A variational formulation of thermomechanical constitutive updates for hyperbolic conservation laws

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Motivations

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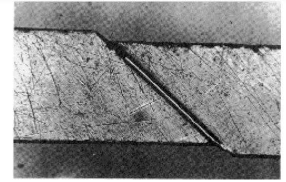
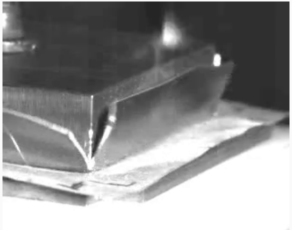
Adiabatic shear bands [1]



Electromagnetic Flanging [2]



Material dynamics / impacts [3]

[1] IM Ward. "Mechanical properties of solid polymers. 2nd Edn Wiley". In : *New York* (1983)

[2] C.T. Sow et al. "Electromagnetic flanging : from elementary geometries to aeronautical components". In : *International Journal of Material Forming* 13 (2020), p. 423-443

[3] *Hypervelocity Impact*. Juin 2013. URL : `http://www.esa.int/ESA_Multimedia/Images/2013/04/Hypervelocity_Impact`

Total Lagrangian modelling in (adiabatic) solid dynamics

Conservation laws [4, 5]

$$\frac{\partial \mathfrak{U}}{\partial t} + \boldsymbol{\nabla}_0 \cdot \mathfrak{F} = 0$$

$$\mathfrak{U} = \begin{Bmatrix} \rho_0 \mathbf{v} \\ \mathbf{F} \\ \mathcal{E} \end{Bmatrix} ; \quad \mathfrak{F} = \begin{Bmatrix} -\mathbf{P} \\ -\mathbf{v} \otimes \mathbf{1} \\ -\mathbf{P}^T \cdot \mathbf{v} \end{Bmatrix}$$

constrained with $\boldsymbol{\nabla}_0 \times \mathbf{F} = \mathbf{0}$

$\mathbf{P}$: 1st Piola-Kirchhoff, $\mathcal{E} = E + \frac{\rho_0 \mathbf{v}^2}{2}$

+Initial and boundary conditions

Rankine-Hugoniot conditions

$$S[\mathfrak{U}] = [\![\mathfrak{F}]\!] \cdot \mathbf{N}$$

Closure equations

$$\mathfrak{F} = \mathfrak{F}(\mathfrak{Q}) \text{ with } \mathfrak{Q} = \begin{Bmatrix} \mathbf{v} \\ \mathbf{P} \\ \eta \end{Bmatrix}$$

$$\mathfrak{U}(\mathfrak{Q}) \Leftrightarrow \mathbf{P}(\mathbf{F}, E(\eta, \mathbf{F}, \mathbf{Z}))$$

$\mathbf{Z}$: set of internal variables

[4] Bradley J Plohr et David H Sharp. “A conservative Eulerian formulation of the equations for elastic flow”. In : *Advances in Applied Mathematics* 9.4 (1988), p. 481 -499

[5] J.A. Trangenstein et P. Collela. “A higher-order Godunov method for modeling finite deformation in elastic-plastic solids”. In : *Communications in Pure Applied mathematics* 47 (1991), p. 41-100

Thermomechanical constitutive framework

Generalized Standard Materials (GSM) [6, 7]

- Helmholtz free energy $W(\mathbf{F}, T, \mathbf{Z})$

$$\mathbf{P}^{\text{rev}} = \frac{\partial W}{\partial \mathbf{F}}; \quad \mathbf{Y}^{\text{rev}} = \frac{\partial W}{\partial \mathbf{Z}}$$

- Dissipation pseudo-potential $\phi(\dot{\mathbf{F}}, \dot{\mathbf{Z}}; \mathbf{F}, \mathbf{Z}, T)$, convex, $\phi \geq 0$, $\phi(0) = 0$

$$\mathbf{P}^{\text{irr}} = \frac{\partial \phi}{\partial \dot{\mathbf{F}}}; \quad \mathbf{Y}^{\text{irr}} = \frac{\partial \phi}{\partial \dot{\mathbf{Z}}}$$

Additive decomposition of thermodynamic forces

$$\mathbf{P} = \mathbf{P}^{\text{rev}} + \mathbf{P}^{\text{irr}}$$
$$\mathbf{Y} = \mathbf{Y}^{\text{rev}} + \mathbf{Y}^{\text{irr}}$$

Since $\mathbf{Y} \cdot \dot{\mathbf{Z}} = 0$, $\mathbf{Y}^{\text{rev}} + \mathbf{Y}^{\text{irr}} = 0$, hence

$$\frac{\partial W}{\partial \mathbf{F}} + \frac{\partial \phi}{\partial \dot{\mathbf{F}}} = 0$$
$$\frac{\partial W}{\partial \mathbf{Z}} + \frac{\partial \phi}{\partial \dot{\mathbf{Z}}} = 0$$

Total dissipation : $\mathcal{D} = \mathbf{P}^{\text{irr}} : \dot{\mathbf{F}} + \mathbf{Y}^{\text{irr}} : \dot{\mathbf{Z}} \geq 0$

[6] Bernard Halphen et Quoc Son Nguyen. “Sur les matériaux standard généralisés”. In : *Journal de mécanique* 14 (1975), p. 39-63
[7] Hans Ziegler. *An introduction to thermomechanics, vol. 21*. 2012

Objectives

Observations

- Constitutive models for dissipative solids use $W(\mathbf{F}, T, \mathbf{Z})$ rather than $E(\mathbf{F}, \eta, \mathbf{Z})$, because T is a measurable quantity.
- Thermomechanical updates are usually driven by the temperature T plus some strain $(\mathbf{F})$ [8]

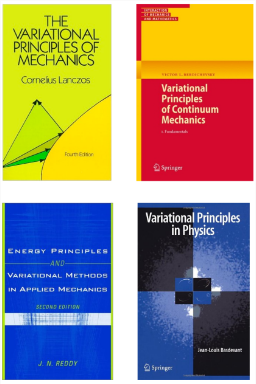
Issues

- How to design thermomechanical updates knowing only updated strain $(\mathbf{F})$ and internal energy E values (i.e. not the temperature) ?
- Especially when the deviatoric component is temperature-dependent (i.e. thermal softening).

