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On Hyperbolicity of Moment Equations

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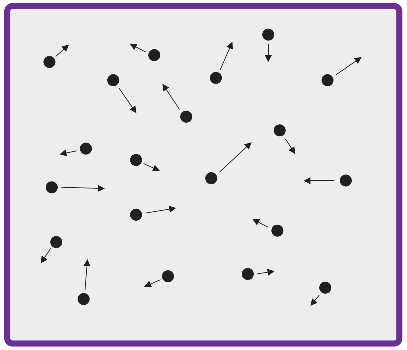
Acknowledgement: Supported by the European Science Foundation (ESF) - EURYI Award 2006

Kinetic Theory

- provides a general modeling framework for multi-scale micro-macro-transitions

Micro-World



stochastic description
distribution function $f(\mathbf{x},t,\mathbf{c})$

mathematical transition

Macro-World

fluid dynamic description with
fields $\rho(\mathbf{x},t), \mathbf{v}(\mathbf{x},t), \theta(\mathbf{x},t)$ etc.

- velocity distribution function $f : \Omega \times [0,\mathcal{T}] \times \mathbb{R}^3 \to \mathbb{R}$ follows (for gases) from

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \int_{\mathbb{R}^5} \left(f' \, f'^1 - f \, f^1 \right) \, g \, b \, db \, d\omega \, d\mathbf{c}_1$$

BOLTZMANN (1872)

- value $f(\mathbf{x},t,\mathbf{c})d\mathbf{c}$ gives the number density of particles with velocity in $[\mathbf{c},\mathbf{c}+d\mathbf{c}]$

Reduction to Moments

- general idea: complexity reduction $f(\mathbf{x}, t, \mathbf{c})\,,\ \mathbf{c} \in \mathbb{R}^3 \leftrightarrow \{F_{i_1 \ldots i_n}(\mathbf{x}, t)\}_{n=0,1,\ldots \mathrm{N}}$
- special spectral method with monomials $c_{i_1} c_{i_2} \cdots c_{i_n}$, $(n = 0,1,\ldots N)$ as test functions
- ansatz function for distribution $f(\mathbf{x}, t, \mathbf{c}) = f^{(\mathrm{model})}\left(\{\lambda_\alpha(\mathbf{x}, t)\}, \mathbf{c}\right) \qquad (|\alpha| = 0,1,\ldots N)$
- change of variables from $\{\lambda_\alpha\}$ to moments $F_{i_1 \ldots i_n} = m \int_{\mathbb{R}^3} c_{i_1} \cdots c_{i_n} \, f \, d\mathbf{c}$
- moment equations:

$$
\begin{aligned}
\left.\begin{aligned}
\partial_t F + \partial_i F_i &= 0 \\
\partial_t F_i + \partial_j F_{ij} &= 0 \\
\partial_t F_{kk} + \partial_i F_{ikk} &= 0
\end{aligned}\right\} &\ \text{conservation laws} \\
\partial_t F_{\langle ij \rangle} + \partial_k F_{\langle ij \rangle k} &= P_{ij} \\
\partial_t F_{ijk} + \partial_l F_{ijkl} &= P_{ijk} \\
\vdots \qquad &\ \ \vdots
\end{aligned}
$$

fluid varables:

$$
\begin{aligned}
F &= \rho \\
F_i &= \rho v_i \\
F_{kk} &= 3\rho\theta + \rho v_k^2 \\
F_{\langle ij \rangle} &\sim \sigma_{ij} \\
F_{ikk} &\sim q_i
\end{aligned}
$$

- hierachical structure: every flux is variable in the next equation

Closure Problem

- closure problem: higher moments, e.g., F_{ijk} or F_{ijkl} describe "fluxes of fluxes" and have to be computed from $f^{(\mathrm{model})}$
- final system of pdes: $$\partial_t U + \underbrace{\mathrm{div}\,\mathcal{F}(U)}_{\text{reversible part}} = \underbrace{\mathcal{P}(U)}_{\text{dissipation}}$$

Some Conditions on the Model

- should produce hyperbolic reversible part, representing microscopic transport

$$\partial_t U + \mathrm{div}\,\mathcal{F}(U) = 0 \quad \leftrightarrow \quad \partial_t f + c_i \partial_{x_i} f = 0$$

- should contain equilibrium (isotropic Gaussians)
- should respect Galilean invariance
- distribution properties: f positive and integrable
- physical richness: heat conduction, viscousity
- admits an entropy function
- should be easy to compute

Two Extreme Cases

- discrete velocity schemes $f^{(\text{discrete})}(\mathbf{c}) = \sum_{n=1}^{N} \lambda_n \, \delta(\mathbf{c} - \mathbf{c}^{(n)})$

⊕ hyperbolicity

⊖ equilibrium not contained

⊖ no Galilean invariance

⊕ easy to compute

⊖ many degrees of freedom needed

⊕ physical richness

- Euler equations of gas dyamics $f^{(\text{Maxwell})}(\mathbf{c}) = \frac{\rho/m}{\sqrt{2\pi\theta}^3} \exp\left(-\frac{(\mathbf{c}-\mathbf{v})^2}{2\theta}\right)$

- based on density, velocity, temperature

$$\rho = m \int f(\mathbf{c})\, d\mathbf{c}, \quad \rho v_i = m \int c_i \, f(\mathbf{c})\, d\mathbf{c}, \quad \frac{3}{2}\rho\theta = m \int \frac{1}{2}(\mathbf{c}-\mathbf{v})^2 f(\mathbf{c})\, d\mathbf{c}$$

⊕ hyperbolicity

⊕ contains equilibrium

⊕ Galilean invariance

⊕ easy to compute

⊕ very few degrees of freedom

⊖ physical richness

Grad's Moment-Equations

- Hermite series expansion $f^{(\mathrm{Grad})}(\mathbf{c}) = f^{(\mathrm{Maxwell})}(\mathbf{c})\left(1 + \sum_{n=1}^{N} \lambda_{i_1 i_2 \cdots i_n} c_{i_1} c_{i_2} \cdots c_{i_n}\right)$
- non-linear in density, velocity, temperature through Maxwellian
- linear in non-equilibrium moments, e.g., pressure tensor, heat flux (with $\mathbf{C} = \mathbf{c} - \mathbf{v}$)

$$p_{ij} = m \int C_i C_j \, f(\mathbf{C}) \, d\mathbf{C}, \quad q_i = m \int \frac{1}{2} \mathbf{C}^2 C_i \, f(\mathbf{C}) \, d\mathbf{C}$$

- variables $(\rho, v_i, \theta, p_{ij}, q_i)$ give "Grad's 13-moment-equations"

