Hyperbolic models for diffusion equations

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Diffusion equations

- Many phenomena in nature are described by diffusion-type equations

1. Fick's second law for particle concentration

$$\frac{\partial \varphi}{\partial t} = \mathrm{div}\left(D \nabla \varphi\right)$$

2. Fourier's law for heat conduction leads to

$$\frac{\partial T}{\partial t} = \mathrm{div}\left(K \nabla T\right)$$

3. etc ...

Very "simple" structure, compares well with experimental observations.

Objective

We would like to provide first-order hyperbolic alternatives to the following systems

1. Euler equations supplemented by Fourier heat conduction

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0, \tag{1a}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + p(\rho, \eta)\mathbf{I}) = 0, \tag{1b}$$

$$\frac{\partial E}{\partial t} + \operatorname{div}(E\mathbf{u} + p(\rho, \eta)\mathbf{u} - K\nabla\theta(\rho, \eta)) = 0. \tag{1c}$$

2. Cahn-Hilliard equations

$$\frac{\partial c}{\partial t} = \Delta\left(c^3 - c - \gamma\Delta c\right). \tag{2}$$

Why are we doing this?

1. Restore the principle of causality :

   information must not travel faster than light speed in vacuum. (Trivially violated by Laplace operator)

2. Symmetric hyperbolic equations are well-posed.
3. Obtain an alternative description of known phenomena.
4. Chance it provides much easier/faster numerical simulations.

Plan of presentation

Objective properties

We want to obtain a model that satisfies the following properties

1. First-order hyperbolic system
2. Can be cast into a Friedrichs symmetric form
3. Total Energy is conserved
4. Compatible with the second law of thermodynamics
5. Gallilean invariant
6. can be derived from a variational principle

About Euler-Lagrange equations

Given a Lagrangian, you can derive the Euler-Lagrange equation

$$\mathcal{L}(q, \dot{q}, \nabla q) \quad \Longrightarrow \quad \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right) + \operatorname{div}\left(\frac{\partial \mathcal{L}}{\partial \nabla q}\right) = \frac{\partial \mathcal{L}}{\partial q}$$

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Things are already more complicated for Euler equations

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

$$\delta\rho = -\mathrm{div}\left(\rho \boldsymbol{\delta x}\right), \quad \delta\mathbf{u} = \frac{\partial \boldsymbol{\delta x}}{\partial t} + \frac{\partial \boldsymbol{\delta x}}{\partial \mathbf{x}}\mathbf{u} - \frac{\partial \mathbf{u}}{\partial \mathbf{x}}\boldsymbol{\delta x}$$

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After a bit of calculus $\quad \Rightarrow \quad \dfrac{\partial \rho\mathbf{u}}{\partial t} + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + \rho^2\dfrac{\partial \varepsilon}{\partial \rho}\mathbf{I}\right) = 0$

Euler equations for compressible fluids

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \mathbf{u}) = 0, \quad \text{(mass)}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \text{div}\,(\rho \mathbf{u} \otimes \mathbf{u} + p(\rho, \eta)\mathbf{I}) = 0, \quad \text{(momentum)}$$

$$\frac{\partial \rho \eta}{\partial t} + \text{div}\,(\rho \eta \mathbf{u}) = 0. \quad \text{(entropy)}$$

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$$\frac{\partial \rho \eta}{\partial t} + \mathrm{div}\,(\rho \eta \mathbf{u}) = 0. \quad \text{(entropy)}$$

Summing up these equations yields the energy conservation equation

$$\frac{\partial E}{\partial t} + \mathrm{div}\,(E\mathbf{u} + p(\rho, \eta)\mathbf{u}) = 0. \quad \text{(Energy)}$$

Thermal displacement (Green-Naghdi 1991)

In this paper :

[1] Green, A. E., & Naghdi, P. (1991). A re-examination of the basic postulates of thermomechanics. Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences, 432(1885), 171-194.

The authors introduce an independent auxiliary potential $\phi(\mathbf{x}, t)$ as a thermal analogue of the kinematic variables such that

$$\dot{\phi}(\mathbf{x}, t) = -\theta(\mathbf{x}, t)$$

One can then write the Lagrangian

$$\mathcal{L}(\rho, \mathbf{u}, \dot{\phi}) = \int_{\Omega} \left(\frac{1}{2}\rho \left|\left|\mathbf{u}\right|\right|^2 - \rho\varepsilon^{\star}(\rho, \dot{\phi}) \right) \, d\Omega,$$

where

$$\varepsilon(\rho, \eta) = \varepsilon^{\star}(\rho, \dot{\phi}) - \eta\dot{\phi}, \quad \text{with} \quad \eta = \frac{\partial \varepsilon^{\star}}{\partial \dot{\phi}}.$$

Entropy as an Euler-Lagrange equation

Given the Lagrangian

$$\mathcal{L}(\rho, \mathbf{u}, \dot{\phi}) = \int_\Omega \left(\frac{1}{2}\rho \left|\left|\mathbf{u}\right|\right|^2 - \rho\varepsilon^\star(\rho, \dot{\phi}) \right) \, d\Omega, \quad \left(\dot{\phi} = \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \right)$$

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One obtains

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \rho^2 \frac{\partial \varepsilon^\star}{\partial \rho} \mathbf{I} \right) = 0, \quad \text{(Euler-Lagrange for } \delta \mathbf{x}\text{)}$$

$$\frac{\partial}{\partial t} \left(\rho \frac{\partial \varepsilon^\star}{\partial \dot{\phi}} \right) + \operatorname{div}\left(\rho \frac{\partial \varepsilon^\star}{\partial \dot{\phi}} \mathbf{u} \right) = 0, \quad \text{(Euler-Lagrange for } \delta \phi\text{)}$$

Entropy as an Euler-Lagrange equation

Given the Lagrangian

$$\mathcal{L}(\rho, \mathbf{u}, \dot{\phi}) = \int_{\Omega} \left(\frac{1}{2}\rho \, ||\mathbf{u}||^2 - \rho\varepsilon^{\star}(\rho, \dot{\phi}) \right) \, d\Omega, \quad \left(\dot{\phi} = \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \right)$$

One obtains

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div} \left(\rho \mathbf{u} \otimes \mathbf{u} + \rho^2 \frac{\partial \varepsilon^{\star}}{\partial \rho} \mathbf{I} \right) = 0, \quad \text{(Euler-Lagrange for } \delta \mathbf{x}\text{)}$$

$$\frac{\partial}{\partial t} (\rho \eta) + \operatorname{div} (\rho \eta \mathbf{u}) = 0, \quad \text{(Euler-Lagrange for } \delta \phi\text{)}$$

$$\frac{\partial \rho}{\partial t} + \operatorname{div} (\rho \mathbf{u}) = 0 \quad \text{(Constraint)}$$

- A similar idea was also used in Lagrangian coordinates in *Peshkov et.al. (2018)*.

