

A Hyperbolic reformulation of the Navier-Stokes-Korteweg equations

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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 stresses are given by:

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

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

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

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**

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

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Main objective

Given the Navier-Stokes-Korteweg system of equations :

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$$(\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \rho \nabla \left(K(\rho) \Delta \rho + \frac{1}{2} K'(\rho) |\nabla \rho|^2 \right) \\ + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} \operatorname{div}(\mathbf{u}) \mathbf{I} \right)$$

- ✓ General model for viscous-dispersive fluid flows.
- ✓ A diffuse interface option for viscous two-phase flows.

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- ✓ A diffuse interface option for viscous two-phase flows.
- ✗ contains high order derivatives (2nd and 3rd order).
 - ⇒ Crippling time-stepping.
 - ⇒ Has non-local operators.
- ✗ Often associated with non-convex equations of state.
 - ⇒ Loss of hyperbolicity in the left-hand side.

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Suggested solution

A first-order hyperbolic reformulation of the NSK system!

Outline

- 1 Hyperbolic reformulation of The Euler-Korteweg system
- 2 Extension to the Navier-Stokes-Korteweg system
- 3 Numerical results

Lagrangian for (EK) system

(EK) system can be derived from the Lagrangian :

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

↓

Hamilton's principle
+
Differential constraint : $\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0$

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

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

Augmented Lagrangian approach

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

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

'Augmented' Lagrangian approach

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla \eta) \quad (\eta \rightarrow \rho)$$

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

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

Preliminary system

Deriving the system of governing equations yields:

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

where:

$$\mathbf{K}_\alpha = \left(\frac{\gamma}{2} |\nabla \eta|^2 - \frac{\eta}{\alpha} \left(1 - \frac{\eta}{\rho}\right) \right) \mathbf{Id} - \gamma \nabla \eta \otimes \nabla \eta$$

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Replacing the relaxation term in the stress tensor yields

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The obtained system :

- ✗ still contains high order derivatives.
- ✗ is not hyperbolic.
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Idea : Include $\dot{\eta}$ into the Lagrangian !

Augmented Lagrangian - Attempt 2

Augmented Lagrangian approach

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

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

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↓ Hamilton's principle : $a = \int_{t_0}^{t_1} \tilde{\mathcal{L}} dt$

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

Order reductions

① We denote $w = \dot{\eta}$. Thus:

$$w = \eta_t + \mathbf{u} \cdot \nabla \eta \quad \implies \quad (\rho\eta)_t + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w$$

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$$\nabla w = \nabla(\eta_t + \mathbf{u} \cdot \nabla \eta)$$

$$\implies \mathbf{p}_t + \operatorname{div}((\mathbf{p} \cdot \mathbf{u} - w)\mathbf{I_d}) = 0$$

Final form of the hyperbolic Euler-Korteweg system

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

$$\mathbf{K}_\alpha = \left(\frac{\gamma}{2} |\mathbf{p}|^2 - \frac{\eta}{\alpha} \left(1 - \frac{\eta}{\rho}\right) \right) \mathbf{Id} - \gamma \mathbf{p} \otimes \mathbf{p}$$

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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 $a_{21} = W''(\rho) + \frac{\eta^2}{\alpha\rho^3}$ 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, $p = \eta_x$)

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

$\color{red}{a^2}$: adiabatic sound speed.

a_γ : wave speed due to capillarity .

a_α and a_β : First and second relaxation speeds.

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$\color{red}{a^2}$: adiabatic sound speed. (**negative in non-convex regions!!**)

a_γ : wave speed due to capillarity .

a_α and a_β : First and second relaxation speeds.

Van der Waals equation of state

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

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2, \quad a > 0, \quad b > 0$$

