Hyperbolic approximation and numerical methods for 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 (dispersive) Korteweg stress tensor is 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

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

Main objective

Given the Navier-Stokes-Korteweg system of equations :

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- ✓ A diffuse interface option for viscous two-phase flows.

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  - ⇒ Has non-local operators.

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  - $\Rightarrow$ Has non-local operators.
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  - $\Rightarrow$ Loss of hyperbolicity in the left-hand side.

Suggested solution

A first-order hyperbolic approximation of the NSK system.

Our model wishlist

We would like a model that

- approximates Euler-Korteweg in some limit.
- is derived from a variational principle (whenever possible).
- is in line with the laws of thermodynamics.
- can be solved numerically with accurate numerical methods.

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Hyperbolic equations

- well-posed IVP (Symmetric Hyperbolic)
- A very rich literature on numerical methods.
- Bounded wave speeds (Principle of causality)

A non-exhaustive subset of connected works and topics

1. A family of Parabolic relaxation models of NSK equations.
   - ⇒ Corli, Rohde, Schleper 2014 (DG for NSK)
   - ⇒ Hitz,Keim,Munz,Rohde 2020 (Barotropic case)
   - ⇒ Keim,Munz,Rohde 2023 [non-Isothermal NSK]

   and many other works...
2. Hyperbolic approximation of Euler-Korteweg equations.
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   - ⇒ Dhaouadi, Gavrilyuk, Vila 2022. (Thin films).
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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

1. Hyperbolic reformulation of the Navier-Stokes-Korteweg system
   - Hyperbolic reformulation of the Euler-Korteweg system
   - Extension to the Navier-Stokes-Korteweg system
   - A few words on hyperbolicity
2. Numerical methods
   - ADER-DG + GLM curl-cleaning
   - Exactly curl-free numerical scheme
   - Some numerical results
3. Conclusion

Dissipationless Euler-Korteweg-Van Der Waals 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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Lagrangian for the Euler-Korteweg-VdW 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 : $\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0$

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

with $P(\rho) = \rho W'(\rho) - W(\rho)$

Augmented Lagrangian approach

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

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

'Augmented' Lagrangian approach [Favrie-Gavrilyuk 2017]

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

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

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

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

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

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

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- Virtual displacement of the continuum ($\delta \mathbf{x}$):
- variation of the independent variable η ($\delta \eta$):

Preliminary system

By applying Hamilton's principle for the Eulerian variations $\delta\mathbf{x}$ and $\delta\eta$ one obtains the system of governing equations

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

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$\operatorname{div}(\mathbf{K}_\alpha) = \gamma\eta\nabla(\Delta\eta),$ original: $\operatorname{div}(\mathbf{K}) = \gamma\rho\nabla(\Delta\rho)$

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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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$\Rightarrow$ Better, but there are still high-order derivatives!

Order reductions

1. We take $w = \dot{\eta}$ as independent variable. Thus:

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

Order reductions

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- IMPORTANT: $\mathbf{p} = \nabla \eta \;\Rightarrow\; \nabla \times \mathbf{p} \equiv 0$

Final form of the approximate Euler-Korteweg system

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\begin{cases}
\rho_t & + \operatorname{div}(\rho \mathbf{u}) = 0 \\
(\rho \mathbf{u})_t & + \operatorname{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + P(\rho)\mathbf{Id} - \mathbf{K}_\alpha\right) = 0 \\
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$\Rightarrow$ Now the system is Gallilean invariant... But is it hyperbolic ?

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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Van der Waals equation of state

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

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

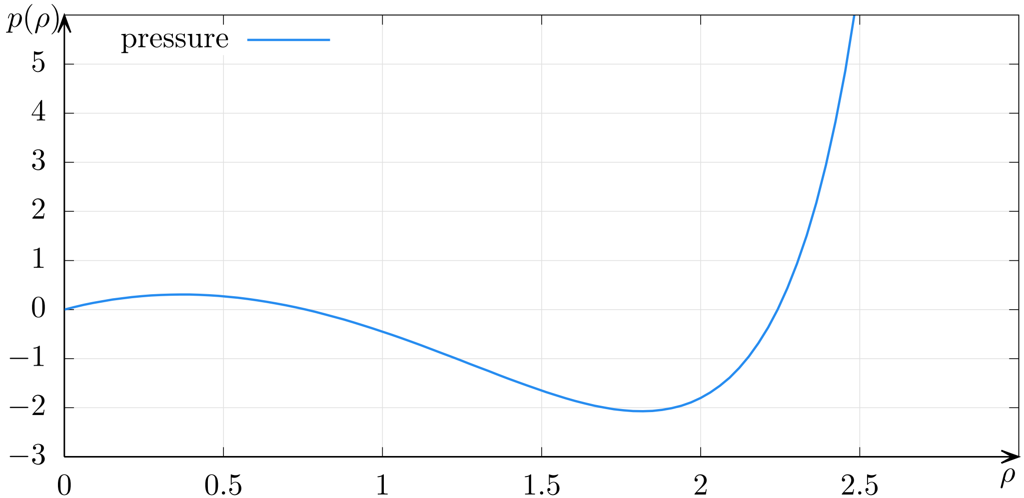

Figure 1: Van der Waals pressure for $T = 0.85, a = 3, b = 1/3, R = 8/3$

What we have so far

- We proposed a first-order hyperbolic reformulation for the dispersive Euler-Korteweg equations.
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$\Rightarrow$ 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:

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

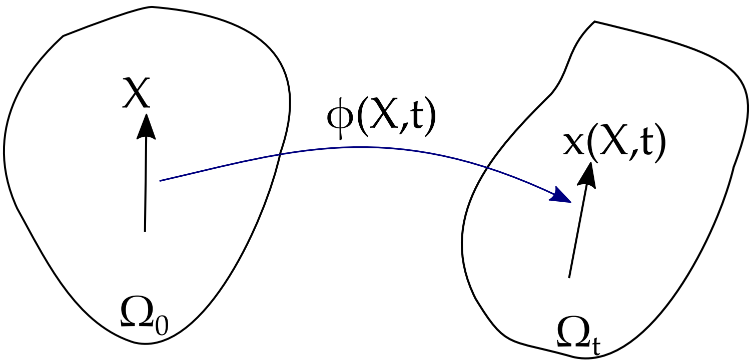
and the (viscous) Navier-Stokes stresses are given by

