

Curl – type involution constraints in multiphase flow modeling

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Physical classification of interfaces

- Diffuse interfaces
- Sharp interfaces



Shock-droplet interaction

(courtesy of G. Jourdan and L. Houas, IUSTI, Marseille)

Multi-phase modeling

The dynamics of interfaces between pure components is the main problem of multi-phase modeling.

Modeling via Hamilton's principle

Definitions

- T – kinetic energy
- W – potential energy
- $L = T - W$ – Lagrangian
- $a = \int_{t_0}^{t_1} \int_{\mathcal{D}(t)} L dD dt$ - Hamilton's action

Hamilton's principle

The governing equations are stationary ‘points’ of Hamilton’s action (under certain constraints to be defined).

Advantages of Hamilton's principle

- Only one scalar function (Lagrangian) determines the governing equations
- Conservation laws and symmetry properties of the governing equations come from the symmetries of Hamilton's action.

Classical diffuse interfaces (Euler–Korteweg–Van de Waals equations)

P. Casal, M. Eglit, H. Gouin, M. Slemrod, L. Truskinovsky, Ph. Le Floch,
D. Jamet, S. Benzoni-Gavage, R. Danchin, Ch. Rohde, D. Bresch, B.
Haspot, ...

- Kinetic energy $T = \int_{\mathcal{D}} \rho \frac{\|\mathbf{u}\|^2}{2} dD,$
- Potential energy $W = \int_{\mathcal{D}} \rho \varepsilon(\rho, \|\nabla \rho\|^2, \eta) dD,$
- Lagrangian $L = T - W,$
- Hamilton's action $a = \int_{t_0}^{t_1} L dt.$

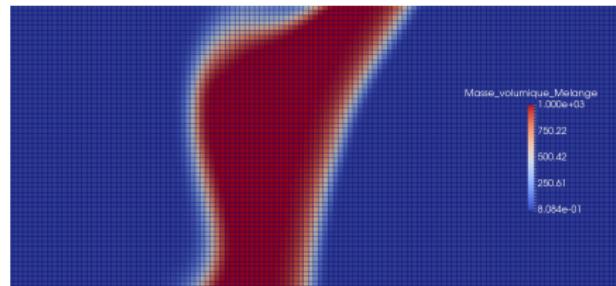
To obtain the governing equations, one uses the Hamilton's principle with the following constraints to respect :

- Conservation of the density
- Conservation of the entropy

Modeling of moving interfaces : multiphase approach

Sharp interfaces as a heterogeneous mixture zone separating two pure fluids (Abgrall and Karni, Saurel and Abgrall), or fluids and solids (Ndanou, Favrie, SG).

- The position of the interface is determined in terms of the volume fraction α_g or mass fraction Y_g .
- The mixture equations of state are formulated in terms of individual equations of state.
- Only the Cauchy problem is solved.



The simplest two-fluid model (A. Kapila et al., 1993)

Originally, it was derived by the averaging procedure.

Variational formulation (SG, 2011).

- $T = \int_{\mathcal{D}} \rho \frac{\|\mathbf{u}\|^2}{2} dD$
- $W = \int_{\mathcal{D}} \rho \varepsilon dD$
- Lagrangian $L = T - W$
- Hamilton's action $a = \int_{t_0}^{t_1} L dt$

Definitions :

- $\rho = \alpha_I \rho_I + \alpha_g \rho_g, \varepsilon = Y_I \varepsilon_I(\rho_I, \eta_I) + Y_g \varepsilon_g(\rho_g, \eta_g),$
- $Y_I = \frac{\alpha_I \rho_I}{\rho}, Y_g = \frac{\alpha_g \rho_g}{\rho}, Y_I + Y_g = 1, \alpha_I + \alpha_g = 1.$

Modeling of capillary effects

The interface energy can be added as

- $W_c = \sigma \int_{\mathcal{D}} \|\nabla \alpha_g\| dD$

Advantage : no scale parameter in the interface modeling.

Problems : the equation for the volume fraction depends on high (second) order derivatives of α_g .

