

An Eulerian hyperbolic model for heat transfer derived via Hamilton's principle

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Diffusion equations

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

- 1 Fick's second law for particle concentration

$$\frac{\partial c}{\partial t} = \operatorname{div} (D \nabla c)$$

- 2 Fourier's law for heat conduction

$$\frac{\partial \theta}{\partial t} = \operatorname{div} (K \nabla \theta)$$

- 3 etc ...

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

Heat conduction in an inviscid compressible flow

Generally described by Euler equation + Fourier's law of heat conduction

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

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

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

System describes conservation of mass, momentum and total energy.

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System describes conservation of mass, momentum and total energy.

Entropy satisfies Clausius-Duhem inequality

$$\frac{\partial \rho \eta}{\partial t} + \operatorname{div} \left(\rho \eta \mathbf{u} - \frac{K}{\theta} \nabla \theta \right) = \frac{K}{\theta^2} \|\nabla \theta\|^2 \geq 0.$$

Objective

We would like to provide first-order hyperbolic alternative to the Euler-Fourier system

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0, \quad (2a)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + p(\rho, \eta) \mathbf{I}) = 0, \quad (2b)$$

$$\frac{\partial E}{\partial t} + \operatorname{div}(E \mathbf{u} + p(\rho, \eta) \mathbf{u} - K \nabla \theta(\rho, \eta)) = 0. \quad (2c)$$

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- 2 Symmetric hyperbolic equations are locally well-posed.
- 3 Obtain an alternative description of known phenomena.
- 4 Chance it provides much easier/faster numerical simulations
(Very often the case, not always).

Plan of presentation

- 1 Model Derivation
- 2 Model analysis and hyperbolicity
- 3 Numerical results

Objective properties

We want to obtain a model that satisfies the following properties

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

Cattaneo's model

Well-known hyperbolic relaxation of heat equation (1948)

$$\frac{\partial \theta}{\partial t} + \operatorname{div}(\mathbf{q}) = 0$$
$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -K \nabla \theta$$

- No underlying variational principle.
- Not Galilean invariant (fixable)
- Generally considered out of the scope of fluid dynamics.
- when coupled with compressible Euler equations
 - 1 Not hyperbolic in multi-D.
 - 2 Does not satisfy Clausius-Duhem inequality.

Cattaneo's model

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0$$

$$\left(\rho \left(\varepsilon + \frac{1}{2} u^2 \right) \right)_t + \left(\rho u \left(\varepsilon + \frac{1}{2} u^2 \right) \right)_x = -(\rho u)_x - q_x$$

$$\tau q_t + \tau u q_x + q = -\kappa \theta_x$$

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$$\tau q_t + \tau u q_x + q = -\kappa \theta_x$$

The Gibbs identity implies that

$$\rho \theta \frac{d\eta}{dt} = -q_x$$

which can be cast in conservative form as

$$(\rho \eta)_t + \left(\rho \eta u + \frac{q}{\theta} \right)_x = -\frac{q \theta_x}{\theta^2} \geq? 0$$

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$$(\rho \eta)_t + \left(\rho \eta u + \frac{q}{\theta} \right)_x = -\frac{q \theta_x}{\theta^2} \stackrel{?}{>} 0$$

not necessarily satisfied because $q \neq -K \theta_x \quad \forall \tau > 0$.

About Euler-Lagrange equations

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

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

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Things are already more complicated for Euler equations

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

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

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After a bit of calculus $\implies \frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div} \left(\rho \mathbf{u} \otimes \mathbf{u} + \rho^2 \frac{\partial \varepsilon}{\partial \rho} \mathbf{I} \right) = 0$

Euler equations for compressible fluids

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

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Summing up these equations yields the energy conservation equation

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

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

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

where

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

Entropy as an Euler-Lagrange equation

Given the Lagrangian

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One obtains

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

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

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

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

- A similar idea was also used in Lagrangian coordinates in *Peshkov, Pavelka, Grmela and Romenski (2018)*.

Extension of Green-Naghdi's philosophy

Consider the Lagrangian

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

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

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

where $P = \rho^2 \frac{\partial\varepsilon^*}{\partial\rho} + \frac{1}{2}(\rho\alpha'(\rho) - \alpha(\rho)) \|\nabla\phi\|^2$

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

Solution: First-order reduction

Recall that

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

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

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Note that since $\mathbf{j} = \nabla \phi$ then \mathbf{j} satisfies

$$\nabla \times \mathbf{j} = 0.$$

Dissipationless system of equations

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

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

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

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

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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Additional term in the energy conservation *should* be the heat flux.