[8] JC Simo et Ch Miehe. "Associative coupled thermoplasticity at finite strains : Formulation, numerical analysis and implementation". In : *Computer Methods in Applied Mechanics and Engineering* 98.1 (1992), p. 41-104

Variational formulation of the thermomechanical constitutive update

On the interest of a variational framework



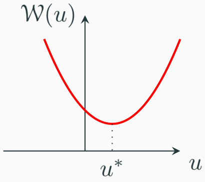
Advantages

- Mathematical
- Physical
- Numerical

Variational formulation

formulating a problem as the optimisation of a scalar functional

$$u^* = \arg\min_u \mathcal{W}(u)$$



Also applied for dissipative problems

- Diffusion problems [9]
- Thermomechanics [10]
- Variational approach to fracture [11]
- Limit analysis
- etc

[9] Jorge de Anda Salazar, Thomas Heuzé et Laurent Stainier. “Multifield variational formulations of diffusion initial boundary value problems”. In : *Continuum Mechanics and Thermodynamics* 33.2 (2021), p. 563-589
[10] Rohit Pethe, Thomas Heuzé et Laurent Stainier. “Remapping-free variational h-adaption for strongly coupled thermo-mechanical problems”. In : *Finite Elements in Analysis and Design* 176 (2020), p. 103435
[11] Blaise Bourdin, Gilles A Francfort et Jean-Jacques Marigo. “The variational approach to fracture”. In : *Journal of elasticity* 91.1-3 (2008), p. 5-148

Basic elements for the variational formulation

Following [12, 13], consider the following functional

$$D(\dot{F}, \dot{\eta}, \dot{Z}, T; \mathbf{F}, \eta, \mathbf{Z}) = \dot{E}(\mathbf{F}, \eta, \mathbf{Z}) - T\dot{\eta} + \phi(\dot{\mathbf{F}}, \dot{\mathbf{Z}}; \mathbf{F}, \mathbf{Z}, T) \equiv \dot{w}_\tau + \phi$$

with $\dot{w}_\tau = \dot{E}(\mathbf{F}, \eta, \mathbf{Z}) - T\dot{\eta} = \mathbf{P}^{\text{rev}} : \dot{\mathbf{F}} + \mathbf{Y}^{\text{rev}} : \dot{\mathbf{Z}}$ is the reversible power per unit volume received by the system.

Comments

- The values of $\dot{E}$ and $\dot{\mathbf{F}}$ are updated by conservation laws.
- Introduce Helmholtz free energy $W(\mathbf{F}, T, \mathbf{Z})$ and hence T with a Legendre transform.
- It is enforced through a Lagrange multiplier λ

[12] Qiang Yang, Laurent Stainier et Michael Ortiz. "A variational formulation of the coupled thermo-mechanical boundary-value problem for general dissipative solids". In : *Journal of the Mechanics and Physics of Solids* 54.2 (2006), p. 401-424

[13] Laurent Stainier. "A Variational Approach to Modeling Coupled Thermo-Mechanical Nonlinear Dissipative Behaviors". In : t. 46. Advances in Applied Mechanics. Elsevier, 2013, p. 69-126

Continuum setting of the variational formulation

Consider the Lagrangian

$$\mathcal{L}(\dot{\mathbf{q}}, \lambda; \mathbf{q}) = \dot{E} - T\dot{\eta} + \phi(\dot{\mathbf{F}}, \dot{\mathbf{Z}}; \mathbf{F}, \mathbf{Z}, T) + \lambda \frac{d}{dt}(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E)$$

with $\mathbf{q} = \{E, \mathbf{F}, \eta, \mathbf{Z}, T\}$ considered known and fixed here

and $\{\dot{\mathbf{F}}, \dot{E}\}$ are assumed fixed and known. Hence, stationarity conditions read

$$\mathcal{W} = \underset{\dot{\eta}, \dot{T}, \lambda}{\text{stat}} \inf_{\dot{\mathbf{Z}}} \mathcal{L}(\dot{\mathbf{q}}, \lambda; \mathbf{q})$$

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$$\mathcal{W} = \underset{\dot{\eta}, \dot{T}, \lambda}{\text{stat}} \ \inf_{\dot{\mathbf{Z}}} \mathcal{L}(\dot{\mathbf{q}}, \lambda; \mathbf{q})$$

Stationarity conditions

- $\underset{\dot{\eta}}{\text{stat}}\, \mathcal{L} \Leftrightarrow -T + \lambda T = 0$, hence $\lambda = 1$
- $\underset{\dot{T}}{\text{stat}}\, \mathcal{L} \Leftrightarrow \lambda \left(\eta + \frac{\partial W}{\partial T}\right) = 0$
- $\underset{\lambda}{\text{stat}}\, \mathcal{L} \Leftrightarrow \frac{d}{dt}(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E) = 0$
- $\inf_{\dot{Z}} \mathcal{L} \Leftrightarrow \dfrac{\partial \phi}{\partial \dot{\mathbf{Z}}} + \lambda \dfrac{\partial W}{\partial \mathbf{Z}} = 0$

Comments

- $\mathcal{L}(\lambda = 1) = \dot{W} + \dot{T}\eta + \phi$, identical to [13]
- $\frac{\partial \mathcal{W}}{\partial \dot{\mathbf{F}}} = \lambda \frac{\partial W}{\partial \mathbf{F}} + \frac{\partial \phi}{\partial \dot{\mathbf{F}}} = \mathbf{P}^{\text{rev}} + \mathbf{P}^{\text{irr}} = \mathbf{P}$

[13] Laurent Stainier. "A Variational Approach to Modeling Coupled Thermo-Mechanical Nonlinear Dissipative Behaviors". In : t. 46. Advances in Applied Mechanics. Elsevier, 2013, p. 69-126

A first order accurate discrete variational constitutive update

Consider the material state $\mathbf{q}_n = \{E_n, \mathbf{F}_n, \eta_n, \mathbf{Z}_n, T_n\}$ known at time t_n, and data $\{E, \mathbf{F}\}_{n+1}$ updated at time t_{n+1} through discrete conservation laws

$$\begin{aligned}\mathcal{J}(\mathbf{q}_{n+1}, \lambda_{n+1}; \mathbf{q}_n) &\approx \int_{t_n}^{t_{n+1}} \mathcal{L}(\dot{\mathbf{q}}(\tau), \lambda(\tau); \mathbf{q}(\tau)) d\tau \\ &= \Delta E - T_n \Delta\eta + \Delta t \phi\left(\frac{\Delta \mathbf{F}}{\Delta t}, \frac{\Delta \mathbf{Z}}{\Delta t}; \mathbf{F}_{n+\alpha}, \mathbf{Z}_{n+\alpha}, T_{n+\alpha}\right) \\ &\quad + \lambda_{n+1}\Delta(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E)\end{aligned}$$

with $(\cdot)_{n+\alpha} = (1-\alpha)(\cdot)_n + \alpha(\cdot)$, $\alpha \in [0,1]$ [14] ; $\Delta(\cdot) = (\cdot)_{n+1} - (\cdot)_n$

Discrete variational principle

$$\mathcal{W}_{n+1} = \underset{(\eta, T, \lambda)_{n+1}}{\text{stat}} \quad \inf_{\mathbf{Z}_{n+1}} \mathcal{J}(\mathbf{q}_{n+1}, \lambda_{n+1}; \mathbf{q}_n)$$

