Derivation and Numerical solution of a multi-phase hyperbolic Model of Continuum Mechanics in the Baer-Nunziato type form

EDP séminaire, IRMA Strasburg

Davide Ferrari
Supervisors M. Dumbser, I. Peshkov

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DICAM, University of Trento

The classical approach for multi-phase mixtures

$\rightarrow$ A multiphase flow can be considered as a set of interacting continua.

Postulating Truesdell (1984, p.81) " a sequence of bodies $\mathcal{B}_n$, all of which ... occupy regions of space ... simultaneously "

C. Truesdell. Rational Thermodynamics, McGraw-Hill, New York, 1984.

Averaging Phases are continua separated by an interface

D.A. Drew, S.L. Passman. Theory of Multicomponent Fluids, Springer, New York, 1999.

The classical approach for multi-phase mixtures

The **averaging** and **postulation** yield the same results

$$\partial_t(\alpha_n\rho_n) + \nabla\cdot(\alpha_n\rho_n \mathbf{v_n}) = \Gamma_n,$$
$$\partial_t(\alpha_n\rho_n \mathbf{v_n}) + \nabla\cdot(\alpha_n\rho_n \mathbf{v_n}\otimes\mathbf{v_n} - \alpha_n \mathbf{T}_n) = \mathbf{M}_n + \Gamma_n \mathbf{v_n},$$
$$\partial_t(\alpha_n\rho_n e_n) + \nabla\cdot(\alpha_n\rho_n e_n \mathbf{v_n} - \alpha_n \mathbf{T}_n\cdot\mathbf{v_n} + \alpha_n \mathbf{q}_n) = E_n + \mathbf{M}_n\mathbf{v_n} + \Gamma_n e_n,$$

This system must be supplemented with

→ **state equations**, $\mathbf{T}_n(S_n), e_n(S_n), \mathbf{q}_n(S_n)$
→ **constitutive equations**, $\Gamma_n(S_1,\dots,S_n), \mathbf{M}_n(S_1,\dots,S_n), E_n(S_1,\dots,S_n)$
→ boundary and initial conditions

The classical approach for multi-phase mixtures

Constitutive equations should be formulated by means of principles

- *well-posedness*
- *separation of components*, self-interaction of phase n are $f(S_n)$
- *Galilean invariance*

$\rightarrow$ constitutive equations must also satisfy the *entropy inequalities*.

A **two-phase** model, $(n = 1,\ 2)$, is the Baer-Nunziato (BN) model

$$
\begin{aligned}
&\partial_t(\alpha_n\rho_n) + \nabla\cdot(\alpha_n\rho_n\mathbf{u_n}) = 0,\\
&\partial_t(\alpha_n\rho_n\mathbf{u_n}) + \nabla\cdot(\alpha_n(\rho_n\mathbf{u_n}\otimes\mathbf{u_n} + p_n\mathbf{I}) = p_I\nabla\alpha_n,\\
&\partial_t(\alpha_n\rho_n E_n) + \nabla\cdot(\alpha_n(\rho_n E_n + p_n)\mathbf{u_n}) = p_I\mathbf{u_I}\cdot\nabla\alpha_1,\\
&\partial_t\alpha_n + \mathbf{u_I}\cdot\nabla\alpha_n = 0.
\end{aligned}
$$

M.R. Baer, J.W. Nunziato. Int. J. Multiph. Flow, 12(6), p. 861–889, 1986.

A different continuum theory for multi-phase mixtures

How, whithin the continuum approach, to

- derive a **closed** form for a multi-phase mixture model
  $\rightarrow$ avoiding the formulation of *constitutive equations*;
- derive a model generalized to an **arbitrary number of constituents**;
- include **multi-material** properties of phases.

Axiom $\rightarrow$ All correct physical theories must be built on a proper mathematical framework

$\rightarrow$ **Symmetric Hyperbolic Thermodynamically Compatible** (SHTC) formulation of continuum mechanics

SHTC formulation of continuum mechanics

The development of a model considers

- causality
- conservation
- thermodynamic principles
- Galilean invariance
- **well-posedness of the initial value problem** (IVP)

How can one guaranty that the IVP for a new nonlinear continuum mechanics model is well-posed?

S. K. Godunov. *An interesting class of quasilinear systems*, Dokl. Akad. Nauk SSSR, 139, 521-523, 1961;
E. I.Romenski et al. J. Sci. Comput. **42**, 68–95 (2010).

