Thermodynamique et Grandes Déformations

ou 30 ans après ...

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Le programme !

1. Thermodynamique et milieux continus
   - Thermostatique
   - Systémes dissipatifs
   - milieux continus
2. Applications
   - Elasticité isotrope
   - Elasticité anisotrope
   - Elasto-Plasticité.
3. En guise de conclusion ...
   - Hors-sujets
   - Un défi

Conservatif - Réversible

Premier principe : $dU = đW + đQ$

Second principe : $dS = đQ/T$

travail élémentaire : $đW = IdC$
$(-pdV)$

variables d'état	
extensives	intensives
U, C, S	T, I

$$dU = IdC + TdS$$

$\rightarrow$ potentiel thermodynamique $U(C, S)$

$$I = \left(\frac{\partial U}{\partial C}\right)_S \qquad T = \left(\frac{\partial U}{\partial S}\right)_C$$

Potentiels thrmodynamiques

énergie interne $U(C,S)$ $\quad dU = IdC + TdS$

Transformation de Legendre

$H = U - CI$: enthalpie $\quad dH = -CdI + TdS$

$$H = H(I,S) \qquad C = -\left(\frac{\partial H}{\partial I}\right)_S \qquad T = \left(\frac{\partial H}{\partial S}\right)_I$$

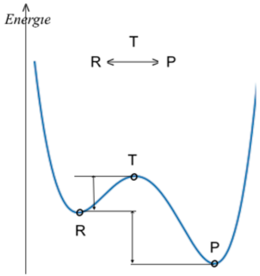
$$\boxed{\begin{array}{c} U, C, S, H, F, G \\ T, I \end{array}}$$

et de même

$F = U - TS = F(C,T)$ énergie libre (Helmholtz)

$G = U - CI - TS = G(I,T)$ enthalpie libre (Gibbs)

zoom : Thermochimie



constante d'équilibre

$$K = \frac{[P]}{[R]} = \exp(\Delta^{RP} G^{\ominus}/RT)$$

vitesse de réaction (Evans-Polanyi)

$$k = d[P]/dt = Cte \; x \exp(\Delta^{RT} G^{\ominus}/RT)$$

où $G^{\ominus}$ est l'**enthalpie libre molaire**

cf *N.Hopper, F.Sidoroff, J.Cayer-Barrioz, D.Mazuyer· W.T.Tysoe : A Molecular-Scale Analysis of Pressure-Dependent Sliding Shear Stresses, Tribology Letters (2023) 71 :121*

En fait $U = U(C, S, n)$ $\quad dU = I\, dC + TdS + \mu dn$ $\quad$ μ : potentiel chimique

$$\mu = \left(\frac{\partial U}{\partial n}\right)_{S,V} = ... = \left(\frac{\partial G}{\partial n}\right)_{T,p} = G/n = G^{\ominus}$$

car $G(p, T, \lambda n) = \lambda G(p, T, n)$

quid des mélanges ? (mélange idéal ?)

$$\boxed{\begin{array}{c} U, C, S, H, F, G, n \\ T, I, \mu \end{array}}$$

Dissipation - Kelvin

Second principe : $dS \geq \text{đ}Q/T \qquad d^{(i)}S = dS - \text{đ}Q/T \geq 0$

dissipation (taux de production interne d'entropie)

$\Phi dt = Td^{(i)}S = TdS - \text{đ}Q = -dU + IdC + TdS \geq 0$

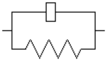
si $U = U(C, S)$

$\Phi = (I - \partial U/\partial C)\dot{C} + \cancel{(T - \partial U/\partial S)}\dot{S}$

$T = \partial U/\partial S \qquad \Phi = I^{(v)}\dot{C}$ dissipation visqueuse (Kelvin-Voigt)

TPI : $\quad I^{(v)} = \partial\Omega/\partial\dot{C} \quad$ ou $\quad \in \partial\Omega(\dot{C})$

$I = I^{(e)} + I^{(v)} = \frac{\partial U}{\partial C} + \frac{\partial \Omega}{\partial \dot{C}}$