A new ‘mixed’ approach : level set + multiphase interface modeling

- The position of the interface is defined by an independent ‘geometric’ parameter c taking the values 0 and 1 in the pure phases which is transported by the flow :

$$\frac{Dc}{Dt} = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla.$$

- The surface energy is taken into account in terms of this parameter :

$$W_c = \sigma \int_{\mathcal{D}} \|\nabla c\| dD.$$

New ‘mixture’ Lagrangian : physics and geometry are separated

- $T = \int_{\mathcal{D}} \rho \frac{\|\mathbf{u}\|^2}{2} dD$
- $W = \int_{\mathcal{D}} (\rho \varepsilon + \sigma \|\mathbf{b}\|) dD, \quad \mathbf{b} = \nabla c$
- Lagrangian $L = T - W$
- Hamilton's action $a = \int_{t_0}^{t_1} L dt$

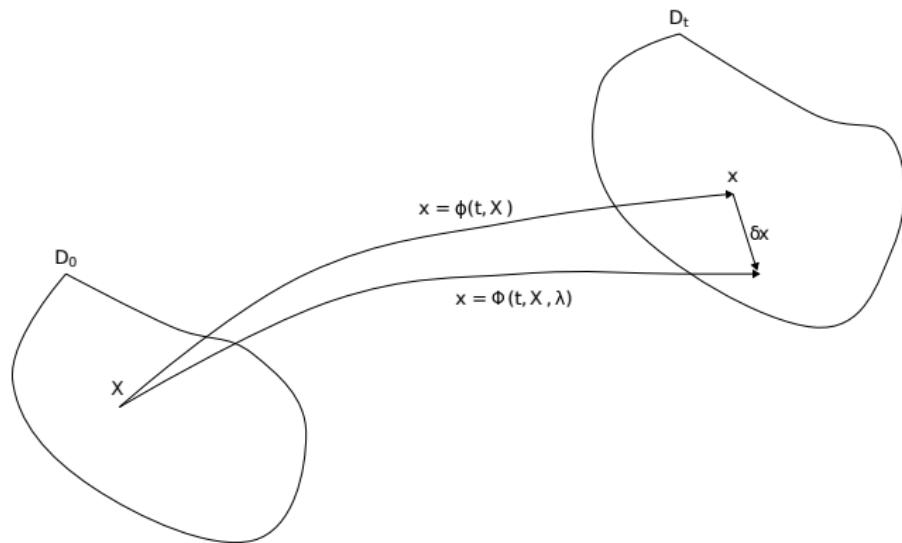
Definitions :

- $\rho = \alpha_I \rho_I + \alpha_g \rho_g, \quad \varepsilon = Y_I \varepsilon_I(\rho_I, \eta_I) + Y_g \varepsilon_g(\rho_g, \eta_g),$
- $Y_I = \frac{\alpha_I \rho_I}{\rho}, \quad Y_g = \frac{\alpha_g \rho_g}{\rho}, \quad Y_I + Y_g = 1, \quad \alpha_I + \alpha_g = 1.$

Constraints

- $\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0,$
- $(\rho Y_i)_t + \operatorname{div}(\rho Y_i \mathbf{u}) = 0, \quad i = l, g,$
- $(\rho \eta_i)_t + \operatorname{div}(\rho \eta_i \mathbf{u}) = 0,$
- $(\rho c)_t + \operatorname{div}(\rho c \mathbf{u}) = 0,$

Virtual motion



Eulerian variations, SG (2011)

Virtial displacements

$$\delta \mathbf{x}(t, \mathbf{X}) = \frac{\partial \Phi}{\partial \lambda} \Big|_{\lambda=0}, \quad \zeta(t, \mathbf{x}) = \delta \mathbf{x}(t, \mathbf{X})|_{\mathbf{X}=\varphi^{-1}(t, \mathbf{x})}. \quad (1)$$

- $\delta \rho = -\operatorname{div}(\rho \zeta),$
- $\delta \eta_i = -\nabla \eta_i \cdot \zeta, \quad \delta Y_i = -\nabla Y_i \cdot \zeta, \quad \delta c = -\nabla c \cdot \zeta,$
- $\delta \mathbf{u} = \frac{D \zeta}{Dt} - \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \zeta, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla.$

Momentum equation

Hamilton's principle :

$$\delta a = \delta \int_{t_0}^{t_1} L dt = \int_{t_0}^{t_1} \int_{\mathcal{D}} \mathbf{M} \cdot \boldsymbol{\zeta} \, dD = 0.$$

Euler-Lagrange equations :

$$(\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} + \Omega) = 0, \quad \Omega = \sigma \|\mathbf{b}\| \left(\frac{\mathbf{b} \otimes \mathbf{b}}{\|\mathbf{b}\|^2} - \mathbf{I} \right)$$

Variation with respect to the volume fraction

$$\rho_I = \rho_g = \rho.$$

As a consequence, one has a differential (non-conservative) equation :

$$\frac{D\alpha_g}{Dt} + K \nabla \cdot \mathbf{u} = 0,$$

$$K = \frac{\rho_g a_g^2 - \rho_I a_I^2}{\frac{\rho_g a_g^2}{\alpha_g} + \frac{\rho_I a_I^2}{\alpha_I}}.$$