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

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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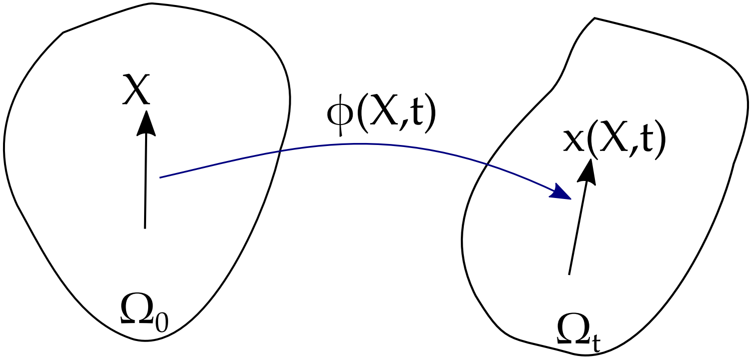

$$\partial_t(\mathbf{A}) + \nabla(\mathbf{A}\mathbf{u}) + \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\right) \cdot \mathbf{u} = 0 \quad \text{(Solids)}$$

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Hyperbolic NSK = Hyperbolic EK + Hyperbolic NS

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

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

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

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

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

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

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

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

Eigenvalues - Hyperbolicity

$\Rightarrow$ 18 Real Eigenvalues (Linearized around $A = \mathbf{I}, \mathbf{p} = (p1, 0, 0)^T$)

Transport: $\lambda_{1-10} = u_1,$

shear waves: $\begin{cases} \lambda_{11-12} = u_1 + c_s, \\ \lambda_{13-14} = u_1 - c_s, \end{cases}$

Mixed waves:

$$\begin{cases} \lambda_{15} = u_1 - \sqrt{Z_1 + Z_2} \\ \lambda_{16} = u_1 - \sqrt{Z_1 - Z_2} \\ \lambda_{17} = u_1 + \sqrt{Z_1 + Z_2} \\ \lambda_{18} = u_1 + \sqrt{Z_1 - Z_2} \end{cases}, \begin{cases} Z_1 = \frac{1}{2}(a_0^2 + a_s^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2), \\ Z_2 = \sqrt{Z_1^2 - a_\beta^2(a_0^2 + a_\alpha^2 + a_s^2)}, \\ a_0 = \sqrt{\rho W''(\rho)}, \quad a_s = \sqrt{\frac{4}{3}c_s^2} \\ a_\alpha = \frac{\eta}{\rho\sqrt{\alpha}}, \quad a_\beta = \sqrt{\frac{\gamma}{\beta\rho}}, \quad a_\gamma = \sqrt{\frac{\gamma}{\rho}p_1^2} \end{cases}$$

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Scaling of relaxations

Representative characteristic velocities

$$\begin{cases} \lambda_{15} = u_1 - \sqrt{Z_1 + Z_2} \\ \lambda_{16} = u_1 - \sqrt{Z_1 - Z_2} \\ \lambda_{17} = u_1 + \sqrt{Z_1 + Z_2} \\ \lambda_{18} = u_1 + \sqrt{Z_1 - Z_2} \end{cases}, \begin{cases} Z_1 = \frac{1}{2}(a_0^2 + a_s^2 + a_\gamma^2 + a_\alpha^2 + a_\beta^2), \\ Z_2 = \sqrt{Z_1^2 - a_\beta^2(a_0^2 + a_\alpha^2 + a_s^2)}, \\ a_0 = \sqrt{\rho W''(\rho)}, \quad a_s = \sqrt{\frac{4}{3}c_s^2} \\ a_\alpha = \frac{\eta}{\rho\sqrt{\alpha}}, \quad a_\beta = \sqrt{\frac{\gamma}{\beta\rho}}, \quad a_\gamma = \sqrt{\frac{\gamma}{\rho}p_1^2} \end{cases}$$

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

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

Dispersion relation

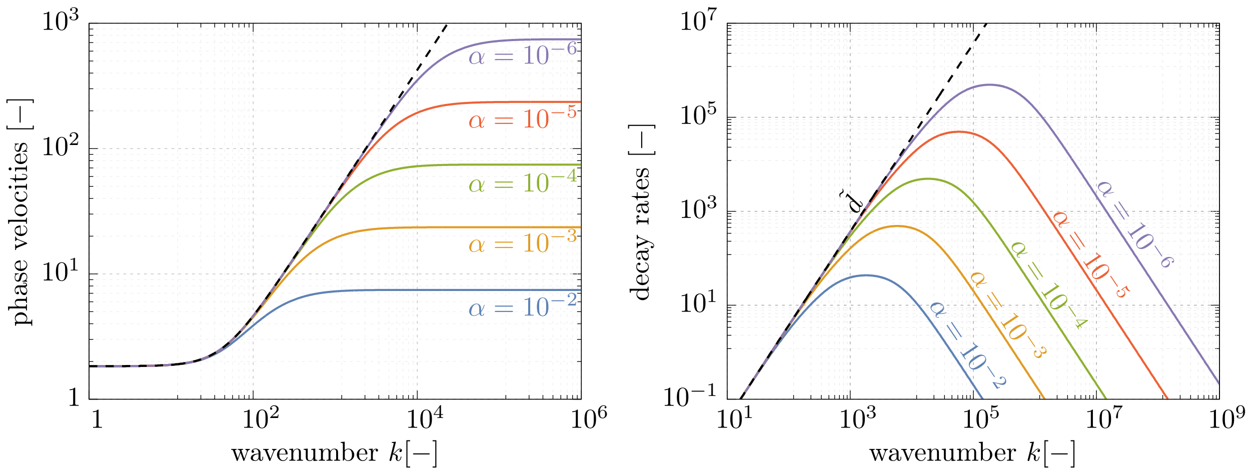

Figure 2: Plot of the phase velocity (left) and the decay rate for several values of α along their counterparts for the Navier-Stokes-Korteweg system. The model parameters are as follows $\gamma = 10^{-3}$, $\mu = 10^{-3}$ and $\rho = 1.8$

Curl-free constraint

We propose two methods to treat the curl-free constraint :

1. ADER-DG + GLM curl-cleaning : Introduce artificial 'cleaning field' to transport the curl errors away

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We propose two methods to treat the curl-free constraint :

1. ADER-DG + GLM curl-cleaning : Introduce artificial 'cleaning field' to transport the curl errors away
2. Exactly curl-free method based on FV : Provide a specific discretization based on staggered grid allowing to conserve the discrete curl-free constraint by construction.

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

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

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

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

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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.

