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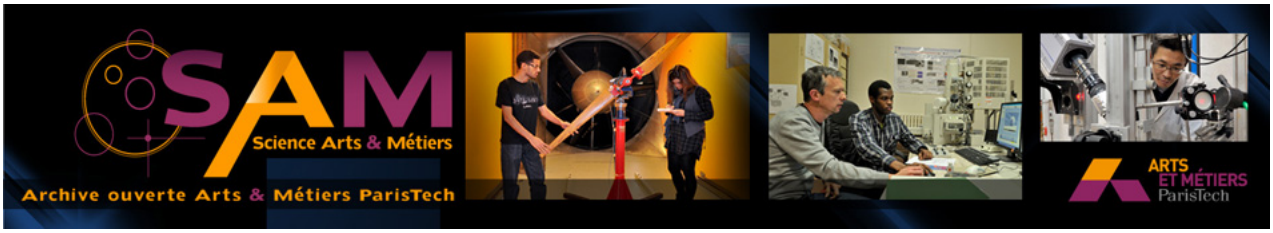

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Modeling and simulation of compressible multi-material interface instabilities

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Abstract. *We aim to simulate the interactions at the material interface of two compressible media. These interactions are modeled by a single fully Eulerian system of conservation laws. The materials differ by their constitutive laws, that can reproduce the mechanical characteristics of fluids or elastic solid. We illustrate the model with simulations of shock waves impinging on undulated interfaces, generating instabilities such as Richtmyer-Meshkov instabilities.*

Keywords: multimaterial coupling; Eulerian frame; elasticity.

1 INTRODUCTION

Physical phenomena that involve several materials are ubiquitous in nature and applications: multiphase flows, fluid-structure interaction, impacts, to cite just a few examples. In recent literature several strategies were proposed to attack these problems: Lagrangian models [11], Arbitrary-Lagrangian-Eulerian (ALE) models [7], Eulerian models [12, 5]. In this context, immersed boundary methods [10] are an option to discretize boundary conditions at the interface, trading off accuracy for mesh generation simplicity.

In this study, we are interested in the numerical simulation of phenomena such as the scattering of shock waves at material interfaces between different fluids or a fluid and an elastic material. These phenomena can be modeled by a fully Eulerian system of conservation laws that applies to every material; only the constitutive law may change, reproducing the mechanical characteristics of the medium under consideration.

The systematic derivation of such models starting from continuum mechanics principles, their thermodynamic consistency and the corresponding wave-propagation patterns were initially studied in [8]. Their numerical simulation is delicate because standard Godunov schemes lead to spurious pressure oscillations at the material contact discontinuity already in the case of multifluids. In [1] the pressure perturbation mechanism at the origin of this phenomenon was explained and a first fix was proposed. An effective remedy to this problem was presented in [6] with the ghost-fluid method (sharp interface between the materials). For multifluids, improvements of this approach requiring less storage were proposed in [2] (diffuse interface) and [4] (sharp interface).

For elastic compressible materials existing methods either rely on the definition of ghost materials [12] or on mixture models and diffuse interfaces [5]. In this presentation we employ a simple, stable and non-oscillatory scheme for multimaterials that avoids the definition of a ghost hyperelastic medium. The equilibrium boundary conditions at the material interface are imposed like in immersed boundary methods, in the same spirit of what is done in [9] for rigid bodies.

2 OVERVIEW OF THE METHOD

2.1 Governing equations in Eulerian frame

Let $\Omega_0 \subset \mathbb{R}^3$ be the reference or initial configuration of a continuous medium and $\Omega_t \subset \mathbb{R}^3$ the deformed configuration at time t. In order to describe the evolution of this medium in the Lagrangian frame we define the forward characteristics $X(\xi, t)$ as the image at time t in the deformed configuration of a material point ξ belonging to the initial configuration, i.e., $X : \Omega_0 \times [0, T] \longrightarrow \Omega_t$, $(\xi, t) \mapsto X(\xi, t)$. The corresponding velocity field u is defined as $u : \Omega_t \times [0, T] \longrightarrow \mathbb{R}^3$, $(x, t) \mapsto u(x, t)$ where $X_t(\xi, t) = u(X(\xi, t), t)$.
To describe the continuous medium in the Eulerian frame, we introduce the backward characteristics $Y(x, t)$ (see [3]) that for a time t and a point x in the deformed configuration, gives the corresponding initial point ξ in the initial configuration, i.e., $Y : \Omega_t \times [0, T] \longrightarrow \Omega_0$, $(x, t) \mapsto Y(x, t)$. Since $Y(X(\xi, t), t) = \xi$, differentiating with respect to time and space in turn we have

$$Y_t + u \cdot \nabla_x Y = 0 \tag{1}$$

The conservation of mass, momentum and energy in the deformed configuration Ω_t is:

$$\begin{cases} \rho_t + \mathrm{div}_x(\rho u) = 0 \\ (\rho u)_t + \mathrm{div}_x(\rho u \otimes u - \sigma) = 0 \\ (\nabla_x Y)_t + \nabla_x(u \cdot \nabla_x Y) = 0 \\ (\rho e)_t + \mathrm{div}_x(\rho e u - \sigma^T u) = 0 \end{cases} \tag{2}$$