[14] Laurence Brassart et Laurent Stainier. "On convergence properties of variational constitutive updates for elasto-visco-plasticity". In : *GAMM-Mitteilungen* 35.1 (2012), p. 26-42

Stationarity conditions in the discrete setting

Stationarity conditions

- $\underset{\eta_{n+1}}{\text{stat}}\, \mathcal{J} \Leftrightarrow -T_n + \lambda_{n+1} T_{n+1} = 0$, hence $\lambda_{n+1} = \frac{T_n}{T_{n+1}}$
- $\underset{T_{n+1}}{\text{stat}}\, \mathcal{J} \Leftrightarrow \eta_{n+1} = -\left.\frac{\partial W}{\partial T}\right|_{n+1} \underbrace{-\frac{T_{n+1}}{T_n} \Delta t \frac{\partial \phi}{\partial T}\left(\frac{\Delta \mathbf{F}}{\Delta t}, \frac{\Delta \mathbf{Z}}{\Delta t}; \mathbf{F}_{n+\alpha}, \mathbf{Z}_{n+\alpha}, T_{n+\alpha}\right)}_{\mathcal{O}(\Delta t)}$
- $\underset{\lambda_{n+1}}{\text{stat}}\, \mathcal{J} \Leftrightarrow \Delta(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E) = 0$
- $\underset{\mathbf{Z}_{n+1}}{\inf}\, \mathcal{J} \Leftrightarrow \frac{\partial \phi}{\partial \dot{\mathbf{Z}}}\left(\frac{\Delta \mathbf{F}}{\Delta t}, \frac{\Delta \mathbf{Z}}{\Delta t}; \mathbf{F}_{n+\alpha}, \mathbf{Z}_{n+\alpha}, T_{n+\alpha}\right) + \frac{T_n}{T_{n+1}} \left.\frac{\partial W}{\partial \mathbf{Z}}\right|_{n+1} = 0$

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Computation of stresses

$$\left.\frac{\partial \mathcal{W}}{\partial \mathbf{F}}\right|_{n+1} = \frac{T_n}{T_{n+1}} \left.\frac{\partial W}{\partial \mathbf{F}}\right|_{n+1} + \frac{\partial \phi}{\partial \dot{\mathbf{F}}}\left(\frac{\Delta \mathbf{F}}{\Delta t}, \frac{\Delta \mathbf{Z}}{\Delta t}; \mathbf{F}_{n+\alpha}, \mathbf{Z}_{n+\alpha}, T_{n+\alpha}\right)$$
$$= \mathbf{P}^{\text{rev}}_{n+1} + \mathbf{P}^{\text{irr}}_{n+1} = \mathbf{P}_{n+1}$$

Variational thermo-(hyper)elastic-viscoplastic solids

Kinematical approach [15]

Choice of internal variables

$$\text{since } \mathbf{L}^p = \dot{p}\mathbf{M}; \qquad \mathbf{L}^p = \dot{\mathbf{F}}^p \cdot (\mathbf{F}^p)^{-1}$$
$$\dot{\mathbf{Z}} = \{\dot{p}, \mathbf{M}\}$$

Solution process

$$\frac{\partial \mathcal{J}}{\partial \lambda} = \Delta(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E) = 0$$
$$\frac{\partial \mathcal{J}}{\partial \Delta p} = \frac{T_n}{T_{n+1}} \left.\frac{\partial W}{\partial \Delta p}\right|_{n+1} + \left[\frac{\partial \phi}{\partial \dot{p}}\left(\frac{\Delta p}{\Delta t}, p_{n+\alpha}, T_{n+\alpha}\right) + \alpha \Delta t \frac{\partial \phi}{\partial p}\left(\frac{\Delta p}{\Delta t}, p_{n+\alpha}, T_{n+\alpha}\right)\right] = 0$$
$$\frac{\partial \mathcal{J}}{\partial \mathbf{M}} = \frac{\partial \Delta W}{\partial \mathbf{M}} = 0, \quad \text{under some constraints}$$

But constrained optimization !

Analytical solution for Mises :

$$\inf_{\mathbf{M}_{n+1}} \mathcal{J}\,;\ \mathbf{M} = \mathbf{M}^T;\ \|\mathbf{M}\| = \sqrt{\frac{3}{2}},\ \text{tr}[\mathbf{M}] = 0$$
$$\Leftrightarrow\ \mathbf{M}_{n+1} = \sqrt{\frac{3}{2}} \left.\frac{\text{dev}[\boldsymbol{\Sigma} - \mathbf{Q}_k]}{\|\text{dev}[\boldsymbol{\Sigma} - \mathbf{Q}_k]\|}\right|_{n+1}^{\text{trial}}$$

Limitations

- additive structure of the updated elastic strain (Hencky hyperelasticity with logarithmic strain)
- associative plasticity
- linear kinematic hardening

[15] Michael Ortiz et Laurent Stainier. "The variational formulation of viscoplastic constitutive updates". In : *Computer methods in applied mechanics and engineering* 171.3-4 (1999), p. 419-444

Parameterization of the flow rule based on pseudo-stresses [16]

Basic idea

Since $\Sigma_{\mathsf{eq}}(c\mathbf{A}) = c\Sigma_{\mathsf{eq}}(\mathbf{A}), \quad \forall c \in \mathbb{R}^+$

$\mathbf{M}(\mathbf{\Sigma} - \mathbf{Q}_k) = \mathbf{M}(\tilde{\mathbf{\Sigma}})$

Advantages

- unconstrained optimization
- possible elastic and plastic anisotropies
- allows non-associative plasticity

[16] J Mosler et OT Bruhns. "On the implementation of rate-independent standard dissipative solids at finite strain–Variational constitutive updates". In : *Computer Methods in Applied Mechanics and Engineering* 199.9-12 (2010), p. 417-429

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Discrete plastic flow rule [17]

$$\mathbf{F}^p_{n+1} = \exp\left(\Delta p \left.\frac{\partial f}{\partial \mathbf{\Sigma}}\right|_{\tilde{\mathbf{\Sigma}}_{n+1}}\right) \cdot \mathbf{F}^p_n$$

$$\mathbf{F}^e_{n+1} = \mathbf{F}^e_{\text{trial}} \cdot \exp\left(-\Delta p \left.\frac{\partial f}{\partial \mathbf{\Sigma}}\right|_{\tilde{\mathbf{\Sigma}}_{n+1}}\right), \quad \mathbf{F}^e_{\text{trial}} = \mathbf{F}_{n+1} \cdot (\mathbf{F}^p_n)^{-1}.$$

[17] Gustavo Weber et Lallit Anand. “Finite deformation constitutive equations and a time integration procedure for isotropic, hyperelastic-viscoplastic solids”. In : *Computer Methods in Applied Mechanics and Engineering* 79.2 (1990), p. 173-202

