INTRODUCTION TO CONTINUUM MECHANICS

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Continuum Media

- Material that can be analysed at the macroscopic level.
- There is no need to consider macroscopic discontinuities.
- The quantities and properties of the medium (temperature, density, displacement…) can be represented by cotinuous functions with the required smoothness.

- Continuum media:
  - solids (with own shape)
  - fluids (liquids, gases)
  - …

Continuum mechanics

1. Equations of motion
2. Kinematics:
   - Lagrangian or material description
   - Eulerian or spatial description
3. Deformations
   - Small deformations
4. Stress tensor

OBJETIVE: write the equilibrium equations that govern continuum media

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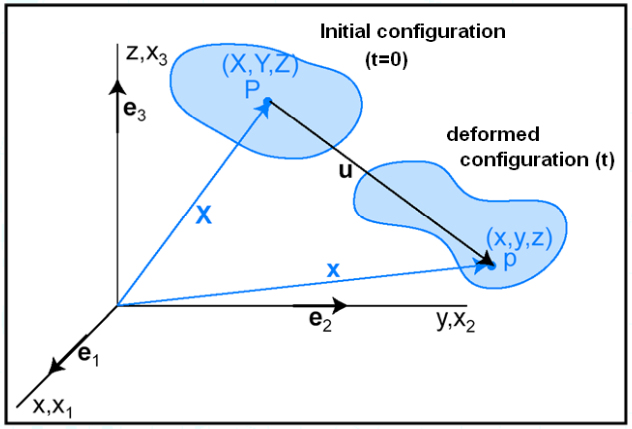
EQUATION OF MOTION



Initial position
$\mathbf{X}=X_i\,\mathbf{e}_i$

Position vector
$\mathbf{x} = x_i\,\mathbf{e}_i$

Displacement
$\mathbf{u} = \mathbf{x} - \mathbf{X}$

Equation of motion: $\boxed{\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X},t)}$

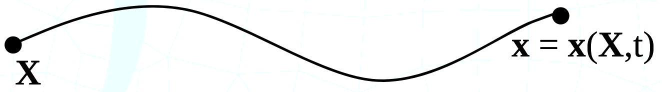
abuse of notation

$\boxed{\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{X},t)}$

- For a fixed t, $\boldsymbol{x} = \varphi(\cdot,t)$ must satisfy:
  - Biunivoc: $\boxed{\det \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \neq 0 \quad \forall t}$
  - Continuity and differentiability
  - $\boxed{\varphi(\boldsymbol{X},0) = \boldsymbol{X}}$

Lagrangian or material description (Euler)

- Physical quantities (and equations) are described with material coordinates **X**. For example, M(**X**,t) represents the physical quantity of the particle that at $t=0$ was at position **X,** and as a function of time.



If we fix **X**, we follow the same material particle at different points of the space.

- Usually employed in solids

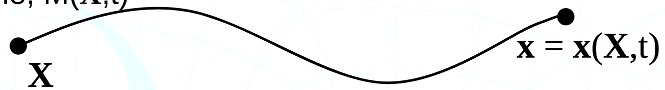
Eulerian or spatial description (Bernoulli & D'Alembert)

- The physical quantitites (and equations) are described with spatial coordinates **x**. For example, m(**x**,t) represents a physical quantity at time t at the spatial position **x**

  If we fix **x**, we are observing the same spatial point, where different material particles may be located at different times.

- Usually employed in fluids

- Once we know the equation of motion, we can swap from the Eulerian description, m(**x**,t), to the Lagrangian one, M(**X**,t)



- Example:

$$\boxed{\begin{array}{c} \boldsymbol{x} = \varphi(\boldsymbol{X},t) \quad \equiv \quad \left\{ \begin{array}{l} x = X + Yt + Zt^2 \\ y = Xt + Y + Zt^2 \\ z = Xt + Yt^2 + Z \end{array} \right. \\ m(\boldsymbol{x},t) = (x+y+z)t \end{array}}$$

Compute M(**X**,t). Compute m((1,2,3),1) and M((1,2,3),1) ¿what does it mean for each case?

Time derivatives (material and spatial)

- Physical quantity
  - Lagrangian or material description $\boxed{M(\boldsymbol{X},t)}$

    material time derivative $\boxed{\frac{d\,\cdot}{dt} := \left.\frac{\partial\,\cdot}{\partial t}\right|_{\boldsymbol{X}}}$

    time variation of a material particle
  - Eulerian or spatial description $\boxed{m(\boldsymbol{x},t)}$

    spatial time derivative $\boxed{\frac{\partial\,\cdot}{\partial t} := \left.\frac{\partial\,\cdot}{\partial t}\right|_{\boldsymbol{x}}}$

    time variation of a fix spatial point

$$\boxed{M(\boldsymbol{X},t) = m(\boldsymbol{x}(\boldsymbol{X},t),t)}$$

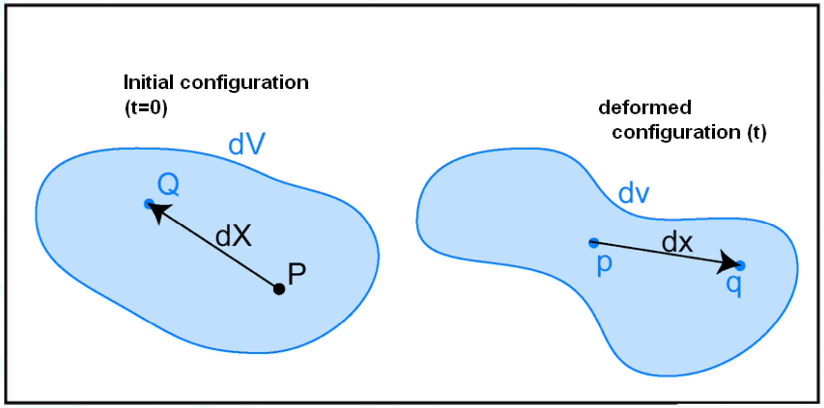
By differentiating we obtain the relation between the material derivative: $\boxed{\frac{d\,\cdot}{dt} := \left.\frac{\partial\,\cdot}{\partial t}\right|_{\boldsymbol{X}}}$ and the spatial $\boxed{\frac{\partial\,\cdot}{\partial t} := \left.\frac{\partial\,\cdot}{\partial t}\right|_{\boldsymbol{x}}}$

$$\boxed{\frac{\partial M}{\partial t} = \frac{\partial m}{\partial t} + \frac{\partial m}{\partial \boldsymbol{x}}\boldsymbol{v}}$$ with $$\boxed{\boldsymbol{v}(\boldsymbol{X},t) = \left.\frac{\partial \boldsymbol{x}}{\partial t}\right|_{\boldsymbol{X}}}$$

(velocity)

Usually we write: $$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} f}$$

DEFORMATION



- Locally, at a point P,

$$\boxed{d\boldsymbol{x} = \boldsymbol{F}\,d\boldsymbol{X}}$$

- **Deformation gradient tensor**

$$\boxed{F = F_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j}$$ $$\boxed{F_{ij} = \frac{\partial x_i}{\partial X_j}}$$

dual basis

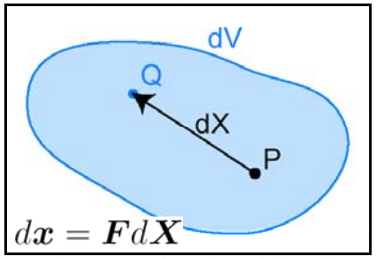
2nd order tensor that is represented with the following matrix:

$$\boxed{F = \begin{pmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} & \frac{\partial x_1}{\partial X_3} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_2}{\partial X_3} \\ \frac{\partial x_3}{\partial X_1} & \frac{\partial x_3}{\partial X_2} & \frac{\partial x_3}{\partial X_3} \end{pmatrix}}$$

Stretch

$$dS = \|d\boldsymbol{X}\|, \quad ds = \|d\boldsymbol{x}\|$$

$$\boldsymbol{T} = \frac{d\boldsymbol{X}}{dS}, \quad \boldsymbol{t} = \frac{d\boldsymbol{x}}{ds}$$



$$d\boldsymbol{x} = \boldsymbol{F}d\boldsymbol{X}$$

Stretch
(lengthening/shortening
per unit of undeformed length)

$$\varepsilon_G := \frac{ds - dS}{dS}$$

$$\begin{aligned} ds^2 - dS^2 &= d\boldsymbol{x}^T d\boldsymbol{x} - d\boldsymbol{X}^T d\boldsymbol{X} \\ &= (\boldsymbol{F}d\boldsymbol{X})^T(\boldsymbol{F}d\boldsymbol{X}) - d\boldsymbol{X}^T d\boldsymbol{X} \\ &= d\boldsymbol{X}^T \left[\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right] d\boldsymbol{X} \end{aligned}$$

- **Deformation gradient (Green)**

$$\boldsymbol{E} := \frac{1}{2}\left[\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right]$$

$$ds^2 - dS^2 = 2d\boldsymbol{X}^T\boldsymbol{E}d\boldsymbol{X}$$

$$\frac{ds^2}{dS^2} = 1 + \frac{ds^2 - dS^2}{dS^2} = 1 + \frac{2d\boldsymbol{X}^T\boldsymbol{E}d\boldsymbol{X}}{dSdS} = 1 + 2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}$$

$$\frac{ds - dS}{dS} = \frac{ds}{dS} - 1 = \sqrt{1 + 2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}} - 1$$

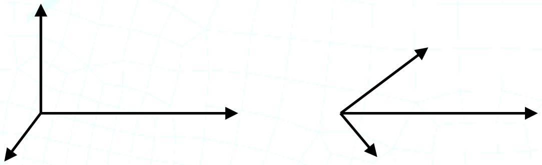
- Stretching: $\varepsilon_G = \sqrt{1 + 2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}} - 1$

Diagonal components of E

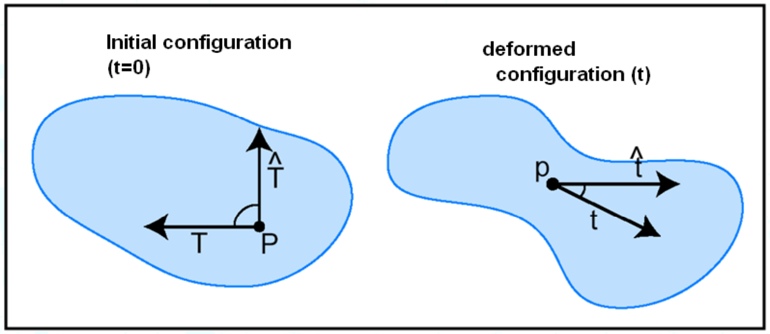
$$\varepsilon_G = \sqrt{1 + 2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}} - 1$$

- The diagonal components of the deformation tensor indicate the stretching along the coordinate axes:

$$\boldsymbol{T} = \boldsymbol{e}_i \quad \rightarrow \quad \varepsilon_G = \sqrt{1 + 2E_{ii}} - 1$$



Shear deformation



$$\cos\theta = \boldsymbol{t}^T\widehat{\boldsymbol{t}} = \frac{d\boldsymbol{x}^T}{ds}\frac{\widehat{d\boldsymbol{x}}}{\widehat{ds}} = \frac{d\boldsymbol{X}^T}{ds}\boldsymbol{F}^T\boldsymbol{F}\frac{\widehat{d\boldsymbol{X}}}{\widehat{ds}} = \boldsymbol{T}^T\left[2\boldsymbol{E} + \boldsymbol{I}\right]\widehat{\boldsymbol{T}}\frac{dS}{ds}\frac{\widehat{dS}}{\widehat{ds}}$$

Non-diagonal components of E

- If $\boxed{\Theta = \frac{\pi}{2}}$, $\boxed{\cos\theta = -\sin(\Delta\theta)}$ and

$$\boxed{\sin(\Delta\theta) = -\frac{\boldsymbol{T}^T[2\boldsymbol{E}+\boldsymbol{I}]\hat{\boldsymbol{T}}}{\sqrt{1+2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}}\sqrt{1+2\hat{\boldsymbol{T}}^T\boldsymbol{E}\hat{\boldsymbol{T}}}}}$$

- The non-linear componets of the deformation gradient indicate the angular distorsion between the coordinate axes.

$$\boxed{\boldsymbol{T} = \boldsymbol{e}_i,\ \hat{\boldsymbol{T}} = \boldsymbol{e}_j \quad \rightarrow \quad \sin(\Delta\theta) = -\frac{2E_{ij}}{\sqrt{1+2E_{ii}}\sqrt{1+2E_{jj}}}}$$

If we work with the displacements $\boxed{\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X}}$:

$$\boxed{\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \frac{\partial(\boldsymbol{X}+\boldsymbol{u})}{\partial \boldsymbol{X}} = \boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}}}$$

- **Displacement gradient tensor** $\boxed{\boldsymbol{J} = \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}}}$

$$\boxed{\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}}$$

$$\boxed{\boldsymbol{E} = \frac{1}{2}\left[\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right]} \quad \boxed{\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{J}^T + \boldsymbol{J}\right) + \frac{1}{2}\boldsymbol{J}^T\boldsymbol{J}}$$

Examples

1. Translation

$$\boxed{\boldsymbol{u}(\boldsymbol{X}) = (1,\ 1)\,, \quad \boldsymbol{\varphi}(\boldsymbol{X}) = (X+1,\ Y+1)}$$

2. Rotation

$$\boxed{\boldsymbol{\varphi}(\boldsymbol{X}) = \boldsymbol{R}\boldsymbol{X}, \quad \boldsymbol{R} = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}$$

3. $\boxed{\boldsymbol{u}(\boldsymbol{X}) = (tY,\ 0)\,, \quad \boldsymbol{\varphi}(\boldsymbol{X}) = (X+tY,\ Y)}$

4. $\boxed{\boldsymbol{\varphi}(\boldsymbol{X}) = (X(1+t/2),\ Y(1-t/2))}$

- We can work with the eulerian formulation:

$$\boxed{d\boldsymbol{X} = \boldsymbol{F}^{-1}d\boldsymbol{x}}$$

Eueleriam deformation tensor (Euler-Almansi) $\boxed{\boldsymbol{e} = \frac{1}{2}\left[\boldsymbol{I} - \boldsymbol{F}^{-T}\boldsymbol{F}^{-1}\right]}$

$$\boxed{ds^2 - dS^2 = 2d\boldsymbol{x}^T\boldsymbol{e}d\boldsymbol{x}}$$

$$\boxed{\varepsilon_{A} = \frac{ds - dS}{ds} = 1 - \sqrt{1 - 2\boldsymbol{t}^T\boldsymbol{e}\boldsymbol{t}}}$$

$$\boxed{\sin(\Delta\theta) = -\frac{\boldsymbol{t}^T[2\boldsymbol{e}+\boldsymbol{I}]\hat{\boldsymbol{t}}}{\sqrt{1-2\boldsymbol{t}^T\boldsymbol{e}\boldsymbol{t}}\sqrt{1-2\hat{\boldsymbol{t}}^T\boldsymbol{e}\hat{\boldsymbol{t}}}}}$$

SMALL DEFORMATION HYPOTHESIS

1. Small displacements: we equalise the initial and deformed configuration, and we set the equilibrium equation and the initial configuration (no update along time)

$$\boxed{\boldsymbol{x} \simeq \boldsymbol{X}}$$

2. Small displacement gradient:

$$\boxed{\left| \frac{\partial u_i}{\partial X_j} \right| << 1}$$

The quadratic terms are neglected and only the linear ones are taken into account.

- Under the small deformation hypothesis,

$$\boxed{E_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_k}{\partial X_i}\frac{\partial u_k}{\partial X_j}\right] \simeq \frac{1}{2}\left[\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i}\right]}$$

- Small deformation tensor

$$\boxed{\boldsymbol{\varepsilon} = \frac{1}{2}\left[\boldsymbol{J} + \boldsymbol{J}^T\right]}$$

$$\boxed{\boldsymbol{\varepsilon} = \frac{1}{2}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}} + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}}\right)^T\right] =: \boldsymbol{\nabla}^s \boldsymbol{u}}$$

(symmetric displacement gradient)

Physical interpretation of the components of ε

- Stretch:

$$\boxed{\sqrt{1+x} = 1 + \frac{1}{2}x + \mathcal{O}(x^2)}$$

$$\boxed{\varepsilon = \sqrt{1 + 2\boldsymbol{T}^T\boldsymbol{E}\boldsymbol{T}} - 1 \simeq 1 + \frac{1}{2}2\boldsymbol{T}^T\boldsymbol{\varepsilon}\boldsymbol{T} - 1 = \boldsymbol{T}^T\boldsymbol{\varepsilon}\boldsymbol{T}}$$

$$\boxed{\boldsymbol{T} = \boldsymbol{e}_i \quad \rightarrow \quad \varepsilon = \varepsilon_{ii}}$$

- Shear (angular distorsion):

$$\boxed{\Delta\theta \simeq \sin(\Delta\theta) \simeq \frac{-2\boldsymbol{T}^T\boldsymbol{\varepsilon}\tilde{\boldsymbol{T}}}{\sqrt{1 + 2\boldsymbol{T}^T\boldsymbol{\varepsilon}\boldsymbol{T}}\sqrt{1 + 2\tilde{\boldsymbol{T}}^T\boldsymbol{\varepsilon}\tilde{\boldsymbol{T}}}} \simeq -2\boldsymbol{T}^T\boldsymbol{\varepsilon}\tilde{\boldsymbol{T}}}$$

$$\boxed{-\frac{\Delta\theta}{2} = \boldsymbol{T}^T\boldsymbol{\varepsilon}\tilde{\boldsymbol{T}}}$$

Small deformation tensor

$$\boxed{\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x & \gamma_{xy}/2 & \gamma_{xz}/2 \\ & \varepsilon_y & \gamma_{yz}/2 \\ (sim) & & \varepsilon_z \end{pmatrix}}$$

- Stretch: ε_*
- Shear: γ_{**}

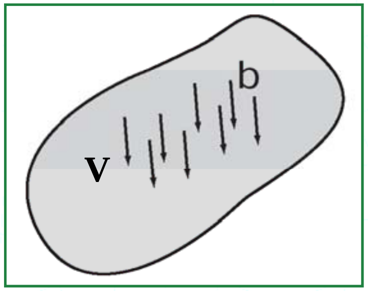
Examples

1. $\boxed{\boldsymbol{J} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}}$ $\boxed{|a|,\ |b| << 1}$

2. $\boxed{\boldsymbol{J} = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}}$ $\boxed{|a| << 1}$

$$\boxed{\begin{aligned} \boldsymbol{F} &= \boldsymbol{I} + \boldsymbol{J} \\ d\boldsymbol{x} &= \boldsymbol{F}\, d\boldsymbol{X} \end{aligned}}$$

STRESS TENSOR
Volumetric loads



They are appied at the volume interior. They are associated to the mass of the continua (gravity, electrostatics…)

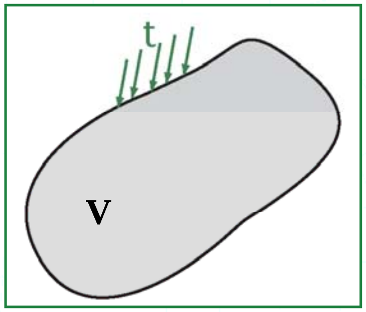
Total load on the whole volume:

$$\boxed{\boldsymbol{f}_V = \int_V \rho \boldsymbol{b}\, dV}$$

b load per unit of mass
ρ density
ρ**b** load per unit of volume

Boundary loads

They are applied at the boundary (surface) of V, S=∂V.

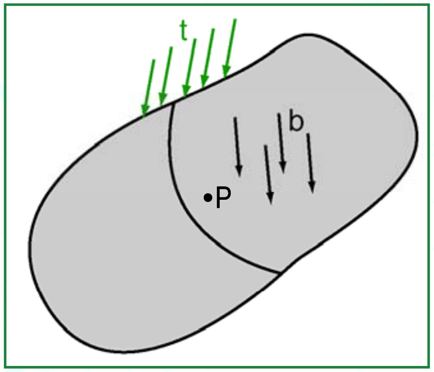


Total load on the surface:

$$\boxed{\boldsymbol{t}_S = \int_S \boldsymbol{t}\, dS}$$

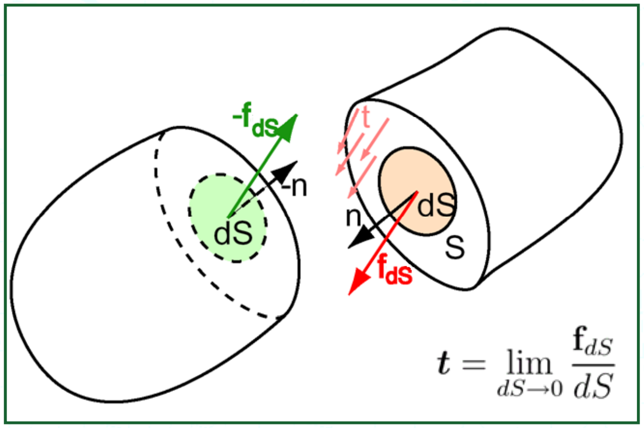
t vectorial field
(force per unit of surface = pressure)

Stress tensor



- Volumetric loads: **b**
- Surface loads: **t**

- Let’s consider a cross-section S of the volume
- The internal forces may be interpreted as a surface load, which at dS are denoted by $\mathbf{f}_{dS}$.



$$\boldsymbol{t} = \lim_{dS\to 0} \frac{\mathbf{f}_{dS}}{dS}$$

- Cauchy’s postulate: the limit

$$\boxed{\boldsymbol{t} = \lim_{dS\to 0} \frac{\mathbf{f}_{dS}}{dS}}$$

depends only on the point $\mathbf{x}$ and the normal vector $\boldsymbol{n}$ (which is independent of the cross-section S).

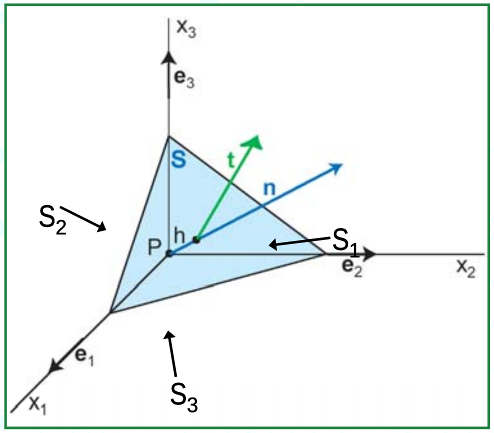
- PROPOSITION: the relation $\mathbf{t}=\mathbf{t}(\mathbf{x},\mathbf{n})$ is linearly dependent on $\mathbf{n}$:

$$\boxed{\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}}$$

Stress tensor

Demostration

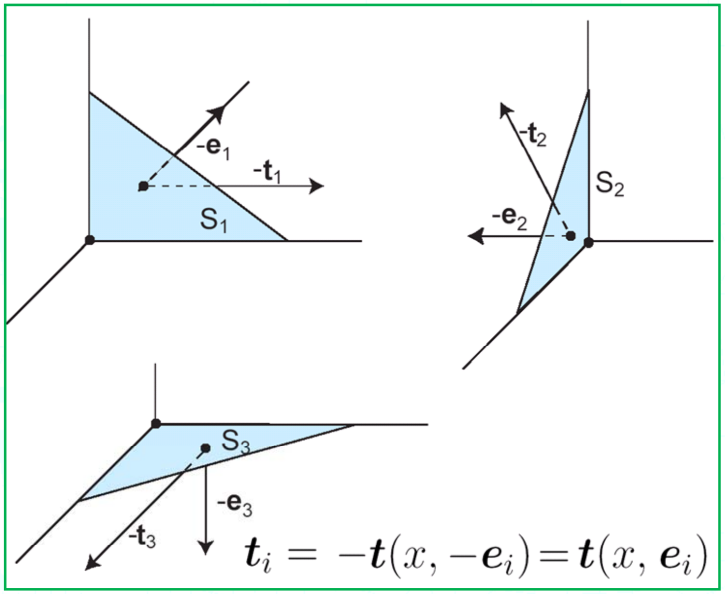
- Let’s consider a vector $\boldsymbol{n}$ at the point P and the tetrahedra formed by the planes x, y, z yand the surface S perpendicular to $\boldsymbol{n}$.



h: distance from P to S

t : surface force on S

S_i : face perpendicular to $\mathbf{e}_i$



$$\boldsymbol{t}_i = -\boldsymbol{t}(x, -\boldsymbol{e}_i) = \boldsymbol{t}(x, \boldsymbol{e}_i)$$

- We impose the conservation of linear momenta to the tetrahedra

$$\boxed{\int_V \rho \boldsymbol{b}\, dV + \int_{\partial V} \boldsymbol{t}\, dS = \int_V \rho \boldsymbol{a}\, dV}$$

$$\Downarrow$$

$$\boxed{\int_S \boldsymbol{t}\, dS - \sum_{i=1}^{3} \int_{S_i} \boldsymbol{t_i}\, dS = \int_V \rho(\boldsymbol{a} - \boldsymbol{b})\, dV}$$

- Using the integral mean value theorem,

$$\boxed{\boldsymbol{t}^* S - \sum_{i=1}^{3} \boldsymbol{t_i}^* S_i = \frac{1}{3} Sh\rho^*(\boldsymbol{a}^* - \boldsymbol{b}^*)}$$

- Taking the limit $h \to 0$

$$\boxed{\boldsymbol{t}(P, \boldsymbol{n}) - \sum_{i=1}^{3} \boldsymbol{t_i} \frac{S_i}{S} = 0}$$

and using the fact that $S_i/S = n_i = \boldsymbol{e}_i \cdot \boldsymbol{n}$

$$\boxed{\boldsymbol{t}(P, \boldsymbol{n}) = \sum_{i=1}^{3} \boldsymbol{t_i}(\boldsymbol{n} \cdot \boldsymbol{e_i}) = \underbrace{\left[\sum_{i=1}^{3} \boldsymbol{t_i} \otimes \boldsymbol{e_i}\right]}_{\boldsymbol{\sigma}} \boldsymbol{n}}$$

$$\boxed{\boldsymbol{t} = \boldsymbol{\sigma n}}$$

- By using the conservation of angular momenta, we can demonstrate that the **stress tensor is symmetric**

$$\boldsymbol{\sigma} = \left(\begin{array}{ccc} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{array}\right)$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ e_1 & e_2 & e_3 \end{array}$$

σ_{**}: normal stresses (tension/compresion)

τ_{**}: shear stresses (tangential to the surface)

CONSERVATION EQUATIONS

Reynolds transport theorem

- Allows us to express the derivative of an integral over a material volume V_t

$$\boxed{\frac{d}{dt} \int_{V_t} f(\boldsymbol{x}, t)\, dV = \underbrace{\int_{V_t} \frac{\partial f(\boldsymbol{x}, t)}{\partial t}\, dV}_{\text{Variation of } f \text{ in } V_t} + \underbrace{\int_{S_t} f(\boldsymbol{x}, t)\, \boldsymbol{v} \cdot \boldsymbol{n}\, dS}_{\text{Flux across } S_t}}$$

where S_t is the boundary of V_t, $\boldsymbol{v}$ is the velocity at S_t and $\boldsymbol{n}$ is the unit external normal vector.

Mass conservation (continuity)

- The mass must be preserved in a material volume:

$$0 = \frac{dM}{dt} = \frac{d}{dt}\int_{V_t} \rho\, dV,$$

where ρ is the density.

- Using Reynolds transport theorem

$$0 = \frac{dM}{dt} = \int_{V_t} \frac{\partial \rho}{\partial t}\, dV + \int_{S_t} \rho\, \boldsymbol{v}\cdot\boldsymbol{n}\, dS = \int_{V_t} \left(\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}) \right) dV$$

- Since the integral must vanish for all V_t

$$\boxed{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}) = 0} \quad \text{o} \quad \boxed{\frac{d\rho}{dt} + \rho\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0}$$

Balance of linear momentum (Cauchy's equation)

- Cauchy's equation equalises the variation of linear momentum and the sum of loads acting on a material volume V_t.
- Using Reynolds transport theorem in vectorial form, the variation of linear momentum results in,

$$\begin{aligned} \frac{d}{dt}\int_{V_t} \rho\boldsymbol{v}\, dV &= \int_{V_t} \frac{\partial \rho \boldsymbol{v}}{\partial t}\, dV + \int_{S_t} (\rho\boldsymbol{v}\otimes\boldsymbol{v})\cdot\boldsymbol{n}\, dS \\ &= \int_{V_t} \left(\frac{\partial \rho\boldsymbol{v}}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}\otimes\boldsymbol{v}) \right) dV, \end{aligned}$$

where $[\mathrm{v}\otimes\mathrm{v}]_{ij} = \mathrm{v}_i \mathrm{v}_j$ and we have used Gauss divergence theorem to transform the integral over S_t into an integral over the volume V_t.

- Using the mass conservation and the relation between the material and spatial derivatives, the variation of linear momentum reads

$$\frac{d}{dt}\int_{V_t} \rho\boldsymbol{v}\, dV = \int_{V_t} \rho \frac{d\boldsymbol{v}}{dt} dV$$

acceleration

- On the material volume V_t we have the following loads:

volume loads $\int_{V_t} \rho\boldsymbol{b}\, dV$ and

surface loads $\int_{S_t} \boldsymbol{\sigma}\cdot\boldsymbol{n}\, dS = \int_{V_t} \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} dV$

- Equalising the variation of linear momentum and the sum of loads over the material volume V_t , we obtain

$$\int_{V_t} \rho \frac{d\boldsymbol{v}}{dt} dV = \int_{V_t} \rho\boldsymbol{b}\, dV + \int_{V_t} \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} dV$$

- Since this holds for arbitrary volume V_t,

$$\boxed{\rho \frac{d\boldsymbol{v}}{dt} = \rho\boldsymbol{b} + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}}$$

Constitutive equation

- As yet we have derived (assuming ρ is known)

$$\boxed{\begin{gathered}\rho\frac{d^2\boldsymbol{u}}{dt^2} = \rho\boldsymbol{b} + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} \\ \boldsymbol{\varepsilon} = \boldsymbol{\nabla}^s\boldsymbol{u}\end{gathered}}$$

- This must be complemented with the constitutive equation

$$\boxed{\boldsymbol{\sigma} = \boldsymbol{f}(\varepsilon), \quad \text{o} \quad \dot{\boldsymbol{\sigma}} = \boldsymbol{f}(\dot{\varepsilon}, \dots)}$$

which characterises the material behaviour.