Thermodynamique des Processus Irreversibles

dissipation $\Phi = X.x$

X forces thermodynamiques
x flux thermdynamiques (souvent $\dot{x}$)

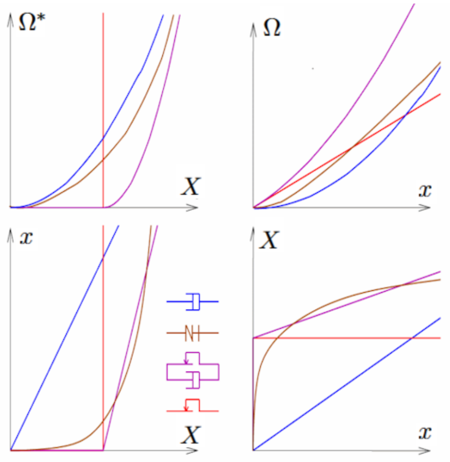
TPI : relation $X \longleftrightarrow x$

relations d'Onsager

$$X_i = L_{ij} x_j \quad L_{ij} = L_{ji}$$

se généralise en $X \in \partial\Omega(x) \quad x \in \partial\Omega^*(X)$

(pseudo)-potentiels de dissipation
(convexes conjuqués)
$\partial\Omega(x)$ et $\partial\Omega^*(X)$ sous-différentiels



Anélasticité - Maxwell

Variables internes   Forces thermodynamiques associées

$$U = U(C, \alpha, S) \qquad A = -\partial U / \partial \alpha$$

$$\Phi = (I - \partial U/\partial C)\dot{C} + A\dot{\alpha} + \cancel{(T - \partial U/\partial S)}\dot{S}$$

$$X = (I^{(v)}, A) \qquad x = (\dot{C}, \dot{\alpha})$$

$$I = \frac{\partial U}{\partial C} + \frac{\partial \Omega}{\partial \dot{C}} \qquad 0 = \frac{\partial U}{\partial \alpha} + \frac{\partial \Omega}{\partial \dot{\alpha}}$$

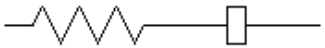
(relaxation)

Anélasticité de Maxwell

$$C = C^e + C^p \qquad U(C^e, S)$$

$$\Phi = (I - \cancel{\partial U/\partial C^e})\dot{C}^e + I\dot{C}^p + (T - \partial U/\partial S)\dot{S}$$

$$I = \partial U/\partial C^e = \partial \Omega/\partial \dot{C}^p$$



Etat local

état local

$$U = \iiint_D \rho\, e\, dv = \iiint_{D_o} \rho_o\, e\, dv_o$$

$$S = \iiint_D \rho \eta\, dv = \iiint_{D_o} \rho_o\, \eta\, dv_o \qquad \text{etc...}$$

ext : U, C, S, H, F, G
exi : e, c, η, h, ψ, g
int : T, I

puissance des efforts intérieurs

$$đW = -\iiint T_{ij}\, D_{ij}\, dv = -\iiint \varpi^{int}\, dv = -\iiint \varpi_o^{int}\, dv_o$$

$$\varpi_o^{int} = J\, \varpi^{int} = J\, \boldsymbol{T} : \boldsymbol{D} = \boldsymbol{\tau} : \boldsymbol{D}$$

inégalité de Clausius-Duhem

$$\phi = -\rho\,(\dot{e} - \theta\,\dot{\eta}) + \boldsymbol{T} : \boldsymbol{D} - \frac{\boldsymbol{q} \cdot grad\,\theta}{\theta} \geq 0$$

<Contraintes,Déformations>

Systéme homogène $\quad đW = V_0\, J\, \boldsymbol{T} : \boldsymbol{D} dt = C.dI \quad ???$

— en HPP : $đW = V_0 \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} dt = V_0\, \boldsymbol{\sigma} : \boldsymbol{d\epsilon}$