[16] J Mosler et OT Bruhns. “On the implementation of rate-independent standard dissipative solids at finite strain–Variational constitutive updates”. In : *Computer Methods in Applied Mechanics and Engineering* 199.9-12 (2010), p. 417-429

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Discrete Euler-Lagrange equations

$$\frac{\partial \mathcal{J}}{\partial \lambda} = \Delta(T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E) = 0$$

$$\frac{\partial \mathcal{J}}{\partial \Delta p} = 0 \text{ with } \left.\frac{\partial W}{\partial \Delta p}\right|_{n+1} = \left.\frac{\partial W^e}{\partial \Delta p}\right|_{n+1} + \left.\frac{\partial W^p}{\partial \Delta p}\right|_{n+1}$$

$$\text{and } \left.\frac{\partial W^e}{\partial \Delta p}\right|_{n+1} = -2\left[\mathbf{C}^e_{\text{trial}} \cdot \exp\left(-\Delta p \left.\frac{\partial f}{\partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}}\right) \cdot \left.\frac{\partial W^e}{\partial \mathbf{C}^e}\right|_{n+1}\right] : D\exp\left(-\Delta p \left.\frac{\partial f}{\partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}}\right) : \left.\frac{\partial f}{\partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}}$$

$$\frac{\partial \mathcal{J}}{\partial \tilde{\boldsymbol{\Sigma}}_{n+1}} = -2\Delta p\left[\mathbf{C}^e_{\text{trial}} \cdot \exp\left(-\Delta p \left.\frac{\partial f}{\partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}}\right) \cdot \left.\frac{\partial W^e}{\partial \mathbf{C}^e}\right|_{n+1}\right] : D\exp\left(-\Delta p \left.\frac{\partial f}{\partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}}\right) : \left.\frac{\partial^2 f}{\partial \boldsymbol{\Sigma} \partial \boldsymbol{\Sigma}}\right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}} = \mathbf{0}$$

solved on $\mathbf{X}_{n+1} = \{T, \Delta p, \tilde{\boldsymbol{\Sigma}}\}|_{n+1}$

[16] J Mosler et OT Bruhns. “On the implementation of rate-independent standard dissipative solids at finite strain–Variational constitutive updates”. In : *Computer Methods in Applied Mechanics and Engineering* 199.9-12 (2010), p. 417-429

Parameterization of pseudo-stresses with spherical coordinates [18]

Enforce $\|\tilde{\mathbf{\Sigma}}\| = 1$

$$\tilde{\mathbf{\Sigma}} = \sum_{k=1}^{3} \tilde{\Sigma}_k(\psi, \rho)\mathbf{B}_k$$

$$\mathbf{B}_k = \mathbf{R}(\varphi_1, \theta_1, \chi_1) \cdot \mathbf{B}_k^{\text{trial}} \cdot \mathbf{R}^T(\varphi_2, \theta_2, \chi_2)$$

solution

$$\frac{\partial \mathfrak{I}}{\partial \boldsymbol{\alpha}} = \frac{\partial \mathfrak{I}}{\partial \tilde{\mathbf{\Sigma}}} : \frac{\tilde{\mathbf{\Sigma}}}{\partial \boldsymbol{\alpha}} = \mathbf{0}$$

$$\text{dime}[\boldsymbol{\alpha}] = 8$$

Elastic isotropy

- $\tilde{\mathbf{\Sigma}} = \tilde{\mathbf{\Sigma}}^T$
- 5 unknowns

Fully isotropic (elastic and plastic) medium

- only 2 unknowns (ψ, ρ) remain
- no tensorial derivatives of the exponential mapping $(\mathbf{B}_k = \mathbf{B}_k^{\text{trial}})$

Pressure independent yield function

- $\mathbf{M} : \mathbf{1} = 0 \Leftrightarrow \text{tr}[\tilde{\mathbf{\Sigma}}] = 0$
- only one unknown (ψ) remain

[18] Nikolaus Bleier et Jörn Mosler. "Efficient variational constitutive updates by means of a novel parameterization of the flow rule". In : *International journal for numerical methods in engineering* 89.9 (2012), p. 1120-1143

Solution algorithm

At each material point, after the thermoelastic prediction

1. Solve for $\mathbf{X} = \{T, \Delta p, \boldsymbol{\alpha}\}$
2. Compute $\tilde{\boldsymbol{\Sigma}}(\boldsymbol{\alpha})$
3. Update $\mathbf{F}^e_{n+1} = \mathbf{F}^e_{\text{trial}} \cdot \exp\left(-\Delta p \left. \frac{\partial f}{\partial \boldsymbol{\Sigma}} \right|_{\tilde{\boldsymbol{\Sigma}}_{n+1}} \right), \quad \mathbf{F}^e_{\text{trial}} = \mathbf{F}_{n+1} \cdot (\mathbf{F}^p_n)^{-1}$
4. Update PK2 stresses $\mathbf{S}_{n+1} = 2 \frac{T_n}{T_{n+1}} \left. \frac{\partial W}{\partial \mathbf{C}} \right|_{n+1} = 2 \frac{T_n}{T_{n+1}} (\mathbf{F}^p_{n+1})^{-1} \cdot \left. \frac{\partial W}{\partial \mathbf{C}^e} \right|_{n+1} \cdot (\mathbf{F}^p_{n+1})^{-T}$
5. Update the entropy density $\eta_{n+1} = - \left. \frac{\partial W}{\partial T} \right|_{n+1} - \frac{T_{n+1}}{T_n} \Delta t \frac{\partial \phi}{\partial T}$
6. Update $\mathcal{I} = \Delta E - T_n \Delta \eta + \Delta t \phi + \frac{T_n}{T_{n+1}} \Delta (T\eta + W(\mathbf{F}, T, \mathbf{Z}) - E)$

Example of thermo-elastic-viscoplastic constitutive model

Free energy

$$W(\boldsymbol{\varepsilon}^e, p, T) = W^e(\mathbf{C}^e, T) + W^p(p, T)$$

$$W^e_{\text{dev}}(\mathbf{C}^e_{\text{dev}}) = \frac{\mu}{2}(\text{tr}[\mathbf{C}^e_{\text{dev}}] - 3);\ \mathbf{C}^e_{\text{dev}} = \frac{\mathbf{C}^e}{|\mathbf{C}^e|^{1/3}}$$

$$W^e_H(J, T):\ \text{EOS}$$

Johnson-Cook constitutive model [19, 20]

$$W^p(p, T) = \frac{B}{n+1} p^{n+1}(1 - \theta_*^q)$$

$$\phi(\dot{p}; p, T) = (A\dot{p} + (A + Bp^n)C\dot{p}_0 \times (\dot{p}_* \ln(\dot{p}_*) - \dot{p}_* + 1)(1 - \theta_*^q)$$

with $\dot{p}_* = \frac{\dot{p}}{\dot{p}_0}$ and $\theta_* = \frac{T - T_t}{T_m - T_t}$