Rayleigh dissipation function

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$$\frac{\partial \rho \eta}{\partial t} + \operatorname{div}(\rho \eta \mathbf{u} + \alpha(\rho) \mathbf{j}) = \frac{\alpha(\rho)}{\theta(\rho, \eta)} \frac{\partial \mathcal{R}}{\partial \mathbf{j}} \cdot \mathbf{j}.$$

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

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

Asymptotic Analysis and compatibility with Fourier's law

we can expand the variables in power series of τ

$$\rho = \rho_0 + O(\tau), \quad \mathbf{u} = \mathbf{u}_0 + O(\tau), \quad \eta = \eta_0 + O(\tau), \quad \mathbf{j} = \mathbf{j}_0 + \tau \mathbf{j}_1 + o(\tau),$$

and we focus on the \mathbf{j} equation

$$\tau \left(\frac{\partial \mathbf{j}_0}{\partial t} + \frac{\partial \mathbf{j}_0}{\partial \mathbf{x}} \mathbf{u}_0 + \left(\frac{\partial \mathbf{u}_0}{\partial \mathbf{x}} \right)^T \mathbf{j}_0 + \nabla \theta(\rho_0, \eta_0) \right) = -(\mathbf{j}_0 + \tau \mathbf{j}_1) + o(\tau).$$

to obtain

$$\mathbf{j}_0 = 0, \quad \mathbf{j}_1 = -\nabla \theta(\rho_0, \eta_0), \quad \implies \boxed{\mathbf{j} = -\tau \nabla \theta(\rho_0, \eta_0) + o(\tau).}$$

Under these considerations, the heat flux vector expresses as

$$\mathbf{q} = -\tau \alpha(\rho_0) \theta(\rho_0, \eta_0) \nabla \theta(\rho_0, \eta_0).$$

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$$\mathbf{q} = -\tau \alpha(\rho_0) \theta(\rho_0, \eta_0) \nabla \theta(\rho_0, \eta_0).$$

compatible with Fourier's law if

$$\tau = \frac{K}{\alpha(\rho_0) \theta(\rho_0, \eta_0)}$$

Energy convexity

Total energy is given by

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

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 is also a convex function of \mathbf{Q} .

We choose a simple function fitting this criterion

$$\alpha(\rho) = \frac{\varkappa^2}{\rho}, \quad \varkappa = \text{cst.}$$

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$$\alpha(\rho) = \frac{\varkappa^2}{\rho}, \quad \varkappa = cst.$$

(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

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

Limiting behavior in 1D

Eigenvalues

$$\lambda_{1,4} = u_1 \pm \sqrt{Z_1 + Z_2}, \quad \lambda_{2,3} = u_1 \pm \sqrt{Z_1 - Z_2}.$$

In the asymptotic limit $\varkappa \rightarrow \infty$ we have

$$\lim_{\varkappa \rightarrow \infty} \chi_{1,8} = \pm \infty, \quad \lim_{\varkappa \rightarrow \infty} \lambda_{2,3} = u_1 \pm a_\theta$$

with a_θ being the isothermal sound speed given by

$$a_\theta = \sqrt{\frac{\partial \tilde{p}(\rho, \theta)}{\partial \rho}} = \sqrt{\frac{\partial p(\rho, \eta)}{\partial \rho} - \frac{\partial p(\rho, \eta)}{\partial \eta} \frac{\partial \theta}{\partial \rho} / \frac{\partial \theta}{\partial \eta}}$$