— fluide $\boldsymbol{T} = -p\,\mathbf{1} \quad đW = -V_0\, p\, J\, tr\boldsymbol{D} dt = -V_0\, p\, dJ = -pdV$

on écrira $đW = C\, dI = V_0\, \Sigma\, .\, d\mathcal{E}$

$>$ comment choisir le couple $\Sigma\,,\, \mathcal{E}$ satisfaisant

$J\, \boldsymbol{T} : \boldsymbol{D}\, dt = \Sigma\, .\, d\mathcal{E}$
$\Sigma(\mathcal{E})$ inversible en $\mathcal{E}(\Sigma)$
ayant (si possible) un sens physique ... pas si simple !!

$$\varpi_o^{int} = J\, \varpi^{int} = J\, T : D = \tau : D = \Pi : \dot{F} = S : \dot{E}$$

$T\,,\,?\; = \tau\,,\,?$ NON

$\Pi\,,\,F$ NON inversible

$S\,,\,E$ oui, mais PK2

etc .... (Seth-Hill,...)

Un exemple

Loi de Hooke-Seth-Hill

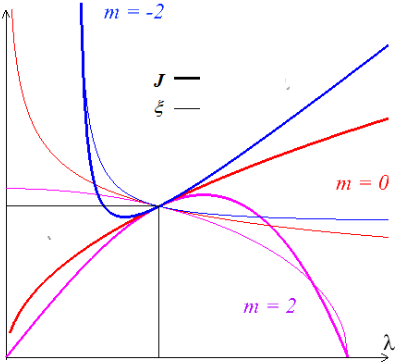
$$E^{(m)} = \frac{1+\nu}{E}\Sigma^{(m)} - \frac{\nu}{E}\left(tr\,\Sigma^{(m)}\right)1$$

$$E^{(m)} = \frac{1}{m}\left(U^m - 1\right) \qquad H = E^{(o)} = \frac{1}{2}\ln C$$

$$\varpi_o^{int} = \Sigma^{(m)} : \dot{E}^{(m)} \qquad \left(S = \Sigma^{(2)}\right)$$

Traction simple

$$F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \xi & 0 \\ 0 & 0 & \xi \end{bmatrix} \qquad T = \begin{bmatrix} \sigma & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



Conclusion: Construire une loi hyperélastique GD "raisonnable" : Pas si simple.....

Quelles conditions imposer à l'énergie élastique ? ("the main unsolved^problem ....")

Dilatation-Distorsion

$$w(\boldsymbol{C}) = w(\boldsymbol{B}) = w(B_I, B_{II}, B_{III}) = w(\lambda_1, \lambda_2, \lambda_3) \qquad \boldsymbol{T} = \frac{2}{J}\,\boldsymbol{B}\,\frac{\partial w}{\partial \boldsymbol{B}}$$

Polyconvexité (J.Ball)

$w(\lambda_1, \lambda_2, \lambda_3)$ fonction convexe de $(\lambda_1, \lambda_2, \lambda_3, \lambda_1\lambda_2, \lambda_2\lambda_3, \lambda_3\lambda_1, \lambda_1\lambda_2\lambda_3)$

ou bien séparer dilatation-distorsion $\boldsymbol{B} = \underbrace{J^{2/3}}_{\text{dilatation}}\underbrace{\overline{\boldsymbol{B}}}_{\text{distorsion}}$ $\quad (\det \overline{\boldsymbol{B}} = 1)$

fluide parfait

$$\boldsymbol{T} = -p(J)\,\mathbf{1}$$

$$p = -\frac{\partial w}{\partial J}$$

$$\boldsymbol{T} = \frac{\partial w}{\partial J}\,\mathbf{1} + \frac{2}{J}\left(\overline{\boldsymbol{B}}\,\frac{\partial w}{\partial \overline{\boldsymbol{B}}}\right)^D$$

$$w = w_s(J) + w_d(\overline{\boldsymbol{B}})$$

incompressible

$$\boldsymbol{T} = -p\,\mathbf{1} + 2\,\boldsymbol{B}\,\frac{\partial w}{\partial \boldsymbol{B}}$$

