Le Centre Francophone en Mathématique a été organisé à Bucarest pour une periode de 4 ans a partir du 1-er Janvier 2017,
par l'Agence Universitaire de la Francophonie et l'Institut de Mathématique Simion Stoilow de l'Académie Roumaine
en parteneriat avec la Faculté de Mathématique et Informatique de l'Université de Bucarest et le GDRI ECO-Math.

Ecole d'été régionale franco-roumaine en mathématiques appliquées, Sinaia, 2 - 11 Juillet 2017

Plasticité des cristaux: une description Eulérienne

Ioan R. Ionescu - *Université Paris Nord*

> Le modèle mécanique Eulerien de plasticité cristalline sera le point de départ et le but final. Pour arriver à faire une résolution numérique d'un problème simple (l'écoulement/déformation d'un cristal dans une filière) on va découvrir d'autres horizons, importants pour la culture générale d'un mathématicien, mais qui seront nos "étapes". On va passer ainsi en revue l'équation de la chaleur, l'écoulement de Stokes et l'équation de transport, qui après une formulation variationnelle seront "résolus" numériquement en utilisant les méthodes des éléments finis et de Galerkin discontinu. On va faire des nombreuses illustrations en s'appuyant sur une programmation FreeFem++ et une visualisation Paraview (ordinateurs portables fortement recommandés) . Seulement à la fin on va tout assembler pour pouvoir résoudre le problème de départ.

Retour

Introduction to continuum mechanics-II

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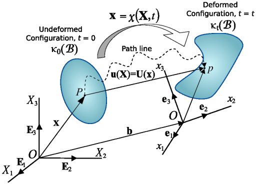
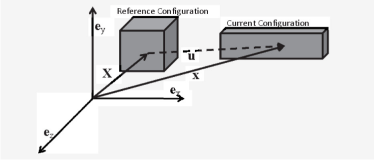
July 3, 2017

Continuum kinematics

- $\mathcal{B}_0$ undeformed/reference configuration, $\mathcal{B}_t$ deformed/actual configuration
- Motion: $\boldsymbol{x}(t, \boldsymbol{X}) = \boldsymbol{X} + \boldsymbol{u}(t, \boldsymbol{X})$ with $\boldsymbol{x}(t, \mathcal{B}_0) = \mathcal{B}_t$.
- Material/Lagrangian coordinates: $\boldsymbol{X} = (X_1, X_2, X_3) \in \mathcal{B}_0$
- Spatial/Eulerian coordinates: $\boldsymbol{x} = (x_1, x_2, x_3) \in \mathcal{B}_t$
- $\boldsymbol{u}(t, \boldsymbol{X}) = \boldsymbol{x}(t, \boldsymbol{X}) - \boldsymbol{X}$ the displacement field





Velocity-acceleration

- velocity (in Lagrange variables) $\boldsymbol{v}(t,\boldsymbol{X}) = \frac{\partial \boldsymbol{x}}{\partial t}(t,\boldsymbol{X})$
- Suppose $\boldsymbol{X} \to \boldsymbol{x}(t,\boldsymbol{X})$ one to one function, then $\exists \quad \boldsymbol{x} \to \boldsymbol{X}(t,\boldsymbol{x})$
- velocity (in Euler variables) $\boldsymbol{v}(t,\boldsymbol{x}) = \boldsymbol{v}(t,\boldsymbol{X}(t,\boldsymbol{x}))$.
- acceleration (in Lagrange variables) $\boldsymbol{a}(t,\boldsymbol{X}) = \frac{\partial^2 \boldsymbol{x}}{\partial^2 t}(t,\boldsymbol{X})$
- acceleration (in Euler variables) $\boldsymbol{a}(t,\boldsymbol{x}) = \boldsymbol{a}(t,\boldsymbol{X}(t,\boldsymbol{x}))$.

Example. Dilatation:

$x_1 = X_1 + \alpha_1 t X_1, \quad x_1 = X_2 + \alpha_2 t X_2, \quad x_3 = X_3 + \alpha_3 t X_3$

- velocity (in Lagrange variables) $\boldsymbol{v}(t,\boldsymbol{X}) = (\alpha_1 X_1, \alpha_2 X_2, \alpha_3 X_3)$
- velocity (in Euler variables) $\boldsymbol{v}(t,\boldsymbol{x}) = (\frac{\alpha_1}{1+\alpha_1 t} x_1, \frac{\alpha_2}{1+\alpha_2 t} x_2, \frac{\alpha_3}{1+\alpha_3 t} x_3)$.

