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# Cell-centered Lagrange+Remap numerical strategy for a multi-material multi-velocity model

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#### ABSTRACT

The present work is devoted to the numerical approximation of multi-material flows. The so-called 6-equation system is considered where each material has its own velocity but shares the same pressure with the rest of the mixture. This model is a necessary building block as dissipation is completely removed outside of shocks. A numerical scheme is then presented and extends the classical "Lagrange+Remap" strategy to a multi-velocity setting. Entropy considerations are the focal point of its derivation as a mean of stabilizing results, ensuring thermodynamical consistency and selecting shocks of interest. Finally the scheme's robustness and ability to deal with the inner stiffness of contrasted mixtures are evaluated on several test cases.

#### 1. Introduction

Multi-material hydrodynamics is of paramount importance for both industrial and academic applications. Applications include, among others, pharmacology, aerodynamics, combustion, astrophysics, and climatology. Although all these applications differ in their physical regimes (*i.e.* material properties, domain and amplitude of physical quantities, dissipation, presence and strength of shocks, ...), the governing equations can be derived in a unified manner. The most common method is based on conditional averaging (Ishii, 1975; Drew and Passman, 1999; Wörner, 2003) of the single-material equations. Averaging, whether performed with respect to space, time, or statistical realizations, produces a mixed zone within which several materials coexist. The physical description and numerical treatment of these diffused interfaces is an active domain of research (Maltsev et al., 2022).

#### 1.1. Multi-material equations

Descriptions of multi-material hydrodynamics are numerous in the literature. The variety of equations stems from two reasons. First, different levels of description (Linga and Flåtten, 2019; Städtke, 2006; Maltsev et al., 2022) exist, from simple 4-equation models to 7-equation models. In the former, the mixture is described by a single equation of state and the interface is tracked with a scalar quantity (usually the mass fraction or the volume fraction). In the latter, each species has its own velocity and equation of state; the most famous instance of such model was introduced by Baer and Nunziato (1986). Obviously, the

more evolution equations are used, the more accurate the description of the mixture is, especially in the case of highly contrasted equations of state (*e.g.* mixtures of air and water). The second reason for the sheer variety of models is the number of system-dependent fluxes, exchange phenomena and closures (dissipative or not, and at large or small scales) such as surface tension, drag, added mass, viscosity, heat flux, etc. Although they are necessary for a complete description of the flow, they are heavily system-dependent. For a given number of variables, infinitely many models can be written depending on the chosen terms and their expression.

In the midst of all different possibilities, thermodynamics is sometimes forgotten in favor of other driving concepts such as hyperbolicity. For example, the Baer–Nunziato model, although well-posed, only conditionally satisfies the second principle of thermodynamics; and it usually does so by introducing an asymmetrical closure on the interface variables (Manach-Pérennou, 2023, §1.2) which prevents it from being universally used outside of its original purpose (namely modeling granular flows). The present work considers instead the so-called 6equation model where each material has its own velocity but shares its pressure with the rest of the mixture. Although its elliptic nature and ill-posedness has sparked controversy (Ramshaw and Trapp, 1978), this model is still relevant as it is formally isentropic and neglects all system-dependent terms. As such, these "backbone" equations consist in the greatest common divisor of all existing models.

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The assumption of pressure equality between all materials is a sensible approximation for numerous systems (Kapila et al., 2001; Manach-Pérennou et al., 2023). Even when it is no longer the case (Zhang et al., 2007), the 6-equation model is still a relevant starting point. Pressure discrepancies must indeed be given a proper phenomenological origin (by the introduction of surface tension for example) whose expression can then be included *a posteriori* into the model. This approach allows for the systematic construction of thermodynamically consistent equations where each additional term must either arise from a potential or be dissipative (and thus produce entropy).

#### 1.2. Numerical discretization

Strategies for the discretization of multi-material multi-velocity flows are numerous in the literature but few actually tackle the 6equation model considered in the present work. Some models are a far cry from the present equations (Saurel and Abgrall, 1999; Del Pino et al., 2018) while others introduce less intrusive modifications (Chang and Liou, 2003). Because the focus is put on hyperbolicity and wellposedness, compliance with the second principle of thermodynamics at the discrete level is a scare sight in the literature (Vazquez-Gonzalez et al., 2020). This challenge is yet all the more relevant in the context of the present work where systems are isentropic (outside of shocks) and thus at the brink of physical inconsistency. This justifies adamant requirements on numerical dissipation and its associated entropy traces as a mean of guaranteeing to be "on the right side on the fence". Apart from providing stability and physically-sound results, control of the numerical dissipation selects solutions inside shocks (Kapila et al., 2001; Heulhard de Montigny and Llor, 2022; Manach-Pérennou et al., 2023). The systematic study and control of discrete entropy traces will be the main guideline of this article.

The present work is an extension of the first-order cell-centered numerical scheme previously presented by the authors for multi-material but single-velocity hydrodynamics (Manach-Pérennou et al., 2023). The previous article focused on the justification and the thermodynamically-consistent treatment of the equality of pressures at the discrete level, in the context of shocks and highly contrasted materials. The present work then builds up on it by incorporating the multi-velocity aspects into the numerical strategy.

The single-velocity scheme is based on a "Lagrange + Remap" splitting (Benson, 1992; Hirt et al., 1974) where physical quantities are first computed on a moving mesh following the flow of the mixture (the Lagrange step) and are then projected on a new mesh whose choice is motivated by various user-controlled criteria (the remapping step). The "Lagrange + Remap" strategy becomes non-trivial in the context of multi-velocity flows as each material possesses its own Lagrangian trajectory. A common Lagrangian frame can be built from any average velocity of the mixture (Chang and Stagg, 2012) or each species can evolve on its own grid (Akselsen and Nydal, 2015). The present work favors an alternative approach where each material evolves in its own Lagrangian frame before being projected back on a common mesh as in Cournède (2001), Enaux (2007) and Del Pino et al. (2018). This socalled "Multi-Lagrange + Remap" formalism allows to exactly isolate the pressure terms in the Multi-Lagrange phase from the convection terms in the remapping phase, thus contributing to the convenient design of thermodynamically-consistent numerical schemes.

Compared to the previously published single-velocity scheme, this new extension to a multi-velocity setting comes with two main difficulties. First, the Lagrange phase of the previous scheme is based on the GLACE/EUCCLHYD method (Maire et al., 2007; Carré et al., 2009; Loubère et al., 2016; Breil, 2016), built on the hyperbolic nature of the equations and heavily relying on the use of approximate Riemann solvers. Such an approach is not compatible with the ellipticity of the 6-equation model. It is however shown in this article that a formal extension is still possible while retaining conservation of mass, momentum and energy, as well as consistency with thermodynamics. The second difficulty comes from the volume-filling condition which is shown to subtly couple the Lagrange and the Remap phases. This renders necessary a new approach to remapping which excludes traditional methods. A solution is here presented and shown to comply with the positiveness of density and volume fraction, as well as with an entropy criterion.

The article is organized as follows. In Section 2, the 6-equation model under consideration is presented. Explicit volume evolution equations are derived from the one-pressure assumption as in Vazquez-Gonzalez et al. (2020) and Heulhard de Montigny and Llor (2022). Shocks and ellipticity are also discussed. In Section 3, the numerical scheme is presented. The consequences and constraints of the multi-velocity aspects on the discretization are emphasized. Finally, the numerical scheme is applied to various one-dimensional and two-dimensional test cases in Section 4. They highlight the scheme's robust behavior in the context of shocks and contrasted mixtures.

#### 2. Multi-velocity model and thermodynamic closures

#### 2.1. Core equations

The present model is written in Lagrangian formalism for an arbitrary number of materials. The notations are standard with  $\alpha^k$ ,  $\rho^k$ ,  $\mathbf{u}^k$ , and  $e^k$  denoting the volume fraction, density, velocity and internal energy of material k. Each material is described by its own equation of state (EOS) which, in particular, defines its pressure  $p^k$  as a function of  $\rho^k$  and  $e^k$ . The EOS are arbitrary, provided they fulfill the thermodynamic constraints such as concavity of entropies  $s^k$  and real speeds of sound  $c^k$ . Because each material possesses its own velocity, it defines its own Lagrangian derivative  $\frac{d^k}{dt} = \frac{\partial}{\partial t} + \mathbf{u}^k \cdot \nabla$ . The mass, momentum, and internal energy equations are thus

$$\alpha^{k}\rho^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\alpha^{k}\rho^{k}}\right)-\nabla\cdot\mathbf{u}^{k}=0,\tag{1a}$$

$$\alpha^{k}\rho^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\mathbf{u}^{k}+\alpha^{k}\nabla p=0, \tag{1b}$$

$$\chi^{k}\rho^{k}\left[\frac{\mathrm{d}^{k}}{\mathrm{d}t}e^{k}+p^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\rho^{k}}\right)\right]=0,\tag{1c}$$

$$p^k(\rho^k, e^k) = p. \tag{1d}$$

**Remark 1.** Eqs. (1) are written in the updated Lagrangian formalism. Although this choice is uncommon, it allows to better clarify the thermodynamical nature of the equations and is consistent with the present numerical strategy. One can easily switch to the Eulerian formalism thanks to

$$\alpha^{k}\rho^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\phi = \frac{\partial}{\partial t}(\alpha^{k}\rho^{k}\phi) + \nabla \cdot (\alpha^{k}\rho^{k}\phi\mathbf{u}^{k}),\tag{2}$$

where  $\phi$  is any function. This identity comes from the definition of the Lagrangian derivative and the mass conservation of material *k*.

Eqs. (1) are commonly obtained through a conditioned averaging procedure introduced by numerous authors, among which (Ishii, 1975; Drew and Passman, 1999) and summarized in Wörner (2003) for non-miscible materials and in Heulhard de Montigny and Llor (2022, app. B) for general mixtures. Single material Euler equations with discontinuous thermodynamic properties are initially considered. These equations undergo a material-conditional averaging procedure which allows specific material quantities to be defined. Finally, if fluctuations appearing in the averaging procedure are neglected the final model is naturally isentropic for each material. The internal energy equation of material *k* thus corresponds to Gibbs identity  $de^k = -p^k d(1/\rho^k) + T^k ds^k$  with  $ds^k = 0$ . Correlation terms or other dissipative effects (*e.g.* viscosity, added mass, ...) can be added separately. Pressure equality (1d) is a sensible first approximation as, in the vast majority of multi-material systems, pressure relaxation processes between

materials occur on time scales much smaller than the characteristic hydrodynamic time scales (Kapila et al., 2001; Städtke, 2006). Alternatively, model (1) can be obtained through a variational principle (Gavrilyuk, 2011). It highlights the reversible, isentropic and geometrical nature of the equations. In this case, pressure equality is a direct consequence of this formalism without any further assumption.