Thermodynamically compatible curl cleaning

The total energy for our system, accounting for the cleaning contribution is given by

$$E = \frac{\rho}{2}|\mathbf{u}|^2 + W(\rho) + \frac{\rho}{4} c_s^2 \mathrm{dev}\mathbf{G} : \mathrm{dev}\mathbf{G} + \frac{\gamma}{2}|\mathbf{p}|^2 + \frac{1}{2\alpha\rho}(\rho-\eta)^2 + \frac{\beta}{2}\rho w^2 + \frac{\rho}{2}|\boldsymbol{\psi}|^2.$$

Accounting for the GLM curl cleaning modifications, an additional scalar balance law for the total energy can be obtained as a consequence of the governing equations and which writes as

$$\partial_t E + \nabla\cdot(E \cdot \mathbf{u} - \mathbf{T}\cdot\mathbf{u} - \gamma w \mathbf{p} + \gamma b_c\, \boldsymbol{\psi} \times \mathbf{p}) = -3 \frac{\det(\mathbf{A})}{\rho \tau c_s^2}^{5/3} \mathcal{E}_{\mathbf{A}} : \mathcal{E}_{\mathbf{A}}$$

where $\mathbf{T} = \Sigma + \mathbf{K} - P \cdot \mathbf{I}$

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

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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:

$$\partial_t(\rho) + \partial_x(\rho u) = 0$$

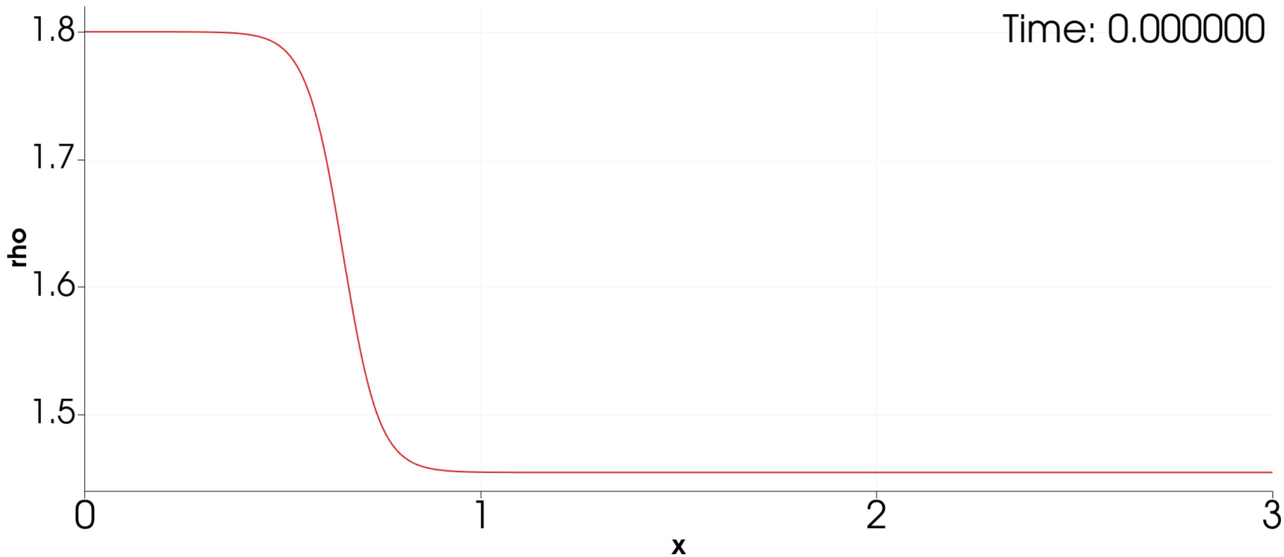
$$\partial_t(\rho u) + \partial_x(\rho u^2 + p(\rho)) = \frac{4}{3}\mu u_{xx} + \gamma \rho \rho_{xxx}$$

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

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

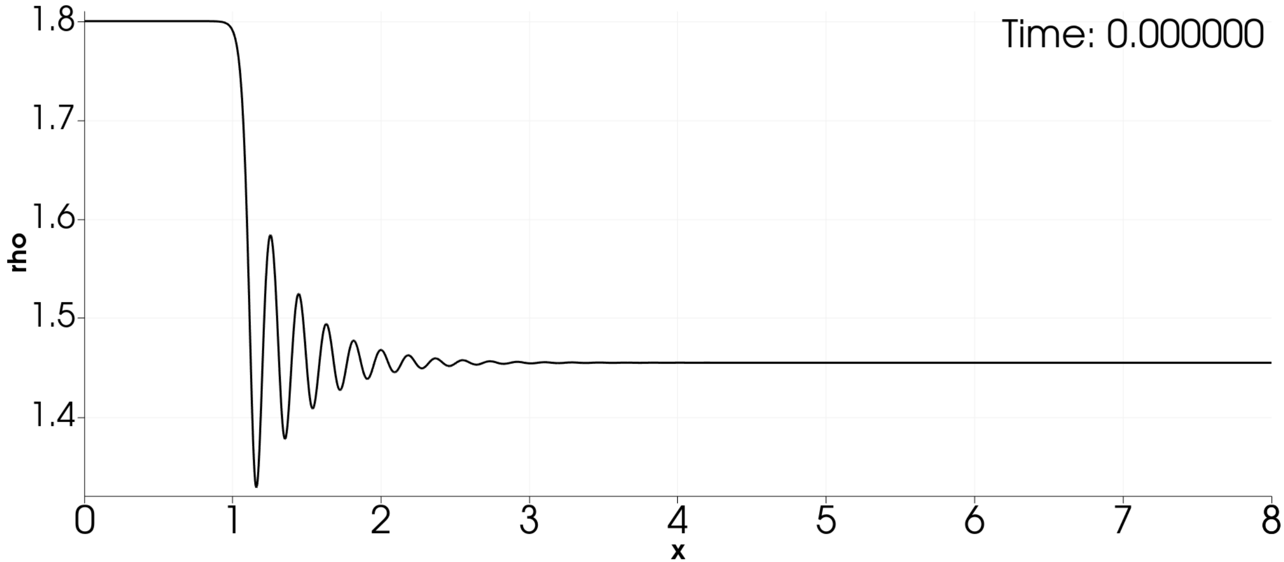
which we solve as a Cauchy problem with a prescribed initial condition $\rho_0 = 1.8$, $\rho_0' = -10^{-10}$, $\rho_0'' = 0$, $u_0 = 0$