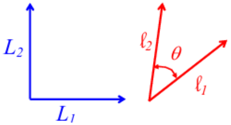
classique

Tissus

Tissu symètrique

$$\lambda_i = \ell_i / L_i$$

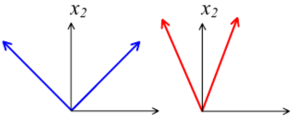
$$\zeta = \cos\theta$$



$$w = \frac{1}{2} k\left[(\lambda_1 - 1)^2 + (\lambda_2 - 1)^2\right] + w_c(\zeta)$$

en biais

$$\lambda_1 = \lambda_2 = \lambda$$



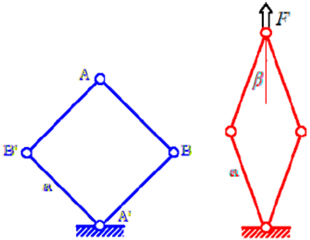
$$\boldsymbol{F} = \begin{bmatrix} f_1 & 0 \\ 0 & f_2 \end{bmatrix} \qquad \boldsymbol{\Pi} = \begin{bmatrix} \pi_1 & 0 \\ 0 & \pi_2 \end{bmatrix}$$

$$f_1 = \lambda\sqrt{1-\zeta} \qquad f_2 = \lambda\sqrt{1+\zeta}$$

$$\pi_1 = \frac{f_1}{\lambda}\left[\frac{1}{2}\frac{\partial w}{\partial \lambda} - \frac{1+\zeta}{\lambda}\frac{\partial w}{\partial \zeta}\right] \qquad \pi_2 = \frac{f_2}{\lambda}\left[\frac{1}{2}\frac{\partial w}{\partial \lambda} + \frac{1-\zeta}{\lambda}\frac{\partial w}{\partial \zeta}\right]$$

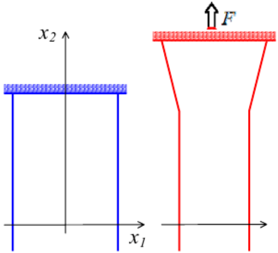
Deux essais

Cisaillement sur cadre



$$F = 2a\cos\beta \; \frac{\partial w}{\partial \zeta}$$

Traction sur biais



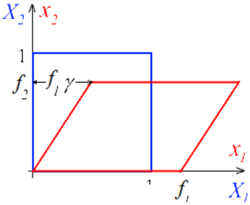
$$\lambda = 1 + \frac{\tau(\zeta)(1+\zeta)}{k}$$

$$\pi_2 = \frac{F}{b_o} = \frac{2\,f_2}{\lambda^2}\,\frac{\partial w_c}{\partial \zeta}$$

Extension-Cisaillement

Extension-Cisaillement

$$x_1 = f_1 X_1 + f_1 \gamma X_2$$
$$x_2 = f_2 X_2 \qquad J = f_1 f_2$$
$$\boldsymbol{F} = \begin{bmatrix} f_1 & f_1\gamma \\ 0 & f_2 \end{bmatrix} \qquad \boldsymbol{T} = \begin{bmatrix} \sigma_1 & \tau \\ 0 & \sigma_2 \end{bmatrix}$$



$$J\,\boldsymbol{T} : d\boldsymbol{F}\,\boldsymbol{F}^{-1} = f_2\, \sigma_1\, df_1 + f_1\, \sigma_2\, df_2 + f_1^2\, \tau\, d\gamma$$

$$\boxed{\Sigma = (f_2\, \sigma_1\ ,\ f_1\, \sigma_2\ ,\ f_1^2\, \tau) \qquad \mathcal{E} = (f_1\ , f_2\ , \gamma)}$$

$$\sigma_1 = \rho_o f_2^{-1}\, \partial u / \partial f_1 = \mathcal{T}_1 (f_1, f_2, \gamma)$$
$$\sigma_2 = \rho_o f_1^{-1}\, \partial u / \partial f_2 = \mathcal{T}_2 (f_1, f_2, \gamma)$$
$$\tau = \rho_o f_1^{-2}\, \partial u / \partial \gamma = \mathcal{T}_3 (f_1, f_2, \gamma)$$