Large-deformation elasticity

Outline

- How to characterize large deformations (revisited)
- Piola-Kirchhoff stress tensors, governing equation of elastodynamics for large deformations
- Constitutive equation for isotropic elastic solid under large deformation

Deformation gradient and Lagrangian strain tensor (revisited)

- Deformation mapping

$$\boldsymbol{x} = \varphi(\boldsymbol{X}, t)$$

- Deformation gradient

$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \qquad F_{iJ} = \frac{\partial x_i}{\partial X_J}$$

- Lagrangian strain tensor

$$\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} - \boldsymbol{I}\right) \qquad E_{IJ} = \frac{1}{2}(F_{kI}F_{kJ} - \delta_{IJ})$$

- Eulerian strain tensor

$$\boldsymbol{e} = \frac{1}{2}\left(\boldsymbol{I} - \boldsymbol{F}^{-\mathrm{T}}\boldsymbol{F}^{-1}\right) \qquad e_{ij} = \frac{1}{2}\left(\delta_{ij} - F^{-1}_{Ki}F^{-1}_{Kj}\right)$$

Remember the summation convention: repeated indices imply summation from 1 to 3

Equation of motion for rigid body motions (revisited)

- Translation

$$\boldsymbol{x} = \boldsymbol{X} + \boldsymbol{c}(t)$$

- Rigid body rotation

$$\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{R}(t)(\boldsymbol{X} - \boldsymbol{b})$$

R: a proper orthogonal tensor (rotation tensor)

$$\boldsymbol{R}^{-1} = \boldsymbol{R}^{\mathrm{T}} \qquad \det \boldsymbol{R} = 1$$

- General rigid body motion

$$\boldsymbol{x} = \boldsymbol{R}(t)(\boldsymbol{X} - \boldsymbol{b}) + \boldsymbol{c}(t)$$

Polar decomposition theorem

- Any real tensor ***F*** with a nonzero determinant can be decomposed into the product of a proper orthogonal tensor and a symmetric tensor:

  $$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U} = \boldsymbol{V}\boldsymbol{R},$$

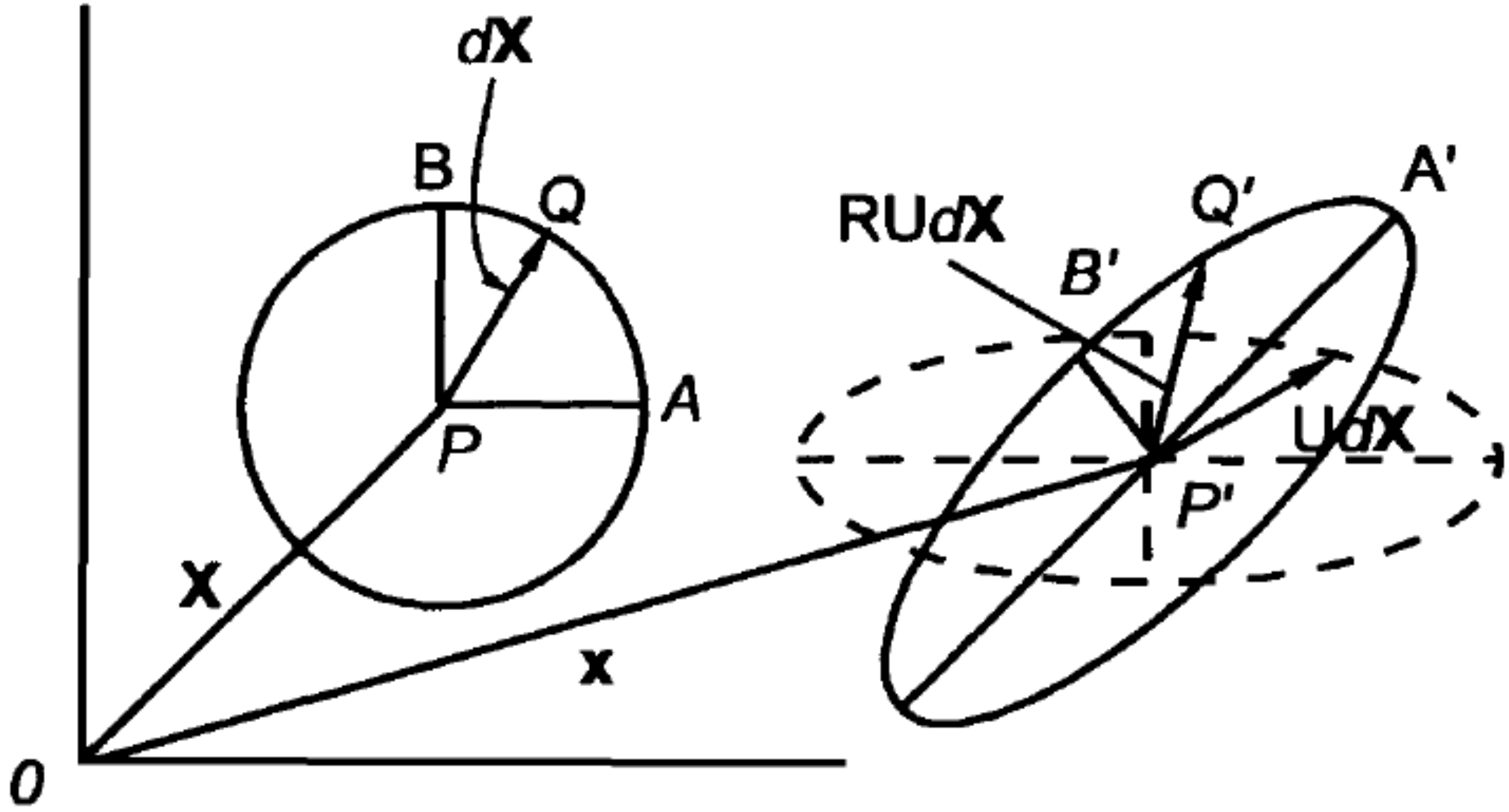
  where ***U*** and ***V*** are positive definite symmetric tensors and ***R*** is a proper orthogonal tensor. The decomposition is unique.

- If ***F*** is the deformation gradient at a certain point, then ***R***, ***U***, and ***V*** are called the rotation tensor, the right stretch tensor, and the left stretch tensor, respectively.

Physical interpretation

$$d\boldsymbol{x} = \boldsymbol{F}\,d\boldsymbol{X} = \boldsymbol{R}\boldsymbol{U}\,d\boldsymbol{X}$$

- The material element *d**X*** first undergoes a pure stretching ***U***, and then rotation ***R***



Physical interpretation (continued)

- Alternatively, we can write

$$d\boldsymbol{x} = \boldsymbol{F} d\boldsymbol{X} = \boldsymbol{V}\boldsymbol{R} d\boldsymbol{X}$$

- First rotate, and then stretch

Calculation of ***U***, ***R***, and ***V*** from ***F***

- Right Cauchy-Green deformation tensor

$$\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} = (\boldsymbol{R}\boldsymbol{U})^{\mathrm{T}}(\boldsymbol{R}\boldsymbol{U}) = \boldsymbol{U}^{\mathrm{T}}\boldsymbol{R}^{\mathrm{T}}\boldsymbol{R}\boldsymbol{U} = \boldsymbol{U}^{\mathrm{T}}\boldsymbol{U}$$

- It can be shown that ***C*** and ***U*** have the same eigenvectors and that the eigenvalues of ***C*** are the squares of those of ***U***, or $\boldsymbol{U} = \boldsymbol{C}^{\frac{1}{2}}$

- That is, if (λ_i^2, $\mathbf{n}_i$), i = 1, 2, 3 are the eigenpairs of ***C***, where $\mathbf{n}_i$ are unit vectors, then

$$\boldsymbol{C} = \sum_{i=1}^{3} \lambda_i^2 \boldsymbol{n}_i \otimes \boldsymbol{n}_i \qquad \boldsymbol{U} = \sum_{i=1}^{3} \lambda_i \boldsymbol{n}_i \otimes \boldsymbol{n}_i$$

Calculation of ***U***, ***R***, and ***V*** from ***F*** (continued)

- Once ***U*** is obtained, ***R*** and ***V*** can be obtained through

$$\boldsymbol{R} = \boldsymbol{F}\boldsymbol{U}^{-1}$$

$$\boldsymbol{V} = \boldsymbol{F}\boldsymbol{R}^{\mathrm{T}} = \boldsymbol{R}\boldsymbol{U}\boldsymbol{R}^{\mathrm{T}}$$

- Left Cauchy-Green deformation tensor

$$\boldsymbol{B} = \boldsymbol{F}\boldsymbol{F}^{\mathrm{T}} = (\boldsymbol{V}\boldsymbol{R})(\boldsymbol{V}\boldsymbol{R})^{\mathrm{T}} = \boldsymbol{V}\boldsymbol{R}\boldsymbol{R}^{\mathrm{T}}\boldsymbol{V}^{\mathrm{T}} = \boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}$$

- Example: Given

$$x_1 = X_1, \quad x_2 = -3X_3, \quad x_3 = 2X_2$$

Find ***F***, ***U***, ***R***, ***V***, ***B***

Change of area due to deformation

- Undeformed differential area element:

$$dA_0 \boldsymbol{n}_0 = d\boldsymbol{X}_1 \times d\boldsymbol{X}_2$$

as a result,

$$\boldsymbol{n}_0 = \frac{d\boldsymbol{X}_1 \times d\boldsymbol{X}_2}{|d\boldsymbol{X}_1 \times d\boldsymbol{X}_2|}$$

- The deformed area element can be simplified to

$$dA\boldsymbol{n} = dA_0(\det \boldsymbol{F})\boldsymbol{F}^{-\mathrm{T}}\boldsymbol{n}_0$$

and its magnitude is given by

$$dA = dA_0(\det \boldsymbol{F})\left|\boldsymbol{F}^{-\mathrm{T}}\boldsymbol{n}_0\right|$$

Change of volume due to deformation

- Differential volume of the deformed configuration

$$dV = (\det \boldsymbol{F}) dV_0$$

where

$$dV_0 = d\boldsymbol{X}_1 \cdot d\boldsymbol{X}_2 \times d\boldsymbol{X}_3$$

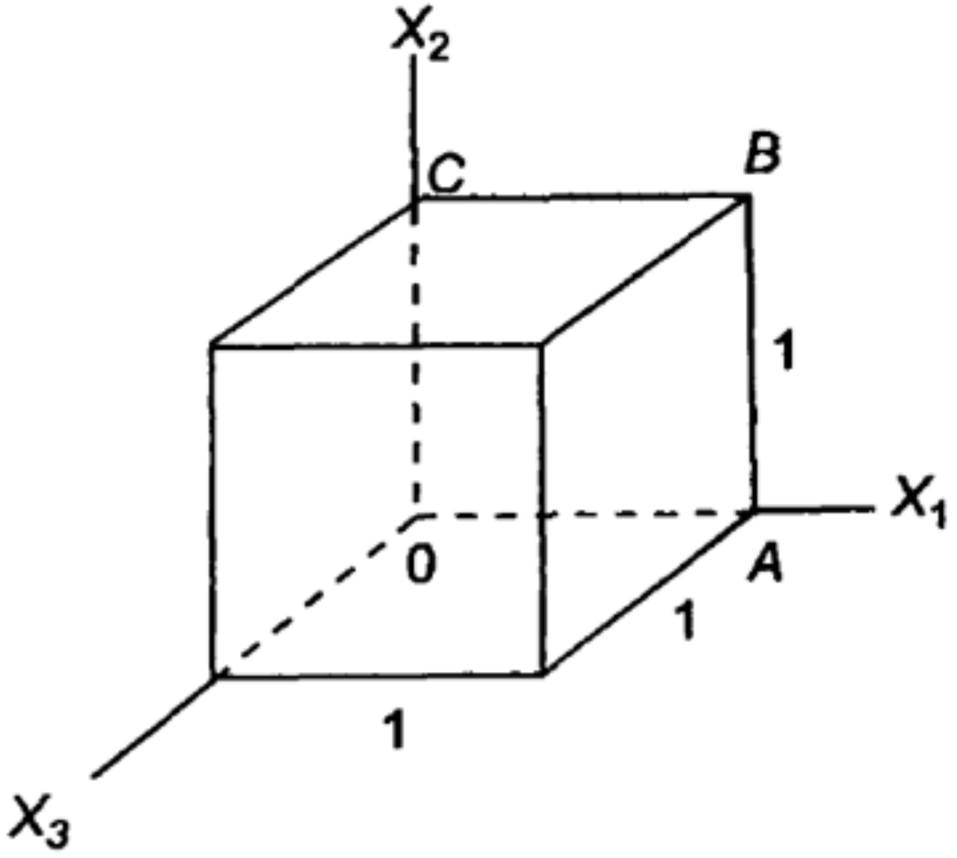
- Hence, incompressibility means

$$\det \boldsymbol{F} = \det \boldsymbol{C} = 1$$

- Consider

$$x_1 = \lambda_1 X_1, \quad x_2 = -\lambda_3 X_3, \quad x_3 = \lambda_2 X_2$$

1. Find the deformed volume of the unit cube
2. Find the deformed area of OABC



Piola-Kirchhoff stress tensors

Revisiting the Cauchy stress tensor

- We have seen the Cauchy stress tensor **σ**, which is a linear transformation such that

$$\boldsymbol{t} = \boldsymbol{\sigma} \boldsymbol{n}$$

- We note that both the direction of the traction ***t*** and the surface normal ***n*** are defined in the deformed configuration.

First Piola Kirchhoff stress tensor

- The first Piola Kirchhoff stress ***P*** relates the undeformed normal to the force in the deformed configuration per undeformed unit area:

$$\boldsymbol{t}_0 = \boldsymbol{P}\boldsymbol{n}_0$$

$$\boldsymbol{df} = \boldsymbol{t}dA = \boldsymbol{t}_0 dA_0$$

- ***P*** is related to **σ** as (show as an exercise):

$$\boldsymbol{P} = (\det \boldsymbol{F})\boldsymbol{\sigma}\boldsymbol{F}^{-\mathrm{T}} \qquad P_{iJ} = (\det \boldsymbol{F})\sigma_{ik}F^{-1}_{Jk}$$

- ***P*** is generally not symmetric

Second Piola-Kirchhoff stress tensor

- The second Piola-Kirchhoff stress tensor ***S*** is defined as

$$\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{P} \qquad\qquad S_{IJ} = F^{-1}_{Ik}P_{kJ}$$

- Motivation: ***Pn***$_0$ gives a vector in the deformed configuration, and hence premultiplying ***F***$^{-1}$ gives a vector in the reference configuration

- ***S*** is related to **σ** as

$$\boldsymbol{S} = (\det \boldsymbol{F})\boldsymbol{F}^{-1}\boldsymbol{\sigma}\boldsymbol{F}^{-\mathrm{T}}$$

- ***S*** is symmetric

Comparison of the stress tensors

- Which ones are symmetric?

- Which ones are physical (i.e., not dependent on the choice of reference configuration)?

Equilibrium equation with respect to the reference configuration

- Cauchy's equation of motion

$$\operatorname{div} \boldsymbol{\sigma} + \rho \boldsymbol{b} = \rho \boldsymbol{a}$$

- From the relation between **σ** and ***P*** we have

$$\operatorname{Div} \boldsymbol{P} + \rho_0 \boldsymbol{b} = \rho_0 \boldsymbol{a}$$

  where ρ_0 is the density at the reference configuration, and Div is the divergence with respect to the material coordinates **X**

- The second equation is more convenient to handle in the reference configuration, since the corresponding weak form involves integrals in the reference configuration

Constitutive equation for isotropic elastic solid under large deformation

Principle of material-frame indifference

- *"An important assumption in continuum mechanics is that two observers in relative motion make equivalent (mathematical and physical) deductions about the macroscopic properties of a material under test. In other words, material properties are unaffected by a superposed rigid motion, and the relation between the stress and the motion has the same form for all observers."* Ogden 1984

Change of frame

- An observer is often referred to as a **frame**
- The most general change of frame is given by

$$\begin{aligned} \boldsymbol{x}^* &= \boldsymbol{c}(t) + \boldsymbol{Q}(t)(\boldsymbol{x} - \boldsymbol{x}_0) \\ \boldsymbol{t}^* &= t - a \end{aligned}$$

where ($\boldsymbol{x}$, t) and ($\boldsymbol{x}^*$, t^*) are observations from the two frames, **c**(t) represents the relative displacement of the base point $\boldsymbol{x}_0$, **Q**(t) is a time-dependent orthogonal tensor, and *a* is a constant.

Frame indifferent (objective)

- Do these depend on the observer?

Position vector of a material point	Yes
Velocity vector of a material point	Yes
Speed of a material point	Yes
The distance between two material points	No
Vector connecting two material points	No

Relation of the same frame-indifferent vector in two frames

- Let the position vectors of two material points be $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ in the unstarred frame and $\boldsymbol{x}_1^*$, $\boldsymbol{x}_2^*$ in the starred frame. Then

$$\boldsymbol{x}_1^* = \boldsymbol{c}(t) + \boldsymbol{Q}(t)(\boldsymbol{x}_1 - \boldsymbol{x}_0)$$
$$\boldsymbol{x}_2^* = \boldsymbol{c}(t) + \boldsymbol{Q}(t)(\boldsymbol{x}_2 - \boldsymbol{x}_0)$$

thus

$$\boldsymbol{x}_1^* - \boldsymbol{x}_2^* = \boldsymbol{Q}(t)(\boldsymbol{x}_1 - \boldsymbol{x}_2)$$

or

$$\boldsymbol{b}^* = \boldsymbol{Q}(t)\boldsymbol{b}$$

Relation of the same frame-indifferent 2nd-order tensor in two frames

- Let ***T*** be the 2nd-order tensor that transforms ***b*** to ***c***, where ***b*** and ***c*** are frame-indifferent vectors:

$$\boldsymbol{c} = \boldsymbol{T}\boldsymbol{b}$$

- In a different frame,

$$\boldsymbol{c}^* = \boldsymbol{T}^*\boldsymbol{b}^*$$

- But since ***c****=***Qc***, ***b****=***Qb***,

$$\boldsymbol{T}^*\boldsymbol{b}^* = \boldsymbol{c}^* = \boldsymbol{Q}\boldsymbol{c} = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{b} = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{b}^*$$

or

$$\boldsymbol{T}^* = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^{\mathrm{T}}$$

Summary of how to change frame

- Scalar

$$\alpha^* = \alpha$$

- Vector

$$\boldsymbol{b}^* = \boldsymbol{Q}(t)\boldsymbol{b}$$

- 2nd-order Tensor

$$\boldsymbol{T}^* = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^{\mathrm{T}}$$

Transforming ***F*** in two frames

- We know

$$d\boldsymbol{x} = \boldsymbol{F} d\boldsymbol{X} \qquad d\boldsymbol{x}^* = \boldsymbol{F}^* d\boldsymbol{X}^*$$

- And

$$d\boldsymbol{x}^* = \boldsymbol{Q}(t) d\boldsymbol{x}$$

- Hence

$$\boldsymbol{Q}(t)\boldsymbol{F} d\boldsymbol{X} = \boldsymbol{F}^* d\boldsymbol{X}^*$$

- At *t* = 0,

$$\boldsymbol{Q}(t_0) d\boldsymbol{X} = d\boldsymbol{X}^*$$

- Setting **Q**(t_0) = **I**, then

$$\boldsymbol{F}^* = \boldsymbol{Q}(t)\boldsymbol{F}$$

Other transformation laws

- Right Cauchy-Green deformation tensor

$$\boldsymbol{C}^* = \boldsymbol{C}$$

- Left Cauchy-Green deformation tensor (objective)

$$\boldsymbol{B}^* = \boldsymbol{Q}(t)\boldsymbol{B}\boldsymbol{Q}(t)^{\mathrm{T}}$$

- Cauchy stress (objective)

$$\boldsymbol{\sigma}^* = \boldsymbol{Q}\boldsymbol{\sigma}\boldsymbol{Q}^{\mathrm{T}}$$

- Second Piola-Kirchhoff stress

$$\boldsymbol{S}^* = \boldsymbol{S}$$

Constitutive equation for an elastic medium under large deformation

- Acceptable constitutive laws:

$$\boldsymbol{S} = f(\boldsymbol{C})$$ (most general anisotropic material)

$$\boldsymbol{\sigma} = f(\boldsymbol{B})$$ (isotropic only)

- The following form of constitutive law is unacceptable, why?

$$\boldsymbol{\sigma} = f(\boldsymbol{C})$$

Constitutive equation for an isotropic elastic medium

- Most general form of constitutive law for isotropy:

$$\boldsymbol{\sigma} = a_0 \boldsymbol{I} + a_1 \boldsymbol{B} + a_2 \boldsymbol{B}^2$$

alternatively,

$$\boldsymbol{\sigma} = \varphi_0 + \varphi_1 \boldsymbol{B} + \varphi_2 \boldsymbol{B}^{-1}$$

where a_0, a_1, a_2, φ_0, φ_1, φ_2 are scalar functions of the scalar invariants of ***B***

Hyperelastic material

- The constitutive relations of such materials are derived from a strain energy density function *W*, e.g., for a compressible hyperelastic material,

$$\boldsymbol{P} = \frac{\partial W}{\partial \boldsymbol{F}} \qquad \boldsymbol{S} = \frac{\partial W}{\partial \boldsymbol{E}} = 2\frac{\partial W}{\partial \boldsymbol{C}}$$

$$P_{iJ} = \frac{\partial W}{\partial F_{iJ}} \qquad S_{IJ} = \frac{\partial W}{\partial E_{IJ}} = 2\frac{\partial W}{\partial C_{IJ}}$$

Example: Compressible Neo-Hookean material

$$W(\boldsymbol{F}) = \frac{\mu}{2}\left(\overline{I}_1 - 3\right) + \frac{\kappa}{2}(J-1)^2$$

where

$$J = \det \boldsymbol{F}$$
$$\overline{I}_1 = J^{-2/3} I_1 = J^{-2/3}\,\mathrm{tr}\,\boldsymbol{B}$$

PARTICLE SYSTEMS
and non-linear dynamics

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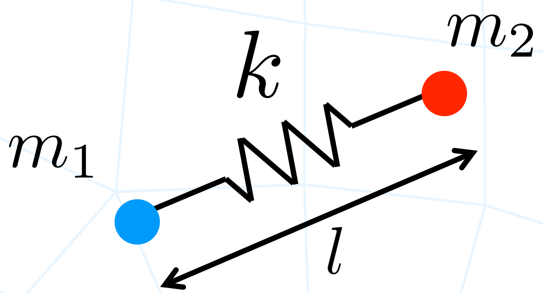
2-particle system

- System of particles:



- Notation: $q = (\boldsymbol{x}_1, \boldsymbol{x}_2)$

  $\dot{q} = (\boldsymbol{v}_1, \boldsymbol{v}_2)$

- Elastic energy: $U(\boldsymbol{q}) = \frac{1}{2}k(l - l_0)^2$

- Kinetic energy: $T(\dot{\boldsymbol{q}}) = \frac{1}{2}m_1||\boldsymbol{v}_1||^2 + \frac{1}{2}m_2||\boldsymbol{v}_2||^2$

- Euler-Lagrange equations (from Hamilton's principle...):

$$\frac{d}{dt}\frac{dL}{d\dot{\boldsymbol{q}}} - \frac{dL}{d\boldsymbol{q}} = \mathbf{0} \Longrightarrow \mathbf{M}\ddot{\boldsymbol{q}} + \nabla_q U(\boldsymbol{q}) = \mathbf{0}$$

2-particle system

- System is Hamiltonian:
  - Define:

$$\boldsymbol{p} = \frac{\partial L}{\partial \boldsymbol{q}}$$

$$H(\boldsymbol{p},\boldsymbol{q}) = \boldsymbol{p}^T\dot{\boldsymbol{q}} - L(\boldsymbol{q},\dot{\boldsymbol{q}})$$

  - Then (Hamilton's equations):

$$\boxed{\begin{aligned}\dot{\boldsymbol{p}} &= -\frac{\partial H}{\partial \boldsymbol{q}}\\ \dot{\boldsymbol{q}} &= \frac{\partial H}{\partial \boldsymbol{p}}\end{aligned}}$$

- Properties:
  - Conservation of total energy: $H(\boldsymbol{p},\boldsymbol{q}) = T(\boldsymbol{p}) + U(\boldsymbol{q})$
  - Conservation of symmetries: linear/angular momentum, simplecticity (conserves area in $(\boldsymbol{p},\boldsymbol{q})$ space)
- **Aim:** analyse time-integration schemes that numerically preserve as many as possible of these constants of motion

Time Integration Schemes (1/2)

- Symplectic Euler (explicit, 1st order)

$$\mathbf{M}\frac{\Delta \boldsymbol{v}}{\Delta t} + \nabla U(\boldsymbol{q}_n) = \mathbf{0}, \qquad \boldsymbol{v}_{n+1} = \frac{\Delta \boldsymbol{q}}{\Delta t}$$

- Trapezoidal Rule (implicit, 2nd order):

$$\mathbf{M}\frac{\Delta \boldsymbol{v}}{\Delta t} + \frac{1}{2}\left(\nabla U(\boldsymbol{q}_{n+1}) + \nabla U(\boldsymbol{q}_n)\right) = \mathbf{0}\ , \quad \boldsymbol{v}_{n+\frac{1}{2}} = \frac{\Delta \boldsymbol{q}}{\Delta t}$$

- Implicit Mid-point rule (implicit, 2nd order, symplectic):

$$\mathbf{M}\frac{\Delta \boldsymbol{v}}{\Delta t} + \nabla U(\boldsymbol{q}_{n+\frac{1}{2}}) = \mathbf{0} \qquad \boldsymbol{v}_{n+\frac{1}{2}} = \frac{\Delta \boldsymbol{q}}{\Delta t}$$

- Störmer-Verlet (explicit 2nd order, symplectic):

$$\boldsymbol{v}_{n+\frac{1}{2}} = \boldsymbol{v}_n - \mathbf{M}^{-1}\frac{\Delta t}{2}\nabla U(\boldsymbol{q}_n), \quad \frac{\Delta q}{\Delta t} = \boldsymbol{v}_{n+\frac{1}{2}}$$

$$\mathbf{M}\frac{\Delta \boldsymbol{v}}{\Delta t} + \frac{1}{2}\left(\nabla U(\boldsymbol{q}_{n+1}) + \nabla U(\boldsymbol{q}_n)\right) = \mathbf{0}$$

Time Integration Schemes (2/2)

- Energy-Conserving:

$$\boxed{\quad \mathbf{R} \equiv \mathrm{M}\frac{\Delta \boldsymbol{v}}{\Delta t} + \bar{\nabla} U(\boldsymbol{q}_n, \boldsymbol{q}_{n+1}) = \mathbf{0} \qquad \boldsymbol{v}_{n+\frac{1}{2}} = \frac{\Delta \boldsymbol{q}}{\Delta t}}$$

- Discrete derivative:

$$\bar{\nabla} U(\boldsymbol{q}_{n+1}, \boldsymbol{q}_n) = \frac{\Delta U}{\Delta \ell} \frac{\Delta \boldsymbol{q}_{n+\frac{1}{2}}}{\ell_{n+\frac{1}{2}}}$$

such that

$$\bar{\nabla} U(\boldsymbol{q}_n, \boldsymbol{q}_{n+1}) \cdot \Delta \boldsymbol{q} = \Delta U$$

- Then,

$$\boldsymbol{v}^T_{n+\frac{1}{2}} \boldsymbol{R} = \frac{\Delta E}{\Delta t}$$

Example:

- Quadratic potential:

$$U(\boldsymbol{q}) = \frac{k}{2}(\ell - \ell_0)^2$$

- Elastic forces (non-linear in 2D or 3D):

$$\nabla U = k\frac{(l - l_0)}{l}\left\{ \begin{array}{c} \boldsymbol{q}_1 - \boldsymbol{q}_2 \\ \boldsymbol{q}_2 - \boldsymbol{q}_1 \end{array} \right\}$$

- Solution of implicit schemes with Newton-Raphson require computation of Jacobian matrix:

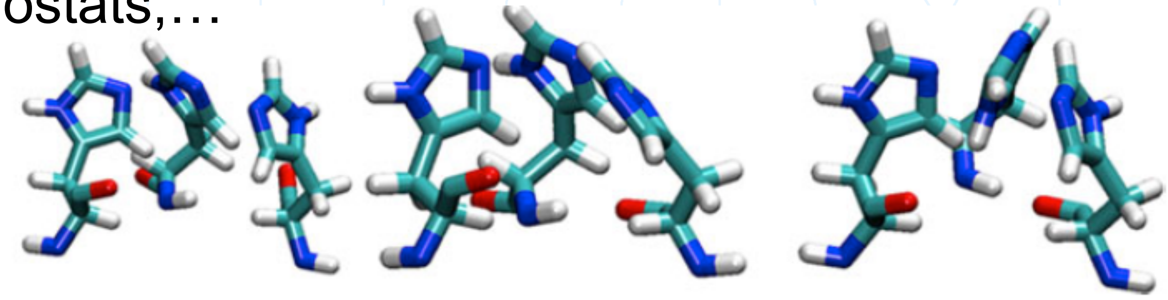
$$\mathbf{J} = \nabla^2 U(\boldsymbol{q}) = \ldots$$