Particular (material, total) derivative

Particular (total) derivative of field K (the particle is followed in its movement) : $K(t, \boldsymbol{X})$ in Lagrange description, $K(t, \boldsymbol{x}) = K(t, \boldsymbol{X}(t, \boldsymbol{x}))$ in Eulerian description

- if K is in Lagrange variables $\dfrac{dK}{dt}(t, \boldsymbol{X}) = \dfrac{\partial K}{\partial t}(t, \boldsymbol{X})$
- if K is in Euler variables $\dfrac{dK}{dt}(t, \boldsymbol{x}) = \dfrac{\partial K}{\partial t}(t, \boldsymbol{x}) + \boldsymbol{v}(t, \boldsymbol{x}) \cdot \nabla_{\boldsymbol{x}} K(t, \boldsymbol{x})$

Examples

- $K = \boldsymbol{x}$: $\quad \dfrac{d\boldsymbol{x}}{dt}(t, \boldsymbol{x}) = \boldsymbol{v}(t, \boldsymbol{x})$
- $K = \boldsymbol{v}(t, \boldsymbol{x})$: $\quad \dfrac{d\boldsymbol{v}}{dt}(t, \boldsymbol{x}) = \boldsymbol{a}(t, \boldsymbol{x}) = \dfrac{\partial \boldsymbol{v}}{\partial t}(t, \boldsymbol{x}) + \boldsymbol{v}(t, \boldsymbol{x}) \cdot \nabla_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x})$

Reynolds's transport theorem

Particular (material, total) derivative of a volume integral
Let $\omega_0 \subset \mathcal{B}_0$ and $\omega_t = \boldsymbol{x}(t, \omega_0) \subset \mathcal{B}_t$ (the subset $\omega_0 \subset \mathcal{B}_0$ is followed in its movement) and $K(t, \boldsymbol{x})$ a field in Eulerian description

$$\frac{d}{dt}\int_{\omega_t} K(t,\boldsymbol{x})\, d\boldsymbol{x} = \int_{\omega_t} \left(\frac{\partial K}{\partial t}(t,\boldsymbol{x}) + div_{\boldsymbol{x}}(K(t,\boldsymbol{x})\boldsymbol{v}(t,\boldsymbol{x})) \right)\, d\boldsymbol{x}$$

$$= \int_{\omega_t} \frac{dK}{dt}(t,\boldsymbol{x}) + K(t,\boldsymbol{x}) div_{\boldsymbol{x}} \boldsymbol{v}(t,\boldsymbol{x})\, d\boldsymbol{x} = \int_{\omega_t} \frac{\partial K}{\partial t}(t,\boldsymbol{x}) + \int_{\partial\omega_t} K(t,\boldsymbol{x})\boldsymbol{v}(t,\boldsymbol{x})\cdot\boldsymbol{n}\, d$$

Examples

- $K \equiv 1$: $\quad \frac{d}{dt} Vol(\omega_t) = \int_{\omega_t} div_{\boldsymbol{x}} \boldsymbol{v}(t,\boldsymbol{x})\, d\boldsymbol{x} = \int_{\partial\omega_t} \boldsymbol{v}(t,\boldsymbol{x}) \cdot \boldsymbol{n}\, dS$
- if $div_{\boldsymbol{x}} \boldsymbol{v}(t,\boldsymbol{x}) = 0$ then the volume is incompressible

Deformation of a continuous body

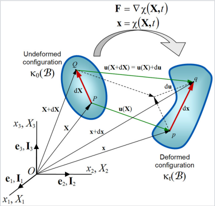


Figure 2. Deformation of a continuum body.

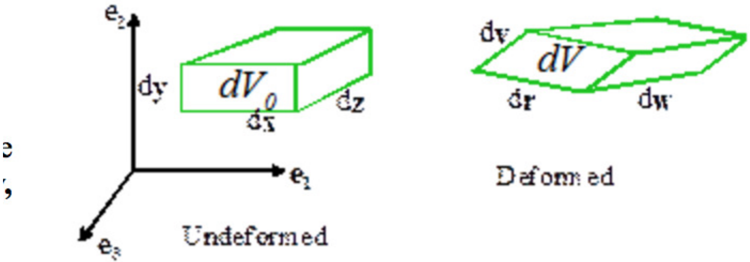
- infinitesimal element of a continuous body $d\boldsymbol{X} = (dX_1, dX_2, dX_3)$
- It is possible to show that (using Taylor expansion around a point of deformation)

$$d\boldsymbol{x} = \boldsymbol{F}(t, \boldsymbol{X})d\boldsymbol{X} = (\boldsymbol{I} + \nabla \boldsymbol{u}(t, \boldsymbol{x}))d\boldsymbol{X}$$