Symmetric hyperbolic systems of PDEs

SHTC formulation of continuum mechanics

If a first order system of conservation laws, for $\mathbf{q} = (q_1, q_2, \ldots, q_n)$,

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathsf{F}^k(\mathbf{q})}{\partial x_k} = 0 \tag{1}$$

admits an extra conservation law for a **strictly convex potential** $E(\mathbf{q})$,

$$\frac{\partial E(\mathbf{q})}{\partial t} + \frac{\partial G^k(\mathbf{q})}{\partial x_k} = 0 \tag{2}$$

Introducing $\mathbf{p} = E_{\mathbf{q}}$, and the potential $L(\mathbf{p}) = \mathbf{q} \cdot \mathbf{p} - E(\mathbf{q})$,
$L^k(\mathbf{p}) = E_{\mathbf{q}} \cdot \mathsf{F}^k(\mathbf{q}) - G^k(\mathbf{q}) = \mathbf{p} \cdot \mathsf{F}^k(\mathbf{q}) - G^k(\mathbf{q})$, eq. (1) reads

$$\frac{\partial L_{\mathbf{p}}}{\partial t} + \frac{\partial L^k_{\mathbf{p}}}{\partial x_k} = 0 \tag{3}$$

SHTC formulation of continuum mechanics

Eq. (3) can be rewritten in a **symmetric quasilinear form** as

$$L_{\mathsf{p}_i\mathsf{p}_j}\frac{\partial p_j}{\partial t} + L^k_{\mathsf{p}_i\mathsf{p}_j}\frac{\partial p_j}{\partial x_k} = 0. \tag{4}$$

The system (1) and the conservation law of the total energy (2) costitute and *overdetermined* system of PDEs

$$E_{\mathbf{q}} \cdot \left(\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathsf{F}^k(\mathbf{q})}{\partial x_k}\right) \equiv \frac{\partial E(\mathbf{q})}{\partial t} + \frac{\partial G^k(\mathbf{q})}{\partial x_k} \tag{5}$$

Thus, this subclass of symmetric hyperbolic PDEs can be associated with the **thermodynamically compatible systems** of first order nonlinear conservation laws.

Composition characteristics

A mixture of N phases denoted by a, where $a = 1, \ldots, N$.
The mass M and the volume V of an infinitesimal element read

$$M = \sum_{a=1}^{N} m_a, \qquad V = \sum_{a=1}^{N} \nu_a, \tag{6}$$

$$\rho = \frac{M}{V} = \frac{m_1 + m_2 + \ldots + m_N}{V} = \sum_{a=1}^{N} \varrho_a, \qquad \text{where} \qquad \varrho_a := \frac{m_a}{V} \tag{7}$$

The volume fraction and the mass fraction read

$$\alpha_a := \frac{\nu_a}{V}, \qquad c_a := \frac{m_a}{M} = \frac{\varrho_a}{\rho}, \qquad \sum_{a=1}^{N} \alpha_a = 1, \qquad \sum_{a=1}^{N} c_a = 1. \tag{8}$$

SHTC multi-phase theory - Definitions of the mixture theory

Composition characteristics

The mass density of the a-th phase of the partial volume ν_a, i.e.

$$\rho_a = \frac{m_a}{\nu_a} = \frac{m_a V}{\nu_a V} = \frac{\varrho_a}{\alpha_a}, \qquad \rightarrow \qquad \varrho_a = \alpha_a \rho_a. \tag{9}$$

The mixture entropy density $\eta = \rho S$ is defined as

$$\eta := \sum_{a=1}^{N} \eta_a = \sum_{a=1}^{N} \varrho_a s_a \tag{10}$$

where s_a is the specific entropy of the a-th phase.

Kinematics of mixtures

The linear momentum $\boldsymbol{U} = \{U_k\}$ is defined as

$$\boldsymbol{U} := \boldsymbol{u}_1 + \boldsymbol{u}_2 + \ldots + \boldsymbol{u}_N = \varrho_1 \boldsymbol{v}_1 + \varrho_2 \boldsymbol{v}_2 + \ldots + \varrho_N \boldsymbol{v}_N. \tag{11}$$

The velocity $\boldsymbol{V} = \{V_k\}$ of the mixture control volume is

$$\boldsymbol{V} := \frac{\boldsymbol{U}}{\rho} = \frac{\varrho_1 \boldsymbol{v}_1 + \varrho_2 \boldsymbol{v}_2 + \ldots + \varrho_N \boldsymbol{v}_N}{\rho} = c_1 \boldsymbol{v}_1 + c_2 \boldsymbol{v}_2 + \ldots + c_N \boldsymbol{v}_N. \tag{12}$$

For the SHTC formulation the relative velocity $\boldsymbol{w} = \{w_{a,k}\}$ is needed

$$\boldsymbol{w}_a = \boldsymbol{v}_a - \boldsymbol{v}_N, \qquad w_{a,k} = v_{a,k} - v_{N,k}, \qquad k = 1, \ldots, 3. \tag{13}$$

which is defined with respect to the N-th constituent that can be chosen arbitrary.