Conservation of material masses and total momentum  $\sum_k \alpha^k \rho^k u^k$  are naturally ensured. So is conservation of total energy. Indeed, defining the volume averaged velocity

$$\overline{\mathbf{u}} = \sum_{k} \alpha^{k} \mathbf{u}^{k}, \tag{3}$$

an using the total volume filling condition  $\sum_k \alpha^k = 1$  gives,

$$\sum_{k} \alpha^{k} \rho^{k} \frac{d^{k}}{dt} e^{k} = -\sum_{k} \alpha^{k} \rho^{k} \frac{d^{k}}{dt} \left(\frac{1}{\rho^{k}}\right)$$

$$= -\sum_{k} \alpha^{k} \rho^{k} \frac{d^{k}}{dt} \left(\frac{1}{\rho^{k}}\right)$$
(4a)

$$= -p \sum_{k} \alpha^{k} \rho^{k} \frac{\mathbf{d}}{\mathbf{d}t} \left( \frac{1}{\rho^{k}} \right)$$
(4b)  
$$= -p \nabla \cdot \overline{\mathbf{u}},$$
(4c)

which eventually yields

$$\sum_{k} \alpha^{k} \rho^{k} \left[ \frac{\mathrm{d}^{k}}{\mathrm{d}t} e^{k} + \frac{\mathrm{d}^{k}}{\mathrm{d}t} \left( \frac{\|\mathbf{u}^{k}\|^{2}}{2} \right) \right] = -\nabla \cdot \left( p \overline{\mathbf{u}} \right).$$
(5)

Although the averaging process alleviates the treatment of interfaces, some details of the flow are lost once correlation terms are neglected and, as such, model (1) is underdetermined. Thermodynamical closures then need to be provided to specify shocks. Indeed, unlike single material shocks, multi-material ones are small-scale dependent which means that no complete jump relationships can be written without knowing the details of what is happening *inside* the shock (Kapila et al., 2001). Mathematically, this property comes from the fact that the system cannot be fully written in conservative form so that no canonical weak formulation exists (Dal Maso et al., 1995).

#### 2.2. Explicit volume closure for the equal pressure assumption

In (1c), the energy evolution is given as a function of the volume evolution, consistently with Gibb's equation. The underlying material expansion rates  $\frac{d^k}{dt}(1/\rho^k)$  associated with the algebraic relationships (1d) can be derived following the ideas introduced in Munkejord et al. (2009) for isentropic flows and extended in Vazquez-Gonzalez et al. (2020, §3.5) for arbitrary entropy productions. This alternate formulation allows to properly factor entropy production inside shocks which is essential to the present numerical strategy.

The coupling of pressures give rise to a linear system, with unknowns  $\frac{d^k}{dt}\rho^k$  and  $\frac{\partial}{\partial t}p$ . The first equation is given by total mass conservation and reads

$$\sum_{k} \left[ \rho^{k} \alpha^{k} \frac{d^{k}}{dt} \left( \frac{1}{\alpha^{k} \rho^{k}} \right) - \nabla \cdot \mathbf{u}^{k} \right] \alpha^{k} = 0$$
$$\iff \sum_{k} \frac{\alpha^{k}}{\rho^{k}} \frac{d^{k}}{dt} \rho^{k} = -\nabla \cdot \overline{\mathbf{u}}.$$
(6)

On the other hand, differentiating (1d) with respect to time gives

$$\frac{\partial}{\partial t}p = \frac{\mathrm{d}^{k}}{\mathrm{d}t}p^{k} - \mathbf{u}^{k} \cdot \nabla p.$$
(7)

Introducing the speed of sound  $c^k$  and the Grüneisen coefficient  $\Gamma^k$  (Menikoff and Plohr, 1989) of material k

$$(c^{k})^{2} = \left. \frac{\partial p^{k}}{\partial \rho^{k}} \right|_{s^{k}}, \quad \Gamma^{k} = \frac{1}{\rho^{k} T^{k}} \left. \frac{\partial p^{k}}{\partial s^{k}} \right|_{\rho^{k}}, \tag{8}$$

pressure derivatives may be written as a function of density and entropy derivatives

$$\frac{\partial}{\partial t}p = (c^k)^2 \frac{\mathrm{d}^k}{\mathrm{d}t} \rho^k + \rho^k \Gamma^k T^k \frac{\mathrm{d}^k}{\mathrm{d}t} s^k - \mathbf{u}^k \cdot \nabla p.$$
(9)

Solving the system formed by Eqs. (6) and (9) eventually yields

$$\alpha^{k}\rho^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\rho^{k}}\right)-\beta^{k}\nabla\cdot\overline{\mathbf{u}}+D^{k}=0,$$
(10)

with

$$D^{k} = \frac{\alpha^{k}}{\rho^{k}(c^{k})^{2}} \sum_{l} \beta^{l} \left[ (\mathbf{u}^{k} - \mathbf{u}^{l}) \cdot \nabla p + \Delta^{kl} \right],$$
(11a)

$$\beta^{k} = \frac{\alpha^{k}}{\rho^{k}(c^{k})^{2}} / \sum_{l} \frac{\alpha^{l}}{\rho^{l}(c^{l})^{2}} , \qquad (11b)$$

$$\Delta^{kl} = \rho^l \Gamma^l T^l \frac{\mathrm{d}^l}{\mathrm{d}t} s^l - \rho^k \Gamma^k T^k \frac{\mathrm{d}^k}{\mathrm{d}t} s^k.$$
(11c)

The term  $\nabla \cdot \overline{\mathbf{u}}$  in Eq. (10) comes from mass conservation and, as such, is purely geometric. It corresponds, in some sense, to a global deformation rate of the mixture which is then shared between materials according to weighting coefficients  $\beta^k$  ( $\beta^k \ge 0$  and  $\sum_k \beta^k = 1$ ). Because of these coefficients and their dependence on the thermodynamic, some stiffness may appear, especially in highly contrasted mixtures (Heulhard de Montigny and Llor, 2022) (*e.g.* air and water when  $\beta^{\text{air}} \gg \alpha^{\text{air}}$ ). The second term,  $D^k$ , corresponds to a volume exchange rate (*i.e.*  $\sum_k D^k =$ 0) and is induced by both the velocity drift between materials and their entropy production.

**Remark 2.** Model (1) is formally isentropic so that the term  $\Delta^{kl}$  is 0. Its incorporation is still relevant (1) inside shocks where reversibility is no longer possible or (2) at the discrete level where some form of numerical dissipation is always needed for stability (even though this term does not modify the formal consistency of the scheme).

#### 2.3. Small-scale effect closure

Shocks are crucial phenomena in most hydrodynamic applications and demand specific care in terms of both physical modeling and numerical treatment. They correspond to zones where quantities vary rapidly or even discontinuously in the vanishing viscosity limit. A notable feature of conservation laws (*e.g.* Euler equations) is that two states connected by a shock do not depend on its profile or on the underlying physical dissipation processes. This property does not extend to systems which are not fully conservative (*e.g.* model (1)) where shocks heavily depend on small-scale effects which do not always explicitly appear in the equations (Kapila et al., 2001). Both from physical and numerical points of view, being able to characterize the range of admissible shocks is a relevant issue.

In the case of the single fluid Euler equations, shocks are completely constrained by conservation of mass, momentum and total energy. Then, the resulting jump relationships (also known as the Rankine–Hugoniot equations in the theory of conservation laws) algebraically close the shock. The set of all right states which can be connected to a given left state through a left-moving or right-moving shock (*i.e.* a 1-shock or a 3-shock in mathematical terms) forms a one dimensional half-curve called the shock locus whose projection on the  $p - 1/\rho$  plane is known as the Hugoniot curve (Menikoff and Plohr, 1989). This essentially means that once the amplitude of the shock is given, other variables, including the shock speed, are immediately recovered as a consequence of conservation.

In the case of multi-material equations, this locus becomes a larger dimension object as illustrated in Fig. 1. The new dimensions offer new degrees of freedom and correspond to the total number of equations of the system minus the number of conserved quantities. For model (1) with *n* materials, this number is 2(n - 1). Hence, for a given amplitude, several shocks are admissible depending on the underlying short-wavelength phenomena. These phenomena may include drag, viscosity, heat exchange, added mass, and surface tension among others. Their number is way larger than the number of degrees of freedom which shows that multiple physical regularizations can define shocks connecting the same left and right states (although the details



**Fig. 1.** Schematic representation of the right states  $U_R$  which can be connected by a shock to a given left state  $U_L$ . Left : the case where all equations are conservation laws. The curve is one dimensional and  $U_R$  is completely determined by the shock amplitude. Right: the case where some equations cannot be written in conservative form. For a given shock amplitude, multiple states  $U_R$  are admissible. The gray region corresponds to the zone inside which each material entropy increases. The larger zone encircled by the dashed lines corresponds to the addition of heat exchange which allows some material entropy to decrease as long as the global entropy still increases.

of the shock's profile may still be different). Generally speaking, the regularized equations read

$$\alpha^{k}\rho^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\mathbf{u}^{k} + \alpha^{k}\nabla p = \varepsilon \mathbf{F}^{k},$$
(12a)

$$^{k}\rho^{k}\left[\frac{\mathrm{d}^{k}}{\mathrm{d}t}e^{k}+p^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\rho^{k}}\right)\right]=\varepsilon\lambda^{k}Q.$$
(12b)

where

α

- $\varepsilon$  is an arbitrarily small parameter controlling the width and steepness of the shock. The smaller  $\varepsilon$  is, the more narrow and steep the shock is.
- The term  $\mathbf{F}^k$  is a global force acting on material k. It may include individual terms (*i.e.* only concerning material k) such as viscosity, as well as exchanges of momentum between materials such as drag. Because of total momentum conservation, the sum  $\sum_k \mathbf{F}^k$  must correspond to a flux, hence the n 1 first degrees of freedom.
- Because of total energy conservation, the sum of powers  $-\sum_k \mathbf{u}^k \cdot \mathbf{F}^k$  is equal, up to a flux, to the total heat deposit Q > 0. It is then distributed among materials with respect to coefficients  $\lambda^k$ . According to Gibb's identity,  $\varepsilon \lambda^k Q$  corresponds to the entropy variation  $\alpha^k \rho^k T^k \frac{d}{dt} s^k$  of material *k*. Coefficients  $\lambda^k$  are such that  $\sum_k \lambda^k = 1$ , hence the remaining n 1 degrees of freedom. If no heat exchange between materials is present (adiabatic closure), coefficients  $\lambda^k$  are also positive.

This interaction between the different terms is represented in Fig. 2. Eq. (12b) and positivity of Q and  $\lambda^k$  shows that material entropies all increase with time which is a sufficient condition for the total entropy to increase, thus complying with the second principle of thermodynamics. Yet, it is not necessary as an additional heat exchange could decrease one material entropy while still inducing a total entropy production. With only incomplete EOS, temperatures are not accessible and there is no way of knowing if a given heat exchange is indeed entropic: this is why it has been excluded here. Nevertheless, it shows that heat exchange could increase the size of the locus defined by conditions (12a) and (12b) as represented by the dashed curves in Fig. 1. It is not a new degree of freedom *per se* as the dimension of the augmented locus remains the same. In this sense, (12)  $\lambda^k \geq 0$  should spread  $U_R$  over all degrees of freedom although not over their entire range.

**Remark 3.** The numerical strategy derived in the next section is consistent with Eqs. (1), which means that no forces  $\mathbf{F}^k$  or associated heat deposit Q are explicitly added inside the equations. The scheme however accounts for numerical dissipation whose form must be consistent with Eqs. (12) and thermodynamics. In this case,  $\varepsilon$  is related to the characteristic length of cells and can become arbitrarily close to



**Fig. 2.** Diagram displaying the physical origin of the different degrees of freedom. They all hinge around total energy conservation which allows some of the total kinetic energy to be transformed into a heat deposit. The loss of kinetic energy and increase in internal energy can both be freely shared among materials. In doing so, each of them provides n - 1 degrees of freedom on the right state of a shock.

zero as the mesh is refined. As such, numerical dissipation is evanescent inside smooth regions of the flow but still controls which shocks are approximated at the discrete level.

