A First-order Hyperbolic Reformulation of the Navier-Stokes-Korteweg Equations

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Joint work with
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Navier-Stokes-Korteweg equations

In general, the equations write

$$\begin{cases} \rho_t + \mathrm{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \underline{\underline{S}} + \underline{\underline{K}} \end{cases}$$

where $\rho = \rho(\mathbf{x}, t)$, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ and $(\mathbf{x}, t) \in \mathbb{R}^d \times [0, T]$
The (viscous) Navier-Stokes contribution is given by

$$\underline{\underline{S}} = \mu \, \mathrm{div} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} \mathrm{div}(\mathbf{u}) \mathbf{I} \right)$$

The (dispersive) Korteweg contribution are given by:

$$\underline{\underline{K}} = \rho \nabla \left(K(\rho) \Delta \rho + \frac{1}{2} K'(\rho) |\nabla \rho|^2 \right)$$

Dissipationless Euler-Korteweg equations

The equations write :

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- $K(\rho) = \gamma$: **Compressible flow with surface tension**

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- $K(\rho) = \frac{1}{4\rho}$: **Quantum hydrodynamics**

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Surface tension / capillarity

- Euler-Korteweg equations : Fluid flow + Surface tension.
- Surface tension = Tendency of a fluid to shrink and minimize its surface.
- Examples in nature : Droplet shape, ripples on the water surface, water striders, etc...



Photos credits : pexels.com

Main objective

Given the Navier-Stokes-Korteweg system of equations :

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Suggested solution

A first-order hyperbolic reformulation of the NSK system!

More generally

We are looking for a new model that:

- approximates Euler-Korteweg in some limit.
- is derived from a variational principle.
- admits no regions of ellipticity.
- is in line with the laws of thermodynamics.
- can be solved numerically with accurate numerical methods.

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Hyperbolic equations

- Mathematically well-posed equations.
- A very rich literature on numerical methods.
- Bounded wave speeds

A subset of connected works and topics

1. A family of Parabolic relaxation of NSK equations.
   - ⇒ Rohde & collaborators [2014 - Now]
   - ⇒ Chertock & Degond & Neusser [2017]
2. Hyperbolic approximation of Euler-Korteweg equations.
   - ⇒ Dhaouadi, Favrie, Gavrilyuk 2019. (Schrödinger equation)
   - ⇒ Dhaouadi, Gavrilyuk, Vila 2022. (Thin films).
   - ⇒ Bourgeois, Lombard, Favrie 2020 (Solids with nonconvex EOS)
   - ⇒ Bresch *et al.*,2020 (2nd Order Hyperbolic)
3. Hyperbolic reformulation of Navier-Stokes equations.
   - ⇒ GPR model of continuum mechanics.[Godunov 1961,Romenski 1998,*Peshkov et al.* 2016]

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Idea

Combine our augmented Lagrangian model with the general *GPR* model of continuum mechanics.

Outline

Lagrangian for the Euler-Korteweg system

(EK) system can be derived from the Lagrangian :

$$\mathcal{L} = \int_{\Omega_t} \left(\frac{\rho \left|\mathbf{u}\right|^2}{2} - W(\rho) - \gamma \frac{\left|\nabla \rho\right|^2}{2} \right) \, d\Omega$$

Variational principle

$+$

Differential constraint : $\rho_t + \mathrm{div}(\rho \mathbf{u}) = 0$

$$(\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla(p(\rho)) = \gamma \rho \nabla(\Delta \rho)$$

with $p(\rho) = \rho W(\rho) - W(\rho)$

Augmented Lagrangian approach

$$\mathcal{L}(\mathbf{u}, \rho, \nabla\rho) = \int_{\Omega_t} \left(\frac{1}{2}\rho\left|\mathbf{u}\right|^2 - W(\rho) - \gamma\frac{\left|\nabla\rho\right|^2}{2} \right) d\Omega$$

$$\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0$$

'Augmented' Lagrangian approach [Favrie-Gavrilyuk 2017]

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta) \qquad (\eta \longrightarrow \rho)$$

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho\frac{\left|\mathbf{u}\right|^2}{2} - W(\rho) - \gamma\frac{\left|\nabla\eta\right|^2}{2} - \frac{1}{2\alpha\rho}\left(\rho - \eta\right)^2 \right) d\Omega$$

$\frac{1}{2\alpha\rho}\left(\rho - \eta\right)^2$: Classical Penalty term

Hints on calculus of variations (For general $K(\rho)$)

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - W(\rho) - K(\rho) \frac{|\nabla \eta|^2}{2} - \frac{\rho}{2\alpha} \left(\frac{\eta}{\rho} - 1 \right)^2 \right) d\Omega$$

$$\tilde{\mathcal{L}}(\overbrace{\mathbf{u}, \rho}^{\delta \mathbf{x}}, \underbrace{\eta, \nabla \eta}_{\delta \eta}) \Rightarrow \text{Two Euler-Lagrange equations}$$

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- Virtual displacement of the continuum ($\delta \mathbf{x}$):

$$(\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla(\rho W'(\rho) - W(\rho))$$
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- η variation ($\delta \eta$):

$$\frac{1}{\alpha} \left(1 - \frac{\eta}{\rho} \right) = - \left(K(\rho) \Delta \eta + K'(\rho) \nabla \rho \cdot \nabla \eta \right)$$

Preliminary system

Deriving the system of governing equations yields:

$$\begin{cases} \rho_t + \mathrm{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u}\right) + \nabla\left(\rho W'(\rho) - W(\rho)\right) = \mathrm{div}(\mathbf{K}_\alpha) \\ -\gamma \Delta \eta = \frac{1}{\alpha}\left(1 - \frac{\eta}{\rho}\right) \end{cases}$$

where:

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Idea : Include $\dot{\eta}$ into the Lagrangian !

Augmented Lagrangian - Attempt 2

Augmented Lagrangian approach

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta, \dot{\eta}) \qquad \alpha, \beta \ll 1$$

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - W(\rho) - \frac{\gamma}{2} |\nabla\eta|^2 - \frac{1}{2\alpha\rho} (\rho - \eta)^2 + \frac{\beta\rho}{2} \dot{\eta}^2 \right) d\Omega$$

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$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - W(\rho) - \frac{\gamma}{2} |\nabla\eta|^2 - \frac{1}{2\alpha\rho} (\rho - \eta)^2 + \frac{\beta\rho}{2} \dot{\eta}^2 \right) d\Omega$$

Variational principle : $a = \int_{t_0}^{t_1} \tilde{\mathcal{L}} \, dt$

$$\begin{cases} \rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \\ (\rho\mathbf{u})_t + \operatorname{div}\left(\rho\mathbf{u} \otimes \mathbf{u} - \mathbf{K}_\alpha(\rho, \eta, \nabla\eta)\right) + \nabla P(\rho) = 0 \\ (\beta\rho\dot{\eta})_t + \operatorname{div}\left(\beta\rho\dot{\eta}\mathbf{u} - \gamma\nabla\eta\right) = \frac{1}{\alpha}\left(1 - \frac{\eta}{\rho}\right) \end{cases}$$

Augmented Lagrangian - Attempt 2

Augmented Lagrangian approach

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta, \dot{\eta}) \qquad \alpha, \beta \ll 1$$

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - W(\rho) - \frac{\gamma}{2} |\nabla\eta|^2 - \frac{1}{2\alpha\rho} (\rho - \eta)^2 + \frac{\beta\rho}{2} \dot{\eta}^2 \right) d\Omega$$

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$\Rightarrow$ There are still high-order derivatives!