Dispersion relation comparison

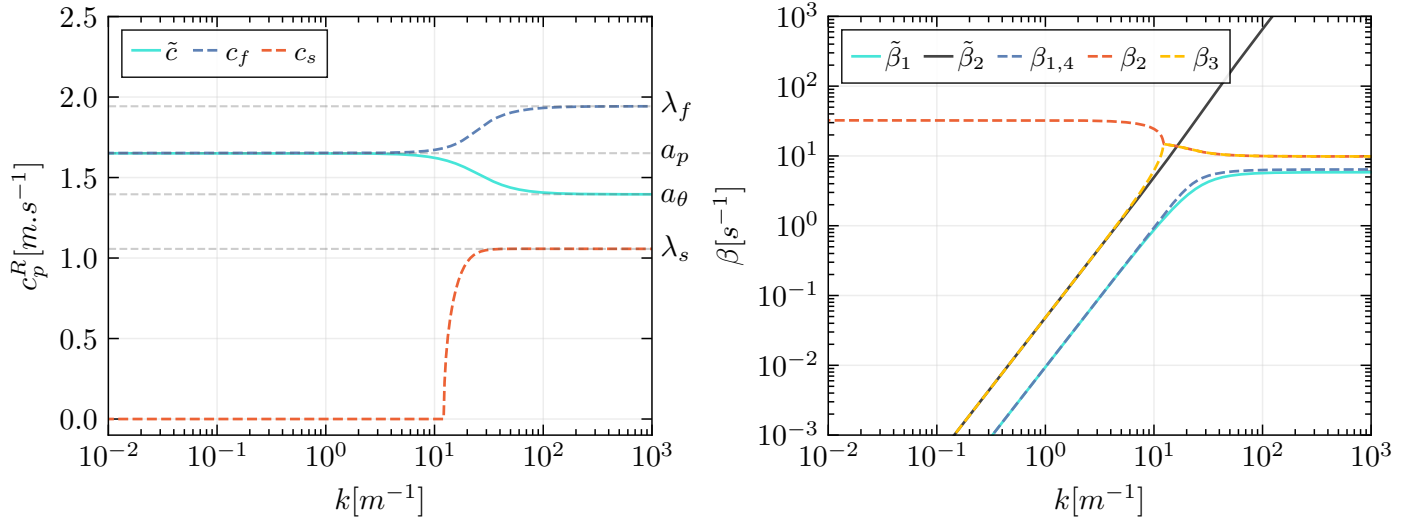


Figure 1: log-linear plot of the norms of the real part of the phase velocities (Left) and log-log plot of the attenuation factors (Right) for both hyperbolic system (Dashed lines) and original Euler-Fourier system (Solid lines).

$$a_p = \sqrt{\frac{\partial p}{\partial \rho}},$$

$$a_\theta = \sqrt{\frac{\partial p}{\partial \rho} - \frac{\partial p}{\partial \eta} \frac{\partial \theta}{\partial \rho} / \frac{\partial \theta}{\partial \eta}}.$$

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

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

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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.
- Eigenfields associated to $\lambda_{2,3}$ are neither genuinely non-linear, neither linearly degenerate.

Rankine-Hugoniot conditions

In one dimension of space the RH conditions write

$$\begin{aligned}
 [\mathcal{M}] &= 0, \\
 \left[p + \frac{\mathcal{M}^2}{\rho} \right] &= 0, \\
 \left[\mathcal{M} \left(\frac{\mathcal{M}^2}{2\rho^2} + \varepsilon + \frac{p}{\rho} + \frac{1}{2} \frac{\varkappa^2}{\rho^2} j^2 \right) + \frac{\varkappa^2}{\rho} \theta j \right] &= 0, \\
 \left[\mathcal{M} \frac{j}{\rho} + \theta \right] &= 0,
 \end{aligned}$$

where we have defined the mass flux across the discontinuity front by $\mathcal{M} = \rho(u - \mathcal{D})$ and \mathcal{D} is the discontinuity speed.

Non-existence of contact discontinuity

On contact discontinuities, that is for $\mathcal{M} = 0$, one obtains by direct substitution