#### 2.4. The elephant in the room : ellipticity of the model

Model (1) is known to display elliptic behavior. This feature sparked much controversy in the community as ellipticity predicts unstable behavior at vanishing small scales, effectively rendering impossible any simulation on a fine mesh (Cournède, 2001). This article does not aim at extensively discussing the complex link between ellipticity and stability in the context of non-linear equations. Contributions may be found in Ramshaw and Trapp (1978), Keyfitz (2001) and Vazquez-Gonzalez et al. (2016). The stance retained in this article follows Vazquez-Gonzalez et al. (2016, app. A and refs therein).

- Model (1) is a *universal* starting point for any description of multi-material flows. Indeed, the model relies on the strong physical basis that is the least action principle (Gavrilyuk, 2011; Vazquez-Gonzalez et al., 2020). It may also be derived through an averaging procedure from the Euler equations whose wellposedness is widely accepted. Hence, the model is essentially correct up to some correlation terms which have been neglected as a first approximation after averaging.
- Small-scale effects (12) then need to be added to amend for the lack of these correlation terms. Apart from providing closures inside shocks (as discussed previously), they also damp short wavelength instabilities. As pointed out in Ramshaw and Trapp (1978), the model is still successful at predicting long wavelength behaviors such as Kelvin–Helmotz instabilities. Consequently, any small-scale effect that should be introduced should not be so intrusive as to seriously modify these phenomena.

That being stated, model (1) will be discretized as it is. In practice, a well-controlled numerical dissipation should mimick Eqs. (12) at the discrete level. In this case,  $\epsilon$  is implicitly related to both the cell characteristic lengths and the order of the scheme. It is also



Fig. 3. Cell notations.

inversely proportional to an underlying cutoff frequency beyond which instabilities are damped. Refining the mesh then allows the growth of instabilities at larger and larger frequencies, to the point where it may abruptly stop the simulation. Results can still be obtained on coarse enough meshes (Vazquez-Gonzalez et al., 2020).

#### 3. Numerical strategy

#### 3.1. Geometry and notations

The notations are similar to those introduced in Maire (2011), Chauvin et al. (2022) and Manach-Pérennou et al. (2023). Each cell is assigned a unique index c and is denoted by  $\omega_c$ . Its volume is  $V_c$ . The two-dimensional cells are assumed to be polygonal so that they are defined by the set of their nodes  $\mathcal{P}(c)$ . For a given node p,  $\mathbf{x}_p$  and  $\mathbf{u}_p$  are its position and velocity while C(p) is the set of cells that contain p. Corner vectors (Goad, 1960) are given by

$$l_{pc}\mathbf{n}_{pc} = \frac{\partial V_c}{\partial \mathbf{x}_p},\tag{13}$$

where  $\mathbf{n}_{pc}$  is a unit vector. They can equivalently be constructed as follows :  $p^+$  is the node in  $\mathcal{P}(c)$  which follows p in counterclockwise order and  $p^-$  the previous node. Let  $\mathbf{n}_{pc}^+$  be the outward normal unit vector to the edge  $pp^+$  and define  $l_{pc}^+ = \frac{1}{2} \|pp^+\|$  ( $\mathbf{n}_{pc}^-$  and  $l_{pc}^-$  are defined accordingly). Finally

$$\mathbf{n}_{pc} = \frac{l_{pc}^{+} \mathbf{n}_{pc}^{+} + l_{pc}^{-} \mathbf{n}_{pc}^{-}}{l_{pc}},$$
(14a)

$$l_{pc} = \left\| l_{pc}^{+} \mathbf{n}_{pc}^{+} + l_{pc}^{-} \mathbf{n}_{pc}^{-} \right\|_{2}.$$
 (14b)

All the notations are illustrated in Fig. 3.

#### 3.2. Global strategy

The present article aims at extending the work introduced in Manach-Pérennou et al. (2023) for a single velocity model. This previous scheme relies on a Lagrange+Remap approach, meaning that each time step consists in two main phases plus an additional pressure equilibration procedure. Here are the summarized the main ingredients of the previously published scheme.

 The Lagrangian phase is based on an extension of the GLACE/EUCCLHYD (Carré et al., 2009; Loubère et al., 2016) scheme to a multi-material one pressure setting. The GLACE/ EUCCLHYD scheme is Lagrangian, cell-centered and allows a semi-discrete entropy production to be written as

$$m_c T_c \frac{\mathrm{d}}{\mathrm{d}t} s_c = m_c \left[ \frac{\mathrm{d}}{\mathrm{d}t} e_c + p_c \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{1}{\rho_c} \right) \right]$$

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$$= \sum_{p \in \mathcal{P}(c)} (\mathbf{u}_p - \mathbf{u}_c) \cdot \mathbf{M}_{pc} (\mathbf{u}_p - \mathbf{u}_c), \tag{15}$$

where  $\mathbf{M}_{pc}$  are symmetric positive matrices ensuring that the entropy increases. Their exact expression is what distinguishes GLACE from EUCCLHYD. The main ingredients of the multimaterial extension concern the evolution equations of the densities and the thermodynamical consistency of the internal energy equations. The density equations ensure equality of pressures up to the time order of the scheme. Once they have been specified, internal energies evolve consequently

$$\frac{\mathrm{d}}{\mathrm{d}t}e_c^k = -p_c \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{\rho_c^k}\right) + T_c^k \frac{\mathrm{d}}{\mathrm{d}t}s_c^k.$$
(16)

where  $\alpha^k \rho^k T^k \frac{d}{dt} s^k$  is taken as an arbitrary portion of the total irreversible work of the scheme (15). This ensures thermodynamic consistency as each material entropy increases over time. The arbitrary distribution of the total irreversible work also allows to capture different solutions in keeping with the discussion of Section 2.3.

- Once all material quantities have evolved on the Lagrangian mesh, they are remapped on the initial mesh. The remapping procedure is essentially independent of the chosen strategy for the Lagrangian step. An Alternate Direction projection (Duboc et al., 2010) is chosen for its entropic character (at first order), easy extensions to second order, and overall simplicity.
- Finally, an equilibration procedure is added so as to enforce pressure equality up to machine precision. This procedure relies on an iterative method (here Newton's method) to solve the following non-linear system of equations

$$\sum_{k} (\alpha \rho)^{k, n+1} e^{k, n+1} = \sum_{k} (\alpha \rho)^{k, n+1} e^{k, \star},$$
(17a)

$$e^{k,n+1} - e^{k,\star} = -p\left(\frac{1}{\rho^{k,n+1}} - \frac{1}{\rho^{k,\star}}\right),$$
 (17b)

$$p = p^{k}(\rho^{k,n+1}, e^{k,n+1}).$$
(17c)

where the exponent  $\star$  is used for the quantities before correction and n + 1 for the corrected variables. This system, by virtue of its implicit pressure work (Lagoutière, 2000; Heulhard de Montigny and Llor, 2022), prevents entropy destruction while conserving total volume and total energy of the system.

Extending this approach to a multi-velocity model is no simple task. The main challenge comes from the very definition of the Lagrangian phase as there exists as many Lagrangian frames as there are materials. The choice retained for this work consists in a "Multi-Lagrange + Remap" approach where all quantities associated with a given material are first computed on its own Lagrangian frame as in Cournède (2001), Enaux (2007) and Del Pino et al. (2018). Quantities then evolve on different frames before being projected on a common mesh, which is here taken as the initial one (see Fig. 4). Finally, the pressure relaxation procedure is not concerned with the multi-velocity aspects and is thus left unchanged. The resulting scheme is only at first order, both in time and space. Extension to higher order is discussed in the conclusion.

The multi-Lagrange and the remapping steps will be presented in Sections 3.4 and 3.5 respectively. During the Lagrangian phase, the main difference with the single-velocity version (Manach-Pérennou et al., 2023) comes from writing individual momentum equations while still algebraically preserving total momentum and total energy conservation. This is shown not to be a trivial matter in the context of the GLACE/EUCCLHYD scheme. As for the remapping procedure, total volume conservation requires some form of consistency with the Lagrange phase. This difficulty is specific to the multi-velocity setting. Before delving into all these issues, a global overview of the scheme's entropy production is given in Section 3.3. It serves as a foundation for the following discussions and justifies the adamant requirements on entropy.



**Fig. 4.** Schematic representation of the "Multi-Lagrange + Remap" approach with two materials. The notation  $L^k$  is used for quantities computed on the Lagrangian frame of material k.

#### 3.3. Considerations on entropy

Control of entropy production is a key ingredient for all multimaterial compressible schemes. It serves two main purposes, namely stabilizing and selecting solutions of interest. Stabilization ensures that numerical simulations do not explode over time, especially around shocks where a strict entropy inequality is required (Von Neumann and Richtmyer, 1950; Lax, 1973). More generally, it ensures that solutions are physically admissible as destroying entropy could create spurious shocks inside what should be rarefaction waves. Secondly, as explained in Section 2.3, ensuring an entropy inequality is not sufficient to fully define solutions; the details of entropy production are then crucial to properly select solutions inside shocks and consist in the second n - 1degrees of freedom identified in Section 2.3.

A comprehensive list of entropy sources in the present numerical scheme is now given.

• The main source of entropy is introduced during the Lagrange phase where some kind of numerical viscosity is added to the pressure work in the internal energy equations by the GLACE/EUCCLHYD scheme procedure. As the total irreversible work *Q* is known explicitly, it may be shared *arbitrarily* among materials

$$\alpha^{k}\rho^{k}\left[\frac{\mathrm{d}^{k}}{\mathrm{d}t}e^{k}+p\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\rho^{k}}\right)\right]=\lambda^{k}Q,$$
(18)

where  $\lambda^k$  are arbitrary coefficients between 0 and 1 whose sum over all materials is 1. Changing the coefficients will change the numerical solution inside shocks, even at convergence (Heulhard de Montigny and Llor, 2022; Manach-Pérennou et al., 2023). Their specification must then be driven by physics and cannot reasonably be determined by numerical considerations alone.

The second main source of entropy (and more generally of numerical diffusion) is the remapping step. A sensible remapping procedure should consist in some sort of averaging. Convex inequalities then ensure that no entropy is destroyed over time. If it provides strong robustness, the remapping procedure may induce accuracy issues as its underlying numerical diffusion pollutes the numerical viscosity terms. Their sum acts as an *effective* viscosity which remains partially uncontrolled, thus inducing some potential convergence issues (LeFloch and Mishra, 2014; Heulhard de Montigny and Llor, 2022) for systems whose shock are small-scale

dependent. These can still be mitigated by a higher order remapping procedure and, more generally, consist in a compromise between accuracy and robustness. This discussion also applies to the following items of the list for which entropy distribution is also not controlled, although their effect is not as substantial as for the remapping procedure.

· The volume-filling condition

$$\frac{\partial}{\partial t}\sum_{k}\alpha^{k} = 0 \tag{19}$$

must be satisfied at the discrete level. If the spatial discretization fails to preserve the sum of volume fractions, one might be tempted to add, what would seem at first, a mere normalization step. However, because masses must be conserved, products  $\alpha^k \rho^k$ cannot be modified. Changes in volume fractions  $\alpha^k$  then carry out as changes in densities  $\rho^k$  which, in turn, alter entropy. More precisely, if the sum  $\sum_k \alpha^k$  is greater than 1 at the end of a time iteration, then normalization will reduce volume fractions and increase densities  $\rho^k$ , thus destroying entropy for all materials (for positive pressures). This issue will be further discussed in Section 3.5.