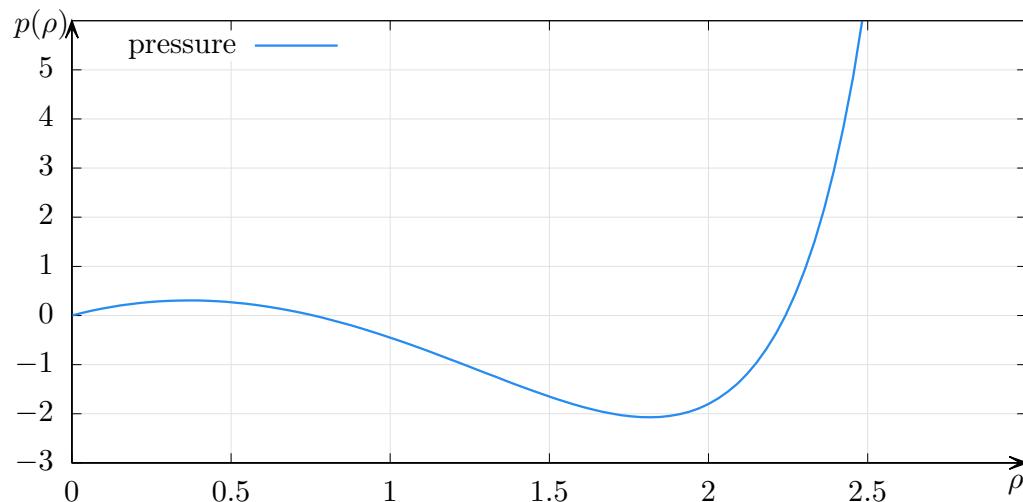


Figure 1: Van der Waals pressure for $T = 0.85, a = 3, b = 1/3, R = 8/3$

Navier-Stokes-Korteweg equations

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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:

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

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Godunov-Peshkov-Romenski Model of continuum mechanics

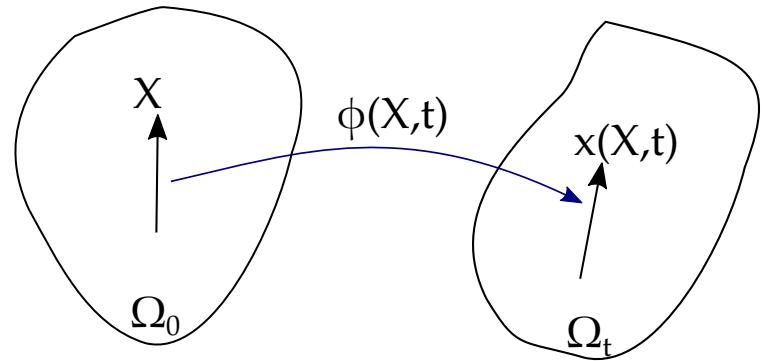
Deformation gradient:

$$\mathbf{F} = \begin{bmatrix} \frac{\partial x_i}{\partial X_j} \end{bmatrix}$$

Inverse Deformation gradient:

$$\mathbf{A} = \mathbf{F}^{-1} = \begin{bmatrix} \frac{\partial X_i}{\partial x_j} \end{bmatrix}$$

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



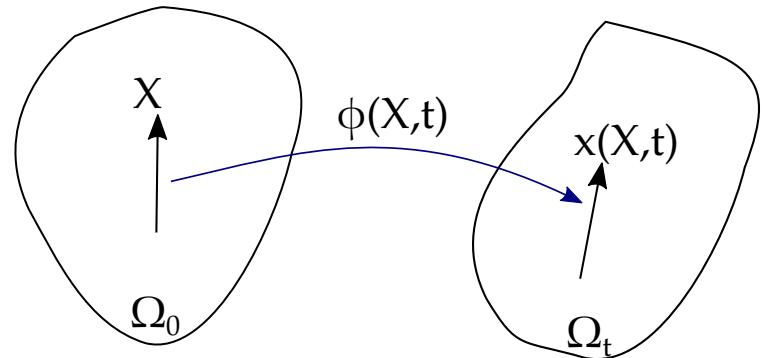
Godunov-Peshkov-Romenski Model of continuum mechanics

Deformation gradient:

$$\mathbf{F} = \begin{bmatrix} \frac{\partial x_i}{\partial X_j} \end{bmatrix}$$

Inverse Deformation gradient:

$$\mathbf{A} = \mathbf{F}^{-1} = \begin{bmatrix} \frac{\partial X_i}{\partial x_j} \end{bmatrix}$$



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

$$\partial_t(\mathbf{A}) + \nabla(\mathbf{A}\mathbf{u}) + \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} \right)^T \right) \cdot \mathbf{u} = \frac{1}{\tau} \mathbf{S}(\mathbf{A}) \quad (\text{Fluids})$$