Extension of Green-Naghdi's philosophy

Consider the Lagrangian

$$\mathcal{L}(\rho, \mathbf{u}, \nabla\phi, \dot{\phi}) = \int_\Omega \left(\frac{1}{2}\rho\left|\left|\mathbf{u}\right|\right|^2 - \rho\varepsilon^\star(\rho, \dot{\phi}) - \frac{1}{2}\alpha(\rho)\left|\left|\nabla\phi\right|\right|^2\right)\, d\Omega,$$

where the function $\alpha(\rho)$ is an arbitrary positive function of density.

Extension of Green-Naghdi's philosophy

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where the function $\alpha(\rho)$ is an arbitrary positive function of density.

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \mathrm{div}\left(\rho\mathbf{u}\right) = 0, \\
&\frac{\partial \rho\mathbf{u}}{\partial t} + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + P(\rho, \nabla\phi)\,\mathbf{I} + \alpha(\rho)\ \nabla\phi\otimes\nabla\phi\right) = 0, \\
&\frac{\partial \rho\eta}{\partial t} + \mathrm{div}\left(\rho\eta\mathbf{u} + \alpha(\rho)\nabla\phi\right) = 0,
\end{aligned}$$

where $P(\rho, \nabla\phi) = \rho^2 \dfrac{\partial \varepsilon^\star}{\partial \rho} + \dfrac{1}{2}(\rho\alpha'(\rho) - \alpha(\rho)) \left|\left|\nabla\phi\right|\right|^2$

Extension of Green-Naghdi's philosophy

Consider the Lagrangian

$$\mathcal{L}(\rho, \mathbf{u}, \nabla\phi, \dot{\phi}) = \int_\Omega \left(\frac{1}{2}\rho \left|\left|\mathbf{u}\right|\right|^2 - \rho\varepsilon^\star(\rho, \dot{\phi}) - \frac{1}{2}\alpha(\rho) \left|\left|\nabla\phi\right|\right|^2 \right) \, d\Omega,$$

where the function $\alpha(\rho)$ is an arbitrary positive function of density.

$$\frac{\partial \rho}{\partial t} + \operatorname{div}\left(\rho\mathbf{u}\right) = 0,$$
$$\frac{\partial \rho\mathbf{u}}{\partial t} + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + P(\rho, \nabla\phi)\,\mathbf{I} + \alpha(\rho)\ \nabla\phi\otimes\nabla\phi\right) = 0,$$
$$\frac{\partial \rho\eta}{\partial t} + \operatorname{div}\left(\rho\eta\mathbf{u} + \alpha(\rho)\nabla\phi\right) = 0,$$

where $P(\rho, \nabla\phi) = \rho^2\dfrac{\partial\varepsilon^\star}{\partial\rho} + \dfrac{1}{2}(\rho\alpha'(\rho) - \alpha(\rho)) \left|\left|\nabla\phi\right|\right|^2$

- Problem : PDE is of second order and depends on $\nabla\phi$.

Solution: First-order reduction

Recall that

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -\theta(\rho, \eta)$$

Solution: First-order reduction

Recall that

$$\nabla \left(\frac{\partial \phi}{\partial t} \right) + \nabla (\mathbf{u} \cdot \nabla \phi) = -\nabla (\theta(\rho, \eta))$$

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Recall that

$$\nabla \left(\frac{\partial \phi}{\partial t}\right) + \nabla(\mathbf{u} \cdot \nabla \phi) = -\nabla(\theta(\rho, \eta))$$

$$\frac{\partial \nabla \phi}{\partial t} + \nabla \left(\mathbf{u} \cdot \nabla \phi + \theta(\rho, \eta)\right) = 0$$

Solution: First-order reduction

Recall that

$$\nabla\left(\frac{\partial\phi}{\partial t}\right)+\nabla(\mathbf{u}\cdot\nabla\phi)=-\nabla(\theta(\rho,\eta))$$

$$\frac{\partial\nabla\phi}{\partial t}+\nabla\left(\mathbf{u}\cdot\nabla\phi+\theta(\rho,\eta)\right)=0$$

Let us introduce $\mathbf{j}=\nabla\phi$ as an independent variable. Then $\mathbf{j}$ satisfies

$$\frac{\partial\mathbf{j}}{\partial t}+\nabla\left(\mathbf{u}\cdot\mathbf{j}+\theta(\rho,\eta)\right)=0$$

Dissipationless system of equations

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0,$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \Pi) = 0, \quad \Pi = P(\rho, \eta, \mathbf{j})\, \mathbf{I} + \alpha(\rho)\, \mathbf{j} \otimes \mathbf{j}$$

$$\frac{\partial \mathbf{j}}{\partial t} + \nabla(\mathbf{j} \cdot \mathbf{u} + \theta(\rho, \eta)) + \left(\frac{\partial \mathbf{j}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{j}}{\partial \mathbf{x}}\right)^T\right) \mathbf{u} = 0,$$

$$\frac{\partial \rho \eta}{\partial t} + \operatorname{div}(\rho \eta \mathbf{u} + \alpha(\rho) \mathbf{j}) = 0.$$

Dissipationless system of equations

$$
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&\frac{\partial \rho \eta}{\partial t} + \operatorname{div}(\rho \eta \mathbf{u} + \alpha(\rho) \mathbf{j}) = 0.
\end{aligned}
$$

Total energy conservation is obtained as a consequence

$$
\frac{\partial E}{\partial t} + \operatorname{div}(E \mathbf{u} + \Pi \mathbf{u} + \mathbf{q}) = 0, \quad \mathbf{q} = \alpha(\rho)\, \theta(\rho, \eta)\, \mathbf{j}
$$

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$$\frac{\partial E}{\partial t} + \mathrm{div}\left(E \mathbf{u} + \Pi \mathbf{u} + \mathbf{q}\right) = 0, \quad \mathbf{q} = \alpha(\rho)\, \theta(\rho, \eta)\, \mathbf{j}$$

Additional term in the energy conservation is heat flux.