- The additional pressure equilibration step (17) also creates an entropy residue. Its sign is always positive thanks to the implicit pressure formulation (Lagoutière, 2000; Heulhard de Montigny and Llor, 2022; Manach-Pérennou et al., 2023). Because pressures are already equal up to the scheme order, this residue may be deemed minor compared to the other entropy contributions.
- In general, time integration induces entropy variations. For instance, time integration of pressure work during Lagrangian phases produces an additional residue whose sign depends on the time at which pressure is taken. Implicit pressure will always result in a positive entropy production while explicit pressure will always destroy entropy (Heulhard de Montigny and Llor, 2022). Once again, this entropy variation is minor compared to the other aforementioned contributions but it still needs to be taken into account for demanding test cases (Heulhard de Montigny and Llor, 2022).

#### 3.4. Multi-Lagrange phase

3.4.1. Numerical viscosity, conservation of total momentum and total energy

Momentum and internal energy equations must be discretized in a consistent manner with (12) so as to produce stable results, particularly in the vicinity of shocks. In the single fluid GLACE/EUCCLHYD scheme, (15) serves this very purpose and may be interpreted as a form of numerical viscosity. However, the exact expression of the numerical viscosity comes from approximate Riemann solvers at the nodes. Consequently, fluxes act as black boxes where both pressure and viscous terms are intertwined. They cannot be separated in the sense that it is not possible to find an estimation of the gradient  $[\nabla p]_c$  such that

$$p_c [\nabla \cdot \mathbf{u}]_c + \mathbf{u}_c \cdot [\nabla p]_c \tag{20}$$

is a flux. Details may be found in Appendix A. This failure has two major consequences: (1) numerical viscosity cannot be removed from the scheme in regions where it is not needed (*e.g.* rarefaction waves); (2) its discretization must take into account that of the pressure terms. (1) and (2) are not specific to this particular scheme and are rather common properties of Godunov-like schemes. The latter consequence heavily constrains the discretization of total momentum and total energy so as to ensure conservation of both. A possibility is to formally replace *u* in the single velocity scheme with  $\overline{u}$ 

$$m_c^k \frac{\mathrm{d}^k}{\mathrm{d}t} \mathbf{u}_c^k = \alpha_c^k \sum_{p \in \mathcal{P}(c)} \mathbf{M}_{pc}(\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c), \tag{21a}$$

=

$$\sum_{k} m_{c}^{k} \frac{\mathbf{d}^{k}}{\mathbf{d}t} e_{c}^{k} = -p_{c} \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \cdot \overline{\mathbf{u}}_{p} + \sum_{p \in \mathcal{P}(c)} (\overline{\mathbf{u}}_{p} - \overline{\mathbf{u}}_{c}) \cdot \mathbf{M}_{pc} (\overline{\mathbf{u}}_{p} - \overline{\mathbf{u}}_{c}).$$
(21b)

**Proposition 1.** Eqs. (21) ensure conservation of both total momentum and total energy provided that

$$\overline{\mathbf{u}}_{p} = \mathbf{M}_{p}^{-1} \sum_{c \in C(p)} \left[ \mathbf{M}_{pc} \overline{\mathbf{u}}_{c} + p_{c} l_{pc} \mathbf{n}_{pc} \right]$$
with  $\mathbf{M}_{p} = \sum_{c \in C(p)} \mathbf{M}_{pc}$ .
(22)

**Proof.** The proof follows the approach introduced in Maire et al. (2007). Node forces are defined by

$$\mathbf{F}_{pc} = -p_c l_{pc} \mathbf{n}_{pc} + \mathbf{M}_{pc} (\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c).$$
(23)

Summing Eq. (21a) over all materials gives the total momentum evolution

$$\sum_{k} m_{c}^{k} \frac{\mathrm{d}^{k}}{\mathrm{d}t} \mathbf{u}_{c}^{k} = \sum_{p \in \mathcal{P}(c)} \mathbf{M}_{pc} (\overline{\mathbf{u}}_{p} - \overline{\mathbf{u}}_{c})$$
(24a)

$$= \sum_{p \in \mathcal{P}(c)} \left[ -p_c l_{pc} \mathbf{n}_{pc} + \mathbf{M}_{pc} (\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c) \right]$$
(24b)

$$= \sum_{p \in \mathcal{P}(c)} \mathbf{F}_{pc}.$$
 (24c)

Pressure terms have been artificially added although they do not contribute to the sum (because  $\sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} = 0$ ). On the other hand, lengthy algebraic computations show that the total energy is given by

$$\sum_{k} m_{c}^{k} \left[ \frac{\mathrm{d}^{k}}{\mathrm{d}t} \frac{|\mathbf{u}_{c}^{k}|^{2}}{2} + \frac{\mathrm{d}^{k}}{\mathrm{d}t} e_{c}^{k} \right] = \sum_{p \in \mathcal{P}(c)} \mathbf{F}_{pc} \cdot \overline{\mathbf{u}}_{c}.$$
(25a)

A local (nodal) conservation property is sought and reads

$$\sum_{c \in \mathcal{C}(p)} \mathbf{F}_{pc} = 0, \tag{26a}$$

$$\sum_{c \in \mathcal{C}(p)} \mathbf{F}_{pc} \cdot \overline{\mathbf{u}}_{c} = 0.$$
(26b)

Factorizing  $\overline{\mathbf{u}}_c$  in (26b) shows that the latter equation is a direct consequence of the former, which is itself satisfied as soon as  $\overline{\mathbf{u}}_p$  is defined by (22).  $\Box$ 

**Remark 4.** It is not immediately clear that the right-hand side of (21a) is consistent with a pressure gradient. Injecting expression (22) in (21a) makes it more apparent. Details may be found in Després (2010) and Appendix A.

#### 3.4.2. Density, internal energy and entropy equations through thermodynamical consistency

The discussion conducted in the previous Section 3.4.1 are deeply tied to the GLACE/EUCCLHYD formalism. Although total momentum and total energy conservation should be a universal concern, the provided answer to this issue is specific to the present approach. The following discussion has however a larger scope. It is rooted in thermodynamical consistency and should apply to a wide array of multi-material schemes (as in Vazquez-Gonzalez et al. (2020) for instance). Internal energy, density, and entropy discretizations are related to each other through Gibbs identity. It is the first step to warrant thermodynamic consistency of the scheme and reads

$$\frac{\mathrm{d}^{k}}{\mathrm{d}t}e_{c}^{k} = -p_{c}\frac{\mathrm{d}^{k}}{\mathrm{d}t}\left(\frac{1}{\rho_{c}^{k}}\right) + T_{c}^{k}\frac{\mathrm{d}^{k}}{\mathrm{d}t}s_{c}^{k}.$$
(27)

Both density and entropy evolution rates are chosen to guarantee that (27) is compatible with (21b). The geometric term  $\nabla \cdot \overline{\mathbf{u}}$  is identified

as  $\sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \overline{\mathbf{u}}_{p}$  in Eq. (21b). It is then shared between materials with respect to coefficients  $\beta_{c}^{k}$ . A consistent discretization  $D_{c}^{k}$  of the exchanges (11a) is added to complete the density evolution

$$m_{c}^{k} \frac{\mathrm{d}^{r}}{\mathrm{d}t} \left(\frac{1}{\rho_{c}^{k}}\right) = \beta_{c}^{k} \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \overline{\mathbf{u}}_{p} + D_{c}^{k}, \qquad (28a)$$
$$D_{c}^{k} = \frac{\alpha_{c}^{k}}{\rho_{c}^{k} (c_{c}^{k})^{2}} \sum_{l} \beta_{c}^{l} \left[ (\mathbf{u}_{c}^{k} - \mathbf{u}_{c}^{l}) \cdot \sum_{p \in \mathcal{P}(c)} \mathbf{M}_{pc} (\overline{\mathbf{u}}_{p} - \overline{\mathbf{u}}_{c}) + \Delta_{c}^{kl} \right], \qquad (28b)$$

$$\Delta_c^{kl} = \frac{\Gamma_c^l}{\alpha_c^l} m_c^l T_c^l \frac{\mathrm{d}^l}{\mathrm{d}t} s_c^l - \frac{\Gamma_c^k}{\alpha_c^k} m_c^k T_c^k \frac{\mathrm{d}^k}{\mathrm{d}t} s_c^k.$$
(28c)

Finally, the total heat deposit is identified in (21b) to be  $\sum_{p \in \mathcal{P}(c)}(\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c) \cdot \mathbf{M}_{pc}(\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c)$ . As in (18), it is shared arbitrarily between materials with respect to coefficients  $\lambda_c^k$ 

$$m_c^k T_c^k \frac{\mathrm{d}^k}{\mathrm{d}t} s_c^k = \lambda_c^k \sum_{p \in \mathcal{P}(c)} (\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c) \cdot \mathbf{M}_{pc} (\overline{\mathbf{u}}_p - \overline{\mathbf{u}}_c).$$
(29)

If both the total heat deposit and coefficients  $\lambda_c^k$  are positive, the next proposition immediately follows.

**Proposition 2.** The semi-discrete Lagrangian procedure increases entropy inside each cell and for each material

$$\frac{d^k}{dt}s_c^k \ge 0. \tag{30}$$

To conclude this section on thermodynamic consistency, the expression of the matrices  $\mathbf{M}_{pc}$  is now discussed. The matrices are symmetric in order to ensure a positive total heat deposit. As in Maire et al. (2007) and Loubère et al. (2016), they are chosen to be proportional to

$$\mathbf{M}_{pc} \propto \left( l_{pc}^{+} \mathbf{n}_{pc}^{+} \otimes \mathbf{n}_{pc}^{+} + l_{pc}^{-} \mathbf{n}_{pc}^{-} \otimes \mathbf{n}_{pc}^{-} \right).$$
(31)

The amplitude must ensure sufficient dissipation so as to produce a stable scheme. It must be consistent with a density times a velocity. As prescribed in Vazquez Gonzalez (2016), it is taken as

$$\left(\sum_{k} \frac{(\beta_c^k)^2}{\alpha_c^k} \rho^k\right) c_{0,c}^2 \tag{32}$$

where  $c_0$  is the mixture speed of sound at zero drag (Martínez Ferrer et al., 2012)

$$c_{0,c}^{2} = \sum_{k} \beta_{c}^{k} (c_{c}^{k})^{2}.$$
(33)

In the case of a light gas flowing against an inert incompressible ( $\beta \rightarrow 0$ ) material, the numerical viscosity on the gas reduces to the singlematerial scheme: the wall has no effect on the dynamics of the system. On the other hand, a mixture of two identical gases (same density, velocity, energy and equation of state but arbitrary volume fraction field) is described, as expected, by the single-material Lagrangian scheme.