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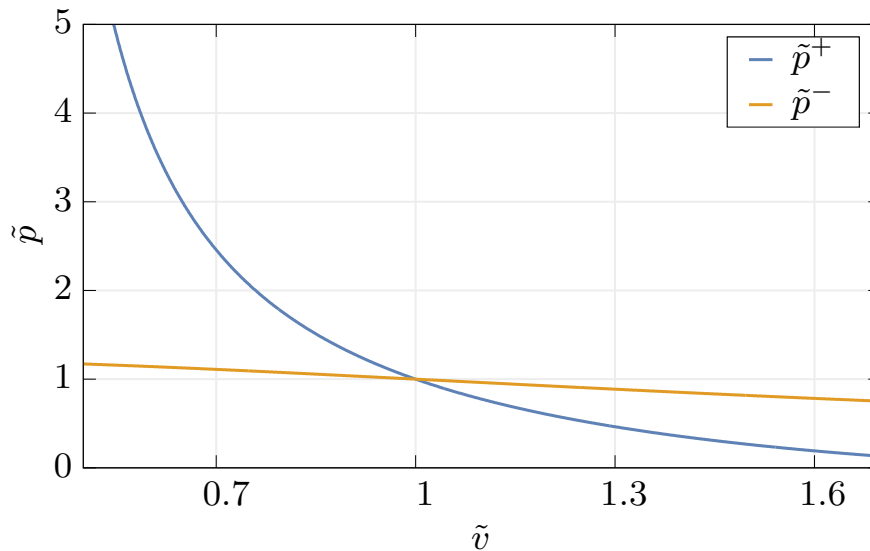
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Since p and θ are continuous across the discontinuity, the density will be as well. Thus:

$$[\rho] = 0, \quad [u] = 0, \quad [\eta] = 0, \quad [j] = 0,$$

Therefore solution is continuous: no contact discontinuities are admissible in this case.

Hugoniot Locus (polytropic gas equation of state)



Study of the Hugoniot curves shows interesting possible solutions:

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

Compound shocks

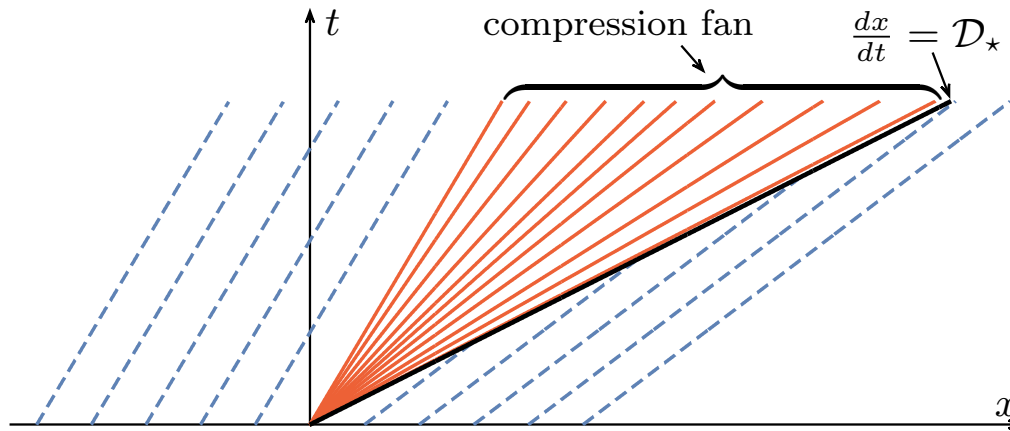


Figure 2: Schematic representation of the wave pattern in the $x - t$ plane, for a compound shock splitting solution. The shock propagates to the right, followed by a right facing compression fan.

