{T} \cdot \mathbf{L} - \rho \dot{\epsilon} + \rho \theta \dot{\eta} - \frac{\mathbf{q} \cdot \operatorname{grad} \theta}{\theta} = \rho \theta \xi := h \ge 0$$
(22)



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$$\mathbf{T} \cdot \mathbf{L} - \rho \dot{\epsilon} + \rho \theta \dot{\eta} - \frac{\mathbf{q} \cdot \operatorname{grad} \theta}{\theta} = \rho \theta \xi := h \ge 0$$
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• For a single constituent and restricting to isothermal processes,



$$\mathbf{T} \cdot \mathbf{L} - \rho \dot{\epsilon} + \rho \theta \dot{\eta} - \frac{\mathbf{q} \cdot \operatorname{grad} \theta}{\theta} = \rho \theta \xi := h \ge 0$$
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• For a single constituent and restricting to isothermal processes, Rate of Dissipation

$$\zeta = \mathbf{T} \cdot \mathbf{D} - \rho \psi \tag{23}$$



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- Suppose the material is incompressible,



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• Maximize rate of dissipation subject to (23) and (24) as constraints:



$$\mathbf{T} \cdot \mathbf{L} - \rho \dot{\epsilon} + \rho \theta \dot{\eta} - \frac{\mathbf{q} \cdot \operatorname{grad} \theta}{\theta} = \rho \theta \xi := h \ge 0$$
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• For a single constituent and restricting to isothermal processes, Rate of Dissipation

$$\zeta = \mathbf{T} \cdot \mathbf{D} - \rho \psi \tag{23}$$

- The above is used as a constraint on the processes. We automatically pick ζ ≥ 0.
- Suppose the material is incompressible,

$$\det \mathbf{F} = 1, \text{ or } \operatorname{tr} \mathbf{D} = 0.$$
 (24)

• Maximize rate of dissipation subject to (23) and (24) as constraints:

$$\Phi := \zeta + \lambda_1 (\zeta - \mathbf{T} \cdot \mathbf{D} + \rho \dot{\psi}) + \lambda_2 (\mathrm{tr} \mathbf{D})$$
(25)

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$$\mathbf{\Gamma} = \mathbf{f}(\rho, \mathbf{L}) \tag{26}$$



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$$\mathbf{T} = \mathbf{f}(\rho, \mathbf{L}) \tag{26}$$

Frame-indifference

$$\mathbf{\mathsf{T}}=\widehat{\mathbf{\mathsf{f}}}(
ho,\mathbf{\mathsf{D}})$$

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$$\mathbf{T} = \mathbf{f}(\rho, \mathbf{L}) \tag{26}$$

Frame-indifference

$$\mathbf{\Gamma} = \hat{\mathbf{f}}(\rho, \mathbf{D}) \tag{2}$$

Isotropy

$$\mathbf{Q}\hat{\mathbf{f}}(
ho, \mathbf{D})\mathbf{Q}^{\mathrm{T}} = \hat{\mathbf{f}}(
ho \mathbf{Q}\mathbf{D}\mathbf{Q}^{\mathrm{T}}), \ \forall \mathbf{Q} \in \mathbf{\Theta}$$
 (28)



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Representation Theorem

$$\hat{\mathbf{f}}(\rho, \mathbf{D}) = \alpha_1 \mathbf{I} + \alpha_2 \mathbf{D} + \alpha_2 \mathbf{D}^2$$



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Representation Theorem

$$\hat{\mathbf{f}}(\rho, \mathbf{D}) = \alpha_1 \mathbf{I} + \alpha_2 \mathbf{D} + \alpha_2 \mathbf{D}^2$$

Linearity in **D**

$$\hat{\mathbf{f}}(\rho, \mathbf{D}) = -p(\rho)\mathbf{I} + \lambda(\rho)\operatorname{trD}\mathbf{I} + 2\mu(\rho)\mathbf{D}$$



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Representation Theorem

$$\hat{\mathbf{f}}(
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Linearity in **D**

$$\hat{\mathbf{f}}(
ho,\mathbf{D})=-oldsymbol{p}(
ho)\mathbf{I}+\lambda(
ho)\mathrm{tr}\mathrm{D}\mathbf{I}+2\mu(
ho)\mathbf{D}$$

Incompressibility

$$\mathbf{\Gamma} = \hat{\mathbf{f}}(\mathbf{D}) = -\rho \mathbf{I} + 2\mu \mathbf{D}$$
(31)

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Q: Can the viscosity of a fluid depend on the pressure?