Rayleigh dissipation function

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0,$$
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P(\rho, \eta, \mathbf{j})\, \mathbf{I} + \alpha(\rho)\, \mathbf{j} \otimes \mathbf{j}) = 0,$$
$$\frac{\partial \mathbf{j}}{\partial t} + \nabla (\mathbf{j} \cdot \mathbf{u} + \theta(\rho, \eta)) + \left(\frac{\partial \mathbf{j}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{j}}{\partial \mathbf{x}} \right)^T \right) \mathbf{u} = -\frac{\partial \mathcal{R}}{\partial \mathbf{j}},$$
$$\frac{\partial \rho \eta}{\partial t} + \operatorname{div}(\rho \eta \mathbf{u} + \alpha(\rho)\mathbf{j}) = \frac{\alpha(\rho)}{\theta(\rho, \eta)} \frac{\partial \mathcal{R}}{\partial \mathbf{j}} \cdot \mathbf{j}.$$

Here $\mathcal{R}$ is the *Rayleigh dissipation* function and which we take in the simplest form as

$$\mathcal{R} = \frac{1}{2\tau} \|\mathbf{j}\|^2, \qquad \frac{\partial \mathcal{R}}{\partial \mathbf{j}} = \frac{1}{\tau}\mathbf{j}$$

Energy convexity

Total energy is given by

$$E(\rho, \mathbf{m}, s, \mathbf{j}) = \frac{1}{2\rho}\left|\left|\mathbf{m}\right|\right|^2 + \rho\varepsilon(\rho, s/\rho) + \frac{1}{2}\alpha(\rho)\left|\left|\mathbf{j}\right|\right|^2, \quad \mathbf{m} = \rho\mathbf{u}, s = \rho\eta$$

Sufficient criterion for energy convexity

$$\text{if } \frac{\partial^2}{\partial\rho^2}\left(\frac{1}{\alpha(\rho)}\right) \leq 0, \quad \text{for } \rho > 0.$$

then E i s also a convex function of $\mathbf{Q}$.

We choose a simple function fitting this criterion

$$\alpha(\rho) = \frac{\varkappa}{\rho}, \quad \varkappa = cst.$$

Energy convexity

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$$\alpha(\rho) = \frac{\varkappa}{\rho}, \quad \varkappa = cst.$$

(Another possibility is $\alpha(\rho) = cst$, taken in *Peshkov et.al. (2018)*)

Hyperbolicity

system can be cast into quasilinear form

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{A}(\mathbf{V})\frac{\partial \mathbf{V}}{\partial \mathbf{x}} = 0$$

where $\mathbf{A}$ admits 8 eigenvalues whose expressions are given by

$$\begin{cases} \chi_1 = u_1 - \sqrt{Z_1 + Z_2}, \\ \chi_2 = u_1 - \sqrt{Z_1 - Z_2}, \\ \chi_{3-6} = u_1, \\ \chi_7 = u_1 + \sqrt{Z_1 - Z_2}, \\ \chi_8 = u_1 + \sqrt{Z_1 + Z_2} \end{cases} \quad \text{where} \begin{cases} Z_1 = \frac{1}{2}\left(a_p^2 + a_T^2 + a_j^2\right), \\ Z_2 = \sqrt{a_{pT}^4 + \frac{1}{4}\left(a_p^2 - a_T^2\right)^2}, \\ a_p^2 = \frac{\partial p}{\partial \rho}, \quad a_T^2 = \frac{\varkappa^2}{\rho^2}\frac{\partial \theta}{\partial \eta}, \\ a_{pT}^4 = \frac{\varkappa^2}{\rho^2}\frac{\partial p}{\partial \eta}\frac{\partial \theta}{\partial \rho}, \quad a_j^2 = \frac{2\varkappa^2}{\rho^2}\left(j_2^2 + j_3^2\right). \end{cases}$$

1D-study: Eigenfields

In one dimension of space, we can write the system as

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0,\\
&\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial \eta}\frac{\partial \eta}{\partial x} = 0,\\
&\frac{\partial \eta}{\partial t} + u\frac{\partial \eta}{\partial x} + \frac{\varkappa^2}{\rho^2}\frac{\partial j}{\partial x} - \frac{\varkappa^2}{\rho^3}j\frac{\partial \rho}{\partial x} = 0,\\
&\frac{\partial j}{\partial t} + j\frac{\partial u}{\partial x} + u\frac{\partial j}{\partial x} + \frac{\partial \theta}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial \theta}{\partial \eta}\frac{\partial \eta}{\partial x} = 0.
\end{aligned}
$$

The eigenvalues are given by

$$
\begin{cases}
\lambda_1 = u - \sqrt{Y_1 + Y_2},\\
\lambda_2 = u - \sqrt{Y_1 - Y_2},\\
\lambda_3 = u + \sqrt{Y_1 - Y_2},\\
\lambda_4 = u + \sqrt{Y_1 + Y_2},
\end{cases}
\quad \text{where} \quad
\begin{cases}
Y_1 = \frac{1}{2}\left(a_p^2 + a_T^2\right),\\
Y_2 = \sqrt{a_{pT}^4 + Y_3^2},\\
Y_3 = \frac{1}{2}\left(a_p^2 - a_T^2\right).
\end{cases}
$$

1D-study: Eigenfields

$$\begin{cases} \lambda_1 = u - \sqrt{Y_1 + Y_2}, \\ \lambda_2 = u - \sqrt{Y_1 - Y_2}, \\ \lambda_3 = u + \sqrt{Y_1 - Y_2}, \\ \lambda_4 = u + \sqrt{Y_1 + Y_2}, \end{cases} \quad \text{where} \quad \begin{cases} Y_1 = \frac{1}{2}\left(a_p^2 + a_T^2\right), \\ Y_2 = \sqrt{a_{pT}^4 + Y_3^2}, \\ Y_3 = \frac{1}{2}\left(a_p^2 - a_T^2\right). \end{cases}$$

Nature of the eigenfields (polytropic gas equation of state):

- System admits full basis of eigenvectors.

