KINETIC RELATIONS FOR UNDERCOMPRESSIVE SHOCKS.
Physical, mathematical, and numerical issues

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Hyperbolic or hyperbolic-elliptic systems of conservation laws with singular perturbation (diffusion, dispersion, etc)

$$u_t^\varepsilon + f(u^\varepsilon)_x = R(\varepsilon u_x^\varepsilon, \varepsilon^2 u_{xx}^\varepsilon, \ldots)_x.$$

- Characterize the limit $u := \lim_{\varepsilon \to 0} u^\varepsilon$. Admissible discontinuities ?
- Second-order: $\alpha(\varepsilon)\, u_{xx}^\varepsilon$.
  Entropy conditions: Lax, Oleinik, Volpert, Kruzkov, Dafermos, Wendroff, TP Liu.
- Third order: $\beta(\varepsilon)\, u_{xxx}^\varepsilon$ and higher-order.
  Oscillations near shocks and competition between small scales.
- Classical compressive + nonclassical undercompressive shocks (or subsonic phase boundaries).

.... Entropy inequality supplemented with a kinetic relation.

PHYSICAL MODELS

- Complex flows. Van der Waals fluid, phase transitions, Nonlinear elasticity, thin liquid film, generalized Camassa-Holm, MHD with Hall effect.

TOWARD A MATHEMATICAL THEORY

- Nonclassical Riemann solver with entropy-compatible kinetics
- Kinetic functions determined by traveling waves
- Dafermos' self-similar regularization of the Riemann problem
- Existence via Glimm-type scheme with generalized TV functionals
- Zero diffusion-dispersion limits for the initial value problem

NUMERICAL APPROXIMATION

- Finite difference schemes with controled dissipation.
- Computing kinetic functions.

Typical model. Materials undergoing phase transitions

$$w_t - v_x = 0$$
$$v_t - \sigma(w)_x = \varepsilon\, v_{xx} - \lambda\, \varepsilon^2\, w_{xxx}$$

v : velocity $w > -1$: deformation gradient $\sigma(w)$: stress
ε : viscosity λ : capillarity

- Slemrod (1984, etc): self-similar solutions
- Shearer (1986, etc.): Riemann problem with $\lambda = 0$.
- Truskinovsky (1987, etc)
- Abeyaratne & Knowles (1990, etc): Riemann problem
- LeFloch (ARMA 1993, etc): mathematical formulation in BV, and Cauchy problem via Glimm scheme.

Active research on undercompressive shocks.

- **Collaborators.** Bedjaoui, Piccoli, Shearer, Joseph, Mohamadian, Laforest, Mishra. **(Former) postdocs and students** Hayes, Kondo, Baiti, Rohde, Mercier, Correia, Thanh, Chalons, Boutin.
- **Related works.** T.-P. Liu, Kulikovskij, Marchesin, Plohr, H.T. Fan, Corli-Tougeron, Benzoni, Metivier-Williams-Zumbrun, Colombo, Bertozzi-Shearer, Y. Wang.

Model with linear diffusion and dispersion.

- Conservation law (with $\alpha > 0$)

$$u_t + f(u)_x = \alpha\, u_{xx} + \beta\, u_{xxx}.$$

(Shearer et al., Hayes-PLF, Bedjaoui-PLF)

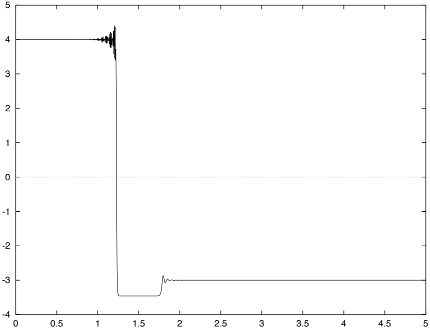
- Single entropy inequality:

$$\left(u^2/2\right)_t + F(u)_x = -D + C_x,$$
$$D := \alpha\, |u_x|^2 \geq 0, \qquad C := \alpha\, u u_x + \beta\left(u\, u_{xx} - (1/2) u_x^2\right).$$

In the (formal) limit $\alpha, \beta \to 0$ one gets $\left(u^2/2\right)_t + F(u)_x \leq 0$,
but no sign for general convex entropies!

- Classical/nonclassical solutions:
  - $\beta << \alpha^2$ (dominant diffusion): classical entropy solutions
  - $\beta >> \alpha^2$ (dominant dispersion): high oscillations, weak convergence (Lax, Levermore)
  - $\beta := \overline{\kappa}\, \alpha^2$ (balanced regime): strong convergence, mild oscillations, nonclassical, depend on $\overline{\kappa}$

$$u_t + (u^3)_x = 0$$



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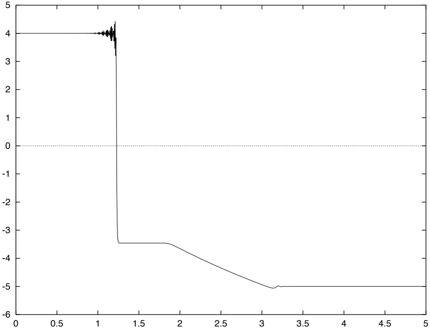


Two shocks — A shock + A rarefaction

The Riemann solutions are distinct from the ones selected by Oleinik's entropy inequalities.

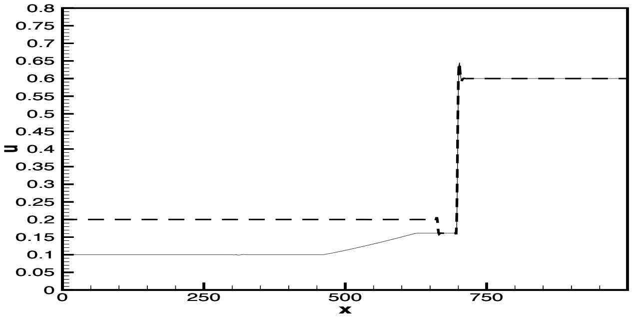
Thin liquid film model.

- Conservation law (with $\alpha, \gamma > 0$)

$$u_t + (u^2 - u^3)_x = \alpha\, u_{xx} - \gamma\, (u^3\, u_{xxx})_x$$

Effect of surface tension
(Bertozzi-Shearer, Zumbrun, Otto-Westdickenberg, PLF-Mohamadian)

- Single entropy inequality: $\left(u \log u - u\right)_t + F(u)_x = -D + C_x$
with $D = \gamma\, |(u^2\, u_x)_x|^2 \geq 0$, thus in the limit $\gamma \to 0$



Oscillations concentrated near shocks.

Generalized Camassa-Holm model.

- Conservation law (with $\alpha > 0$)

$$u_t + f(u)_x = \alpha\, u_{xx} + \beta\left(u_{txx} + 2u_x\, u_{xx} + u\, u_{xxx}\right)$$

Shallow water model for wave breaking
(Bressan-Constantin, Karlsen-Coclite, Raynaud, PLF-Mohamadian)

- Single entropy inequality:

$$\left((u^2 + \alpha\,|u_x|^2)/2\right)_t + F(u)_x = -\,\alpha\,|u_x|^2 + C_x.$$

Here, numerical solutions are similar to, but do not coincide with, the ones obtained with the linear diffusion-dispersion model.

Limiting solutions depend on the regularization.

Van der Waals fluids.