#### 3.4.3. Lagrangian volume and node velocities

The derivation of Lagrangian volume equations are quite straightforward. The only essential modification from the single material scheme is the fact that as many equations as there are materials are now needed.

$$m_{c}^{k} \frac{\mathrm{d}^{k}}{\mathrm{d}t} \left( \frac{1}{(\alpha \rho)_{c}^{k}} \right) = \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k}.$$
(34)

The term  $l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k}$  is a node flux ensuring conservation of total volume. The conservation is local as the sum of fluxes over all cells of a given node is zero (as in the proof of Proposition 1). Eq. (34) may be seen as a consistent discretization of Eq. (1a). It also corresponds to the derivative of the Lagrangian volume, using the chain rule and the formula  $\frac{\partial V_{c}}{\partial \mathbf{x}_{p}} = l_{pc} \mathbf{n}_{pc}$ . This double interpretation is why Eq. (34) is often referred to as the Geometric Conservation Law (Thomas and Lombard, 1979). The remaining difficulty lies in the definition of material node velocities  $\mathbf{u}_p^k$ . Up until now, only the average node velocity  $\overline{\mathbf{u}}_p$  is known (22). It is then natural to enforce equality

$$\overline{\mathbf{u}}_{p} = \sum_{k} \alpha_{p}^{k} \mathbf{u}_{p}^{k}, \tag{35}$$

where node estimates of volume fractions  $a_p^k$  still need to be specified. Eq. (35) will be shown to have profound consequences on the remapping procedure and  $a_p^k$  will only then be defined. From (35), material node velocities are taken as

$$\mathbf{u}_{p}^{k} = \mathbf{M}_{p}^{-1} \sum_{c \in \mathcal{C}(p)} \left[ \mathbf{M}_{pc} \mathbf{u}_{c}^{k} + p_{c} l_{pc} \mathbf{n}_{pc} \right] + C_{p},$$
(36a)

$$C_{p} = \sum_{k} \mathbf{M}_{p}^{-1} \left[ \sum_{c \in C(p)} \mathbf{M}_{pc} \alpha_{c}^{k} \mathbf{u}_{c}^{k} - \alpha_{p}^{k} \sum_{c \in C(p)} \mathbf{M}_{pc} \mathbf{u}_{c}^{k} \right].$$
(36b)

 $C_p$  is a covariance term that may also be written  $\sum_k \mathbb{E}_p[\alpha^k \mathbf{u}^k] - \mathbb{E}_p[\alpha^k]\mathbb{E}_p[\mathbf{u}^k]$  where  $\mathbb{E}_p[X]$  is some node estimation of *X*. It is necessary for (35) but might be negligible in practice.

#### 3.4.4. Time integration

A standard Euler forward strategy is chosen for the time discretization. The scheme is then explicit, all spatial terms derived in the previous sections being taken at the initial time. In keeping with (Cheng et al., 2012), some caution still needs to be exercised on the velocity  $\bar{\mathbf{u}}_c$  for discrete total energy conservation.

$$m_{c}^{k} \frac{e_{c}^{k,L^{k}} - e_{c}^{k,n}}{\Delta t} = -p_{c}^{n} \frac{m_{c}^{k}}{\Delta t} \left( \frac{1}{\rho_{c}^{k,L^{k}}} - \frac{1}{\rho_{c}^{k,n}} \right) + \lambda_{c}^{k} \sum_{p \in \mathcal{P}(c)} (\overline{\mathbf{u}}_{p}^{n} - \overline{\mathbf{u}}_{c}^{n}) \cdot \mathbf{M}_{pc}^{n} \left( \overline{\mathbf{u}}_{p}^{n} - \frac{\overline{\mathbf{u}}_{c}^{n} + \overline{\mathbf{u}}_{c}^{L}}{2} \right).$$
(37)

The exponent  $L^k$  is used for the quantities computed in the Lagrangian frame of material k and

$$\overline{\mathbf{u}}_{c}^{L} = \sum_{k} \alpha_{c}^{k,n} \mathbf{u}_{c}^{k,L^{k}}.$$
(38)

The resulting scheme is still fully explicit as velocities are computed before internal energies. As stated earlier, although the semi-discrete scheme is strictly entropic for each material, time integration may destroy small amounts of entropy. It does so through the explicit time integration of pressure work (Heulhard de Montigny and Llor, 2022) and the discrete energy deposit in (37) where the half sum  $(\overline{\mathbf{u}}_c^n + \overline{\mathbf{u}}_c^L)/2$  prevents it from being a perfect squared norm.

The time step  $\Delta t$  is subject to two constraints. First, a CFL-like condition accounts for the propagation of acoustic waves. It reads

$$\Delta t = \text{CFL} \times \min_{k,c} \left( \frac{V_c}{P_c(c_{0,c} + \|\mathbf{u}_c^k\|)} \right),$$
(39)

where  $V_c$  is the volume of the cell,  $P_c$  its perimeter and  $c_{0,c}$  the speed of sound of the mixture (33). CFL is a parameter, of the order of 1, which must be tuned. Additionally,  $\Delta t$  is chosen so as to prevent cell volumes and volume fractions from becoming negative.

#### 3.5. Remap phase : Lagrange/remap consistency and volume conservation

The following discussion is restricted to the one dimensional scheme where cells are ordered from left to right by indexes  $i \in \mathbb{Z}$  while nodes are denoted by half-integers  $i + \frac{1}{2}$ . The one dimensional setting is sufficient to illustrate the necessity of some form of consistency between the Lagrange and the remapping, as well as how the issue was tackled in the present work. The general multi-dimensional remapping procedure may be found in Appendix B.

#### 3.5.1. From volume conservation to a common diffusion

In the context of a Multi-Lagrange+Remap approach, enforcing the volume filling condition (19) at the discrete level is no simple matter. Because each  $\alpha^k$  is first computed on its own Lagrangian frame, the sum may not be conserved during the Lagrange step, nor may it be maintained during the remapping step. It is then crucial to ensure that both steps compensate each other as best as possible. Failing to do so would make the normalization step all the more intrusive which, as explained in 3.3, may jeopardize the scheme stability and its consistency with thermodynamics.

In practice, the divergence term  $\nabla \cdot \mathbf{\bar{u}}$  appearing in the Lagrange step (6) must cancel with the sum of the remapping fluxes for the volume fractions  $\sum_{k} \nabla \cdot (\alpha^{k} \mathbf{u}^{k})$ . It should not come as a surprise considering the computations performed in (6) and the geometric nature of the term  $\nabla \cdot \mathbf{\bar{u}}$ . In one dimension, the sum over all materials of Eq. (10) yields

$$\sum_{k} \left( V_i^{k,L^k} - V_i^{k,n} \right) = \Delta t \left( \overline{\overline{u}}_{i+\frac{1}{2}} - \overline{\overline{u}}_{i-\frac{1}{2}} \right), \tag{40}$$

while a generic remapping procedure should be written

$$\sum_{k} \left( V_{i}^{k,n+1} - V_{i}^{k,L^{k}} \right) = -\Delta t \sum_{k} \left( (\alpha u)_{i+\frac{1}{2}}^{k} - (\alpha u)_{i-\frac{1}{2}}^{k} \right),$$
(41)

where  $(\alpha u)_{i+\frac{1}{2}}^{k}$  are node flux estimations. Total volume conservation means that fluxes from Eqs. (40) and (41) should cancel out. It yields the following equation which is to be compared with (35)

$$\overline{\mathbf{u}}_{i+\frac{1}{2}} = \sum_{k} (\alpha \mathbf{u})_{i+\frac{1}{2}}^{k}.$$
(42)

Remap procedures often consist in upwinding physical quantities as it provides stability while still remaining quite simple. In a multi-velocity setting, two major choices exist.

• Physical quantities are upwinded with respect to their respective material velocities. Then

$$(\alpha \mathbf{u})_{i+\frac{1}{2}}^{k} = \alpha_{i+\frac{1}{2},\mathbf{u}p^{k}}^{k} \mathbf{u}_{i+\frac{1}{2}}^{k},$$
(43)

with  $\alpha_{i+\frac{1}{2},up^k}^k = \alpha_i^k$  if  $u_{i+\frac{1}{2}}^k \ge 0$  and  $\alpha_{i+\frac{1}{2},up^k}^k = \alpha_{i+1}^k$  if not. This is a robust choice as it generates convex combinations. However, because volume fractions are upwinded with respect to different velocities, their value may come from different cells. As such, their sum needs not be one at a given node. Apart from inducing potentially dubious geometrical interpretations, it prevents the Lagrange volume evolution rate  $\nabla \cdot \overline{\mathbf{u}}$  from being translation invariant as

$$\sum_{k} \alpha_{i+\frac{1}{2}, up^{k}}^{k} (u_{i+\frac{1}{2}}^{k} - u_{0}) = \sum_{k} \alpha_{i+\frac{1}{2}, up^{k}}^{k} u_{i+\frac{1}{2}}^{k} - u_{0} \sum_{k} \alpha_{i+\frac{1}{2}, up^{k}}^{k}, \quad (44)$$

may differ from  $\overline{u}_{i+\frac{1}{2}} - u_0$ .

• Physical quantities are upwinded with respect to a common velocity *U*. Node volume fractions now come from the same cell so that translation symmetry is recovered. However convex combinations are lost for material whose velocities are opposite to *U*, leading to possible stability issues.

In order to correct these shortcomings, upwind fluxes (43) are written in the alternate form

$$\alpha_{i+\frac{1}{2}}^{k,\mathrm{up}^{k}}\mathbf{u}_{i+\frac{1}{2}}^{k} = \mathbf{u}_{i+\frac{1}{2}}^{k} \frac{\alpha_{i}^{\kappa} + \alpha_{i+1}^{\kappa}}{2} + \left|\mathbf{u}_{i+\frac{1}{2}}^{k}\right| \frac{\alpha_{i}^{\kappa} - \alpha_{i+1}^{\kappa}}{2},$$
(45)

which can be interpreted as the sum of a centered flux (for which the sum of volume fractions adds up to one) and a diffusion flux, necessary for stability. When summing these fluxes over all materials, the effective nodal volume fractions are not centered because diffusion fluxes do not cancel out. It shows that the diffusion level must be the same for all materials. Consequently, fluxes are replaced with

$$(\alpha \mathbf{u})_{i+\frac{1}{2}}^{k} = u_{i+\frac{1}{2}}^{k} \frac{\alpha_{i}^{k} + \alpha_{i+1}^{k}}{2} + w_{i+\frac{1}{2}} \frac{\alpha_{i}^{k} - \alpha_{i+1}^{k}}{2},$$
(46)

where  $w_{i+\frac{1}{2}}$  no longer depends on material *k*. Then constraint (42) becomes consistent with translation symmetry. Stability is discussed in the next Section 3.5.2; it is shown to hold for a specific value of  $w_{i+\frac{1}{2}}$ .

**Remark 5.** Eq. (46) implies that node volume fractions used in (36) are

$$\alpha_{i+\frac{1}{2}}^{k} = \frac{\alpha_{i}^{k} + \alpha_{i+1}^{k}}{2}.$$
(47)

Although probably negligible, the correlation term (36b) is non-zero. Enforcing  $C_p = 0$  is possible (at least in one dimension) but at the cost of introducing thermodynamics inside the remapping procedure. It has been excluded so as to keep the projection purely geometrical.

**Remark 6.** Consistency between the volume-filling constraint and the upwinding is recurring issue in multi-material schemes (Cournède, 2001; Vazquez-Gonzalez et al., 2020) whatever their approach (Eulerian, Lagrangian, with remap, ...). It appears to be generally solved with decomposition "tricks" similar to (46).

#### 3.5.2. From a common diffusion to stability

All Eulerian quantities  $\phi \in \{1, \alpha, \alpha\rho, \alpha\rho u, \alpha\rho e\}$  are treated in the same manner

$$V_{i}^{n+1}\phi_{i}^{k,n+1} - V_{i}^{L^{k}}\phi_{i}^{k,L^{k}} = -\Delta t \left(F_{i+\frac{1}{2}}^{k}(\phi) - F_{i-\frac{1}{2}}^{k}(\phi)\right),$$
(48)

with

$$F_{i+\frac{1}{2}}^{k}(\phi) = u_{i+\frac{1}{2}}^{k} \frac{\phi_{i}^{k} + \phi_{i+1}^{k}}{2} + w_{i+\frac{1}{2}} \frac{\phi_{i}^{k} - \phi_{i+1}^{k}}{2}.$$
(49)

The following proposition shows that the "global-upwinding"

$$w_{i+\frac{1}{2}} = \max_{l} \left| u_{i+\frac{1}{2}}^{l} \right|$$
(50)

is sufficient to ensure stability in the sense detailed in the next proposition.