- $dx_i = F_{ik}dX_k = (\delta_{ik} + \dfrac{\partial u_i}{\partial X_k})dX_k$

Volume change

- Consider a differential material volume dV at some material point that goes to dv after deformation
- How to measure the volume change ?
- Reference volume: $dV_0 = d\mathbf{Z} \cdot (d\mathbf{X} \times d\mathbf{Y})$
- Deformed volume: $dv = d\mathbf{W} \cdot (d\mathbf{R} \times d\mathbf{V})$
- $J(t, \boldsymbol{X}) = det(\boldsymbol{F}(t, \boldsymbol{X}))$ Jacobien of the trasformation
- It is easy to show that the volume change: $dv = JdV$



Polar decomposition theorem

- A rotation matrix: $\boldsymbol{R}$ such that $\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{R}^T\boldsymbol{R}$=**I** ($det\boldsymbol{R} = I$).
- Polar decomposition theorem: For any matrix **F** with $det\mathbf{F} > \mathbf{0}$, there exists an unique rotation $\boldsymbol{R}$ and an unique positive-definite symmetric matrix $\boldsymbol{U}$ such that

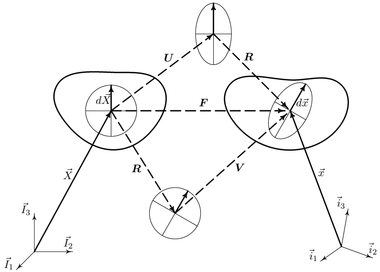
$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U}$$

- how to calculate it ? Calculate the Cauhy-Green strain tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$ and then $\boldsymbol{U} = \sqrt{\boldsymbol{C}}$, i.e. Find the eigenvalues $\{\gamma_1, \gamma_2, \gamma_3\}$ and eigenvectors $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3\}$ of $\boldsymbol{C}$ calculate $\mu_i = \sqrt{\gamma_i}$ and then $\boldsymbol{U}$ is the matrix with eigenvalues $\{\mu_1, \mu_2, \mu_3\}$ and the corresponding eigenvectors such that

$$\boldsymbol{U} = \mu_1\boldsymbol{u}_1 \otimes \boldsymbol{u}_1 + \mu_2\boldsymbol{u}_2 \otimes \boldsymbol{u}_2 + \mu_3\boldsymbol{u}_3 \otimes \boldsymbol{u}_3$$

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

Polar decomposition theorem



Velocity gradient

Velocity gradient tensor $\boldsymbol{L} = \boldsymbol{L}(t, \boldsymbol{x}) = \nabla_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x}), \quad L_{ij} = \frac{\partial v_i}{\partial x_j}$

$$\boldsymbol{L} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} = (\frac{d}{dt}\boldsymbol{F})\boldsymbol{F}^{-1}$$

$$\boldsymbol{L} = \dot{\boldsymbol{R}}\boldsymbol{R}^T + \boldsymbol{R}\dot{\boldsymbol{U}}\boldsymbol{U}^{-1}\boldsymbol{R}^T$$

Strain rate (stretching, rate of deformation) tensor $\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{v})$

$$\boldsymbol{D} = \boldsymbol{D}(t, \boldsymbol{x}) = \frac{1}{2}(\nabla_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x}) + \nabla_{\boldsymbol{x}}^T \boldsymbol{v}(t, \boldsymbol{x})), \quad D_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$$

Spin tensor $\boldsymbol{W} = \boldsymbol{W}(\boldsymbol{v})$

$$\boldsymbol{W} = \boldsymbol{W}(t, \boldsymbol{x}) = \frac{1}{2}(\nabla_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x}) - \nabla_{\boldsymbol{x}}^T \boldsymbol{v}(t, \boldsymbol{x})), \quad W_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i})$$

$$\boldsymbol{L} = \boldsymbol{D} + \boldsymbol{W}, \quad \boldsymbol{D}^T = \boldsymbol{D}, \quad \boldsymbol{W}^T = -\boldsymbol{W}$$

$$\boldsymbol{\omega}(t, \boldsymbol{x}) = curl_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x}), \quad \boldsymbol{W}\boldsymbol{c} = \frac{1}{2}\boldsymbol{\omega} \times \boldsymbol{c}, \quad \forall \boldsymbol{c}$$

Rate of Change of Length and Orientation.

$$d\boldsymbol{x} = \boldsymbol{F} d\boldsymbol{X}, \boldsymbol{L} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} \Longrightarrow \frac{d}{dt}(d\boldsymbol{x}) = \boldsymbol{L} d\boldsymbol{x}$$