SHTC multi-phase theory - Formulation

Define a vector of conserved variables $\boldsymbol{Q}$,

$$\boldsymbol{Q} = \{\rho, \boldsymbol{U}, \phi_1, \ldots, \phi_{N-1}, \varrho_1, \ldots, \varrho_{N-1}, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{N-1}, \eta_1, \ldots, \eta_N\}, \qquad (14)$$

and the vector of primitive variables $\boldsymbol{P}$

$$\boldsymbol{P} = \{\rho, \boldsymbol{V}, \alpha_1, \ldots, \alpha_{N-1}, c_1, \ldots, c_{N-1}, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{N-1}, s_1, \ldots, s_N\}, \qquad (15)$$

which are related as

$$\phi_a = \rho\alpha_a, \qquad \boldsymbol{U} = \rho\boldsymbol{V}, \qquad \varrho_a = \rho c_a \qquad \eta_a = \rho s_a. \qquad (16)$$

SHTC multi-phase theory - Formulation

The total energy density $\mathcal{E}$ of the mixture

$$\mathcal{E} = \sum_{a=1}^{N} \mathcal{E}_a = \sum_{a=1}^{N} \left(\varepsilon_a + \frac{1}{2\varrho_a} \|\boldsymbol{u}_a\|^2 \right), \tag{17}$$

then can be expressed in the SHTC state variables

$$\mathcal{E}(Q) = \sum_{a=1}^{N} \varepsilon_a + W(\rho, \varrho_1, \ldots, \varrho_{N-1}, \boldsymbol{w}_a, \ldots, \boldsymbol{w}_{N-1}) + \frac{1}{2\rho} \sum_{k=1}^{3} U_k^2, \tag{18}$$

where the relative kinetic energy W is defined as

$$W := \frac{1}{2} \sum_{k=1}^{3} \sum_{a=1}^{N-1} \varrho_a w_{a,k}^2 - \frac{1}{2\rho} \sum_{k=1}^{3} \left(\sum_{a=1}^{N-1} \varrho_a w_{a,k} \right)^2. \tag{19}$$

The internal energies $\varepsilon_a = \varrho_a e_a$, in eq.(18)

$$\varepsilon_a(\rho, \varrho_a, \eta_a) = \hat{\varepsilon}_a(\rho_a, s_a) = \hat{\varepsilon}_a \left(\frac{\varrho_a \rho}{\phi_a}, \frac{\eta_a}{\varrho_a} \right), \tag{20}$$

SHTC multi-phase theory - Formulation

In the SHTC theory, the thermodynamic pressure of the mixture

$$P(\mathbf{Q}) := \rho\mathcal{E}_\rho + U_i\mathcal{E}_{U_i} + \phi_a\mathcal{E}_{\phi_a} + \varrho_a\mathcal{E}_{\varrho_a} + \eta_a\mathcal{E}_{\eta_a} - \mathcal{E}, \qquad (21)$$

The partial derivatives of the total mixture energy with respect to the state vector $\mathbf{Q}$ are, e.g.

$$\frac{\partial\mathcal{E}}{\partial\rho} = \sum_{a=1}^{N-1}\frac{\partial\hat{\varepsilon}_a}{\partial\rho_a}\frac{\varrho_a}{\phi_a} + \frac{\partial\hat{\varepsilon}_N}{\partial\rho_N}\left(\frac{\rho\phi_N - \rho\varrho_N + \varrho_N\phi_N}{\phi_N^2}\right) - \frac{\partial\hat{\varepsilon}_N}{\partial s_N}\frac{\eta_N}{\varrho_N^2} + \qquad (22)$$

$$+ \frac{1}{2\rho^2}\sum_{k=1}^{3}\sum_{a=1}^{N}(\varrho_a w_{a,k})^2 - \frac{1}{2\rho^2}\sum_{k=1}^{3}U_k^2,$$

$$\frac{\partial\mathcal{E}}{\partial U_i} = \frac{1}{\rho}U_i. \qquad (23)$$

SHTC multi-phase theory - Formulation

The SHTC multi-phase system for of N phases, $a = 1, \dots, N$,

$$\frac{\partial U_i}{\partial t} + \frac{\partial \left(U_i V_k + P\delta_{ik} + w_{a,i}\mathcal{E}_{w_{a,k}} \right)}{\partial x_k} = 0, \tag{24a}$$

$$\frac{\partial w_{a,k}}{\partial t} + \frac{\partial \left(w_{a,l} V_l + \mathcal{E}_{\varrho_a} \right)}{\partial x_k} - V_l \left(\frac{\partial w_{a,k}}{\partial x_l} - \frac{\partial w_{a,l}}{\partial x_k} \right) = 0, \tag{24b}$$

$$\frac{\partial \varrho_a}{\partial t} + \frac{\partial \left(\varrho_a V_k + \mathcal{E}_{w_{a,k}} \right)}{\partial x_k} = 0, \tag{24c}$$

$$\frac{\partial \phi_a}{\partial t} + \frac{\partial \left(\phi_a V_k \right)}{\partial x_k} = 0 \tag{24d}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho V_k \right)}{\partial x_k} = 0, \tag{24e}$$

$$\frac{\partial \eta_a}{\partial t} + \frac{\partial (\eta_a V_k)}{\partial x_k} = 0, \tag{24f}$$