Extended system

One has

$$\frac{Dc}{Dt} = 0.$$

It implies

$$\frac{\partial \mathbf{b}}{\partial t} + \nabla(\mathbf{b} \cdot \mathbf{u}) = 0, \quad \mathbf{b} = \nabla c.$$

It is equivalent to

$$\frac{\partial \mathbf{b}}{\partial t} + \left(\frac{\partial \mathbf{b}}{\partial \mathbf{x}} \right)^T \mathbf{u} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^T \mathbf{b} = 0.$$

Not Galilean invariant! One uses $\text{curl}(\mathbf{b}) = 0$:

$$\frac{\partial \mathbf{b}}{\partial t} + \nabla(\mathbf{b} \cdot \mathbf{u}) + \left(\frac{\partial \mathbf{b}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{b}}{\partial \mathbf{x}} \right)^T \right) \mathbf{u} = 0 \quad \Leftrightarrow \frac{D\mathbf{b}}{Dt} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^T \mathbf{b} = 0.$$

Galilean invariant!

Galilean invariant governing equations *curl*-type involution constraint

$$\frac{D\alpha_g}{Dt} + K \nabla \cdot \mathbf{u} = 0,$$

$$(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \mathbf{u}) = 0, \quad \frac{D\eta_k}{Dt} = 0, \quad k = l, g.$$

$$(\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} + \Omega) = 0, \quad \Omega = \sigma \|\mathbf{b}\| \left(\frac{\mathbf{b} \otimes \mathbf{b}}{\|\mathbf{b}\|^2} - \mathbf{I} \right),$$

$$\frac{\partial \mathbf{b}}{\partial t} + \nabla (\mathbf{b} \cdot \mathbf{u}) + \left(\frac{\partial \mathbf{b}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{b}}{\partial \mathbf{x}} \right)^T \right) \mathbf{u} = 0.$$

Energy equation :

$$(\rho E + \sigma \|\mathbf{b}\|)_t + \nabla \cdot ((\rho E + \sigma \|\mathbf{b}\| + p) \mathbf{u} + \Omega \mathbf{u}) = 0,$$

$$E = \frac{\|\mathbf{u}\|^2}{2} + \sum_k Y_k \varepsilon_k(\rho_k, \eta_k).$$

Characteristic speeds : 1D case

Unknowns

$$\mathbf{U} = (\alpha_I, u, v, w, P, b_1, b_2, b_3, c, \eta_1, \eta_2, Y_I)^T \quad (2)$$

$$u - a_s < u - a_c \leq u \leq u + a_c < u + a_s \quad (3)$$

Eigenvectors

For the multiple eigenvalue $\lambda = u$ one eigenvector is missing. The system is only weakly hyperbolic.

Example

$$\rho_t + (\rho u)_x = 0, \quad (\rho u)_t + (\rho u^2)_x = 0.$$

Linearization $\rho = \rho_0 = \text{const}$, $u = 0$.

Unbounded solution for perturbations :

$$u'(t, x) = u'(0, x), \quad \rho'(t, x) = \rho'(0, x) - t \rho_0 u'(0, x)$$

Remark To obtain a hyperbolic system one has to add the terms of $\text{curl}(b)$ type into the momentum and energy equation - type into the governing system (see S. Chiocchetti, M. Dumbser, I. Peshkov, SG, 2020.)

Clearning procedure

The idea comes from Munz *et al.* 2000 for the MHD equations.

$$\frac{D\alpha_l}{Dt} - K \nabla \cdot \mathbf{u} = 0,$$

$$(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \mathbf{u}) = 0, \quad \frac{D\eta_k}{Dt} = 0, \quad k = l, g.$$

$$(\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} + \Omega) = 0, \quad \Omega = \sigma \|\mathbf{b}\| \left(\frac{\mathbf{b} \otimes \mathbf{b}}{\|\mathbf{b}\|^2} - \mathbf{I} \right),$$

$$\frac{D\mathbf{b}}{Dt} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^T \mathbf{b} = C \|\mathbf{b}\| \operatorname{curl}(\psi), \quad \rho \frac{D\psi}{Dt} = -\sigma C \operatorname{curl}(\mathbf{b}), \quad C \gg 1.$$

Energy equation :

$$(\rho(E + \|\psi\|^2/2) + \sigma \|\mathbf{b}\|)_t$$

$$+ \nabla \cdot ((\rho(E + \|\psi\|^2/2) + \sigma \|\mathbf{b}\| + p) \mathbf{u} + \Omega \mathbf{u} + \sigma C \mathbf{b} \times \psi) = 0,$$

Clearning procedure

1. Such an extended system is hyperbolic, a pair of additional large eigenvalues is only added.
2. It is thermodynamically consistent (the energy is conserved).