**Proposition 3.** The remapping procedure (48)–(50) consists in convex combinations under a CFL-like condition on the time step. They ensure positivity of the densities and volume fractions as well as positive entropy production for each material in the sense that

$$\sum_{i\in\mathbb{Z}} \left( m^{k,n+1} s_i^{k,n+1} - m^{k,n} s_i^{k,L^k} \right) \ge 0.$$
(51)

**Proof.** Eq. (48), together with (49), yields

$$V_{i}^{n+1}\phi_{i}^{k,n+1} = \left(V_{i}^{L^{k}} - \Delta t(u_{i+\frac{1}{2}}^{k} + w_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}^{k} + w_{i-\frac{1}{2}})\right)\phi_{i}^{k,L^{k}} + V_{i-\frac{1}{2}}^{n}\phi_{i+1}^{k,L^{k}} + V_{i+\frac{1}{2}}^{n}\phi_{i+1}^{k,L^{k}},$$
(52a)

$$V_{i\pm\frac{1}{2}}^{n} = \frac{\Delta t}{2} \left( w_{i\pm\frac{1}{2}} - u_{i\pm\frac{1}{2}}^{k} \right).$$
(52b)

With the choice (50), all coefficients are positive under a CFL-like condition which is essentially (but not exactly) the same global restriction which would have resulted from an upwind remapping procedure on each material. Dividing (52a) by the very same equation for  $\phi = 1$  gives convex combinations on the Eulerian variables  $\phi$ . It ensures positivity of the volume fraction. Alternatively, dividing (52a) by the very same equation for  $\phi = \alpha \rho$  gives convex combinations on the Lagrangian variables  $\phi/(\alpha \rho)$  which ensures positivity of the density. In particular, for  $\phi = \alpha$  and  $\phi = \alpha \rho e$ , it reads

$$\frac{1}{\rho_i^{k,n+1}} = \left(1 - \kappa_{i-\frac{1}{2}}^n - \kappa_{i+\frac{1}{2}}^n\right) \frac{1}{\rho_i^{k,L^k}} + \kappa_{i-\frac{1}{2}}^n \frac{1}{\rho_{i-1}^{k,L^k}} + \kappa_{i+\frac{1}{2}}^n \frac{1}{\rho_{i+1}^{k,L^k}},$$
(53a)

$$e_{i}^{k,n+1} = \left(1 - \kappa_{i-\frac{1}{2}}^{n} - \kappa_{i+\frac{1}{2}}^{n}\right)e_{i}^{k,L^{k}} + \kappa_{i-\frac{1}{2}}^{n}e_{i-1}^{k,L^{k}} + \kappa_{i+\frac{1}{2}}^{n}e_{i+1}^{k,L^{k}},$$
(53b)

with  $\kappa_{i\pm\frac{1}{2}}^{n} = \Delta V_{i\pm\frac{1}{2}}^{n} / V_{i}^{k,n+1}$ . By concavity of the function  $s^{k}(1/\rho^{k}, e^{k})$  $s_{i}^{k,n+1} \ge \left(1 - \kappa_{i-\frac{1}{2}}^{n} - \kappa_{i+\frac{1}{2}}^{n}\right) s_{i}^{k,L^{k}} + \kappa_{i-\frac{1}{2}}^{n} s_{i-1}^{k,L^{k}} + \kappa_{i+\frac{1}{2}}^{n} s_{i+1}^{k,L^{k}}.$  (54)

Unwinding all the previous computations eventually gives

$$m^{k,n+1}s_{i}^{k,n+1} - m^{k,L^{k}}s_{i}^{k,L^{k}} \ge -\Delta t \left(F_{i+\frac{1}{2}}^{k}(\alpha\rho s) - F_{i-\frac{1}{2}}^{k}(\alpha\rho s)\right),$$
(55)

which is consistent with the continuous inequality  $\partial_t(\alpha^k \rho^k s^k) + \partial_x(\alpha^k \rho^k s^k u^k) \ge 0$ . Summing over all cells, it implies the weaker global result (51).  $\Box$ 

Going beyond the previous result, some nuances are brought to the discussion in the following remarks. They also hold for the multidimensional extension presented in Appendix B.

**Remark 7.** The remapping fluxes depend on the Lagrangian values. Enforcing Eq. (42) would require a global implicitation of the volume fraction during the Lagrange step. It has been excluded for the sake of simplicity and computation time. Consequently, Eq. (42) is verified only up to a  $O(\Delta t)$  residue. Then, a normalization step is added at the end of the remapping; it will be shown in Section 4.2 that it is however now significantly less intrusive. Just as for the Lagrange step, the semi-discrete remapping step is strictly entropic for each material but integration in time may induce small entropy destruction after normalization.

**Remark 8.** While some entropy destruction cannot be completely excluded, the remapping procedure should actually be quite diffusive as all material quantities are now diffused with respect to the maximum velocity and no longer with their own. It may cause singular asymptotic behavior when a high-velocity phase disappears (*i.e.*  $u^k$  large and  $\alpha^k \rightarrow 0$ ), effectively driving the dissipation of the whole mixture. A possible answer is to replace the diffusion coefficient max<sub>l</sub>  $|u_{i+\frac{1}{2}}^l|$  in (49)

with some weighted average

$$\sum_{l} \theta^{l} \left| u_{i+\frac{1}{2}}^{l} \right|, \tag{56}$$

where  $\theta^l \to 0$  as  $\alpha^l \to 0$ . Then the proof of Proposition 3 is no longer valid and entropy might be destroyed over time for the fastest materials. However, convex combinations are sufficient for the proof but perhaps not necessary. Besides, the second principle of thermodynamics only requires an increase in total entropy so that an entropy destruction for a fast disappearing material might not be such a concern. The general issue of phase disappearance is a painful recurring hassle in several situations. It is usually taken care of by a brute force clipping below some threshold (Paulin et al., 2022, §1).

**Remark 9.** Conservation of total energy is not given *a priori*. The issue comes from the difference between projected kinetic energy and kinetic energy computed from the projected velocities (DeBar, 1974). A solution is to look at the gap between the two and dump it into the internal energy. Convexity of the square function ensures that the correction does not destroy entropy.

#### 4. Numerical results

The various test cases presented in this section are concerned with stiffened gas and perfect gas equations of state (EOS). The stiffened gas EOS (of which the perfect gas EOS is simply a specific case) is presented in Appendix C. The CFL parameter is 0.45 in all test cases (unless specified otherwise).

The different test cases aim at highlighting the multi-velocity aspects of the equations. Materials (up to nine) are made to cross each other and such results could not be obtained with a single-velocity scheme.

#### Table 1

Initial c	conditions	and	equations	of	state	for	the	double	shock	problem.	
-----------	------------	-----	-----------	----	-------	-----	-----	--------	-------	----------	--

	$u_L$	$u_R$	$\rho_L=\rho_R$	$p_L = p_R$	$\alpha_L = \alpha_R$	γ
Gas 1 Gas 2	5	-5	1	1	$1 - 10^{-5}$ $10^{-5}$	1.4 2

Table 2

Initial conditions inside the domain for the Ransom faucet problem.	
---	--

	ρ	и	р	α
Air	1	0	105	0.2
Water	1000	10	105	0.8

#### 4.1. Double shock through a mixture of perfect gases

The first test case considers two perfect gases and consists in a Riemann problem whose solution displays two symmetric shocks. Equations of state and initial conditions can be found inside Table 1.

This test case aims at measuring the effect of correlation closures on the solutions inside shocks. Consistently with the discussion of Section 2.3, no analytical solution can exist as shocks depend on the details of the correlation terms; those are here tweaked in two different manners. First, the total heat deposit is distributed either with respect to mass fractions ( $\lambda_1 = \alpha^1 \rho^1 / \rho$ ) or entirely on the first material ( $\lambda_1 = 1$ ). Second, an additional drag force can couple the fluid velocities. The modified equations read

$$\alpha^{1}\rho^{1}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}^{1} = -\alpha^{1}\nabla p + \nu\rho\left(\mathbf{u}^{2} - \mathbf{u}^{1}\right),$$
(57a)

$$\alpha^2 \rho^2 \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{u}^2 = -\alpha^2 \nabla p + \nu \rho \left( \mathbf{u}^1 - \mathbf{u}^2 \right).$$
(57b)

Numerically, time integration of the drag force is implicit, resulting in a local 2 × 2 linear system which can easily be inverted by hand. Three values of the drag coefficient v are here considered: v = 0 (no drag),  $v = 10^{-4}$  and  $v = 10^{10}$ . The latter is essentially infinite and recovers the single-velocity limit.

Density and velocity results for all six combinations of closures are compiled inside Fig. 5. As gas 1 has a volume fraction close to one, its post-shock state is almost independent of the chosen closure (apart from a distinct wall-heating phenomenon in the single-velocity limit). By contrast, gas 2 displays radically different behaviors on its density (and thus internal energy because its pressure is that of gas 1) and velocity. Its velocity is completely decoupled when no drag force is applied; it slowly relaxes to the same value with an average drag coefficient  $v = 10^{-4}$ ; finally, both velocities are equal with an almost infinite drag  $v = 10^{10}$ . Notably, in the two first cases, gas 2 is pushed toward the center of the domain while gas 1 is slowly evacuated. It leads to some form of contact waves associated with the saturated elliptic modes of the equations, as described in Keyfitz (2001). This phenomena is however slow enough not to be visible.

Differences resulting from different closures may be deemed minor at first as gas 2 has no relevant effect on the dynamic of the mixture. They however become all the more necessary to take into account when additional phenomena such as chemical reactions are considered. In this case, capturing accurate energy levels is crucial as being below or above reaction thresholds can radically change the physics of the system.

#### 4.2. Ransom water faucet problem

The Ransom water faucet problem is a standard benchmark in multi-velocity two-phase numerical simulations (Ransom, 1987; Vazquez Gonzalez, 2016; Vazquez-Gonzalez et al., 2016). A 12m long vertical pipe is filled with an initially homogeneous mixture of air and water whose properties are detailed in Table 2. Air and water are respectively described by a perfect gas ( $\gamma = 1.4$ ) and a

stiffened gas ( $\Gamma = 3.4$  and  $\pi = 10^9$ ) equations of state. At the top of the tube, water is injected at 10 m.s<sup>-1</sup> with a volume fraction of 0.8, density of 1000 Kg.m<sup>-3</sup> and pressure  $p = 10^5$  Pa. The bottom of the tube is left opened at atmospheric pressure  $p = 10^5$  Pa. Additionally, a downward gravity force g = 10 m.s<sup>-2</sup> is applied to the mixture.

Because of the highly contrasted equations of state, water behaves in an almost incompressible manner while its dynamics is essentially insensitive to that of air. The dynamics of water can then be approximated with a free fall. Because its upstream velocity is constant, the newly injected water lags behind the continuously accelerated stream. As a result, the water stream narrows while the space left unoccupied is filled with air.

Fig. 6 displays the numerical results for the air volume fraction and the water velocity. Good agreement with the semi-analytical solution is observed. For finer meshes, an undershoot appears upstream of the contact wave. This instability is not numerical but rather comes from the elliptic nature of the model itself. This well-known issue echoes the discussion in Section 2.4 and is also largely examined in Vazquez-Gonzalez et al. (2016) and references therein.