Tribologie
(plan invariant)

$$x_1 = X_1, \quad x_2 = X_2$$
$$x_3 = \gamma_1 X_1 + \gamma_2 X_2 + f_3 X_3$$
$$\boldsymbol{F} = \begin{pmatrix} 1 & 0 & \gamma_1 \\ 0 & 1 & \gamma_2 \\ 0 & 0 & f_3 \end{pmatrix}$$
$$\boldsymbol{T} = \begin{pmatrix} \sigma_1 & \tau_{12} & \tau_{13} \\ \tau_{12} & \sigma_2 & \tau_{23} \\ \tau_{13} & \tau_{23} & \sigma_3 \end{pmatrix}.$$
$$\tau_{13} d\gamma_1 + \tau_{23} d\gamma_2 + \sigma_3 df_3$$

$$\boxed{\begin{aligned} \Sigma &= (\sigma_3, \tau_{13}, \tau_{23}) \\ \mathcal{E} &= (f_3, \gamma_1, \gamma_2) \end{aligned}}$$

Description directionnelle

Loi de comportement (élastique par exemple) $\boldsymbol{T} = \mathcal{T}(\boldsymbol{F})$.

Objectivité $\mathcal{T}(\boldsymbol{QF}) = \boldsymbol{Q}\,\mathcal{T}(\boldsymbol{F})\,\boldsymbol{Q}^T$

usuellement : $\boldsymbol{Q} = \boldsymbol{R}^T$ conduit à $\boldsymbol{S} = \mathcal{S}(\boldsymbol{E})$

maintenant $\boldsymbol{Q} = \boldsymbol{R}_1{}^T$

$$\boldsymbol{F} = \boldsymbol{R}_1\,\boldsymbol{F}_1 = \begin{bmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{bmatrix} \begin{bmatrix} f_1 & f_1\gamma \\ 0 & f_2 \end{bmatrix}$$

$$\theta_1 = angle\ (\boldsymbol{e}_1 = \boldsymbol{F}\boldsymbol{E}_1,\ \boldsymbol{E}_1) = Arctan\ (F_{21}/F_{11})$$

$$\boldsymbol{T} = \mathcal{T}(\boldsymbol{F}) = \boldsymbol{R}_1\,\mathcal{T}(\boldsymbol{F}_1)\,\boldsymbol{R}_1{}^T$$

$$= \begin{bmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{bmatrix} \begin{bmatrix} \sigma_1^{(1)} & \tau^{(1)} \\ \tau^{(1)} & \sigma_2^{(1)} \end{bmatrix} \begin{bmatrix} \cos\theta_1 & \sin\theta_1 \\ -\sin\theta_1 & \cos\theta_1 \end{bmatrix}$$

$$\sigma_1{}^{(1)} = \mathcal{T}_1(f_1, f_2, \gamma) \qquad \sigma_2{}^{(1)} = \mathcal{T}_2(f_1, f_2, \gamma) \qquad \tau^{(1)} = \mathcal{T}_3(f_1, f_2, \gamma)$$

ViscoPlasticité

$$\phi = \mathbf{S} : \dot{\mathbf{E}} - \dot{\mathbf{w}}$$

Kelvin $\quad w = w(\mathbf{E})$

$$\phi = (\mathbf{S} - \partial \mathbf{w}/\partial \mathbf{E}) : \dot{\mathbf{E}}$$

$$\mathbf{S} = \partial \mathbf{w}/\partial \mathbf{E} + \partial \Omega(\mathbf{E}; \dot{\mathbf{E}})/\partial \dot{\mathbf{E}}$$

Maxwell $\quad w = w(\mathbf{E^e})$

$$\mathbf{E} = \mathbf{E^e} + \mathbf{E^p}$$

$$\phi = (\mathbf{S} - \cancel{\partial \mathbf{w}/\partial \mathbf{E^e}}) : \dot{\mathbf{E}}^{\mathbf{e}} + \mathbf{S} : \dot{\mathbf{E}}^{\mathbf{p}}$$

$$\mathbf{S} = \partial \mathbf{w}/\partial \mathbf{E^e} = \partial \Omega/\partial \dot{\mathbf{E}}^{\mathbf{p}}$$

