Schemes with Well-Controlled Dissipation (WCD)

Jan Ernest

Seminar of Applied Mathematics (SAM),
ETH Zürich, Switzerland

Joint work with

- Siddhartha Mishra
  - Center of Mathematics for Applications (CMA), University of Oslo, Norway.
- Philippe G. LeFloch
  - Laboratoire Jacques-Louis Lions, Centre National de la Recherche Scientifique, Université Pierre et Marie Curie, Paris, France.

Scope of the Talk

Hyperbolic conservation law

$$u_t + f(u)_x = 0, \qquad u = u(x,t), \qquad (x,t) \in \mathbb{R} \times \mathbb{R}_+.$$

Scope of the Talk

Hyperbolic conservation law with small-scale effects

$$u_t^\varepsilon + f(u^\varepsilon)_x = \mathcal{R}^\varepsilon(u^\varepsilon), \qquad u^\varepsilon = u^\varepsilon(x,t), \qquad (x,t) \in \mathbb{R} \times \mathbb{R}_+.$$

Interested in limit as $\varepsilon \to 0$.

Scope of the Talk

Two cases:

1. diffusive-dispersive regularization

$$\mathcal{R}^{\varepsilon}(u) = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

Scope of the Talk

Two cases:

1. diffusive-dispersive regularization

$$\mathcal{R}^{\varepsilon}(u) = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

2. pseudo-parabolic regularization

$$\mathcal{R}^{\varepsilon}(u) = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxt}$$

Scope of the Talk

Two cases:

1. diffusive-dispersive regularization

$$\mathcal{R}^{\varepsilon}(u) = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

2. pseudo-parabolic regularization

$$\mathcal{R}^{\varepsilon}(u) = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxt}$$

Goal: Approximate solutions for fixed δ and $\varepsilon \to 0$ numerically.

Classical vs. Nonclassical Solutions

Why interesting?

- Classical and Nonclassical shock waves may arise depending on value of δ

Classical vs. Nonclassical Solutions

Why interesting?

- Classical and Nonclassical shock waves may arise depending on value of δ

- Classical solutions
  - satisfy Lax / Oleinik entropy inequalities
  - $S(u)_t + Q(u)_x \leq 0$ for **all** entropy pairs (S, Q)
  - are TVD

Classical vs. Nonclassical Solutions

Why interesting?

- Classical and Nonclassical shock waves may arise depending on value of δ

- Classical solutions
  - satisfy Lax / Oleinik entropy inequalities
  - $S(u)_t + Q(u)_x \leq 0$ for **all** entropy pairs (S, Q)
  - are TVD

- Nonclassical solutions
  - do not satisfy Lax / Oleinik entropy conditions
  - satisfy $S(u)_t + Q(u)_x \leq 0$ for a **single** entropy pair (S, Q)
  - not TVD
  - additional criterion for uniqueness: Kinetic relation (Hayes & LeFloch (1997))
    - Controls entropy dissipation at a shock as a function of the shock speed.

Example: Cubic Conservation Law

Regularized cubic conservation law:

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \delta \varepsilon^2 u_{xxx}$$

Jacobs, McKinney, Shearer (1995):

- Systematic study of traveling wave solutions
- Analytic expressions for nonclassical solutions

Cubic CL: Classical Solution

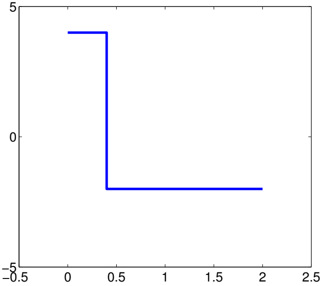
Classical solution ($\delta = 0$):

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx}$$

Cubic CL: Classical Solution

Classical solution ($\delta = 0$):

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx}$$

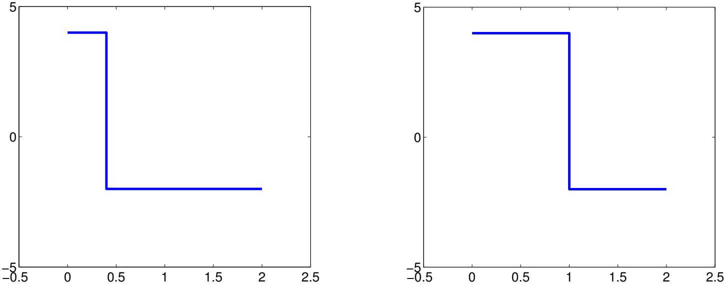


(a) $t = 0$

Cubic CL: Classical Solution

Classical solution ($\delta = 0$):

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx}$$



(a) $t = 0$ (b) $t = 0.05$

Cubic CL: Nonclassical Solution

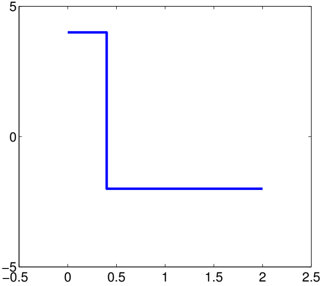
Nonclassical solution ($\delta = 1$):

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \varepsilon^2 u_{xxx}$$

Cubic CL: Nonclassical Solution

Nonclassical solution ($\delta = 1$):

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \varepsilon^2 u_{xxx}$$

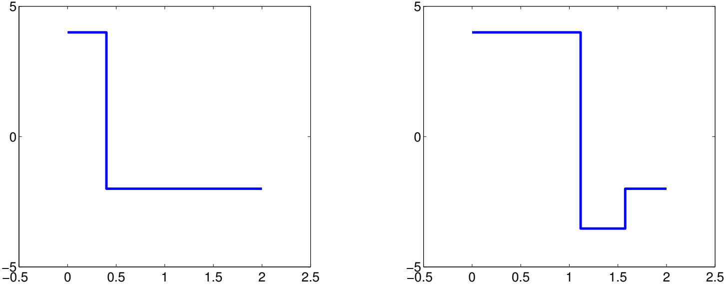


(a) $t = 0$

Cubic CL: Nonclassical Solution

Nonclassical solution ($\delta = 1$):