Viscous TW solution



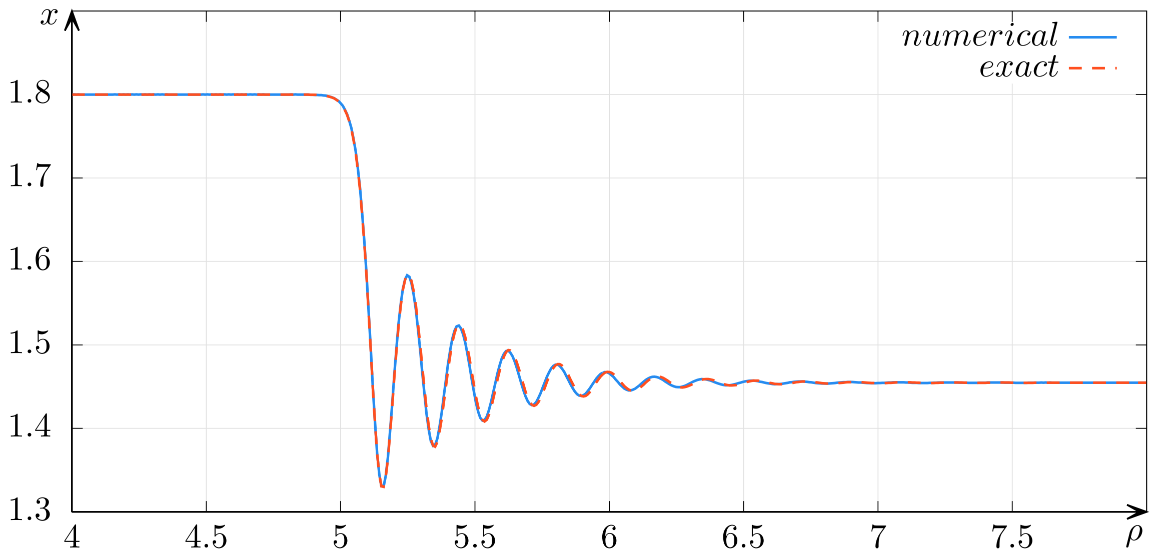
Viscous shock traveling wave solution to the original NSK (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.2$, $\alpha = 0.001$, $\beta = 0.00001$)

Oscillatory TW solution



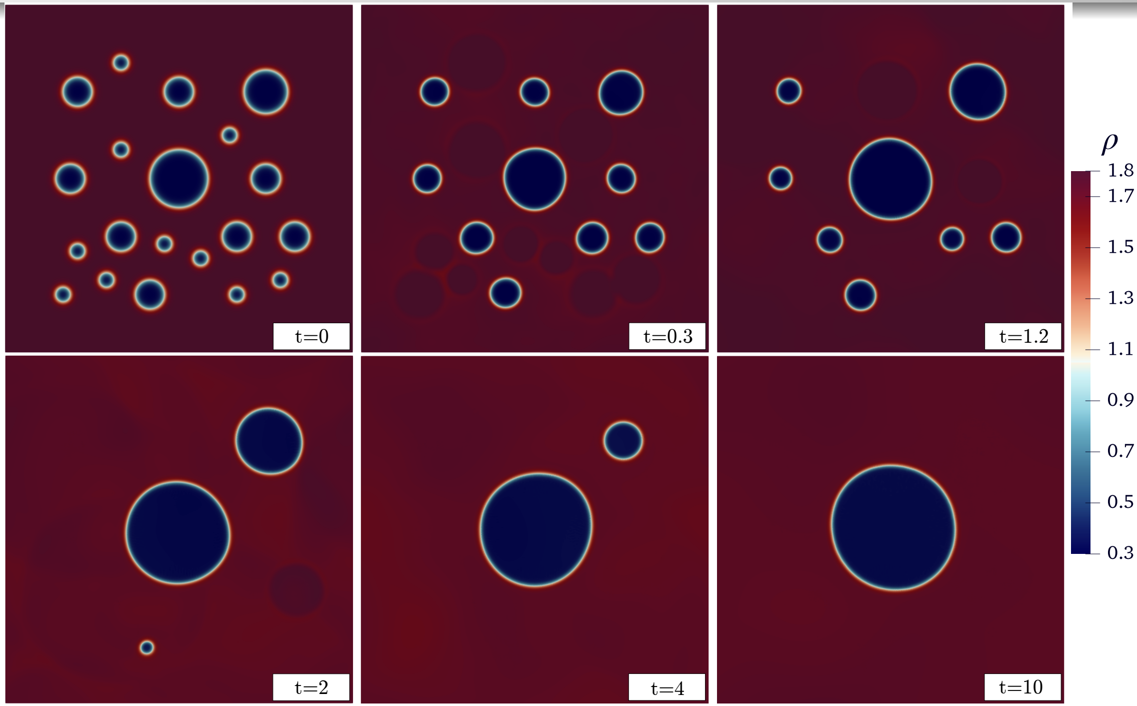
Dispersive traveling wave solution to the original NSK (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.0075$, $\alpha = 0.001$, $\beta = 0.00001$)

Oscillatory TW solution



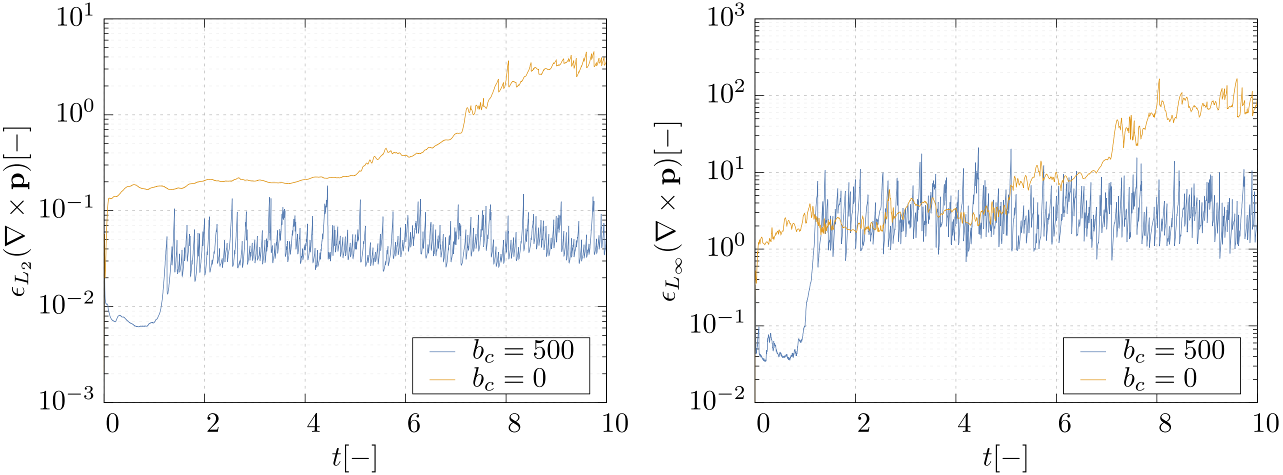
Superimposed numerical solution and exact solution of original model at t=4. (Obtained with a P_4P_4 ADER-DG scheme + WENO3 subcell limiting on a grid with 512 cells with $\gamma = 0.001$,$\mu = 0.0075$, $c_s = 10$, $\alpha = 0.001$, $\beta = 0.00001$)

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).