Recovery of Fourier law: Shock tube problem

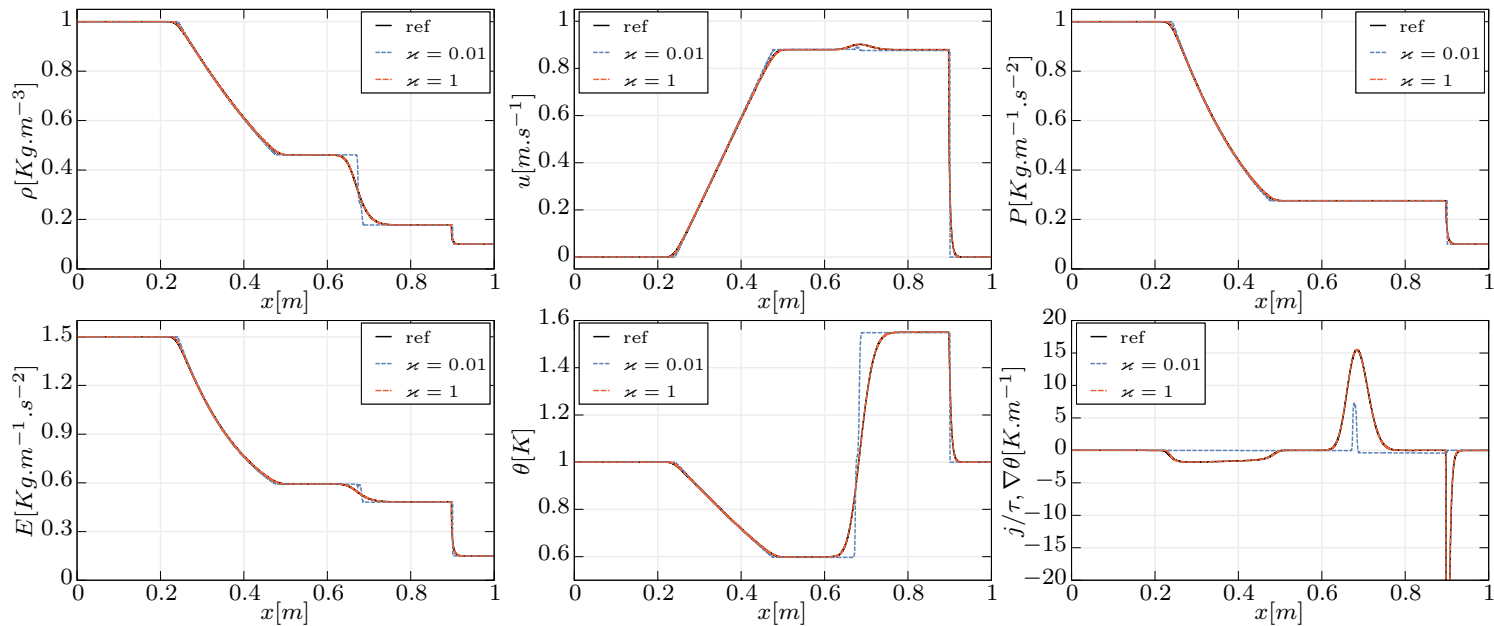


Figure 3: Shock tube with heat conduction. The solution is given at final time $t = 0.2$. Parameters: $\text{CFL} = 0.9$, $\gamma = 5/3$, $c_V = 3/2$, $K = 10^{-3}$. Relaxation time is taken as $\tau = \frac{K}{\alpha(\rho_0)\theta(\rho_0, \eta_0)}$