Extension with a relaxation equation for α_I

$$\frac{D\alpha_I}{Dt} = \mu(p_I - p_g), \quad \mu > 0.$$

This procedure is compatible with the entropy inequality.

Numerical methods

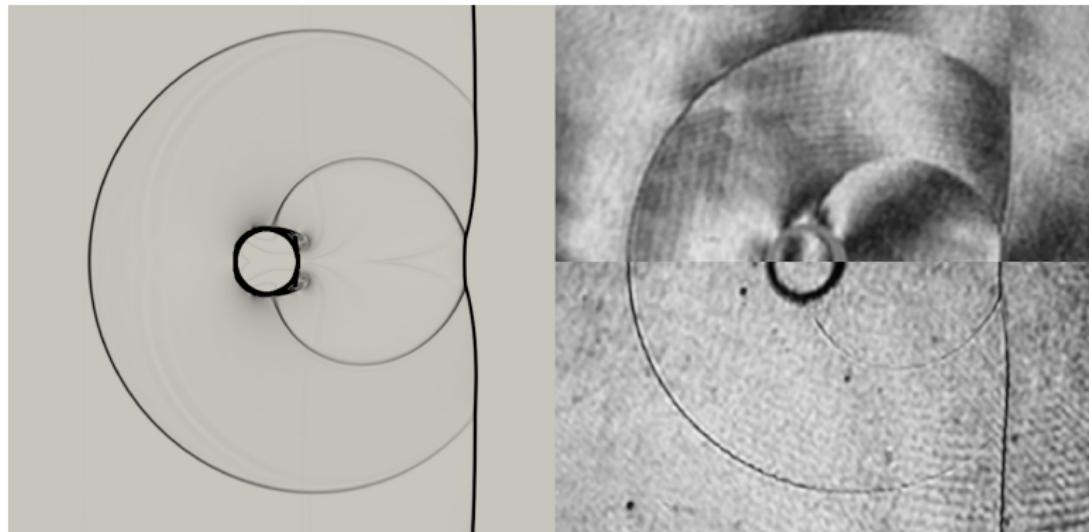
I. Splitting method for weakly hyperbolic system (Schmidmayer, Daniel, Petitpas, Favrie, SG, 2017)

- Hyperbolic sub-system for compression waves
- Weakly hyperbolic sub-system for capillary waves
- Relaxation

II. ADER schemes + clearing procedure (Simone Chiocchetti, Michael Dumbser, Ilya Peshkov, SG, 2020).

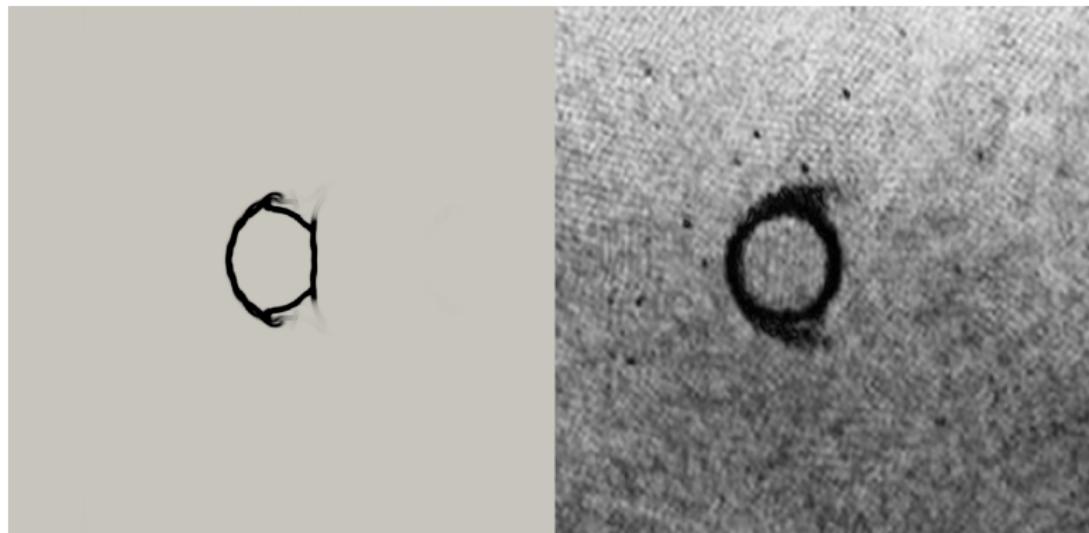
Shock-droplet interaction

Mach number 1.3, drop's diameter 6.4 mm, number of mesh cells 3200x1200 for a physical domain 220 mm x 82,5 mm at time instant 55 μs .