Order reductions

1. We denote $w = \dot{\eta}$. Thus:

$$w = \eta_t + \mathbf{u} \cdot \nabla \eta \quad \Longrightarrow \quad \boxed{(\rho\eta)_t + \mathrm{div}(\rho\eta\mathbf{u}) = \rho w}$$

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$$\Longrightarrow \quad \boxed{\mathbf{p}_t + \nabla(\mathbf{p} \cdot \mathbf{u} - w) = 0}$$

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Important !

Initial data must be such that:

$$\mathbf{p}(\mathbf{x}, 0) = \nabla \eta(\mathbf{x}, 0), \quad w(\mathbf{x}, 0) = \dot{\eta}(\mathbf{x}, 0)$$

Final form of the hyperbolic Euler-Korteweg system

$$
\begin{cases}
\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\
(\rho \mathbf{u})_t + \operatorname{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + (\rho W'(\rho) - W(\rho))\, \mathbf{Id} - \mathbf{K}_\alpha\right) = 0 \\
(\beta \rho w)_t + \operatorname{div}\left(\beta \rho w \mathbf{u} - \gamma \mathbf{p}\right) = \frac{1}{\alpha}\left(1 - \frac{\eta}{\rho}\right) \\
\mathbf{p}_t + \operatorname{div}((\mathbf{p} \cdot \mathbf{u} - w)\mathbf{Id}) = 0, \quad \operatorname{curl}(\mathbf{p}) = 0 \\
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$$

$$
\mathbf{K}_\alpha = \left(\frac{\gamma}{2}|\mathbf{p}|^2 - \frac{\eta}{\alpha}\left(1 - \frac{\eta}{\rho}\right)\right)\mathbf{Id} - \gamma \mathbf{p} \otimes \mathbf{p}
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- Main question : Is this system hyperbolic ?

Hyperbolicity in 1D

1D case: $\mathbf{u} = (u,0,0)^T$ and $\mathbf{p} = (p,0,0)^T$: We can write the system in its quasi-linear form

$$\mathbf{Q}_t + \mathbf{A}(\mathbf{Q})\mathbf{Q}_x = \mathbf{S}(\mathbf{Q})$$

where $\mathbf{Q}$ is the vector of primitive variables, $\mathbf{A} = \mathbf{A}(\mathbf{Q})$ is the jacobian matrix of the flux, and $\mathbf{S} = \mathbf{S}(\mathbf{Q})$ is the vector of source terms, all of which are given by

$$\mathbf{A} = \begin{pmatrix} u & \rho & 0 & 0 & 0 \\ a_{21} & u & 0 & \frac{\gamma p}{\rho} & a_{25} \\ 0 & 0 & u & -\frac{\gamma}{\beta\rho} & 0 \\ 0 & p & -1 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{pmatrix}, \quad \mathbf{Q} = \begin{pmatrix} \rho \\ u \\ w \\ p \\ \eta \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{\alpha\beta\rho}\left(1 - \frac{\eta}{\rho}\right) \\ 0 \\ w \end{pmatrix}$$

with $a_{21} = \rho^2 P'(\rho) + \frac{\eta^2}{\alpha\rho^3}$ and $a_{25} = \frac{1}{\alpha}\left(1 - \frac{2\eta}{\rho}\right)$

Hyperbolicity in 1-D

$\mathbf{A}$ admits 5 eigenvalues that can be expressed as follows :
Reminder ($P(\rho)$: hydrostatic pressure, $p = \eta_x$)

$$\xi = \begin{pmatrix} u \\ u + \sqrt{\psi_1 + \psi_2} \\ u + \sqrt{\psi_1 - \psi_2} \\ u - \sqrt{\psi_1 + \psi_2} \\ u - \sqrt{\psi_1 - \psi_2} \end{pmatrix} \text{ with } \begin{cases} \psi_1 = \frac{1}{2}(a^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2) \\ \psi_2 = \frac{1}{2}\sqrt{(a^2 + a_\gamma^2 + a_\alpha^2 - a_\beta^2)^2 + 4a_\beta^2 a_\gamma^2} \\ a = \sqrt{P'(\rho)}, \quad a_\gamma = \sqrt{\dfrac{\gamma}{\rho} p^2} \\ a_\alpha = \dfrac{\eta}{\rho\sqrt{\alpha}}, \quad a_\beta = \sqrt{\dfrac{\gamma}{\beta\rho}} \end{cases}$$

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a^2: adiabatic sound speed. (negative in non-convex regions!!)
a_γ: wave speed due to capillarity .
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Van der Waals equation of state

In the context of two-phase flows, the equation of state is non-convex

$$p = \frac{\rho R T}{1 - b\rho} - a\rho^2, \qquad a > 0,\ b > 0$$

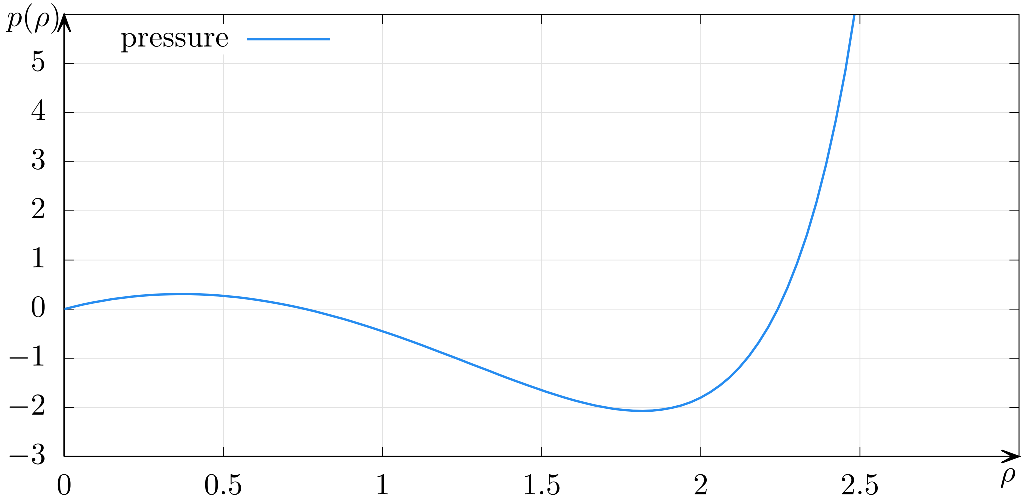

Figure 1: Van der Waals pressure for $T = 0.85, a = 3, b = 1/3, R = 8/3$

Hyperbolicity in 1-D: proof

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3. If $\rho^2 P'(\rho) < 0$, one can take α such that $a^2 + a_\alpha^2 > 0$.

$\Rightarrow$ Eigenvalues are always real for a reasonable choice of α.