Exactly-curl free numerical scheme

A set of classical conservation laws:

$$\begin{aligned}
\partial_t(\rho) &\quad + \operatorname{div}(\rho\mathbf{u}) = 0\\
\partial_t(\rho\mathbf{u}) &\quad + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + P(\rho)\mathbf{Id} - K_\alpha - \sigma\right) = 0\\
\partial_t(\rho\eta) &\quad + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w\\
\partial_t(\rho w) &\quad + \operatorname{div}\left(\rho w\mathbf{u} - \gamma\mathbf{p}/\beta\right) = (\alpha\beta)^{-1}\left(1 - \eta/\rho\right)
\end{aligned}$$

A set of potentially curl constrained vectors:

$$\begin{aligned}
\partial_t(\mathbf{p}) &\quad + \nabla\left(\mathbf{p}\cdot\mathbf{u} - w\right) + \left(\nabla\times\mathbf{p}\right)\times\mathbf{u} = 0,\\
\partial_t(\mathbf{A_1}) &\quad + \nabla(\mathbf{A_1}\cdot\mathbf{u}) + (\nabla\times\mathbf{A}_1)\times\mathbf{u} = -\frac{1}{\tau}\mathbf{S}_1\\
\partial_t(\mathbf{A_2}) &\quad + \nabla(\mathbf{A_2}\cdot\mathbf{u}) + (\nabla\times\mathbf{A}_2)\times\mathbf{u} = -\frac{1}{\tau}\mathbf{S}_2\\
\partial_t(\mathbf{A_3}) &\quad + \nabla(\mathbf{A_3}\cdot\mathbf{u}) + (\nabla\times\mathbf{A}_3)\times\mathbf{u} = -\frac{1}{\tau}\mathbf{S}_3
\end{aligned}$$

Exactly-curl free numerical scheme

A set of classical conservation laws: MUSCL-Hancock FV scheme

$$\begin{aligned}
&\partial_t(\rho) && + \operatorname{div}(\rho\mathbf{u}) = 0 \\
&\partial_t(\rho\mathbf{u}) && + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + P(\rho)\mathbf{Id} - K_\alpha - \sigma\right) = 0 \\
&\partial_t(\rho\eta) && + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w \\
&\partial_t(\rho w) && + \operatorname{div}\left(\rho w\mathbf{u} - \gamma\mathbf{p}/\beta\right) = (\alpha\beta)^{-1}\left(1-\eta/\rho\right)
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\end{aligned}$$

A set of potentially curl constrained vectors: VIP Treatment

$$\begin{aligned}
&\partial_t(\mathbf{p}) && + \nabla\left(\mathbf{p} \cdot \mathbf{u} - w\right) + (\nabla \times \mathbf{p}) \times \mathbf{u} = 0,\\
&\partial_t(\mathbf{A_1}) && + \nabla(\mathbf{A_1} \cdot \mathbf{u}) + (\nabla \times \mathbf{A}_1) \times \mathbf{u} = -\frac{1}{\tau}\mathbf{S}_1\\
&\partial_t(\mathbf{A_2}) && + \nabla(\mathbf{A_2} \cdot \mathbf{u}) + (\nabla \times \mathbf{A}_2) \times \mathbf{u} = -\frac{1}{\tau}\mathbf{S}_2\\
&\partial_t(\mathbf{A_3}) && + \nabla(\mathbf{A_3} \cdot \mathbf{u}) + (\nabla \times \mathbf{A}_3) \times \mathbf{u} = -\frac{1}{\tau}\mathbf{S}_3
\end{aligned}$$

Exactly curl-free scheme: Staggered Grid

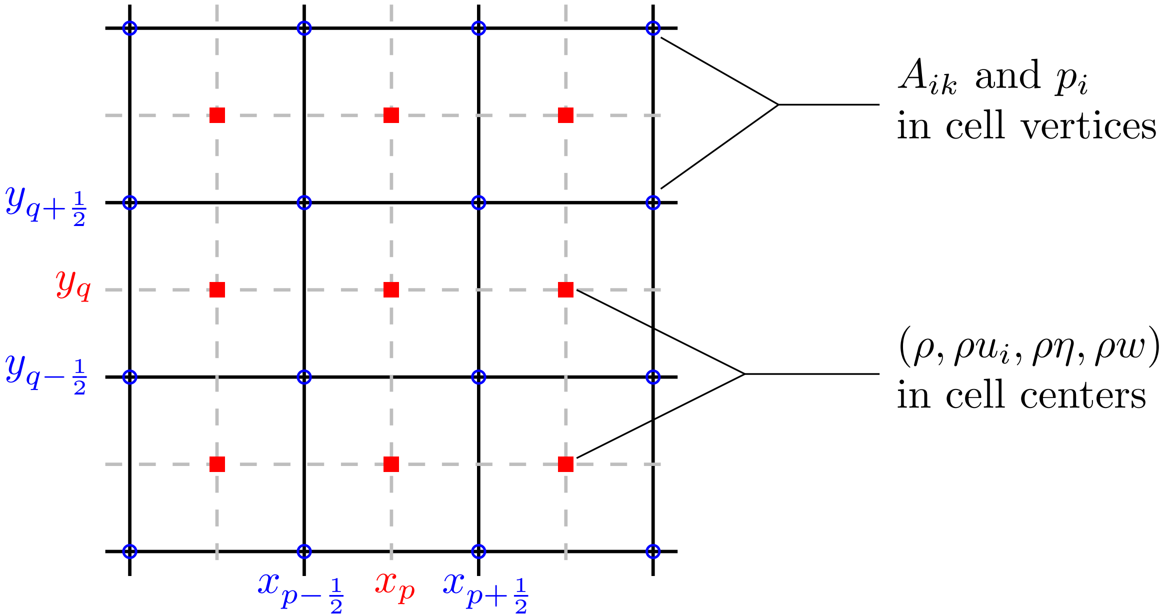
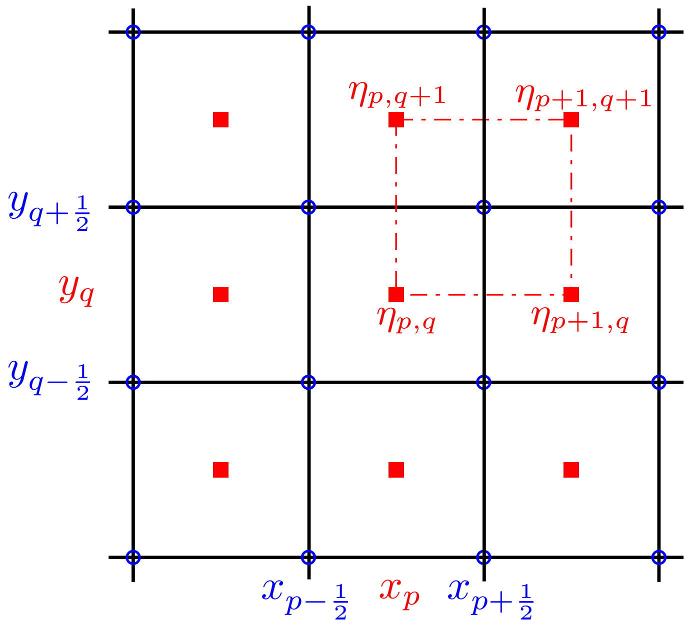