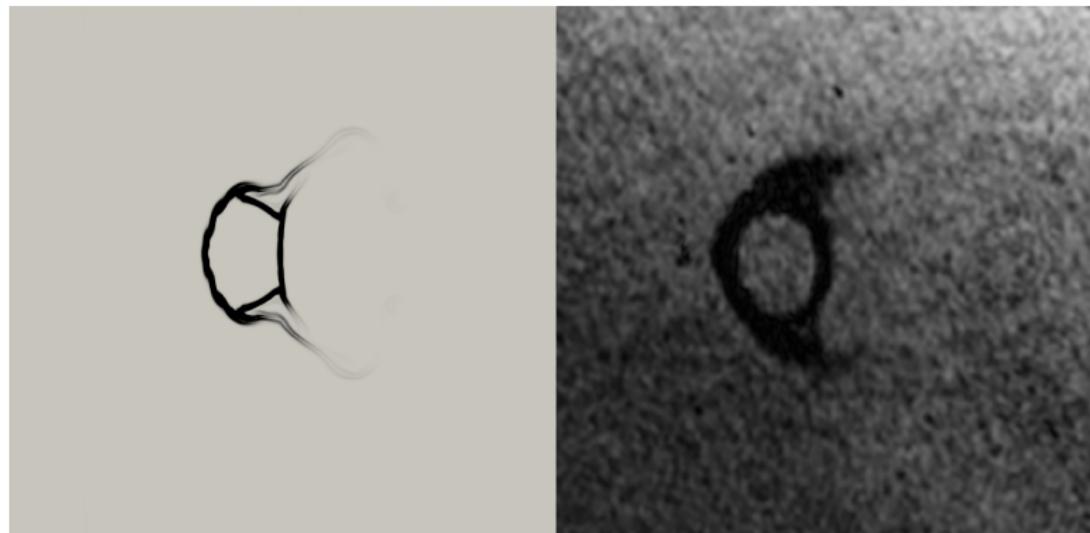
Shock-droplet interaction

Mach number 1.3, drop's diameter 6.4 mm, number of mesh cells 3200x1200 for a physical domain 220 mm x 82,5 mm at time instant 200 μ s.



Shock-droplet interaction

Mach number 1.3, drop's diameter 6.4 mm, number of mesh cells 3200x1200 for a physical domain 220 mm x 82,5 mm at time instant 300 μ s.



Shock-droplet interaction

Hyperbolic version of the Euler-Van-der Waals - Korteweg-van der Waals equations

A priori, the dispersive equations have nothing to do with the hyperbolic equations.

Cubic defocusing NLS equation

$$i\psi_t + \frac{1}{2}\Delta\psi - |\psi|^2\psi = 0.$$

- A wide range of applications : quantum fluids, nonlinear optics, surface gravity waves
- Advantage : the equation is integrable in 1D case [Zakharov, Manakov 1974]

A first order hyperbolic reformulation of the Navier-Stokes-Korteweg system based on the GPR model and an augmented Lagrangian approach

Cubic defocusing NLS equation

- A wide range of applications : quantum fluids, nonlinear optics, surface gravity waves
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The Madelung transform

$$\psi(x, t) = \sqrt{\rho(x, t)} e^{i\theta(x, t)} \quad u = \nabla\theta$$

$$\begin{cases} \rho_t + \operatorname{div}(\rho u) = 0 \\ (\rho u)_t + \operatorname{div}(\rho u \otimes u + \Pi) = 0 \end{cases}$$

with : $\Pi = \left(\frac{\rho^2}{2} - \frac{1}{4}\Delta\rho \right) \operatorname{Id} + \frac{1}{4\rho} \nabla\rho \otimes \nabla\rho$

Lagrangian for NLS equation

For the previous set of equations, we can construct the Lagrangian :

$$L = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla \rho|^2}{2} \right) d\Omega_t$$