⊖ hyperbolicity

⊕ contains equilibrium

⊕ Galilean invariance

⊖ distribution negative

⊕ easy to compute

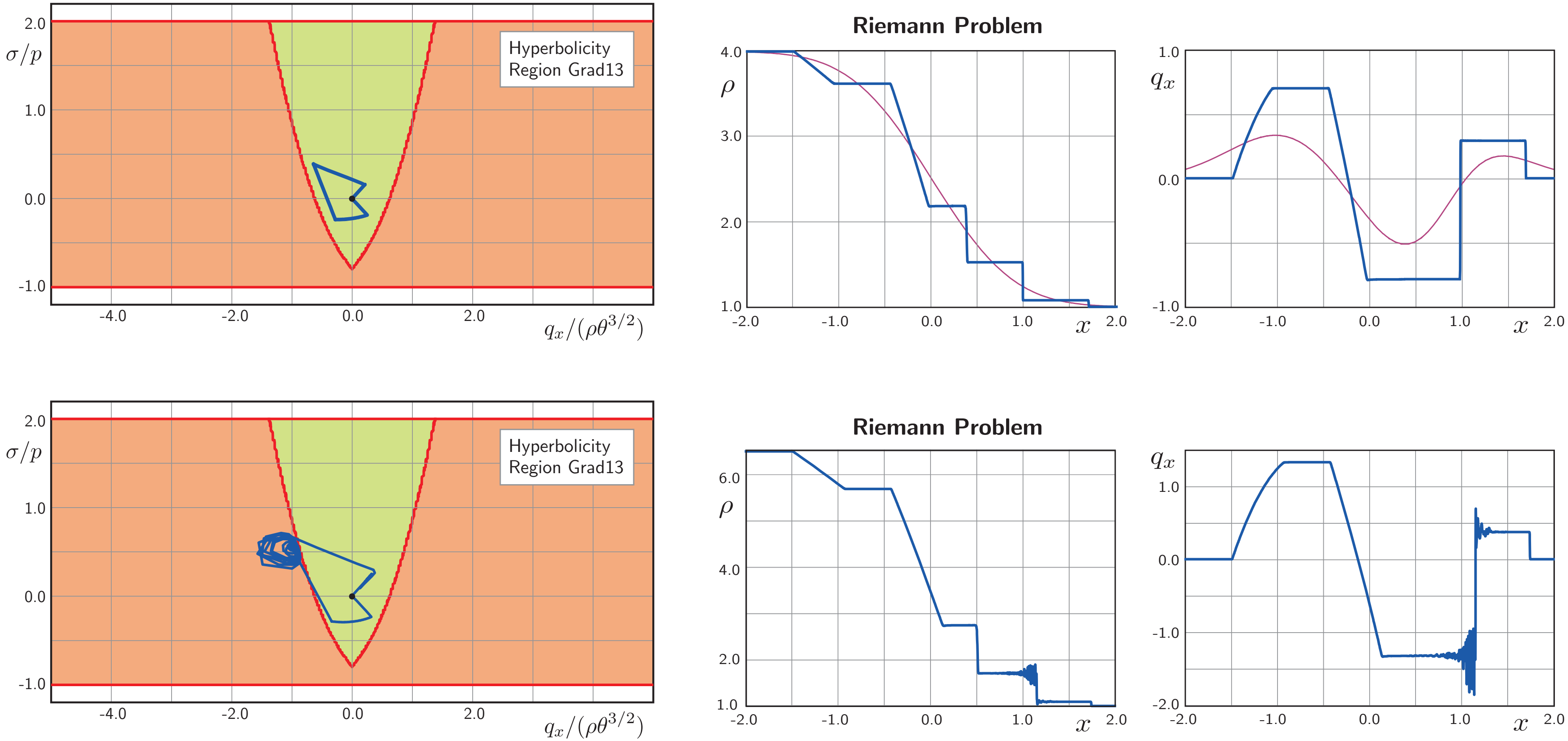
⊕ very few degrees of freedom

⊕ physical richness

⊖ no entropy

Grad13: Loss of Hyperbolicity

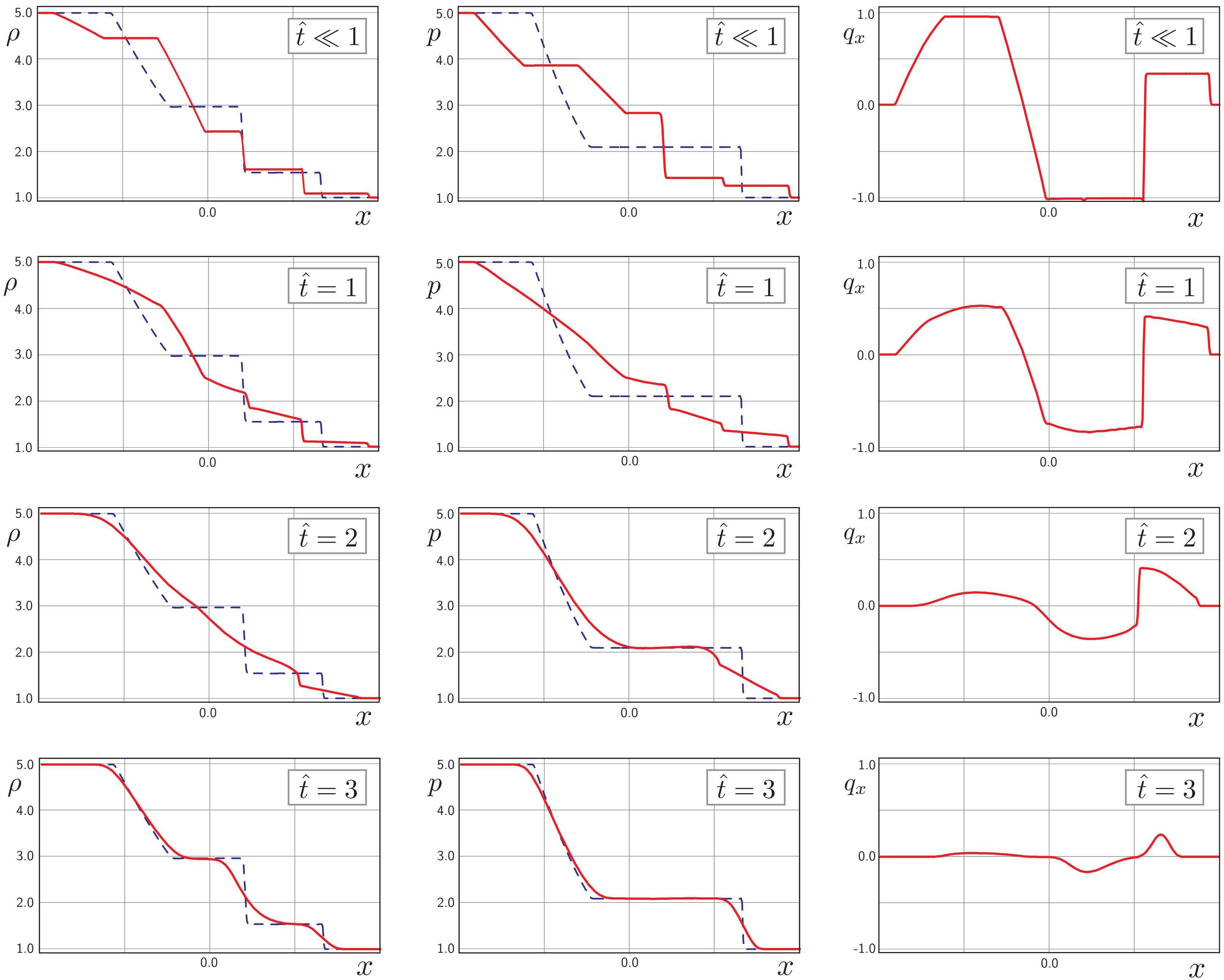
- test reversible part, i.e., homogeneous equations, on Riemann problems (shock tube)
- hyperbolicity is given only close to equilibrium (linear regime)



lack of hyperbolicity is crucial in strong non-equilibrium, non-linear, high-velocity processes (e.g., hypersonics), and for robustness of numerical simulations