Regarding the sum of volume fractions and Remark 7, the performance of the present strategy is also assessed without any normalization step. Results are shown on Fig. 7 for different CFL numbers  $(5 \cdot 10^{-1}, 5 \cdot 10^{-2} \text{ and } 5 \cdot 10^{-3})$ . As expected, taking smaller time steps reduces the error (dividing the time step by a factor 10 also divides the error by 10, consistently with the fact that the scheme is first order in time). Results with a traditional upwind strategy (43) has also been included. The error is larger as it accounts for an additional space residue (that the present method eliminated) which also prevents convergence to zero when the time step is decreased. Overall, with a reasonable CFL of 0.5, the volume-filling condition is only violated by around 0.001% *at the end* of the simulation (t = 0.6).

#### 4.3. Air-water shock tube

This test case from Chang and Liou (2003) consists in shock tube of air and water. The water equation of state is the same as in the previous test case while the air (or vapor in the original instance of the test case) is a perfect gas with  $\gamma = 1.0942$ . Initial conditions can be found in Table 3. Both the air EOS and part of the initial conditions are probably not exactly the same as in Chang and Liou (2003) where they are missing; more generally, EOS and initial conditions seems to vary in other instances of this test case (Toumi, 1996; Paillère et al., 2003; Tiselj and Petelin, 1997) (some even consider an initial velocity difference between the two fluids).

On Fig. 8 are displayed the results at t = 0.005 with and without an interfacial pressure term (Stuhmiller, 1977; Bestion, 1990) supplementing Eq. (1) as well as with different mesh sizes. The solution consists in a left rarefaction wave and a right shock. The results without the additional term are somewhat jagged; it seems that the elliptic instabilities appear before a clean transient convergence can be observed. This is probably exacerbated by the air EOS which is close to the thermodynamical singularity  $\gamma = 1$ . Water and air both experience a spurious velocity peak. It is all the more pronounced as the mesh is refined and, again, ellipticity is to be blamed.

In Chang and Liou (2003), this very same artefact is observed and is eliminated by the introduction of the interfacial pressure which restores hyperbolicity of the model. When incorporated into the present scheme, it stabilizes the solution and allows convergence as shown on Fig. 8. It must be stressed out that this term has been chosen for convenience and its mathematical properties rather than for any physical reason. In particular, it is not consistent with thermodynamics as it may induce losses of entropy.



**Fig. 5.** Results of the double shock problem at t = 0.15 with 500 cells. Left: density. Right: Velocity. Top: without drag (v = 0). Middle: with a drag coefficient  $v = 10^{-4}$ . Bottom: with an infinite drag coefficient ( $v = 10^{10}$ ) effectively recovering the single-velocity limit. Gas 1 (the dominant material) is essentially not affected by small-scale closures while post-shock density levels of gas 2 are heavily dependent on them.

Initial	conditions	and	equations	of	state	for	the	air-water	shock	tube	problem.	
munu	contaitions	unu	equations	01	otute	101	unc	un water	onoci	lube	problem.	

	и	$\rho_L$	$\rho_R$	$p_L$	$p_R$	$\alpha_L$	$\alpha_R$
Air Water	0	75 1000	37.5 1000	$2\cdot 10^7$	107	0.1 0.9	0.25 0.75

#### Table 4

Initial conditions inside the domain for the sedimentation problem.

	ρ	и	р	α
Air	1	0	105	0.5
Water	1000	0	10-	0.5

#### 4.4. Sedimentation problem

This numerical test case from Städtke (2006) studies the evolution of a mixture of water and air in a vertical column [0,7]. Equations of state are the same as in the Ransom faucet problem. At first, the mixture is homogeneous and at rest; its characteristics are detailed in Table 4. Wall conditions are set on each side. The mixture is set into motion by gravity and density contrast: the denser water moves downwards while air goes upwards. As a consequence, a volume fraction wave forms on each side and both eventually merge into an interface between the then fully separated air and water. Fig. 9 shows the air volume fraction profile at different times obtained with 200 cells. The expected behavior is reproduced at the discrete level leading to the total separation of air and water.



Fig. 6. Air volume fraction (left) and water velocity (right) profiles displayed at time t = 0.6. With 1200 cells, an undershoot appears on the upstream state of the volume fraction wave.



**Fig. 7.** The distance between the sum of volume fractions and 1 for 200 cells and different CFL numbers. The results with the present strategy and a traditional upwind discretization (43) are included. Error decreases with the present strategy (elimination of the space residue) and with a smaller CFL number (smaller time residue).

#### 4.5. Crossing clouds

From Vazquez Gonzalez (2016) is considered a test case consisting in the crossing of water droplet clouds ( $\rho = 1000$ ) at supersonic speeds in air ( $\rho = 1$ ). The equations of state are the same as in the Ransom faucet problem. The volume fraction profile of each cloud is Gaussian

$$\alpha(\mathbf{x}, 0) = 0.12 \exp\left(\frac{(\mathbf{x}_0 - \mathbf{x})^2}{0.08}\right).$$
(58)

The initial position  $\mathbf{x}_0$  and velocity of the clouds can be found in Fig. 10. The pressure is initially homogeneous throughout the domain with  $P = 10^5$ .

The particles then move steadily until crossing each other in the center at  $t = 10^{-3}$ . There, their movement remains unperturbed as air inhibits all pressure perturbations. Although such behavior may seem counter-intuitive, one has to remember that the model has been stripped of all dissipative terms so as to focus on the universal features of dissipation-free multi-material flows. A complete physical description would include exchanges of momentum such as drag which would slow the clouds down upon crossing each other, the form and amplitude of such exchanges being heavily system-dependent. Just as for the Ransom faucet and the sedimentation problems, the solution is only semi-analytical in the sense that it predicts an idealized behavior of the water alone. The air actually undergoes a more chaotic flow, including shock waves. The water is basically oblivious to these pressure waves

and to the medium behavior because of the high contrast in densities and compressibilities.

Numerical results at different times are displayed on Fig. 11. At  $t = 2 \cdot 10^{-3}$ , the clouds have reached the other side, modified only by the numerical diffusion induced by the remapping step. It is worth noticing that the resulting smearing seems isotropic (*i.e.* their circular shape is preserved). With usual remapping procedures, diffusion is only observed in the direction of the propagation. Here, it is common to all materials, including those moving horizontally and those moving vertically. As a result, all materials are equally subject to both horizontal and vertical diffusion. Overall, the numerical scheme shows good robustness with respect to the supersonic velocities of the droplets, to the highly contrasted equations of state, as well as to the small values reached by the air volume fraction when the particles are all superimposed at  $t = 10^{-3}$ .

#### 5. Conclusion

A numerical scheme was presented for a multi-material multivelocity one-pressure system of equations. The model is isentropic and thus completely reversible for smooth solutions. On the other hand, thermodynamically-consistent dissipation must be added so as to specify the solutions inside shocks. The numerical scheme is based on a splitting which consists in a extension for multi-velocity flows of the so-called "Lagrange+Remap" strategy. A Lagrangian phase is first performed in parallel on each material; all quantities are then projected back to a common mesh. For both steps, a large emphasis is put on discrete thermodynamic consistency and on entropy as a mean of stabilizing the scheme and selecting the solutions of interest inside shocks. More precisely

- Space integration of both the Lagrange phase and the remapping is shown to be strictly entropic.
- Entropic solutions are not unique and the main source of entropy (namely the Lagrangian numerical viscosity) can be arbitrarily shared between materials, a key feature allowing the approximation of different shocks.

Pressure equality is guaranteed even in the context of contrasted mixtures (*e.g.* air and water) thanks to a local implicit equilibration step. The numerical scheme is benchmarked on several test cases assessing its robustness to shocks and contrasted equations of state.

The present work paves the way for further studies. First, properly tuning the numerical viscosity is a self-standing question, seldom studied in the context of multi-velocity equations. Beyond its expression, incorporation in a given scheme is not necessarily trivial as it was shown that Godunov-type schemes produce intricate compensations between pressure gradients and numerical viscosity. Being able to



**Fig. 8.** Results of the air-water shock tube problem at t = 0.0005 with 250 and 1000 cells. The results for the unaltered model (1) ( $\sigma = 0$ ) displays a velocity overshoot in the middle whose amplitude grows with the mesh resolution. This is due to the elliptic nature of the equations and the artefact is removed as an interfacial term ( $\sigma = 2$ ) is added.

streamline cell-centered schemes by properly separating both phenomena would allow for both an easier integration of various numerical dissipation terms and their removal where they are not needed (e.g.inside rarefaction waves).

If robustness is the focal point of this article, accuracy is still a relevant and desirable property of numerical schemes. While shocks uncompromisingly need dissipation, reversibility of smooth solutions advocates for a strict zero entropy production. Excessive dissipation then enhances robustness inside shocks but can also degrade solutions elsewhere. The aforementioned issue of separating numerical viscosity from pressure gradients could help solving this almost schizophrenic behavior, in the spirit of Von Neumann and Richtmyer (1950) and Vazquez-Gonzalez et al. (2020). Alternatively, extension to second or higher order (both in time and space) would also substantially improve the quality of the solutions, especially during the remapping step where limiters could be used (Paulin et al., 2022). It should still be stressed out that careless high-order strategies can destroy thermodynamic consistency (Marboeuf, 2018).

Finally, the performances of the present scheme could be evaluated on more demanding test cases as in Heulhard de Montigny and Llor



Fig. 9. Air volume fraction profile at different times for the sedimentation problem. The mesh contains 200 cells. Air and water are eventually completely separated.



**Fig. 10.** Geometry and initial velocities for the crossing particle test. Only the information for two out of six particles is given; the rest can be deduced from symmetry considerations (namely invariance with respect to repeated  $90^{\circ}$  rotations and reflections through the *x*-axis).

(2022). A virtually infinite amount of test cases also includes real-world applications, together with their respective closures of the correlation terms.

#### CRediT authorship contribution statement

**B. Manach-Pérennou:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **R. Chauvin:** Writing – review & editing, Supervision, Software, Methodology, Investigation, Formal analysis, Conceptualization. **S. Guisset:** Writing – review & editing, Supervision, Software, Methodology, Investigation, Formal analysis, Conceptualization. **A. Llor:** Writing – review & editing, Supervision, Methodology, Investigation, Formal analysis, Conceptualization.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Appendix A. GLACE/EUCCLHYD and discrete integration by part failure

The single-fluid GLACE/EUCCLHYD scheme, written in internal energy, reads

$$n_c \frac{\mathrm{d}}{\mathrm{d}t} \left( \frac{1}{\rho_c} \right) = \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_p, \tag{A.1a}$$

$$m_c \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{u}_c = \sum_{p \in \mathcal{P}(c)} \mathbf{M}_{pc} (\mathbf{u}_p - \mathbf{u}_c), \qquad (A.1b)$$

$$\begin{aligned} \int_{c} \frac{\mathbf{d}}{\mathbf{d}t} e_{c} &= -p_{c} \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p} \\ &+ \sum_{p \in \mathcal{P}(c)} (\mathbf{u}_{p} - \mathbf{u}_{c}) \cdot \mathbf{M}_{pc} (\mathbf{u}_{p} - \mathbf{u}_{c}), \end{aligned} \tag{A.1c}$$

$$\mathbf{u}_{p} = \mathbf{M}_{p}^{-1} \sum_{c \in C(p)} \left[ \mathbf{M}_{pc} \mathbf{u}_{c} + p_{c} l_{pc} \mathbf{n}_{pc} \right], \qquad (A.1d)$$

$$\mathbf{M}_{p} = \sum_{c \in C(p)} \mathbf{M}_{pc}.$$
 (A.1e)

The discrete divergence of the velocity  $[\nabla \cdot \mathbf{u}]_c$  directly comes from the Geometric Conservation Law (GCL) in Eq. (A.1a).