Figure 3: Schematic of the computational domain featuring the grid points and the staggered dual grid points. Red squares are barycenters and blue circles are the vertexes of the computational cells.

Exactly curl-free scheme: Compatible gradient stencil



$$
\begin{cases}
(\partial_x^h \phi)^{p+\frac{1}{2},q+\frac{1}{2}} = \frac{1}{2}\frac{\phi^{p+1,q}-\phi^{p,q}}{\Delta x} + \frac{1}{2}\frac{\phi^{p+1,q+1}-\phi^{p,q+1}}{\Delta x}, \\
(\partial_y^h \phi)^{p+\frac{1}{2},q+\frac{1}{2}} = \frac{1}{2}\frac{\phi^{p,q+1}-\phi^{p,q}}{\Delta y} + \frac{1}{2}\frac{\phi^{p+1,q+1}-\phi^{p+1,q}}{\Delta y}.
\end{cases}
$$

Figure 4: Stencil of the gradient field computed in every corner

Exactly curl-free scheme: Compatible curl stencil

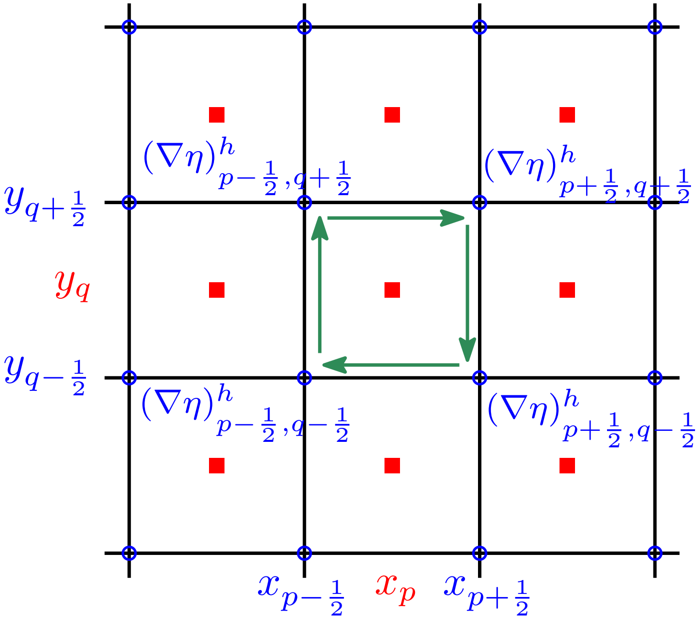


Figure 5: Stencil of the curl operator computed in every cell-center

Compatible discrete curl-operator

Based on this corner gradient, one can now define a compatible discrete curl operator such that $(\nabla^h \times \nabla^h \phi)^{p,q} \cdot \mathbf{e_z}$ is given by

$$\frac{(\partial_y^h \phi)^{p+\frac{1}{2},q+\frac{1}{2}} - (\partial_y^h \phi)^{p+\frac{1}{2},q-\frac{1}{2}}}{2\Delta y} + \frac{(\partial_y^h \phi)^{p-\frac{1}{2},q+\frac{1}{2}} - (\partial_y^h \phi)^{p-\frac{1}{2},q-\frac{1}{2}}}{2\Delta y}$$
$$-\frac{(\partial_x^h \phi)^{p+\frac{1}{2},q+\frac{1}{2}} - (\partial_x^h \phi)^{p-\frac{1}{2},q+\frac{1}{2}}}{2\Delta x} - \frac{(\partial_x^h \phi)^{p+\frac{1}{2},q-\frac{1}{2}} - (\partial_x^h \phi)^{p-\frac{1}{2},q-\frac{1}{2}}}{2\Delta x}.$$

It is straightforward to prove that

$$\nabla^h \times \nabla^h \phi \equiv 0$$

Update formulas ($h = \min(\Delta x, \Delta y)$)

- For the conserved variables $\rho, \mathbf{u}, \rho\eta, \rho w$:
  $\Rightarrow$ Classical MUSCL-Hancock scheme.