1D-study: Eigenfields

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Nature of the eigenfields (polytropic gas equation of state):

- System admits full basis of eigenvectors.
- Eigenfields associated to $\lambda_{1,4}$ are genuinely non-linear.

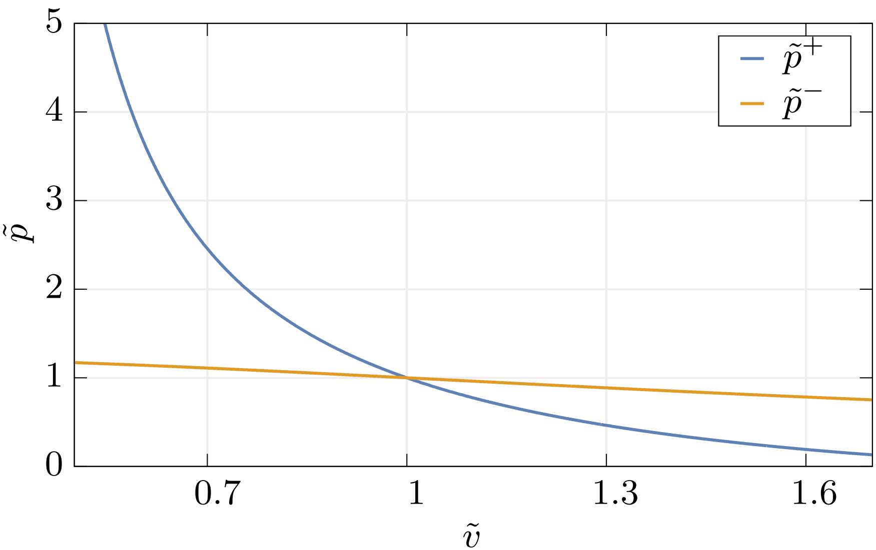
1D-study: Eigenfields

$$\begin{cases} \lambda_1 = u - \sqrt{Y_1 + Y_2}, \\ \lambda_2 = u - \sqrt{Y_1 - Y_2}, \\ \lambda_3 = u + \sqrt{Y_1 - Y_2}, \\ \lambda_4 = u + \sqrt{Y_1 + Y_2}, \end{cases} \quad \text{where} \quad \begin{cases} Y_1 = \frac{1}{2}\left(a_p^2 + a_T^2\right), \\ Y_2 = \sqrt{a_{pT}^4 + Y_3^2}, \\ Y_3 = \frac{1}{2}\left(a_p^2 - a_T^2\right). \end{cases}$$

Nature of the eigenfields (polytropic gas equation of state):

- System admits full basis of eigenvectors.
- Eigenfields associated to $\lambda_{1,4}$ are genuinely non-linear.
- Eigenfields associated to $\lambda_{2,3}$ are neither genuinely non-linear, neither linearly degenerate.

Hugoniot Locus (polytropic gas equation of state)



Study of the Hugoniot curves shows interesting possible solutions:

- Expansion shocks,
- Compression fans,
- Compound shocks.

Compound shocks

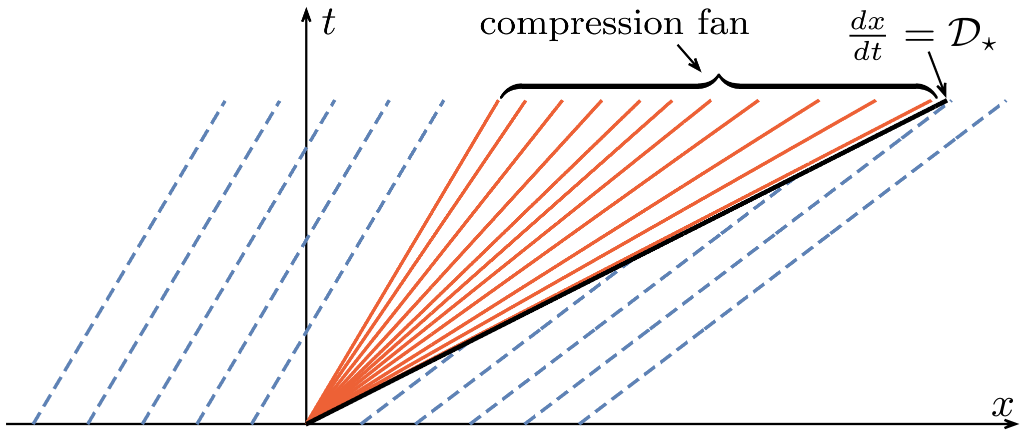


Figure 1: Schematic representation of the wave pattern in the $x - t$ plane, for a compound shock splitting solution. The shock propagates to the right, followed by a right facing compression fan.