The SHTC multi-phase system for of N phases, $a = 1, \ldots, N$,

$$\frac{\partial U_i}{\partial t} + \frac{\partial \left(U_i V_k + P\delta_{ik} + w_{a,i}\mathcal{E}_{w_{a,k}} \right)}{\partial x_k} = 0, \tag{25a}$$

$$\frac{\partial w_{a,k}}{\partial t} + \frac{\partial \left(w_{a,l} V_l + \mathcal{E}_{\varrho_a} \right)}{\partial x_k} - V_l \left(\frac{\partial w_{a,k}}{\partial x_l} - \frac{\partial w_{a,l}}{\partial x_k} \right) = -\Lambda_{a,k}, \tag{25b}$$

$$\frac{\partial \varrho_a}{\partial t} + \frac{\partial \left(\varrho_a V_k + \mathcal{E}_{w_{a,k}} \right)}{\partial x_k} = -\chi_a, \tag{25c}$$

$$\frac{\partial \phi_a}{\partial t} + \frac{\partial \left(\phi_a V_k \right)}{\partial x_k} = -\Phi_a, \tag{25d}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho V_k \right)}{\partial x_k} = 0, \tag{25e}$$

$$\frac{\partial \eta_a}{\partial t} + \frac{\partial (\eta_a V_k)}{\partial x_k} = \Pi_a - \pi_a, \tag{25f}$$

SHTC multi-phase theory - Formulation

Various dissipative processes can be considered

Φ_a pressure relaxation

$$\Phi_a = \rho \sum_{b=1}^{N-1} \phi_{ab} \mathcal{E}_{\phi_b}, \qquad \mathcal{E}_{\phi_a} = \frac{\partial \mathcal{E}}{\partial \phi_a} = -\frac{p_a - p_N}{\rho}, \tag{26}$$

$\Lambda_{a,k}$ relative velocity relaxation

$$\Lambda_{a,k} = \frac{1}{\rho} \sum_{b=1}^{N-1} \lambda_{ab,k} \mathcal{E}_{w_{b,k}}, \qquad \mathcal{E}_{w_{b,k}} = \frac{\partial \mathcal{E}}{\partial w_{b,k}} = \varrho_b (v_{b,k} - V_k), \tag{27}$$

$\rightarrow$ they diminish the thermodynamic forces $\mathcal{E}_{\phi_a}$, $\mathcal{E}_{w_{a,k}}$.

$\rightarrow$ Π_a serve the goal of making the system compatible with the **second law of thermodynamic**.

SHTC multi-phase theory - A different form

Is it possible to write this system in a different form?

→ Recall the BN-type model

$$
\begin{aligned}
&\partial_t(\alpha_n\rho_n) + \nabla\cdot(\alpha_n\rho_n\mathbf{u_n}) = 0,\\
&\partial_t(\alpha_n\rho_n\mathbf{u_n}) + \nabla\cdot(\alpha_n(\rho_n\mathbf{u_n}\otimes\mathbf{u_n} + p_n\mathbf{I}) = p_I\nabla\alpha_n,\\
&\partial_t(\alpha_n\rho_n E_n) + \nabla\cdot(\alpha_n(\rho_n E_n + p_n)\mathbf{u_n}) = p_I\mathbf{u_I}\cdot\nabla\alpha_1,\\
&\partial_t\alpha_n + \mathbf{u_I}\cdot\nabla\alpha_n = 0.
\end{aligned}
$$

→ A conservation equation of mass, momentum, energy and volume fraction for each phase + inter-phase terms

SHTC multi-phase theory - A different form

The **phase volume fraction equations** from the eq. (25d) and (25e)

$$\frac{\partial \alpha_a}{\partial t} + V_k \frac{\partial \alpha_a}{\partial x_k} = -\frac{1}{\rho}\Phi_a \tag{28}$$

The **phase mass equations** (25c) can be rewritten as

$$\frac{\partial \varrho_a}{\partial t} + \frac{\partial \left(\varrho_a v_{a,k}\right)}{\partial x_k} = -\chi_a. \tag{29}$$

The **phase momentum equations**, after lengthy manipulations

$$\frac{\partial u_{a,i}}{\partial t} + \frac{\partial}{\partial x_k}\left(u_{a,i}v_{a,k} + P_a\delta_{ki}\right) = -c_a \sum_{b=1}^{N} p_b \frac{\partial \alpha_b}{\partial x^i} + p_a \frac{\partial \alpha_a}{\partial x^i} \tag{30a}$$

$$- c_a \sum_{b=1}^{N} \varrho_b \bar{v}_{b,k}\omega_{b,k,i} + \varrho_a \bar{v}_{a,k}\omega_{a,k,i} \tag{30b}$$

$$-c_a \sum_{b=1}^{N} \varrho_b s_b \frac{\partial T_b}{\partial x^i} + \varrho_a s_a \frac{\partial T_a}{\partial x^i} \tag{30c}$$

$$+c_a \sum_{b=1}^{N} \varrho_b \Lambda_{b,i} - \varrho_a \Lambda_{a,i} \tag{30d}$$

$$+c_a \sum_{b=1}^{N} v_{b,i}\chi_b - v_{a,i}\chi_a, \tag{30e}$$

SHTC - Extension to elasto-plastic solids and viscous fluid

Thanks to Eulerian hyperelasticity equations of Godunov and Romenski (GPR)

S.K. Godunov and E.I.Romenski. Non stationary equations of the non linear theory of elasticity in Euler coordinates. Journal of Applied Mechanics and Technical Physics, 13:868–885, 1972.