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- For the curl-free vector $\mathbf{p}$

$$p_k^{p+\frac{1}{2},q+\frac{1}{2},n+1} = p_k^{p+\frac{1}{2},q+\frac{1}{2},n} - \Delta t\, \nabla_k^h \left(p_j u_j - w\right)^{p+\frac{1}{2},q+\frac{1}{2},n}$$

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$$p_k^{p+\frac{1}{2},q+\frac{1}{2},n+1} = p_k^{p+\frac{1}{2},q+\frac{1}{2},n} - \Delta t\, \nabla_k^h \left(p_j u_j - w - h\; c^* \nabla_j^h p_j \right)^{p+\frac{1}{2},q+\frac{1}{2},n}$$

- Lastly, for $\mathbf{A}$

$$\begin{aligned} A_{ik}^{p+\frac{1}{2},q+\frac{1}{2},n+1} = A_{ik}^{p+\frac{1}{2},q+\frac{1}{2},n} &- \Delta t (\nabla_k^h (A_{ij} u_j) - h\; c^* \nabla_j^h A_{ij})^{p+\frac{1}{2},q+\frac{1}{2}} \\ &- \Delta t\; h\; c^* \varepsilon_{kj3} \nabla_j^{p+\frac{1}{2},q+\frac{1}{2},n} \left(\varepsilon_{3lm} \nabla_l^h A_{im} \right) \\ &- \frac{\Delta t}{4} \sum_{r=0}^{1} \sum_{s=0}^{1} u_m^{p+r,q+s,n} \left((\nabla_m^h A_{ik})^{p+\frac{1}{2},q+\frac{1}{2}} - (\nabla_k^h A_{im})^{p+\frac{1}{2},q+\frac{1}{2}} \right) \\ &- \Delta t \frac{1}{3\tau} \det(\mathbf{A}^{p+\frac{1}{2},q+\frac{1}{2},n+1})^{5/3} A_{im}^{p+\frac{1}{2},q+\frac{1}{2},n+1} \mathring{G}_{mk}^{p+\frac{1}{2},q+\frac{1}{2},n+1}. \end{aligned}$$

Near equilibrium bubble: density field

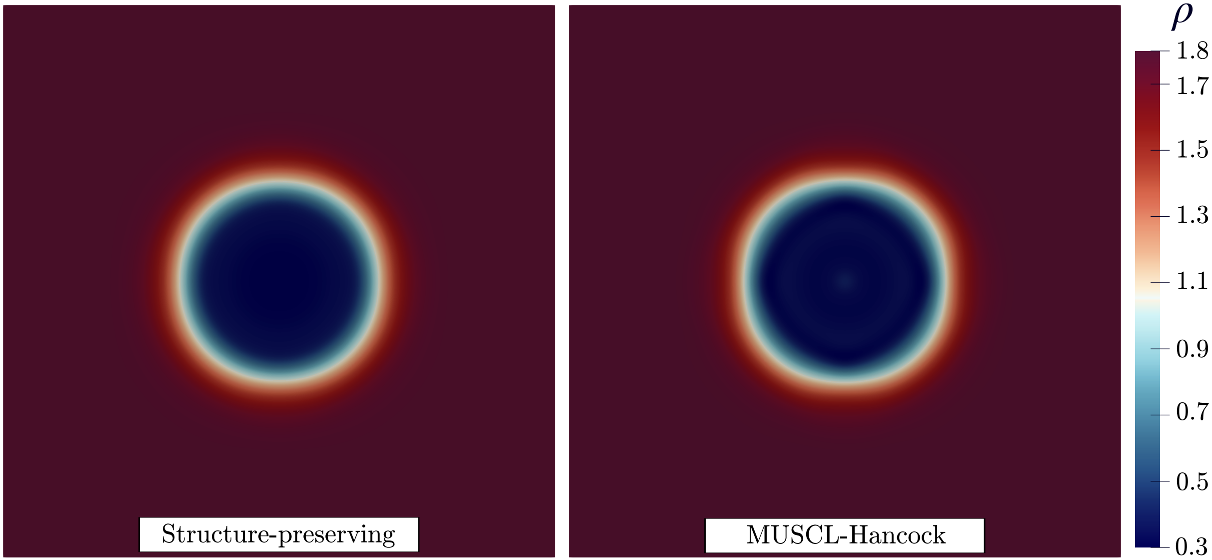

Figure 6: Results are shown for $t = 2$ on a 512×512 grid. With $\gamma = 2.10^{-4}$, $\alpha = 10^{-2}$, $\beta = 10^{-5}$, $\mu = 10^{-2}, c_s = 10$. The computational domain is $\Omega_c = [-0.25, 0.25] \times [-0.25, 0.25]$.

Near equilibrium bubble: gradient field

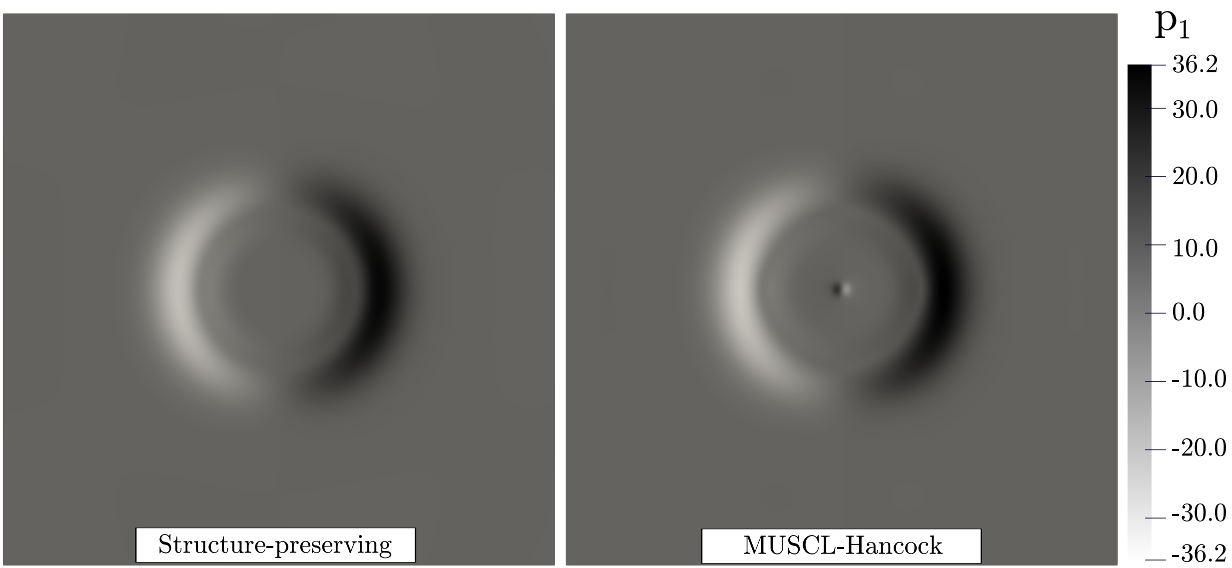

Figure 7: Results are shown for $t = 2$ on a 512×512 grid. With $\gamma = 2.10^{-4}$, $\alpha = 10^{-2}$, $\beta = 10^{-5}$, $\mu = 10^{-2}, c_s = 10$. The computational domain is $\Omega_c = [-0.25, 0.25] \times [-0.25, 0.25]$.

