A Hyperbolic reformulation of the Navier-Stokes-Korteweg equations

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Navier-Stokes-Korteweg equations

In general, the equations write

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

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 stresses are given by

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

The (dispersive) Korteweg stresses are given by:

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

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 :

$$
\begin{aligned}
&\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\
&(\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \rho \nabla \left(K(\rho)\Delta\rho + \frac{1}{2}K'(\rho)|\nabla\rho|^2 \right) \\
&\qquad\qquad + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3}\operatorname{div}(\mathbf{u})\mathbf{I} \right)
\end{aligned}
$$

- ✓ 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

Lagrangian for the Euler-Korteweg 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 : $\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0$

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

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

Augmented Lagrangian approach

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

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

'Augmented' Lagrangian approach

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

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

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

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:

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

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Replacing the relaxation term in the stress tensor yields

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Reminder: Original Korteweg stress tensor

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$$\mathrm{div}(\mathbf{K}) = \gamma \rho \nabla(\Delta \rho), \quad \mathrm{div}(\mathbf{K}_\alpha) = \gamma \eta \nabla(\Delta \eta)$$

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The obtained system :

- ✗ still contains high order derivatives.
- ✗ is not hyperbolic.
- ✗ has an elliptic constraint.

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

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

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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2. We denote $\mathbf{p} = \nabla \eta$. Again take :

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2. We denote $\mathbf{p} = \nabla \eta$. Again take :

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

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

Final form of the hyperbolic Euler-Korteweg system

$$
\begin{cases}
\rho_t + \mathrm{div}(\rho \mathbf{u}) = 0 \\
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(\beta \rho w)_t + \mathrm{div}\left(\beta \rho w \mathbf{u} - \gamma \mathbf{p}\right) = \frac{1}{\alpha}\left(1 - \frac{\eta}{\rho}\right) \\
\mathbf{p}_t + \mathrm{div}((\mathbf{p}\cdot\mathbf{u} - w)\mathbf{Id}) = 0, \quad \mathrm{curl}(\mathbf{p}) = 0 \\
(\rho\eta)_t + \mathrm{div}(\rho\eta\mathbf{u}) = \rho w
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$$
\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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$$\mathbf{K}_\alpha = \left(\frac{\gamma}{2}|\mathbf{p}|^2 - \frac{\eta}{\alpha}\left(1 - \frac{\eta}{\rho}\right)\right)\mathbf{Id} - \gamma \mathbf{p} \otimes \mathbf{p}$$

- 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, $p = \eta_x$)

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

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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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

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

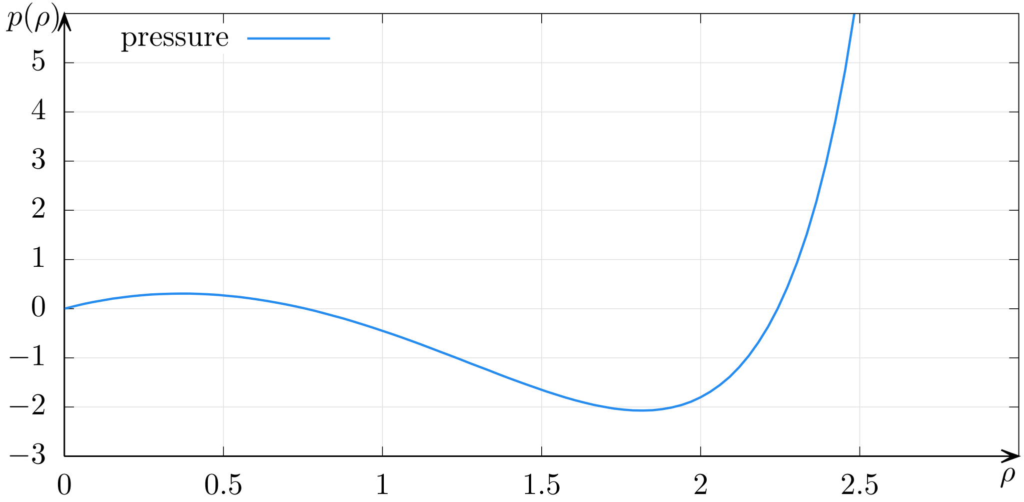

Figure 1: Van der Waals pressure for $T = 0.85, a = 3, b = 1/3, R = 8/3$

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:

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

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

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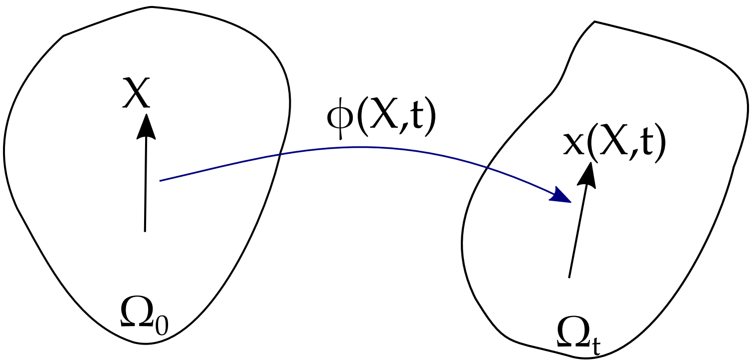
Godunov-Peshkov-Romenski Model of continuum mechanics

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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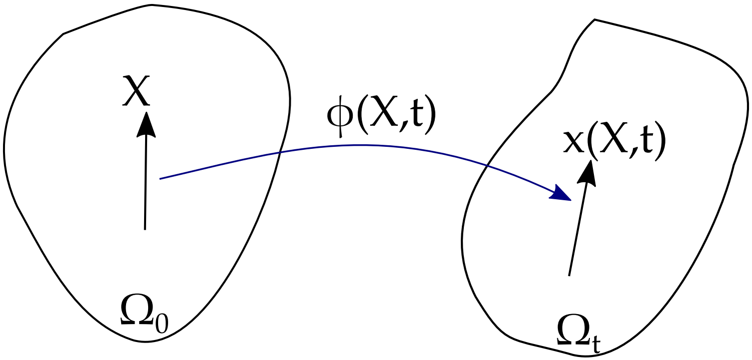
Inverse Deformation gradient:

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



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

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

Hyperbolic NSK = Hyperbolic EK + Hyperbolic NS

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

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

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

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

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

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

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

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

Reformulation of the NSK system

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

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

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

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

$\psi = (\psi_1, \psi_2, \psi_3)^T$: 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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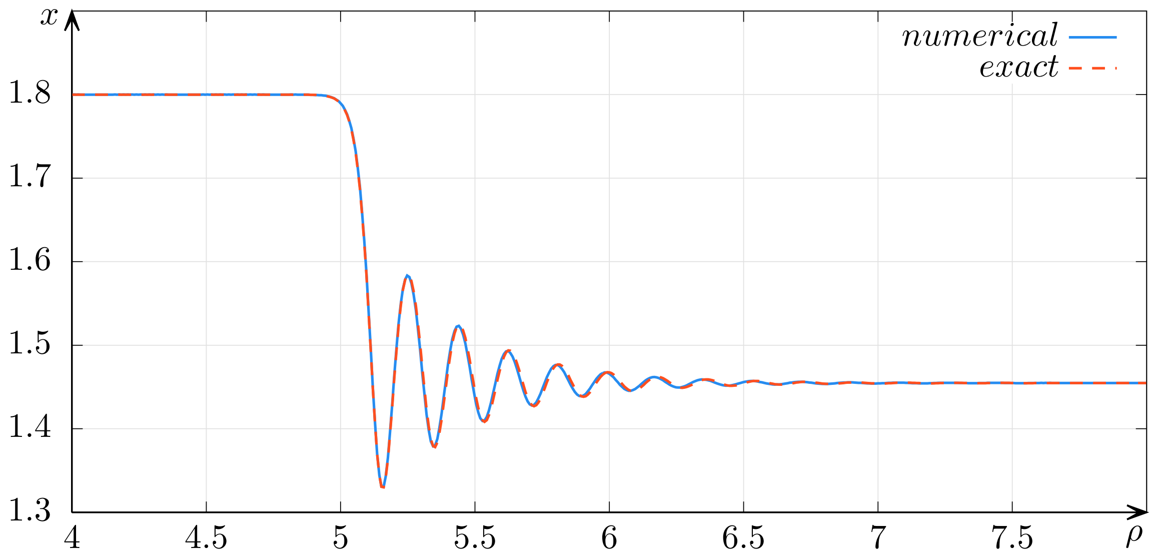
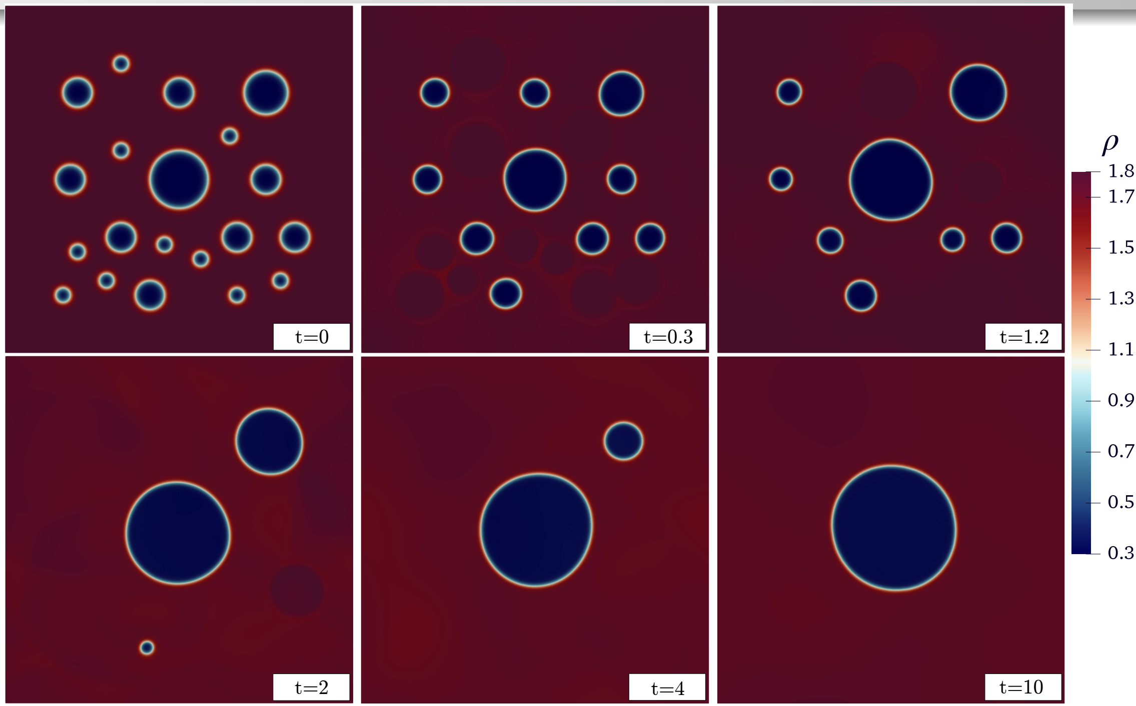
- *A posteriori* Weno limiting (MOOD approach) is considered.
- We use the Rusanov solver for the conservative fluxes.
- Path-conservative method for non-conservative terms.
- Mesh: Uniform cartesian Grid.