Strength criteria

Hill

$$\boldsymbol{\Sigma} : \mathbb{H} : \boldsymbol{\Sigma} = \sigma_0^2$$

$$F(\Sigma_{22} - \Sigma_{33})^2 + G(\Sigma_{11} - \Sigma_{33})^2 + H(\Sigma_{22} - \Sigma_{11})^2 + 2L\Sigma_{23}^2 + 2M\Sigma_{13}^2 + 2N\Sigma_{12}^2 = \sigma_0^2$$

Mises : $F = G = H = \frac{1}{2},\ L = M = N = \frac{3}{2}$

Mises

$$3J_2(\text{dev}[\boldsymbol{\Sigma}]) = \sigma_0^2$$

$$\frac{1}{2}\left[(\Sigma_{22} - \Sigma_{33})^2 + (\Sigma_{11} - \Sigma_{33})^2 + (\Sigma_{22} - \Sigma_{11})^2 + 6(\Sigma_{23}^2 + \Sigma_{13}^2 + \Sigma_{12}^2\right] = \sigma_0^2$$

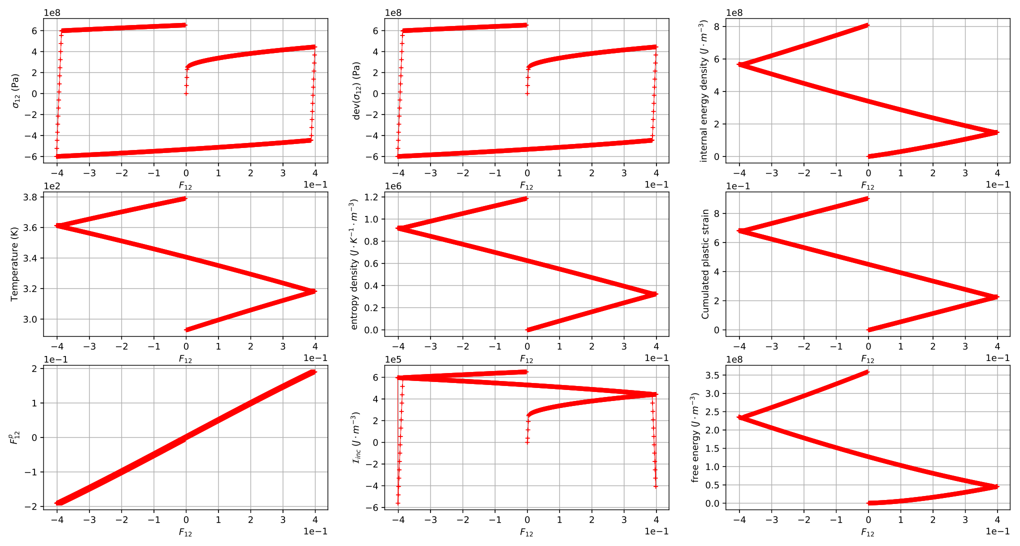
[19] G. R. Johnson et W. H. Cook. “A constitutive model and data for metals subjected to large strains, high strain rates and high temperatures”. In : *Proceedings of the 7th International Symposium on Ballistics* (1983), p. 541-547

[20] Nicolas Ranc et André Chrysochoos. “Calorimetric consequences of thermal softening in Johnson–Cook’s model”. In : *Mechanics of Materials* 65 (2013), p. 44-55

Numerical examples with Mises criterion

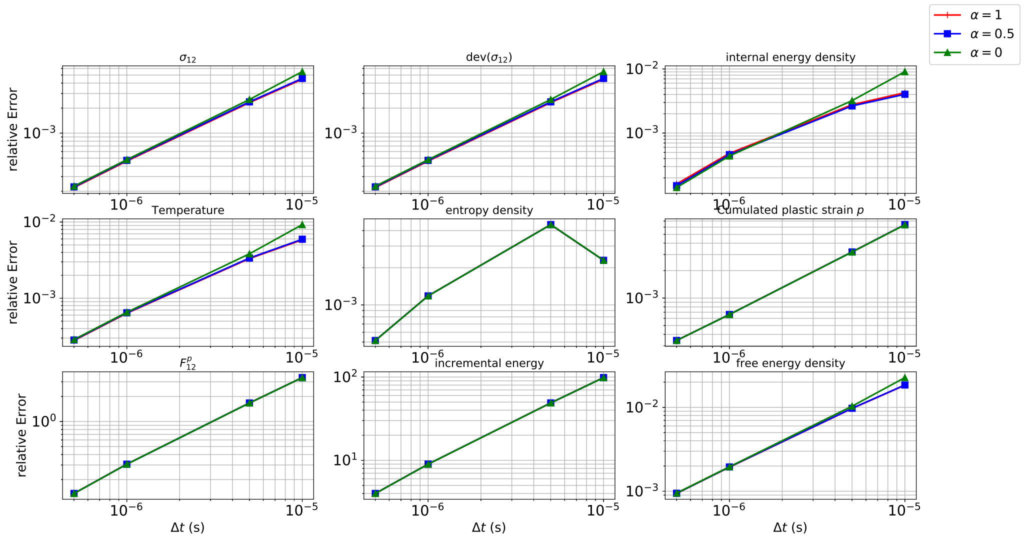
Material point : pure shear test case $\mathbf{F} = \mathbf{1} + \mathbf{F}_{12}\mathbf{e}_1 \otimes \mathbf{e}_2$, $\dot{F}_{12} = 10^3\mathbf{s}^{-1}$

The internal energy balance $\Delta E = \mathbf{P} : \Delta\mathbf{F}$ is enforced solving $\mathbf{P}_{n+1} = \frac{\partial}{\partial \mathbf{F}}\left[\mathcal{W}\left(\Delta E, \frac{\Delta \mathbf{F}}{\Delta t}\right)\right]\Big|_{n+1}$ through a fixed point loop. (smooth solution assumed)

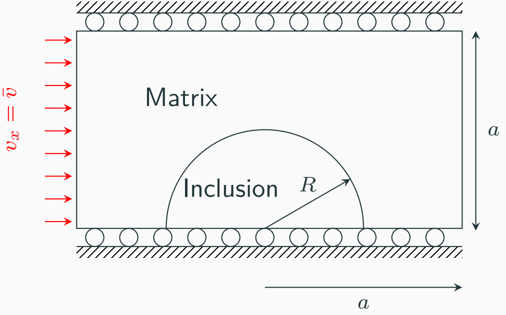


Convergence curves : pure shear test case

- Many values of α are considered
- A convergence rate of one is found as expected.