Near equilibrium bubble: Discrete curl error over time

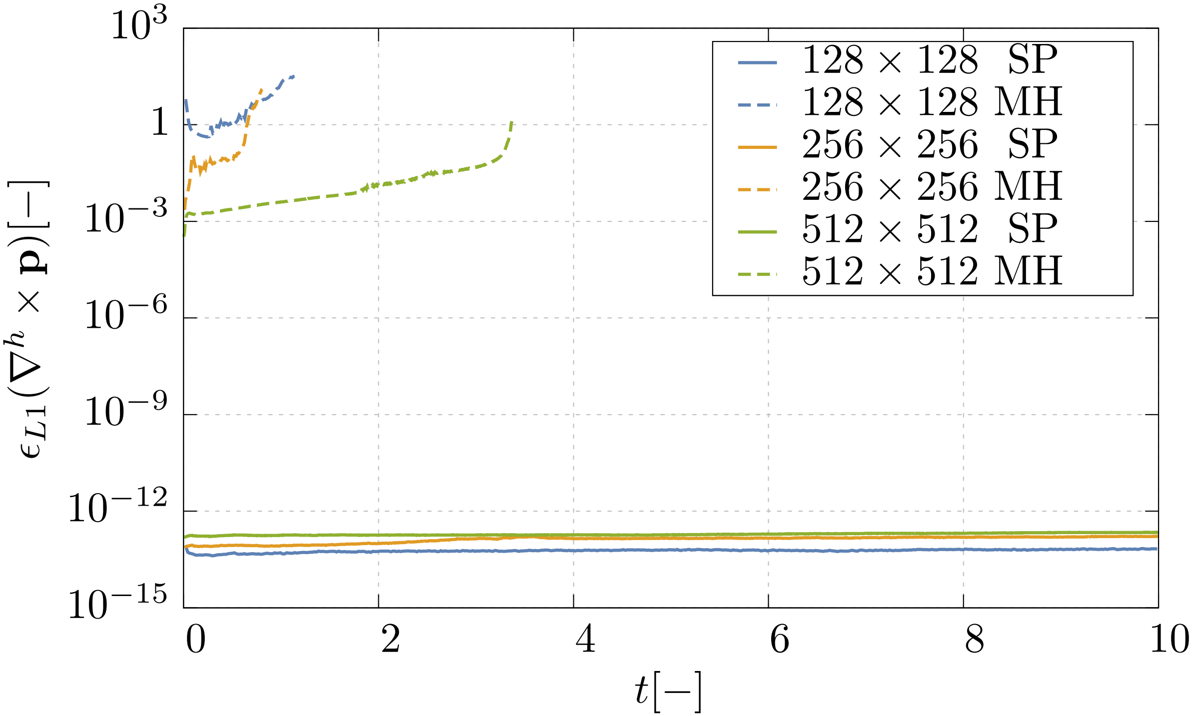

Figure 8: Time-evolution of the L_1 norm of the discrete curl errors on different mesh sizes.

2D Ostwald Ripening

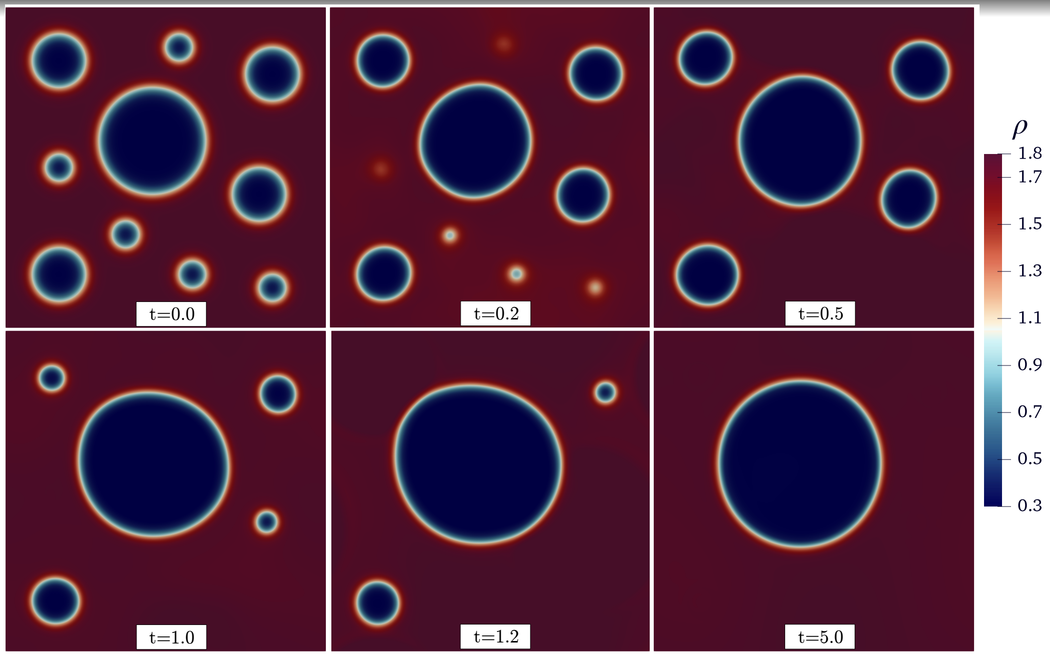

Figure 9: Values used here are $\rho_l = 1.8$, $\rho_v = 0.3$, $\gamma = 2.10^{-4}$, $\alpha = 10^{-2}$, $\beta = 10^{-5}$, $c_s = 10$ and an effective viscosity of $\mu = 10^{-2}$. The total domain is $\Omega = [-0.6, +0.6] \times [-0.6, +0.6]$ discretized over a 4096×4096 uniform grid with periodic boundary conditions.

Conclusion and Perspectives

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Perspectives

- Extension to non-isothermal flows (by using a hyperbolic heat transfer model [3]).
- Splitting of the fluxes for semi-implicit discretization
- Higher-order extension of the scheme
- Investigation of Laplace jumps... etc
- Study of convergence towards original model

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.

[3] Dhaouadi, Firas, and Sergey Gavrilyuk. "An Eulerian hyperbolic model for heat transfer derived via Hamilton's principle: analytical and numerical study." Proceedings of the Royal Society A 480.2283 (2024): 20230440.

And references therein.

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Invitation to ProHyp 2024

SCAN ME

- **22 to 26 April 2024**. (In 1.5 months)
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We will be happy to welcome you!