- Gravity may be added by adding potential:

$$U_g(\boldsymbol{q}) = -\boldsymbol{g}^T\boldsymbol{q}$$

Remarks:

- Applications:
    - Granular materials: contact detection, large scale computations (explicit)…
    - Astrophysics, celestial mechanics: long time simulations, accuracy (Conserving schemes,…)
    - Molecular Dynamics: specific potentials (Lennard-Jones, rotations, …), thermostats,…



- Deformable bodies:
    - Use elastic potential (large-deformations, non-linear , …)
    - Similar structure: Hamiltonian,
    - Conserving schemes provide stability in non-linear dyanmics.
    - Also conserving schemes available (not everything can be conserved, but …)

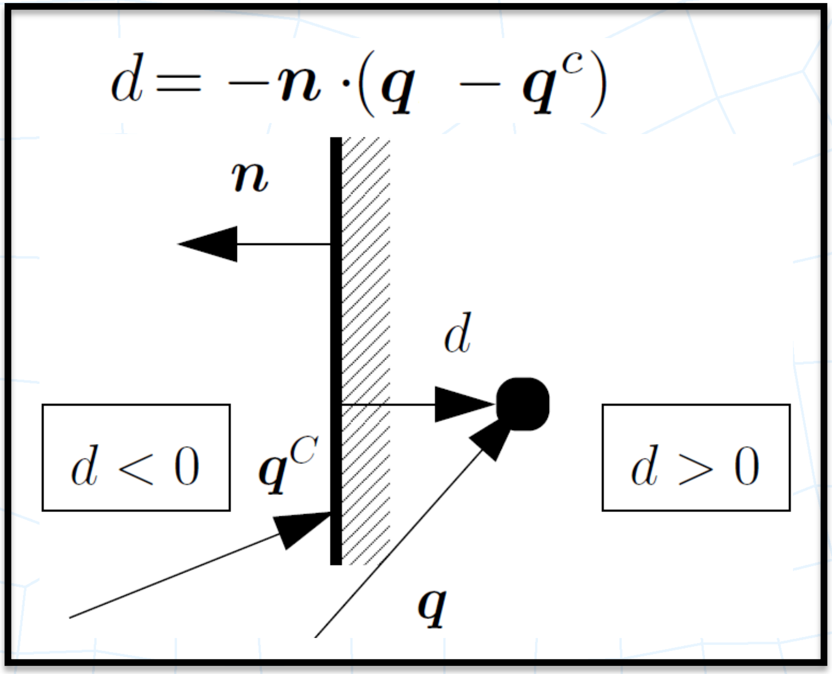
Adding constraints: Contact

- Unilateral contact: constraint with inequality
- Statics:

$$\min_{\boldsymbol{q}} U(\boldsymbol{q})$$
$$s.t.\quad d(\boldsymbol{q}) < 0$$

- Dynamics:

$$\mathbf{M}\ddot{\boldsymbol{q}} + \nabla_q U(\boldsymbol{q}) = \mathbf{0}$$
$$d(\boldsymbol{q}) < 0$$



•General approach:

$$\mathbf{M}\ddot{\boldsymbol{q}} + \nabla_q U(\boldsymbol{q}) + \boxed{\boldsymbol{g}^c} = \mathbf{0}$$

Contact

- General idea: add pot. energy: $$U^c = \frac{1}{2} p \langle d \rangle^2$$
  ⇒new residual component:

$$\boldsymbol{g}^c = \nabla_q U^c = -p \langle d_i \rangle \boldsymbol{n}$$

- Dissipative penalty:

$$\boldsymbol{g}^c = -H(d_{n+1}) p \langle \dot{d}_{n+\frac{1}{2}} \rangle \boldsymbol{n}$$

with $\dot{d}_{n+\frac{1}{2}} = -\boldsymbol{v}^T_{n+\frac{1}{2}} \boldsymbol{n}$

- Conserving penalty (Armero’98):

$$\bar{\nabla} U^c_p = -\frac{\Delta U^c_p}{\Delta d} \boldsymbol{n}$$

Contact

- Lagrange multipliers:

$$\max_{\boldsymbol{\lambda}} \min_{\boldsymbol{q}} U(\boldsymbol{q}) + \lambda d$$

KKT condit:

$$\lambda \geq 0$$

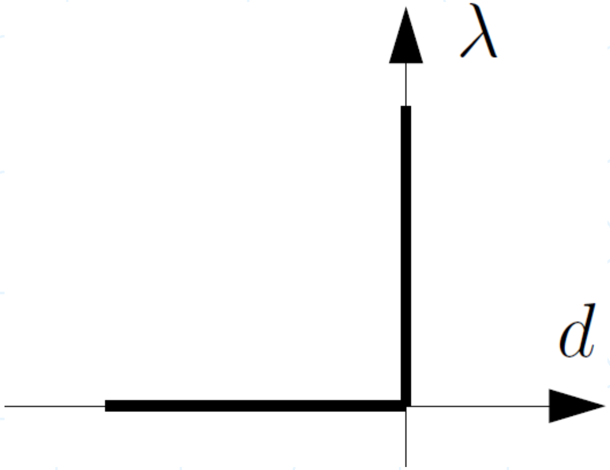
$$d \leq 0$$

Complem. c.

$$\lambda d = 0$$

Persistency c.

$$\lambda \dot{d} \leq 0$$



- Implementation:

$$U^c = \langle \lambda_i \rangle d_i$$

$$\boldsymbol{g}^c = -\langle \lambda_i \rangle \boldsymbol{n}$$

- Solution: -Uzawa algorithm

  - λ prediction (reactions)

COMPUTATIONAL PLASTICITY

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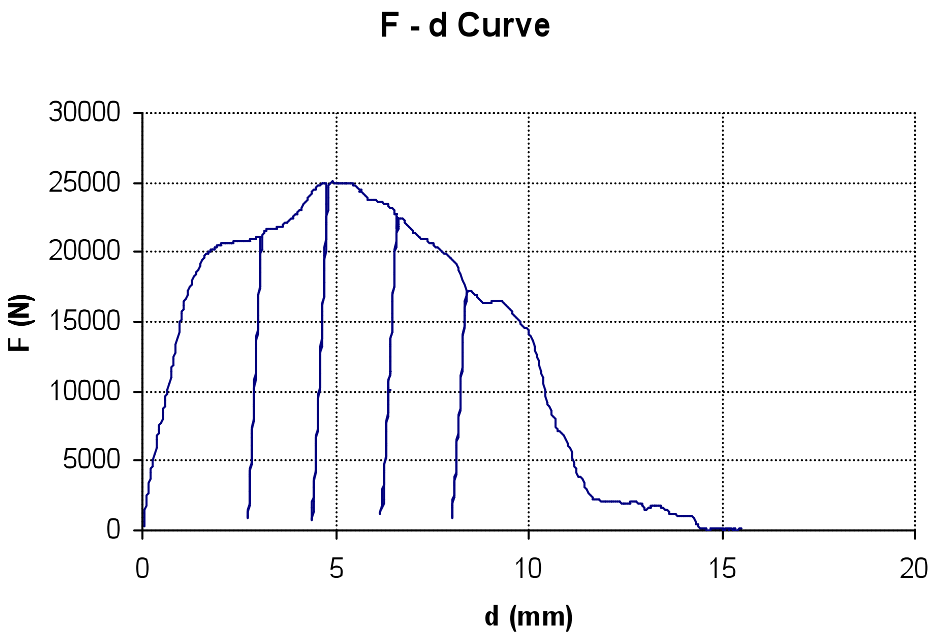
Crash-tests

Motivation

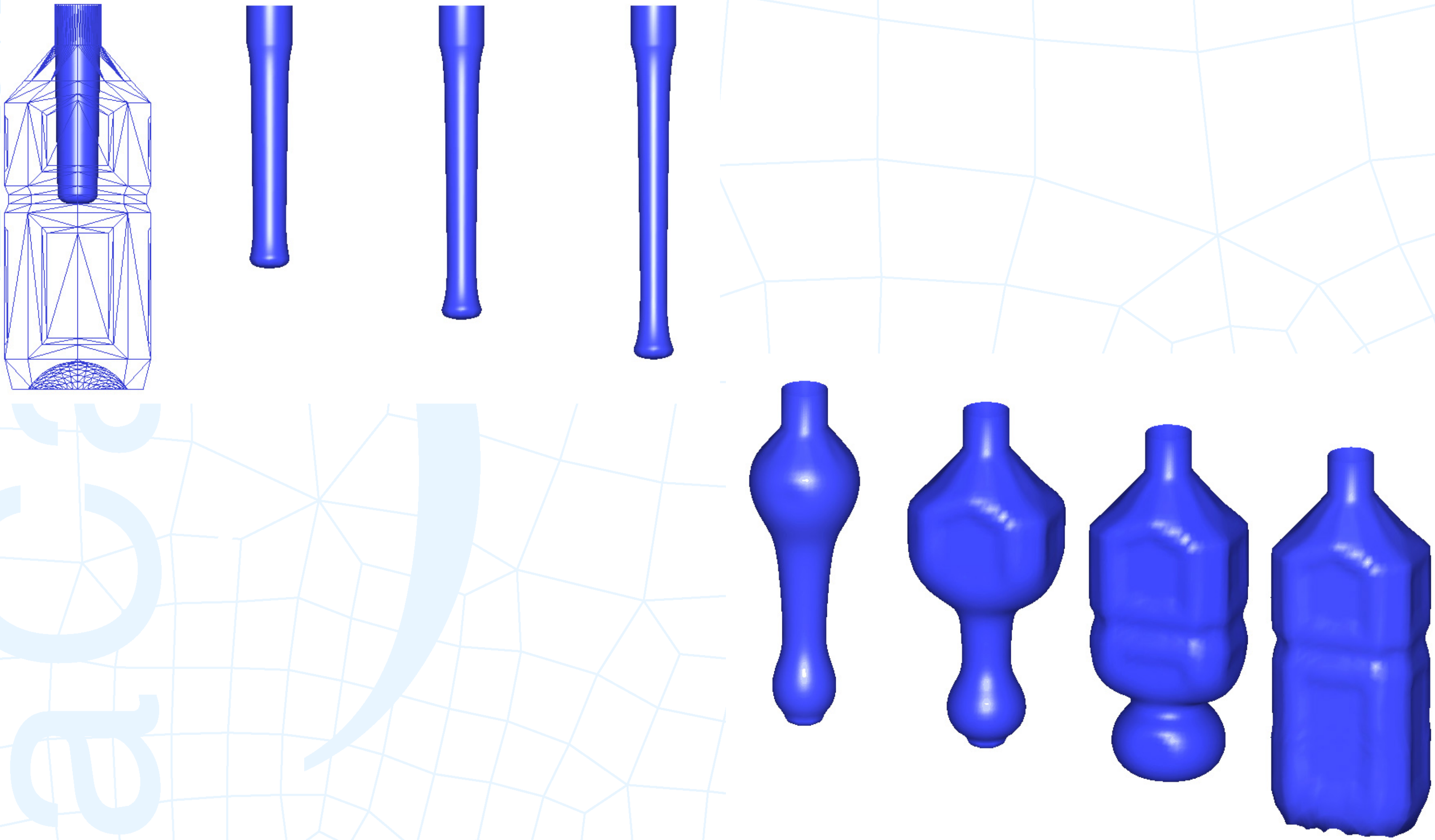


Tensile tests in lightweight steel joints

Motivation

Accidental collapse of a crane

Motivation

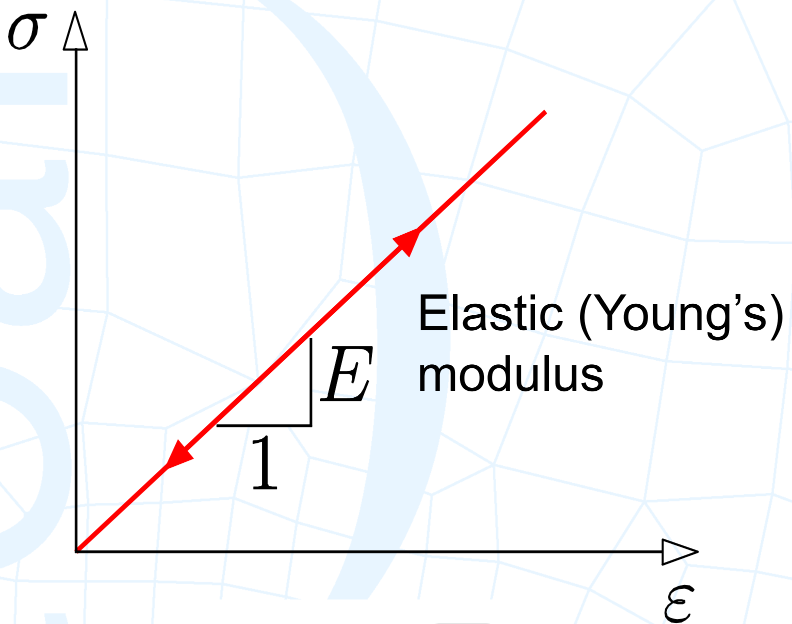


Blow moulding of a plastic bottle

(www.riken.go.jp/lab-www/mat-fab/blow/PETBlow.html)

Elasticity vs. plasticity

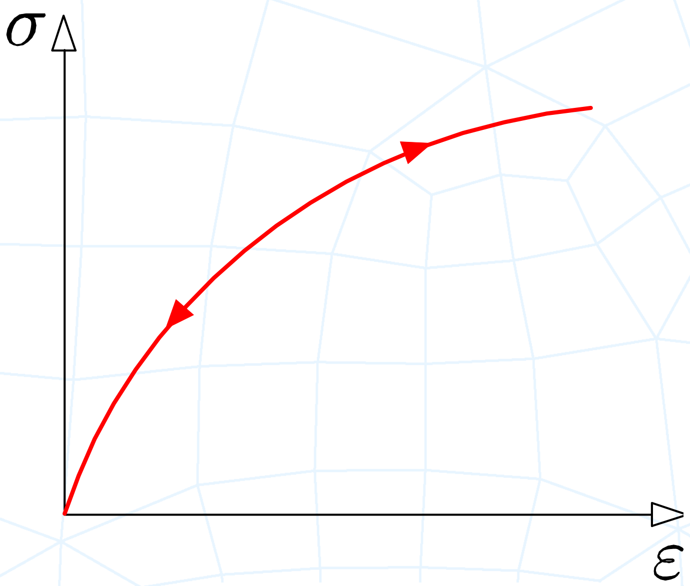
Elasticity



Elastic (Young's) modulus

$$\sigma = E\varepsilon$$

Linear elasticity

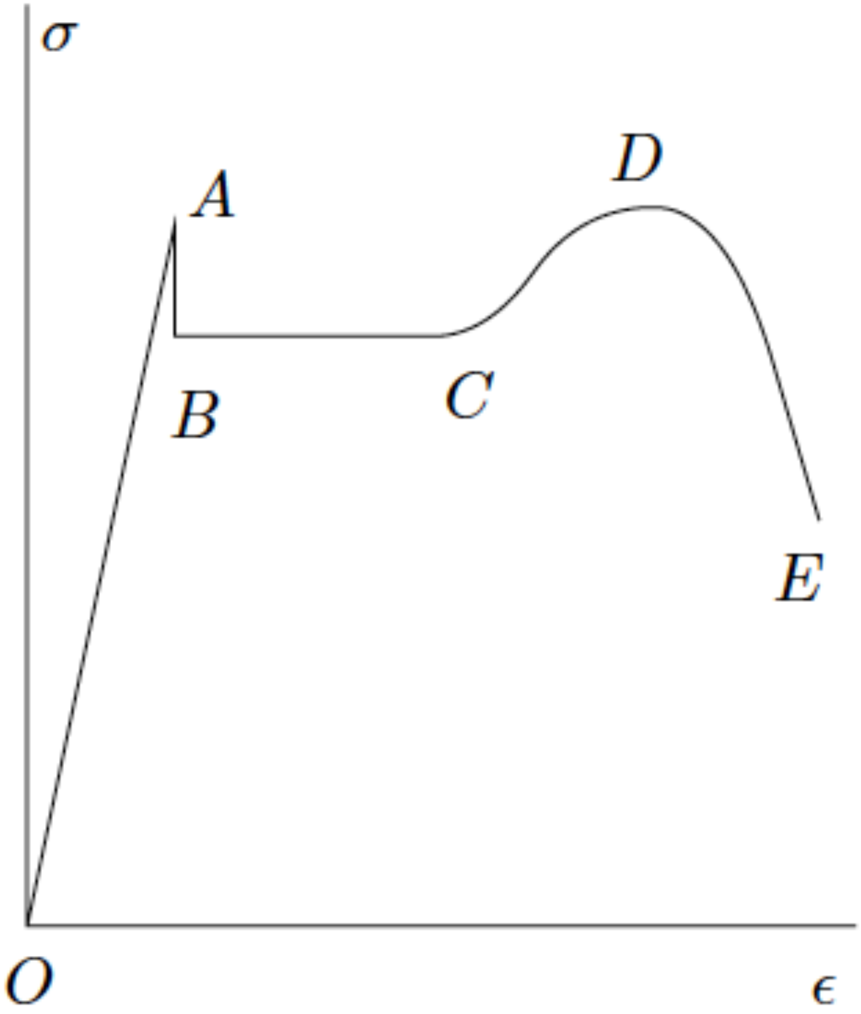


$$\sigma = F(\varepsilon)$$

Nonlinear elasticity

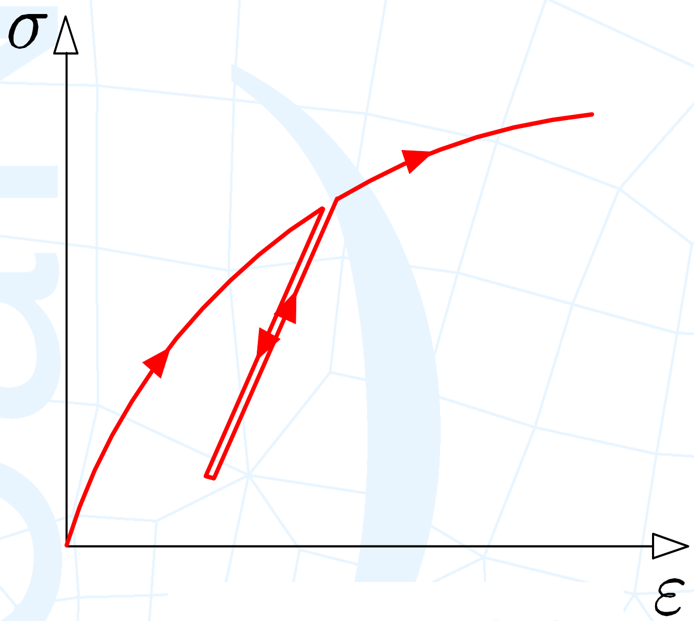
Elasticity vs. plasticity

- Stress-strain curve of a mild steel



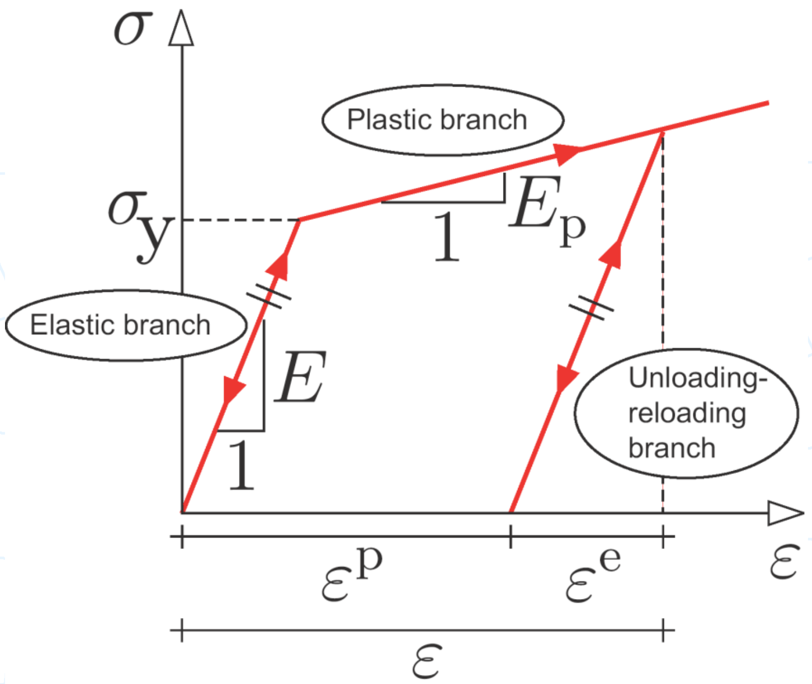
Elasticity vs. plasticity

Plasticity (or elastoplasticity)



$$\dot{\sigma} = F(\dot{\varepsilon})$$

No one-to-one relation between strain ε and stress σ



ε^e : elastic (reversible) strain

ε^p : plastic (irreversible) strain

E : elastic modulus

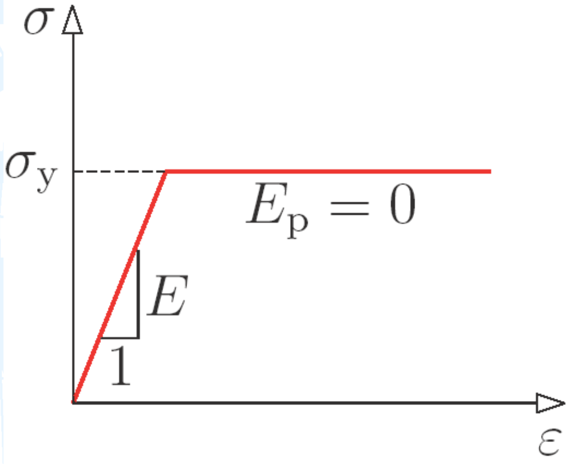
E_p : elastoplastic modulus

σ_y : yield stress

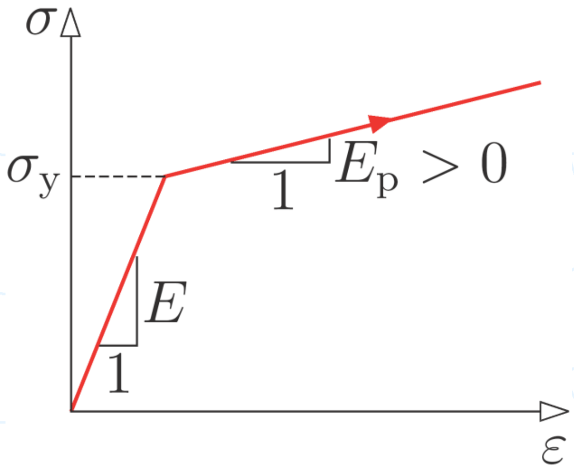
Plasticity is characterized by the ability of deforming permanently

Elasticity vs. plasticity

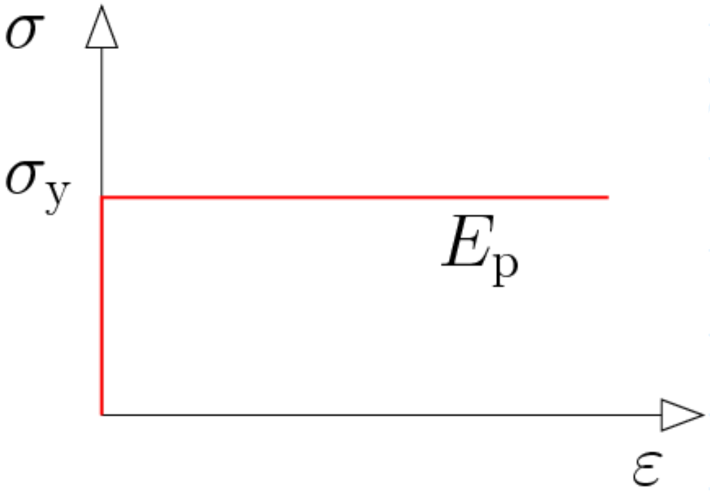
Types of plasticity



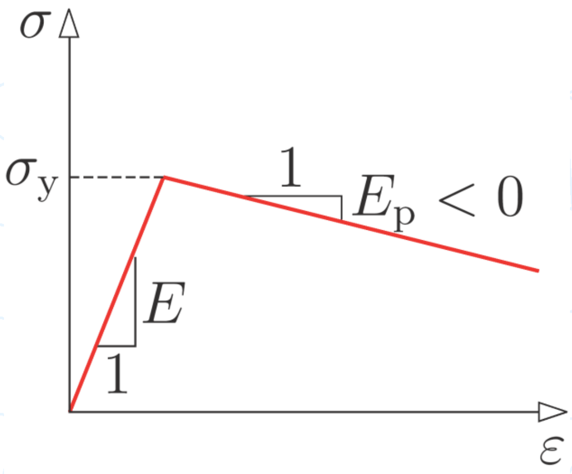
Perfect plasticity



Hardening plasticity



Rigid-Plastic (limit analysis)

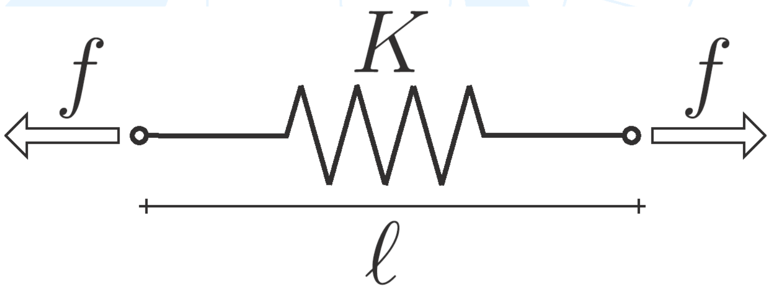


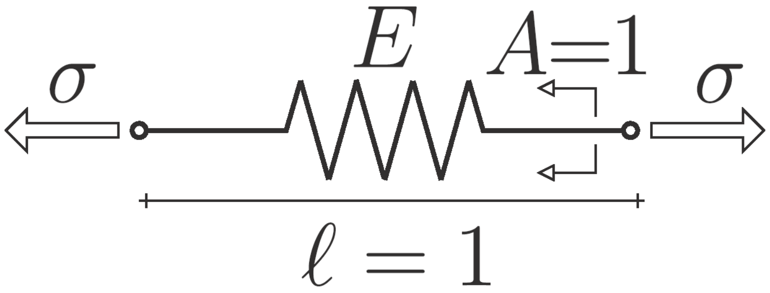
Softening plasticity

Virtual model of 1D perfect plasticity

Ref: Simo JC & Hughes TJR, *Computational Inelasticity*, Springer, 1998

Linear elasticity





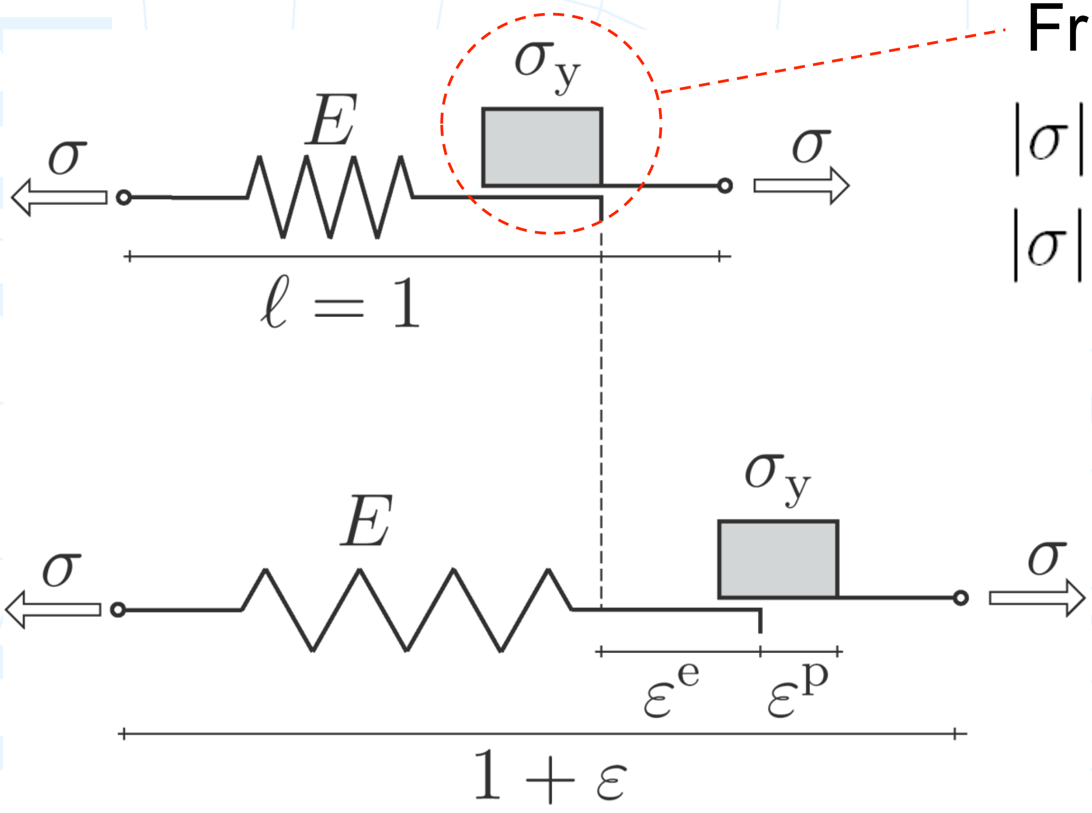
$$f = K\Delta\ell$$ (Hooke's law)

$$\left.\begin{array}{l} A = 1 \Longrightarrow \sigma = \dfrac{f}{A} = f \\ \ell = 1 \Longrightarrow \varepsilon = \dfrac{\Delta\ell}{\ell} = \Delta\ell \end{array}\right\} \Longrightarrow$$

$$K = \frac{f}{\Delta\ell} = \frac{\sigma}{\varepsilon} = E$$

Virtual model of 1D perfect plasticity

Perfect plasticity



Frictional device

$|\sigma| \geq \sigma_y$: free sliding

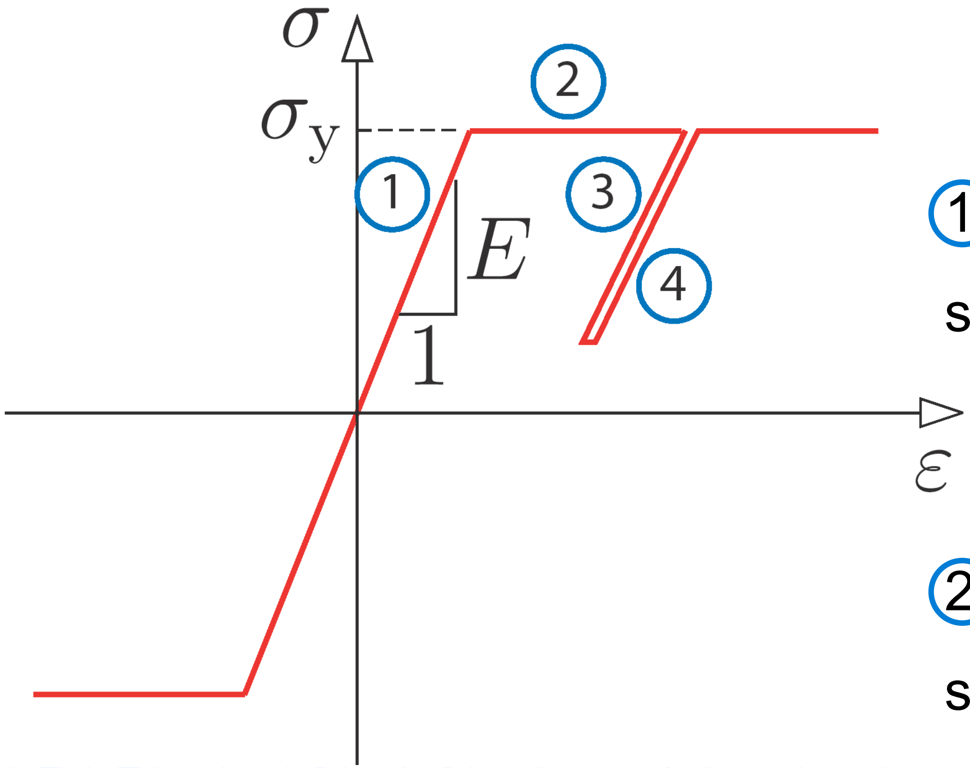
$|\sigma| < \sigma_y$: friction prevents sliding