Sudden velocity loading and unloading of a heterogeneous volume



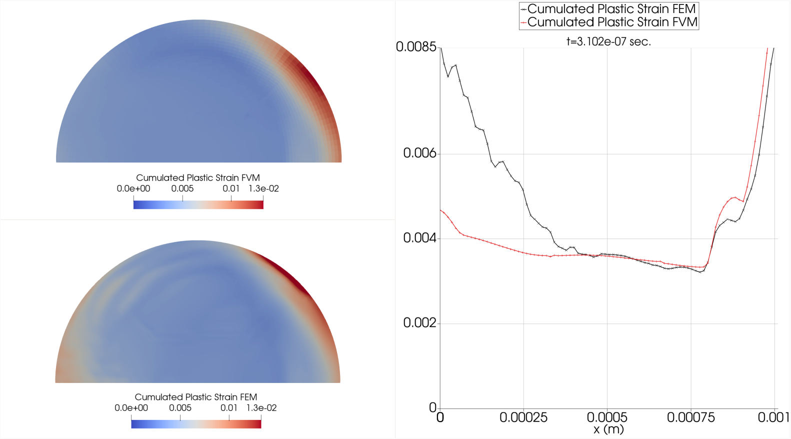
[21] R J Leveque. “Wave propagation algorithms for multidimensional hyperbolic systems”. In : *Journal of Computational physics* 131 (1997), p. 327-353
[22] T. Heuzé. “Simulation of impacts on elastic–viscoplastic solids with the flux-difference splitting finite volume method applied to non-uniform quadrilateral meshes”. In : *Advanced Modeling and Simulation in Engineering Sciences* 5.1 (2018), p. 9
[23] *ZorgLib*. User’s manual. L. Stainier. 2020
[13] Laurent Stainier. “A Variational Approach to Modeling Coupled Thermo-Mechanical Nonlinear Dissipative Behaviors”. In : t. 46. Advances in Applied Mechanics. Elsevier, 2013, p. 69-126

Small strain computation

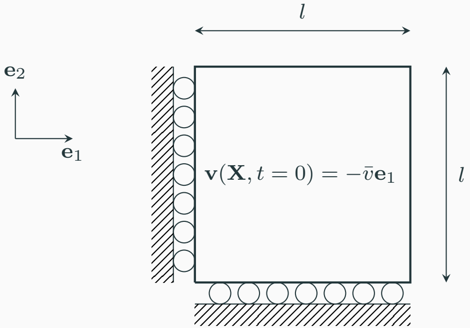
- Thermoelastic matrix (steel)
- Inclusion with Johnson-Cook model (alu)
- explicit FVM solver [21, 22]/ variational solver (E, ε)
- explicit (central difference) FEM /variational solver (T, ε)[23, 13]

Sudden velocity loading and unloading of a heterogeneous volume

Sudden velocity loading and unloading of a heterogeneous volume



2D Taylor-like impact



- J-C Viscoplasticity with linear isotropic hardening
- Hencky hyperelasticity [24]

  $W^e(\mathbf{C}^e) = W^v(J) + \mu(\text{dev}[\boldsymbol{\epsilon}^e] : \text{dev}[\boldsymbol{\epsilon}^e])$

  with $\boldsymbol{\epsilon}^e = \dfrac{1}{2}\log[\mathbf{C}^e]$

-

$$\mathcal{U} = \begin{Bmatrix} \rho_0 \mathbf{v} \\ \mathbf{F} \\ J \\ \mathcal{E} \end{Bmatrix}$$

for quasi-incompressibility

Comparison

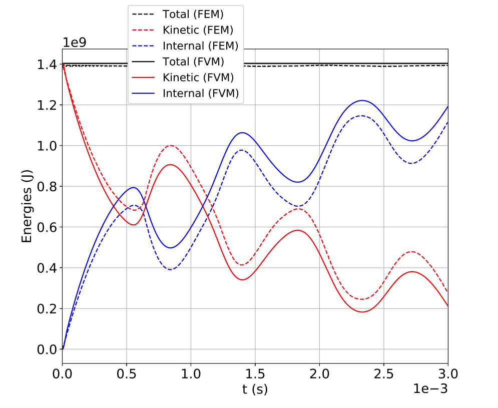
Method	CFL
explicit FVM / VF $(E, \mathbf{F})$	0.4
explicit FEM / VF $(T, \mathbf{F})$ [23]	0.8

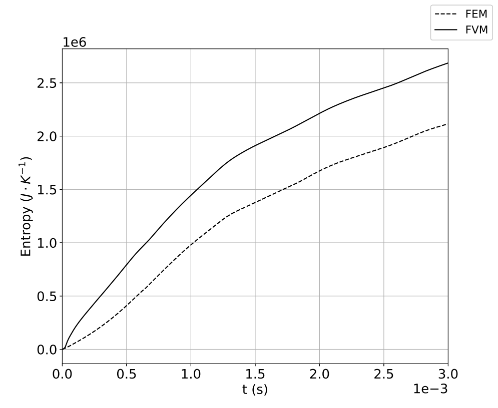
[23] *ZorgLib*. User's manual. L. Stainier. 2020

[24] Eduardo Fancello, Jakson M. Vassoler et Laurent Stainier. "A variational constitutive update algorithm for a set of isotropic hyperelastic–viscoplastic material models". In : *Computer Methods in Applied Mechanics and Engineering* 197.49 (2008), p. 4132 -4148. ISSN : 0045-7825. DOI : https://doi.org/10.1016/j.cma.2008.04.014