The unknowns are the density $\rho(x, t)$, the velocity $u(x, t)$, the backward characteristics of the problem $Y(x, t)$ and the total energy per unit mass $e(x, t)$. Here $\sigma(x, t)$ is the Cauchy stress tensor in the physical domain. Together with equations of mass, momentum and energy conservation, the additional equation (1) is required in order to record the deformation in the Eulerian frame. However, since σ will directly depend on $\nabla_x Y$ we take the gradient of (1) as a governing equation and obtain a system in conservative form.
The initial density $\rho(x, 0)$, the initial velocity $u(x, 0)$, the initial total energy $e(x, 0)$ and $\nabla_x Y(x, 0) = I$ are given together with appropriate boundary conditions.

2.2 Constitutive law

The internal energy per unit mass $\varepsilon(x, t)$ is defined as

$$\varepsilon = e - \frac{1}{2}|u|^2 = \frac{\kappa(s)}{\gamma - 1}\left(\frac{1}{\rho} - b\right)^{1-\gamma} - a\rho + \frac{p_\infty}{\rho} + \frac{\chi}{\rho_0}(\mathrm{Tr}(\overline{B}) - 2) \tag{3}$$

where $\kappa(s) = \exp\left(\frac{s}{c_v}\right)$ and c_v, γ, p_∞, a, b, $\chi \in \mathbb{R}^+$ are constants that characterize a given material. The constant χ is the shear elastic modulus and the other constants have the usual meaning. Other energy functions can be envisaged to mitigate or accentuate certain aspects of the resulting non-linear relation between stress and deformation. Note that $\overline{B} = \frac{B}{\det(B)^{\frac{1}{2}}}$ where B is the left Cauchy-Green tensor in a two-dimensional problem, so that $\det(\overline{B}) = 1$. Classical models are obtained by particular choices of the coefficients. For example, the stiffened gas model is obtained by taking $a = 0$, $b = 0$ and $\chi = 0$ in (3). The Van Der Waals gas model is obtained taking $p_\infty = 0$ and $\chi = 0$.

2.3 Multimaterial solver

The numerical scheme in two or three space dimensions is based on the solution of one-dimensional problems in the direction orthogonal to the cell sides of a uniform Cartesian mesh. In this framework, to simplify notation, we consider the discrete problem in the direction of one axis of the canonical basis in space. Also, we initially focus on a first order explicit scheme in space and time. Second order is obtained by classical MUSCL reconstructions.
We assume that the conservative variables at the n-th time step are known. Let φ_k^n be the signed distance of the cell center k from the material interface, i.e., $\varphi_k^n > 0$ corresponds to one material, $\varphi_k^n < 0$ corresponds to the other. Let Ψ_k^n be a piece-wise constant function representing the conservative variables at time step n and at the cell k.
Whenever $\varphi_k^n\, \varphi_{k+1}^n > 0$ and $\varphi_k^n\, \varphi_{k-1}^n > 0$ (same material), the space and time discretization is as follows

$$\frac{\Psi_k^{n+1} - \Psi_k^n}{\Delta t} = -\frac{\mathcal{F}_{k+1/2}^n(\Psi_k^n, \Psi_{k+1}^n) - \mathcal{F}_{k-1/2}^n(\Psi_{k-1}^n, \Psi_k^n)}{\Delta x} \tag{4}$$

where Δt is the time step, Δx the uniform grid size, $\mathcal{F}_{k-1/2}^n$ and $\mathcal{F}_{k+1/2}^n$ are the numerical fluxes evaluated at the cell interfaces respectively located to the left and to the right of the cell center k. The numerical flux function $\mathcal{F}$ is defined thanks to a special form of the HLLC approximation of the Riemann problem.
Let us focus on $\mathcal{F}_{k+1/2}^n(\Psi_k^n, \Psi_{k+1}^n)$. The HLLC solver defines two intermediate states $(\Psi^-)^n$ and $(\Psi^+)^n$ as a function of Ψ_k^n and Ψ_{k+1}^n. The material velocity, $(u_1^\star)^n$, is continuous across the states $(\Psi^-)^n$ and $(\Psi^+)^n$. Let us assume that $(\Psi^-)^n$ is the state to the left of the contact discontinuity and $(\Psi^+)^n$ to the right.
The main idea of the multimaterial solver is that whenever $\varphi_k^n\,\varphi_{k+1}^n < 0$ (material interface to the right of cell k) instead of (4) we have

$$\frac{\Psi_k^{n+1} - \Psi_k^n}{\Delta t} = -\frac{\mathcal{F}_-^n((\Psi^-)^n) - \mathcal{F}_{k-1/2}^n(\Psi_{k-1}^n, \Psi_k^n)}{\Delta x} \tag{5}$$

or if $\varphi_k^n\,\varphi_{k-1}^n < 0$ (material interface to the left of cell k), instead of (4) we have