I. Peshkov and E.I. Romenski. A hyperbolic model for viscous Newtonian flows. Continuum Mechanics and Thermodynamics, 28:85–104, 2016.

An evolution equation for a matrix value field A_a, called **distortion matrix** or **cobasis**, should be added for each phase.

$\rightarrow$ In solid mechanics is the inverse of the deformation gradient.

$\rightarrow$ In visco-plastic flows is a local field of the material element.

A_a satisfies the convection-relaxation

$$\frac{\partial A_{a,i,k}}{\partial t} + \frac{\partial \left(A_{a,i,m} v_{a,m}\right)}{\partial x_k} + v_{a,m}\left(\frac{\partial A_{a,i,k}}{\partial x_m} - \frac{\partial A_{a,i,m}}{\partial x_k}\right) = Z_{a,i,k}, \qquad (31)$$

in which the stiff *strain relaxation source term* Z_a is

$$\mathsf{Z}_a = -\frac{3}{\tau_a}\left(\det \mathsf{A}_a\right)^{5/3} \mathsf{A}_a \operatorname{dev}\left(\mathsf{A}_a^{\mathsf{T}} \mathsf{A}_a\right). \qquad (32)$$

The total energy potential $\mathcal{E}$ should be augmented with ε_a^s

$$\mathcal{E} = \sum_{a=1}^{N}(\varepsilon_a + \varepsilon_a^s) + W(\rho, \varrho_a, \boldsymbol{w}_a) + \frac{1}{2\rho}\|\boldsymbol{U}\|^2. \qquad (33)$$

SHTC - Extension to elasto-plastic solids and viscous fluid

ε_a^s is assumed to be

$$\varepsilon_a^s = \varrho_a \, Cs_a^2 \, \frac{\mathrm{tr}\,(\mathrm{dev}\,\mathsf{G}_a \; \mathrm{dev}\,\mathsf{G}_a)}{4}, \qquad \text{with} \qquad \mathsf{G}_a = \mathsf{A}_a^{\mathsf{T}}\mathsf{A}_a \tag{34}$$

For this choice of elastic-shear energy potential, the elastic-shear stress tensor reads

$$\boldsymbol{\sigma}_a := -\varrho_a \mathsf{A}^T \frac{\partial \mathcal{E}}{\partial A} = -\varrho_a \, Cs_a^2 \, (\mathsf{G}_a \; \mathrm{dev}\,\mathsf{G}_a). \tag{35}$$

Numerical Method - A simplified model

A simplified mathematical model is addressed, for $N = 3$, $a = 1, 2, 3$

$$
\begin{aligned}
\frac{\partial \varrho_a}{\partial t} + \frac{\partial u_{a,k}}{\partial x_k} &= \; 0 \\
\frac{\partial u_{a,i}}{\partial t} + \frac{\partial}{\partial x_k}\left(u_{a,i} v_{a,k} + P_a \delta_{i,k} - \sigma_{a,k,i}\right) &= -c_a \sum_{b=1}^{N} p_b \frac{\partial \alpha_b}{\partial x^i} + p_a \frac{\partial \alpha_a}{\partial x^i} \\
&\quad - c_a \sum_{b=1}^{N} \varrho_b \bar{v}_{b,k} \omega_{b,k,i} + \varrho_a \bar{v}_{a,k} \omega_{a,k,i} + c_a \sum_{b=1}^{N} \lambda_b \varrho_b \bar{v}_{b,k} - \lambda_a \varrho_a \bar{v}_{a,k}, \\
\frac{\partial s_a}{\partial t} + V_k \frac{\partial s_a}{\partial x_k} &= \frac{\lambda_a}{T_a} c_a \bar{v}_{a,k}^2, \\
\frac{\partial \alpha_a}{\partial t} + V_k \frac{\partial \alpha_a}{\partial x_k} &= \; 0, \\
\frac{\partial A_{a,i,k}}{\partial t} + \frac{\partial (A^m_{a,i} v^m_a)}{\partial x_k} + v^m_a \left(\frac{\partial A_{a,i,k}}{\partial x^m} - \frac{\partial A^m_{a,i}}{\partial x_k} \right) &= \; Z_{a,i,k},
\end{aligned}
$$

Numerical Method - Matrix-vector notation

A compact matrix-vector notation can be defined as

$$\partial_t \mathsf{Q}_a + \nabla \cdot \mathsf{F}(\mathsf{Q}_a) + \mathsf{B}(\mathsf{Q}_a) \cdot \nabla \mathsf{Q}_a = \mathsf{S}(\mathsf{Q}_a) \tag{37}$$

with a vector of conserved Q_a and primitive V_a variables for each phase

$$\mathsf{Q}_a = (\varrho_a, \mathsf{u}_a, s_a, \alpha_a, A_a), \qquad \mathsf{V}_a = (\rho_a, \mathsf{v}_a, P_a, \alpha_a, A_a)^\top, \tag{38}$$

which are related by operators

$$\mathsf{Q}_a(x,y) = \mathcal{C}[\mathsf{V}_a(x,y)], \qquad \text{and} \qquad \mathsf{V}_a(x,y) = \mathcal{P}[\mathsf{Q}_a(x,y)]. \tag{39}$$