- Two conservation laws (also the energy equation may be included):

$$v_t - u_x = 0$$
$$u_t + p(v)_x = \big(\mu(v)\, u_x\big)_x + \Big(\lambda'(v)\, \frac{v_x^2}{2} - \big(\lambda(v)\, v_x\big)_x\Big)_x$$

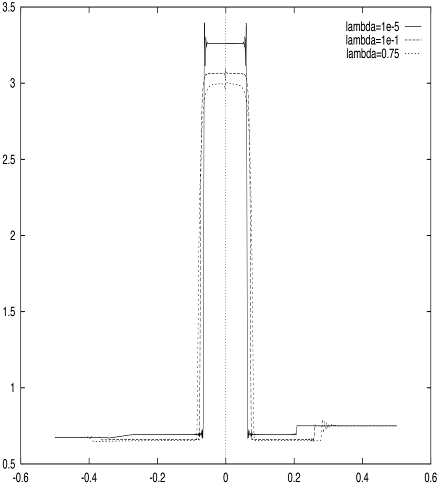
v : specific volume u : velocity
$\mu(v)$: viscosity $\lambda(v)$: capillarity

$p(v,T) = \frac{RT}{v-b} - \frac{a}{v^2}$. Hyperbolic when T sufficiently large. Of mixed type otherwise.

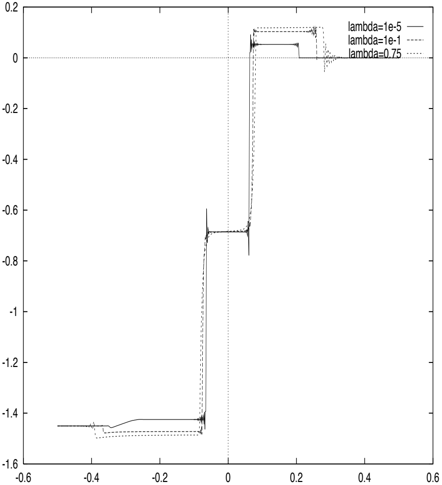
- Single entropy inequality:

$$\Big(\varepsilon(v) + \frac{u^2}{2} + \lambda(v)\, \frac{v_y^2}{2}\Big)_t + \big(p(v)\, u\big)_x = -\,\mu(v)\, u_x^2 + C_x.$$

Nonclassical behavior for Van der waals fluids



Specific volume v ,



Velocity u

Solutions depend upon the ratio

(viscosity)^2/capillarity.

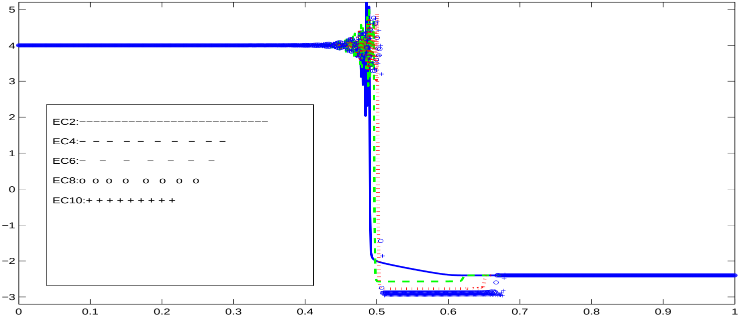
Ideal magnetohydrodynamics with Hall effect. (simplified version)

$$v_t + ((v^2 + w^2)\, v)_x = \varepsilon\, v_{xx} + \alpha\epsilon\, w_{xx}$$
$$w_t + ((v^2 + w^2)\, w)_x = \varepsilon\, w_{xx} - \alpha\epsilon\, v_{xx}$$

(v, w): transverse components of the magnetic field.
ε: magnetic resistivity, α: Hall parameter (solar wind).

$$(1/2)\,(v^2 + w^2)_t + (3/4)\,((v^2 + w^2)^2)_x = -\,\varepsilon\,(v_x^2 + w_x^2) + C_x.$$

When $\alpha = 0$: Brio, Hunter, Freistühler, Pitman, Panov, Wu, Kennel.
When $\alpha \neq 0$: PLF-Mishra — Radius variable $r = (v^2 + w^2)^{1/2}$.



Solutions depend on the (order of the) scheme.

Further regularizations and models.

- Buckley-Leverett equation for two-phase flows in porous media (Hayes-Shearer, van Duijn, Peletier, Pop, Y. Wang)
- Quantum hydrodynamics (Marcati, Jerome)
- Suliciu model (Tzavaras, Bouchut, Frid).
- Phase field models
- Integral regularization terms (Rohde, Kissling, PLF, etc)
- Fractional regularization (Karlsen, etc)
- Discrete molecular models (Truskinovsky, Weinan E, etc).

FOR ALL THESE MODELS

- Complex wave patterns
- Different ratio/regularizations/schemes yield different solutions.
- Non-convex flux-functions. A single entropy inequality.

FOR CONVEX FLUX-FUNCTIONS

- One entropy is sufficient (Panov; Delellis, Otto, Westdickenberg)
- Shocks are regularization-independent.
- Classical entropy solutions (compressive shocks, Lax inequalities).

WHAT WE NEED

- Include macro-scale effects without resolving the small-scales.
- Encompass nonclassical entropy solutions containing undercompressive shocks having fewer impinging characteristics.

No "universal" admissibility criterion
but "several hyperbolic theories", each being determined by specifying a physical regularization. .... KINETIC RELATION

NONCLASSICAL RIEMANN SOLVER

For simplicity in the presentation, consider

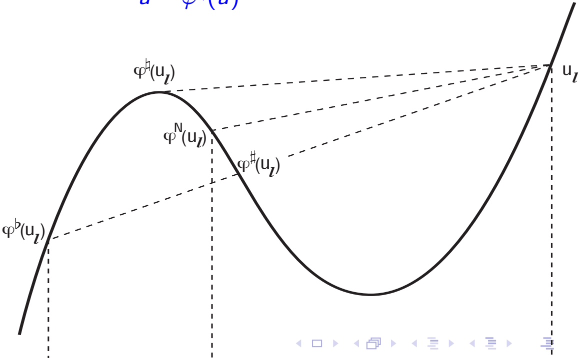
$$u_t + f(u)_x = 0$$

- Concave-convex flux

$$u\, f''(u) > 0 \quad \text{for } u \neq 0$$
$$f'''(0) \neq 0, \qquad \lim_{u \to \pm\infty} f'(u) = +\infty$$

- Tangent function $\varphi^\natural : \mathbb{R} \to \mathbb{R}$ and its inverse $\varphi^{-\natural}$

$$f'(\varphi^\natural(u)) = \frac{f(u) - f(\varphi^\natural(u))}{u - \varphi^\natural(u)}, \qquad u \neq 0$$



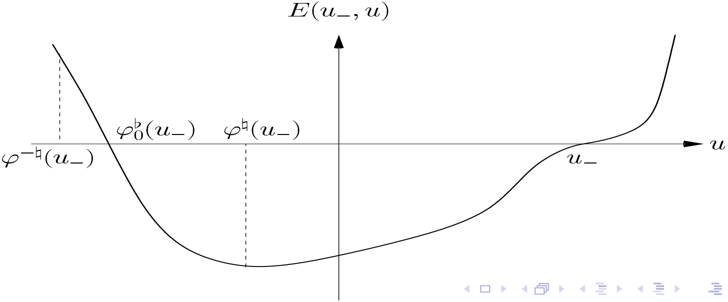
Entropy inequality for a shock wave (u_-, u_+):

$$U(u)_t + F(u)_x \leq 0, \qquad U'' > 0, \qquad F'(u) := f'(u)\, U'(u)$$

$$E(u_-, u_+) := -\frac{f(u_-) - f(u_+)}{u_- - u_+} \left(U(u_+) - U(u_-)\right) + F(u_+) - F(u_-)$$
$$\leq 0$$

Zero entropy dissipation function $\varphi_0^\flat : \mathbb{R} \mapsto \mathbb{R}$.

$$E(u, \varphi_0^\flat(u)) = 0, \qquad \varphi_0^\flat(u) \neq u \quad (\text{ when } u \neq 0)$$
$$(\varphi_0^\flat \circ \varphi_0^\flat)(u) = u.$$



Riemann problem.

$$u(x,0) = \begin{cases} u_l, & x < 0 \\ u_r, & x > 0 \end{cases}$$

A single entropy inequality allows for:

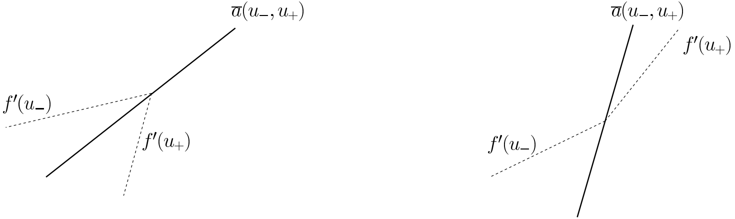
- Classical compressive shocks (satisfying Lax inequalities)

$$u_- > 0, \qquad \varphi^\natural(u_-) \leq u_+ \leq u_-.$$

- Nonclassical undercompressive shocks

$$u_- > 0, \qquad \varphi_0^\flat(u_-) \leq u_+ \leq \varphi^\natural(u_-).$$

- Rarefaction waves



However, *the Riemann problem admits (up to) a one-parameter family of solutions satisfying a single entropy inequality.*

Entropy-compatible kinetic function.