Expansion shock solution

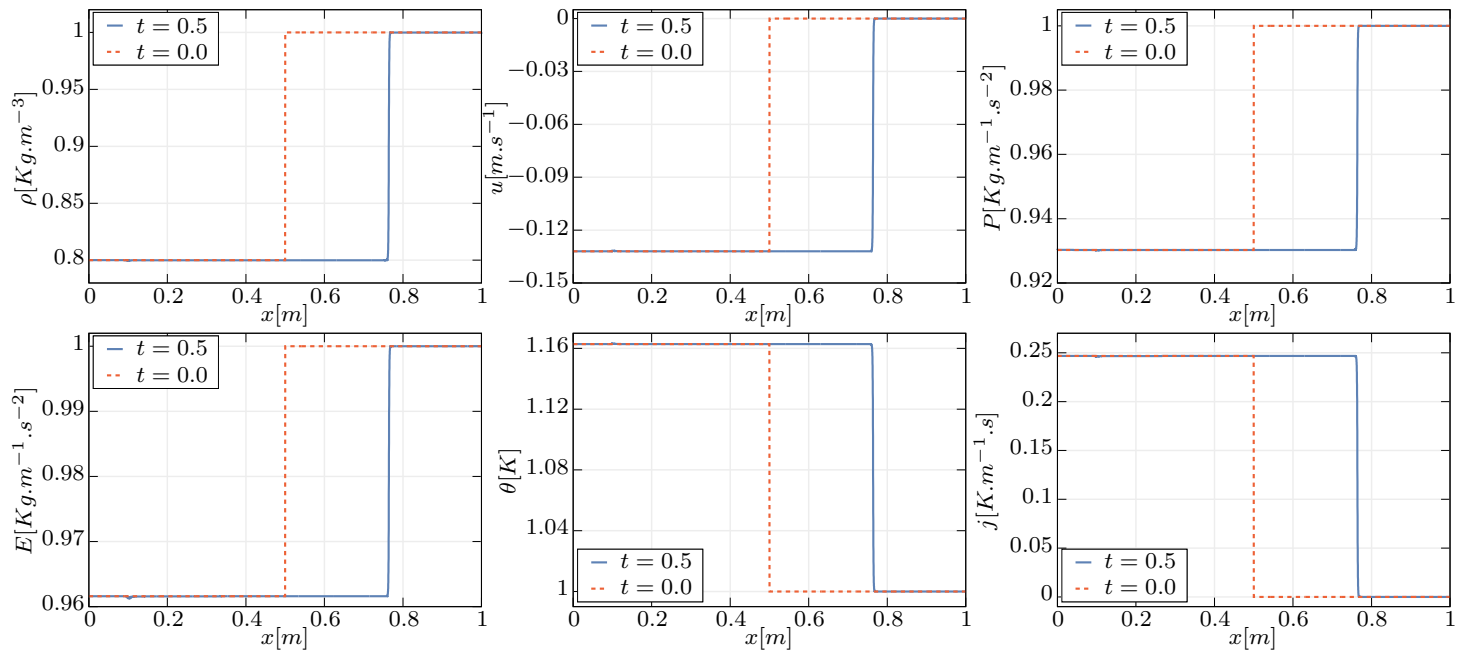


Figure 4: Numerical result for an expansion shock solution on the computational domain $[0, 1]$, discretized over $N = 10000$ cells displayed at final time $t = 0.5$. Parameters: $\text{CFL} = 0.9$, $\gamma = 2$, $c_V = 1$, $\varkappa = 0.8$.

Compression fan

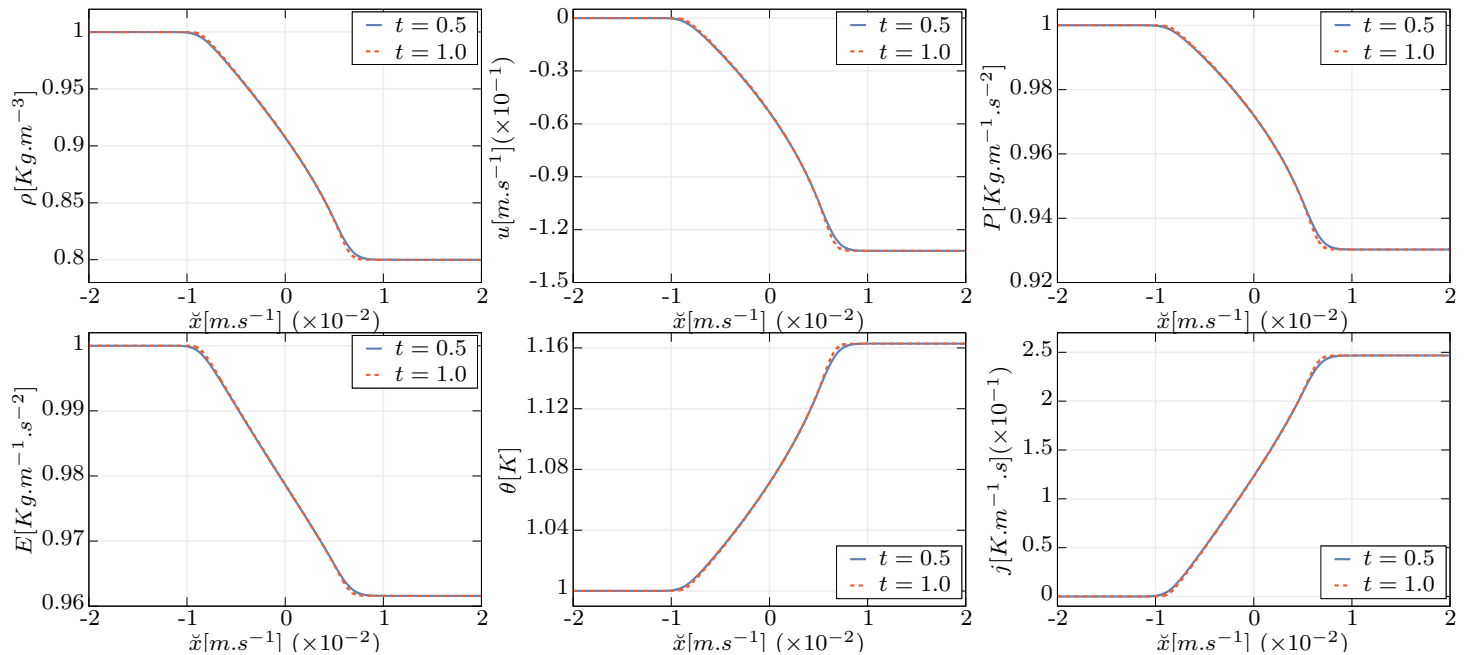


Figure 5: Numerical result for a compression fan solution. Parameters: $CFL = 0.9$, $\gamma = 2$, $c_V = 1$, $\varkappa = 0.8$