Energy conservation law :

$$\frac{\partial \rho \mathcal{E}}{\partial t} + \operatorname{div} \left(\rho \mathcal{E} \mathbf{u} + \Pi \mathbf{u} - \frac{1}{4} \frac{D\rho}{Dt} \nabla \rho \right) = 0$$

where

$$\rho \mathcal{E} = \rho \frac{|\mathbf{u}|^2}{2} + \frac{\rho^2}{2} + \frac{1}{4\rho} \frac{|\nabla \rho|^2}{2}$$

Idea

1. Smooth initial data are needed for dispersive systems. But, sometimes, one needs to solve the equations with discontinuous data (ex. shock pulses generated by a laser drive). Not well posed for dispersive equations ...
2. Difficulties in formulating “transparent” boundary conditions (C. Besse, M. Ehrhardt, P. Noble, M. Kazakova, ...)
3. Sometimes the computations are expensive (elliptic operators should be inverted, ...)

Hyperbolic equations are better then ! Godunov type methods could be used !

Hyperbolic regularisation

Cattaneo relaxation approach for the heat equation

$$u_t = q_x, \quad q_t = \frac{u_x - q}{\tau}, \quad 0 < \tau \ll 1$$

Energy equation

$$\left(\frac{u^2}{2} + \tau \frac{q^2}{2} \right)_t - (uq)_x = -q^2$$

New idea for dispersive equations coming from Hamilton's principle :

modify the 'master' Lagrangian (Favrie and SG, 2017 ; Dhaouadi, Favrie, SG, 2019).

'Augmented' Lagrangian

'Master' Lagrangian :

$$L = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla \rho|^2}{2} \right) d\Omega_t$$

'Augmented' Lagrangian : F. Dhaouadi, N. Favrie, SG (SAM, 2019)

$$\hat{L} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\mathbf{p}|^2}{2} - \frac{\lambda}{2} \rho \left(\frac{\eta}{\rho} - 1 \right)^2 + \frac{\beta\rho}{2} \mathbf{w}^2 \right) d\Omega_t$$

$$\mathbf{p} = \nabla \eta \quad \mathbf{w} = \frac{D\eta}{Dt}$$

$$\frac{\lambda}{2} \rho \left(\frac{\eta}{\rho} - 1 \right)^2 : \text{Penalty}$$

$$\frac{\beta\rho}{2} \left(\frac{D\eta}{Dt} \right)^2 : \text{Regularizer}$$

Augmented Lagrangian

'Augmented' Lagrangian :

$$\hat{L} = \int_{\Omega_t} \left(\rho \frac{|\boldsymbol{u}|^2}{2} + \frac{\beta\rho}{2} w^2 - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\boldsymbol{p}|^2}{2} - \frac{\lambda}{2} \rho \left(\frac{\eta}{\rho} - 1 \right)^2 \right) d\Omega_t$$

The constraint :

$$\rho_t + \operatorname{div}(\rho \boldsymbol{u}) = 0$$

Augmented Euler–Lagrange equations

- Virtual displacements of the continuum :

$$(\rho \mathbf{u})_t + \operatorname{div} (\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = 0$$

with : $\mathbf{P} = \left(\frac{\rho^2}{2} - \frac{1}{4\rho} |\mathbf{p}|^2 + \eta \lambda \left(1 - \frac{\eta}{\rho} \right) \right) \mathbf{I} + \frac{1}{4\rho} \mathbf{p} \otimes \mathbf{p}$

- Variations with respect to η :

$$\frac{D\eta}{Dt} = w, \quad (\rho w)_t + \operatorname{div} \left(\rho w \mathbf{u} - \frac{1}{4\rho\beta} \mathbf{p} \right) = \frac{\lambda}{\beta} \left(1 - \frac{\eta}{\rho} \right)$$

Weakly hyperbolic Galilean invariant augmented system

$$\left\{ \begin{array}{l} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = 0 \\ (\rho \eta)_t + \operatorname{div}(\rho \eta \mathbf{u}) = \rho w \\ (\rho w)_t + \operatorname{div}\left(\rho w \mathbf{u} - \frac{1}{4\rho\beta} \mathbf{p}\right) = \frac{\lambda}{\beta} \left(1 - \frac{\eta}{\rho}\right) \\ \frac{\partial \mathbf{p}}{\partial t} + \nabla \cdot (\mathbf{p} \cdot \mathbf{u} - w) + \left(\frac{\partial \mathbf{p}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{p}}{\partial \mathbf{x}}\right)^T\right) \mathbf{u} = 0. \end{array} \right.$$

$$(\rho \mathcal{E})_t + \nabla \cdot \left(\rho \mathbf{u} \mathcal{E} + \mathbf{P} \mathbf{u} - \frac{1}{4\rho} w \mathbf{p} \right) = 0,$$

$$\mathcal{E} = \frac{|\mathbf{u}|^2}{2} + \frac{\beta}{2} w^2 + \frac{\rho}{2} + \frac{1}{4\rho^2} \frac{|\mathbf{p}|^2}{2} + \frac{\lambda}{2} \left(\frac{\eta}{\rho} - 1\right)^2$$