Proof of hyperbolicity in 1D

Since $\psi_1 > 0$ and $\psi_2 \geq 0$, the eigenvalues are ordered as follows:

$$u - \sqrt{\psi_1 + \psi_2} \leq u - \sqrt{\psi_1 - \psi_2} < u < u + \sqrt{\psi_1 - \psi_2} \leq u + \sqrt{\psi_1 + \psi_2}$$

- Multiple eigenvalues for $\psi_2 = 0$.
- We can show that in this case, we still have a full basis of right eigenvectors:

$$\xi = \begin{pmatrix} u \\ u + \sqrt{\psi_1} \\ u + \sqrt{\psi_1} \\ u - \sqrt{\psi_1} \\ u - \sqrt{\psi_1} \end{pmatrix}, \quad \Lambda = \begin{pmatrix} -\frac{\rho - 2\eta}{\alpha a_\beta^2} & 0 & \frac{\rho}{a_\beta} & 0 & -\frac{\rho}{a_\beta} \\ 0 & 0 & 1 & 0 & 1 \\ 0 & -a_\beta & 0 & a_\beta & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

This concludes the proof (works for general $K(\rho)$ [Dhaouadi 2020])

Some numerical results for hyperbolic EK equations

Preliminary test: The nonlinear Schrödinger equation

$$K(\rho) = \frac{1}{4\rho}, \quad W(\rho) = \rho^2/2$$

$$\begin{cases} \rho_t + \mathrm{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \left(\frac{\rho^2}{2} - \frac{1}{4}\Delta\rho \right) \mathbf{Id} + \frac{1}{4\rho} \nabla\rho \otimes \nabla\rho \right) = 0 \end{cases}$$

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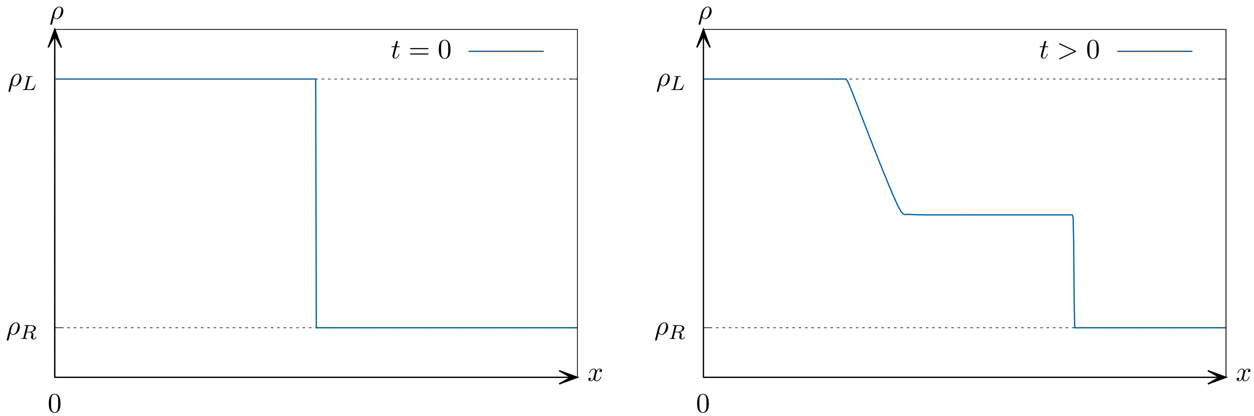
with

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

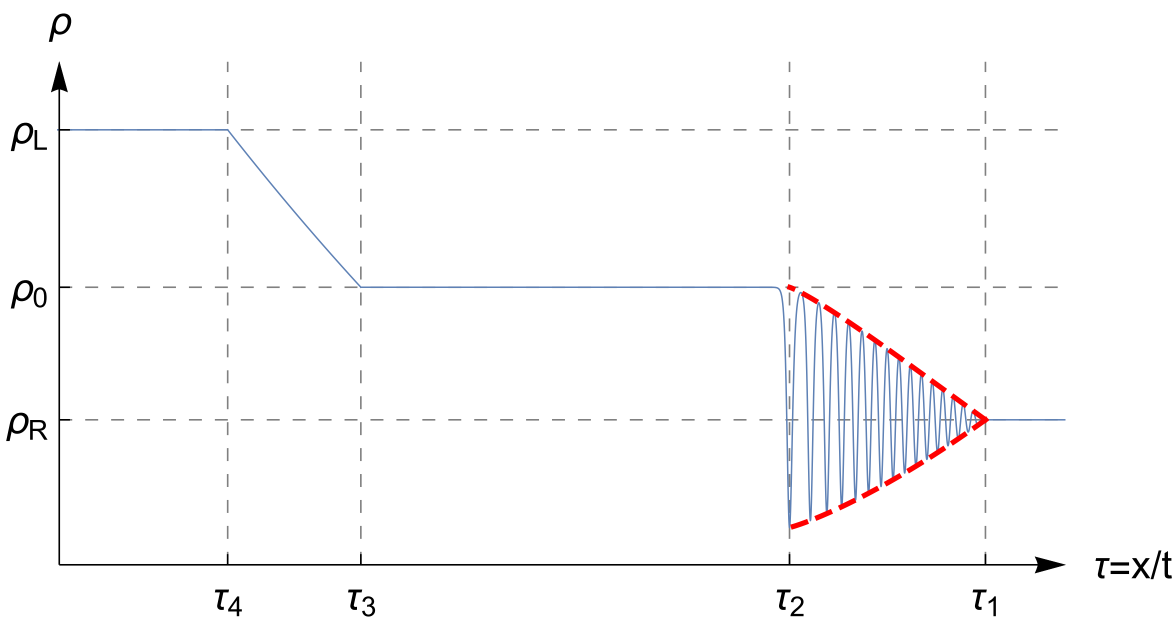
Shock waves for Euler equations

Riemann problem in dispersionless hydrodynamics governed by Euler Equations :



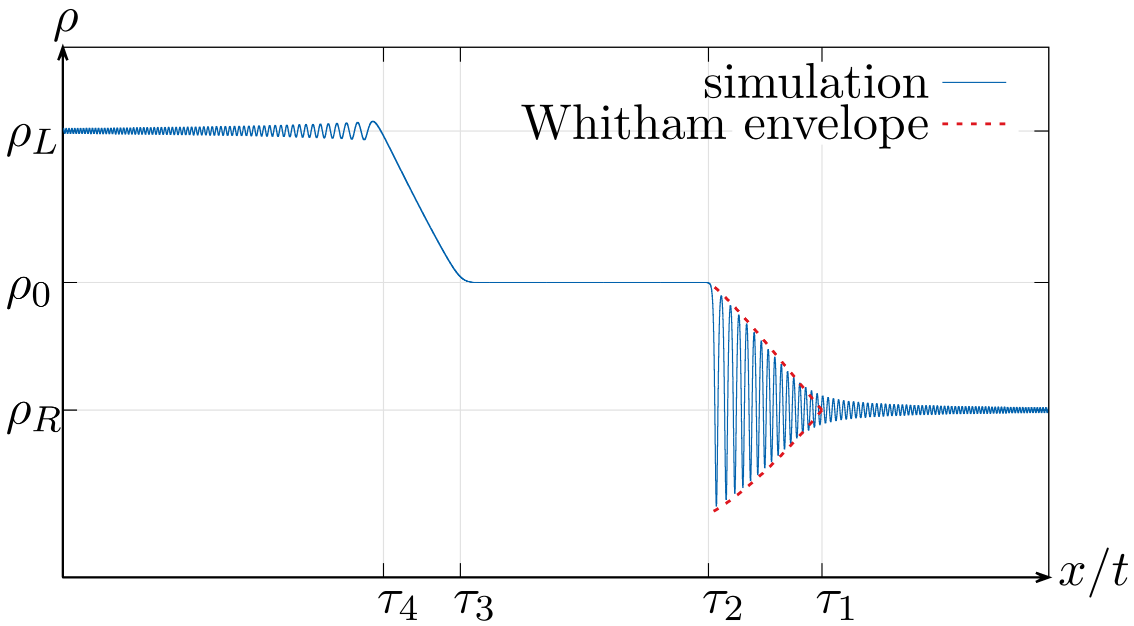
Rarefaction-Shock solution to a Riemann problem for Euler Equations.