$$\frac{\Psi_k^{n+1} - \Psi_k^n}{\Delta t} = -\frac{\mathcal{F}_{k+1/2}^n(\Psi_k^n, \Psi_{k+1}^n) - \mathcal{F}_+^n((\Psi^+)^n)}{\Delta x} \tag{6}$$

where $\mathcal{F}_\pm^n((\Psi^\pm)^n) = F((\Psi^\pm)^n)$. As for ghost-fluid methods, the scheme is locally non conservative since $\mathcal{F}_+^n \neq \mathcal{F}_-^n$, but it is consistent since $\mathcal{F}_\pm^n$ are regular enough functions of the states to the left and to the right of the interface, and $\mathcal{F}_+^n = \mathcal{F}_-^n$ when those states are identical. As shown in the numerical test section the error in conservation is negligible: the shock speeds and positions are correctly predicted. Indeed, the number of cell interfaces for which a non-conservative numerical flux is employed is always negligible compared to the total number of mesh cells.
The interface position is advected using the material velocity field. For numerical stability, the integration step is limited by the fastest characteristics over the grid points. Hence, the interface position will belong to the same interval between two grid points for more than one time step. When the physical interface overcomes a grid point, the corresponding conservative variables, say Ψ_k^{n+1}, do not correspond anymore to the material present at that grid point before the integration step. When the physical interface moves to the right, then we take $\Psi_k^{n+1} = (\Psi^-)^n$, whereas if it moves to the left $\Psi_k^{n+1} = (\Psi^+)^n$.
Compared to the ghost-fluid method and its improvements and variants [6, 2, 4], this scheme is simpler as it does not require the storage of any additional variables or equation of state relative to a ghost fluid to treat the material interface, nor the solution of additional Riemann problems, each relative to a different material at the interface. Our scheme only relies on the intermediate states $(\Psi^-)^n$ and $(\Psi^+)^n$ that are anyway computed at every cell interface.

3 RESULTS

We show here an example of simulations involving an undulated interface separating two different compressible materials over which a shock wave is impinging. In fluid mechanics these phenomena are known as Richtmeyer-Meshkov instabilities. See Fig. 1.

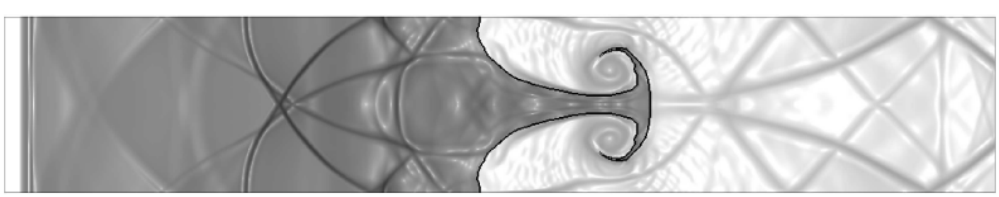

Figure 1: A shock wave traveling from air to helium at M=2.1 impinges on an initially undulated interface. Interface at later times.

These instabilities can affect also the interface between a compressible fluid and a compressible elastic material [13]. The simulations in Fig. 2 are, as far as we know, among the first accurate computational examples of such instabilities.

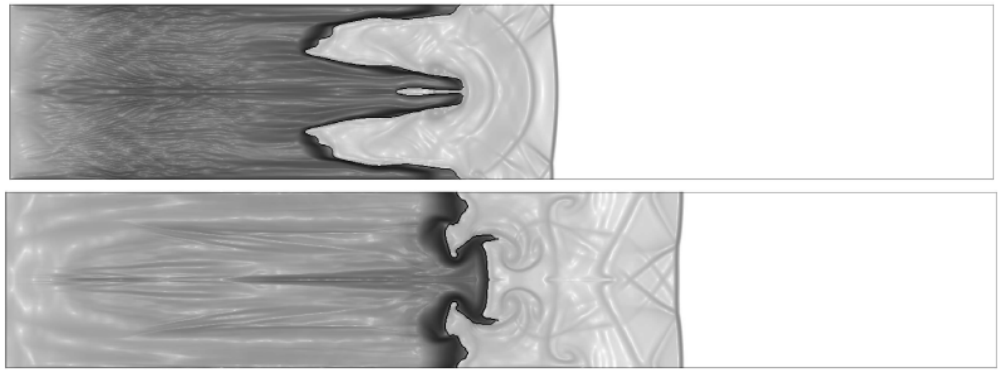

Figure 2: Upper picture: a shock wave traveling from the elastic material to air impinges on an initially undulated interface. The shear modulus of the material is 10^2 times smaller than that of copper, the compression rigidity the same. Bottom: as before, but the shear modulus of the material is now 10^4 times smaller than that of copper. Interfaces at later times.

4 CONCLUSIONS

We presented a simple method to model interactions of compressible multimaterials. As shown by the illustrations, the model captures well the scattering of shock waves and is able to recover the Richtmyer-Meshkov instabilities at the interface between two fluids. Instabilities in the case of elastic media and properties of plasticity are under current investigations.

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