$\varepsilon = \varepsilon^e + \varepsilon^p$: Straining caused by (i) spring elongation (ε^e) and (ii) sliding (ε^p)

$$\sigma = E\varepsilon^e$$
$$= E(\varepsilon - \varepsilon^p)$$
: Same stress in (sequentially connected) spring and frictional device

Virtual model of 1D perfect plasticity

Response of virtual device



① Elastic response for $|\sigma| < \sigma_{\mathrm{y}}$

spring elongation, no sliding

② Plastic response for $|\sigma| = \sigma_{\mathrm{y}}$

sliding at constant stress

③-④ Unloading-reloading

spring contraction-elongation, no sliding

Virtual model of 1D perfect plasticity

Irreversible frictional response

Assumptions:

1. Stress in frictional device cannot exceed σ_{y} : $\sigma \in [-\sigma_{\mathrm{y}}, \sigma_{\mathrm{y}}]$

$$E_\sigma = \{\sigma \in \mathbb{R} \quad | \quad f(\sigma) := |\sigma| - \sigma_{\mathrm{y}} \leq 0\}$$

Set of admissible stresses (closed set)

$f(\sigma)$: yield function

$$\begin{cases} f(\sigma) \leq 0 : \text{yield condition} \\ f(\sigma) > 0 : \text{stress is not admissible} \end{cases}$$

2. Stress below yield stress $\Longrightarrow$ no change in plastic strain

$$\dot{\varepsilon}^{\mathrm{p}} = 0 \quad \text{if} \quad f(\sigma) < 0 \quad ; \quad f(\sigma) < 0 \Longrightarrow \dot{\sigma} = E\dot{\varepsilon}$$

(elastic instantaneous response)

$$\mathrm{int}(E_\sigma) = \{\sigma \in \mathbb{R} \quad | \quad f(\sigma) := |\sigma| - \sigma_{\mathrm{y}} < 0\}$$

Elastic range (open set)

Virtual model of 1D perfect plasticity

3. Change in plastic strain only possible if $f(\sigma) = 0$

$$\partial E_\sigma = \{\sigma \in \mathbb{R} \quad | \quad f(\sigma) := |\sigma| - \sigma_\mathrm{y} = 0\}$$

Yield surface
(two points in 1D)

$\gamma \geq 0$: absolute value of the slip rate

$$\left.\begin{array}{lll} \dot{\varepsilon}^\mathrm{p} = \gamma \geq 0 & \text{if} & \sigma = \sigma_\mathrm{y} > 0 \\ \dot{\varepsilon}^\mathrm{p} = -\gamma \leq 0 & \text{if} & \sigma = -\sigma_\mathrm{y} < 0 \end{array}\right\} \qquad \dot{\varepsilon}^\mathrm{p} = \gamma \, \mathrm{sgn}(\sigma)$$

Virtual model of 1D perfect plasticity

Determination of the slip rate

(i) $\gamma \geq 0$ (absolute value) and $f(\sigma) \leq 0$ (yield condition)

(ii) $\gamma f(\sigma) = 0$ Kuhn-Tucker conditions

$\gamma > 0$ and $f(\sigma) < 0$ not possible:

$\gamma > 0 \Longrightarrow f(\sigma) = 0$ by assumption 3

$f(\sigma) < 0 \Longrightarrow \gamma = 0$ by assumption 2

γ is the (plastic) multiplier associated to constraint $f(\sigma) \leq 0$

(iii) $\gamma \dot{f}(\sigma) = 0 \quad (\text{if } f(\sigma) = 0)$ Plastic persistency

$\gamma > 0 \Longrightarrow \dot{f} = 0$ plastic slip only on yield surface

$\dot{f} < 0 \Longrightarrow \gamma = 0$ no plastic slip if yield function decreases

Note: $f(\sigma(t))$

Virtual model of 1D perfect plasticity

Determination of the slip rate (continued)

Two possible cases:

(a) $\gamma > 0 \quad , \quad \dot{f} = 0$ purely plastic strain variation

$$0 = \dot{f} = \frac{\partial f}{\partial \sigma}\dot{\sigma} = \mathrm{sgn}(\sigma)E(\dot{\varepsilon} - \dot{\varepsilon}^{\mathrm{p}}) = \mathrm{sgn}(\sigma)E\dot{\varepsilon} - \underbrace{[\mathrm{sgn}(\sigma)]^2}_{=1} E\gamma$$

$$\Rightarrow \begin{cases} \gamma = \mathrm{sgn}(\sigma)\dot{\varepsilon} \\ \dot{\varepsilon}^{\mathrm{p}} = \dot{\varepsilon} \\ \dot{\varepsilon}^{\mathrm{e}} = 0 \end{cases}$$

(b) $\gamma = 0 \quad , \quad \dot{f} \le 0$ purely elastic strain variation

$$\Rightarrow \begin{cases} \gamma = 0 \\ \dot{\varepsilon}^{\mathrm{p}} = 0 \\ \dot{\varepsilon}^{\mathrm{e}} = \dot{\varepsilon} \end{cases}$$

Numerical integration of constitutive equations

Constitutive equations (1D perfect plasticity)

$\dot{\sigma} = E(\dot{\varepsilon} - \dot{\varepsilon}^{\mathrm{p}})$	Generalized Hooke's law
$\dot{\varepsilon}^{\mathrm{p}} = \gamma \, \mathrm{sgn}(\sigma)$	Flow rule
$f(\sigma) := \lvert\sigma\rvert - \sigma_{\mathrm{y}} \leq 0$	Yield condition
$\gamma \geq 0 \, ; \; f \leq 0 \, ; \; \gamma f = 0$	Kuhn-Tucker conditions
$(\text{if } f = 0) \; \gamma \dot{f} = 0$	Plastic persistency

System of differential-algebraic equations (DAE)

Numerical integration of constitutive equations

Efficient form of Kuhn-Tucker conditions

Given admissible σ and prescribed $\dot{\varepsilon}$:

1. Compute $\dot{\sigma}_{\text{trial}} = E\dot{\varepsilon}$ Elastic prediction

2. If $f(\sigma) < 0$ or ($f(\sigma) = 0$ and $\operatorname{sgn}(\sigma)\dot{\sigma}_{\text{trial}} \leq 0$)
   then
   $$\dot{\sigma} = \dot{\sigma}_{\text{trial}}$$
   (Elastic process)

3. If $f(\sigma) = 0$ and $\operatorname{sgn}(\sigma)\dot{\sigma}_{\text{trial}} > 0$ Plastic correction

   then $\dot{\sigma} = \dot{\sigma}_{\text{trial}} - \gamma E \operatorname{sgn}(\sigma)$
   with $\gamma = \dfrac{\operatorname{sgn}(\sigma)\dot{\sigma}_{\text{trial}}}{E}$ (Plastic process)

Remark: plastic correction results in $\dot{\sigma} = 0$
(plastic flow at constant stress in perfect plasticity)

Numerical integration of constitutive equations

Numerical time-integration of initial-value problems

Initial value problem

$$\dot{x}(t) = F\big(x(t)\big) \qquad \text{in } (0,T)$$
$$x(0) = x_0 \qquad \text{initial condition}$$

Generalized mid-point rule

$$^{n+1}x = {}^{n}x + \Delta t F\big(^{n+\theta}x\big)$$
$$^{n+\theta}x = \theta\, ^{n+1}x + (1-\theta)\, ^{n}x \quad \text{with} \quad \theta \in [0,1]$$

Forward Euler method

(*θ* = 0)

$$^{n+1}x = {}^{n}x + \Delta t F\big(^{n}x\big)$$

Explicit $\mathcal{O}(\Delta t)$

Backward Euler method

(*θ* = 1)

$$^{n+1}x = {}^{n}x + \Delta t F\big(^{n+1}x\big)$$

Implicit $\mathcal{O}(\Delta t)$

Mid-point rule

(*θ* = 1/2)

$$^{n+1}x = {}^{n}x + \Delta t F\big(^{n+1/2}x\big)$$
$$^{n+1/2}x = \frac{1}{2}\big(^{n}x + {}^{n+1}x\big)$$

Implicit $\mathcal{O}(\Delta t^2)$

Numerical integration of constitutive equations

Backward Euler time-stepping

BE is common in plasticity:

- Good stability properties
- Order 1 is OK (small Δt for convergence in global problem)

Generic time-step

- Inputs: state at beginning of time-step $^{n}\sigma$, $^{n}\varepsilon$, $^{n}\varepsilon^{\mathrm{p}}$

  increment of total strain $\Delta\varepsilon$

  time-step Δt

- Output: state at end of time-step $^{n+1}\sigma$, $^{n+1}\varepsilon$, $^{n+1}\varepsilon^{\mathrm{p}}$

Numerical integration of constitutive equations

Backward Euler time stepping leads to:

$$^{n+1}\varepsilon = {}^{n}\varepsilon + \Delta\varepsilon$$

(trivial update of total strain)

$$^{n+1}\sigma = E\left({}^{n+1}\varepsilon - {}^{n+1}\varepsilon^{\mathrm{p}}\right)$$

$$^{n+1}\varepsilon^{\mathrm{p}} = {}^{n}\varepsilon^{\mathrm{p}} + \underbrace{\Delta t\, {}^{n+1}\gamma}_{\Delta\gamma}\, \mathrm{sgn}({}^{n+1}\sigma)$$

Restrictions (Kuhn-Tucker):

$$^{n+1}f := |{}^{n+1}\sigma| - \sigma_{\mathrm{y}} \leq 0 \quad ; \quad \Delta\gamma \geq 0 \quad ; \quad \Delta\gamma\, {}^{n+1}f = 0$$

The problem has a unique solution

Numerical integration of constitutive equations

Predictor-corrector strategy

1. Elastic prediction (Hypothesis: $\Delta\gamma = 0$)

$$^{n+1}\varepsilon^{\mathrm{p}}_{\mathrm{trial}} = {}^{n}\varepsilon^{\mathrm{p}}$$ (no change in plastic strain)

$$^{n+1}\sigma_{\mathrm{trial}} = E\left({}^{n+1}\varepsilon - {}^{n+1}\varepsilon^{\mathrm{p}}_{\mathrm{trial}}\right) = {}^{n}\sigma + E\Delta\varepsilon$$

$$^{n+1}f_{\mathrm{trial}} = \left|{}^{n+1}\sigma_{\mathrm{trial}}\right| - \sigma_{\mathrm{y}}$$

2. Check the elastic prediction

a) $^{n+1}f_{\mathrm{trial}} \leq 0$: elastic trial is admissible

$\Delta\gamma = 0$ and trial values solve the problem

step is incrementally elastic

b) $^{n+1}f_{\mathrm{trial}} > 0$: elastic trial is not admissible

compute $\Delta\gamma > 0$ such that $^{n+1}f = 0$

(return to yield surface)

step is incrementally plastic

Numerical integration of constitutive equations

Predictor-corrector strategy (continued)

3. Plastic correction (case b): $\Delta\gamma > 0$ unknown

$$ {}^{n+1}\varepsilon^{\mathrm{p}} = {}^{n}\varepsilon^{\mathrm{p}} + \Delta\gamma \,\mathrm{sgn}({}^{n+1}\sigma) $$

$$ {}^{n+1}\sigma = E({}^{n+1}\varepsilon - {}^{n+1}\varepsilon^{\mathrm{p}}) = {}^{n+1}\sigma_{\mathrm{trial}} - \Delta\gamma E \,\mathrm{sgn}({}^{n+1}\sigma) $$

Rearranging and using that $a = |a| \,\mathrm{sgn}(a)$:

$$ \underbrace{\left[|{}^{n+1}\sigma| + E\Delta\gamma \right]}_{>0} \mathrm{sgn}({}^{n+1}\sigma) = \underbrace{|{}^{n+1}\sigma_{\mathrm{trial}}|}_{>0} \mathrm{sgn}({}^{n+1}\sigma_{\mathrm{trial}}) $$

$$ \Longrightarrow \begin{cases} \mathrm{sgn}({}^{n+1}\sigma) = \mathrm{sgn}({}^{n+1}\sigma_{\mathrm{trial}}) & \text{(sign of prediction OK)} \\ |{}^{n+1}\sigma| + E\Delta\gamma = |{}^{n+1}\sigma_{\mathrm{trial}}| \end{cases} $$

Correction is completed by prescribing ${}^{n+1}f = 0$:

$$ 0 = {}^{n+1}f = |{}^{n+1}\sigma| - \sigma_{\mathrm{y}} = |{}^{n+1}\sigma_{\mathrm{trial}}| - \sigma_{\mathrm{y}} - E\Delta\gamma \Longrightarrow \boxed{\Delta\gamma = \frac{{}^{n+1}f_{\mathrm{trial}}}{E}} $$

Numerical integration of constitutive equations

- Finishing the plastic step

$$
{}^{n+1}\sigma = {}^{n+1}\sigma_{\text{trial}} - \Delta\gamma E \operatorname{sgn} {}^{n+1}\sigma_{\text{trial}}
$$

$$
{}^{n+1}\varepsilon^{\text{p}} = {}^{n}\varepsilon^{\text{p}} + \Delta\gamma \operatorname{sgn} {}^{n+1}\sigma_{\text{trial}}
$$

Hardening plasticity

Constitutive equations (1D hardening plasticity)

$\dot{\sigma} = E(\dot{\varepsilon} - \dot{\varepsilon}^{\mathrm{p}})$	Generalized Hooke's law
$\dot{\varepsilon}^{\mathrm{p}} = \gamma \, \mathrm{sgn}(\sigma)$	Flow rule
$\dot{\alpha} = \gamma$	Hardening law
$f(\sigma, \alpha) := \lvert\sigma\rvert - (\sigma_{\mathrm{y}} + K\alpha) \leq 0$	Yield condition
$\gamma \geq 0\,;\ f \leq 0\,;\ \gamma f = 0$	Kuhn-Tucker conditions
(if $f = 0$) $\gamma \dot{f} = 0$	Plastic persistency

α : internal hardening variable
K : plastic modulus

Numerical time-integration: similar to perfect plasticity

Numerical integration of constitutive equations

Predictor-corrector strategy

1. Elastic prediction (Hypothesis: $\Delta\gamma = 0$)

$$^{n+1}\varepsilon^{\mathrm{p}}_{\mathrm{trial}} = {}^{n}\varepsilon^{\mathrm{p}}$$ (no change in plastic strain)

$$^{n+1}\sigma_{\mathrm{trial}} = E\left({}^{n+1}\varepsilon - {}^{n+1}\varepsilon_{\mathrm{trial}}\right)$$

$$^{n+1}\alpha_{\mathrm{trial}} = {}^{n}\alpha$$

$$^{n+1}f_{\mathrm{trial}} = \left|{}^{n+1}\sigma_{\mathrm{trial}}\right| - (\sigma_{\mathrm{y}} + K\,{}^{n+1}\alpha_{\mathrm{trial}})$$

2. Check the elastic prediction

a) $^{n+1}f_{\mathrm{trial}} \leq 0$: elastic trial is admissible

$\Delta\gamma = 0$ and trial values solve the problem

step is incrementally elastic

b) $^{n+1}f_{\mathrm{trial}} > 0$: elastic trial is not admissible

compute $\Delta\gamma > 0$ such that $^{n+1}f = 0$

(return to yield surface)

step is incrementally plastic

Numerical integration of constitutive equations

Predictor-corrector strategy (continued)

3. Plastic correction (case b): $\Delta\gamma > 0$ unknown

The same argument as in the case of perfect plasticity yields

$$\begin{cases} \operatorname{sgn}({}^{n+1}\sigma) = \operatorname{sgn}({}^{n+1}\sigma_{\text{trial}}) \\ |{}^{n+1}\sigma| + E\Delta\gamma = |{}^{n+1}\sigma_{\text{trial}}| \end{cases}$$

Correction is completed by prescribing ${}^{n+1}f = 0$:

$$\begin{aligned} 0 = {}^{n+1}f &= |{}^{n+1}\sigma| - (\sigma_{\text{y}} + K\,{}^{n+1}\alpha) \\ &= |{}^{n+1}\sigma_{\text{trial}}| - E\Delta\gamma - (\sigma_{\text{y}} + K\,{}^{n+1}\alpha) \\ &= \underbrace{|{}^{n+1}\sigma_{\text{trial}}| - (\sigma_{\text{y}} + K\,{}^{n}\alpha)}_{{}^{n+1}f_{\text{trial}}} - E\Delta\gamma + K\underbrace{({}^{n+1}\alpha - {}^{n}\alpha)}_{\Delta\gamma} \end{aligned}$$

$$\Longrightarrow \quad \boxed{\Delta\gamma = \frac{{}^{n+1}f_{\text{trial}}}{E+K}}$$

Numerical integration of constitutive equations

- Finishing the plastic step

$$
\begin{aligned}
{}^{n+1}\sigma &= {}^{n+1}\sigma_{\mathrm{trial}} - \Delta\gamma E \,\mathrm{sgn}\, {}^{n+1}\sigma_{\mathrm{trial}} \\
{}^{n+1}\varepsilon^{\mathrm{p}} &= {}^{n}\varepsilon^{\mathrm{p}} + \Delta\gamma \,\mathrm{sgn}\, {}^{n+1}\sigma_{\mathrm{trial}} \\
{}^{n+1}\alpha &= {}^{n}\alpha + \Delta\gamma
\end{aligned}
$$

- Remark: we can rewrite the expression for ${}^{n+1}\sigma$ as

$$
{}^{n+1}\sigma = \left[1 - \frac{\Delta\gamma E}{\left|{}^{n+1}\sigma_{\mathrm{trial}}\right|}\right] {}^{n+1}\sigma_{\mathrm{trial}}
$$

"[T]he final stress state is the projection of the trial stress onto the yield surface." (Simo & Hughes)
Hence this algorithm is called a return-mapping algorithm.

COMPUTATIONAL PLASTICITY

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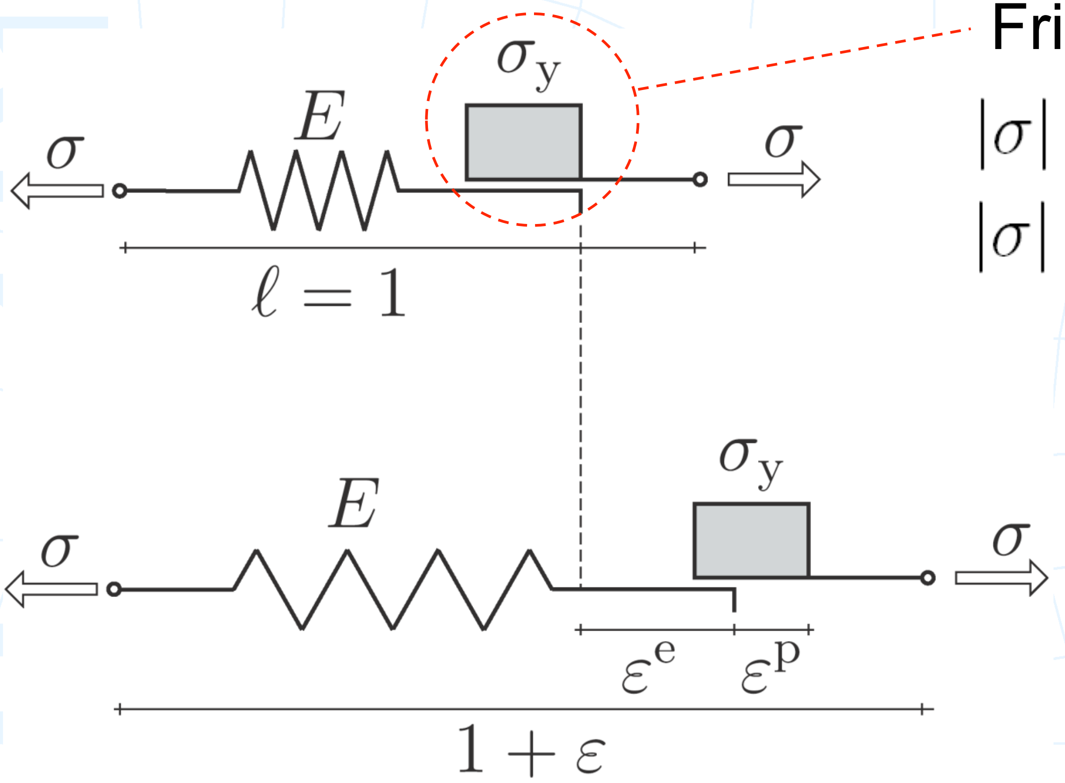
Recall: Virtual model of 1D perfect plasticity

Perfect plasticity



Frictional device

$|\sigma| \geq \sigma_y$: free sliding

$|\sigma| < \sigma_y$: friction prevents sliding

$\varepsilon = \varepsilon^e + \varepsilon^p$: Straining caused by (i) spring elongation (ε^e) and (ii) sliding (ε^p)

$$\sigma = E\varepsilon^e = E(\varepsilon - \varepsilon^p)$$

: Same stress in (sequentially connected) spring and frictional device

Recall: Constitutive equations

Constitutive equations (1D perfect plasticity)

$\dot{\sigma} = E(\dot{\varepsilon} - \dot{\varepsilon}^{\mathrm{p}})$	Generalized Hooke's law
$\dot{\varepsilon}^{\mathrm{p}} = \gamma \, \mathrm{sgn}(\sigma)$	Flow rule
$f(\sigma) := \lvert\sigma\rvert - \sigma_{\mathrm{y}} \leq 0$	Yield condition
$\gamma \geq 0\,;\; f \leq 0\,;\; \gamma f = 0$	Kuhn-Tucker conditions
$(\text{if } f = 0)\; \gamma \dot{f} = 0$	Plastic persistency

System of differential-algebraic equations (DAE)

Isotropic hardening plasticity

Constitutive equations (1D isotropic hardening plasticity)

$\dot{\sigma} = E(\dot{\varepsilon} - \dot{\varepsilon}^{\mathrm{p}})$	Generalized Hooke's law
$\dot{\varepsilon}^{\mathrm{p}} = \gamma \, \mathrm{sgn}(\sigma)$	Flow rule
$\dot{\alpha} = \gamma$	Hardening law
$f(\sigma, \alpha) := \lvert\sigma\rvert - (\sigma_{\mathrm{y}} + K\alpha) \leq 0$	Yield condition
$\gamma \geq 0\,;\; f \leq 0\,;\; \gamma f = 0$	Kuhn-Tucker conditions
$(\text{if } f = 0)\; \gamma \dot{f} = 0$	Plastic persistency

α : internal hardening variable
K : plastic modulus

Numerical time-integration: similar to perfect plasticity

Numerical integration of constitutive equations

Predictor-corrector strategy

1. Elastic prediction (Hypothesis: $\Delta\gamma = 0$)

$$ {}^{n+1}\varepsilon^{\mathrm{p}}_{\mathrm{trial}} = {}^{n}\varepsilon^{\mathrm{p}} \qquad \text{(no change in plastic strain)} $$

$$ {}^{n+1}\sigma_{\mathrm{trial}} = E\left({}^{n+1}\varepsilon - {}^{n+1}\varepsilon_{\mathrm{trial}}\right) $$

$$ {}^{n+1}\alpha_{\mathrm{trial}} = {}^{n}\alpha $$

$$ {}^{n+1}f_{\mathrm{trial}} = \left|{}^{n+1}\sigma_{\mathrm{trial}}\right| - \left(\sigma_{\mathrm{y}} + K\,{}^{n+1}\alpha_{\mathrm{trial}}\right) $$

2. Check the elastic prediction
   a) ${}^{n+1}f_{\mathrm{trial}} \leq 0$: elastic trial is admissible

   $\Delta\gamma = 0$ and trial values solve the problem

   step is incrementally elastic

   b) ${}^{n+1}f_{\mathrm{trial}} > 0$: elastic trial is not admissible

   compute $\Delta\gamma > 0$ such that ${}^{n+1}f = 0$
   (return to yield surface)

   step is incrementally plastic

Numerical integration of constitutive equations

Predictor-corrector strategy (continued)

3. Plastic correction (case b): $\Delta\gamma > 0$ unknown

The same argument as in the case of perfect plasticity yields

$$\begin{cases} \operatorname{sgn}({}^{n+1}\sigma) = \operatorname{sgn}({}^{n+1}\sigma_{\text{trial}}) \\ |{}^{n+1}\sigma| + E\Delta\gamma = |{}^{n+1}\sigma_{\text{trial}}| \end{cases}$$

Correction is completed by prescribing ${}^{n+1}f = 0$:

$$\begin{aligned} 0 = {}^{n+1}f &= |{}^{n+1}\sigma| - (\sigma_{\text{y}} + K\,{}^{n+1}\alpha) \\ &= |{}^{n+1}\sigma_{\text{trial}}| - E\Delta\gamma - (\sigma_{\text{y}} + K\,{}^{n+1}\alpha) \\ &= \underbrace{|{}^{n+1}\sigma_{\text{trial}}| - (\sigma_{\text{y}} + K\,{}^{n}\alpha)}_{{}^{n+1}f_{\text{trial}}} - E\Delta\gamma - K\underbrace{({}^{n+1}\alpha - {}^{n}\alpha)}_{\Delta\gamma} \end{aligned}$$

$$\Longrightarrow \quad \boxed{\Delta\gamma = \frac{{}^{n+1}f_{\text{trial}}}{E+K}}$$

Numerical integration of constitutive equations

- Finishing the plastic step

$$
\begin{aligned}
{}^{n+1}\sigma &= {}^{n+1}\sigma_{\text{trial}} - \Delta\gamma E \operatorname{sgn} {}^{n+1}\sigma_{\text{trial}} \\
{}^{n+1}\varepsilon^{\text{p}} &= {}^{n}\varepsilon^{\text{p}} + \Delta\gamma \operatorname{sgn} {}^{n+1}\sigma_{\text{trial}} \\
{}^{n+1}\alpha &= {}^{n}\alpha + \Delta\gamma
\end{aligned}
$$

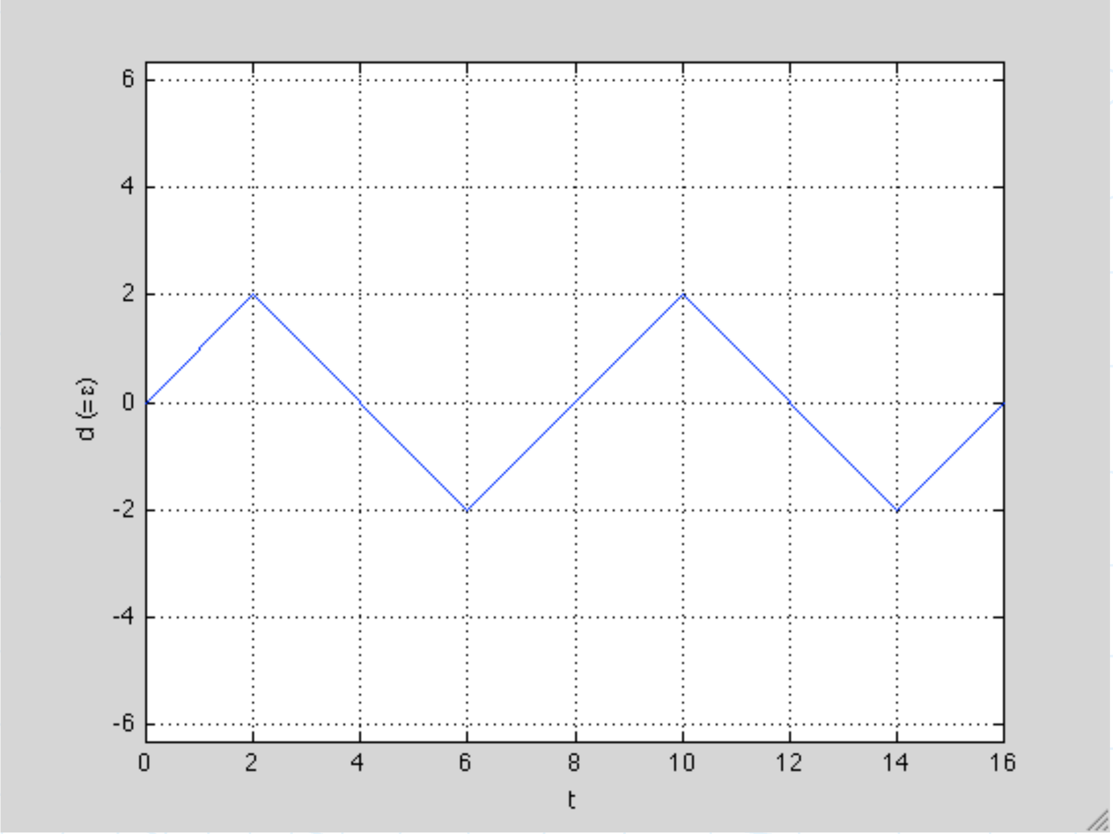
- Remark: we can rewrite the expression for $^{n+1}\sigma$ as

$$
{}^{n+1}\sigma = \left[1 - \frac{\Delta\gamma E}{\left|{}^{n+1}\sigma_{\text{trial}}\right|}\right] {}^{n+1}\sigma_{\text{trial}}
$$

"[T]he final stress state is the projection of the trial stress onto the yield surface." (Simo & Hughes)
Hence this algorithm is called a return-mapping algorithm.