Orientation and length of the infinitesimal vectors

$$d\boldsymbol{x} = \boldsymbol{n} ds, d\boldsymbol{x}^1 = \boldsymbol{n}^1 ds^1, d\boldsymbol{x}^2 = \boldsymbol{n}^2 ds^2$$

Rate of change of orientation $\frac{d}{dt}(\boldsymbol{n}) = \boldsymbol{L}\boldsymbol{n} - (\boldsymbol{D}\boldsymbol{n} \cdot \boldsymbol{n})\boldsymbol{n}$

$$\frac{d}{dt}(d\boldsymbol{x}^1 \cdot d\boldsymbol{x}^2) = 2\boldsymbol{D}\boldsymbol{x}^1 \cdot d\boldsymbol{x}^2$$

Rate of change of length

$$d\boldsymbol{x}^1 = d\boldsymbol{x}^2 = \boldsymbol{n} ds \Longrightarrow \frac{d}{dt}(\ln ds) = \frac{1}{ds}\frac{d}{dt}(ds) = \boldsymbol{D}\boldsymbol{n} \cdot \boldsymbol{n}$$

Rate of change of angles

$$\frac{d}{dt}(\boldsymbol{n}^1 \cdot \boldsymbol{n}^2) = 2\boldsymbol{D}\boldsymbol{n}^1 \cdot \boldsymbol{n}^2 - \left(\boldsymbol{D}\boldsymbol{n}^1 \cdot \boldsymbol{n}^1 + \boldsymbol{D}\boldsymbol{n}^2 \cdot \boldsymbol{n}^2\right) \boldsymbol{n}^1 \cdot \boldsymbol{n}^2$$

Mass conservation law

Let $\rho_0 : \boldsymbol{\mathcal{B}}_0 \to \mathbb{R}_+$, *and* $\rho(t, \cdot) : \boldsymbol{\mathcal{B}}_t \to \mathbb{R}_+$ be the **mass density** such that

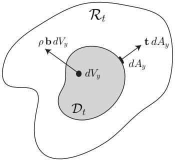
$$mass(\omega_0) = \int_{\omega_0} \rho_0(\boldsymbol{X}) \, d\boldsymbol{X}, \quad mass(\omega_t) = \int_{\omega_t} \rho(t, \boldsymbol{x}) \, d\boldsymbol{x}$$

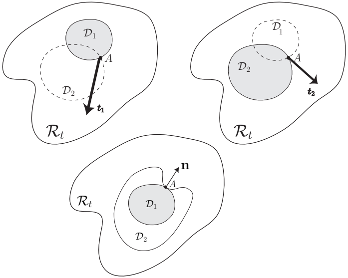
for all $\omega_0 \subset \boldsymbol{\mathcal{B}}_0$ and $\omega_t = \boldsymbol{x}(t, \omega_0) \subset \boldsymbol{\mathcal{B}}_t$.

- **Mass conservation law:** $mass(\omega_0) = mass(\omega_t)$ for all $\omega_0 \subset \boldsymbol{\mathcal{B}}_0$.
- Lagrangian description $\rho(t, \boldsymbol{x}) J(t, \boldsymbol{X}) = \rho_0(\boldsymbol{X})$ for all $\boldsymbol{X} \in \boldsymbol{\mathcal{B}}_0$
- Eulerian description $\dfrac{d}{dt}\rho(t, \boldsymbol{x}) + \rho(t, \boldsymbol{x}) div_{\boldsymbol{x}} \boldsymbol{v}(t, \boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \boldsymbol{\mathcal{B}}_t$
- Eulerian description $\dfrac{\partial}{\partial t}\rho(t, \boldsymbol{x}) + div_{\boldsymbol{x}}(\rho(t, \boldsymbol{x}) \boldsymbol{v}(t, \boldsymbol{x})) = 0$

Consequence: $\dfrac{d}{dt} \displaystyle\int_{\omega_t} \rho(t, \boldsymbol{x}) K(t, \boldsymbol{x}) \, d\boldsymbol{x} = \int_{\omega_t} \rho(t, \boldsymbol{x}) \frac{d}{dt} K(t, \boldsymbol{x}) \, d\boldsymbol{x}$