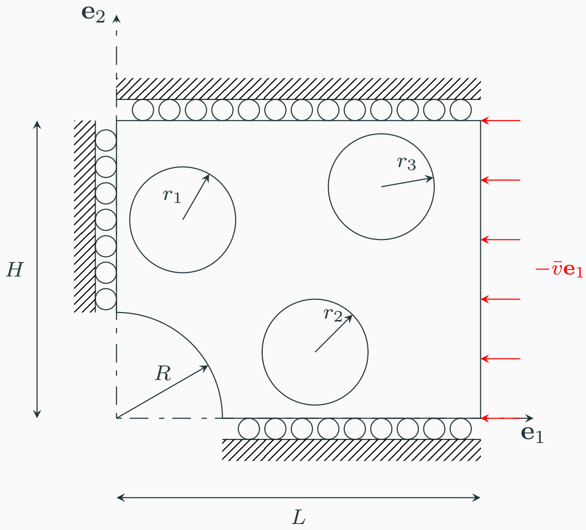
2D Taylor-like impact

2D Taylor-like impact





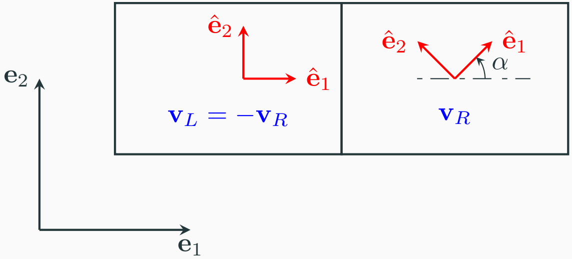
Multi-holed elementary cell



Multi-holed elementary cell

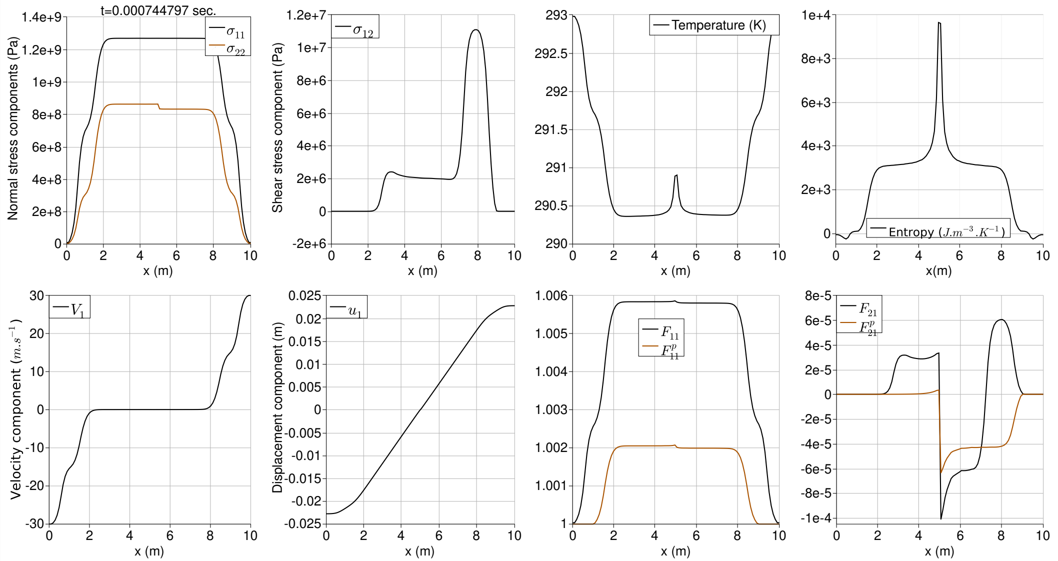
Numerical examples with Hill criterion

Simple Riemann-type 1D test case

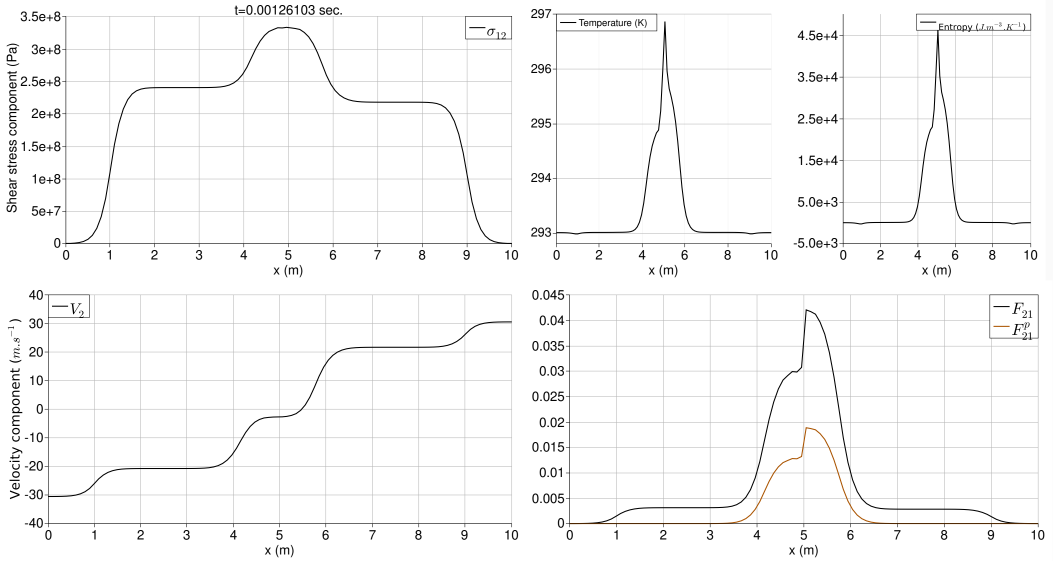


Plastic flow convected by waves ?

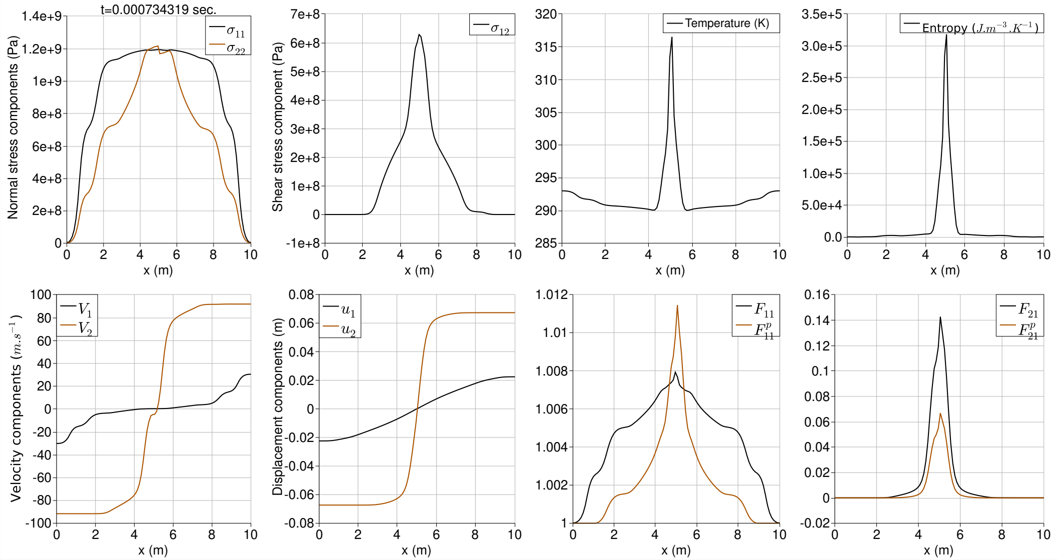
Tension : $\mathbf{v}_R = \frac{2Y_H}{\rho_0 c_L}\mathbf{e}_1$



Shear : $\mathbf{v}_R = \frac{2Y_H}{\rho_0 c_L}\mathbf{e}_2$



Tension + shear : $\mathbf{v}_R = \frac{3Y_H}{\rho_0 c_L}\mathbf{e}_1 + \frac{2Y_H}{\rho_0 c_L}\mathbf{e}_2$