- A monotone decreasing, Lipschitz continuous function $\varphi^\flat : \mathbb{R} \mapsto \mathbb{R}$

$$\varphi_0^\flat(u) < \varphi^\flat(u) \le \varphi^\natural(u), \quad u > 0$$

- The kinetic relation $u_+ = \varphi^\flat(u_-)$ singles out one nonclassical shock.

Observe that:

- Extremal choices:

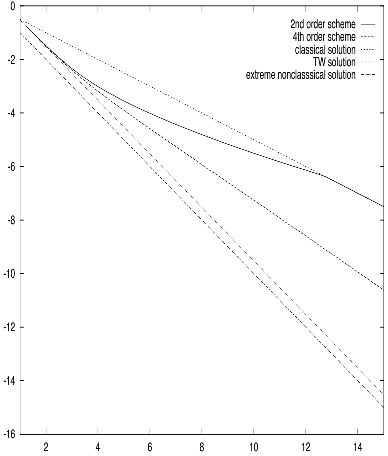
$$\varphi^\flat = \varphi^\natural \qquad \text{(classical solution, all convex entropies)}$$
$$\varphi^\flat = \varphi_0^\flat \qquad \text{(dissipation-free, one entropy equality)}$$

- Equivalently, prescribe the entropy dissipation rate.

- The property $(\varphi_0^\flat \circ \varphi_0^\flat)(u) = u$ implies the contraction property

$$|\varphi^\flat(\varphi^\flat(u))| < |u|, \quad u \ne 0.$$

Notation: Companion (threshold) function $\varphi^\sharp : \mathbb{R} \to \mathbb{R}$


2nd order scheme
4th order scheme
classical solution
TW solution
extreme nonclasssical solution
0
-2
-4
-6
-8
-10
-12
-14
-16
2
4
6
8
10
12
14

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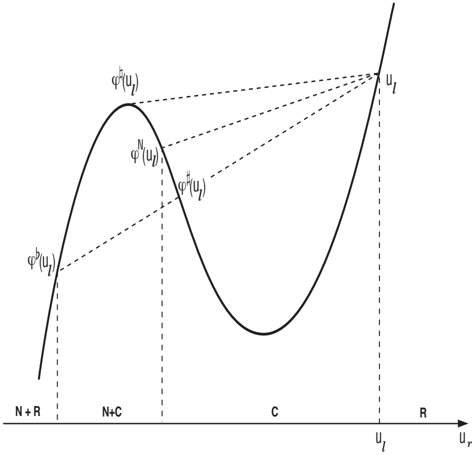
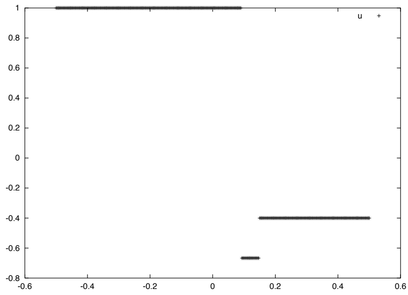
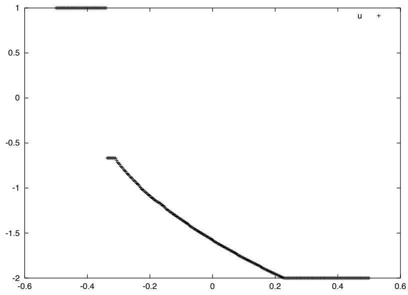

$\varphi^\natural(u_l)$
u_l
$\varphi^N(u_l)$
$\varphi^\sharp(u_l)$
$\varphi^\flat(u_l)$
N + R
N+C
C
R
u_l
u_r

Nonclassical Riemann solver. For instance, suppose $u_l > 0$.

- $u_r \geq u_l$: rarefaction wave.
- $u_r \in [\varphi^\sharp(u_l), u_l)$: classical shock.
- $u_r \in (\varphi^\flat(u_l), \varphi^\sharp(u_l))$: nonclassical shock $\big(u_l, \varphi^\flat(u_l)\big)$ + classical shock $\big(\varphi^\flat(u_l), u_r\big)$.
- $u_r \leq \varphi^\flat(u_l)$: nonclassical shock $\big(u_l, \varphi^\flat(u_l)\big)$ + rarefaction wave.





Conclusion.

Given a kinetic function $\varphi^\flat$ compatible with an entropy, the Riemann problem admits a unique solution, satisfying :

- *hyperbolic conservation law with Riemann initial data*
- *single entropy inequality plus a kinetic relation $u_+ = \varphi^\flat(u_-)$*

L^1 *continuous dependence (but spikes – some states are discontinuous).*

Generalization (piecewise smooth solutions to the Riemann problem).

- 2×2 isentropic Euler equations and nonlinear elasticity or phase transition system
  – uniqueness if hyperbolic
  – non-uniqueness if hyperbolic-elliptic
  (Slemrod, Truskinovsky, Shearer et al., PLF-Thanh, Hattori, Mercier-Piccoli, Corli-Tougeron)
- $N \times N$ strictly hyperbolic systems of conservation laws. Hayes-PLF (SIAM J. Math. Anal., 2000).

Derivation of kinetic functions.

Characterizes the dynamics of nonclassical shocks.

TW analysis, Explicit formula, physical experiments, numerical experiments.

For simplicity in the presentation, consider

$$u_t + f(u)_x = \alpha \left(|u_x|^p \, u_x\right)_x + u_{xxx}$$

$$f \;\text{ concave-convex}, \quad \alpha > 0, \quad p \geq 0.$$

More generally

$$u_t + f(u)_x = \alpha \left(b(u, u_x) \, |u_x|^p \, u_x\right)_x + \left(c_1(u) \, (c_2(u) \, u_x)_x\right)_x$$

Main issues.

- Kinetic function $\varphi^\flat$ associated to this model ?
- Monotonicity ?
- Behavior near $u = 0$?

Earlier result for the cubic flux. Explicit formulas

- $p = 0$: Shearer et al. (1995)
- $p = 1$: Hayes - PLF (1997). Here, ${\varphi^\flat}'(0) = \varphi_0^\flat(0) = -1$.

Traveling wave analysis.

- Second-order ODE

$$u(x,t) = u(y), \qquad y = x - \lambda\, t$$
$$-\lambda\,(u - u_-) + f(u) - f(u_-) = \alpha\,|u'|^p\,u' + u''$$

with boundary conditions $\lim_{y \to \pm\infty} u(y) = u_\pm$ and data $u_\pm, \lambda$ satisfying the Rankine-Hugoniot relation.

- Phase plane analysis:
  - First-order system in the plane (u, u').
  - Existence of saddle-node (classical shocks) and saddle-saddle (nonclassical shocks) connections.
  - Dependence upon u_0, λ, α, p.