Grad13: Waves and Dissipation

- comparison with Euler-solution:
- dissipation damps the wave for large times



Maximized Entropy Distribution

DREYER (1985)

- constrained entropy maximization yields $f^{(\mathrm{ME})}(\mathbf{c}) = \exp\left(1 + \sum_{n=1}^{N} \lambda_{i_1 i_2 \cdots i_n} c_{i_1} c_{i_2} \cdots c_{i_n}\right)$
- LEVERMORE (1996) worked out a formal theory including hyperbolicity and entropy
- JUNK (1998) showed that the mapping $\{F_\alpha\} \leftrightarrow \{\lambda_\alpha\}$ is highly ill-conditioned even close to equilibrium

⊕ hyperbolicity	⊖ extremely complicated to compute
⊕ contains equilibrium	⊕ very few degrees of freedom
⊕ Galilean invariance	⊕ physical richness
? distribution integrable	⊕ entropy

- the case $N = 2$ is feasible (Gaussian 10-moment-case), but does not contain heat conduction

⊕ hyperbolicity	⊕ easy to compute
⊕ entropy	⊖ physical richness

Pearson-Type-IV Distribution in 1D

PEARSON (1895)/(1901)/(1916)

- Pearson in 1D uses a translation λ, a scale a, a skewness ν, and a shape factor m

$$f^{(\mathrm{P1})}(c\,;\lambda,a,m,\nu) = \frac{1}{a\,k}\,\frac{\exp\left(-\nu\,\arctan\left(\frac{c-\lambda}{a}\right)\right)}{\left(1+\left(\frac{c-\lambda}{a}\right)^2\right)^m} \qquad (k \text{ norm. constant})$$

- moments $\mu_n = \int_{-\infty}^{\infty} (c-v)^n\, f^{(\mathrm{P1})}(c)\,dc$ can be computed analytically

- they satisfy the recursion $\mu_n = \frac{a(n-1)}{r-(n-1)}\left(\left(1+\left(\frac{\nu}{r}\right)^2\right)a\,\mu_{n-2} - \frac{2\nu}{r}\mu_{n-1}\right)$

- define variance $\theta = \mu_2$ and scaled moments $Q = \frac{\mu_3}{\mu_2^{3/2}}$, $\;D = \frac{\mu_4}{\mu_2^2}$

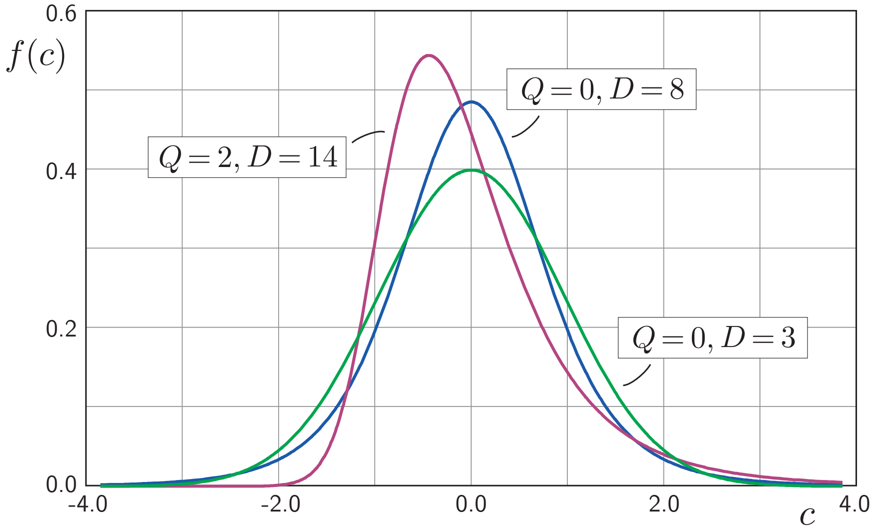
- all parameters can be computed explicitly from the first moments

$$r = 2(m-1) = \frac{6(D-Q^2-1)}{2D-3Q^2-6} \qquad \nu = -\frac{r(r-2)Q}{\sqrt{16(r-1)-Q^2(r-2)^2}}$$

$$a = \sqrt{\theta}\sqrt{r-1-\tfrac{1}{16}Q^2(r-2)^2} \qquad \lambda = v - \tfrac{1}{4}(r-2)Q\sqrt{\theta}$$

Pearson-Type-IV Distribution in 1D

- examples of Pearson distributions:



- for $Q=0,\ D=3$ (i.e., $\nu=0,\ m\to\infty$) Pearson-IV-distribution reduces to a Gaussian

$$\lim_{m\to\infty} f^{(\mathrm{P1})}(c;\lambda,a,m,0) = \lim_{m\to\infty} \frac{1}{a\,k}\frac{1}{\left(1+\left(\frac{c-\lambda}{a}\right)^2\right)^m} = \frac{1}{\sqrt{2\pi\theta}}\exp\left(-\frac{(c-\lambda)^2}{2\theta}\right)$$

- for $m<\infty$ the distribution is heavy-tailed

Model-Problem: Kinetic Theory in 1D

- one-dimensional particle velocity space $\partial_t f + c\,\partial_x f = 0 \quad (c \in \mathbb{R})$
- consider moments $m\int_{-\infty}^{\infty}(c-v)^n f(c)\,dc$ denoted by $\big(\rho, v, \theta, q, \Delta, R\big)$
- with moment system:

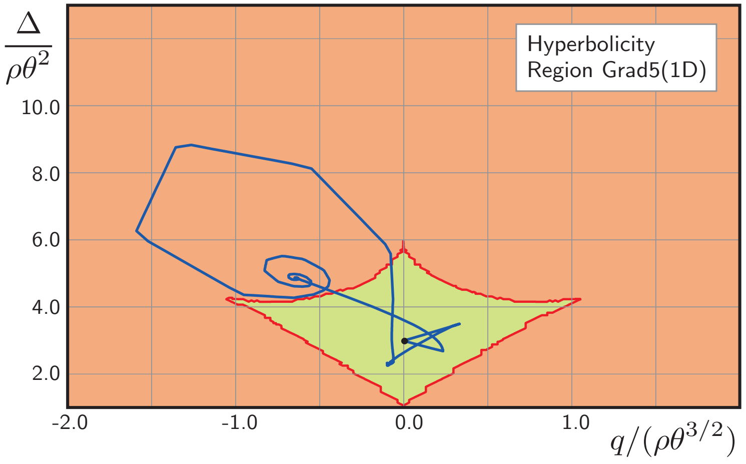
$$
\begin{aligned}
\partial_t \rho + \partial_x \rho v &= 0\\
\partial_t \rho v + \partial_x \left(\rho v^2 + \rho\theta\right) &= 0\\
\partial_t \left(\rho v^2 + \rho\theta\right) + \partial_x \left(\rho v^3 + 3\rho\theta\, v + q\right) &= 0\\
\partial_t \left(\rho v^3 + 3\rho\theta v + q\right) + \partial_x \left(\rho v^4 + 6\rho\theta\, v^2 + 4q\, v + \Delta\right) &= 0\\
\partial_t \left(\rho v^4 + 6\rho\theta\, v^2 + 4\, q\, v + \Delta\right) + \partial_x \left(\rho v^5 + 10\rho\theta\, v^3 + 10 q\, v^2 + 5\Delta\, v^2 + R\right) &= 0
\end{aligned}
$$

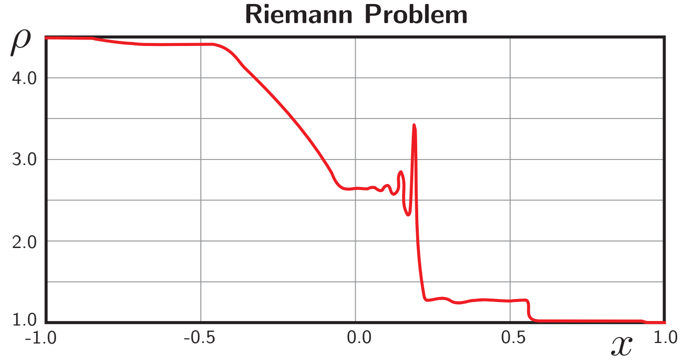
- Grad closure $R^{(\mathrm{Grad})} = 10\,\theta\, q$
- Pearson closure $R^{(\mathrm{Pearson5})}(Q,D) = 2\,\theta\, q\,\dfrac{D^2 - 3Q^2 + 7D}{3Q^2 - D + 9}$

  with scaled moments $Q = \dfrac{q}{\rho\theta^{3/2}},\ D = \dfrac{\Delta}{\rho\theta^2}$

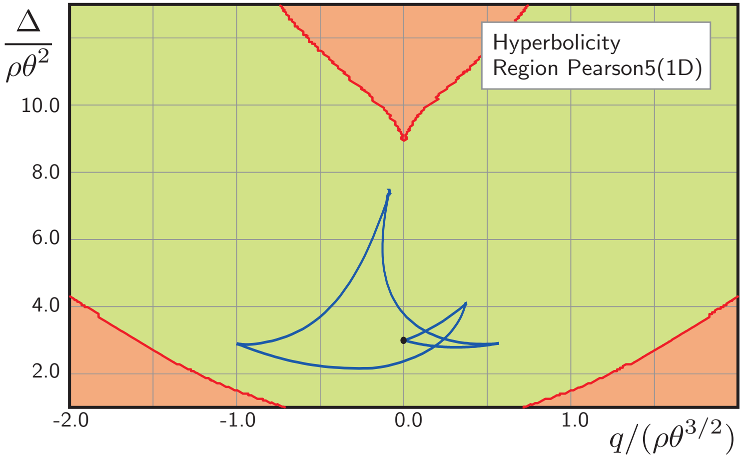
1D-Kinetic Theory: Riemann Problem

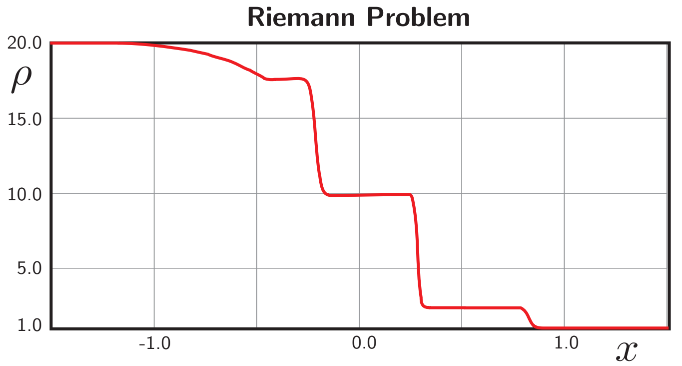
- the Grad closure shows loss of hyperbolicity





- Pearson extends the hyperbolicity region and allows stronger Riemann problems



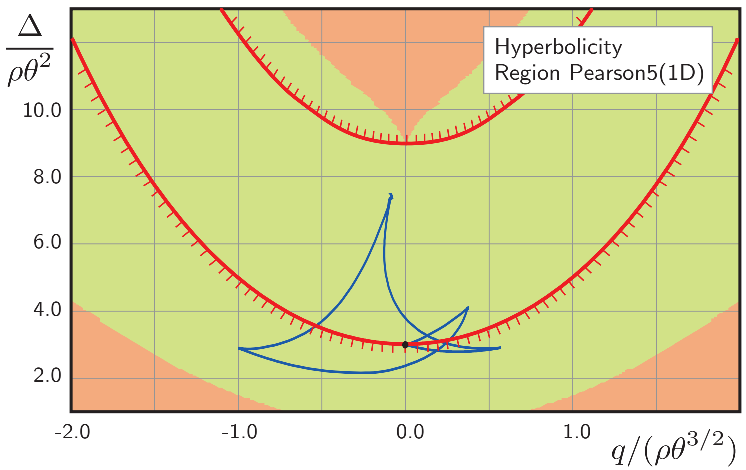


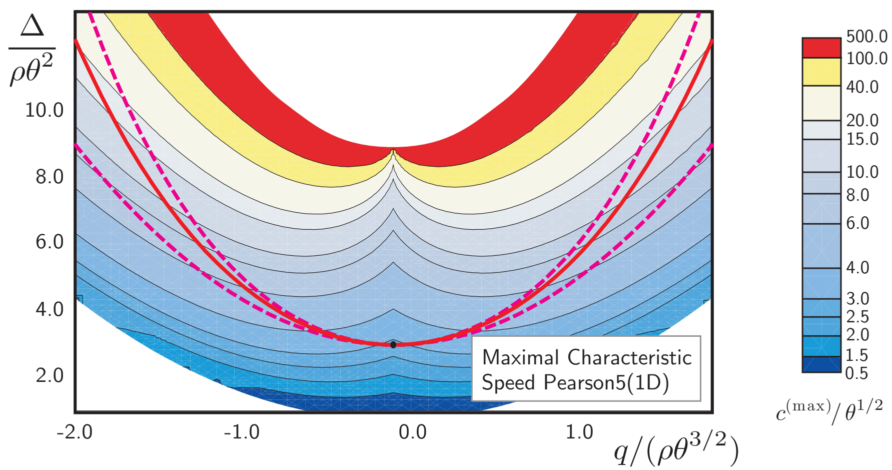
1D-Kinetic Theory: Pearson Realizability