Conclusion

Conclusion

Summary

- Introduction of a variational formulation of thermomechanical constitutive update driven by some strain ($\mathbf{F}$) and internal energy (E) values
- Right shock speeds are then ensured to be computed.
- Application to thermo-(hyper)elastic-viscoplastic solids (Johnson-Cook) in small and large strains

Outlooks

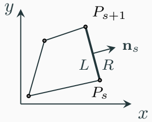
- Recast the formulation in the initial and current settings
- Describe other dissipative mechanisms (damage, gradient plasticity, etc)
- Higher order discrete variational principles can be derived

[25] Thomas Heuzé et Laurent Stainier. "A variational formulation of thermomechanical constitutive update for hyperbolic conservation laws". In : *Computer Methods in Applied Mechanics and Engineering* 394 (2022), p. 114893

Appendix : Flux difference splitting finite volume method

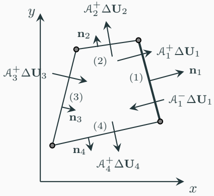
Flux-difference splitting finite volume method [21]

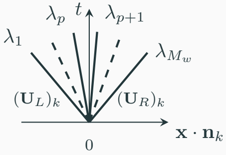
Conservation laws



$$\int_\Omega \frac{\partial \mathfrak{U}}{\partial t} d\Omega + \int_{\partial\Omega} \mathfrak{F}\cdot\mathbf{n} dS = \mathbf{0} \quad \Rightarrow \left(\frac{d\mathbf{U}}{dt}\right)_i = -\frac{1}{|A_i|}\sum_{s=1}^{N} L_s \mathbf{F}_s$$

Decomposition in waves and fluctuations





$$\Delta\mathbf{U}_k = \sum_{p=1}^{M_w} \mathcal{W}_k^{(p)} = \sum_{p=1}^{M_w} \alpha_k^{(p)}\mathbf{R}_k^{(p)} = \mathbf{R}_k\boldsymbol{\alpha}_k$$

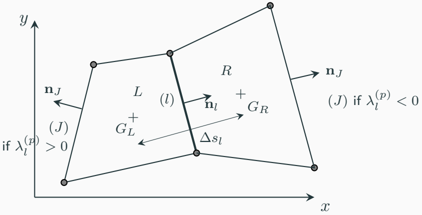
$$\sum_{s=1}^{N} L_s\mathbf{F}_s = \sum_{k=1}^{P} L_k\mathcal{A}_k^+\Delta\mathbf{U}_k + \sum_{l=1}^{Q} L_l\mathcal{A}_l^-\Delta\mathbf{U}_l$$

$$\mathcal{A}_k^\pm\Delta\mathbf{U}_k = \sum_{p=1}^{M_w}\lambda_p^\pm\mathcal{W}_k^{(p)} = \sum_{p=1}^{M_w}\lambda_p^\pm\alpha_k^{(p)}\mathbf{R}_k^{(p)}$$

[21] R J Leveque. "Wave propagation algorithms for multidimensional hyperbolic systems". In : *Journal of Computational physics* 131 (1997), p. 327-353

High order fluxes

Comparison between upwind and downwind waves



$$\theta_l^{(p)} = \frac{\mathcal{W}_J^{(p)}(\mathbf{n}_l) \cdot \mathcal{W}_l^{(p)}}{\|\mathcal{W}_l^{(p)}\|^2}$$

$$\boldsymbol{\alpha}_J(\mathbf{n}_l) = \mathbf{R}^{-1}(\mathbf{n}_l) \cdot \Delta\mathbf{U}_J$$

$$\mathbf{W}_J(\mathbf{n}_l) = \text{diag}\ (\boldsymbol{\alpha}_J(\mathbf{n}_l)) \cdot \mathbf{R}(\mathbf{n}_l)$$
$$= \left[\text{diag}\ ([\mathbf{R}(\mathbf{n}_l)]^{-1} \cdot \Delta\mathbf{U}_J)\right] \cdot \mathbf{R}(\mathbf{n}_l)$$

TVD limiter [26]

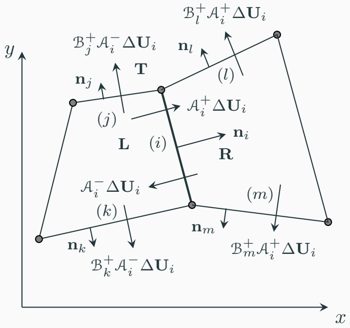
$$\tilde{\alpha}_l^{(p)} = \phi(\theta_l^{(p)})\alpha_l^{(p)}$$
$$\phi(\theta) = \text{minmod}(1, \theta) \quad \text{(minmod)}$$

High order flux

$$\tilde{\mathbf{F}}_l^{\text{HO}} = \frac{1}{2}\sum_{p=1}^{M_w} |\lambda_l^{(p)}| \left(1 - \frac{\Delta t}{\Delta s_l}|\lambda_l^{(p)}|\right) \tilde{\mathcal{W}}_l^{(p)}$$

[26] P.K. Sweby. "High resolution schemes using flux limiters for hyperbolic conservation laws". In : *SIAM Journal on Numerical Analysis* 21 (1984), p. 995-1011

Corner Transport Upwind (CTU) method [27]



Interest

- Allows to account for waves propagating in bias / each grid cell
- Improve the CFL condition

Transverse Riemann solver

$$\mathcal{A}_i^-\Delta\mathbf{U}_i = \sum_{p=1}^{M_w} \beta_p \mathbf{R}_j^{(p)} = \mathbf{R}(\mathbf{n}_j)\boldsymbol{\beta}$$

For edge j (outward normal) :

$$\mathcal{B}_j^+\mathcal{A}_i^-\Delta\mathbf{U}_i = c_L \mathcal{W}^{(2)} + c_s \mathcal{W}^{(4)}$$

the additional flux reads :

$$\tilde{\mathbf{F}}_j^{\text{tran}} = \frac{\Delta t}{2\Delta s_j}\mathcal{B}_j^+\mathcal{A}_i^-\Delta\mathbf{U}_i$$

[27] Phillip Colella. “Multidimensional upwind methods for hyperbolic conservation laws”. In : *Journal of Computational Physics* 87.1 (1990), p. 171-200

Final update

$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{|A_i|}\left(\sum_{k=1}^{P} L_k \mathcal{A}_k^+\Delta\mathbf{U}_k + \sum_{l=1}^{Q} L_l \mathcal{A}_l^-\Delta\mathbf{U}_l\right) - \frac{\Delta t}{|A_i|}\left(\sum_{k=1}^{P} L_k \tilde{\mathbf{F}}_k^{\text{out}} - \sum_{l=1}^{Q} L_l \tilde{\mathbf{F}}_l^{\text{in}}\right) ; \quad \tilde{\mathbf{F}}_l^{\text{in}} = \tilde{\mathbf{F}}_l^{\text{HO}} + \tilde{\mathbf{F}}_l^{\text{tran}}.$$