- Admissible shocks

$$S(u_-) := \{ u_+ \; / \; \text{there exists a TW connecting } u_\pm \}$$

Theorem. (Bedjaoui - PLF, 2001 & 2004).
(i) Kinetic function $\varphi^\flat : \mathbb{R} \to \mathbb{R}$, strictly decreasing,

$$S(u) = \{\varphi^\flat(u)\} \cup \left(\varphi^\sharp(u), u\right], \qquad u > 0$$
$$\varphi_0^\flat(u) < \varphi^\flat(u) \le \varphi^\natural(u), \qquad u > 0$$

(ii) Threshold function $A^\natural$ such that

- $0 \le p \le 1/3$:

$$A^\natural : \mathbb{R} \to [0, \infty) \text{ Lipschitz continuous}, \quad A^\natural(0) = 0$$
$$\varphi^\flat(u) = \varphi^\natural(u) \quad \text{iff} \;\; \alpha \ge A^\natural(u)$$

- $p > 1/3$:

$$\varphi^\flat(u) \ne \varphi^\natural(u) \qquad (u \ne 0)$$

(iii) Behavior of infinitesimally small shocks:

- $p = 0$:

$$\varphi^{\flat\,\prime}(0) = \varphi^{\natural\,\prime}(0) = -1/2$$
$$A^\natural(0) = 0, \qquad A^{\natural\,\prime}(0\pm) \ne 0$$

- $0 < p \leq 1/3$: $${\varphi^\flat}'(0) = -1/2$$ $$A^\natural(0) = 0, \quad {A^\natural}'(0\pm) = +\infty$$

- $1/3 < p < 1/2$: $${\varphi^\flat}'(0) = -1/2$$

- $p = 1/2$: $${\varphi^\flat}'(0) \in \left({\varphi_0^{-\flat}}'(0), -1/2\right) = (-1, -1/2)$$

$$\lim_{\alpha \to 0+} {\varphi^\flat}'(0) = -1, \qquad \lim_{\alpha \to +\infty} {\varphi^\flat}'(0) = -1/2$$

- $p > 1/2$: $${\varphi^\flat}'(0) = -1$$

Special case of the cubic flux. Explicit formula

- $p = 1/2$: Linear kinetic function

$$\varphi^\flat(u) = -c_\alpha\, u, \qquad c_\alpha \in (1/2, 1).$$

Conclusion.
To the augmented model one can associate a unique kinetic function which is monotone and satisfies all the assumptions required in the theory of the Riemann problem.

Generalizations.

- 2×2 Nonlinear elasticity/Euler equations (non-nec. monotone)
  (PLF-Bedjaoui, Truskinovsky, Benzoni, Shearer)
- 2×2 Van de Waals model (two inflection points) (multiple solutions)
  (Bedjaoui-Chalons-Coquel-PLF).

Partial results (on traveling waves).

- Thin liquid film model
  (Bertozzi, Shearer, Münch).
- Generalized Camassa-Holm model
  (Constantin, Strauss, Lenells).

BV EXISTENCE THEORY

Glimm-type scheme based on a nonclassical Riemann solver.

- lack of monotonicity and increase of the total variation.
- for systems, lack of regularity of the wave curves.

For simplicity, consider

$$\begin{aligned}&\partial_t u + \partial_x f(u) = 0\\ &u(x,0) = u_0(x) \qquad u_0 \in BV(\mathbb{R}),\\ &f \text{ concave-convex.}\end{aligned}$$

Assumptions.

- $\varphi^\flat : \mathbb{R} \to \mathbb{R}$: Lipschitz continuous, monotone decreasing.
- The second iterate of $\varphi^\flat$ is a strict contraction: for $K \in (0,1)$

$$\left|\varphi^\flat \circ \varphi^\flat(u)\right| \leq K|u|, \qquad u \neq 0.$$

Remark. Since $\left|\varphi^\flat \circ \varphi^\flat(u)\right| < |u|$ for $u \neq 0$, this is only a condition at $u = 0$, about nonclassical shocks with infinitesimally small strength.

Notion of generalized wave strength

$$\sigma(u_-, u_+) = |\psi(u_-) - \psi(u_+)|, \qquad \text{with} \qquad \psi(u) = \begin{cases} u, & u > 0, \\ \varphi_0^\flat(u), & u < 0. \end{cases}$$

Properties.

- Equivalence with the standard strength:

$$\underline{C}\,|u_- - u_+| \le \sigma(u_-, u_+) \le \overline{C}\,|u_- - u_+|.$$

- Continuity as u_+ crosses $\varphi^\sharp(u_-)$ during a transition from a single crossing shock to a two wave pattern:

$$\begin{aligned}\sigma(u_-, \varphi^\sharp(u_-)) &= \left|u_- - \varphi_0^\flat \circ \varphi^\sharp(u_-)\right| \\ &= \left|u_- - \varphi_0^\flat \circ \varphi^\flat(u_-)\right| + \left|\varphi_0^\flat \circ \varphi^\flat(u_-) - \varphi_0^\flat \circ \varphi^\sharp(u_-)\right| \\ &= \sigma(u_-, \varphi^\flat(u_-)) + \sigma(\varphi^\flat(u_-), \varphi^\sharp(u_-)).\end{aligned}$$

Generalized TV functional.

For a piecewise constant function $u = u(t, \cdot)$ made of shock or rarefaction fronts (u_-^α, u_+^α)

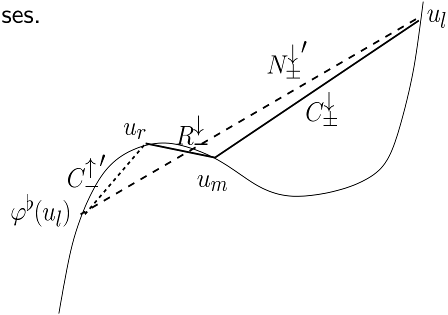
$$V\big(u(t)\big) := \sum_\alpha \sigma(u_-^\alpha, u_+^\alpha),$$

equivalent to the total variation

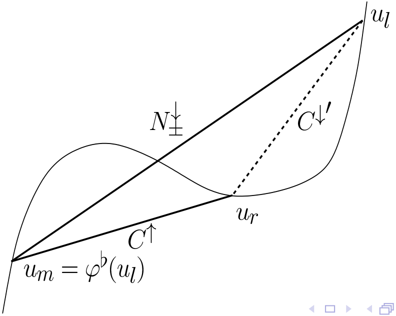
$$TV\big(u(t)\big) := \sum_\alpha \big|u_-^\alpha - u_+^\alpha\big|.$$

Classification of wave interaction patterns. 20 cases...

Case CR-4. $(C^{\downarrow}_{\pm} R^{\downarrow}_{-})$–$({N^{\downarrow}_{\pm}}' {C^{\uparrow}_{-}}')$ (monotone to non-monotone) The total variation increases.



Case NC. $(N^{\downarrow}_{\pm} C^{\uparrow})$–$({C^{\downarrow}}')$ (non-monotone to monotone) The total variation decreases.



Proposition. [Laforest - PLF (2009)]
The generalized total variation functional $V = V\big(u^h(t)\big)$ is non-increasing along a sequence of front tracking approximations. At each interaction

$$[V] \le \begin{cases} -2\,\sigma(R^{in}), & \text{Cases RC-1, RC-3, CR-1, CR-2, CR-4,} \\ -C\,\sigma(R^{in}), & \text{Cases RC-2, RN,} \\ -2\big(\sigma(R^{in}) - \sigma(R^{out})\big), & \text{Case CR-3,} \\ 0, & \text{all other cases,} \end{cases}$$

where R^{in} and R^{out} denote the incoming/outgoing rarefactions, and

$$C := \frac{\mathrm{Lip}\big((\varphi_0^\flat - \varphi_0^\flat \circ \varphi^\flat)^{-1}\big)}{\mathrm{Lip}(\varphi_0^\flat)}.$$

Theorem [Existence of nonclassical entropy solutions, Baiti-PLF-Piccoli (2001), Laforest -PLF (2009)].

$$\|u^h(t)\|_{L^\infty(\mathbb{R})} \lesssim \|u_0\|_{L^\infty(\mathbb{R})},$$
$$TV(u^h(t)) \lesssim TV(u_0),$$
$$\|u^h(t) - u^h(s)\|_{L^1(\mathbb{R})} \lesssim |t - s|,$$

and u^h converge in L^1 to a weak solution satisfying the entropy inequality and the kinetic relation.