- closure relation remains finite only for $m > 3$, i.e., $D < 9 + 3Q^2$
- maximal characteristic speed becomes infinite (robust loss of hyperbolicity)
- Pearson distribution is realizable only for moments satisfying $\nu \in \mathbb{R}$, i.e.,

$$D \geq D^{(\mathrm{crit})} = \frac{48 + 39Q^2 + 6\sqrt{(4+Q^2)^3}}{32 - Q^2} \qquad |Q| < \sqrt{32}$$

- realizability is ignored by solution of the moment system



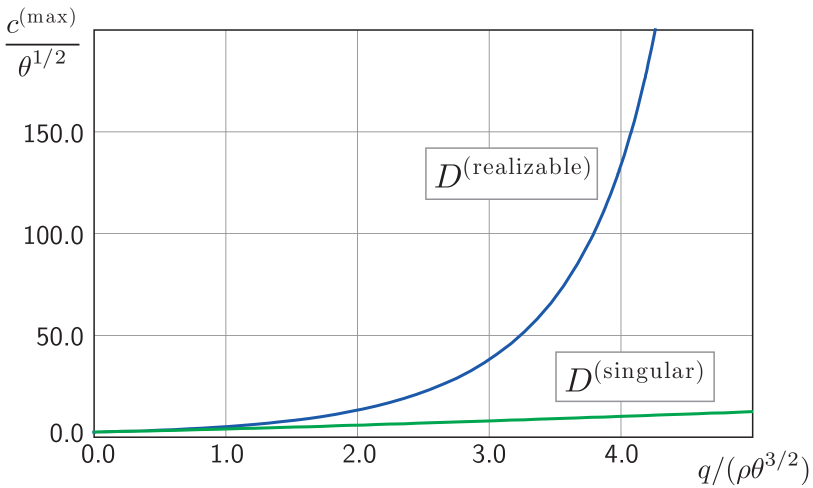


- idea: reduce moment system by one variable and slave Pearson parameter

$$D = D^{(\mathrm{closure})}(Q)$$

1D-Kinetic Theory: Parameter Slaving

- set of variables (ρ, v, θ, q) with closure $\Delta(\rho, \theta, q) = \rho\theta^2 D^{(\mathrm{closure})}\left(q/(\rho\theta^{3/2})\right)$
- Grad closure: $D^{(\mathrm{Grad})} = 3$ with hyperbolicity $\left|\frac{q}{\rho\theta^{3/2}}\right| \lesssim 0.9$
- realizable closure: $D^{(\mathrm{realizable})} = 3(1 + Q^2\frac{22+Q^2}{32-Q^2})$ with hyperbolicity $\left|\frac{q}{\rho\theta^{3/2}}\right| < \sqrt{32}$
- singular closure: $D^{(\mathrm{singular})} = 3(1 + \frac{1}{2}Q^2)$ with hyperbolicity $\left|\frac{q}{\rho\theta^{3/2}}\right| < \infty$
- the singular closure formally corresponds to Pearson distributions with exponential decay



Extension: Pearson-Type-IV in 3D

- Pearson in 3D uses a translation $\boldsymbol{\lambda} \in \mathbb{R}^3$, a scale tensor $\mathbf{A} \in \mathbb{R}^{3\times 3}$, a skewness and a shape factor $\nu, m \in \mathbb{R}$, and a direction of skewness $\mathbf{n} \in S^2$

$$f^{(\mathrm{P3})}\left(\mathbf{c}\,;\boldsymbol{\lambda},\mathbf{A},m,\nu,\mathbf{n}\right) = \frac{1}{\det\left(\mathbf{A}\right)K}\,\frac{\exp\left(-\nu\ \arctan\left(\mathbf{n}^T\mathbf{A}^{-1}\left(\mathbf{c}-\boldsymbol{\lambda}\right)\right)\right)}{\left(1+\left(\mathbf{c}-\boldsymbol{\lambda}\right)^T\mathbf{A}^{-2}\left(\mathbf{c}-\boldsymbol{\lambda}\right)\right)^m} \qquad (K \text{ norm. constant})$$

- all moments can be explicitly computed, for example (with $N_i = \Theta^2_{ij} n_j$)

$$\Theta_{ij} = \frac{1}{2m-5}\left(1+\left(\frac{\nu}{2m-4}\right)^2\right)A^2_{ij}$$

$$M_{ijk} = \frac{1}{2}Q\left(-N_iN_jN_k + 3\,N_{(i}\,\Theta_{jk)}\right)$$

$$M_{ijkl} = \left(D-\frac{3}{4}Q^2\right)\Theta_{(ij}\Theta_{kl)} + \frac{3}{4}Q^2\left(-N_iN_jN_kN_l + 2N_{(i}N_j\Theta_{kl)}\right)$$

- analogously to 1D we have a mapping of the parameters $(Q,D) \leftrightarrow (\nu,m)$

- for $\nu = 0,\ m \to \infty$ Pearson $f^{(\mathrm{P3})}$ reduces to the Gaussian 10-moment distribution

Pearson13 Closure

- including density, the Pearson distribution in 3D has 14 parameter
- choose 13 moments $(\rho, v_i, \theta, p_{ij}, q_i)$, the remaining parameter is slaved for realizability
- temperature tensor is given by $\Theta_{ij} = p_{ij}/\rho$
- the parameters Q and n_i follow from the non-linear equation

$$q_i = \frac{\rho}{2} Q\, \Theta_{ij}^{1/2} \left(\tfrac{1}{2} \left(3\theta - n_l \Theta_{lm} n_m\right) \delta_{jk} + \Theta_{jk} \right) n_k$$

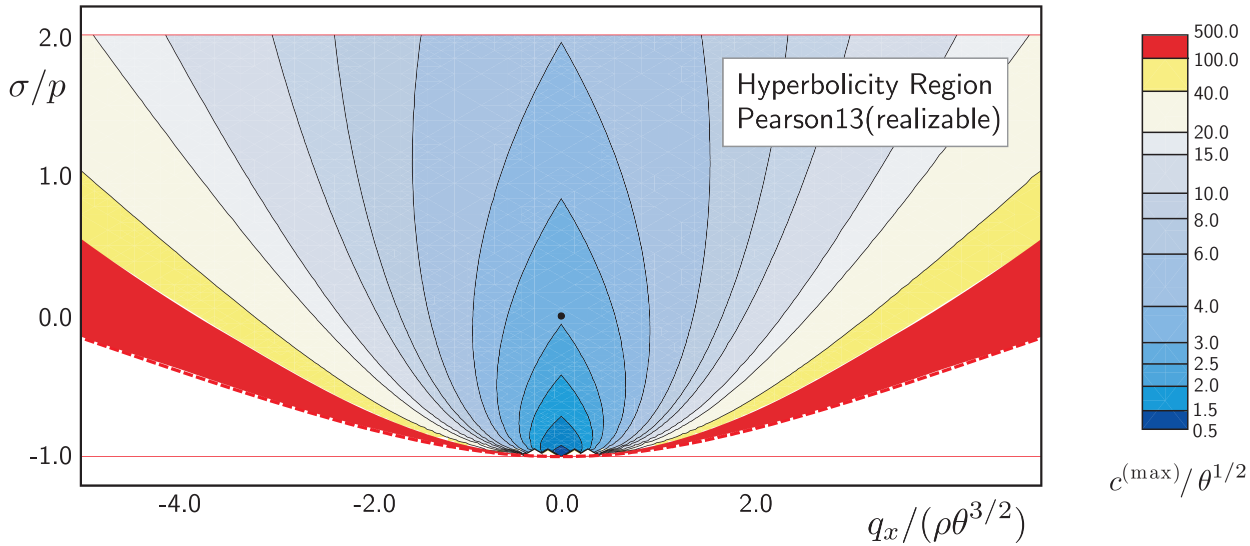
- the parameter D follows from $D = D^{(\text{closure})}(Q)$
- explicit closure relations for 13-moment-equations