Dispersive Shock waves



Asymptotic profile of the solution to NLS equation (continuous line) for the Riemann problem $\rho_L = 2$, $\rho_R = 1$, $u_L = u_R = 0$. Oscillations shown at t=70

DSW Numerical results



Comparison of the numerical result (ρ) with the Whitham modulational profile of the DSW at $t = 70$. $\beta = 2.10^{-5}$, $\alpha = 10^{-3}$, $N = 100000$. The computational domain is $[-500, 500]$

So far

- We proposed a first-order hyperbolic reformulation for the dispersive part of the equations.
- This reformulation remains hyperbolic even in non-convex regions of the free energy.
- No dissipation taken into account.

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- We proposed a first-order hyperbolic reformulation for the dispersive part of the equations.
- This reformulation remains hyperbolic even in non-convex regions of the free energy.
- No dissipation taken into account.

$\Rightarrow$ Let us extend this model to the Navier-Stokes-Korteweg system.

Navier-Stokes-Korteweg equations

In general, the equations write

$$\begin{cases} \rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \\ (\rho\mathbf{u})_t + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p(\rho) = \underline{\underline{S}} + \underline{\underline{K}} \end{cases}$$

where $\rho = \rho(\mathbf{x}, t)$, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ and $(\mathbf{x}, t) \in \mathbb{R}^d \times [0, T]$
The (dispersive) Korteweg stress tensor is given by:

$$\underline{\underline{K}} = \rho\nabla\left(\gamma\Delta\rho + \frac{1}{2}K'(\rho)|\nabla\rho|^2\right)$$

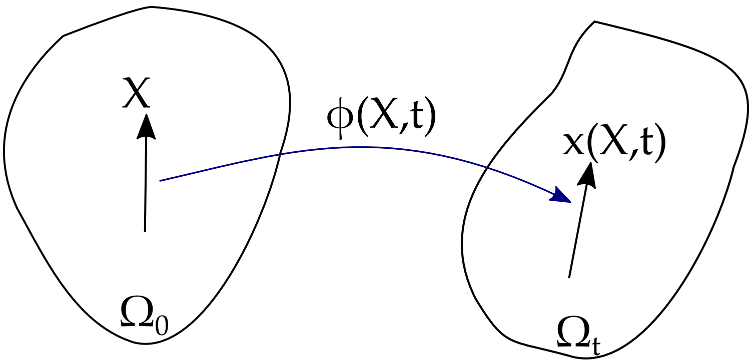
and the (viscous) Navier-Stokes stresses are given by

$$\underline{\underline{S}} = \mu \operatorname{div}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T - \frac{2}{3}\operatorname{div}(\mathbf{u})\mathbf{I}\right)$$

Godunov-Peshkov-Romenski Model of continuum mechanics

Deformation gradient:

$$\mathbf{F} = \left[\frac{\partial x_i}{\partial X_j}\right]$$



Inverse Deformation gradient:

$$\mathbf{A} = \mathbf{F}^{-1} = \left[\frac{\partial X_i}{\partial x_j}\right]$$

$$\partial_t(\mathbf{A}) + \nabla(\mathbf{A}\mathbf{u}) + \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\right) \cdot \mathbf{u} = 0 \quad \text{(Solids)}$$

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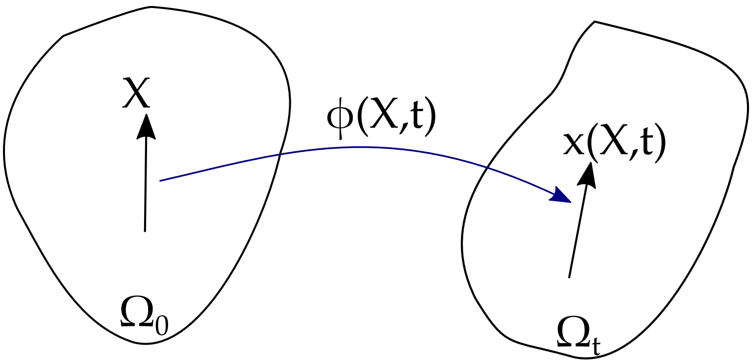

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Hyperbolic NSK = Hyperbolic EK + Hyperbolic NS

(Black: Euler part, Red: Dispersive part, Blue: Viscous part.)

$$\partial_t(\rho) + \operatorname{div}(\rho\mathbf{u}) = 0$$

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + (\rho W'(\rho) - W(\rho))\mathbf{Id} - K_\alpha - \sigma\right) = 0$$

$$\partial_t(\rho\eta) + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w$$

$$\partial_t(\rho w) + \operatorname{div}\left(\rho w\mathbf{u} - \frac{\gamma}{\beta}\mathbf{p}\right) = \frac{1}{\alpha\beta}\left(1 - \frac{\eta}{\rho}\right)$$

$$\partial_t(\mathbf{p}) + \nabla\left(\mathbf{p}\cdot\mathbf{u} - w\right) + \left(\frac{\partial\mathbf{p}}{\partial\mathbf{x}} - \left(\frac{\partial\mathbf{p}}{\partial\mathbf{x}}\right)^T\right)\cdot\mathbf{u} = 0,$$

$$\partial_t(\mathbf{A}) + \nabla(\mathbf{A}\mathbf{u}) + \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}} - \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\right)\cdot\mathbf{u} = -\frac{3}{\tau}\det(\mathbf{A})^{5/3}\mathbf{A}\operatorname{dev}(\mathbf{G})$$

where $\begin{cases}\sigma = -\rho c_s^2\mathbf{G}\operatorname{dev}(\mathbf{G}) \text{ where } \mathbf{G} = \mathbf{A}^T\mathbf{A} \\ \mathbf{K}_\alpha = -\gamma\mathbf{p}\otimes\mathbf{p} + \left(\frac{\gamma}{2}|\mathbf{p}|^2 - \frac{\eta}{\alpha}\left(1 - \frac{\eta}{\rho}\right)\right)\mathbf{Id}\end{cases}$

GLM curl cleaning [Munz *et al.*, 2000]

Black: Euler, Red: Dispersive, Blue: Viscous, Green: Curl Cleaning

$$\partial_t(\rho) + \mathrm{div}(\rho\mathbf{u}) = 0$$

$$\partial_t(\rho\mathbf{u}) + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + (\rho W'(\rho) - W(\rho))\mathbf{Id} - K_\alpha - \sigma\right) = 0$$

$$\partial_t(\rho\eta) + \mathrm{div}(\rho\eta\mathbf{u}) = \rho w$$

$$\partial_t(\rho w) + \mathrm{div}\left(\rho w\mathbf{u} - \frac{\gamma}{\beta}\mathbf{p}\right) = \frac{1}{\alpha\beta}\left(1 - \frac{\eta}{\rho}\right)$$

$$\mathbf{p}_t - \nabla w + \left(\frac{\partial\mathbf{u}}{\partial\mathbf{x}}\right)^T\mathbf{p} + \left(\frac{\partial\mathbf{p}}{\partial\mathbf{x}}\right)\mathbf{u} + 2a_c\,\nabla\times\psi = 0$$

$$\psi_t + \left(\frac{\partial\psi}{\partial\mathbf{x}}\right)^T\mathbf{u} - a_c\sqrt{\frac{\gamma}{\rho}}\,\nabla\times\mathbf{p} = 0$$

$$\partial_t(\mathbf{A}) + \nabla(\mathbf{A}\mathbf{u}) + \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}} - \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\right)\cdot\mathbf{u} = -\frac{3}{\tau}\det(\mathbf{A})^{5/3}\mathbf{A}\,\mathrm{dev}(\mathbf{G})$$

$\psi = (\psi_1, \psi_2, \psi_3)^T$: Curl cleaning field.