The quasi-linear form

$$\partial_t \mathsf{V}_a + \mathsf{C}\nabla \mathsf{V}_a = \mathsf{S}(\mathsf{V}_a), \ \text{with} \ \mathsf{C} = \frac{\partial \mathsf{Q}_a}{\partial \mathsf{V}_a}^{-1} \left(\frac{\partial \mathsf{F}(\mathsf{Q}_a)}{\partial \mathsf{V}_a} + \mathsf{B}(\mathsf{Q}_a) \frac{\partial \mathsf{Q}_a}{\partial \mathsf{V}_a} \right). \tag{40}$$

An **operator splitting** approach is employed.

→ first the *homogeneous* part of the system is solved

$$\partial_t \mathbf{Q} + \nabla \cdot \mathbf{F}(\mathbf{Q}) + \mathbf{B}(\mathbf{Q}) \cdot \nabla \mathbf{Q} = \mathbf{0}, \qquad \to \qquad \mathbf{Q}_{ij}^{(1)} \tag{41}$$

→ then the Cauchy problem for the *ODEs* system

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} = \mathbf{S}_v(\mathbf{Q}_a) + \mathbf{S}_s(\mathbf{Q}_a), \qquad \mathbf{Q}(t^n) = \mathbf{Q}^{(1)}, \qquad \to \qquad \mathbf{Q}_{ij}^{n+1} \tag{42}$$

$$\mathbf{S}_v(\mathbf{Q}_a) = \begin{pmatrix} 0 \\ +c_a \sum_{b=1}^{N} \lambda_b \varrho_b \bar{v}_{b,k} - \lambda_a \varrho_a \bar{v}_{a,k} \\ 0 \\ \frac{\lambda_a}{T_a} c_a \bar{v}_{a,k}^2 \\ \mathbf{0} \end{pmatrix}, \quad \mathbf{S}_s(\mathbf{Q}_a) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mathbf{Z}_a \end{pmatrix}, \tag{43}$$

A path-conservative MUSCL-Hancock method

$$\begin{aligned}
\mathsf{Q}_{i,j}^{(1)} = \mathsf{Q}_{i,j}^{n} &- \frac{\Delta t}{\Delta x}\left(\mathsf{F}_{i+1/2,j}^{RS} - \mathsf{F}_{i-1/2,j}^{RS} + \mathsf{D}_{i+1/2,j} + \mathsf{D}_{i-1/2,j}\right) + \\
&- \frac{\Delta t}{\Delta y}\left(\mathsf{F}_{i,j+1/2}^{RS} - \mathsf{F}_{i,j-1/2}^{RS} + \mathsf{D}_{i,j+1/2} + \mathsf{D}_{i,j-1/2}\right) + \\
&+ \frac{\Delta t}{\Delta x}\mathsf{B}_1\left[\mathsf{V}_{i,j}^{r}\left(t^{\,n+1/2}, x_i, y_j\right)\right]\Delta \mathsf{V}_i + \\
&+ \frac{\Delta t}{\Delta y}\mathsf{B}_2\left[\mathsf{V}_{i,j}^{r}\left(t^{\,n+1/2}, x_i, y_j\right)\right]\Delta \mathsf{V}_j .
\end{aligned} \tag{44}$$

Fluxes and non-conservative products are evaluated in the **primitive space of the variable**.

The conservative numerical flux F^{RS}

$$\begin{aligned}\mathsf{F}^{RS}_{i+1/2,j}(\mathsf{v}_L,\mathsf{v}_R) &= \frac{1}{2}\Big(\mathsf{F}_1(\mathsf{v}_L)+\mathsf{F}_1(\mathsf{v}_R)\Big)-\frac{1}{2}s_1^{\max}\Big(\mathcal{C}[\mathsf{v}_R]-\mathcal{C}[\mathsf{v}_L]\Big),\\ \mathsf{F}^{RS}_{i,j+1/2}(\mathsf{v}_L,\mathsf{v}_R) &= \frac{1}{2}\Big(\mathsf{F}_2(\mathsf{v}_L)+\mathsf{F}_2(\mathsf{v}_R)\Big)-\frac{1}{2}s_2^{\max}\Big(\mathcal{C}[\mathsf{v}_R]-\mathcal{C}[\mathsf{v}_L]\Big)\end{aligned} \tag{45}$$

The path integrals $\mathsf{D}_{i+1/2,j}$ and $\mathsf{D}_{i,j+1/2}$

$$\mathsf{D}_{\Psi}(\mathsf{v}_L,\mathsf{v}_R)\cdot\hat{\mathsf{n}} = \frac{1}{2}\int_0^1 \mathsf{B}\left[\Psi(\mathsf{v}_L,\mathsf{v}_R,s)\right]\cdot\hat{\mathsf{n}}\frac{\partial\Psi}{\partial s}ds \tag{46}$$

in which the segment path $\Psi(\mathsf{v}_L,\mathsf{v}_R,s)=\mathsf{v}_L+s(\mathsf{v}_R-\mathsf{v}_L)$