$$\begin{aligned} m_{ijk}^{(\text{Pearson13})} &= \frac{\rho}{2} Q \left(- N_i N_j N_k + 3\, N_{(i}\, \Theta_{jk)} \right) \\ R_{ij}^{(\text{Pearson13})} &= \rho \left(D - \tfrac{3}{4} Q^2 \right) \left(\Theta_{ij} \theta + \tfrac{2}{3} \Theta_{ij}^2 \right) \\ &\quad + \rho \tfrac{1}{4} Q^2 \left(3 \left(\theta - \mathbf{N}^2 \right) N_i N_j + \mathbf{N}^2 \Theta_{ij} + 4 N_k \Theta_{k(i} N_{j)} \right) \end{aligned}$$

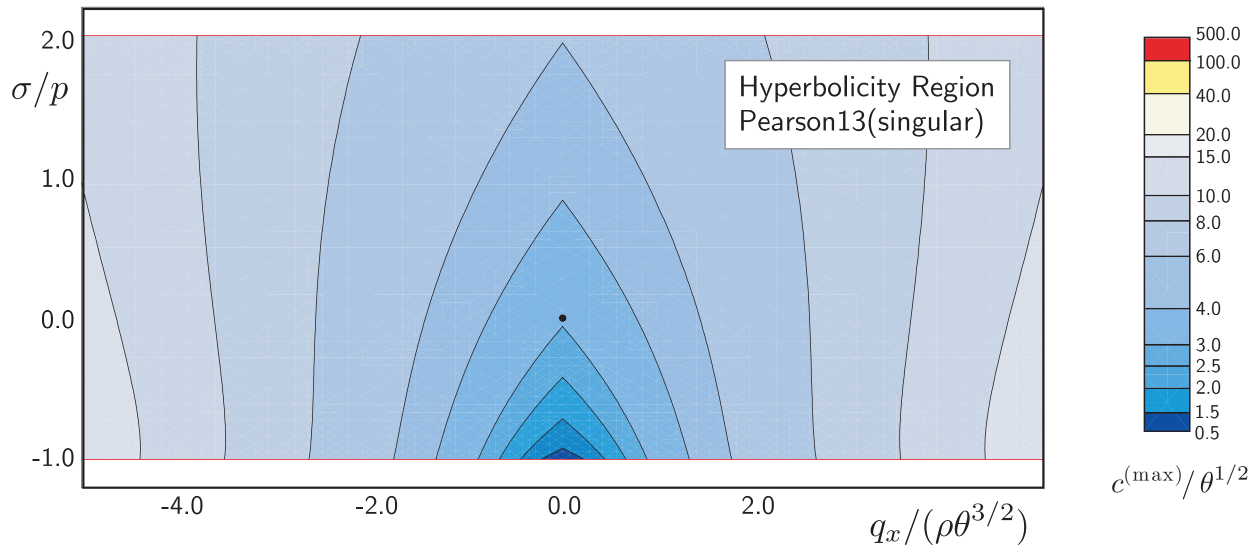
Pearson-Closure: Hyperbolicity

- contours show maximal characteristic speed of the system

- realizable closure shows robust loss of hyperbolicity for extreme values

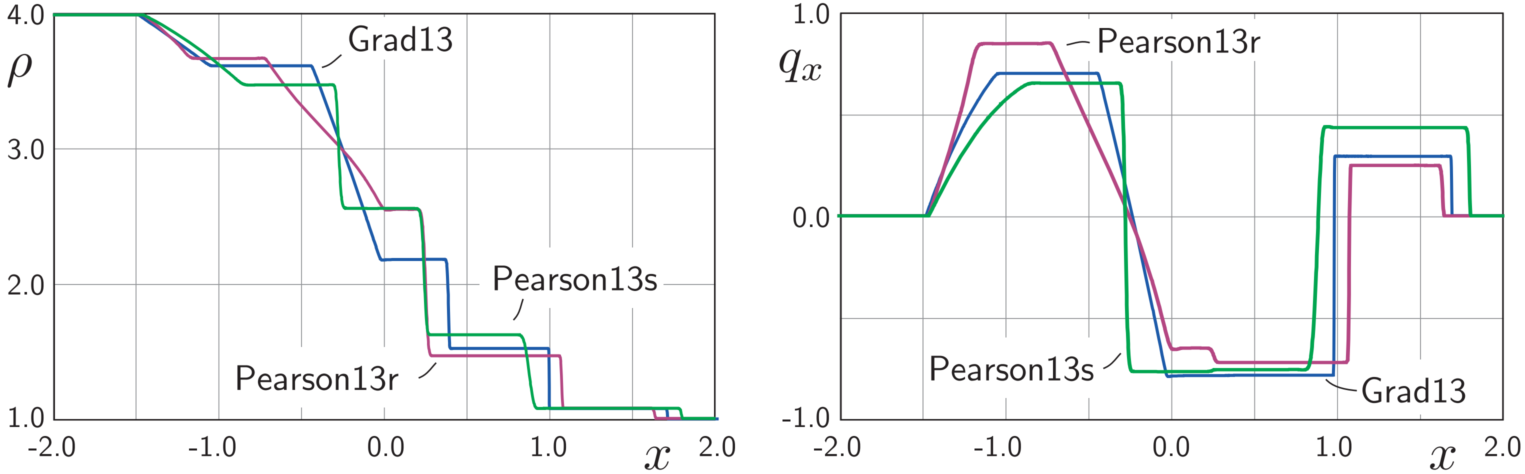


- singular closure remains hyperbolic apparently for all physical variable states