Eigenvalues - Hyperbolicity

$\Rightarrow$ 21 Eigenvalues (Linearized around $A = \mathbf{I}, \mathbf{p} = (p1, 0, 0)^T$)

Transport: $\lambda_{1-9} = u_1,$

shear waves: $\begin{cases} \lambda_{10-11} = u_1 + c_s, \\ \lambda_{12-13} = u_1 - c_s, \end{cases}$

Cleaning waves: $\begin{cases} \lambda_{14-15} = u_1 - \sqrt{\gamma/\rho}\, a_c, \\ \lambda_{16-17} = u_1 + \sqrt{\gamma/\rho}\, a_c, \end{cases}$

Mixed waves:

$$\begin{cases} \lambda_{18} = u_1 - \sqrt{Z_1 + Z_2} \\ \lambda_{19} = u_1 - \sqrt{Z_1 - Z_2} \\ \lambda_{20} = u_1 + \sqrt{Z_1 + Z_2} \\ \lambda_{21} = u_1 + \sqrt{Z_1 - Z_2} \end{cases}, \begin{cases} Z_1 = \frac{1}{2}(a_0^2 + a_s^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2), \\ Z_2 = \sqrt{Z_1^2 - a_\beta^2(a_0^2 + a_\alpha^2 + a_s^2)}, \\ a_0 = \sqrt{\rho W''(\rho)}, \quad a_s = \sqrt{\frac{4}{3}c_s^2} \\ a_\alpha = \frac{\eta}{\rho\sqrt{\alpha}}, \quad a_\beta = \sqrt{\frac{\gamma}{\beta\rho}}, \quad a_\gamma = \sqrt{\frac{\gamma}{\rho}p_1^2} \end{cases}$$

Brief summary of the numerical method

We are interested in general hyperbolic equations of the form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) + \mathbf{B}(\mathbf{U}) \cdot \nabla \mathbf{U} = \mathbf{S}(\mathbf{U}).$$

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- We use a one-step fully explicit ADER-DG scheme, based on a weak formulation of the PDE in space-time

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_i} \varphi_k \left(\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) + \mathbf{B}(\mathbf{U}) \cdot \nabla \mathbf{U} \right) d\Omega \, dt = \int_{t^n}^{t^{n+1}} \int_{\Omega_i} \varphi_k \left(\mathbf{S}(\mathbf{U}) \right) d\Omega \, dt.$$

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- *A posteriori* Weno limiting (MOOD approach) is considered.
- We use the Rusanov solver for the conservative fluxes.
- Path-conservative method for non-conservative terms.
- Mesh: Uniform cartesian Grid.

1D Traveling wave solutions for original NSK

1D NSK system reduces to:

$$\partial_t(\rho) + \partial_x(\rho u) = 0$$
$$\partial_t(\rho u) + \partial_x(\rho u^2 + p(\rho)) = \frac{4}{3}\mu u_{xx} + \gamma\rho\rho_{xxx}$$

Traveling wave assumption: $\rho(x,t) = \rho(x-st)$, $u(x,t) = u(x-st)$

$$\begin{cases} \rho''' = \frac{1}{\lambda\rho}\left(\left(p'(\rho) - (u-s)^2\right)\rho' - \frac{4}{3}\mu(u-s)(2\frac{\rho'^2}{\rho^2} - \frac{\rho''}{\rho})\right) \\ u' = (s-u)\frac{\rho'}{\rho} \end{cases}$$

which we solve as a Cauchy problem with a prescribed initial condition $\rho_0 = 1.8$, $\rho_0' = -10^{-10}$, $\rho_0'' = 0$, $u_0 = 0$

Traveling wave solutions

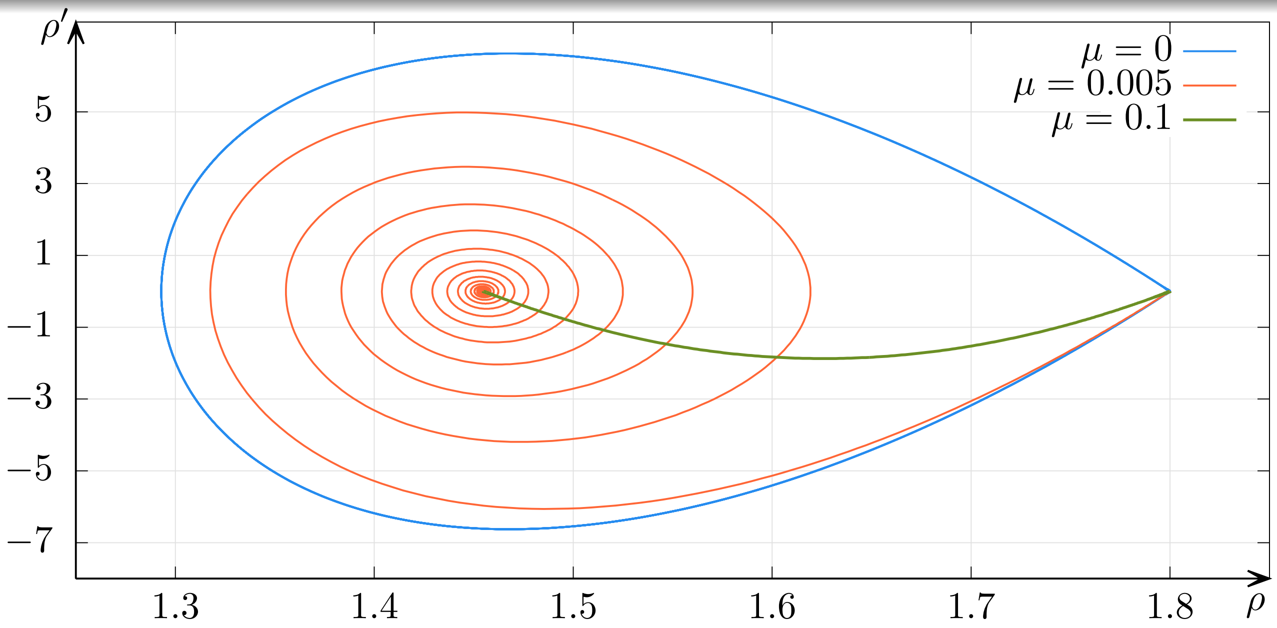
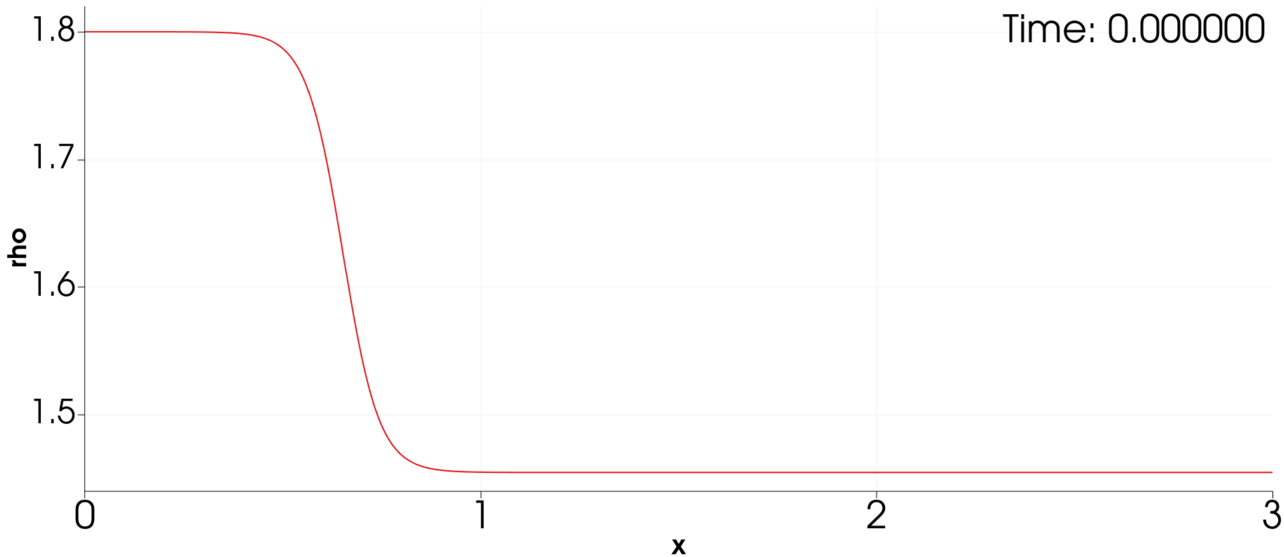