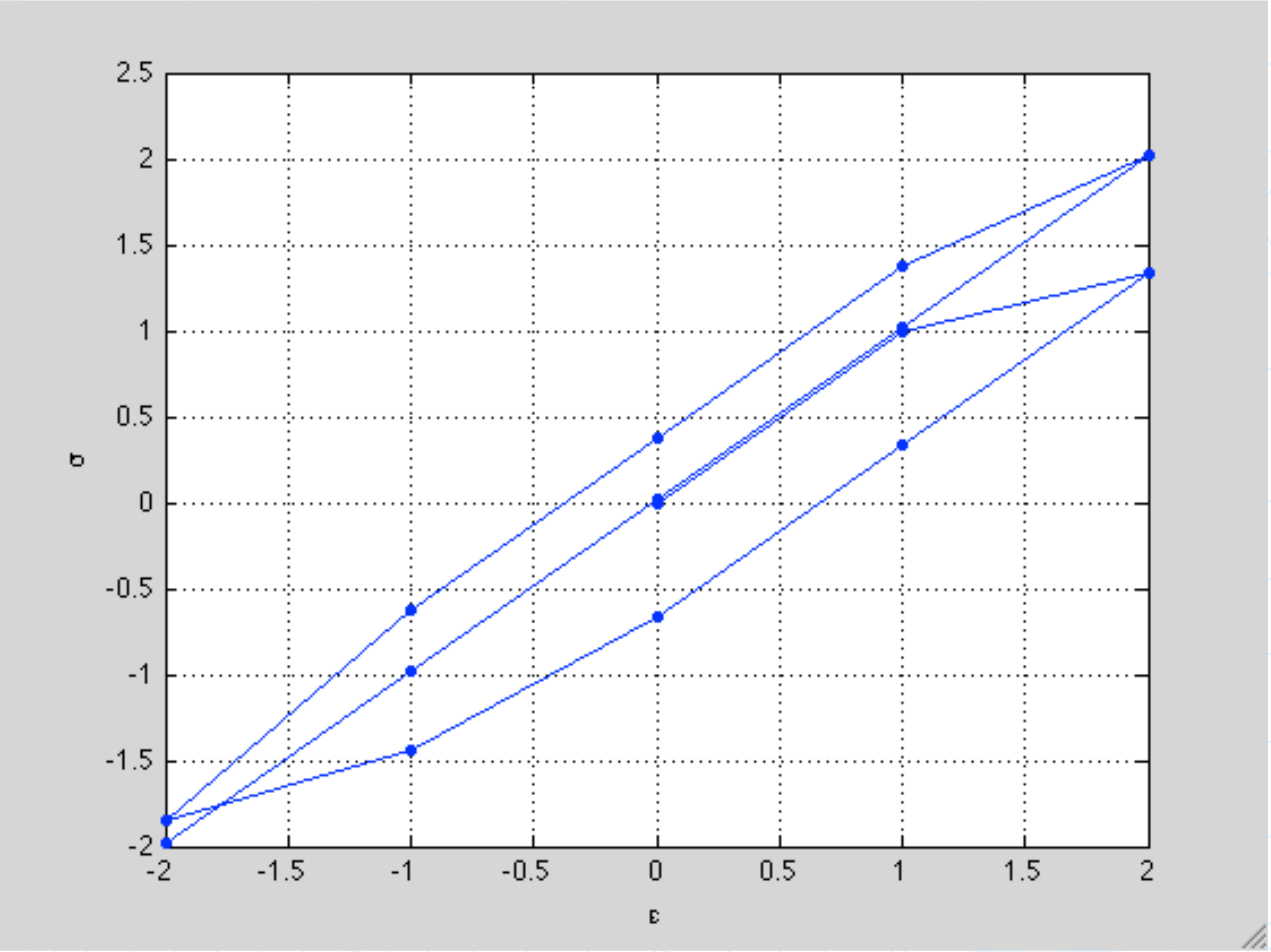
Example for illustrating the algorithm for isotropic hardening plasticity

- Repeat the same exercise with $K = 0.5$, ${}^{0}\alpha=0$. Take $\Delta t = 1$.



*The evolution of α also has to be kept track of.

- With the result, we can plot σ vs ε



Kinematic hardening

- In many metals subjected to cyclic loading, it is experimentally observed that the center of the yield surface experiences a motion in the direction of the plastic flow.
- The yield condition is modified as

$$f(\sigma,q,\alpha) := |\sigma - q| - \left(\sigma_{\mathrm{y}} + K\alpha\right)$$

where the evolution of the *back stress* *q* is defined by Ziegler's rule as

$$\dot{q} = H\dot{\varepsilon}^{\mathrm{p}} = \gamma H \,\mathrm{sgn}(\sigma - q)$$

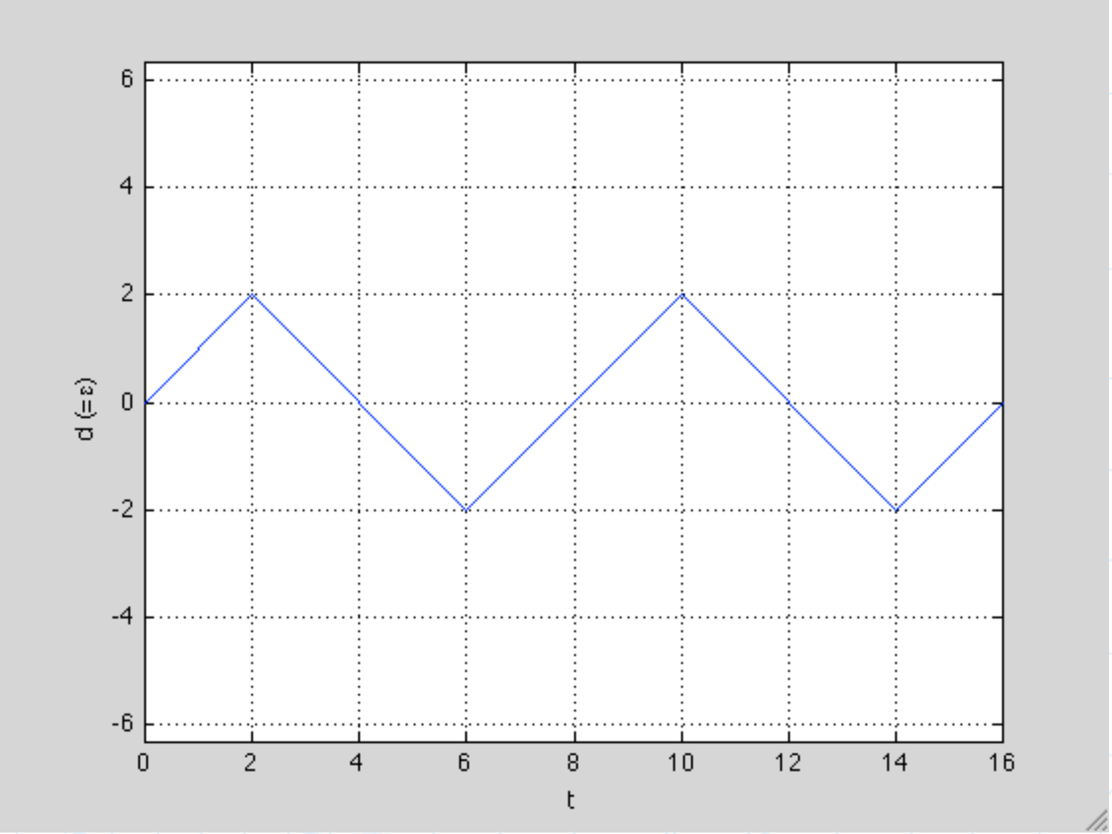
H: kinematic hardening modulus

- The other conditions (Hooke's law, hardening law for α, Kuhn-Tucker, plastic consistency) remain unchanged
- Backwared Euler algorithm step:

$$\Delta\gamma = \frac{{}^{n+1}f^{\mathrm{trial}}}{E + H + K}$$

Example for illustrating the algorithm for isotropic and kinematic hardening plasticity

- Derive the backward Euler algorithm (elastic prediction and plastic correction)
- Repeat the same exercise with $K = H = 0.5$, ${}^0\alpha=0$, ${}^0q=0$. Take $\Delta t = 1$.



*The evolution of *α* and *q* also has to be kept track of.

1D INITIAL BOUNDARY VALUE PROBLEM WITH PLASTICITY

Strong form

- Having discussed the virtual model of the frictional device, let's see what it takes to model plasticity in a 1D continuum, where *each* point has to obey the yield condition, Kuhn-Tucker condition, etc.
- In a 1D problem, the stress and the strain tensors both have only one component, but may vary with *x*.
- We consider the interval B=(0, *L*).
- Pointwise relations
  - Momentum equation:

$$\frac{\partial \sigma}{\partial x} + \rho b = \rho \frac{\partial v}{\partial t}$$

  - Kinematic relation; velocity field

$$\varepsilon = \frac{\partial u}{\partial x} \qquad v = \frac{\partial u}{\partial t}$$

- Initial conditions

$$u(x,0) = u_0(x) \quad v(x,0) = v_0(x)$$

- Boundary conditions. There are many possibilities, e.g.,

$$u(0,t) = \overline{u}(t) \quad \sigma(L,t) = \overline{\sigma}(t)$$

Dirichlet Neumann

- Questions:
  - Can the initial and boundary conditions be arbitrarily prescribed?
  - What is missing to completely define the evolution of the system?

Weak form

- Weak form to get a matrix equation:

trial space $S_t = \left\{ u(\cdot,t) \in H^1(B) \mid u(0,t) = \bar{u}(t) \right\}$

test space $V = \left\{ \eta \in H^1(B) \mid \eta(0) = 0 \right\}$

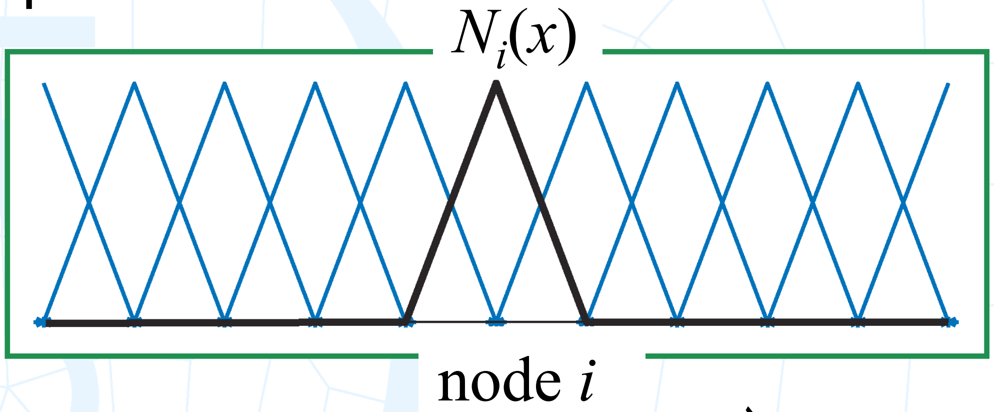
Find $u \in S_t$ such that for all $\eta \in V$ and all $t \in [0, T]$,

$$\int_B \rho \frac{\partial v}{\partial t} \eta dx + \int_B \sigma \frac{d\eta}{dx} dx - \int_B \rho b \eta dx - \bar{\sigma} \eta(L) = 0$$

Note: This is exactly the same equation for elastodynamics, except that we don't have a simple constitutive relation between σ and ε.

Matrix equation

With the finite element basis functions, we can rewrite the weak form as the following (semi-discrete) matrix equation:



$$u^h(x,t) = \bar{u}(t)N_0(x) + \sum_i N_i(x)u_i(t)$$

$$\eta^h(x) = \sum_i N_i(x)\eta_i$$

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{F}^{\text{int}}\left(\sigma^h\right) - \mathbf{F}^{\text{ext}}\left(t\right) = 0$$

Quasi-static problem:

$$\mathbf{F}^{\text{int}}\left(\sigma^h\right) - \mathbf{F}^{\text{ext}}\left(t\right) = 0$$

$$M_{ij} = \int_B \rho N_i N_j dx$$

$$F_i^{\text{int}}\left(\sigma^h\right) = \int_B \sigma^h \frac{dN_i}{dx} dx$$

internal work of
virtual displacement

$$F_i^{\text{ext}}(t) = \int_B \rho N_i\left(b - \ddot{u} N_0\right) dx + \overline{\sigma} N_i(L)$$

external work of
virtual displacement

Solution strategy for quasi-static analysis

- We discretize in time and use the backward Euler method. The solution procedure is stated as:
  Given the state at time step *n*, find the displacement at the next time step ${}^{n+1}u$ and the variables $\{\varepsilon^p, \alpha, q, \sigma\}$ at time step *n*+1 such that both the constitutive relation and the equilibrium equation are satisfied at time *n*+1.

- For practical reasons, the constitutive relation is enforced only at the Gauss quadrature points, while equilibrium is enforced in the sense of

$$\mathbf{F}^{\text{int}}\left(\sigma^{h}\right)-\mathbf{F}^{\text{ext}}\left(t\right)=0$$

or its dynamic version with backward Euler approximation

Below we drop the superscript h which denotes the finite element mesh.

Due to the nonlinearity, an iterative solution procedure is needed:

- Make a guess of ${}^{n+1}u$, compute the corresponding ${}^{n+1}\varepsilon$
- At the Gauss quadrature points, find values of ${}^{n+1}\{\varepsilon^{p}, \alpha, q, \sigma\}$ according to the plasticity constitutive relation (elastic prediction-plastic correction)
- Check whether equilibrium is satisfied (within tolerance). If yes, start the next time step; otherwise, make another guess and start over.

MULTI-DIMENSIONAL PLASTICITY

Principal values and principal directions of real symmetric tensors

- Important properties of a real symmetric matrix (tensor)
  - The eigenvalues of any real symmetric matrix are all real. (simple proof on the board)
  - A real symmetric matrix is always diagonalizable. For a proof, see http://www.mathresource.iitb.ac.in/linear%20algebra/proof10.3.4.html

- Thus, there exist three mutually orthogonal eigenvectors for any given real symmetric tensor **T** (such as the stress and strain tensors). We call them the principal directions of **T**, and the corresponding eigenvalues the principal values.

- For repeating eigenvalues, the choice of the corresponding principal directions is not unique

Principal scalar invariants of a tensor

- The characteristic equation of a tensor T is

$$\det\left(\mathbf{T}-\lambda\mathbf{I}\right)=0$$

- It can be written as

$$\lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 = 0$$

where

$$I_1 = \operatorname{tr}\mathbf{T} = \lambda_1 + \lambda_2 + \lambda_3$$

$$I_2 = \frac{1}{2}\left[\left(\operatorname{tr}\mathbf{T}\right)^2 - \operatorname{tr}\mathbf{T}^2\right] = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3$$

$$I_3 = \det\mathbf{T} = \lambda_1\lambda_2\lambda_3$$

Remark: other definitions of I_1 , I_2 and I_3 can be found in the literature

Principal stresses and principal strains

- The principal directions of the stress tensor and those of the strain tensor coincide for an isotropic linear elastic material. To see this, consider the strain tensor at some point. With its principal directions as coordinate axes, we can write

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}$$

In the same coordinate system, the stress is then given by

$$\sigma = \begin{bmatrix} \lambda\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right)+2\mu\varepsilon_{xx} & 0 & 0 \\ 0 & \lambda\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right)+2\mu\varepsilon_{yy} & 0 \\ 0 & 0 & \lambda\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right)+2\mu\varepsilon_{zz} \end{bmatrix}$$

which is also diagonal.

Multi-dimensional plasticity

Stress invariants

$$\sigma_{\mathrm{m}} = \frac{1}{3} I_1$$

mean stress

$$\boldsymbol{\sigma}' \equiv \boldsymbol{\sigma}^{\mathrm{dev}} := \boldsymbol{\sigma} - \sigma_{\mathrm{m}} \boldsymbol{I}$$

deviatoric stress tensor

J are used to denote the invariants of the deviatoric tensor:

$$J_1 := \mathrm{tr}(\boldsymbol{\sigma}') = \mathrm{tr}(\boldsymbol{\sigma}) - 3\sigma_{\mathrm{m}} = 0$$

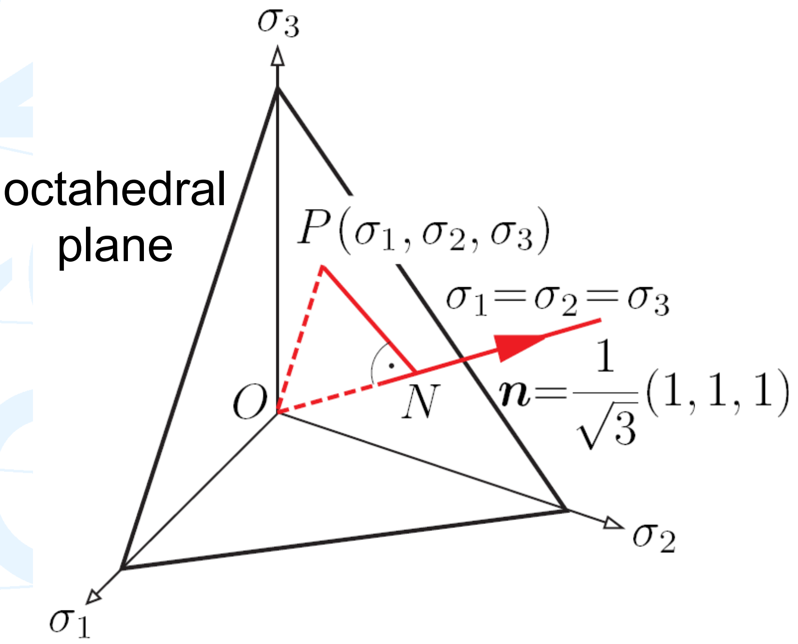
$$J_2 := \frac{1}{2}\boldsymbol{\sigma}' : \boldsymbol{\sigma}' = \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{\sigma} - \frac{3}{2}\sigma_{\mathrm{m}}^2 = \frac{1}{3}I_1^2 - I_2$$

$$= \frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2\right]$$

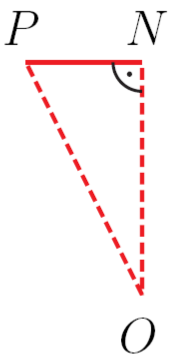
Remark: The definition of J_2 as a function of invariants may vary depending on how the invariants are defined.

Multi-dimensional plasticity

Space of principal stresses



Stress states with the same I_1 are on the same octahedral plane



$$|\overline{OP}| = \sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}$$

$$|\overline{ON}| = \overline{OP} \cdot \boldsymbol{n} = \frac{I_1}{\sqrt{3}}$$

$$|\overline{PN}|^2 = |\overline{OP}|^2 - |\overline{ON}|^2 = 2J_2$$

- The first invariant of the stress tensor, I_1, indicates the distance from the octahedral plane to the origin
- The second invariant of the deviatoric tensor, J_2, indicates the distance to the spherical (hydrostatic) stress state (σ_1=σ_2=σ_3)

Multi-dimensional plasticity

Von Mises plasticity (J_2 plasticity)

- Typically used for metals
- Yield function defined as $f(\boldsymbol{\sigma}) := \sqrt{\frac{3}{2}}\|\boldsymbol{\sigma}'\| - \sigma_{\mathrm{y}} = \sqrt{3J_2} - \sigma_{\mathrm{y}}$

  Equivalent (or von Mises) stress: $\sigma_{\mathrm{eq}} = \sqrt{3J_2}$
- Question: what is the shape of the yield surface $f(\boldsymbol{\sigma}) = 0$?

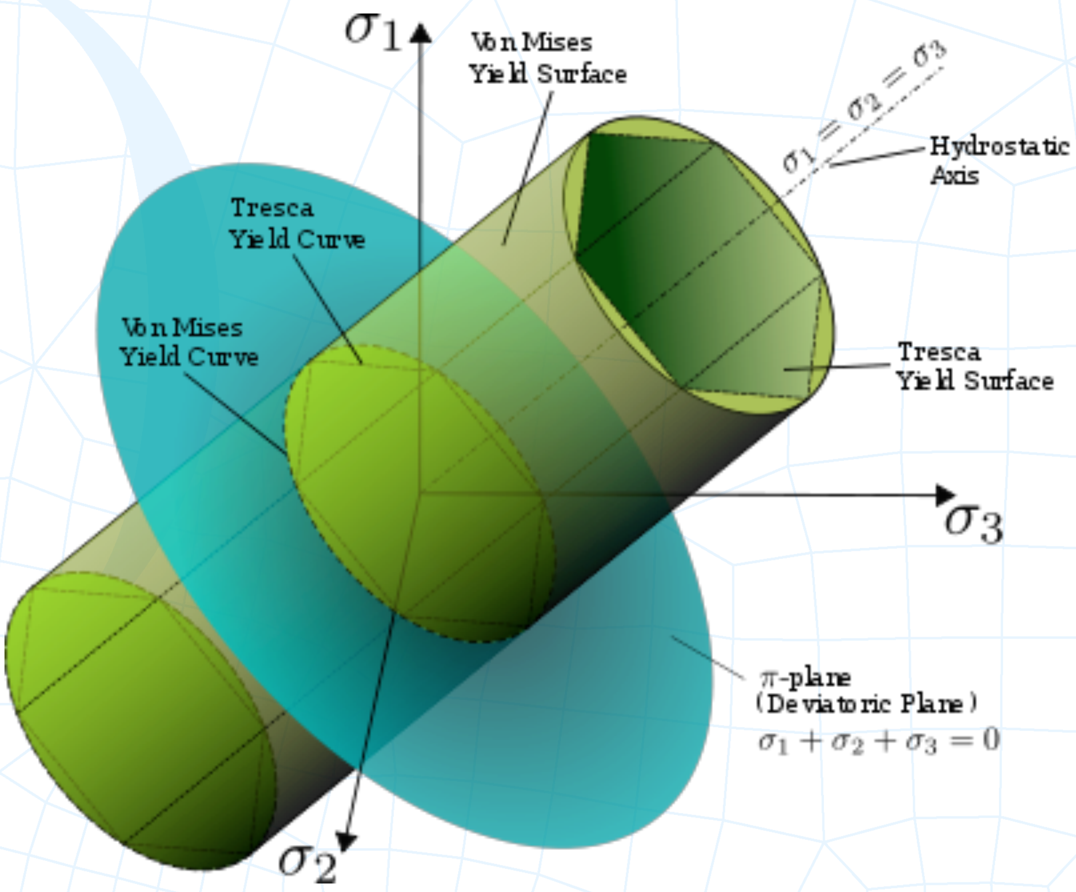
Tresca plasticity

$$f(\boldsymbol{\sigma}) = \max\{|\sigma_1 - \sigma_2|, |\sigma_1 - \sigma_3|, |\sigma_2 - \sigma_3|\} - \sigma_{\mathrm{y}}$$

Other yield criteria: Mohr-Coulomb, Drucker-Prager

Shape of the yield surface

- A cylindrical surface whose axis is given by the line pointing the direction (1,1,1).



The numerical procedure is similar as for 1D problems

ELASTICITY

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Isotropic Linear Elasticity

Linear elasticity

1. Elasticity: one-to-one relation between stress and deformation
2. Linear: small deformations and natural configuration ε=0, σ=0

$$\boxed{\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\varepsilon}}$$

$$\boxed{\sigma_{ij} = C_{ijkl}\varepsilon_{kl}}$$

C is a 4th order tensor (81 components) with symmetries

$$\boxed{\begin{array}{ll} C_{ijkl} = C_{ijlk} & \text{(symmetry of } \varepsilon\text{)} \\ C_{ijkl} = C_{jikl} & \text{(symmetry of } \sigma\text{)} \\ C_{ijkl} = C_{klij} & \text{(major symmetry)} \end{array}}$$

⇨ 21 material parameters!