Remarks.

- Behavior near $u = 0$ important to prevent TV blow-up.
- Assumption $\varphi^{\flat\prime}(0-)\,\varphi^{\flat\prime}(0+) < 1$, satisfied by kinetic functions generated by nonlinear diffusion-dispersion

$$\alpha\left(b(u, u_x)\,|u_x|^p\,u_x\right)_x + \left(c_1(u)\,(c_2(u)\,u_x)_x\right)_x$$

provided $p < 1/2$.

Generalization.

- Kinetics and nucleation: PLF-Shearer (2005).
- Hyperbolic systems:
  - Perturbation of a nonclassical wave
    PLF (1993), Corli-Tougeron (2002), Colombo-Corli (2002), Hattori (2003), Laforest-PLF (2009).
  - The new functional opens the way to further investigations.

Uniqueness.

- Classical setting: Bressan-LeFloch (1997, tame variation), extended by Bressan with Goatin and Lewicka.
- Nonclassical setting:
  Baiti-PLF-Piccoli (JDE, 2001)

L^1 **continuous dependence.**

- Classical setting : Bressan et al., LeFloch et al., Liu-Yang.
- Nonclassical setting: open problem.

Further reading. Lect. in Math., ETH Zürich, Birkhäuser.
Download at http://www.ann.jussieu.fr/~lefloch

VANISHING DIFFUSION-DISPERSION LIMITS

- Tartar's compensated compactness method.
  - 1D scalar equations:
    Schonbek (1982)
    Hayes - PLF (1997), PLF - Natalini (1999)
  - 2×2 elasticity system: Hayes - PLF (2000)
  - Camassa-Holm equation : Coclite - Karlsen (2006)

- DiPerna's measure-valued solutions.
  - Multidimensional conservation laws:
    Correia - PLF (1999), Kondo - PLF (2001)
  - With discontinuous flux:
    Holden - Karlsen - Mitrovic (2009)

- Lions-Perthame-Tadmor 's kinetic formulation.
  - Multidimensional conservation laws:
    Hwang - Tzavaras (2002), Hwang (2004)
    Kissling - PLF - Rohde (2009) (non-local regularization)

SCHEMES WITH PRESCRIBED DISSIPATION

For simplicity in the presentation, consider

$$\partial_t u + \partial_x f(u) = \alpha\, \varepsilon\, u_{xx} + \varepsilon^2\, u_{xxx}$$

- u_α: the limit when $\varepsilon \to 0$.
- $\varphi^\flat_\alpha$: the associated kinetic function.

Can we design schemes converging to u_α ?

Glimm scheme and front tracking schemes.

- Theoretical convergence results
- Numerical experiments:
  Chalons and LeFloch, Interfaces and Free Boundaries (2003).

Finite difference schemes.

Hayes-LeFloch (SINUM, 1998).

- $u_\alpha^{\Delta x}$: numerical solution
  $v_\alpha := \lim_{\Delta x \to 0} u_\alpha^{\Delta x}$: the limit of the scheme.
  $\psi_\alpha^\flat$: the numerical kinetic function.

- Observation:

$$v^\alpha \neq u^\alpha, \qquad \psi_\alpha^\flat \neq \varphi_\alpha^\flat$$

  - even if the scheme is "conservative", "consistent", "high-order", etc.
  - Small scale effects play a critical role in the selection of shocks.
  - The discrete dissipation $\neq$ discrete dissipation.

Proposed criterion: $\psi_\alpha^\flat$ should be an accurate approximation of $\varphi_\alpha^\flat$.

Capillarity terms create oscillations, not captured by standard TVD schemes.

Schemes with prescribed dissipation.

- High-order accurate, entropy conservative, discrete flux.
- Discrete version of the physically relevant entropy inequality. Hence, preserve exactly (and globally in time) an approximate entropy balance
- Equivalent equation coincide with the augmented model, given by the physical modeling, up to a sufficiently high order.

  For instance, for

$$\partial_t u + \partial_x f(u) = \alpha\, \epsilon\, u_{xx} + \epsilon^2\, u_{xxx}$$

we require

$$\partial_t u + \partial_x f(u) = \alpha\, \Delta x\, u_{xx} + (\Delta x)^2\, u_{xxx} + O(\Delta x)^p,$$

for $p \geq 3$ at least.

Theorem (Second-order, Tadmor, 1984). Two-point numerical flux

$$g^*(v_0, v_1) = \int_0^1 g(v_0 + s\,(v_1 - v_0))\,ds, \qquad v_0, v_1 \in \mathbb{R}^N,$$

where v is the entropy variable associated with a strictly convex entropy.

- Entropy conservative scheme, satisfying

$$\frac{d}{dt}U(u_j) + \frac{1}{h}\left(G^*_{j+1/2} - G^*_{j-1/2}\right) = 0,$$

  with

$$\begin{aligned} G^*(v_0, v_1) =& \frac{1}{2}(G(v_0) + G(v_1)) + \frac{1}{2}(v_0 + v_1)\, g^*(v_0, v_1) \\ & - \frac{1}{2}\Big(v_0 \cdot g(v_0) + v_1 \cdot g(v_1)\Big). \end{aligned}$$

- Second-order accurate, with (conservative) equivalent equation

$$\partial_t u + \partial_x f(u) = \frac{h^2}{6}\,\partial_x\Big(- g(v)_{xx} + \frac{1}{2}\, v_x \cdot \partial_x Dg(v)\Big).$$

Theorem. (High-order, PLF - Rohde, 2000) Given any symmetric $N \times N$ matrices $B^*(v_{-p+2}, \cdots, v_p)$, the $(2p+1)$-point scheme associated with

$$g^*(v_{-p+1}, \cdots, v_p) = \int_0^1 g(v_0 + s\,(v_1 - v_0))\,ds - \frac{1}{12}\Big((v_2 - v_1)\cdot B^*(v_{-p+2}, \cdots, v_p) - (v_0 - v_{-1})\cdot B^*(v_{-p+1}, \cdots, v_{p-1})\Big)$$

is entropy conservative, with entropy flux

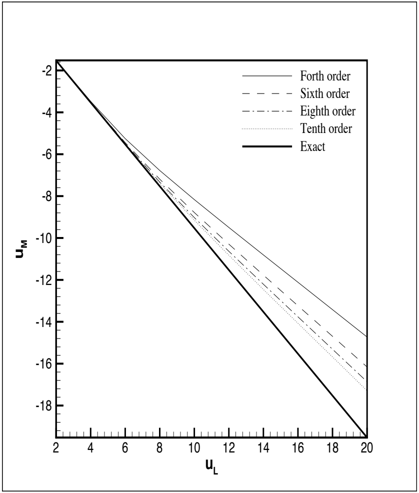
$$G^*(v_{-p+1}, \cdots, v_p) = \frac{1}{2}(v_0 + v_1)\cdot g^*(v_{-p+1}, \cdots, v_p) - \frac{1}{2}\Big(\psi^*(v_{-p+2}, \cdots, v_p) + \psi^*(v_{-p+1}, \cdots, v_{p-1})\Big).$$

When $p = 2$ and $B^*(v, v, v) = B(v)\Big(= Dg(v)\Big)$, this five-point scheme is third-order, at least.