$$[\nabla \cdot \mathbf{u}]_c = \sum_{p \in \mathcal{P}(c)} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_p.$$
(A.2)

Having the same in the energy Eq. (A.1c) is desirable to properly mimic Gibbs identity and ensure consistency with thermodynamics. Excluding viscous terms (*i.e.* the entropy production) in (A.1c), total energy conservation advocates for the existence of a discrete pressure gradient  $[\nabla p]_c$  such that

$$m_c \frac{\mathrm{d}}{\mathrm{d}t} |\mathbf{u}_c|^2 + m_c \frac{\mathrm{d}}{\mathrm{d}t} e_c = \mathbf{u}_c \cdot [\nabla p]_c + p_c [\nabla \cdot \mathbf{u}]_c$$
(A.3)

can be written in terms of fluxes. Injecting (A.1d) in (A.2) gives

$$\nabla \cdot \mathbf{u}]_{c} = \sum_{p \in \mathcal{P}(c)} \sum_{d \in \mathcal{C}(p)} l_{pc} \mathbf{n}_{pc}^{\mathrm{T}} \mathbf{M}_{p}^{-1} \mathbf{M}_{pd} \mathbf{u}_{d} + \sum_{p \in \mathcal{P}(c)} \sum_{d \in \mathcal{C}(p)} p_{d} l_{pc} l_{pd} \mathbf{n}_{pc}^{\mathrm{T}} \mathbf{M}_{p}^{-1} \mathbf{n}_{pd}.$$
(A.4)

The first part only depends on the velocity and is consistent with  $\nabla \cdot \mathbf{u}$  (Després, 2010). The second part only depends on the pressure and comes from approximate Riemann solvers at the nodes. It is this second part which does not allow the discrete integration by parts (A.3). Neglecting boundary conditions, for (A.3) to imply conservation, it would require that

$$\sum_{c} \left( \mathbf{u}_{c} \cdot [\nabla p]_{c} + p_{c} [\nabla \cdot \mathbf{u}]_{c} \right) = 0.$$
(A.5)

Using the fact that

n

$$\sum_{c} \sum_{p \in \mathcal{P}(c)} \sum_{d \in \mathcal{C}(p)} = \sum_{p} \sum_{c, d \in \mathcal{C}(p)}$$
(A.6)

and the symmetry of matrices  $\mathbf{M}_{pc}$  when switching between indexes c and d, it eventually leads to

$$\sum_{c} \mathbf{u}_{c} \cdot \left[ [\nabla p]_{c} + \sum_{p \in \mathcal{P}(c)} \sum_{d \in \mathcal{C}(p)} p_{d} l_{pd} \mathbf{M}_{pc} \mathbf{M}_{p}^{-1} \mathbf{n}_{pd} \right]$$
  
+ 
$$\sum_{p} \sum_{c,d \in \mathcal{C}(p)} p_{c} p_{d} l_{pc} l_{pd} \mathbf{n}_{pc}^{\mathrm{T}} \mathbf{M}_{p}^{-1} \mathbf{n}_{pd} = 0.$$
(A.7)

As stated earlier, no pressure gradient can compensate for the pressure terms in the second part of the equation. In the GLACE/EUCCLHYD scheme, conservation of total energy is obtained through subtle compensations between the work of pressure forces and the numerical viscosity. In other words, both terms do not individually generate a flux; they only generate a global flux together.



Fig. 11. Medium volume fraction profile with  $1200 \times 1200$  cells.

#### Appendix B. Multi-dimensional remapping procedure

In order to extend the one-dimensional remapping procedure of Section 3.5, the following generic scheme is written

$$V_{c}^{n+1}\phi_{c}^{k,n+1} = V_{c}^{L^{k}}\phi_{c}^{k,L^{k}} - \Delta t \sum_{p \in \mathcal{P}(c)} F_{pc}^{k}(\phi),$$
(B.1)

with  $\phi \in \{1, \alpha, \alpha\rho, \alpha\rho \mathbf{u}, \alpha\rho e\}$ . Node fluxes are chosen instead of face fluxes because consistency with the Lagrange step is needed. It will be seen that a remapping procedure with face fluxes is actually not compatible with volume conservation. As in the one-dimensional case, fluxes are written as the sum of a centered and a diffusion contribution

$$F_{pc}^{k}(\boldsymbol{\phi}) = \boldsymbol{\phi}_{p}^{k,L^{k}} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k} + \sum_{d \in C(p)} w_{dpc} \left( \boldsymbol{\phi}_{c}^{k,L^{k}} - \boldsymbol{\phi}_{d}^{k,L^{k}} \right).$$
(B.2)

Node estimations  $\phi_p^{k,L^k}$  are given as convex combinations over the surrounding cells

$$\phi_p^{k,L^k} = \sum_{d \in \mathcal{C}(p)} \theta_{dp} \phi_d^{k,L^k} \tag{B.3}$$

with positive coefficients  $\theta_{dp}$  summing up to one. They are assumed to only depend on the geometry of the initial mesh, hence being the same

for all materials. This is essential to ensure that the sum of node volume fractions ( $\phi = \alpha$ ) over all materials equals one. As for the diffusion coefficients  $w_{dpc}$ , necessary for stability, they are also assumed not to depend on the material so as to ensure their sum over all materials is zero for  $\phi = \alpha$ . Both parameters answer to different constraints:

- (i) Consistency needs to be ensured.
- (ii)  $F_{nc}^{k}(\phi)$  must be fluxes. A local conservation property is sought

$$\sum_{c \in C(p)} F_{pc}^k(\phi) = 0.$$
(B.4)

(iii) Lagrangian quantities  $\psi_c^{n+1} = \phi_c^{n+1}/(\alpha \rho)_c^{n+1} \in \{1/\alpha \rho, 1/\rho, 1, \mathbf{u}, e\}$  are convex combinations of the initial values (under a CFL-like condition). In this case, the proof of 3 extends naturally to the multi-dimensional case.

In the following, the exponent  $L^k$  will be omitted for readability purposes. Condition (i) is automatically recovered as long as  $w_{dpc}$  are  $\mathcal{O}(h)$  with *h* a characteristic length of the cells. Condition (ii) reads

$$\sum_{c \in C(p)} \left( l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_p^k \phi_p^k + \sum_{d \in C(d)} w_{dpc} (\phi_c^k - \phi_d^k) \right) = 0,$$
(B.5a)

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$$\mathbf{u}_{p}^{k}\boldsymbol{\phi}_{p}^{k}\cdot\sum_{c\in\mathcal{C}(p)}l_{pc}\mathbf{n}_{pc}+\sum_{c,d\in\mathcal{C}(p)}w_{dpc}(\boldsymbol{\phi}_{c}^{k}-\boldsymbol{\phi}_{d}^{k})=0, \tag{B.5b}$$

$$\sum_{\{c,d\}} (w_{dpc} - w_{cpd})(\phi_c^k - \phi_d^k) = 0.$$
 (B.5c)

It is then natural to enforce symmetry of the coefficients  $w_{dpc} = w_{cpd}$ . In regards to condition (iii), Eq. (B.1) may be written

$$V_{c}^{n+1}\phi_{c}^{k,n+1} = \left(V_{c} - \Delta t \sum_{p \in \mathcal{P}(c)} \left(\theta_{cp}l_{pc}\mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k} + w_{dpc}\right)\right)\phi_{c}^{k} + \Delta t \sum_{d \neq c} \left(\sum_{p \in \mathcal{P}(c) \cap \mathcal{P}(d)} \left(w_{dpc} - \theta_{dp}l_{pc}\mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k}\right)\right)\phi_{d}^{k}.$$
 (B.6)

Dividing (B.6) for an arbitrary  $\phi$  by the same equation for  $\phi = 1$  then gives a convex combination provided that

$$V_{c} - \Delta t \sum_{p \in \mathcal{P}(c)} \left( \theta_{cp} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k} + \sum_{d \in C(p)} w_{dpc} \right) \ge 0,$$
(B.7a)

$$\sum_{p \in \mathcal{P}(c) \cap \mathcal{P}(d)} \left( w_{dpc} - \theta_{dp} l_{pc} \mathbf{n}_{pc} \cdot \mathbf{u}_{p}^{k} \right) \ge 0.$$
(B.7b)

Eq. (B.7a) is essentially a CFL-like restriction on the time step. Eq. (B.7b) gives a lower-bound for the diffusion coefficient. In the present work, only regular cartesian meshes are considered. In all test cases, node estimations were given by

$$\theta_{cp} = 1/4. \tag{B.8}$$

As for the diffusion coefficients  $w_{dc}$ , constraint (B.7b) is saturated so that

$$\sum_{p \in \mathcal{P}(c) \cap \mathcal{P}(d)} w_{dpc} = \frac{1}{4} \max_{k} \max_{e \in \{c,d\}} \left( \sum_{p \in \mathcal{P}(c) \cap \mathcal{P}(d)} l_{pe} \mathbf{n}_{pe} \cdot \mathbf{u}_{pe}^{k} \right).$$
(B.9)

The sum contains one or two terms depending on if the cells c and d share a face or only a single node.

**Remark 10.** With a usual remapping procedure based on face fluxes, no flux exists between two cells only sharing one node (and no face). Here, it is worth noticing that for all materials not satisfying the maximum  $\max_k$  in (B.9), the flux between two such cells is non-zero. This is necessary to comply with the constraints on total volume conservation.

#### Appendix C. Stiffened gas equation of state

A stiffened gas (Menikoff and Plohr, 1989) is described by two constant coefficients  $\varGamma$  and  $\pi$ 

$$p = \Gamma e \rho - (\Gamma + 1)\pi. \tag{C.1}$$

The parameter  $\Gamma$  coincides with the Grüneisen coefficient  $\Gamma = \partial_s p|_{\rho}/(\rho T)$  while the parameter  $\pi$ , homogeneous to a pressure, allows to take into account attraction between molecules. For any EOS, the following relationships stand Menikoff and Plohr (1989)

$$dp = c^2 d\rho + \rho \Gamma T ds, \tag{C.2a}$$

$$=c^{2}d\rho+\rho\Gamma\left(de-\frac{p}{\rho^{2}}d\rho\right),$$
(C.2b)

$$= \left(c^2 - \frac{I\rho}{\rho}\right)d\rho + \rho\Gamma de.$$
(C.2c)

On the other hand, Eq. (C.1) yields

$$dp = \Gamma e d\rho + \rho \Gamma de. \tag{C.3}$$

Identifying Eqs. (C.2c) and (C.3) confirms the fact that the parameter  $\Gamma$  in (C.1) is indeed the Grüneisen coefficient. It also gives the expression of the speed of sound

$$c^{2} = \partial_{\rho} p \Big|_{s} = (\Gamma + 1) \frac{p + \pi}{\rho}.$$
 (C.4)

Because the speed of sound is real, Eq. (C.4) implies the thermodynamic consistency condition

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$$p + \pi > 0. \tag{C.5}$$

Integrating the equation  $dp = c^2 d\rho$  shows that the product

$$(p+\pi)\rho^{-(I+1)}$$
 (C.6)

is a constant along isentropic curves. Because  $\Gamma > 0$ , an entropy for the stiffened gas needs to be an increasing function of (C.6).

**Remark 11.** When  $\pi = 0$ , the stiffened gas EOS reduces to the perfect gas EOS. The perfect gas EOS is generally written with the adiabatic exponent  $\gamma$  which, in this case, is equal to  $\Gamma + 1$ 

$$p = (\Gamma - 1)\rho e. \tag{C.7}$$

#### Data availability

Data will be made available on request.

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