Isotropy

The behaviour is independent of the orientation. The expression of $\boldsymbol{C}$ does not depend on the orthogonal coordinate system ⇒ $\boldsymbol{C}$ does not depend on the basis considered:

$$\boxed{C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \omega\left(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\right)}$$

$\Downarrow$ Major symmetry

$$\boxed{C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)}$$

$\boxed{\lambda,\ \mu}$ Lamé constants (material parameters)

- **Lamé equations** (linear isotropic elasticity)

$$\boxed{\boldsymbol{\sigma} = \lambda\, tr(\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}}$$

- Inverse Lamé equations:

$$\boxed{\boldsymbol{\varepsilon} = \frac{-\lambda\, tr(\boldsymbol{\sigma})}{2\mu(3\lambda + 2\mu)}\boldsymbol{I} + \frac{1}{2\mu}\boldsymbol{\sigma}}$$

- Usually, the following parameters are used:

$$\boxed{\begin{aligned} G &= \mu \\ E &= \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \\ \nu &= \frac{\lambda}{2(\lambda + \mu)} \end{aligned}}$$

Shear modulus

Young's modulus

Poisson's ratio

Relations:

$$\boxed{G = \frac{E}{2(1 + \nu)}}$$

Limiting values:

$$\boxed{E > 0, \quad G > 0, \quad -1 < \nu < 0.5}$$

- Inverse relations:

$$\boxed{\begin{aligned}\lambda &= \frac{E\nu}{(1+\nu)(1-2\nu)}\\ \mu &= \frac{E}{2(1+\nu)}\end{aligned}}$$

Note: $\nu \rightarrow 0.5 \Leftrightarrow \lambda \rightarrow \infty$

Full incompressiblity is imposed with an adidtional constraint

$$tr(\varepsilon) = 0$$

- Constitutive equation:

$$\boxed{\boldsymbol{\varepsilon} = -\frac{\nu}{E}\,tr(\boldsymbol{\sigma})\boldsymbol{I} + \frac{1+\nu}{E}\boldsymbol{\sigma}}$$

- For each component:

$$\begin{array}{ll}
\varepsilon_{xx} = \dfrac{1}{E}\left[\sigma_{xx} - \nu(\sigma_{yy} + \sigma_{zz})\right] & \varepsilon_{xy} = \frac{1}{2G}\sigma_{xy} \\
\varepsilon_{yy} = \dfrac{1}{E}\left[\sigma_{yy} - \nu(\sigma_{xx} + \sigma_{zz})\right] & \varepsilon_{xz} = \frac{1}{2G}\sigma_{xz} \\
\varepsilon_{zz} = \dfrac{1}{E}\left[\sigma_{zz} - \nu(\sigma_{xx} + \sigma_{yy})\right] & \varepsilon_{yz} = \frac{1}{2G}\sigma_{yz}
\end{array}$$

Physical interpretations of E, G and ν

- Shear modulus:

$$\boxed{\varepsilon_{xy} = \frac{1}{2G}\sigma_{xy}}$$

G: stiffness of shear deformation

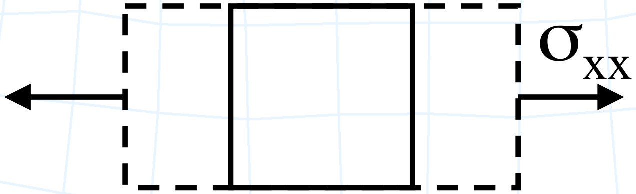
- Young or elastic modulus:

$$\boxed{\boldsymbol{\varepsilon} = -\frac{\nu}{E}\, tr(\boldsymbol{\sigma})\boldsymbol{I} + \frac{1+\nu}{E}\boldsymbol{\sigma}}$$

E: stiffness

- Poisson coefficient:
  - ν=0:

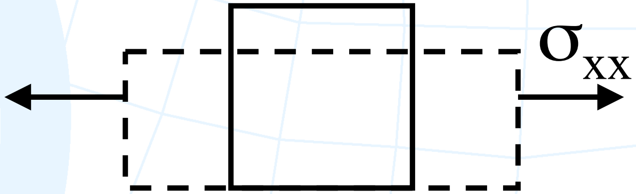
$$\boxed{\begin{aligned}\varepsilon_{xx} &= \frac{1}{E}\sigma_{xx}\\ \varepsilon_{yy} &= \frac{1}{E}\sigma_{yy}\end{aligned}}$$



$$\boxed{\sigma_{yy} = 0 \;\Rightarrow\; \varepsilon_{yy} = 0}$$

- ν≠0: **Poisson effect**

$$\boxed{\sigma_{yy} = \sigma_{zz} = 0,\ \sigma_{xx} \neq 0\ \Rightarrow\ \varepsilon_{yy} = -\frac{\nu}{E}\sigma_{xx}}$$



- Incompressibility when: ν ➔ 0.5

$$\boxed{tr(\boldsymbol{\varepsilon}) = 0} \qquad \boxed{\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0}$$

- Usually, the symmetric tensors σ and ε are written as 6-dimensional vectors (3-dimensional in 2D):

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x & \gamma_{xy}/2 & \gamma_{xz}/2 \\ & \varepsilon_y & \gamma_{yz}/2 \\ \text{(sym)} & & \varepsilon_z \end{pmatrix} \rightarrow \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{xz} \\ \gamma_{yz} \end{pmatrix}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ & \sigma_y & \tau_{yz} \\ \text{(sym)} & & \sigma_z \end{pmatrix} \rightarrow \boldsymbol{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{yz} \end{pmatrix}$$

- Constitutive equations:

$$\boldsymbol{\varepsilon} = \begin{pmatrix} 1/E & -\nu/E & -\nu/E & & & \\ -\nu/E & 1/E & -\nu/E & & & \\ -\nu/E & -\nu/E & 1/E & & & \\ & & & 1/G & & \\ & & & & 1/G & \\ & & & & & 1/G \end{pmatrix} \boldsymbol{\sigma}$$

- Constitutive equations:

$$\boldsymbol{\sigma} = \lambda \mathrm{tr}(\boldsymbol{\varepsilon})\mathbf{I} + 2\mu\boldsymbol{\varepsilon} = \boldsymbol{C}\boldsymbol{\varepsilon}$$

$$C = \frac{E}{(1+\nu)(1-2\nu)}\begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}$$

LINEAR ISOTROPIC ELASTICITY EQUATIONS

- Unknowns: displacements
- Equations:

$$\boxed{\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)}$$

(1) Equilibrium equations

(2) Kinematic relations

(3) Constitutive equations

$$\rho \boldsymbol{b} + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \rho \frac{d^2 \boldsymbol{u}}{dt^2}$$

$$\boldsymbol{\varepsilon} = \boldsymbol{\nabla}^s \boldsymbol{u}$$

$$\boldsymbol{\sigma} = \lambda \, \mathrm{tr}(\boldsymbol{\varepsilon}) \boldsymbol{I} + 2\mu \boldsymbol{\varepsilon}$$

- By substituting (2) in (3), and (3) in (1) we obtain the **Navier equations**

$$\boxed{(\lambda + \mu) \nabla (\nabla \cdot \boldsymbol{u}) + \mu \Delta \boldsymbol{u} + \rho \boldsymbol{b} = \rho \frac{d^2 \boldsymbol{u}}{dt^2}}$$

- **Initial conditions** $\boxed{\boldsymbol{u}(\boldsymbol{x},0)=\boldsymbol{u}_0(\boldsymbol{x})}$ **and initial velocity**

  Example: undeformed and unstressed configuration:

$$\boxed{\boldsymbol{u}(\boldsymbol{x},0)=\mathbf{0},\ \boldsymbol{\varepsilon}(\boldsymbol{x},0)=\mathbf{0},\ \boldsymbol{\sigma}(\boldsymbol{x},0)=\mathbf{0}}$$

- **Boundary conditions**:

1. Prescribed conditions:

$$\boxed{\boldsymbol{u}(\boldsymbol{x},t)=\boldsymbol{u}^D(\boldsymbol{x},t),\ \boldsymbol{x}\in\Gamma^D}$$

2. Boundary loads:

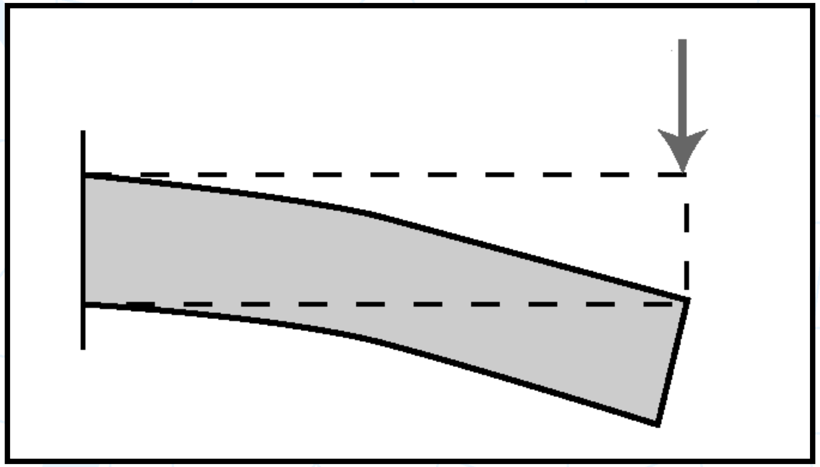
$$\boxed{\boldsymbol{t}(\boldsymbol{x},t):=\boldsymbol{\sigma}(\boldsymbol{x},t)\cdot\boldsymbol{n}=\boldsymbol{t}^N(\boldsymbol{x},t),\ \boldsymbol{x}\in\Gamma^N}$$

3. Mixed conditions:

$$\boxed{\begin{array}{l} u_i(\boldsymbol{x},t)=u_i^D(\boldsymbol{x},t),\ \boldsymbol{x}\in\Gamma^M \\ t_j(\boldsymbol{x},t)=t_j^N(\boldsymbol{x},t),\ \boldsymbol{x}\in\Gamma^M \end{array}}$$

PROBLEM STATEMENT IN ELASTOSTATICS

1. We are only interested in the stationary (final configuration is in equilibrium)



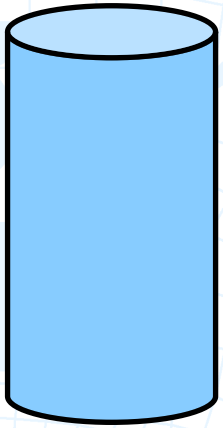
2. Negligible inertial forces:

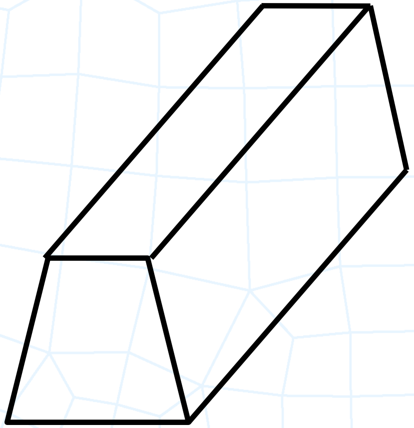
$$\boxed{\rho \boldsymbol{b} + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0}$$

PLANE ELASTICITY

- Plane strain

“If the deformation of a cylindrical body is such that there is no axial components of the displacement and that the other components do not depend on the axial coordinate, then the body is said to be in a state of plane strain. Such a state of strain exists for example in a cylindrical body whose end faces are prevented from moving axially and whose lateral surface are acted on by loads that are independent of the axial position and without axial components.”





Plane strain hypothesis

- Hypothesis:
  - $\boxed{\boldsymbol{u} = \boldsymbol{u}(x, y)}$ (independent of z)
  - $\boxed{u_z = 0}$
- Then,

$$\boxed{\varepsilon_z = \gamma_{xz} = \gamma_{yz} = 0}$$

$$\boxed{\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{pmatrix}}$$

$$\boxed{\begin{aligned} \sigma_x &= (\lambda + 2\mu)\varepsilon_x + \lambda\varepsilon_y \\ \sigma_y &= \lambda\varepsilon_x + (\lambda + 2\mu)\varepsilon_y \\ \tau_{xy} &= \mu\gamma_{xy} \end{aligned}}$$

$$\boxed{\begin{aligned} &\sigma_z = \lambda\left(\varepsilon_x + \varepsilon_y\right) = \nu(\sigma_x + \sigma_y) \\ &\tau_{xz} = \tau_{yz} = 0 \end{aligned}}$$

$$\boldsymbol{\sigma} = \boldsymbol{C}^{P\varepsilon}\,\boldsymbol{\varepsilon}$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{pmatrix} \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{pmatrix}, \qquad \sigma_z = \nu(\sigma_x + \sigma_y)$$

$$\boldsymbol{C}^{P\varepsilon} = \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \\ \nu & 1-\nu & \\ & & (1-2\nu)/2 \end{pmatrix}$$

Plane stress hypothesis

- Hypothesis:
  - $\boxed{\boldsymbol{u} = \boldsymbol{u}(x, y)}$ (independent of z)
  - Loads applied only on the xy-plane, plane stresses only
  - Appropriate for thin structures
- Then,

$$\boxed{\sigma_z = \tau_{xz} = \tau_{yz} = 0}$$

$$\boxed{\boldsymbol{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{pmatrix}}$$

$$\boxed{\begin{aligned} \varepsilon_x &= (\sigma_x - \nu\sigma_y)/E \\ \varepsilon_y &= (\sigma_y - \nu\sigma_x)/E \\ \gamma_{xy} &= \tau_{xy}/\mu \end{aligned}}$$

$$\boxed{\begin{aligned} &\varepsilon_z = -\frac{\nu}{E}(\sigma_x + \sigma_y) = -\frac{\nu}{1-\nu}(\varepsilon_x + \varepsilon_y) \\ &\gamma_{xz} = \gamma_{yz} = 0 \end{aligned}}$$

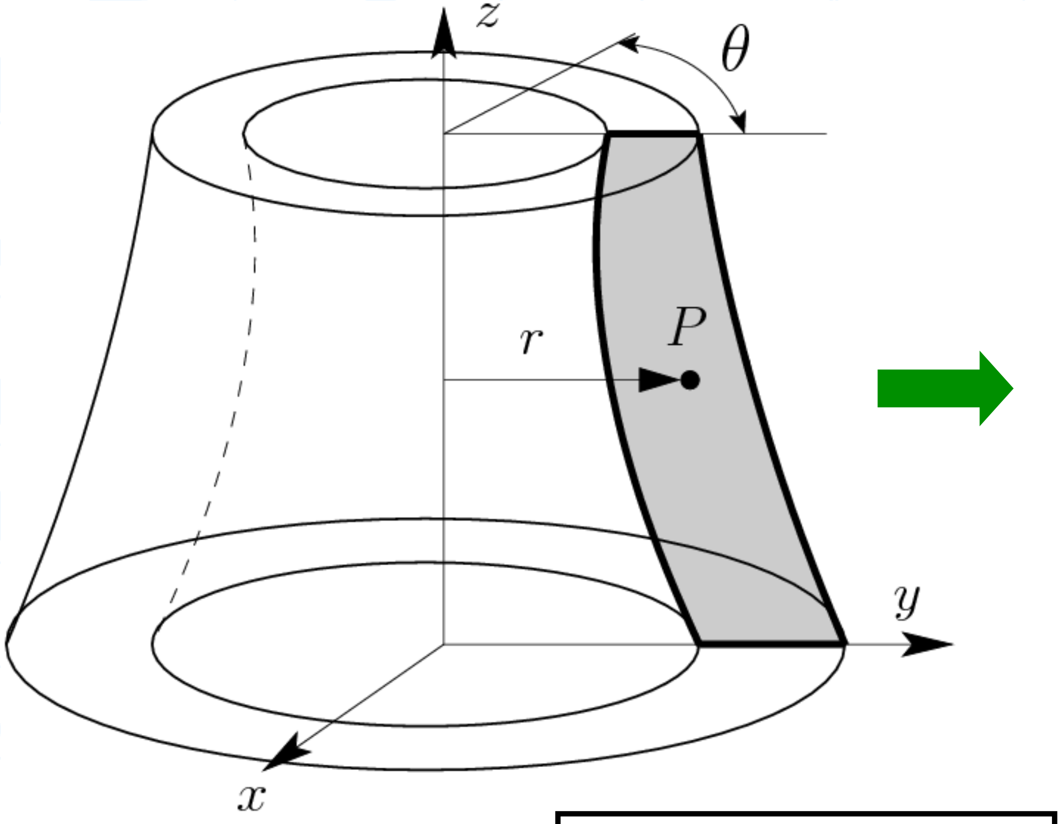
$$\boldsymbol{\sigma} = \boldsymbol{C}^{P\sigma}\,\boldsymbol{\varepsilon}$$

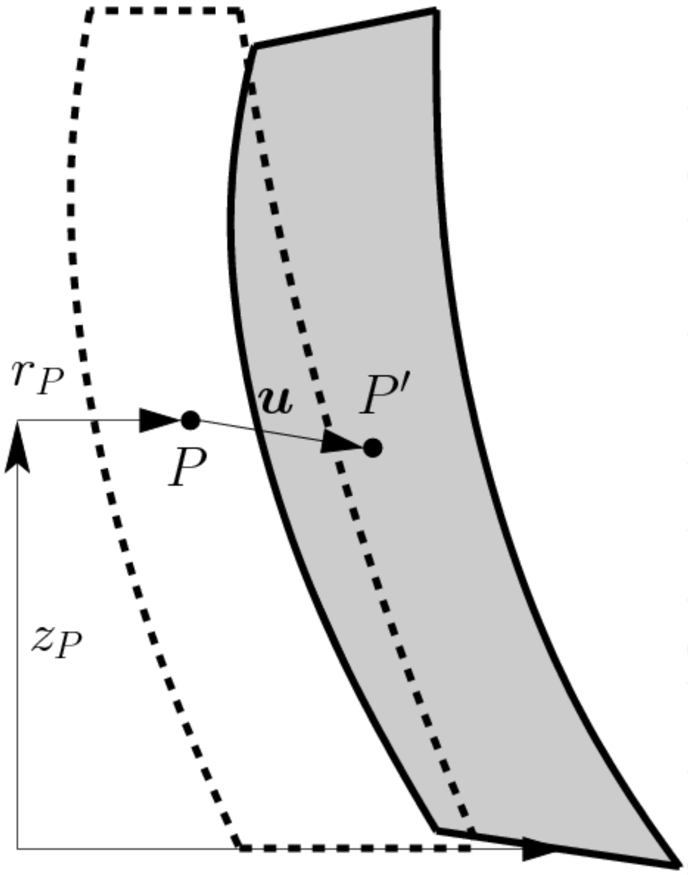
$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{pmatrix} \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{pmatrix} \quad \varepsilon_z = -\frac{\nu}{1-\nu}(\varepsilon_x + \varepsilon_y)$$

$$\boldsymbol{C}^{P\sigma} = \frac{E}{1-\nu^2} \begin{pmatrix} 1 & \nu & \\ \nu & 1 & \\ & & (1-\nu)/2 \end{pmatrix}$$

AXISYMMETRIC ELASTICITY

Axial symmetry : The geometry, material and boundary conditions are independent of θ :





$$\boxed{\boldsymbol{u} = \left\{ \begin{array}{c} u_r(r,z) \\ u_z(r,z) \end{array} \right\}}$$

AXISYMMETRIC ELASTICITY

Strains:

- Radial:

$$\boxed{\varepsilon_r = \frac{\partial u_r}{\partial r}}$$

- Shear:

$$\boxed{\gamma_{rz} = \frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}}$$

- Axial:

$$\boxed{\varepsilon_z = \frac{\partial u_z}{\partial z}}$$

- Circumferential:

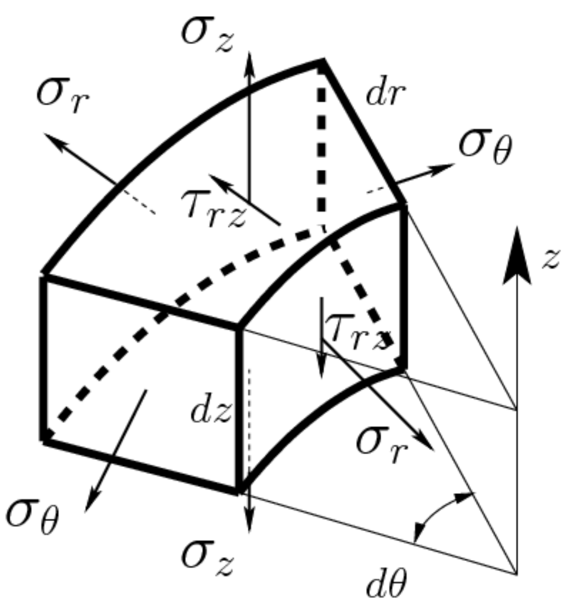
$$\boxed{\varepsilon_\theta = \frac{2\pi(r+u_r) - 2\pi r}{2\pi r} = \frac{u_r}{r}}$$

$$\boxed{\boldsymbol{\varepsilon}^t = \{\varepsilon_r \ \varepsilon_z \ \varepsilon_\theta \ \gamma_{rz}\}}$$

AXISYMMETRIC ELASTICITY

Stresses:

- In $dV = r\ d\theta\ dr\ dz$



$$\boldsymbol{\sigma}^t = \{\sigma_r\ \sigma_z\ \sigma_\theta\ \tau_{rz}\}$$

$$\boldsymbol{\sigma} = \boldsymbol{C}^{AX}\boldsymbol{\varepsilon}$$

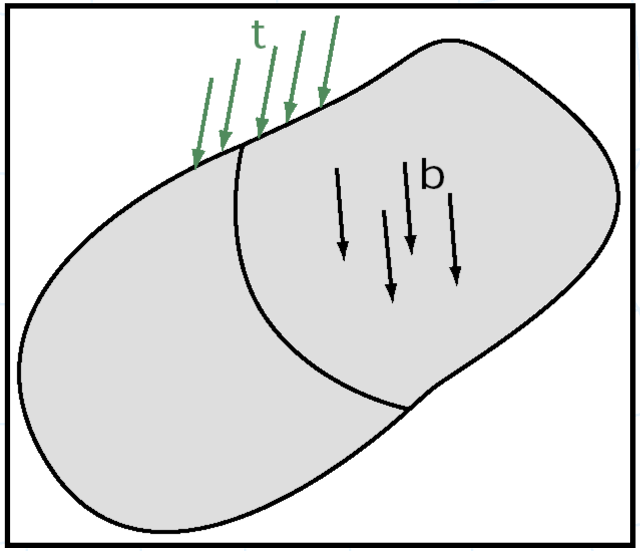
$$\boldsymbol{C}^{AX} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 \\ \nu & 1-\nu & \nu & 0 \\ \nu & \nu & 1-\nu & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}$$

WEAK FORM

WEAK FORM

Equilibrium + boundary c.:

$$
\begin{aligned}
&\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b} = \rho \ddot{\boldsymbol{u}} && \text{in } V \\
&\boldsymbol{u} = \boldsymbol{u}_D && \text{on } \Gamma^d \\
&\boldsymbol{\sigma n} = \boldsymbol{t} && \text{on } \Gamma^n
\end{aligned}
$$



Method of weighted residuals

1. Multiply by a test function, $\boldsymbol{v}$ with $\boldsymbol{v} = 0$ on Γ^d :

$$\int_V \boldsymbol{v} \cdot (\nabla \cdot \boldsymbol{\sigma}) + \int_V \rho \boldsymbol{v} \cdot \boldsymbol{b} = \int_V \rho \boldsymbol{v} \cdot \ddot{\boldsymbol{u}}, \ \forall \boldsymbol{v} \in \left[\boldsymbol{\mathcal{H}}^1(V)\right]^d$$

d: number of spatial dimensions (2 or 3)

WEAK FORM

2. Taking into account that $\nabla \cdot (\boldsymbol{v} \cdot \boldsymbol{\sigma}) = \nabla \boldsymbol{v} : \boldsymbol{\sigma} + \boldsymbol{v} \cdot (\nabla \cdot \boldsymbol{\sigma})$

$$\boxed{\int_V \nabla \cdot (\boldsymbol{v} \cdot \boldsymbol{\sigma}) - \int_V \nabla \boldsymbol{v} : \boldsymbol{\sigma} + \int_V \rho \boldsymbol{v} \cdot \boldsymbol{b} = \int_V \rho \boldsymbol{v} \cdot \ddot{\boldsymbol{u}}}$$

3. Using the divergence theorem in the first integral, the boundary conditions, and the fact that $\boldsymbol{v} = 0$ on Γ^d :

$$\boxed{\int_V \rho \boldsymbol{v} \cdot \ddot{\mathrm{u}} + \int_V \nabla \boldsymbol{v} : \boldsymbol{\sigma} = \int_V \rho \boldsymbol{v} \cdot \boldsymbol{b} + \int_{\Gamma^n} \boldsymbol{t} \cdot \boldsymbol{v}, \ \forall \boldsymbol{v} \in \left[\boldsymbol{\mathcal{H}}^1(V)\right]^d}$$

WEAK FORM

Can also be deduced from the principle of virtual work (PVW):

- Virtual displacements $\boldsymbol{v}$.
- $\boldsymbol{\sigma}$ is symmetric $\Rightarrow \nabla\boldsymbol{v} : \boldsymbol{\sigma} = \nabla^s\boldsymbol{v} : \boldsymbol{\sigma} = \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{\sigma}$,therefore:

$$\boxed{\underbrace{\int_V \rho\boldsymbol{v}\cdot\ddot{\boldsymbol{u}}}_{\text{VW of inertial forces}} + \underbrace{\int_V \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{\sigma}}_{\text{VW of internal (elastic) forces}} = \underbrace{\underbrace{\int_V \rho\boldsymbol{v}\cdot\boldsymbol{b}}_{\text{VW of volumetric loads}} + \underbrace{\int_{\Gamma^n} \boldsymbol{t}\cdot\boldsymbol{v}}_{\text{VW of boundary loads}}}_{\text{VW of external loads}}}$$

DISCRETIZATION

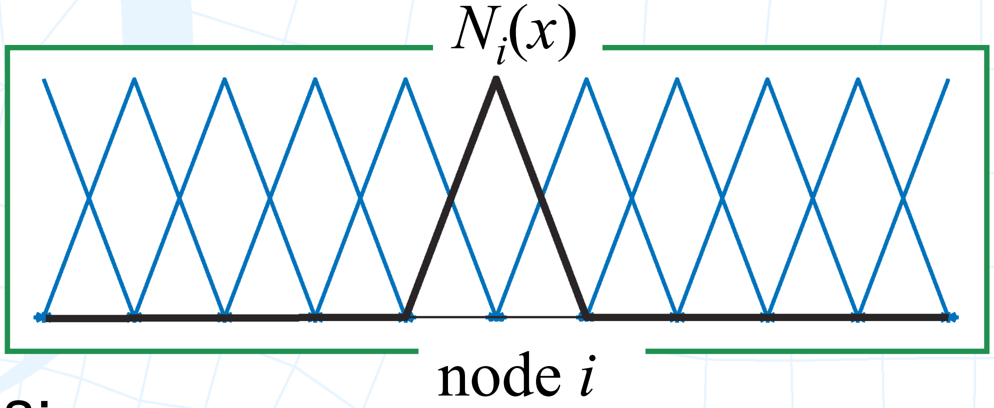
Idea of discretisation

- The unknown displacement field ***u***(t) (for a fixed t) and the virtual displacement field ***v*** can vary in an infinite number of ways
- To obtain a manageable system, we ask ***u***(t) and ***v*** to take specific forms, i.e., as linear combinations of a chosen set of basis functions
- This is called the *semi-discretized* weak form, because time is still continuous. The semi-discretized weak form can be rewritten as a coupled system of ordinary differential equations
- The discretization in time will be discussed in the next class

Typical finite element interpolation in 1D

- Each unknown field is interpolated with hat functions (linear C^0, quadratic C^0, cubic C^0 or C^1,…):

$$\boxed{u(x) \simeq u^h(x) = \sum_i u_i N_i(x)}$$

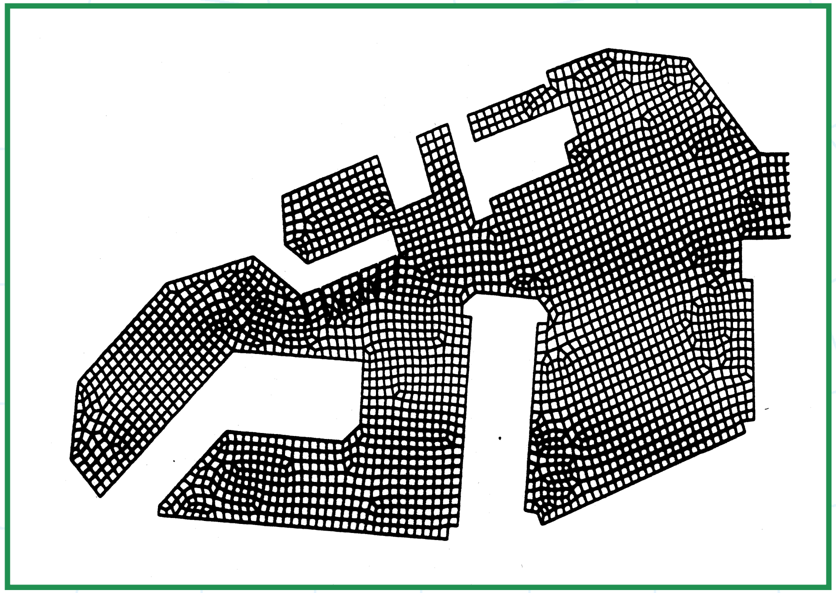


- Advantages:
  - Compact support (local bases) ⇒ sparse matrices
  - Easy to integrate
  - Physical meaning of the coefficients u_i, since $N_i(x_j) = \delta_{ij}$

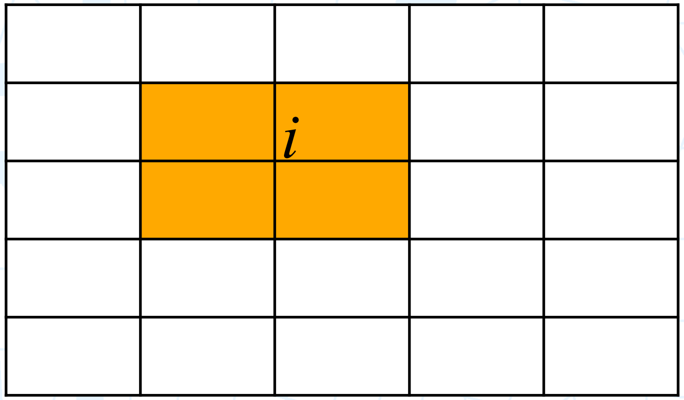
$$u^h(x_i) = u_i$$

DISCRETIZATION

- Each node *i* is associated with a basis function (“shape function”) N_i such that
  - $N_i(\mathbf{x}_j) = \delta_{ij}$, where $\mathbf{x}_j$ is the coordinate of node *j*
  - $N_i = 0$ in the elements that do not have node *i* as their node



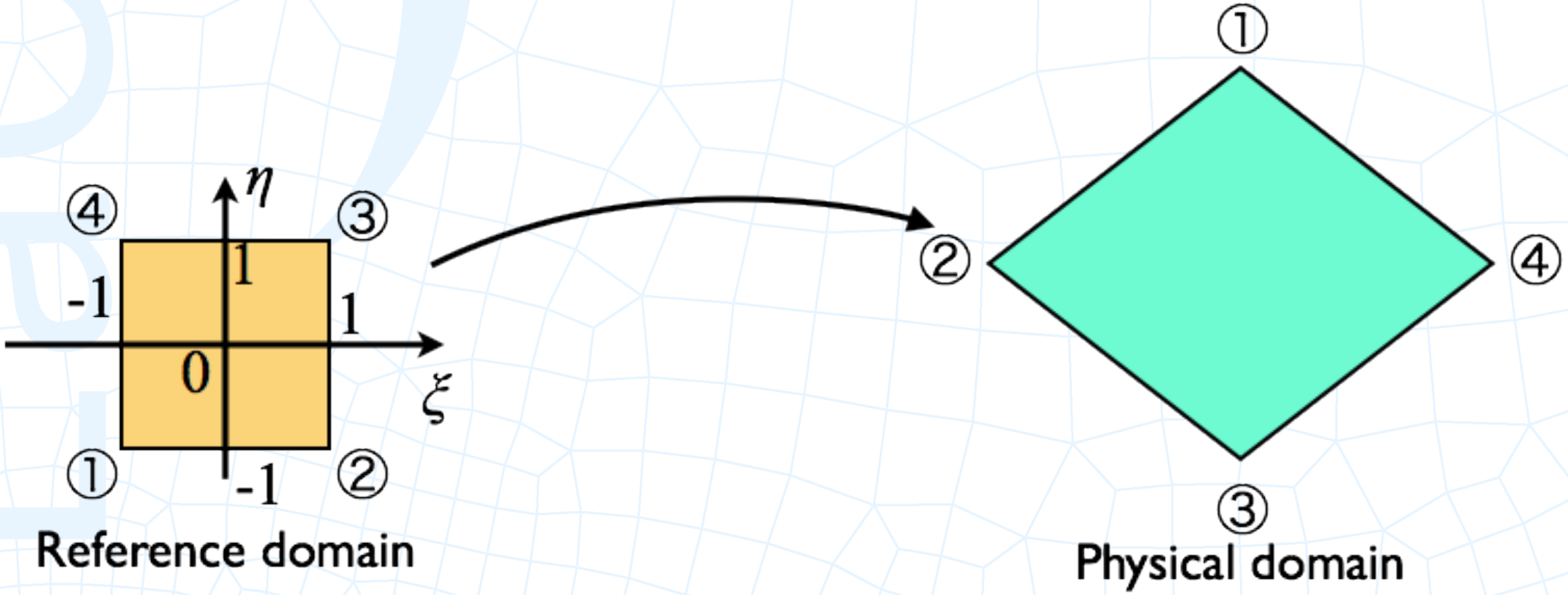
A 2D mesh with quadrilaterals



🟧 The support of N_i (region on which $N_i \neq 0$)