Compound shock solution

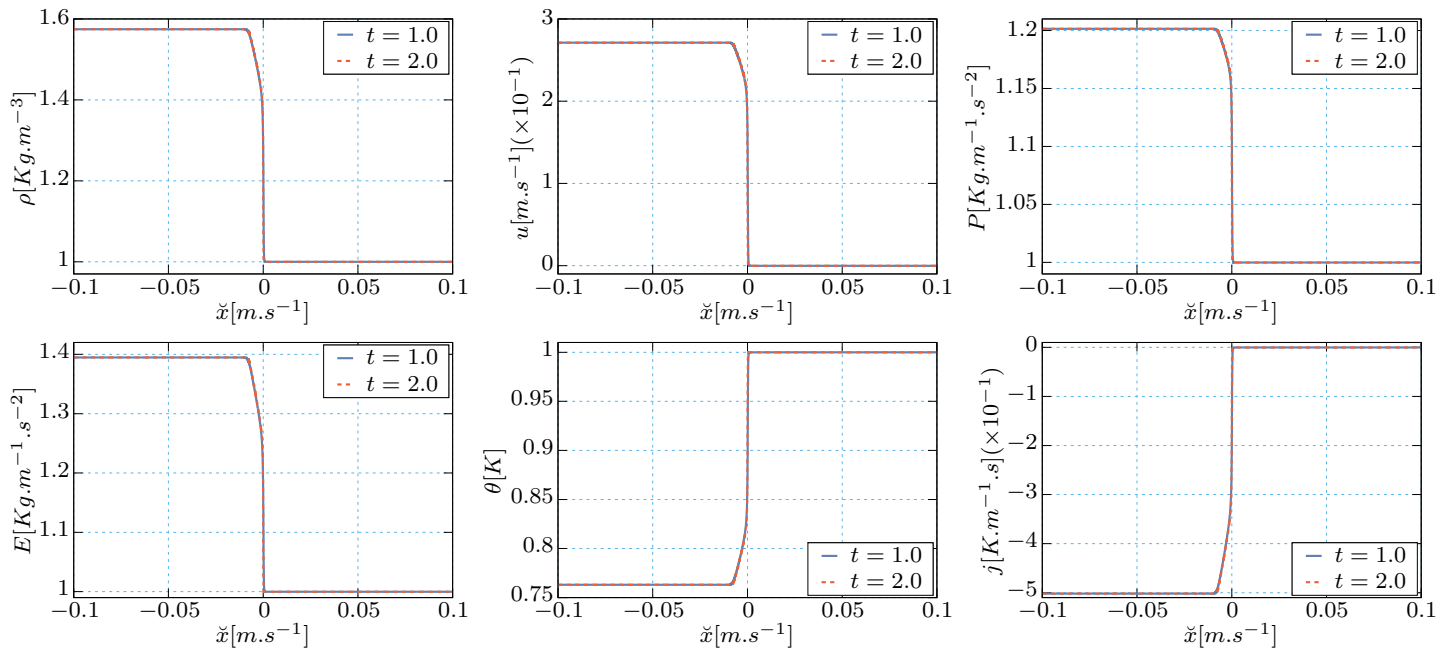


Figure 6: Compound shock plotted as a function of the self-similar coordinate $\check{x} = (x - D_{\star}t)/t$. CFL = 0.9, $\gamma = 2$, $c_V = 1$, $\varkappa = 1.3$.

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- Multi-D simulations (accounting for curl-involutions, etc)
- Rigorous Justification of the relaxation limit
- Further optimization at the numerical level (semi-implicit discretization, etc)
- Further study of the Riemann problem.

Thank you for your attention !

[1] Dhaouadi, Firas, and Sergey Gavriluk. "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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