Recovery of Fourier law: Shock tube problem

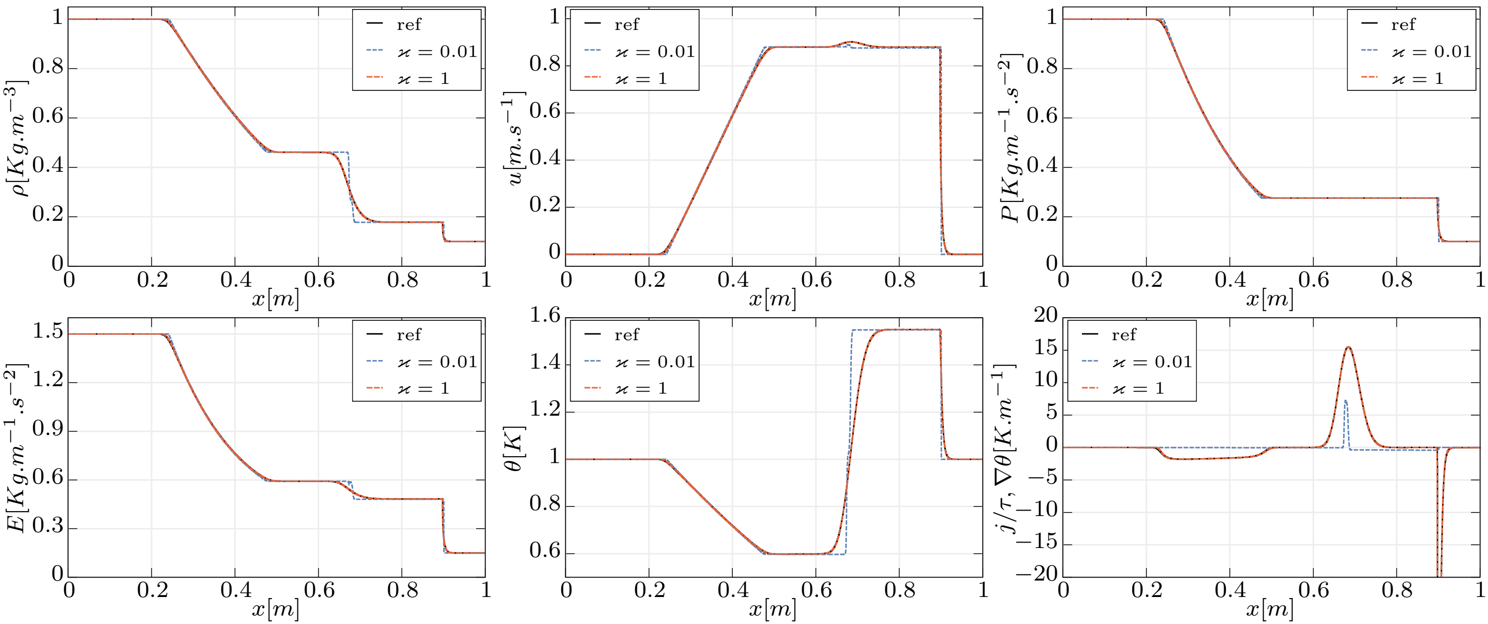


Figure 2: Shock tube with heat conduction. The solution is given at final time $t = 0.2$. Parameters: $\mathrm{CFL} = 0.9$, $\gamma = 5/3$, $c_V = 3/2$, $K = 10^{-3}$. Relaxation time is taken as $\tau = \frac{K}{\alpha(\rho_0)\,\theta(\rho_0,\eta_0)}$

Expansion shock solution

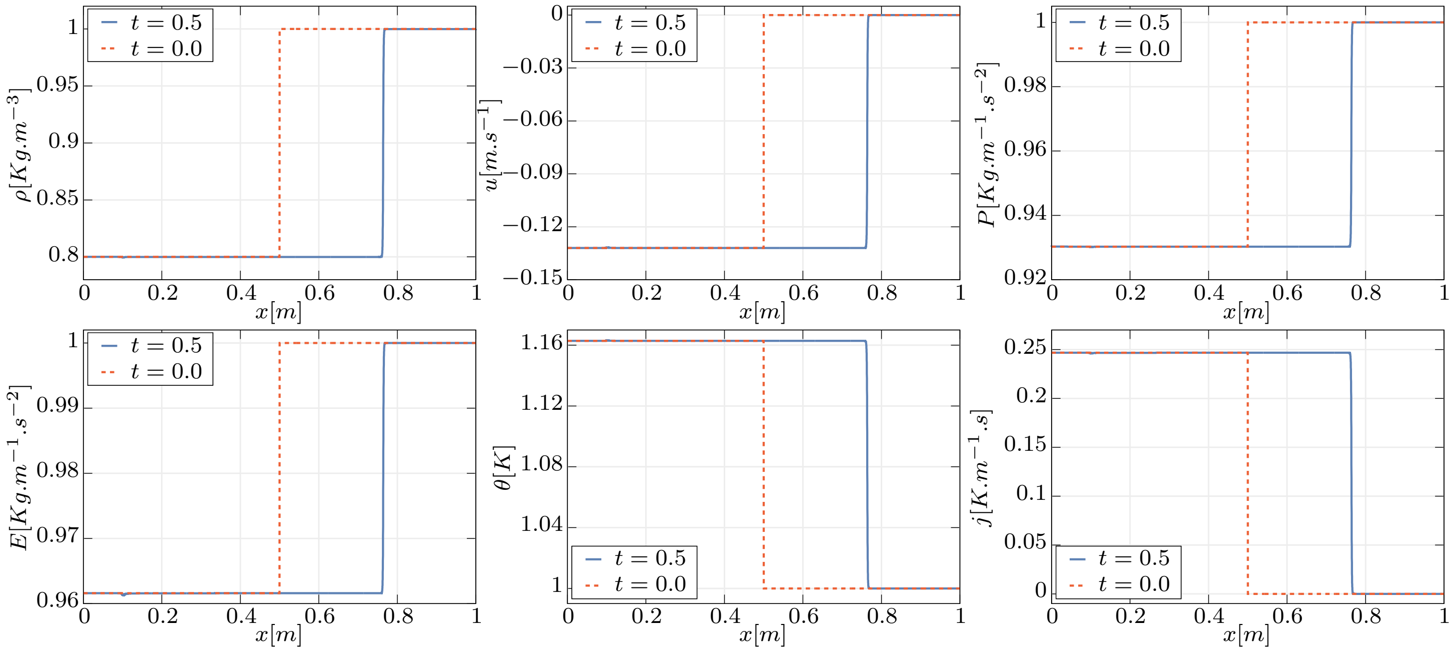


Figure 3: Numerical result for an expansion shock solution on the computational domain $[0, 1]$, discretized over $N = 10000$ cells displayed at final time $t = 0.5$. Parameters: $\mathrm{CFL} = 0.9$, $\gamma = 2$, $c_V = 1$, $\varkappa = 0.8$.