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Q: Can the viscosity of a fluid depend on the pressure? **A:** Yes.



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- **Q:** Can the viscosity of a fluid depend on the pressure? **A:** Yes.
- **Q:** Is it reasonable to assume that a liquid is incompressible and its viscosity depends on the pressure (normal stress)?



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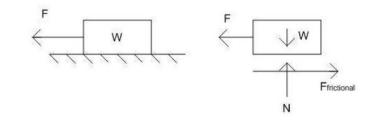
- **Q:** Can the viscosity of a fluid depend on the pressure? **A:** Yes.
- **Q**: Is it reasonable to assume that a liquid is incompressible and its viscosity depends on the pressure (normal stress)?

A: Yes.

• Density changes in liquids in certain applications(wherein the pressure (normal stresses) changes by several orders of magnitude) are of the order of a few percent, while the viscosity changes by factor of 10⁷ to 10⁸ !!!

- Elastohydrodynamic Lubrication, Szeri (1998)





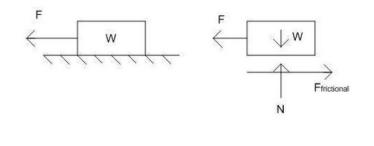


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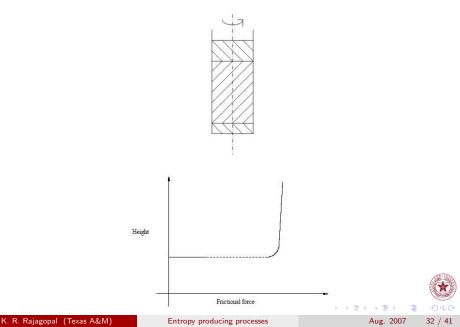
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• Frictional force definitely depends on the normal force for solids. Why should it be any different for fluids?

• Coulombs erroneous conclusions on the basis of his experiments:



• Stokes recognized that the viscosity can depend on the pressure for incompressible liquids:



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• Stokes recognized that the viscosity can depend on the pressure for incompressible liquids:

If we suppose μ to be independent of pressure also, and substitute \ldots



• Stokes recognized that the viscosity can depend on the pressure for incompressible liquids:

If we suppose μ to be independent of pressure also, and substitute \ldots

Let us now consider in what cases it is allowable to suppose μ to be independent of the pressure. It has been concluded by Du Buat from his experiments on the motion of water in pipes and canals, that the total retardation of the velocity due to friction is not increased by increasing the pressure... I shall therefore suppose that for water, and by analogy for other incompressible fluids, μ is independent of the pressure



. . .

Barus (1891)

$\mu = A \exp(\alpha p), \quad \alpha - \text{constant}, \quad \alpha \ge 0$



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$$\mathbf{T} = -\rho \mathbf{I} + \hat{\alpha_1} \mathbf{D} + \hat{\alpha_2} \mathbf{D}^2$$
(33)

Image: A matrix

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$$\mathbf{T} = -\rho \mathbf{I} + \hat{\alpha_1} \mathbf{D} + \hat{\alpha_2} \mathbf{D}^2$$
(33)

$$\hat{\alpha}_i = \hat{\alpha}_i \left(p, II_D, III_D \right) \tag{34}$$

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Entropy producing processes

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$$\mathbf{T} = -\rho \mathbf{I} + \hat{\alpha_1} \mathbf{D} + \hat{\alpha_2} \mathbf{D}^2$$
(33)

$$\hat{\alpha}_i = \hat{\alpha}_i \left(\boldsymbol{p}, \boldsymbol{II}_D, \boldsymbol{III}_D \right) \tag{34}$$

Q: Does the constraint response do no work(DAlembert, Bernoulli, Lagrange)?