Numerical Method - Discretization of the homogenous part

The **cell-local space-time predictor** in the primitive space variable

$$\mathsf{V}^r_{i,j}(x,y,t) = \mathsf{V}_{i,j} + (x - x_{i,j})\frac{\Delta\mathsf{V}_i}{\Delta x} + (y - y_{i,j})\frac{\Delta\mathsf{V}_j}{\Delta y} + (t - t^n)\,\partial_t\mathsf{V}_{i,j}, \quad (47)$$

$\rightarrow \widetilde{\Delta\mathsf{V}}_i$, by means of *Generalised minmod slope limiter*

$\rightarrow \Delta\mathsf{V}_i$ positivity preserving limiting

$\rightarrow \partial_t\mathsf{V}_{i,j}$ approximated with finite difference from (40)
+ source contribution

Numerical Method - Discretization of the source contribution

Source related to the velocity relaxation process

$$\frac{\mathrm{d}\mathsf{V}}{\mathrm{d}t} = \mathsf{S}_v(\mathsf{V}), \qquad \mathsf{V}(t^n) = \mathcal{P}[\mathsf{Q}_{ij}^{(1)}] = \mathsf{V}_{ij}^{(1)}, \qquad \rightarrow \qquad \mathsf{V}_{ij}^{n+1} \tag{48}$$

$$\text{with} \qquad \mathsf{S}_v(\mathsf{V}_a) = \begin{pmatrix} 0 \\ +\sum_{b=1}^{N} \lambda_b c_b \bar{v}_{b,k} - \lambda_a \bar{v}_{a,k} \\ 0 \\ \frac{\lambda_a}{T_a} c_a \bar{v}_{a,k}^2 \\ \mathbf{0} \end{pmatrix}. \tag{49}$$

$\rightarrow$ for each direction, an independent system for $\widetilde{\mathsf{V}}_1 = (v_{1,1}, v_{2,1}, v_{3,1})^{\mathsf{T}}$

$\rightarrow$ Backward Euler dicretization

$$\widetilde{\mathsf{V}}_1^{n+1} = \widetilde{\mathsf{V}}_1^{(1)} - \Delta t\, \mathcal{M}\, \widetilde{\mathsf{V}}_1^{n+1} \quad \rightarrow \quad \widetilde{\mathsf{V}}_1^{n+1} = (I - \Delta t\, \mathcal{M})^{-1}\, \widetilde{\mathsf{V}}_1^{(1)} \tag{50}$$

$\rightarrow$ for entropy analytical solution $\mathsf{S}_v(\widetilde{\mathsf{V}}_1^{n+1}, T_a^n)$

Numerical Method - Discretization of the source contribution

Source related to the distortion matrix

$$\partial_t \mathsf{A}_a + \nabla\left(\mathsf{A}_a \cdot \mathsf{v}_a\right) + \left(\nabla \mathsf{A}_a - \nabla \mathsf{A}_a^{\mathsf{T}}\right) \cdot \mathsf{v}_a = \frac{-3}{\tau_a} \left(\det \mathsf{A}_a\right)^{5/3} \mathsf{A}_a \mathrm{dev} \mathsf{G}_a, \quad (51)$$

$\rightarrow$ highly non-linear, stiff, wide range of time scales,

$\rightarrow$ in multi-phase context $\tau_a(\alpha_a) = \tau_a^{\xi(\alpha_a)} \, \tau_0^{1-\xi(\alpha_a)}$,

$\rightarrow$ an robust method to solve the strain relaxation source [1]

S. Chiocchetti, M. Dumbser. An exactly curl-free staggered semi-implicit finite volume scheme for a first order hyperbolic model of viscous two-phase flows with surface tension. Journal of Scientific Computing, 94:24, 2023.

Source related to the distortion matrix

The problem is simplified by *polar decomposition*, recalling that the metric tensor $\mathsf{G}_a = \mathsf{A}_a^T \mathsf{A}_a$,

$$\mathsf{A}_a = \mathsf{R}_a \, \mathsf{G}_a^{1/2} \quad \text{with} \quad \mathsf{G}_a^{1/2} = \mathsf{E}_a \, \hat{\mathsf{G}}_a^{1/2} \, \mathsf{E}_a^{-1} \quad \rightarrow \quad \mathsf{R}_a = \mathsf{A}_a \, \mathsf{G}_a^{-1/2}, \tag{52}$$

$\rightarrow$ rotational component are invariant under strain relaxation

$\rightarrow$ thus the following nonlinear ODE system is solved

$$\frac{\mathrm{d}\mathsf{G}_a}{\mathrm{d}t} = \frac{\mathsf{G}_a^{(1)} - \mathsf{G}_a^{(n)}}{\Delta t} - \frac{6}{\tau_a} \left(\det \mathsf{G}_a \right)^{5/6} \mathsf{G}_a \, \mathrm{dev}\, \mathsf{G}_a \,, \tag{53}$$