Pearson-Grad Comparison

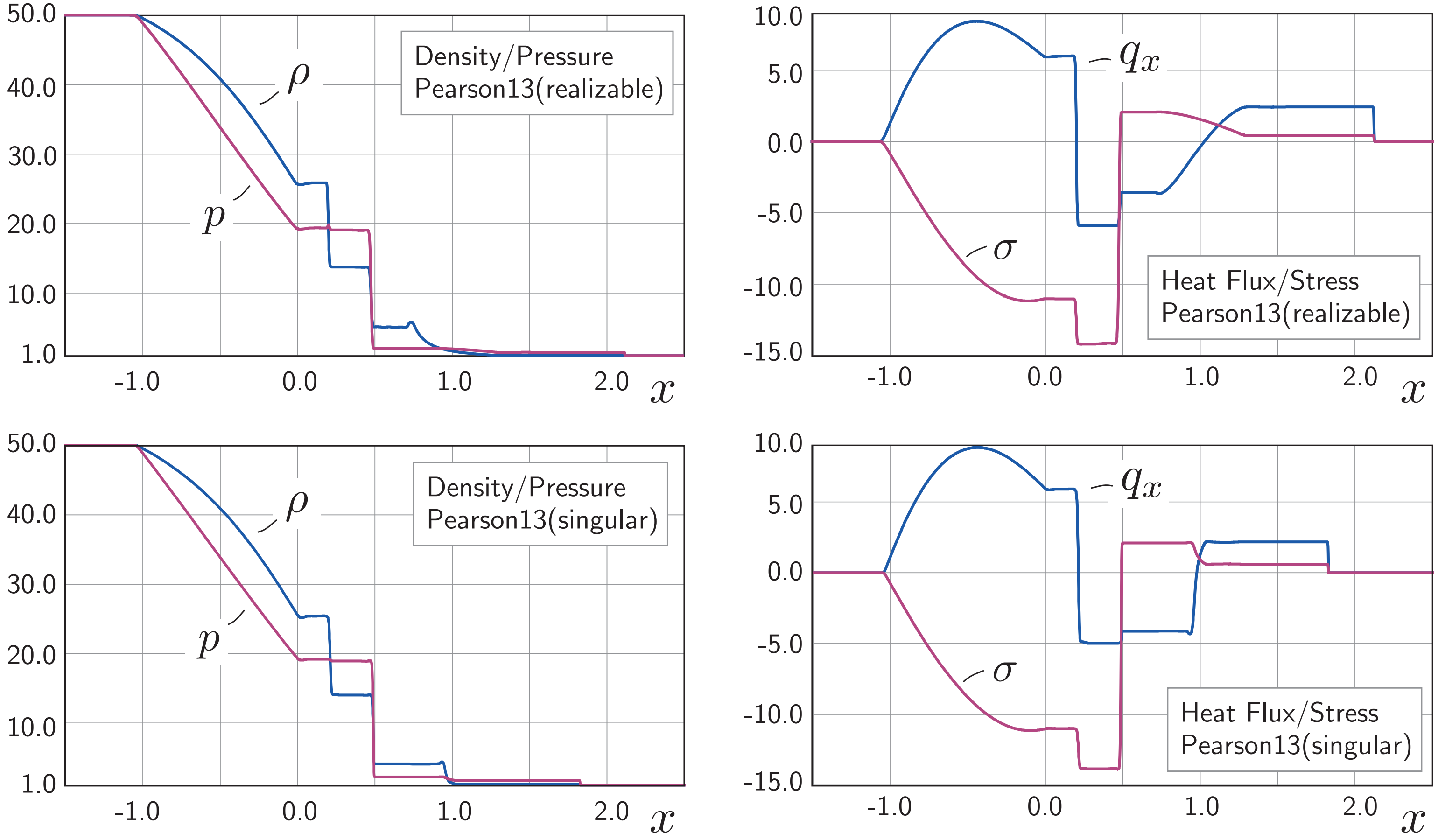
- for a weak Riemann problem comparison between Pearson and Grad is possible
- roughly identical wave structure, but differences in details



- in one space dimension the Pearson closure can be shown to reduce to Grad close to equilibrium

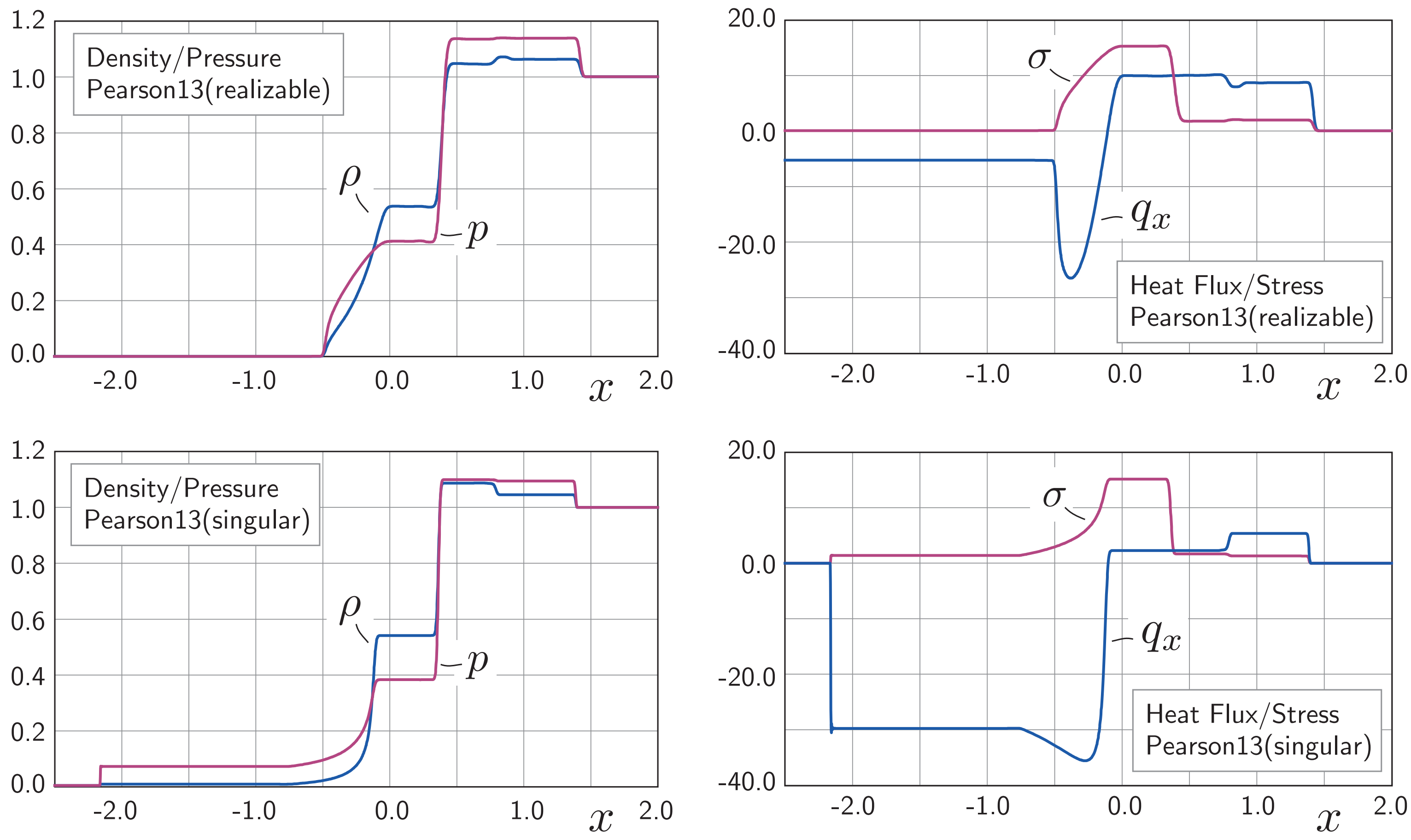
Riemann Problem: Shock Tube

- shock tube problem with initially zero velocity, constant temperature, strong density jump
- the realizable closure shows a faster wave to the right