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Q: Can the material moduli depend on the Lagrange multiplier? **A:** Yes.

$$\mathbf{T} = -\rho \mathbf{I} + \hat{\alpha_1} \mathbf{D} + \hat{\alpha_2} \mathbf{D}^2$$
(33)

$$\hat{\alpha}_i = \hat{\alpha}_i \left(\boldsymbol{p}, \boldsymbol{II}_D, \boldsymbol{III}_D \right) \tag{34}$$

- **Q:** Does the constraint response do no work(DAlembert, Bernoulli, Lagrange)?
- A: It is not correct to make such an assumption. Moreover, it depends on what one means by the constraint response.



• The following representation stems from assuming that the constraint response does no work, in this case the constraint being tr D = 0;



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• The following representation stems from assuming that the constraint response does no work, in this case the constraint being tr D = 0;

$$\mathbf{T} = -\rho \mathbf{I} + 2\mu \mathbf{D} \tag{35}$$



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• Goldstein (1981):



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• Goldstein (1981):

We now restrict ourselves to systems for which the net virtual work of forces of constraint is zero. We have seen that this condition holds for rigid bodies and it is valid for a large number of other constraints. Thus, if a particle is constrained to move on a surface, the force of constraint is perpendicular to the surface, while the virtual displacement must be tangent to it, and hence the virtual work vanishes. This is no longer true if sliding friction forces are present, and we must exclude such systems from our formulation.



• **Gauss** (1829 - Translated into English and published in the Philosophical Magazine in 1841):



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• **Gauss** (1829 - Translated into English and published in the Philosophical Magazine in 1841):

The motion of a system of material points connected together in any manner whatsoever, whose motions are modified by any external restraints whatsoever, proceeds in every instance in the greatest possible accordance with free motion, or under the least possible constraint; the measure of the constraint which the whole system suffers in every particle of time being considered equal to the sum of products of the square of the deviation of every point from its free motion into its mass.



• **SIMPLY PUT**: The constraint force ought to be the least force to enforce the constraint.



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- **SIMPLY PUT**: The constraint force ought to be the least force to enforce the constraint.
 - Rajagopal & Srinivasa, Proc. Roy. Soc. London (2004): Implications for Continua.



- **SIMPLY PUT**: The constraint force ought to be the least force to enforce the constraint.
 - Rajagopal & Srinivasa, Proc. Roy. Soc. London (2004): Implications for Continua.
 - Rajagopal, Applications of Mathematics (2003): Constraints and their consequences for implicit constitutive theories.



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$$\mathbf{T} = -\rho \mathbf{I} + 2\mu(\rho, |\mathbf{D}|^2)\mathbf{D} \text{ with } \mathrm{tr}\mathbf{D} = 0$$
(36)



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$$\mathbf{T} = -\boldsymbol{p}\mathbf{I} + 2\mu(\boldsymbol{p}, |\mathbf{D}|^2)\mathbf{D} \text{ with } \mathrm{tr}\mathbf{D} = 0$$
(36)

• Thus $p = -\frac{1}{3} \text{tr} \mathbf{T}$ and equation(36) takes the form,



$$\mathbf{\Gamma} = -\mathbf{p}\mathbf{I} + 2\mu(\mathbf{p}, |\mathbf{D}|^2)\mathbf{D} \text{ with } \mathrm{tr}\mathbf{D} = 0$$
(36)

• Thus $p = -\frac{1}{3} \text{tr} \mathbf{T}$ and equation(36) takes the form,

$$\mathbf{f}(\mathbf{T},\mathbf{D}) = \mathbf{0} \tag{37}$$



Thank You



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