Hyperbolic NSK = Hyperbolic EK + Hyperbolic NS

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

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

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

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

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

$$\partial_t(\mathbf{p}) + \nabla(\mathbf{p} \cdot \mathbf{u} - w) = 0, \quad \nabla \times \mathbf{p} = 0$$

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

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

Reformulation of the NSK system

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

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

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

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

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

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

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

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

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

Eigenvalues - Hyperbolicity

$\Rightarrow 21$ Eigenvalues (Linearized around $A = \mathbf{I}$, $\mathbf{p} = (p_1, 0, 0)^T$)

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

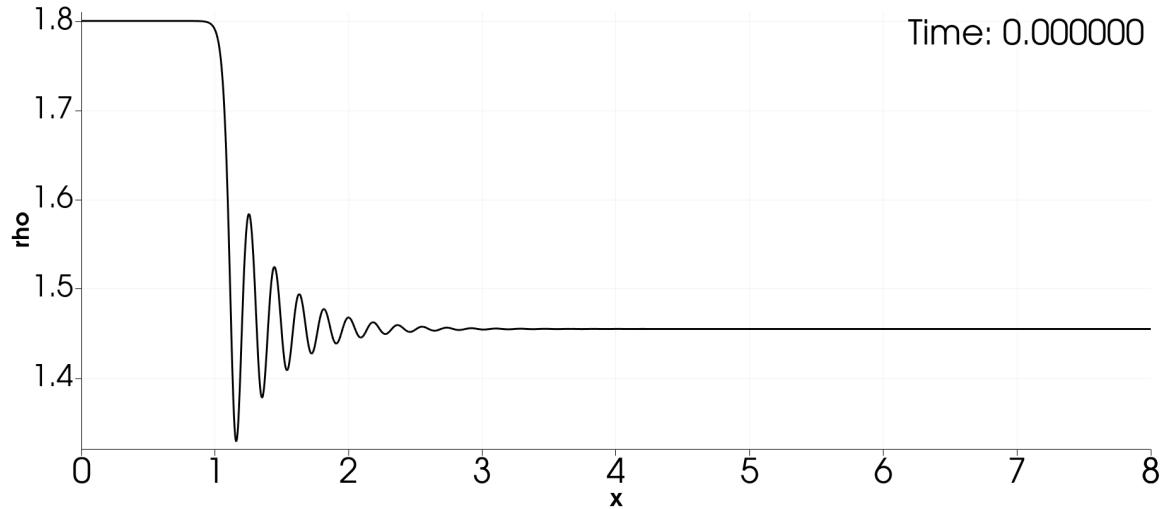
shear waves:
$$\begin{cases} \lambda_{10-11} = u_1 + c_s, \\ \lambda_{12-13} = u_1 - c_s, \end{cases}$$

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:

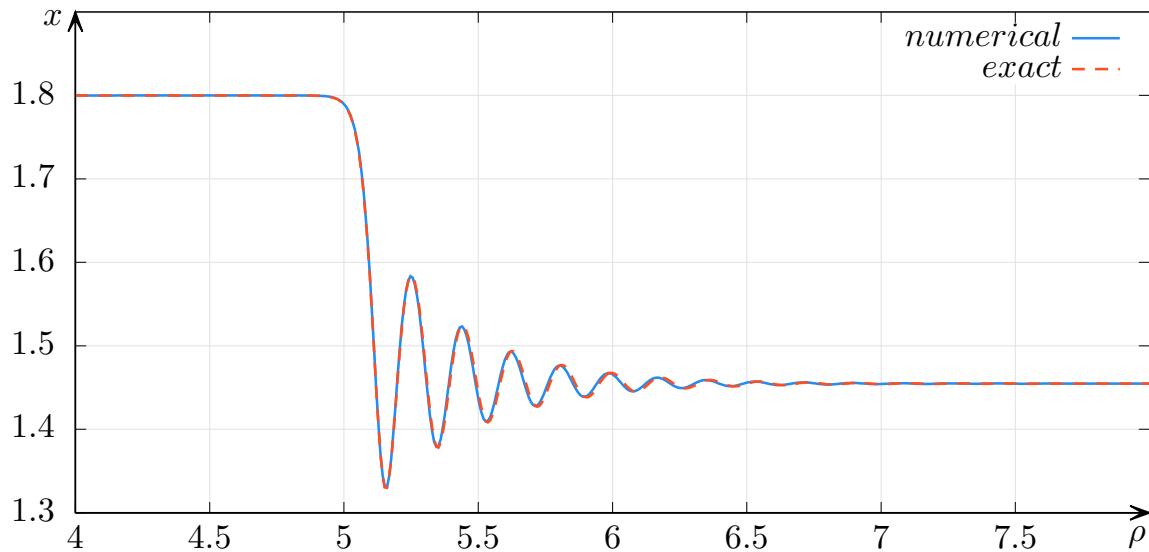
$$\left\{ \begin{array}{l} \lambda_{18} = u_1 - \sqrt{Z_1 + Z_2} \\ \lambda_{19} = u_1 - \sqrt{Z_1 - Z_2} \\ \lambda_{20} = u_1 + \sqrt{Z_1 + Z_2} \\ \lambda_{21} = u_1 + \sqrt{Z_1 - Z_2} \end{array} \right. , \left\{ \begin{array}{l} Z_1 = \frac{1}{2}(a_0^2 + a_s^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2),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