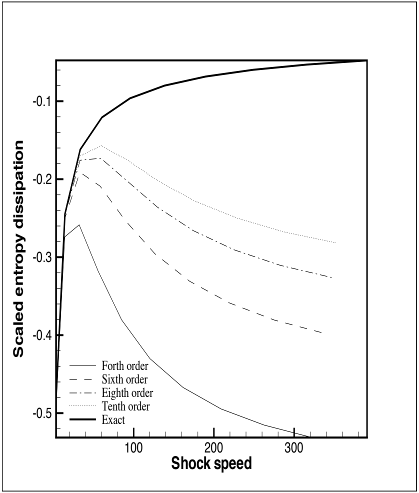
Convergence of the kinetic function.

LeFloch-Mohamadian (JCP, 2008)

Cubic conservation law with (relatively) large diffusion $\alpha = 1$.



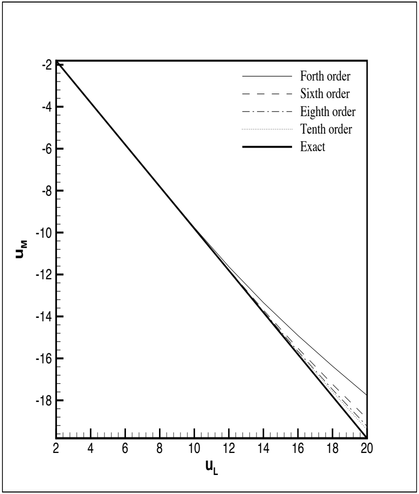
Kinetic function

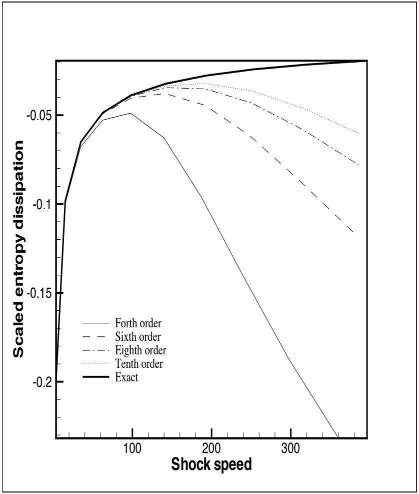


Scaled entropy dissipation

$\phi(s)/s^2$ (versus shock speed s)

Cubic conservation law with (relatively) large diffusion $\alpha = 1/6$.





Kinetic function

Scaled entropy dissipation

APPLICATION. Generalized Camassa-Holm model

$$u_t + (u^3)_x = \alpha\, u_{xx} + \beta\,\big(u_{txx} + 2u_x\, u_{xx} + u\, u_{xxx}\big)$$

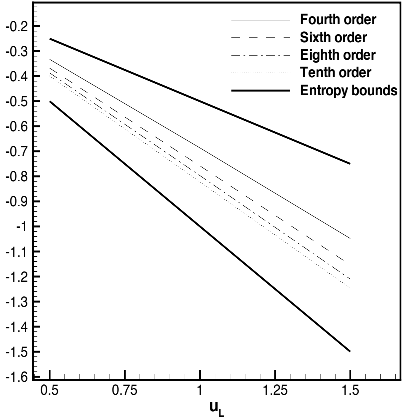
Theory.

- Well-posedness for the initial-value problem
  Bressan, Constantin, Karlsen, Coclite, Raynaud.
- Kinetic relations via traveling wave analysis: open problem.

Numerical investigation

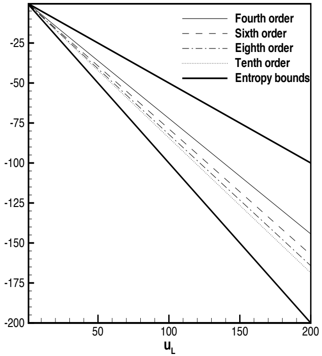
- Existence of a kinetic function ? Globally monotone ?
- Relation with the linear diffusive-dispersive model ?

Shocks with moderate strength.

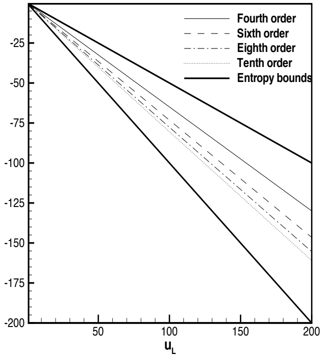


The kinetic functions
for the linear diffusion-dispersion and Camassa-Holm models
essentially coincide for shocks with moderate strength.

Shocks with large strength.



Linear diffusion-dispersion model

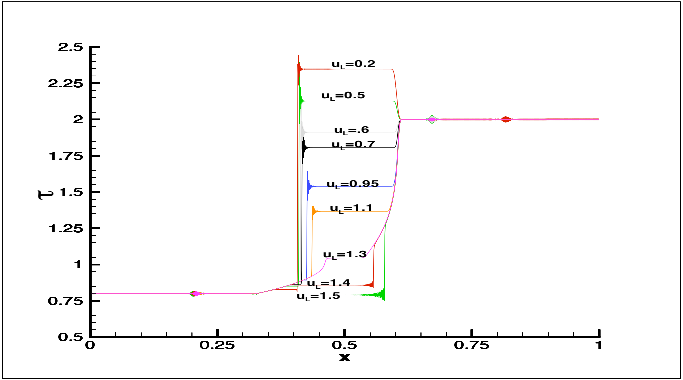


Camassa-Holm model

APPLICATION. Van der Waals fluids.

Complex wave structure.

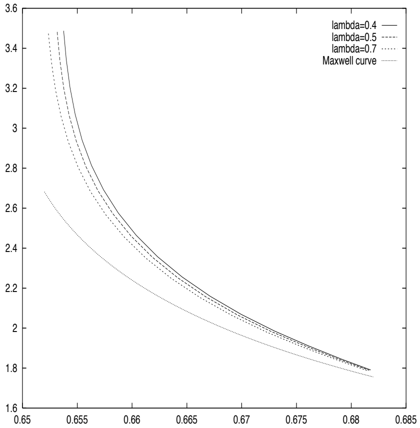
Initial data $\tau_L = 0.8$, $\tau_R = 2$, $u_R = 1$ with variable left-hand data u_L.



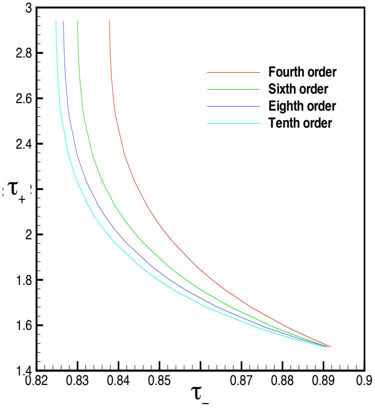
Better described... with the kinetic function.

Kinetic function.

For τ near to 1: existence and monotonicity.



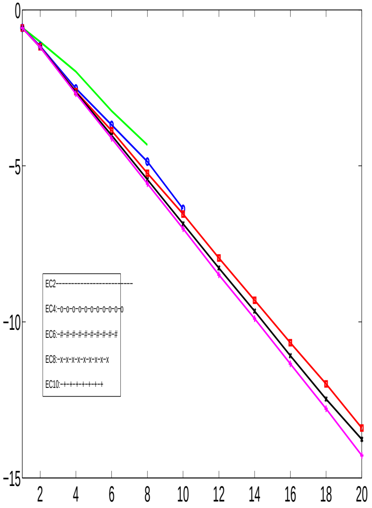
Varying the capillarity coefficient

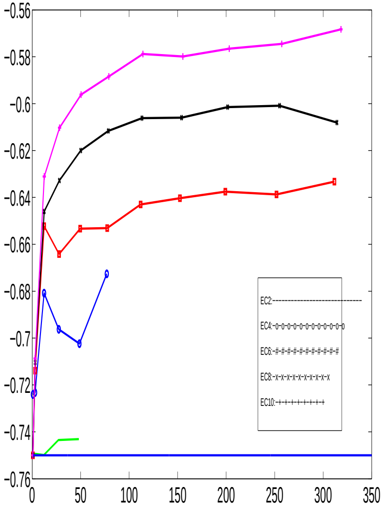


Varying the order of the discretization.