Clearning procedure (hyperbolic system)

$$\left\{ \begin{array}{l} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = 0 \\ (\rho \eta)_t + \operatorname{div}(\rho \eta \mathbf{u}) = \rho w \\ (\rho w)_t + \operatorname{div}\left(\rho w \mathbf{u} - \frac{1}{4\rho\beta} \mathbf{p}\right) = \frac{\lambda}{\beta} \left(1 - \frac{\eta}{\rho}\right) \\ \frac{D\mathbf{p}}{Dt} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{p} - \nabla w + 2a_c \rho \operatorname{curl}(\psi) = 0 \\ \rho \frac{D\psi}{Dt} - \frac{a_c}{2} \operatorname{curl}(\mathbf{p}) = 0. \end{array} \right.$$

$$\mathbf{P} = \left(\frac{\rho^2}{2} - \frac{1}{4\rho} |\mathbf{p}|^2 + \eta \lambda \left(1 - \frac{\eta}{\rho}\right) \right) \mathbf{I} + \frac{1}{4\rho} \mathbf{p} \otimes \mathbf{p}$$

Energy equation

$$\left(\rho(\mathcal{E} + |\psi|^2/2) \right)_t + \nabla \cdot \left(\rho \mathbf{u} (\mathcal{E} + |\psi|^2/2) + \mathbf{P} \mathbf{u} - \frac{1}{4\rho} w \mathbf{p} + \frac{a_c}{2} \psi \times \mathbf{p} \right) = 0,$$

$$\mathcal{E} = \frac{|\mathbf{u}|^2}{2} + \frac{\beta}{2} w^2 + \frac{\rho}{2} + \frac{1}{4\rho^2} \frac{|\mathbf{p}|^2}{2} + \frac{\lambda}{2} \left(\frac{\eta}{\rho} - 1 \right)^2$$

Values of λ and β

- Values have to be assigned : a criterion is needed.
- We can base this choice, for example, on the dispersion relation.

DSW Numerical results : ρ

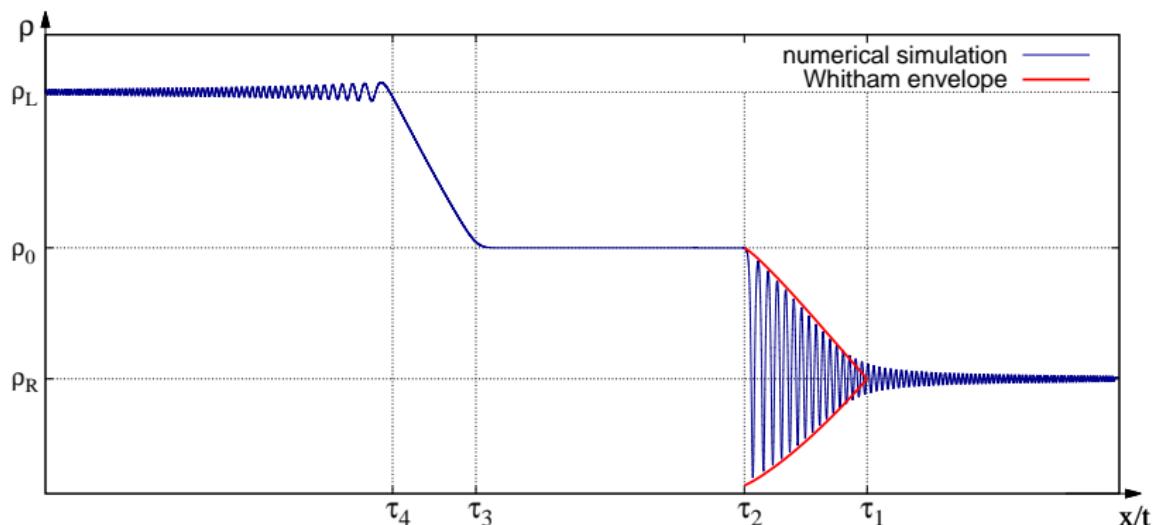


Figure – Comparison of the numerical result $\rho(x, t) = f(x/t)$ (blue line) with the asymptotic profile of the oscillations from Whitham's theory of modulations (M. Pavlov, 1987). $t=70$ (F. Dhaouadi, N. Favrie, SG, 2019).