Elasto-plasticité d'après Naghdi

La matière est lagrangienne,
la physique est eulérienne

Fluide incompressible

$$\phi = \boldsymbol{\sigma}^D : \boldsymbol{D} \qquad \boldsymbol{\sigma} = -p\boldsymbol{1} + \boldsymbol{\tau}(\boldsymbol{D})$$

$$\Omega(\boldsymbol{D}) = \Omega(d) \qquad d = |\boldsymbol{D}|$$

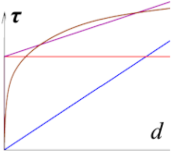
$$\boldsymbol{\tau} = \Omega'(d)\frac{\boldsymbol{D}}{d} = 2\mu(d)\boldsymbol{D}$$

fluide newtonien

fluide viscoplastique

Bingham

Norton-Hoff



fluide plastique de von Mises

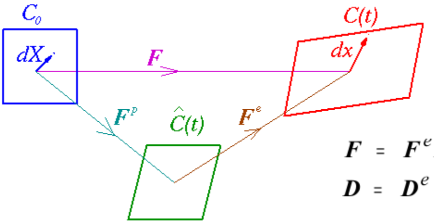
$$\boldsymbol{\tau} = \sqrt{\frac{2}{3}}\, Y_o \frac{\boldsymbol{D}}{d} \qquad |\boldsymbol{\sigma}^D| = \sqrt{\frac{2}{3}}\, Y_o$$

Elasto-Plasticité isotrope

$$u = u^e(\boldsymbol{B}^e) + \hat{u}(p)$$

$$\phi = \boldsymbol{\sigma} : \boldsymbol{D} - \rho\, \dot{u}$$

$$R = \rho \frac{d\hat{u}}{dp}$$



$$\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p$$

$$\boldsymbol{D} = \boldsymbol{D}^e + \left(\boldsymbol{F}^e \boldsymbol{L}^p \boldsymbol{F}^{e-1}\right)^S$$

$$\phi = \left(\boldsymbol{\sigma} - \cancel{2\rho \frac{\partial u^e}{\partial \boldsymbol{B}^e} \boldsymbol{B}^e}\right) : \boldsymbol{D}^e + \boldsymbol{\sigma} : \boldsymbol{F}^e \boldsymbol{L}^p \boldsymbol{F}^{e-1} - R\,\dot{p}$$

$$\downarrow \qquad\qquad \downarrow$$

$$\boldsymbol{\sigma} = 2\rho \frac{\partial u}{\partial \boldsymbol{B}^e} \boldsymbol{B}^e \longrightarrow \boldsymbol{\sigma} : \boldsymbol{R}^e \boldsymbol{D}^p \boldsymbol{R}^{eT} - R\,\dot{p}$$

dualité $(\boldsymbol{\sigma}, R) \Leftrightarrow \left(\overline{\boldsymbol{D}}^p = \boldsymbol{R}^e \boldsymbol{D}^p \boldsymbol{R}^{eT}, -\dot{p}\right)$

Trièdre Directeur

$$F = A P$$

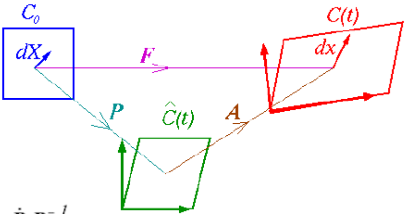
$$\Delta^e = \frac{1}{2}\left(A^T A - 1\right)$$

$$u = u^e(\Delta^e) + R(p)$$

$$\phi = \left(\cancel{\sigma - \rho A \frac{\partial u^e}{\partial \Delta^e} A^T}\right) : \dot{A} A^{-1} + A^T \sigma A^{-T} : \dot{P} P^{-1}$$

$$\Downarrow$$

$$\sigma = \rho A \frac{\partial u^e}{\partial \Delta^e} A^T$$



dualité $\Sigma = A^T \sigma A^{-T} \Leftrightarrow \dot{P} P^{-1} = D^p + W^p$

$\uparrow$

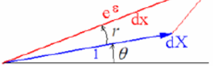
spin plastique

référentiel tournant (Zaremba-Jaumann, Naghdi, ...)
théorèmes de représentation
la Physique (monocristal)