Compound shock solution

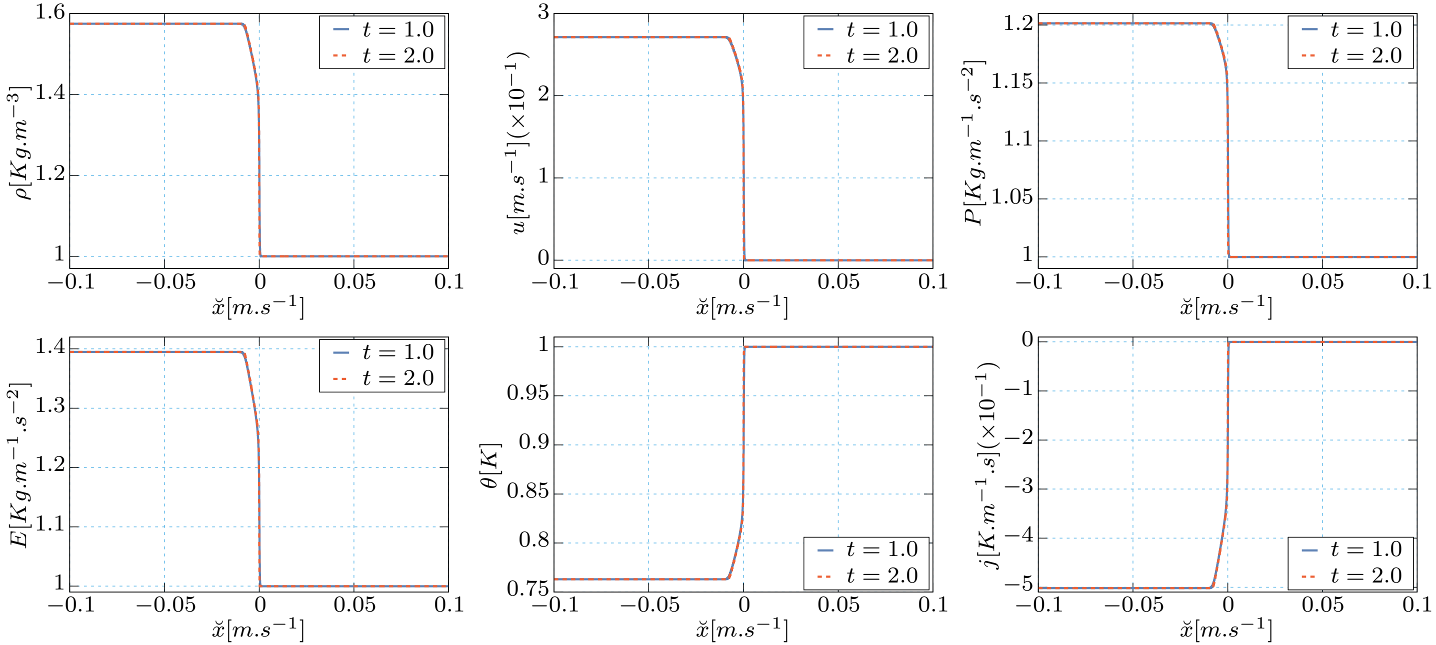


Figure 4: Compound shock plotted as a function of the self-similar coordinate $\breve{x} = (x - \mathcal{D}_\star t)/t$. $\mathrm{CFL} = 0.9$, $\gamma = 2$, $c_V = 1$, $\varkappa = 1.3$.

Plan

About Cahn-Hilliard equations

The Cahn-Hilliard equation is given by

$$\frac{\partial c}{\partial t} = \Delta\left(c^3 - c - \gamma \Delta c\right).$$

It admits the following Lyapunov functional $\left(\frac{dF}{dt} \leq 0\right)$

$$F = \int_{\mathcal{D}} f(c, \nabla c)\, d\Omega, \quad f(c, \nabla c) = \frac{\left(c^2 - 1\right)^2}{4} + \frac{\gamma}{2} \left|\left|\nabla c\right|\right|^2$$

The C-H can also be written in conservative form as

$$\frac{\partial c}{\partial t} + \operatorname{div}(\mathbf{j}) = 0, \quad \mathbf{j} = \nabla\left(\frac{\partial f}{\partial c} - \operatorname{div}\left(\frac{\partial f}{\partial \nabla c}\right)\right)$$

Proposed action

Let us introduce the following action

$$a = \int_t \int_{\mathcal{D}} \mathcal{L}\, d\Omega\, dt, \quad \mathcal{L} = \frac{\left(c^2-1\right)^2}{4} + \frac{\gamma}{2}\left|\left|\nabla \varphi\right|\right|^2 + \frac{\lambda}{2}(c-\varphi)^2 - \frac{\beta}{2}\varphi_t^2$$

- φ is the new order parameter (distinguishes the phases).
- $\frac{\lambda}{2}(c-\varphi)^2$ is a classical penalty term.

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$$\frac{\partial c}{\partial t} = \operatorname{div}\left(\nabla\left(\frac{\partial \mathcal{L}}{\partial c}\right)\right), \implies \quad \frac{\partial c}{\partial t} = \Delta\left(c^3 - c + \lambda\left(c-\varphi\right)\right)$$

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$$\frac{\partial c}{\partial t} = \operatorname{div}\left(\nabla\left(\frac{\partial \mathcal{L}}{\partial c}\right)\right), \qquad \Longrightarrow \qquad \frac{\partial c}{\partial t} = \Delta\left(c^3 - c + \lambda\left(c - \varphi\right)\right)$$

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \varphi_t}\right) + \operatorname{div}\left(\frac{\partial \mathcal{L}}{\partial \nabla \varphi}\right) = \frac{\partial \mathcal{L}}{\partial \varphi} \quad \Longrightarrow \quad \beta \frac{\partial \varphi_t}{\partial t} - \operatorname{div}\left(\gamma \nabla \varphi\right) = \lambda(c - \varphi)$$

Cattaneo-type relaxation for first equation

We start from

$$\frac{\partial c}{\partial t} = \mathrm{div}\left(\nabla\left(c^3 - c + \lambda\left(c - \varphi\right)\right)\right)$$

We apply classical relaxation ($\tau \ll 1$ is a characteristic time)

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\frac{1}{\tau}\mathbf{q}\right) = 0,$$
$$\frac{\partial \mathbf{q}}{\partial t} + \nabla\left(c^3 - c + \lambda\left(c - \varphi\right)\right) = -\frac{1}{\tau}\mathbf{q},$$

Order reduction for second equation

We start from

$$\beta \frac{\partial \varphi_t}{\partial t} - \operatorname{div}(\gamma \nabla \varphi) = \lambda (c - \varphi)$$

We denote

$$w = \beta \frac{\partial \varphi_t}{\partial t}, \quad \mathbf{p} = \nabla \varphi.$$

Thus obtaining the system

$$\frac{\partial w}{\partial t} - \operatorname{div}(\gamma \mathbf{p}) = -\lambda(\varphi - c)$$
$$\frac{\partial \mathbf{p}}{\partial t} - \frac{1}{\beta} \nabla w = 0$$
$$\frac{\partial \varphi}{\partial t} = \frac{1}{\beta} w$$