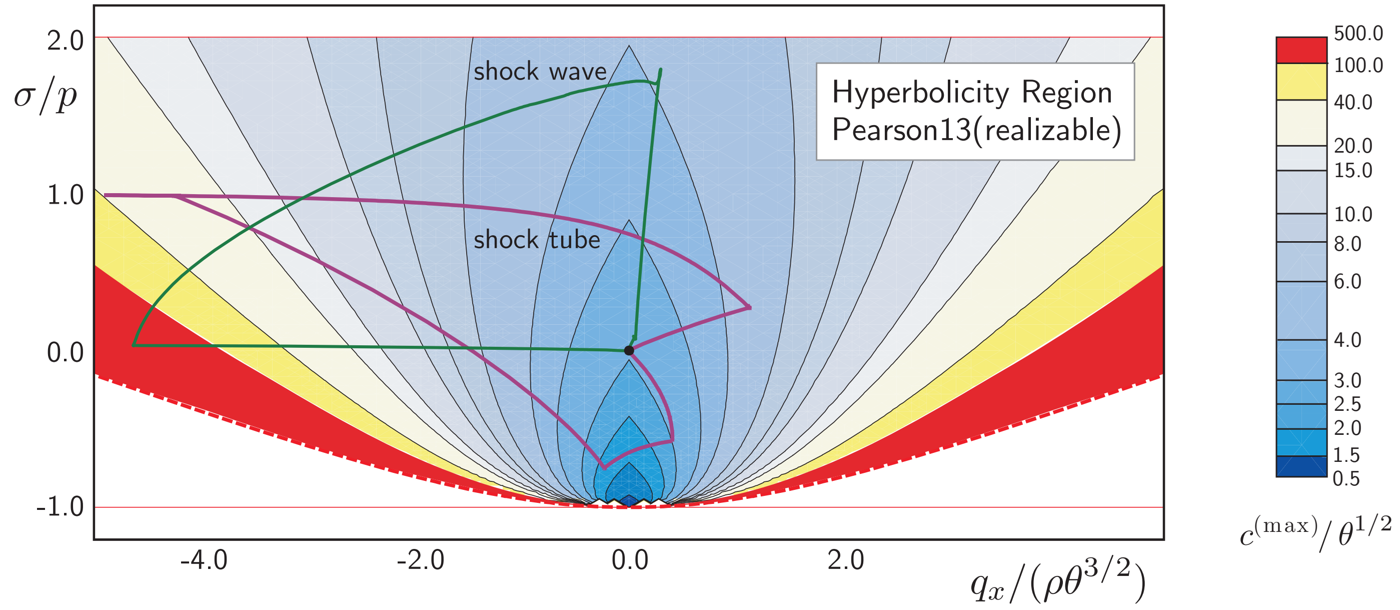


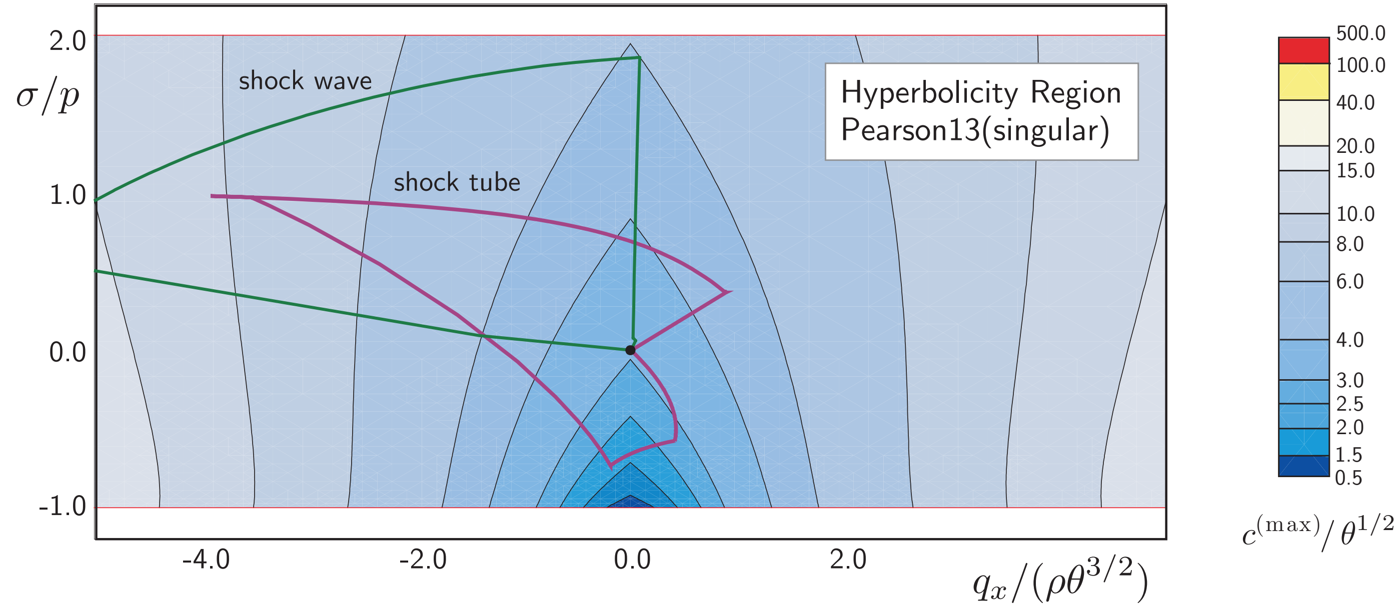
Riemann Problem: Shock Wave

- Rieman problem with initial Rankine-Hugoniot conditions for a $M_0 = 4$ shock wave
- pressure and density profiles normalized
- realizable closure exhibits a very fast wave requiring a 20x stronger CFL condition than the singular closure



Hyperbolicity Regions





Conclusions and Outlook

- Pearson offers a hyperbolic alternative to Grad which is fully explicit in contrast to maximum-entropy
- in the realizable regime Pearson is based on a positive and integrable distribution which admits an entropy $\eta = \int f \ln f \, d\mathbf{c}$

⊕ hyperbolicity	⊕ easy to compute
⊕ contains equilibrium	⊕ very few degrees of freedom
⊕ Galilean invariance	⊕ physical richness
⊕ positive distribution	⊕ entropy

- there is some trade-off between realizability and hyperbolicity
- equations need to be investigated and tested in two and more space dimensions