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 $\gamma = 0.0002$,$\mu = 0.01$, $c_s = 10$, $\alpha = 0.001$, $\beta = 0.00001$)

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

Thank you for your attention !

Dispersion relation

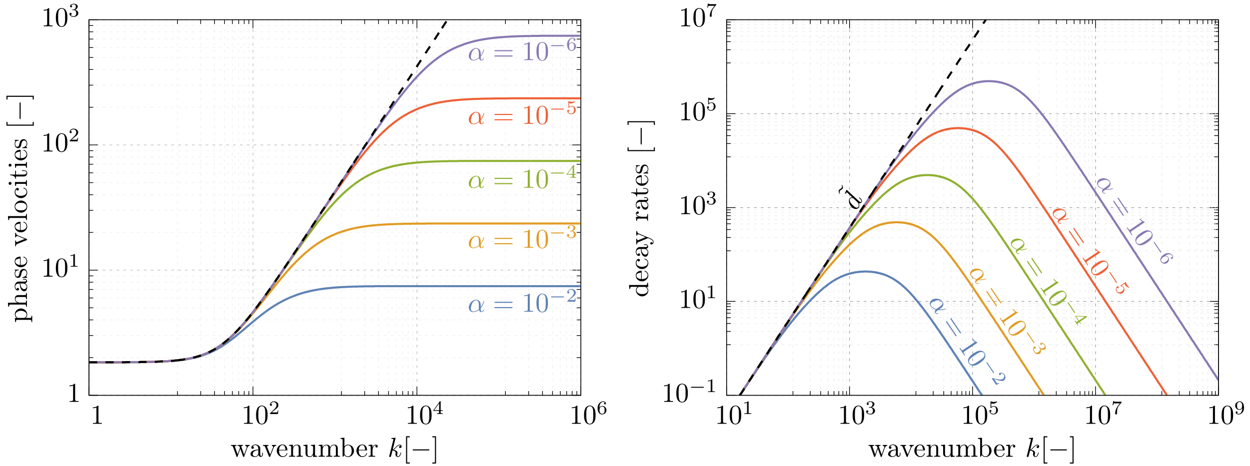

Figure 2: Plot of the phase velocity (left) and the decay rate for several values of α along their counterparts for the Navier-Stokes-Korteweg system. The model parameters are as follows $\gamma = 10^{-3}$, $\mu = 10^{-3}$ and $\rho = 1.8$

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 contriobutions at the same order of magnitude, we can take for example

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