Figure 2: Nature of travelling wave solutions at fixed dispersion ($\gamma = 0.001$), for the original NSK equations.

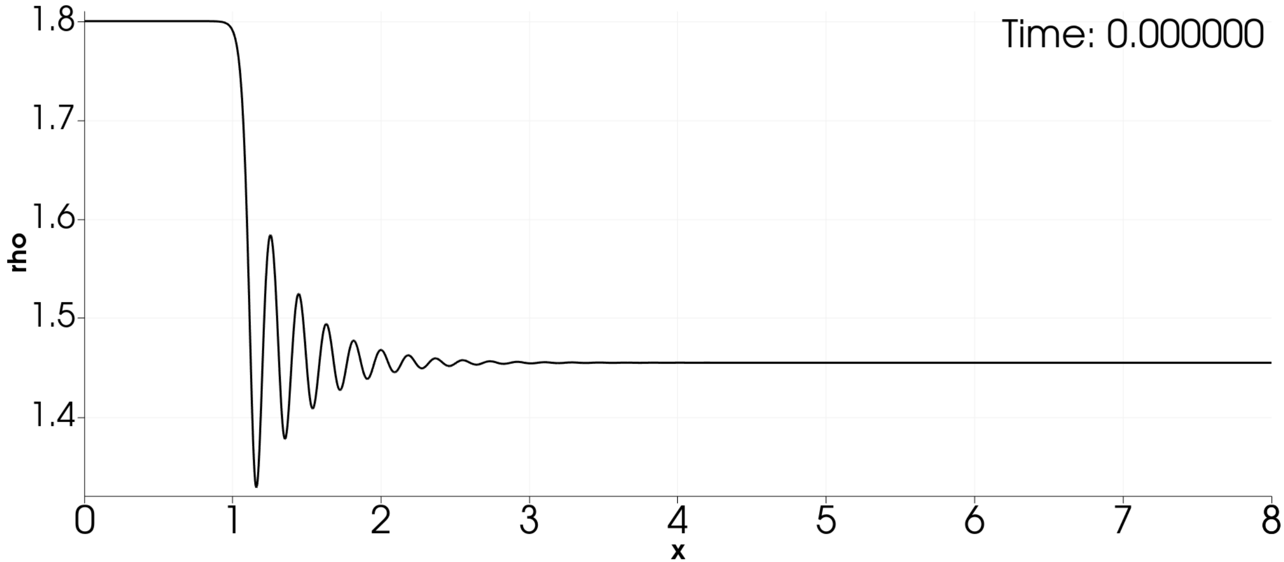
See [Affouf & Caflisch 1991] for a discussion on the nature of the solutions for a simplified system.

Viscous TW solution



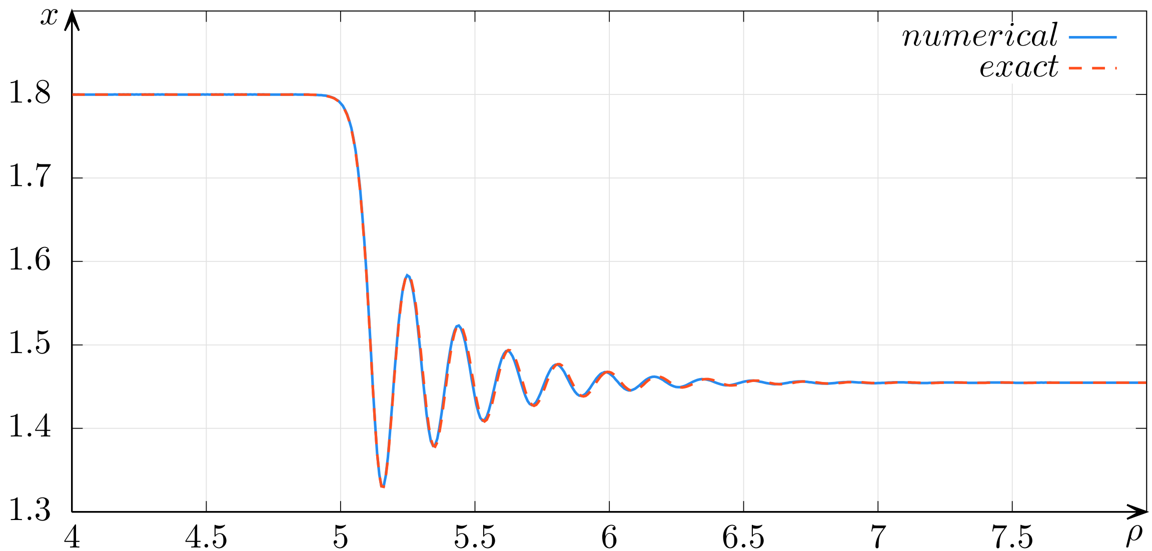
Viscous shock traveling wave solution to the original NSK (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.2$, $\alpha = 0.001$, $\beta = 0.00001$)