Oscillatory TW solution



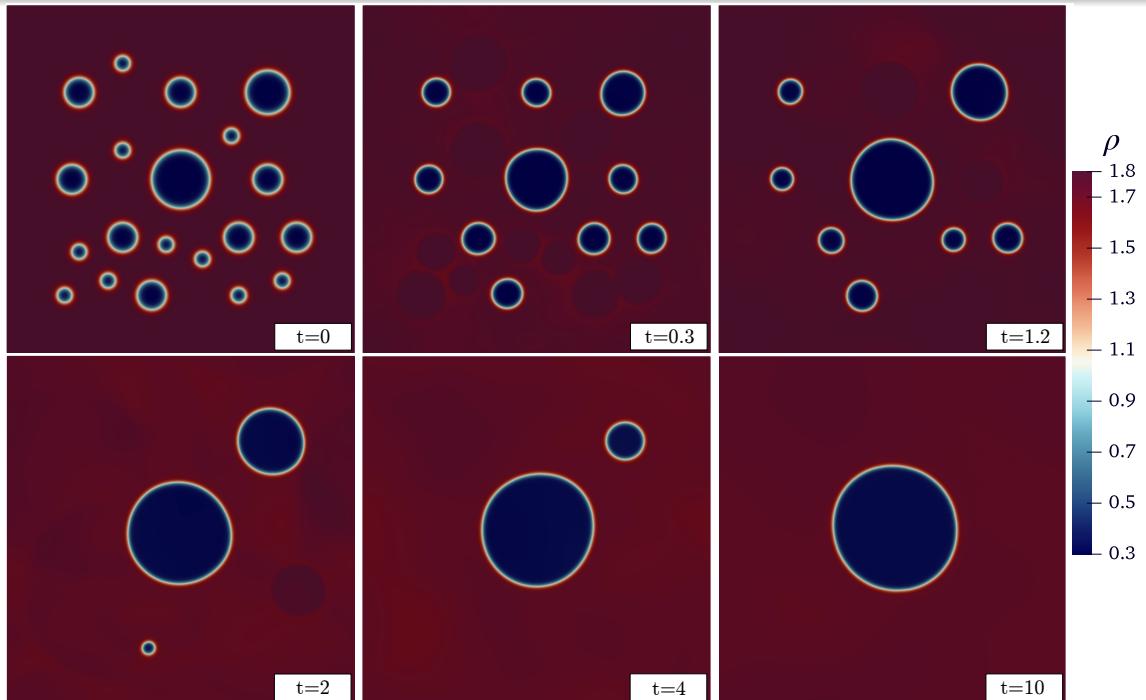
Dispersive shock traveling wave solution to the original NSK (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$, $\mu = 0.0075$, $\alpha = 0.001$, $\beta = 0.00001$)

Dispersive shock wave



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 $\gamma = 0.001$, $\mu = 0.0075$, $\alpha = 0.001$, $\beta = 0.00001$)

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 $\gamma = 0.0002$, $\mu = 0.01$, $\alpha = 0.001$, $\beta = 0.00001$)

Conclusion and Perspectives

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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 ($\gamma \rightarrow 0$) and Asymptotic Preserving schemes.
- Generalization of the hyperbolic model to the non-isothermal case.

Thank you for your attention !