First-order hyperbolic system for C-H equations

Regrouping all equations we get

$$
\begin{aligned}
&\frac{\partial c}{\partial t} + \operatorname{div}\left(\frac{1}{\tau}\mathbf{q}\right) = 0 \\
&\frac{\partial \mathbf{q}}{\partial t} + \nabla\left(c^3 - c + \lambda(c-\varphi)\right) = -\frac{1}{\tau}\mathbf{q} \\
&\frac{\partial w}{\partial t} - \operatorname{div}\left(\gamma \mathbf{p}\right) = -\lambda(\varphi - c) \\
&\frac{\partial \mathbf{p}}{\partial t} - \frac{1}{\beta}\nabla w = 0 \\
&\frac{\partial \varphi}{\partial t} = \frac{1}{\beta} w
\end{aligned}
$$

Energy decay

One can obtain an decay law for the total energy given by

$$\frac{\partial E}{\partial t} + \mathrm{div}\left(\frac{\partial E}{\partial c}\frac{\partial E}{\partial \mathbf{q}} - \frac{\partial E}{\partial w}\frac{\partial E}{\partial \mathbf{p}}\right) = -\left|\left|\frac{\partial E}{\partial \mathbf{q}}\right|\right|^2 \leq 0.$$

where the total energy E is

$$E(c, \varphi, w, \mathbf{p}, \mathbf{q}) = \frac{\left(c^2 - 1\right)^2}{4} + \frac{\gamma}{2}\left|\left|\mathbf{p}\right|\right|^2 + \frac{\lambda}{2}(c - \varphi)^2 + \frac{1}{2\beta}w^2 + \frac{1}{2\tau}\left|\left|\mathbf{q}\right|\right|^2$$

Hyperbolicity

In three dimensions of space, the eigenvalues are given by

$$
\begin{aligned}
\xi_{1-5} &= 0 \\
\xi_6 &= -\frac{\sqrt{3c^2+\lambda-1}}{\sqrt{\tau}} \\
\xi_7 &= \frac{\sqrt{3c^2+\lambda-1}}{\sqrt{\tau}} \\
\xi_8 &= -\frac{\sqrt{\gamma}}{\sqrt{\beta}} \\
\xi_9 &= \frac{\sqrt{\gamma}}{\sqrt{\beta}},
\end{aligned}
$$

for which a full basis of real eigenvectors exist.

Implicit fourth order FD on staggered grids for the original Cahn-Hilliard equations

$$\frac{\partial c}{\partial t} - \operatorname{div}(\chi \nabla c) + \gamma \Delta\Delta c = 0, \quad \chi = 3c^2 - 1$$

We propose the following scheme

$$c_{i,j}^{n+1} = c_{i,j}^{n} + \frac{\Delta t}{\Delta x}\left(\mathcal{F}_{i+\frac{1}{2},j}^{n+1} - \mathcal{F}_{i-\frac{1}{2},j}^{n+1}\right) + \frac{\Delta t}{\Delta y}\left(\mathcal{G}_{i,j+\frac{1}{2}}^{n+1} - \mathcal{G}_{i,j-\frac{1}{2}}^{n+1}\right) - \gamma \Delta\Delta_h c_{i,j}^{n+1}$$

$$\mathcal{F}_{i+\frac{1}{2},j}^{n+1} = \chi_{i+\frac{1}{2},j}^{n+1,r} \left(\nabla_x c\right)_{i+\frac{1}{2},j}^{n+1},$$

where

$$\begin{cases} \chi_{i+\frac{1}{2},j}^{n+1,r} \simeq \dfrac{1}{12}\left(7\,\chi_{i,j}^{n+1,r} - \chi_{i-1,j}^{n+1,r} + 7\,\chi_{i+1,j}^{n+1,r} - \chi_{i+2,j}^{n+1,r}\right) \\ \left(\nabla_x c\right)_{i+\frac{1}{2},j}^{n+1} \simeq -\dfrac{1}{12\,\boldsymbol{\delta x}}\left(15\,c_{i-1,j}^{n+1} - 15\,c_{i,j}^{n+1} + c_{i+1,j}^{n+1} - c_{i-2,j}^{n+1}\right) \end{cases}$$

(The same for $\mathcal{G}^{n+1}$)

$\Delta\Delta_h c_{i,j}^{n+1}$ is a discretization of the bi-Laplacian operator in the cell-centers as follows

$$\begin{aligned}\Delta\Delta_h c_{i,j}^{n+1} =& -\frac{\Delta t}{\Delta x^4}\left(c_{i-2,j}^{n+1} - 4c_{i-1,j}^{n+1} + 6c_{i,j}^{n+1} - 4c_{i+1,j}^{n+1} + c_{i+2,j}^{n+1}\right)\\ & -\frac{\Delta t}{\Delta y^4}\left(c_{i,j-2}^{n+1} - 4c_{i,j-1}^{n+1} + 6c_{i,j}^{n+1} - 4c_{i,j+1}^{n+1} + c_{i,j+2}^{n+1}\right)\\ & -\frac{2\Delta t}{\Delta x^2\Delta y^2}\big(c_{i-1,j-1}^{n+1} - 2c_{i,j-1}^{n+1} + c_{i+1,j-1}^{n+1} - 2c_{i-1,j}^{n+1}\\ & \qquad + 4c_{i,j}^{n+1} - 2c_{i+1,j}^{n+1} + c_{i-1,j+1}^{n+1} - 2c_{i,j+1}^{n+1} + c_{i+1,j+1}^{n+1}\big)\end{aligned}$$