APPLICATION. Magnetohydrodynamics with Hall effect.

LeFloch - Mishra (2009)





Kinetic function , Scaled entropy dissipation

Schemes with controled dissipation.

- No convergence to the analytical solution.
- Practically useful schemes.

  The numerical kinetic function approaches the exact kinetic function.

- Kinetic functions exist and are monotone for large classes of physically relevant models:
  - thin liquid films, generalized Camassa-Holm, nonlinear phase transitions, van der Waals fluids (small shocks), magnetohydrodynamics (more challenging).

- Computing the kinetic function. Useful to investigate:
  - Effects of the diffusion/dispersion ratio, regularization, order of accuracy of the schemes.
  - Efficiency of the schemes.

Remark. Kinetic functions associated with schemes.

- Beam-Warming scheme (for concave-convex flux) produces non-classical shocks.
- No such shocks observed with the Lax-Wendroff scheme.

All of this depends crucially on the sign of the numerical dispersion coefficient !

- T.Y. Hou and P.G. LeFloch, `Why nonconservative schemes converge to wrong solutions. Error analysis`, Math. of Comput. 62 (1994), 497–530.

- B.T. Hayes and P.G. LeFloch, `Nonclassical shocks and kinetic relations. Finite difference schemes`, SIAM J. Numer. Anal. 35 (1998), 2169–2194.

- P.G. LeFloch, J.-M. Mercier, and C. Rohde, `Fully discrete entropy conservative schemes of arbitrary order`, SIAM J. Numer. Anal. 40 (2002), 1968–1992.

- P.G. LeFloch and M. Mohamadian, `Why many theories of shock waves are necessary. Fourth-order models, kinetic functions, and equivalent equations`, J. Comput. Phys. 227 (2008), 4162–4189.

NON-UNIQUENESS – Two (or more) inflection points

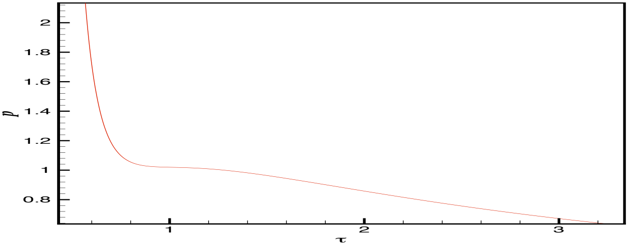
Van der Waals fluids (undergoing phase transitions) with viscosity and capillarity

$$\tau_t - u_x = 0$$
$$u_t + p(\tau)_x = \alpha\big(\beta(\tau)\,|\tau_x|^q\,u_x\big)_x - \tau_{xxx}$$

- τ : specific volume $\quad u$: velocity
- α : viscosity/capillarity, $\quad q \geq 0, \quad \beta > 0$

- Convex/concave/convex pressure law :

$$p''(\tau) \geq 0, \quad \tau \in (0,a) \cup (c,+\infty)$$
$$p''(\tau) \leq 0, \quad \tau \in (a,c), \qquad p'(a) > 0$$



Main issues.

- existence of classical / nonclassical traveling waves
- existence of a kinetic function ?
- monotonicity ?
- dependence in α ?

Already known for the 2×2 system with concave-convex flux:
Bedjaoui - PLF (2004).
Also, contributions by Truskinovsky, Shearer, Benzoni, etc.

How about two inflection points ?

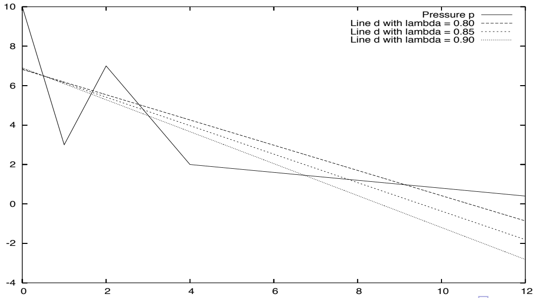
Traveling wave analysis.

2-wave issuing from (τ_0, u_0) at $-\infty$ and with speed $\lambda > 0$:

$$\lambda\,(\tau - \tau_0) + u - u_0 = 0$$
$$\lambda\,(u - u_0) - p(\tau) + p(\tau_0) = -\alpha\,\beta(\tau)|\tau'|^q u' + \tau''.$$

Phase plane analysis in the plane (τ, τ'):

- Second-order differential equation + an algebraic equation.
- Fix a left-hand state τ_0 and a speed λ within the interval where there exist three other equilibria τ_1, τ_2, τ_3.



Entropy inequality.

$$-\lambda\,\widetilde{U}' + \widetilde{F}' = -\alpha\,\beta(\tau)|\tau'|^q(u')^2 < 0$$

$$\widetilde{U} := -\int^{\tau} p(s)\,ds + \frac{u^2}{2} + \frac{(\tau')^2}{2}$$

$$\widetilde{F} := u\,p(\tau) + \lambda\,(\tau')^2 + u\,\tau'' - u\,\alpha\,\beta(\tau)\,|\tau'|^q\,u'.$$

Lemma. (Classification of the equilibrium points.)

- For all $q \geq 0$, the equilibria $(\tau_0, 0)$ and $(\tau_2, 0)$ are *saddle* points (two real eigenvalues with opposite signs).

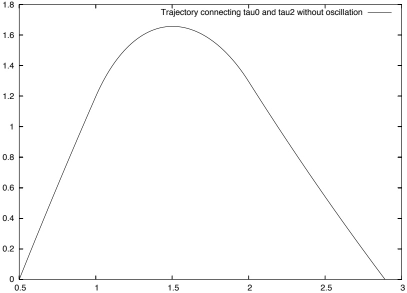
- For $q = 0$ and $i = 1, 3$, the point $(\tau_i, 0)$ is :
  - a stable *node* (two negative eigenvalues) if $p'(\tau_i) + \lambda^2 \leq (\alpha\lambda\beta(\tau_i))^2/4$
  - a stable spiral (two eigenvalues with the same negative real part and with opposite sign and non-zero imaginary parts) if $p'(\tau_i) + \lambda^2 > (\alpha\lambda\beta(\tau_i))^2/4$.

- For $q > 0$ the equilibria $(\tau_1, 0)$ and $(\tau_3, 0)$ are centers (two purely imaginary eigenvalues).

Theorem. (Bedjaoui, Chalons, Coquel, PLF, 2005). There exists a decreasing sequence of diffusion/dispersion ratio $\alpha_n(\tau_0, \lambda) \to 0$ such that:

- $\alpha = \alpha_n$ (nonclassical) TW with n oscillations connecting τ_0 to τ_2.
- $\alpha \in (\alpha_{2n+2}, \alpha_{2n+1}) \cup (\alpha_0, +\infty)$ (classical) TW connecting τ_0 to τ_1.
- $\alpha \in (\alpha_{2n+1}, \alpha_{2n})$ (classical) TW connecting τ_0 to τ_3.

Nonclassical trajectories. Infinitely many, associated to a sequence $\alpha_n \to 0$:



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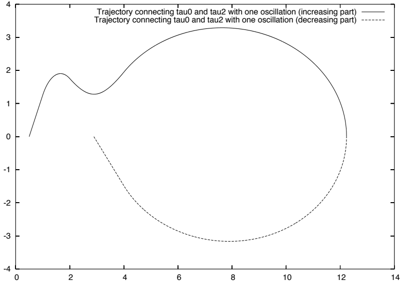

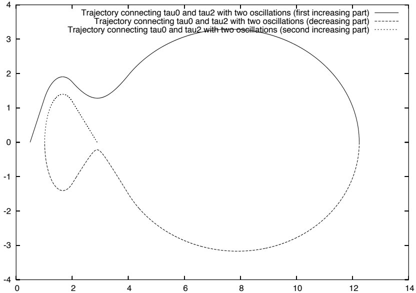

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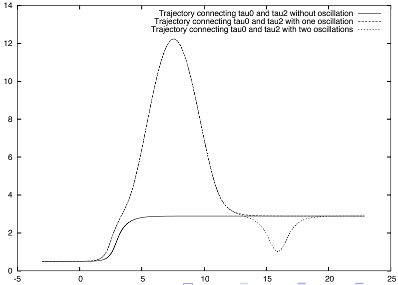


New features found with the van der Waals model.