Numerical experiments - Lid driven cavity

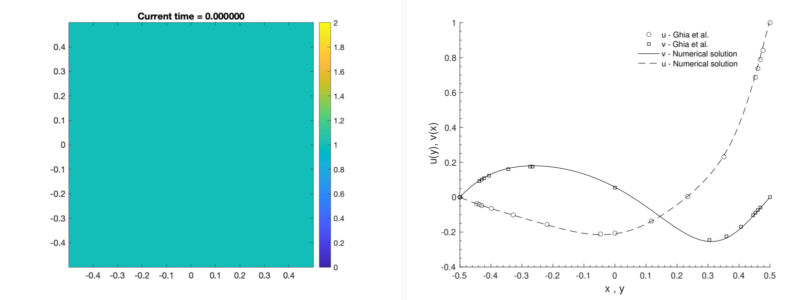

Figure 1: Rotations (Left), comparison velocity components in x and y-direction (Right)

Numerical experiments - Berilum bending plate

This problem simulates the elastic (reversible) vibrations of a beryllium bar after an initial velocity impulse

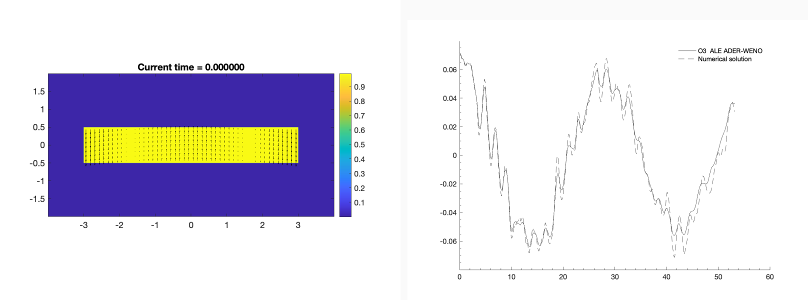

Figure 2: Volume fractions (Left), comparison velocity component in y-direction (Right)

Numerical experiments - Three phases 2D Riemann problem

This problem tests the ability of a model to propagate shock waves into different phases.

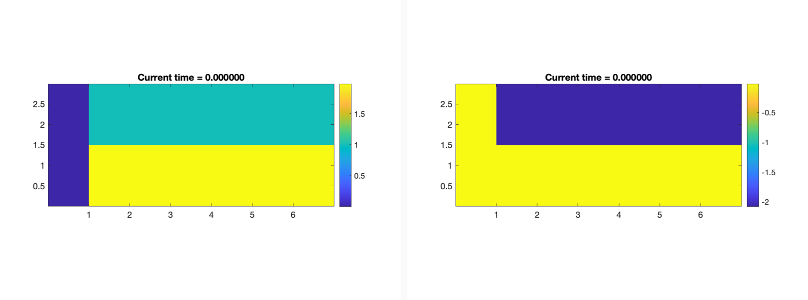

Figure 3: Volume fractions (Left), densities (Right)

Numerical experiments - Three phases 2D Riemann problem

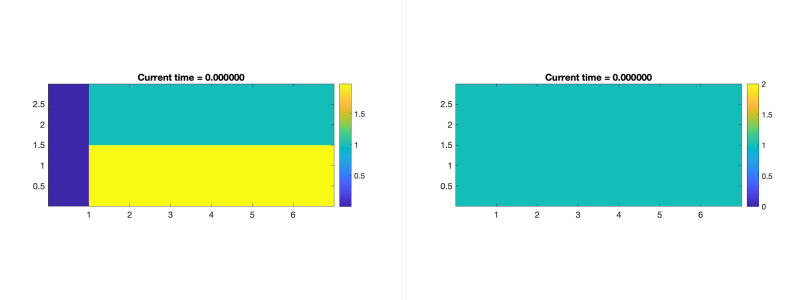

Figure 4: Volume fractions (Left), rotations (Right)

Numerical experiments - A complex configuration

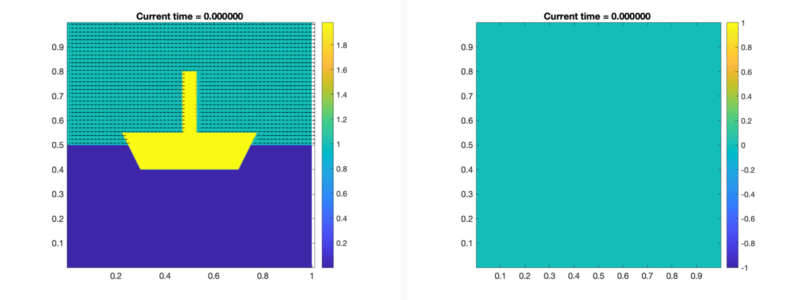

Figure 5: Volume fractions (Left), stress (Right)

Research directions

Some future research directions are:

- development of a **Hyperbolic Thermodynamically Compatible** (HTC) numerical scheme for the SHTC multiphase model, considering more than two phases;
- extension of the multi-phase SHTC model to include phenomena such as **phase change** and **surface tension**;
- development of a **structure-preserving** numerical scheme to account for different **involution constraints** present in SHTC systems;