Comparison of hyperbolic and original CH: ODE solution

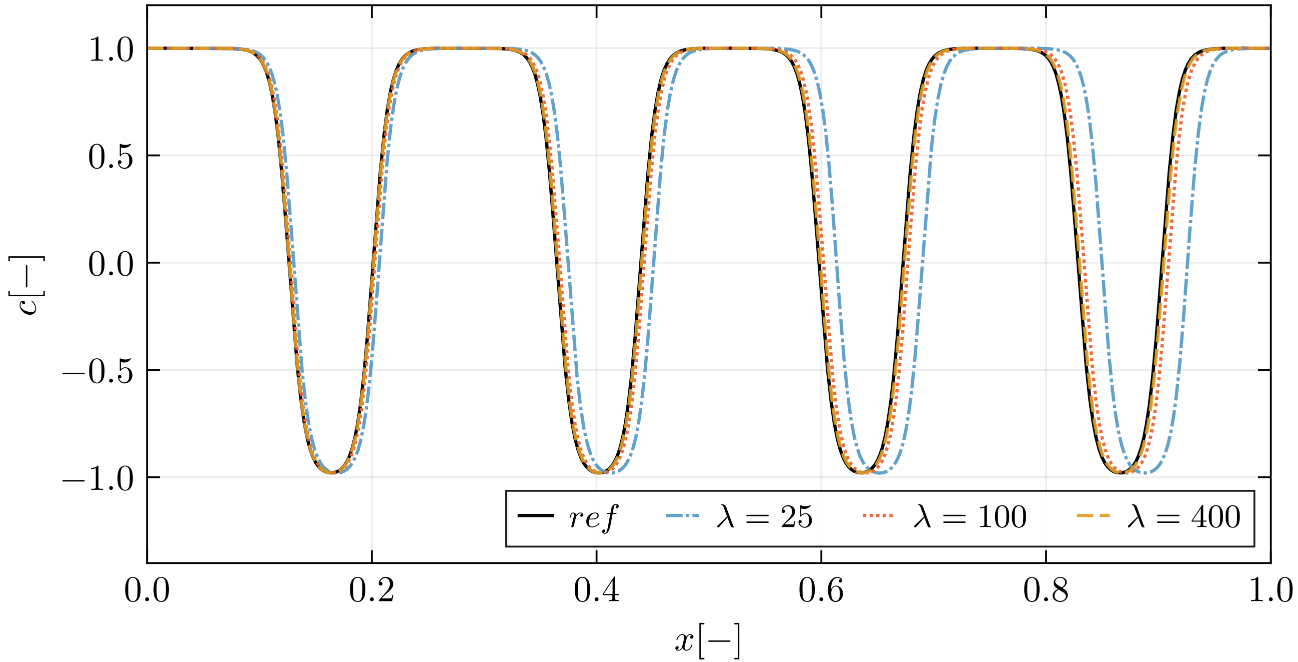


Figure 5: Comparison of a stationary solution of the hyperbolic model with the original counterpart for different values of λ.

Comparison of hyperbolic and original CH: 1D Ostwald Ripening

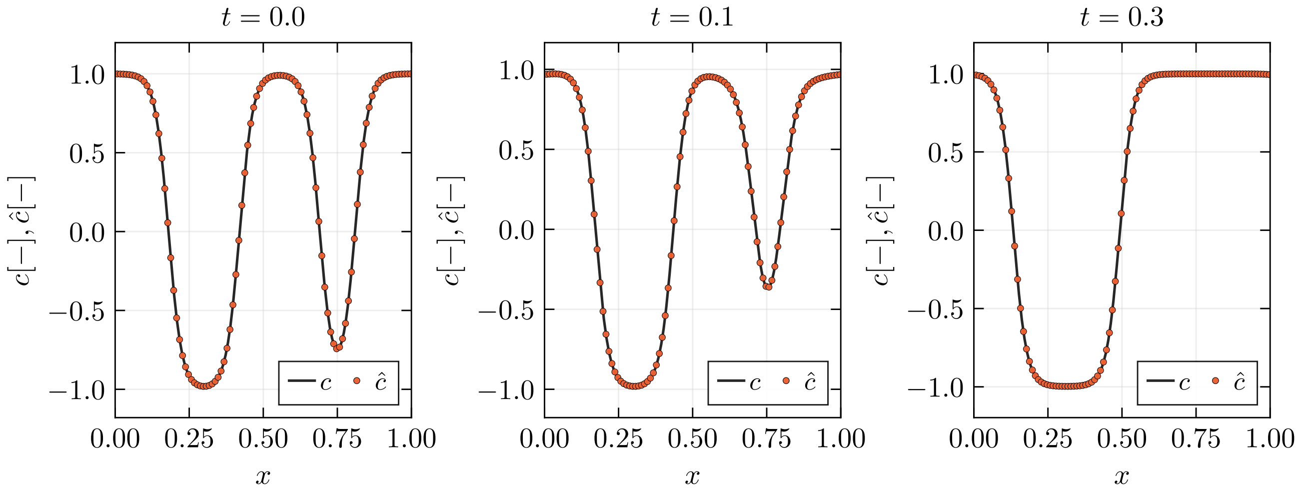
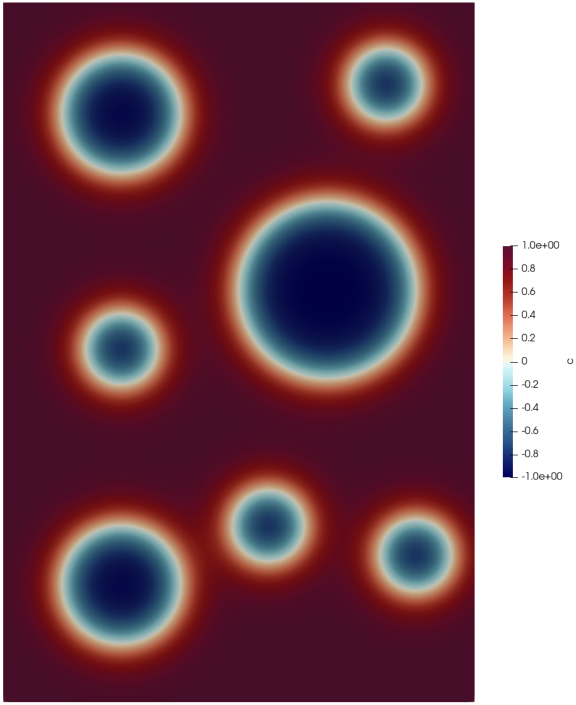


Figure 6: Comparison of Ostwald Ripening solution of the hyperbolic model with the original counterpart. Parameters are

Preliminary results for 2D Ostwald Ripening



Results obtained using explicit one-step fourth order ADER-DG.

Conclusion and Perspectives

- Heat conduction can be modeled by hyperbolic equations.
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Perspectives

- Multi-D simulations for heat equation (accounting for curl-involutions, etc)
- Rigorous Justification of the relaxation limit
- Further optimization at the numerical level (semi-implicit discretization, etc)
- Preserving $-1 \leq c \leq 1$ numerically

Thank you for your attention !

[1] 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.

[2] Dhaouadi firas, Michael Dumbser and Sergey Gavrilyuk, "A first-order hyperbolic approximation to the Cahn-Hilliard equation". To be submitted.
And references therein.

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