Oscillatory TW solution



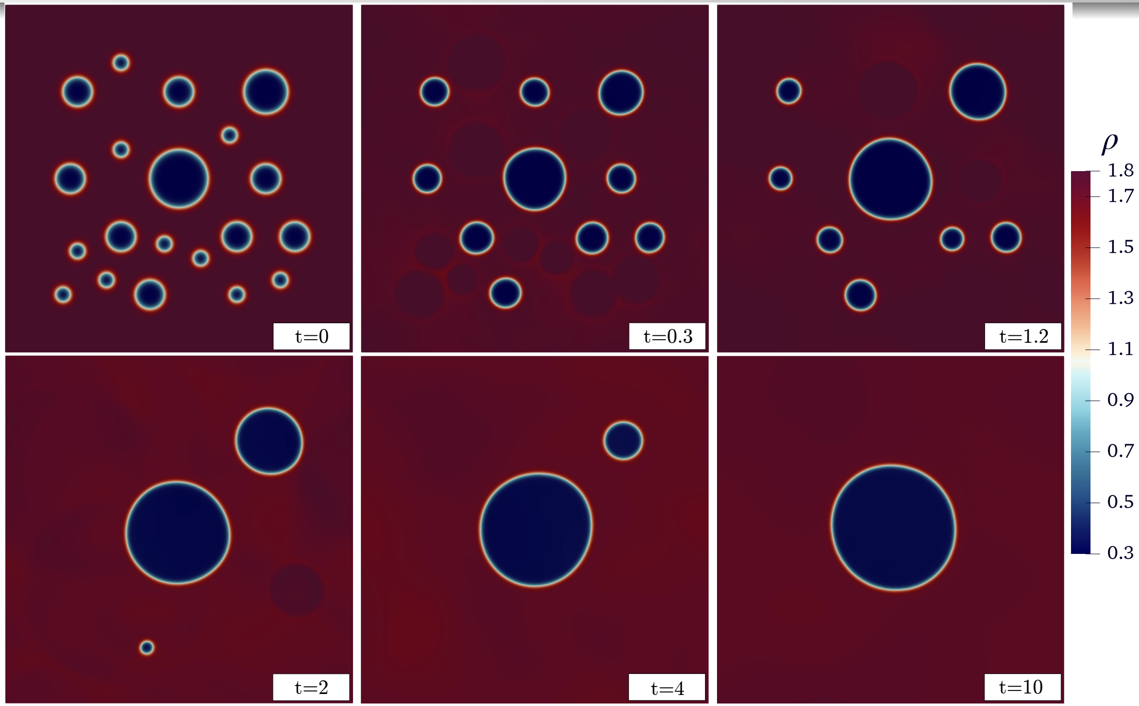
Dispersive traveling wave solution to the original NSK (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.0075$, $\alpha = 0.001$, $\beta = 0.00001$)

Oscillatory TW solution



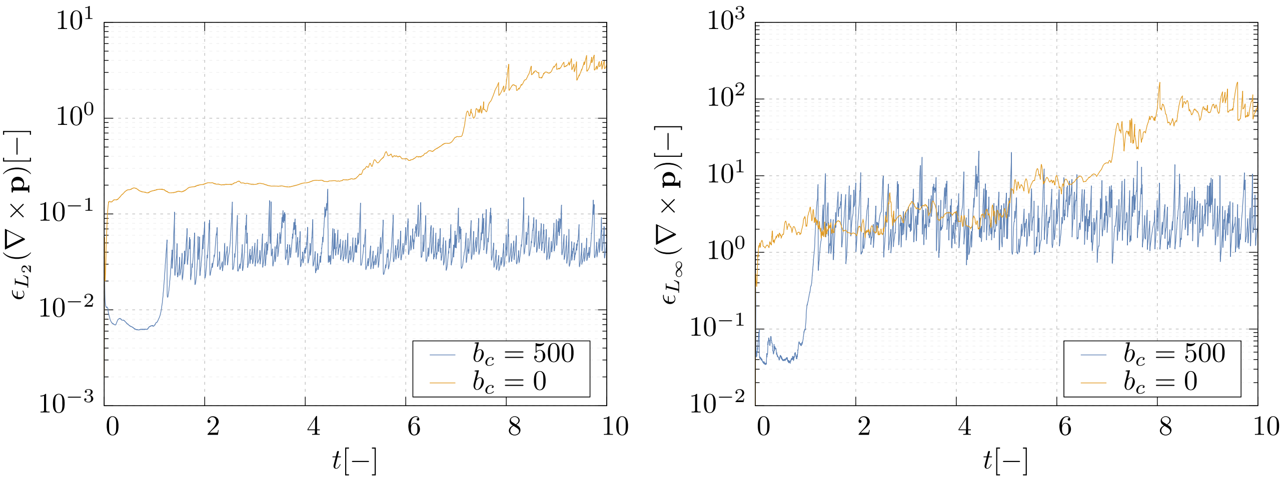
Superimposed numerical solution and exact solution of original model at t=4. (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.0075$, $c_s = 10$, $\alpha = 0.001$, $\beta = 0.00001$)

2D Ostwald Ripening



20 Bubbles result (Obtained with a P_3P_3 ADER-DG scheme + Periodic boundary conditions + WENO3 subcell limiting on a 288×288 grid with $\gamma = 0.0002$,$\mu = 0.01$, $c_s = 10$, $\alpha = 0.001$, $\beta = 0.00001$)

Curl errors



Comparison of the time evolution of the curl errors for two simulations with cleaning (blue line) and without cleaning (orange line).

Conclusion and Perspectives

Conclusion

- We presented a hyperbolic relaxation to the Navier-Stokes-Korteweg equations.
- Numerical results showed promise.

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Perspectives

- ✓ Application of structure preserving schemes, in particular exactly curl-free schemes.
- Splitting of the fluxes to separate fast waves for less constraining time-steps (IMEX, Semi-Implicit, ...)
- Investigation of the sharp interface limit ($\gamma \to 0$) and Asymptotic Preserving schemes.
- Generalization of the hyperbolic model to the non-isothermal case.

Some results using exactly curl-free schemes

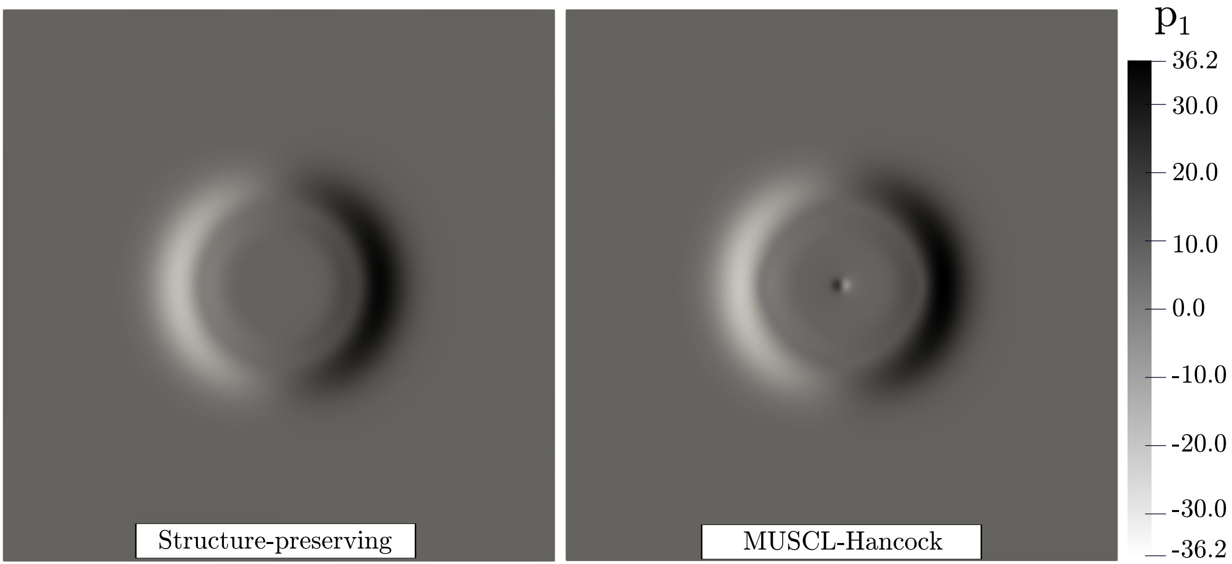

Figure 3: Comparison of the overall shape of the gradient field component p_1 with both a staggered curl-free discretization (left) and with a MUSCL-Hancock scheme (right). Results are shown for $t = 2$ on a 512×512 grid.