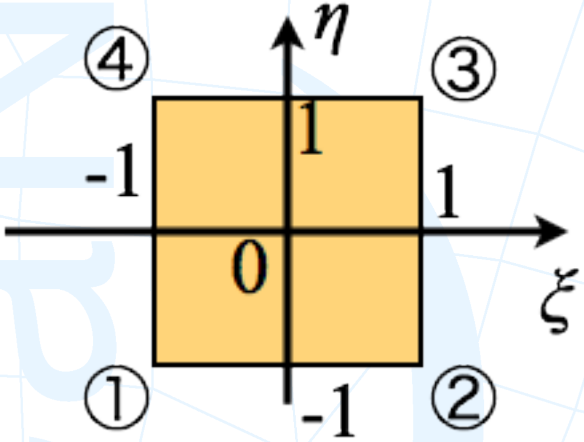
DISCRETIZATION

- Especially in multidimensions, the shape functions are normally not written in the physical coordinates *x*, *y* (, *z*).
- Instead, we define a reference domain that can be mapped to all elements, each with a different mapping.
- If we want to evaluate the shape function of a given point (*x*, *y*), we need to first find the corresponding (*ξ*, *η*)



DISCRETIZATION

Interpolation in 2D:

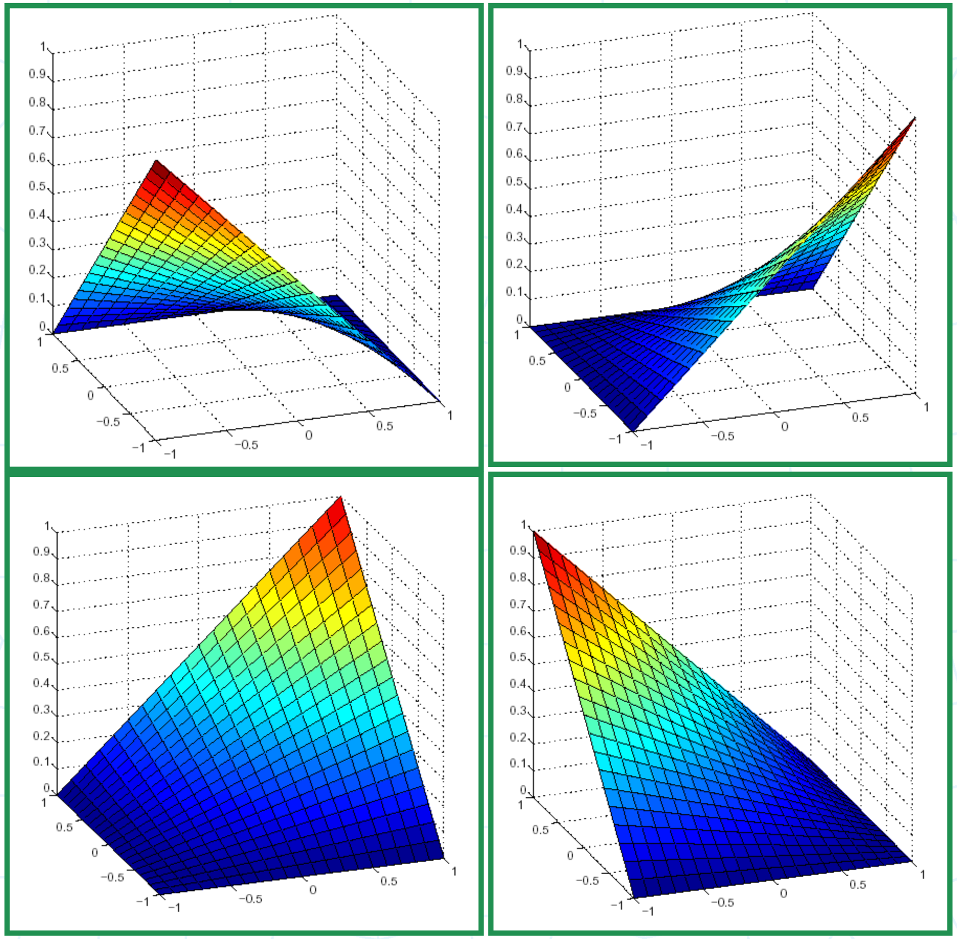


$$N_1 = \frac{1}{4}(1-\xi)(1-\eta)$$

$$N_2 = \frac{1}{4}(1+\xi)(1-\eta)$$

$$N_3 = \frac{1}{4}(1+\xi)(1+\eta)$$

$$N_4 = \frac{1}{4}(1-\xi)(1+\eta)$$



Remark: $$\sum_{i=1}^{4} N_i(\xi,\eta) = 1$$

DISCRETIZATION

Dirichlet boundary conditions:

- The prescribed values u_D are used in the interpolation:

$$\boxed{\boldsymbol{u}^h(x) = \sum_{i \notin \Gamma^d} \boldsymbol{u}_i N_i(x) + \underbrace{\sum_{j \in \Gamma^d} \boldsymbol{u}_D(x_j) N_j(x)}_{\boldsymbol{\phi}(x)}}$$

- $\boldsymbol{u}^h(\boldsymbol{x})$ satisfies (up to interpolation error) the Dirichlet (or essential) boundary condition $\boldsymbol{u} = \boldsymbol{u}_D$ on Γ^d .
- Test functions: $\boldsymbol{v}^h(\boldsymbol{x}) = \sum_{i \notin \Gamma^d} \boldsymbol{v}_i N_i(\boldsymbol{x})$; hence $\boldsymbol{v}^h(\boldsymbol{x}_i) = 0$ for $\boldsymbol{x}_i \in \Gamma^d$.
- There are other techniques to impose Dirichlet boundary conditions: Lagrange multipliers, penalty methods, Nitsche's method...

DISCRETIZATION

Small deformation hypothesis:

- Contitutive law:

d-dimensional vector

$$\boxed{\boldsymbol{\sigma}^h = \mathcal{C} : \boldsymbol{\varepsilon}(\boldsymbol{u}^h) = \boldsymbol{C} \sum_j \mathbf{B}_j(\boldsymbol{x}) \boldsymbol{u}_j}$$

with:

$$\boxed{\mathbf{B}_j(\boldsymbol{x}) = \begin{bmatrix} \dfrac{\partial N_j(\boldsymbol{x})}{\partial x} & 0 \\ 0 & \dfrac{\partial N_j(\boldsymbol{x})}{\partial y} \\ \dfrac{\partial N_j(\boldsymbol{x})}{\partial y} & \dfrac{\partial N_j(\boldsymbol{x})}{\partial x} \end{bmatrix}}$$

for 2D

- *Semi-discretized* weak form (spatial discretization, no temporal discretization):

$$\boxed{\int_V \rho \boldsymbol{v}^h \cdot \ddot{\boldsymbol{u}}^h + \int_V \boldsymbol{\varepsilon}(\boldsymbol{v}^h) : \boldsymbol{\sigma}^h = \int_V \rho \boldsymbol{v}^h \cdot \boldsymbol{b} + \int_{\Gamma^n} \boldsymbol{t} \cdot \boldsymbol{v}^h, \ \forall \boldsymbol{v}^h}$$

Exercise

- Write down the $\mathbf{B}_j$ matrix for 3D and axisymmetric settings

SEMI-DISCRETIZED WEAK-FORM SOLUTION

- Using $u^h(x)$ and $v^h(x)$ in the weak form we obtain:

$$\boxed{\boldsymbol{v}_i \cdot \left(\sum_j \mathbf{m}_{ij} \ddot{\boldsymbol{u}}_j + \sum_j \mathbf{k}_{ij} \boldsymbol{u}_j \right) = \boldsymbol{v}_i \cdot \boldsymbol{f}_i, \ \forall \boldsymbol{v}_i}$$

where,

$d \times d$ $$\mathbf{m}_{ij} = \int_V \rho N_i(\boldsymbol{x}) N_j(\boldsymbol{x}) \mathbf{I} dV$$

$d \times d$ $$\mathbf{k}_{ij} = \int_V \mathbf{B}_i(\boldsymbol{x})^T \mathbf{C} \mathbf{B}_j(\boldsymbol{x}) dV$$

$d \times 1$ $$\mathbf{f}_i = \int_V \rho N_i(\boldsymbol{x}) \boldsymbol{b} dV + \int_{\Gamma^n} N_i(\boldsymbol{x}) \boldsymbol{t} d\Gamma - \int_V \mathbf{B}_i(\boldsymbol{x})^T \mathbf{C} \varepsilon(\phi) dV - \int_V \rho N_i(\boldsymbol{x}) \ddot{\boldsymbol{\phi}}(\boldsymbol{x}) dV$$

SEMI-DISCRETIZED WEAK-FORM SOLUTION

- Since this must be satisfied for all v_i , we end up with the following system of equations:

$$\boxed{\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}}$$

where,

$$\mathbf{u} = \left\{ \begin{array}{c} \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_{nnodes} \end{array} \right\}, \qquad \mathbf{f} = \left\{ \begin{array}{c} \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_{nnodes} \end{array} \right\}$$

$$\mathbf{M} = \mathop{\mathsf{A}}_{i,j=1}^{nnodes} \mathbf{m}_{ij} \quad , \qquad \mathbf{K} = \mathop{\mathsf{A}}_{i,j=1}^{nnodes} \mathbf{k}_{ij}$$

A means “assemble,” superposing elemental contributions to the global matrices **M** and **K**

NUMERICAL INTEGRATION

- Numerical integration with weights W_g and $nint$ points $\boldsymbol{x}_g$:

$$\mathbf{m}_{ij} = \sum_{g=1}^{nint} W_g \rho_g N_i(\boldsymbol{x}_g) N_j(\boldsymbol{x}_g)\mathbf{I}$$

$$\mathbf{k}_{ij} = \sum_{g=1}^{nint} W_g \mathbf{B}_i(\boldsymbol{x}_g)^T \mathbf{C}\mathbf{B}_j(\boldsymbol{x}_g)$$

$$\mathbf{f}_i = \sum_{g=1}^{nint} W_g \rho_g N_i(\boldsymbol{x}_g)\boldsymbol{b}_g + \sum_{g=1}^{nint} W_g N_i(\boldsymbol{x}_g)\boldsymbol{t}_g - \cdots$$

- The stresses are also evaluated at $\boldsymbol{x}_g$:

$$\boldsymbol{\sigma}(\boldsymbol{x}_g) = \boldsymbol{C}\sum_j \mathbf{B}_j(\boldsymbol{x}_g)\boldsymbol{u}_j$$

Solving the system of equations

- Static problems (no need to compute matrix *M*)
  - Solve the matrix equation (direct solver vs iterative solver)

$$\boxed{\mathbf{K}\mathbf{u} = \mathbf{f}}$$

- Dynamic problems: the discretised equations are a coupled set of ordinary differential equations

$$\boxed{\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}}$$

  - Select a time step Δt
  - Adopt an algorithm to advance in discrete time steps Δt, $2\Delta t$, $3\Delta t$….
  - Stability and accuracy need to be considered (next class)

Linear vs Non-linear elasticity

- Linear elasticity

$$\boldsymbol{x} \approx \boldsymbol{X}, |\partial_i u_j| << 1$$

$$w^{el} = \frac{1}{2}\boldsymbol{\varepsilon} : \mathcal{C} : \boldsymbol{\varepsilon}$$

$$\boldsymbol{\sigma} = \frac{\partial w^{el}}{\partial \boldsymbol{\varepsilon}} = \mathcal{C} : \boldsymbol{\varepsilon}$$

$$\delta W^{el} = \int_V \delta\boldsymbol{\varepsilon} : \boldsymbol{\sigma} dV$$

- Non-linear elasticity

$$\boldsymbol{x} = \boldsymbol{X} + \boldsymbol{u}$$

$$w^{el}(\mathbf{C}, \mathbf{E}, J, ..)$$

$$\mathbf{S} = \frac{\partial w^{el}}{\partial \mathbf{E}} = 2\frac{\partial w^{el}}{\partial \mathbf{C}}$$

$$\boldsymbol{\sigma} = J^{-1}\mathbf{F}\mathbf{S}\mathbf{F}^T$$

$$\delta W^{el} = \int_V \frac{\partial w^{el}}{\partial \mathbf{C}} : \delta\mathbf{C} dV$$

$$= \int_V \frac{1}{2}\mathbf{S} : \delta\mathbf{C} dV = \int_v \boldsymbol{\sigma} : \nabla_x \delta\boldsymbol{v} dv$$

Linear vs Non-linear elasticity

$$\boxed{\boldsymbol{g}_i := \frac{\partial(\delta W^{el} - \delta W^{ext} + \delta W^{dyn})}{\partial \delta \boldsymbol{v}_i} = \mathbf{0}\ ,\ \mathbf{K}_{ij} = \frac{\partial \delta W^{el}}{\partial \delta \boldsymbol{v}_i \partial \boldsymbol{x}_j}}$$

- Linear elasticity

$$\boldsymbol{g}_i^e = \int_{V^e} \boldsymbol{\sigma} \nabla N_i dV$$

$$\boldsymbol{g}_i^e = \mathbf{K}_{ij}^e \boldsymbol{u}_j$$

$$\mathbf{K}_{ij}^e = \int_{V^e} \mathbf{B}_i^T \mathbf{C} \mathbf{B}_j dV$$

- Non-linear elasticity

$$\delta \mathbf{F} = \delta \boldsymbol{x}_i \otimes \nabla_X N_i = \delta \boldsymbol{x}_i \otimes \mathbf{F}^T \nabla_x N_i$$
$$= \delta \boldsymbol{x}_i \otimes \nabla_x N_i \mathbf{F}$$

$$\boldsymbol{g}_i^e = \int_{V_0^e} \boxed{\mathbf{F}}\boxed{\mathbf{S}} \nabla_X N_i dV_0 = \int_{V^e} \boxed{\boldsymbol{\sigma}}\boxed{\nabla_x N_i}\boxed{dV}$$

Non-linear

$$\boxed{\mathbf{K}_{ij}^e = \frac{\partial \boldsymbol{g}_i^e}{\partial \boldsymbol{x}_j}}$$

Non-constant

Meaning of $\mathbf{SN}$, $\mathbf{PN}$, and $\boldsymbol{\sigma}\mathbf{n}$?

Modeling and simulation of convection-diffusion-reaction of hydrocarbons

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Sponsors

EXPERT COMPONENTS S.A.

MINISTERIO DE CIENCIA Y TECNOLOGÍA

The problem: impact of automobile in environment

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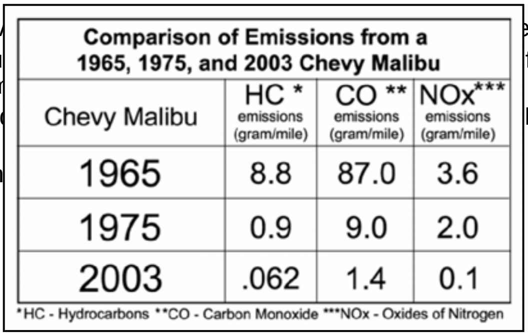

Comparison of Emissions from a 1965, 1975, and 2003 Chevy Malibu

Chevy Malibu	HC * emissions (gram/mile)	CO ** emissions (gram/mile)	NOx*** emissions (gram/mile)
1965	8.8	87.0	3.6
1975	0.9	9.0	2.0
2003	.062	1.4	0.1

*HC - Hydrocarbons **CO - Carbon Monoxide ***NOx - Oxides of Nitrogen

Cal/EPA: 1 car built in 1965 polluted as much as 40 cars built in 1998; 1 LEV I car pollutes as 5 LEV II cars

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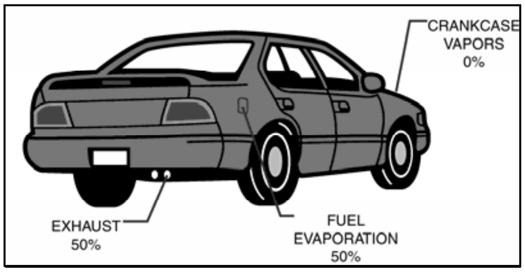
Vehicle emissions

Today
Before



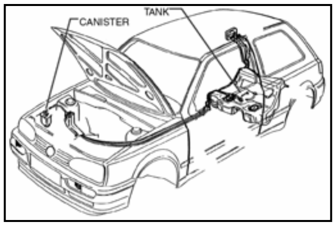
Fuel evaporation accounts for 50% of vehicle emissions

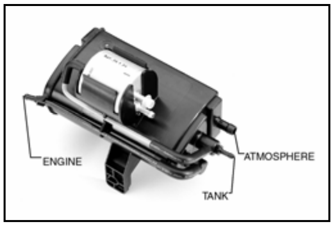
Today an average car pollutes as much parked on the street (fuel evaporation) as running (exhaust)

LEV II imposes almost zero evaporative emissions

Emission control: active carbon filters (1)

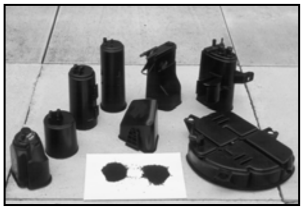
- Active carbon filters mitigate evaporative emissions
- Canister of injected plastic with three openings: tank, atmosphere, engine
- Different materials: active carbon, plastic, air chambers, foams, fleece.



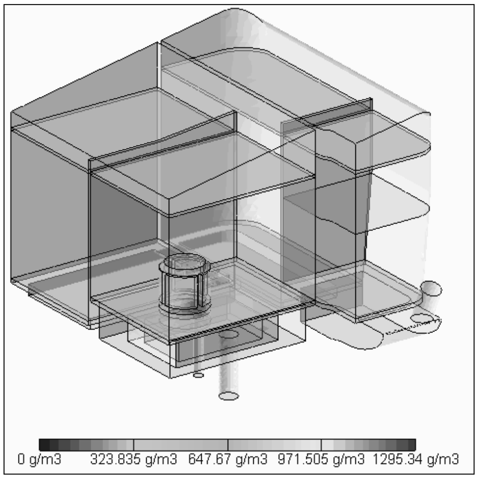


Difficulties in canister design

- Complex 3D geometries
  - Volkswagen Polo
  - Audi A8
- Different materials
- Strict design requirements:
  - Pressure drop
  - Breakthrough and working capacity
  - Bleed emissions (three-diurnal test)



Porche Boxster:



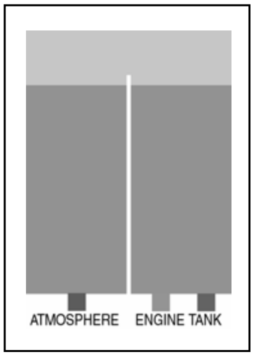
SUMMARY: definition of the problem

- Critical modeling: almost zero emissions for an equipment that controls 50% of hydro-carbon pollution.
- Complex 3D geometries
- Multiphysics (flow, diffusion, convection, reaction, ...)
- Two length scales: local (active carbon pellets; mm)
  global (canister, dm)
- Transient and non-uniform problem
- Two time scales: due to the wide range of flow rates e.g. working capacity test
  - Loading at 0.2 l/min ⟹ reaction is “instantaneous”
  - Purge at 22.7 l/min ⟹ reaction takes time

“Simplified” model: Flow of fuel vapor and
Mass transfer of hydro-carbons between air and pellets

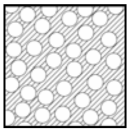
Flow of fuel vapor

- Active carbon: porous media theory
  v is Darcy velocity
- Air chambers: potential flow
  prescribed pressure drop
- Air-carbon interface: uniform pressure
  continuity of vapor flow



Mass transfer of hydro-carbons (1)

- Two-porosity model



Interparticle porosity

$$\varepsilon_e = \frac{\mathrm{V}_{\text{interparticle fluid}}}{\mathrm{V}_{\text{total}}}$$

Intraparticle porosity

$$\varepsilon_p = \frac{\mathrm{V}_{\text{intraparticle fluid}}}{\mathrm{V}_{\text{particle}}}$$

- Three fractions of hydro-carbons (HC)
  - ✓In interparticle fluid (air): concentration $\boxed{\mathrm{c} \quad [\mathrm{g/m^3}]}$
  - ✓In intraparticle fluid (pores): concentration $\boxed{\mathrm{c_{pore}} \quad [\mathrm{g/m^3}]}$
  - ✓Adsorbed in active carbon (AC): ratio $\boxed{\mathrm{q} \quad [\mathrm{g\ HC/g\ AC}]}$

Mass transfer of hydro-carbons (2)

- Mass conservation: mass transfer mechanism ($\underbrace{\text{diffusion + convection}}_{\textbf{only air fraction}}$ + “local” mass variation)

$$\boxed{\frac{1}{\varepsilon_{\mathrm{e}}}\frac{\partial \mathrm{m}}{\partial \mathrm{t}} = \boldsymbol{\nabla}\cdot(D\boldsymbol{\nabla}\mathrm{c}) - \boldsymbol{v}\cdot\boldsymbol{\nabla}\mathrm{c}}$$

Mass of hydro-carbons is a combination of the three species

$$\boxed{\mathrm{m} = \underbrace{\rho_{\mathrm{s}}(1-\varepsilon_{\mathrm{e}})(1-\varepsilon_{\mathrm{p}})\mathrm{q}_{\square}}_{\textbf{adsorbed}} + \underbrace{(1-\varepsilon_{\mathrm{e}})\,\varepsilon_{\mathrm{p}}\mathrm{c}_{\mathrm{P}}}_{\textbf{pores}} + \underbrace{\varepsilon_{\mathrm{e}}\,\mathrm{c}}_{\textbf{air}}}$$

Mass transfer of hydro-carbons (3)

- Mass transfer mechanisms: global level

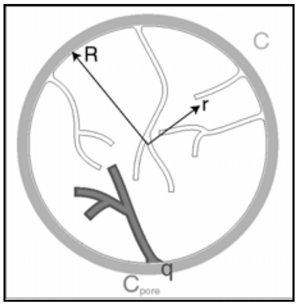
$$\boxed{\varepsilon_{\mathrm{e}}\frac{\partial c}{\partial t} + \underbrace{\mathbf{v}\cdot\nabla c}_{\text{convection}} - \underbrace{\varepsilon_{\mathrm{e}}\nu\nabla^2 c}_{\text{diffusion}} + \overbrace{\underbrace{\sigma[q(c), c_{\text{pore}}(c)]c}_{\text{reaction}} = \underbrace{f[q(c), c_{\text{pore}}(c)]}_{\text{source}}}^{\text{adsorption/desorption}}}$$

- Reaction term
  - models adsorption/desorption
  - couples local and global levels
  - is nonlinear: $\boxed{c_{\text{pore}} = c_{\text{pore}}(c),\ q = q(c)}$
- Diffusion term
  - tiny (important in localized areas)
  - renders the problem parabolic
- Convection term
  - models fuel vapor motion
  - **v** computed before mass transfer

Mass transfer of hydro-carbons (5)

- Mass transfer mechanisms at local level:
  Radial surface diffusion

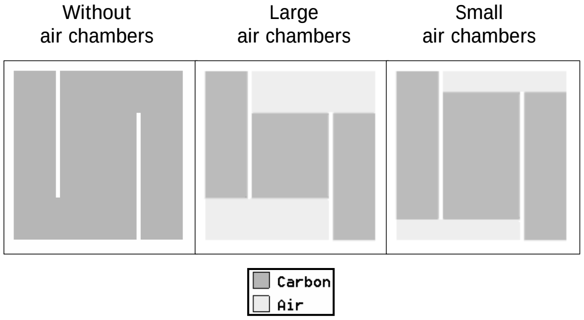
$$\boxed{\frac{\partial q}{\partial t} = D_p \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial q}{\partial r}\right)}$$



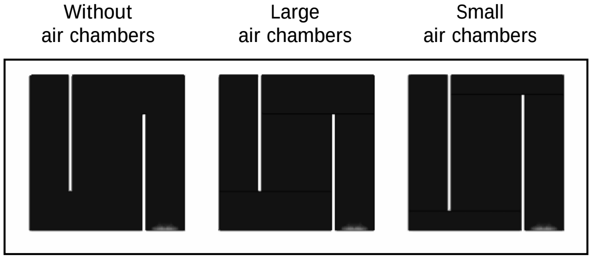
Symmetry at center: $\boxed{D_p \frac{\partial q}{\partial r}\Big|_{r=0} = 0}$

Film mass transfer: Robin B.C. $\boxed{D_p \frac{\partial q}{\partial r}\Big|_{r=R} = \frac{K_f}{\rho_s(1-\varepsilon_p)}\left(c(R) - c_{\text{pore}}(R)\right)}$

The smoothing effect of air chambers (1)

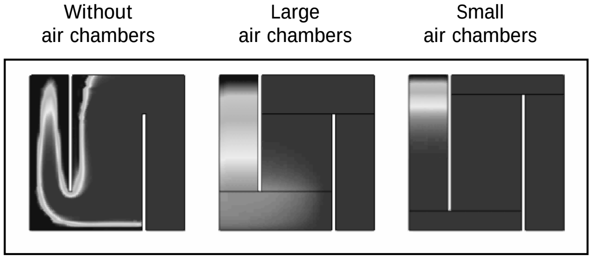


The smoothing effect of air chambers (2)



Adsorption

The smoothing effect of air chambers (3)



Desorption

Numerical simulation

- Transient convection-diffusion-reaction (non-linear):
  - Accuracy
  - Stabilization

  Need high-accuracy and stabilization?
- Wide range of flow rates: e.g. working capacity test
  - Loading at 0.2 l/min $\Longrightarrow$ diffusion-reaction dominated
  - Purge at 22.7 l/min $\Longrightarrow$ convection dominated

True or False?

- Complex 3D geometries $\Longrightarrow$ mesh adaption
- Local problem must be solved efficiently (at each node or Gauss point) $\Longrightarrow$ homogenize (non-linear ODE…)
- Is the advancing front controlled by the convection velocity?

Numerical simulation

- Transient convection-diffusion-reaction (non-linear):
  - Accuracy
  - Stabilization

  Need high-accuracy and stabilization?
- Wide range of flow rates: e.g. working capacity test
  - Loading at 0.2 l/min $\Longrightarrow$ Vertical front
  - Purge at 22.7 l/min $\Longrightarrow$ Smooth front

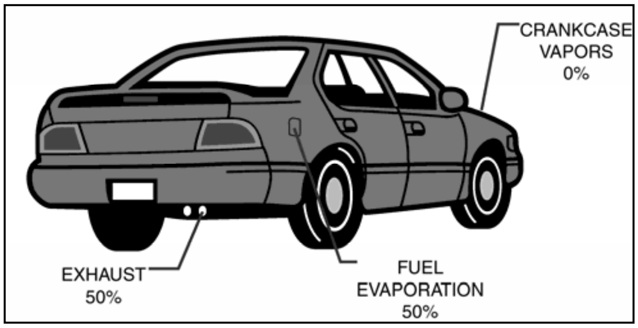
True or False?

- Complex 3D geometries $\Longrightarrow$ mesh adaption
- Local problem must be solved efficiently (at each node or Gauss point) $\Longrightarrow$ homogenize (non-linear ODE…)
- Is the advancing front controlled by the convection velocity?