Clearning procedure

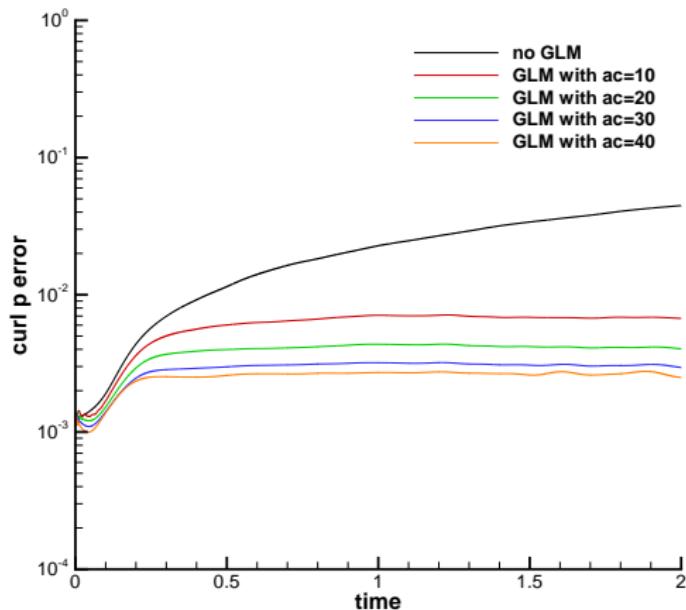


Figure – L_2 norm of $\text{curl}(p)$ as a function of the cleaning speed a_c . An exact solution was tested (S. Bustos, C. Escalante, M. Dumbser, N. Favrie, SG et al. 2021)

DSW Numerical results

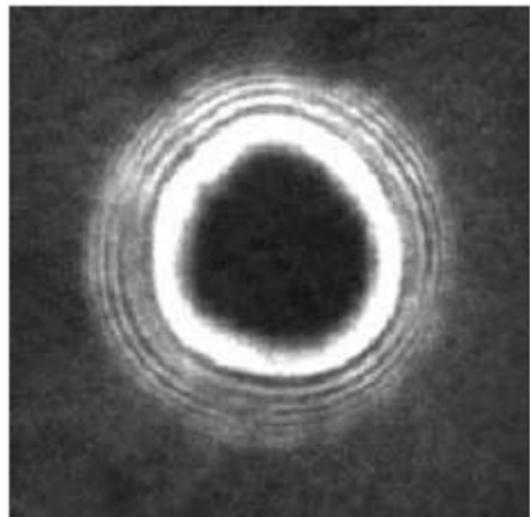
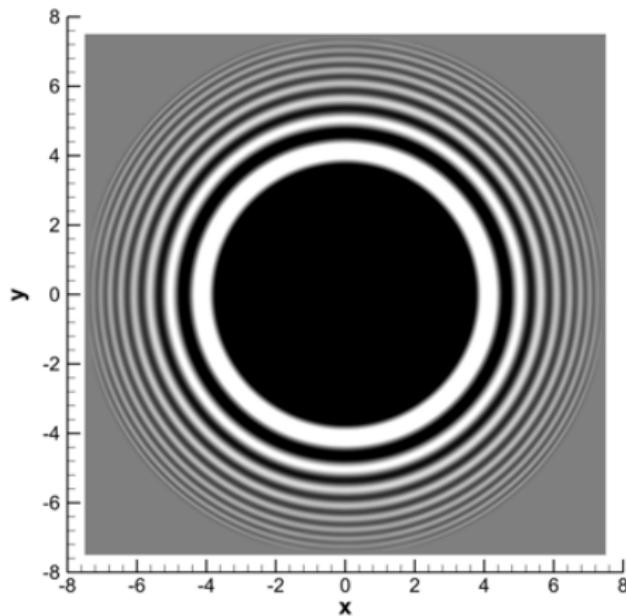


Figure – Explosion in Bose-Einstein condensates (S. Busto *et al.* 2021)

This approach was extended by F. Dhaouadi, M. Dumbser, J. Comp. Physics 2022 **470** to the capillary fluids with the van der Waals type (non-monotonic) equation of state.

Conclusion

- Two weakly hyperbolic systems with *curl* - type involution constraints are derived : a two–fluid system with capillary effects and a hyperbolic approximation of the Euler–van der Waals–Korteweg equations.
- Energy compatible clearing procedure is proposed.