Cercloïde de Mohr

$$\varepsilon(\boldsymbol{n}) = \ln(d\boldsymbol{x}/d\boldsymbol{X})$$

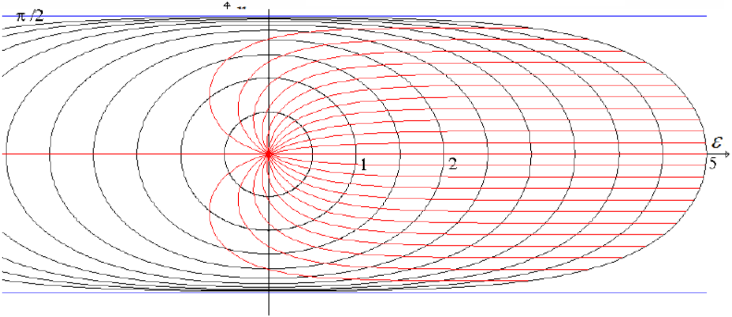
$$r(\boldsymbol{n}) = (d\boldsymbol{x}, d\boldsymbol{X})$$



$$\boldsymbol{F} = \boldsymbol{RU} = rot(\psi)\, rot(\theta_1) \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} rot(-\theta_1)$$

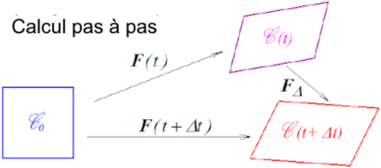
$$\lambda_1 = e^{a+d} \qquad \lambda_2 = e^{a-d}$$

$$\boxed{r = \psi \pm Arc\cos \frac{\cosh(\varepsilon - a)}{\cosh(d)}}$$



Chemins d'interpolation

Calcul pas à pas



Loi incrémentale
(intégrateur comportemental)

$$T(t+\Delta t) = t\left(T(t), F(t), \alpha(t) ; F(t+\Delta t)\right)$$

1/ un <u>chemin d'interpolation</u> $f(s)$

$$F(t+s\Delta t) = f(s)\, F(t)$$

$$f(0) = 1 \qquad f(1) = F_\Delta$$

2/ un algorithme d'intégration

<u>*chemin linéaire*</u> $\quad f(s) = (1-s)\,1 + s\,F_\Delta$

(ne reconnaît pas la rotation
pas l'incompressibilité)

<u>*chemin exponentiel*</u> $\quad f(s) = exp(s\,h_\Delta) \qquad h_\Delta = ln\, F_\Delta$

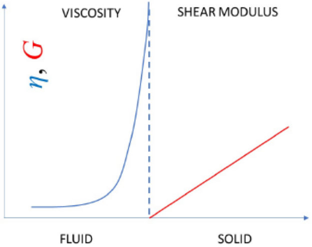
<u>*chemin géodésique*</u> $\quad f(s) = exp(s\Omega_\Delta)\, exp(sD_\Delta) \qquad \Omega_\Delta = ln\, R_\Delta \quad D_\Delta = ln\, U_\Delta$

Transition Vitreuse

Complete mathematical theory of the jamming transition

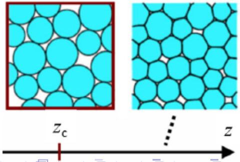
Alessio Zaccone

`https://arxiv.org/abs/2410.21439v1`



z average coordination number

Défi : modéle thermomécanique minimal ?



- quelle viscoélasticité ?
- Pression comme variable thermodynamique
- matériau incompressible dilatable $J = J(\theta)$
- matériau quasi-incompressible