Some results using exactly curl-free schemes

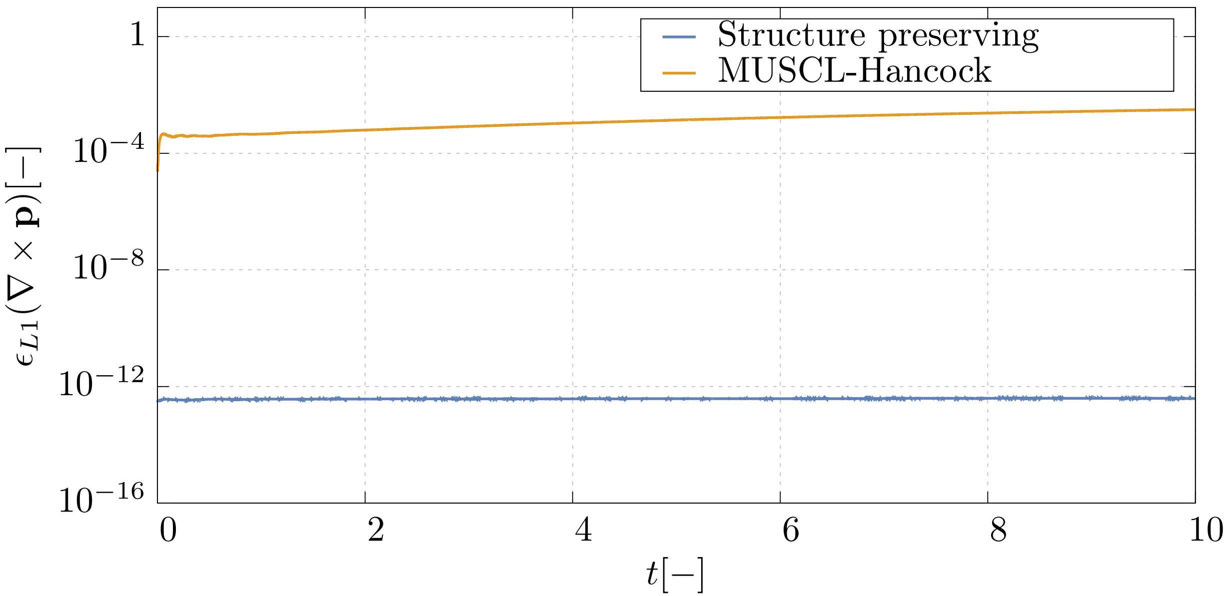

Figure 4: Comparison of the discrete curl errors over time.

Thank you for your attention !

[1] Dhaouadi, Firas, and Michael Dumbser. "A first order hyperbolic reformulation of the Navier-Stokes-Korteweg system based on the GPR model and an augmented Lagrangian approach." *Journal of Computational Physics* 470 (2022): 111544.

[2] Dhaouadi, Firas, and Michael Dumbser. "A Structure-Preserving Finite Volume Scheme for a Hyperbolic Reformulation of the Navier–Stokes–Korteweg Equations." *Mathematics* 11.4 (2023): 876.

(Check also the references therein).

Dispersion relation

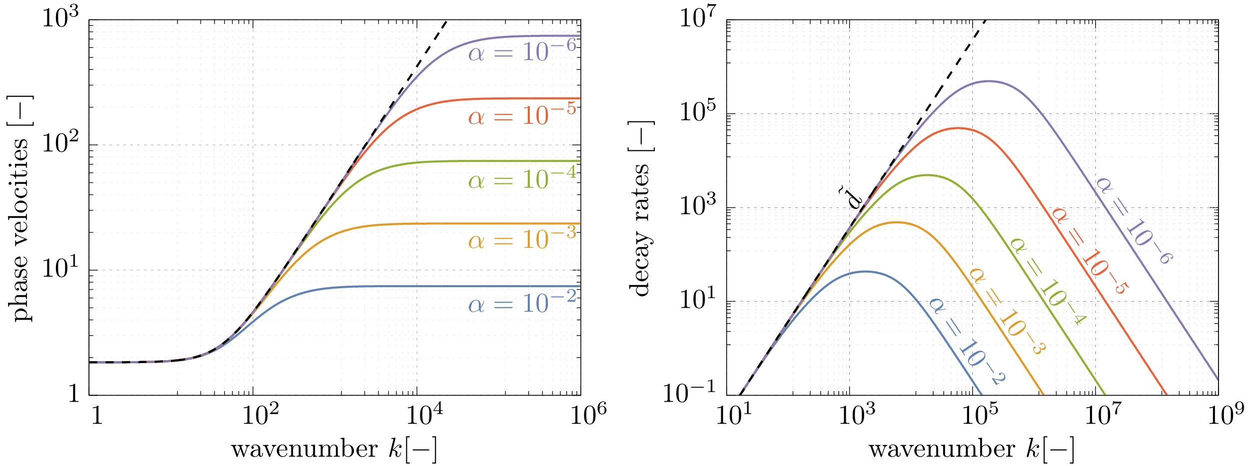

Figure 5: Plot of the phase velocity (left) and the decay rate for several values of α along their counterparts for the Navier-Stokes-Korteweg system. The model parameters are as follows $\gamma = 10^{-3}$, $\mu = 10^{-3}$ and $\rho = 1.8$

Scaling of relaxations

Representative characteristic velocities

$$\begin{cases} \lambda_{18} = u_1 - \sqrt{Z_1 + Z_2} \\ \lambda_{19} = u_1 - \sqrt{Z_1 - Z_2} \\ \lambda_{20} = u_1 + \sqrt{Z_1 + Z_2} \\ \lambda_{21} = u_1 + \sqrt{Z_1 - Z_2} \end{cases}, \quad \begin{cases} Z_1 = \frac{1}{2}(a_0^2 + a_s^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2), \\ Z_2 = \sqrt{Z_1^2 - a_\beta^2(a_0^2 + a_\alpha^2 + a_s^2)}, \\ a_0 = \sqrt{\rho W''(\rho)}, \quad a_s = \sqrt{\frac{4}{3}c_s^2} \\ a_\alpha = \frac{\eta}{\rho\sqrt{\alpha}}, \quad a_\beta = \sqrt{\frac{\gamma}{\beta\rho}}, \quad a_\gamma = \sqrt{\frac{\gamma}{\rho}p_1^2} \end{cases}$$

The different relaxation contributions scale as

$$a_\alpha^2 \sim \frac{1}{\alpha}, \quad a_\beta^2 \sim \frac{\gamma}{\beta\rho}, \quad a_s^2 \sim c_s^2$$

To keep the contributions at the same order of magnitude, we can take for example

$$\beta = \gamma\alpha, \quad c_s = \frac{1}{\sqrt{\alpha}}$$