- Non-classical trajectories may be non-monotone.
- Several kinetic functions : $u_+ = \varphi^\flat_\alpha(u_-)$, that is, the right-hand side is not unique.
- Non-uniqueness of Riemann solutions.

NON-UNIQUENESS – Nucleation criterion

Joint work with M. Shearer (scalar equations) and M. Laforest (systems).

Available shocks after imposing the kinetic relation.

- All nonclassical shocks (u_-, u_+) satisfy the kinetic relation $u_+ = \varphi^\flat(u_-)$.
- All classical shocks : $\varphi^\natural(u_-) \leq u_+ \leq u_-$.

Riemann problem. Given data u_l, u_r with $u_l > 0$ there are still two solutions for every $u_r < \varphi^\sharp(u_l)$:

- Classical Riemann solution:
  - Single shock (if $u_r > \varphi^\natural(u_l)$),
  - or (right-characteristic) shock plus rarefaction (if $u_r < \varphi^\natural(u_l)$).

- Nonclassical Riemann solution:
  Undercompressive shock $(u_l, \varphi^\flat(u_l))$ and faster wave $(\varphi^\flat(u_l), u_r)$, which is
  - either a classical shock (if $u_r > \varphi^\flat(u_l)$)
  - or a rarefaction (if $u_r < \varphi^\flat(u_l)$).

Nucleation criterion.

- Nucleation threshold:
  Lipschitz continuous function φ^N satisfying
  $\varphi^\natural(u_l) \leq \varphi^N(u_l) \leq \varphi^\sharp(u_l)$ for $u_l > 0$.

- We impose the criterion

  If $u_r \leq \varphi^N(u_l)$, the solution is nonclassical;

  it is classical, otherwise.

- A large initial jump always "nucleates".
  Similar criterion proposed in material science: nucleation in austenite-martensite materials (Abeyaratne - Knowles)

- Extremal choices :

$$\varphi^N = \varphi^\natural \text{ (fully classical)}$$
$$\varphi^N = \varphi^\sharp \text{ (fully nonclassical)}$$

Splitting-merging initial data.

- Fix $u_* > 0$ and $u_0(x) = u_0^N(x) + v_0(x)$

$$u_0^N(x) := \begin{cases} u_*, & x < 0 \\ \varphi^N(u_*), & x > 0 \end{cases}$$

- Two parameters in the problem : $\eta << \varepsilon$

$$TV(v_0) < \varepsilon << 1$$
$$\eta := \varphi^\sharp(u_*) - \varphi^N(u_*) << 1$$

- The initial data u_0^N gives rise to two distinct solutions made of admissible waves.

Example. $v_0(x) = \begin{cases} 0, & x < 0 \\ \delta, & x > 0 \end{cases}$

- When $\delta > 0$, a single classical shock $C^\downarrow$:

$$u^\downarrow(x,t) := \begin{cases} u_*, & x < s\,t \\ \varphi^N(u_*) + \delta, & x > s\,t \end{cases}$$

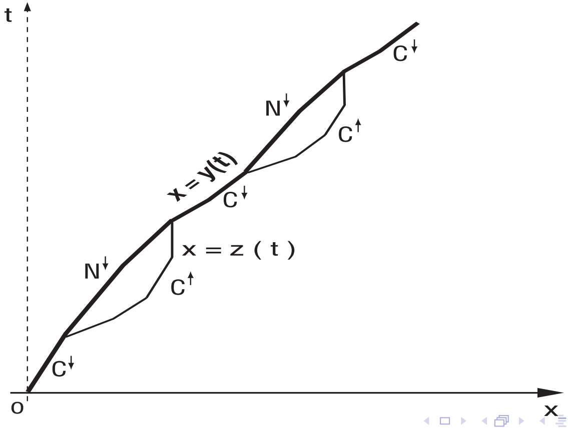
- When $\delta < 0$, a two-wave solution $u^{\downarrow\uparrow}$ consisting of an undercompressive shock $N^\downarrow$ plus a classical shock $C^\uparrow$.

Splitting/merging structure.

- One or two big waves at each time $t > 0$.
- Solution close to a one-wave solution $u^{\downarrow}$ or a two-wave solution $u^{\downarrow\uparrow}$
- Notation: $x = y(t)$: locus of big shocks $N^{\downarrow}$ and $C^{\downarrow}$

  $x = z(t)$: locus of the big shock $C^{\uparrow}$

Main issue. Generalized TV functional for front tracking solutions $u^h = u^h(t, x)$



Generalized wave strength.

$$V(t) := \sum_{\text{jumps}(u_-, u_+)} \sigma(u_-, u_+)$$

- Generalized strengths of the big increasing classical shock located at $z = z(t)$
$$\sigma^C(u_-, u_+) := \varphi^\flat(u_-) - \varphi^\flat(u_+) > 0.$$

- Nonclassical shock at $y = u(t)$
$$\sigma^{NC}(u) := (u - \psi(u)) - (\varphi^\flat \circ \psi(u) - \varphi^\flat \circ \varphi^\flat(u))$$

- Standard definition for the big decreasing classical shock.

Properties.

- Continuity/decreasing properties above, since for $u > 0$

$$\psi(u) < \varphi^\flat \circ \psi(u) < \varphi^\flat \circ \varphi^\flat(u) < u.$$

- The generalized strength $\sigma(u)$ is strictly positive.

Notation.

- Total strength of small waves in each region :

$$V^h_{\text{left}}(t) := TV_{-\infty}^{y^h(t)}(u^h(t)), \qquad V^h_{\text{middle}}(t) := TV_{y^h(t)}^{z^h(t)}(u^h(t))$$

$$V^h_{\text{right}}(t) := TV_{y^h(t)}^{+\infty}(u^h(t))$$

$$V^h(t) = V^h_{\text{left}}(t) + \kappa_0 \, V^h_{\text{middle}}(t) + \kappa_0 \, V^h_{\text{right}}(t)$$

- Total strength of big waves : $W^h(t)$

Theorem [LeFloch - Shearer]

- Front tracking solutions $u^h = u^h(x,t)$ have the splitting/merging structure, with

$$V^h(t) + \kappa_2\, W^h(t) \le V^h(0) + \kappa_2\, W^h(0)$$
$$V^h_{\text{left}}(t) \le V^h_{\text{left}}(0),$$
$$V^h_{\text{right}}(t) \le V^h_{\text{right}}(0)$$
$$V^h_{\text{left}}(t) + \kappa_1\, V^h_{\text{middle}}(t) \le V^h_{\text{left}}(t) + \kappa_1\, V^h_{\text{middle}}(t)$$

- The limit $h \to 0$ yields an exact, splitting/merging solution $u = u(x,t)$ made of admissible waves, only.

- At each splitting, $V^h(t) + \kappa_2 W^h(t)$ decreases by at least $\psi(u_*) - \varphi^N(u_*)$.
  At each merging, it decreases by at least $\varphi^\sharp(u_*) - \psi(u_*)$.

- If $\varphi^N(u_*) \neq \varphi^\sharp(u_*)$, *only finitely many mergings/splittings* and the solution eventually settles to a solution having a specified (one-wave or two-wave) structure.

- When $\varphi^N(u_*) = \varphi^\sharp(u_*)$, the *splittings/mergings may continue for all times.*

Generalization to strictly hyperbolic systems. Laforest - PLF.