Forces acting on the body





Assumptions

- **Body forces** $\rho \boldsymbol{b} d\boldsymbol{x}$: $\boldsymbol{b} = \boldsymbol{b}(t, \boldsymbol{x})$
- **Surface forces** $\boldsymbol{t} dS$ acting on $\partial \mathcal{D}_t$: the action of $\boldsymbol{\mathcal{B}}_t \setminus \mathcal{D}_t$ on $\mathcal{D}_t$ can be replaced by the distribution of the **Cauchy stress vector** $\boldsymbol{t}$
- **Cauchy's hypothesis**: $\boldsymbol{t} = \boldsymbol{t}(t, \boldsymbol{x}, \boldsymbol{n})$

The Balance of Momentum Principles

Balance principle for linear momentum (Newton's law):

$$\frac{d}{dt}\int_{\omega_t}\rho(t,\boldsymbol{x})\boldsymbol{v}(t,\boldsymbol{x})\,d\boldsymbol{x}=\int_{\omega_t}\rho(t,\boldsymbol{x})\boldsymbol{b}(t,\boldsymbol{x})\,d\boldsymbol{x}+\int_{\partial\omega_t}\boldsymbol{t}(t,\boldsymbol{x},\boldsymbol{n})\,dS$$

Balance principle for angular momentum (Newton's law):

$$\frac{d}{dt}\int_{\omega_t}\rho(t,\boldsymbol{x})\boldsymbol{x}\wedge\boldsymbol{v}(t,\boldsymbol{x})\,d\boldsymbol{x}=\int_{\omega_t}\rho(t,\boldsymbol{x})\boldsymbol{x}\wedge\boldsymbol{b}(t,\boldsymbol{x})\,d\boldsymbol{x}+\int_{\partial\omega_t}\boldsymbol{x}\wedge\boldsymbol{t}(t,\boldsymbol{x},\boldsymbol{n})\,dS$$

for all $\omega_t\subset\boldsymbol{\mathcal{B}}_t$.

Consequences of balance principles and stress tensor

Consequences of linear momentum balance principle + Cauchy's hypothesis

- $\boldsymbol{n} \to \boldsymbol{t}(t, \boldsymbol{x}, \boldsymbol{n})$ is linear and there exists $\boldsymbol{\sigma}(t, \boldsymbol{x})$ **Cauchy stress tensor** such that

$$\boldsymbol{t}(t, \boldsymbol{x}, \boldsymbol{n}) = \boldsymbol{\sigma}(t, \boldsymbol{x})\boldsymbol{n}$$

- Equation of motion

$$\rho(t, \boldsymbol{x})\frac{d}{dt}\boldsymbol{v}(t, \boldsymbol{x}) = div_{\boldsymbol{x}}\boldsymbol{\sigma}(t, \boldsymbol{x}) + \rho(t, \boldsymbol{x})\boldsymbol{b}(t, \boldsymbol{x})$$

Consequence of angular momentum balance principle

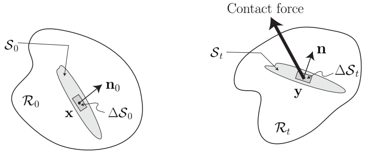
- Cauchy stress tensor is symetric

$$\boldsymbol{\sigma}^T(t, \boldsymbol{x}) = \boldsymbol{\sigma}(t, \boldsymbol{x})$$

Equation of motion in Lagrange formulation

First Piola-Kirchhoff stress tensor (non-symmetric !)

$$\boldsymbol{\Pi}(t, \boldsymbol{X}) = J(t, \boldsymbol{X})\boldsymbol{\sigma}(t, \boldsymbol{x}(t, \boldsymbol{X}))\boldsymbol{F}^{-T}(t, \boldsymbol{X})$$



Nanson's formula $\boldsymbol{n}dS = J\boldsymbol{F}^{-T}\boldsymbol{n}_0 dS_0 \Longrightarrow \boldsymbol{\sigma}(t, \boldsymbol{x})\boldsymbol{n}dS = \boldsymbol{\Pi}(t, \boldsymbol{X})\boldsymbol{n}_0 dS_0$

$$\rho_0(\boldsymbol{X})\frac{d}{dt}\boldsymbol{v}(t, \boldsymbol{X}) = div_{\boldsymbol{X}}\boldsymbol{\Pi}(t, \boldsymbol{X}) + \rho_0(\boldsymbol{X})\boldsymbol{b}(t, \boldsymbol{X})$$

Equilibrium equation $div_{\boldsymbol{X}}\boldsymbol{\Pi}(t, \boldsymbol{X}) + \rho_0(\boldsymbol{X})\boldsymbol{b}(t, \boldsymbol{X}) = 0$
Second Piola-Kirchhoff tensor (symmetric !) $\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{\Pi}$

Examples of stress tensors