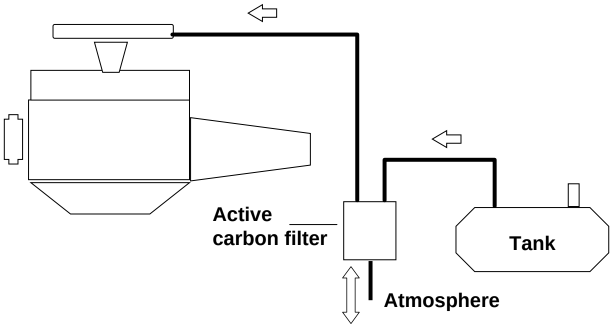
Concluding remarks

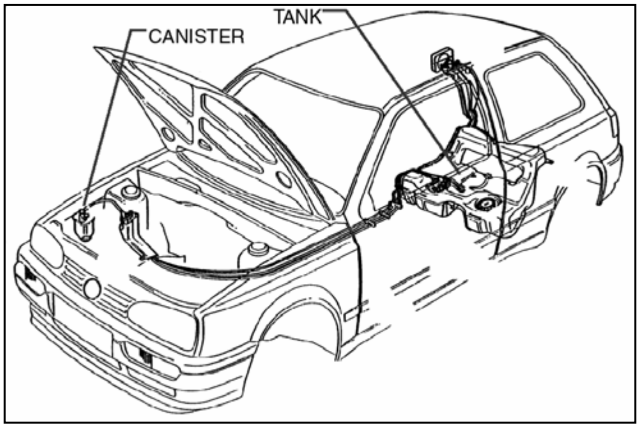
Finite element model of evaporative emission canisters:

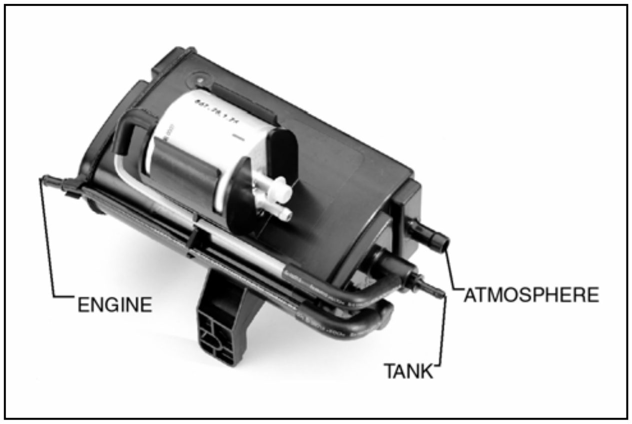
- Realistic modeling of multi-physics: flow, convection, diffusion at local and global levels, nonlinear reaction (adsorption/desorption),…
- Challenging numerical issues: 3D, stabilization of convective term, accurate time-stepping, different time and length scales,…
- Valuable tool for canister design



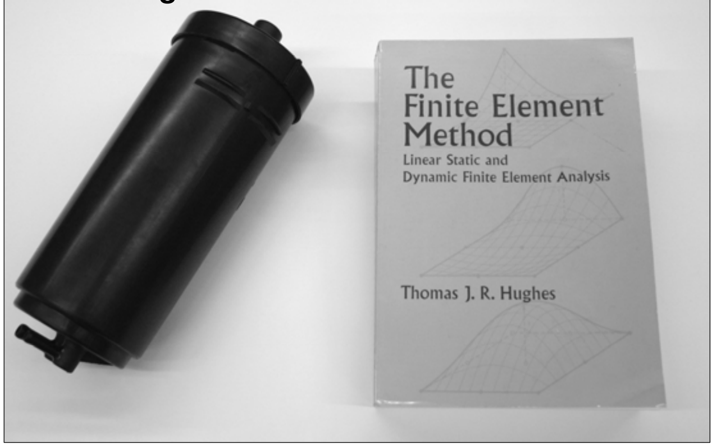
Evaporative emission system





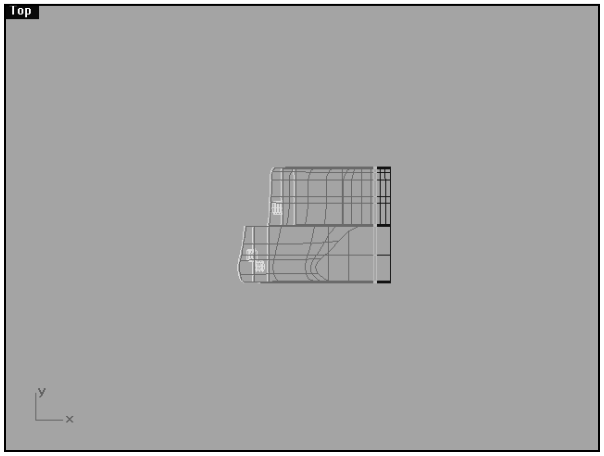


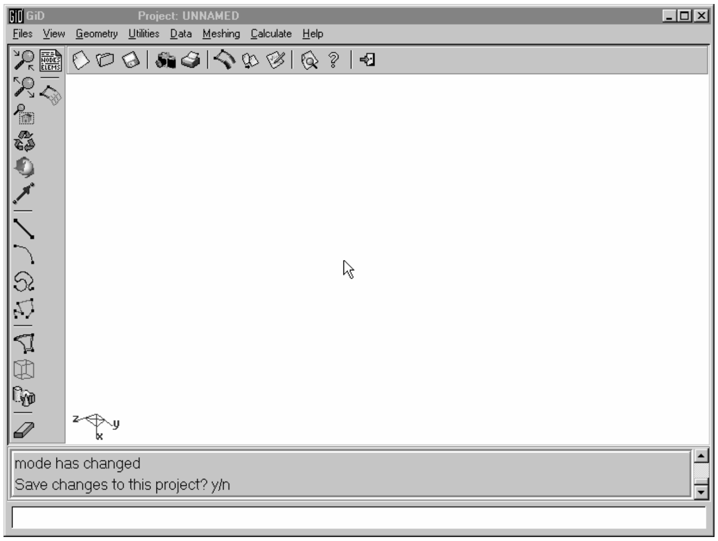
Volkswagen Polo



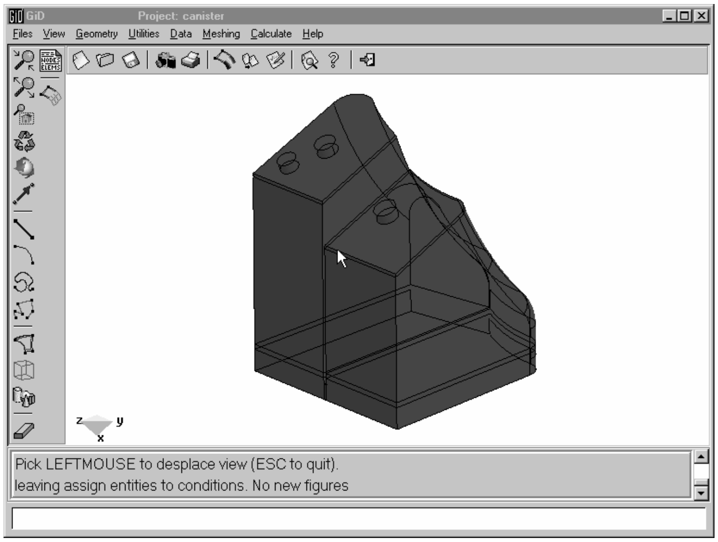
Audi A8

Audi A8

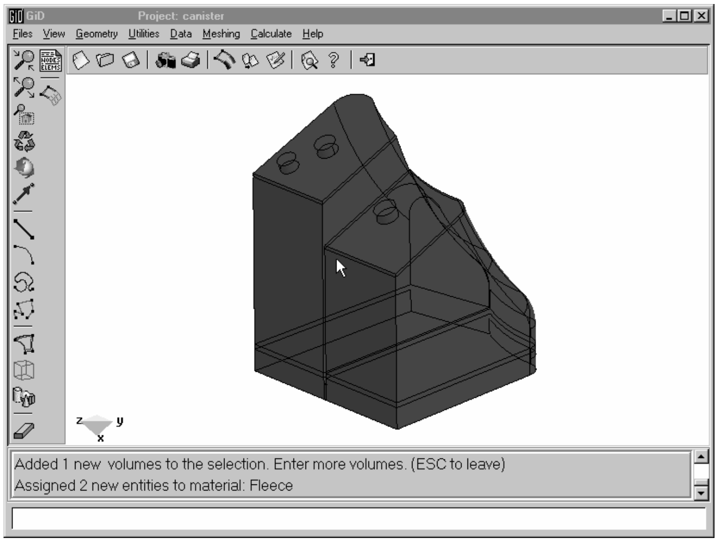




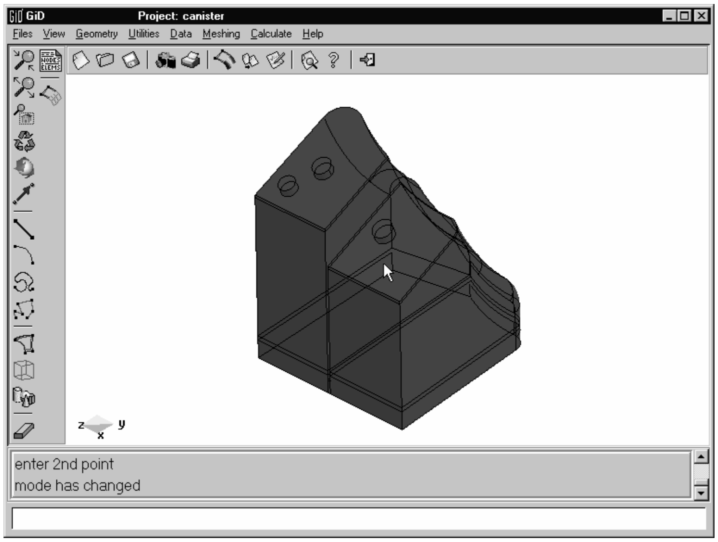
mode has changed
Save changes to this project? y/n



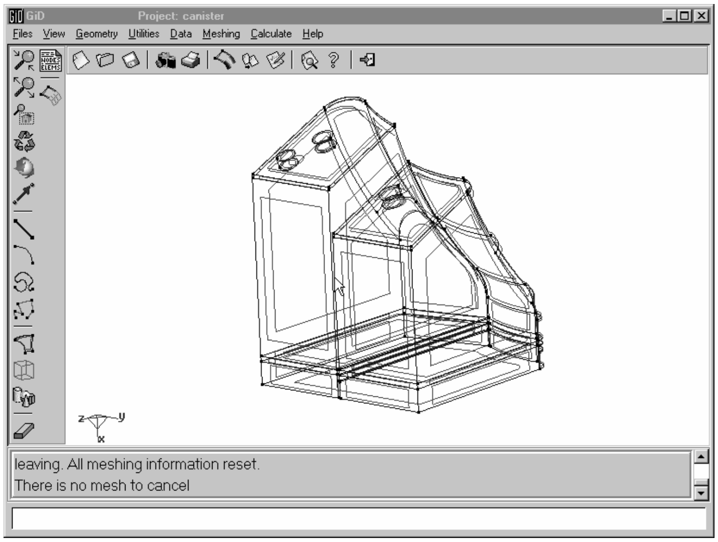
Pick LEFTMOUSE to desplace view (ESC to quit).
leaving assign entities to conditions. No new figures



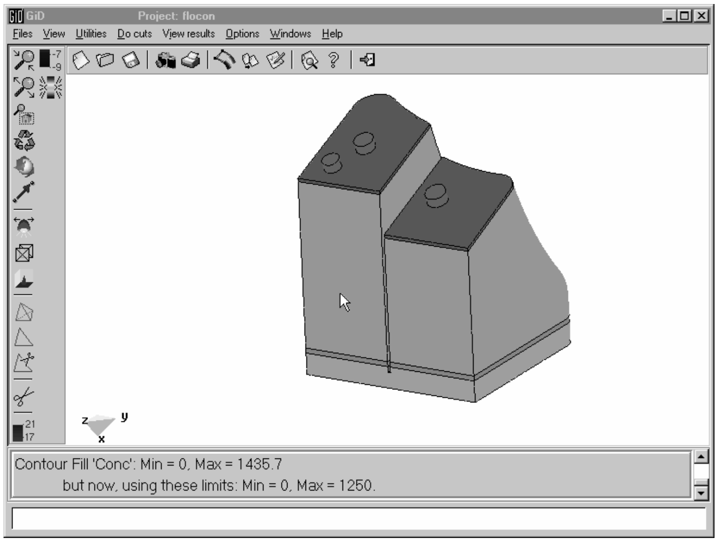
Added 1 new volumes to the selection. Enter more volumes. (ESC to leave)
Assigned 2 new entities to material: Fleece



enter 2nd point
mode has changed

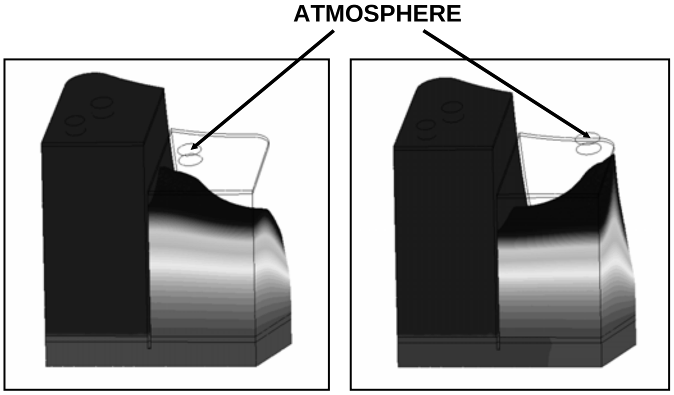


leaving. All meshing information reset.
There is no mesh to cancel



Contour Fill 'Conc': Min = 0, Max = 1435.7
but now, using these limits: Min = 0, Max = 1250.

Design capabilities



Unsteady convection-diffusion

Com. NME **18**/8 (2002)

$$u_t + \mathbf{a} \cdot \nabla u - \nu \nabla^2 u = s$$

$$u_t + \mathcal{L}(u) = s$$ where $$\mathcal{L} := \mathbf{a} \cdot \nabla - \nu \nabla^2$$

Implicit multi-stage schemes
(IRK, Padé …)

$$\frac{\Delta \mathbf{u}}{\Delta t} - \mathbf{W} \Delta \mathbf{u}_t = \mathbf{w} u_t^n$$

$$\mathcal{R}(\Delta \mathbf{u}) := \frac{\Delta \mathbf{u}}{\Delta t} - \mathbf{W} \Delta \mathbf{u}_t - \mathbf{w} u_t^n$$

- CRANK-NICOLSON (n_{stg}=1)

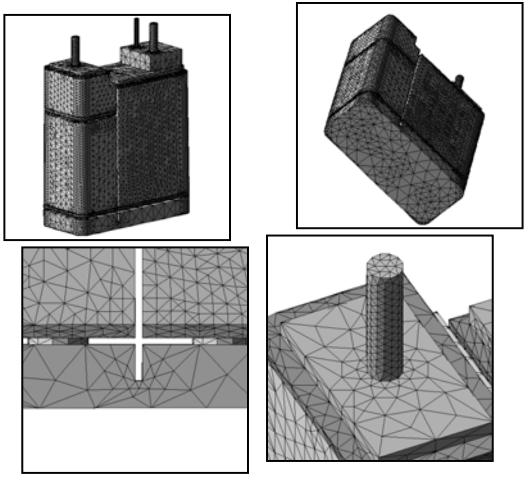
$$\begin{array}{ll} \Delta \mathbf{u} = u^{n+1} - u^n, & \Delta \mathbf{s} = s^{n+1} - s^n, \\ \mathbf{W} = \frac{1}{2} & \mathbf{w} = 1. \end{array}$$

It can be seen as a 2ond order Padé approximation : R_{11}

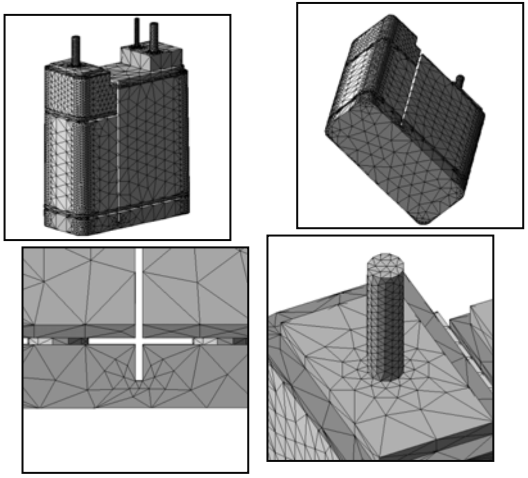
- 4th ORDER PADÉ APPROXIMATION: R_{22} (n_{stg}=2)

$$\begin{array}{ll} \Delta \mathbf{u} = \left\{ \begin{array}{c} u^{n+\frac{1}{2}} - u^n \\ u^{n+1} - u^{n+\frac{1}{2}} \end{array} \right\}, & \Delta \mathbf{s} = \left\{ \begin{array}{c} s^{n+\frac{1}{2}} - s^n \\ s^{n+1} - s^{n+\frac{1}{2}} \end{array} \right\}, \\ \mathbf{W} = \frac{1}{24} \left[\begin{array}{cc} 7 & -1 \\ 13 & 5 \end{array} \right], & \mathbf{w} = \frac{1}{2} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\}. \end{array}$$

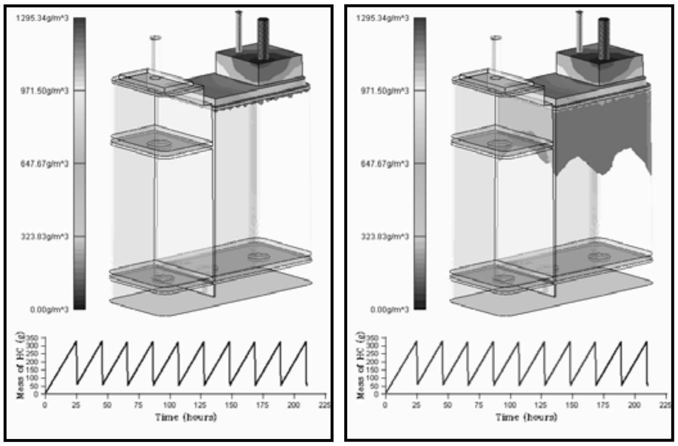
GM light truck: Load mesh



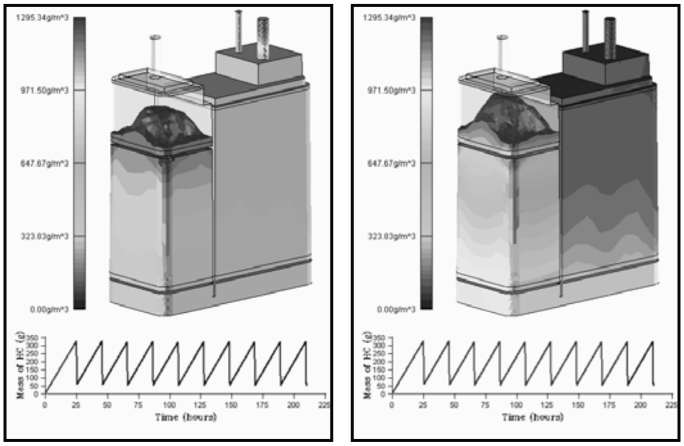
GM light truck: Purge mesh



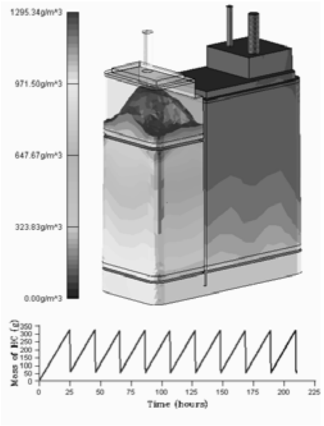
Loading: concentration of HC (1)

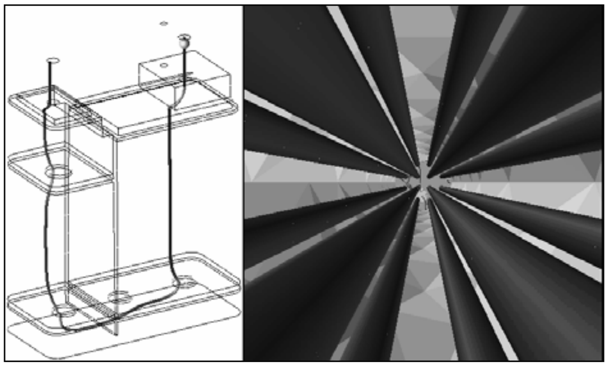


Loading: concentration of HC (2)



Purge





- Galerkin weak form

$$\boxed{(\mathbf{v}, \frac{\Delta \mathbf{u}}{\Delta t})_\Omega - (\mathbf{v}, \mathrm{W}\Delta\mathbf{u}_t)_\Omega = (\mathbf{v}, \mathrm{w}u_t^n)_\Omega}$$

- Stabilized weak form

$$\boxed{(\mathbf{v}, \frac{\Delta \mathbf{u}}{\Delta t})_\Omega - (\mathbf{v}, \mathbf{W}\Delta\mathbf{u}_t)_\Omega + \sum_e \tau(\mathcal{P}(\mathrm{v}), \mathcal{R}(\Delta\mathrm{u}))_{\Omega^e} = (\mathbf{v}, \mathbf{w}u_t^n)_\Omega}$$

  – Streamline-Upwind Petrov-Galerkin: $\boxed{\mathcal{P}(\mathrm{v}) := \mathbf{W}(a \cdot \nabla)\mathbf{v}}$

  – Least-Squares (LS): $\boxed{\tau\mathcal{P}(\mathrm{v}) := \Delta t \mathbf{W}\mathcal{L}(\mathbf{v})}$

- Stabilization terms:

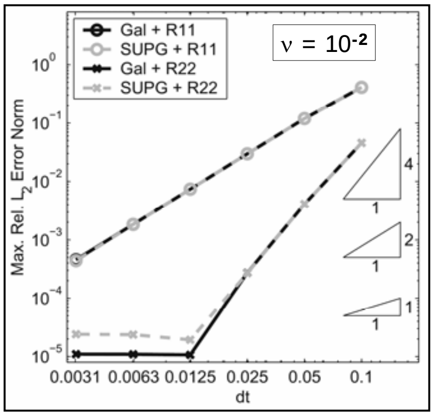
$$\boxed{\underbrace{\tau\,(\mathbf{a}\cdot\nabla v, \mathbf{a}\cdot\nabla u)_{\Omega_e}}_{\text{extra diffusion}} + \underbrace{\tau\,(\mathbf{a}\cdot\nabla v, \nu\nabla^2 u)_{\Omega_e}}_{\text{high order derivatives}} + \ldots}$$

  – With linear FE, terms with high order derivatives are neglected or under-represented.

  – The lack of consistency leads to errors of order $\boxed{\mathcal{O}(\tau)}$

  – In order to preserve the convergence rates:
    - ✓$\boxed{\tau}$ must be defined such that it behaves as $\boxed{\mathcal{O}(\Delta t^{2\mathrm{n_{stg}}})}$
    - ✓Second derivatives can be approximated (iterative computation), Jansen et al. *CMAME* 174 (1999).

Consistent stabilization: is it crucial?



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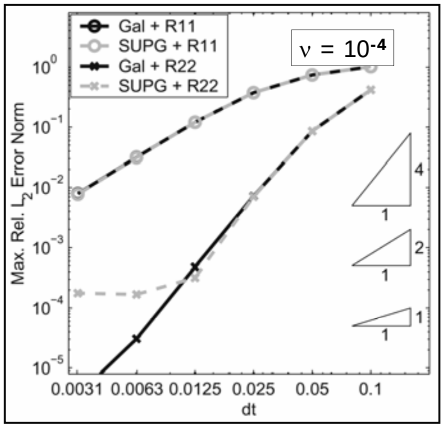
Consistent stabilization: is it crucial?



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Modeling: dimensionless analysis (1)

- General equations

$$\boxed{\begin{aligned}
\frac{\partial \mathrm{c}'}{\partial \mathrm{t}'} &= \boldsymbol{\nabla}'\cdot\left(\frac{1}{P_\mathrm{e}}\boldsymbol{\nabla}'\mathrm{c}'\right) - (\boldsymbol{v}'\cdot\boldsymbol{\nabla}')\mathrm{c}' - 3\left(S_\mathrm{t} + \frac{S_\mathrm{h}E_\mathrm{d}\mathrm{r}_{\varepsilon_\mathrm{p}}}{n\bar{\mathrm{q}}'}\sqrt[n]{\frac{\bar{\mathrm{q}}'}{A'}}\right)(\mathrm{c}' - \mathrm{L}'(\mathrm{q}'_\mathrm{R}))\\
\frac{\partial \bar{\mathrm{q}}'}{\partial \mathrm{t}'} &= 3S_\mathrm{h}E_\mathrm{d}(\mathrm{c}' - \mathrm{L}'(\mathrm{q}'_\mathrm{R}))\\
\frac{\partial \mathrm{q}'_\mathrm{R}}{\partial \mathrm{t}'} &= 10S_\mathrm{h}E_\mathrm{d}(\mathrm{c}' - \mathrm{L}'(\mathrm{q}'_\mathrm{R})) + 35E_\mathrm{d}(\bar{\mathrm{q}}' - \mathrm{q}'_\mathrm{R})
\end{aligned}}$$

- Dimensionless variables

$\boxed{P_\mathrm{e} = \frac{VL}{D}}$ $\boxed{S_\mathrm{t} = \frac{k_\mathrm{f}L(1-\varepsilon_\mathrm{e})}{VR\varepsilon_\mathrm{e}}}$ $\boxed{E_\mathrm{d} = \frac{LD_\mathrm{s}}{VR^2}}$ $\boxed{S_\mathrm{h} = \frac{Rk_\mathrm{f}c_\mathrm{ref}}{D_\mathrm{s}\rho_\mathrm{s}(1-\varepsilon_\mathrm{p})q_\mathrm{ref}}}$

$\boxed{\mathrm{r}_{\varepsilon_\mathrm{p}} = \frac{(1-\varepsilon_\mathrm{e})\varepsilon_\mathrm{p}}{\varepsilon_\mathrm{e}}}$ $\boxed{A' = A\frac{c_\mathrm{ref}^n}{q_\mathrm{ref}}}$

$$\boxed{\begin{aligned}\bar{\mathrm{c}}'_\mathrm{p} &= \mathrm{L}'(\bar{\mathrm{q}}') = \sqrt[n]{\frac{\bar{\mathrm{q}}'}{A'}}\\ \bar{\mathrm{q}}' &= \mathrm{L}'^{-1}(\bar{\mathrm{c}}'_\mathrm{p}) = A'(\bar{\mathrm{c}}'_\mathrm{p})^n\end{aligned}}$$

Modeling: dimensionless analysis (2)

- Compute dimensionless parameters and neglect terms **<<** 1.
- Assume simplifying hypothesis for isotherm: fast intraparticle diffusion

$$\boxed{\left\{\begin{array}{l}\boxed{q' = \bar{\mathrm{q}}' = \mathrm{q}'_{\mathrm{R}}}\\ \boxed{\bar{\mathrm{c}}'_{\mathrm{P}} = \mathrm{c}'}\end{array}\right. \text{then } \bar{\mathrm{q}}' = \mathrm{L}'^{\text{-}1}(\mathrm{c}')}$$

LOADING!

- Solve:

$$\boxed{\left(1 + \mathrm{r}_{\varepsilon_{\mathrm{P}}} + \frac{S_{\mathrm{t}}}{S_{\mathrm{h}}E_{\mathrm{d}}}\frac{\partial \mathrm{L}'^{\text{-}1}(\mathrm{c}')}{\partial \mathrm{c}'}\right)\frac{\partial \mathrm{c}'}{\partial \mathrm{t}'} = \boldsymbol{\nabla}' \cdot \left(\frac{1}{P_{\mathrm{e}}}\boldsymbol{\nabla}'\mathrm{c}'\right) - (\boldsymbol{v}' \cdot \boldsymbol{\nabla}')\mathrm{c}'}$$

- or

$$\boxed{\frac{\partial u}{\partial t} + \boldsymbol{a}(u) \cdot \boldsymbol{\nabla} u - \boldsymbol{\nabla} \cdot \big(\nu(u)\boldsymbol{\nabla} u\big) = 0} \quad \text{with} \quad \boxed{\begin{array}{l}\nu(u) \ll 1\\ \boldsymbol{a}(u) \propto u\boldsymbol{v}\end{array}}$$

Modeling: dimensionless analysis (3)

- Loading induces Burgers' equation!

$$\boxed{u_t + uu_x - \epsilon u_{xx} = 0}$$

- Recall behavior of inviscid Burgers' $\boxed{u_t + uu_x = 0}$

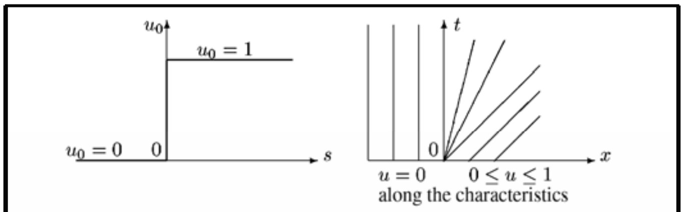
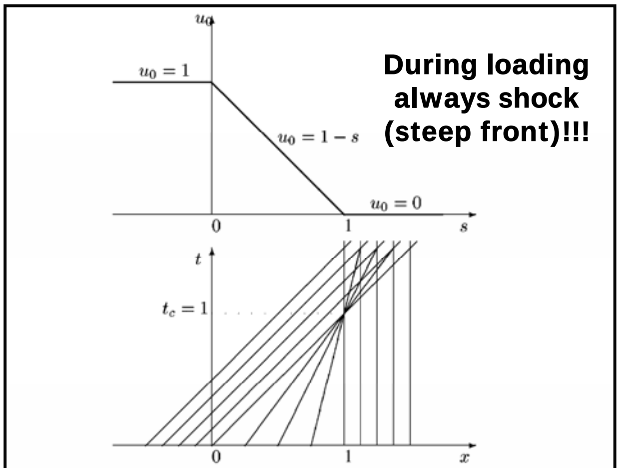


Fig. 4.2 Increasing discontinuous initial data produce a continuous solution to Burgers' equation.

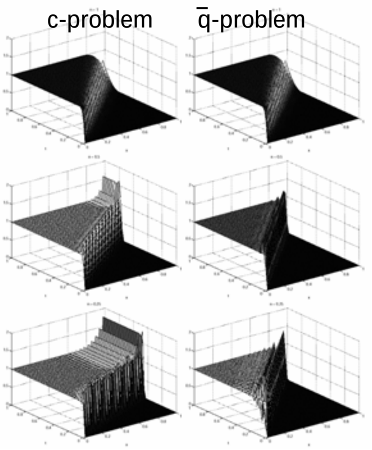


During loading always shock (steep front)!!!

Fig. 4.3 With decreasing initial data the characteristics $x = s + u_0(s)\,t$ intersect causing the solution to become discontinuous.

Modeling: dimensionless analysis (4)

- Moreover, as in other nonli choice of the right conserva
- For usual isotherms the **q̄**-p



c-problem q̄-problem