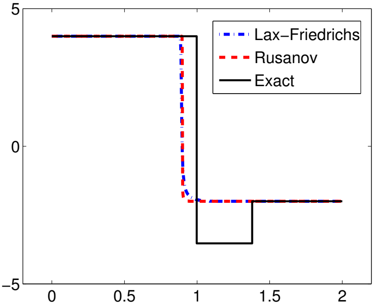
$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \varepsilon^2 u_{xxx}$$



(a) $t = 0$ (b) $t = 0.05$

Numerical Approximation

Standard schemes fail to approximate nonclassical solutions completely. They always converge to the classical solution ($\delta = 0$).



$\Rightarrow$ Design schemes that approximate correct solution for $\delta \neq 0$.

Approaches to Resolve Nonclassical Shocks

Numerical solvers for regularized cubic conservation law:

- Kissling & Rohde (2010): Heterogeneous multiscale approach
- LeFloch & Mohammadian (2008): High-order finite difference schemes with controlled dissipation

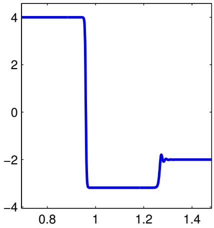
$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p} \alpha_j (u^3)_{i+j}\right) + \frac{\varepsilon}{(\Delta x)^2}\left(\sum_{j=-p}^{j=p} \beta_j u_{i+j}\right) + \frac{\delta\varepsilon^2}{(\Delta x)^3}\left(\sum_{j=-p}^{j=p} \gamma_j u_{i+j}\right)$$

  - α_j, β_j and γ_j chosen such that scheme is of order $2p$ and leading order terms in equivalent equation match the small-scale effects.

Failure at Strong Shocks

Observation:

Approximations for $\varepsilon = 5 \cdot 10^{-3} dx$.

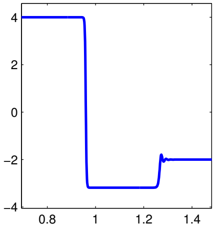


(a) $u_L = 4$

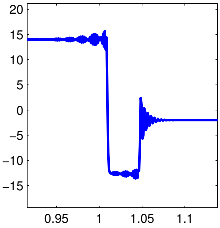
Failure at Strong Shocks

Observation:

Approximations for $\varepsilon = 5 \cdot 10^{-3} dx$.



(a) $u_L = 4$

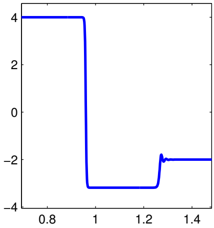


(b) $u_L = 14$

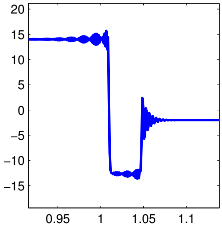
Failure at Strong Shocks

Observation:

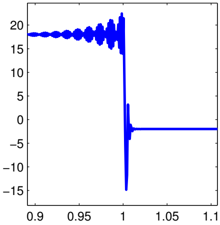
Approximations for $\varepsilon = 5 \cdot 10^{-3} dx$.



(a) $u_L = 4$



(b) $u_L = 14$

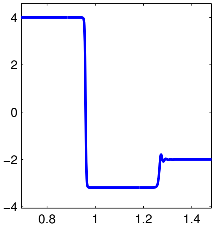


(c) $u_L = 18$

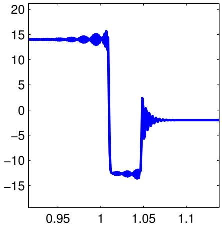
Failure at Strong Shocks

Observation:

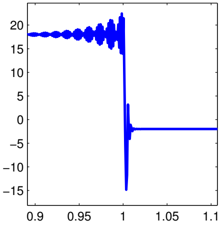
Approximations for $\varepsilon = 5 \cdot 10^{-3} dx$.



(a) $u_L = 4$



(b) $u_L = 14$



(c) $u_L = 18$

- Scheme performs well for small shocks but fails for large shocks.

Construction of Schemes with Well-Controlled Dissipation

Cubic conservation law:

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

Idea 1 (Controlled Dissipation):
Develop schemes such that leading-order terms of equivalent equation match the regularizing terms **exactly**.

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p} \alpha_j (u^3)_{i+j}\right) + \frac{c}{\Delta x}\left(\sum_{j=-p}^{j=p} \beta_j u_{i+j}\right) + \frac{\delta c^2}{\Delta x}\left(\sum_{j=-p}^{j=p} \gamma_j u_{i+j}\right)$$

Construction of Schemes with Well-Controlled Dissipation

Cubic conservation law:

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

Idea 1 (Controlled Dissipation):
Develop schemes such that leading-order terms of equivalent equation match the regularizing terms **exactly**.

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p}\alpha_j (u^3)_{i+j}\right) + \frac{\mathbf{c}}{\Delta x}\left(\sum_{j=-p}^{j=p}\beta_j u_{i+j}\right) + \frac{\delta \mathbf{c}^2}{\Delta x}\left(\sum_{j=-p}^{j=p}\gamma_j u_{i+j}\right)$$

Equivalent Equation

Cubic conservation law:

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

Equivalent equation:

$$u_t = \underbrace{-(u^3)_x + c\Delta x u_{xx} + \delta c^2 \Delta x^2 u_{xxx}}_{\textit{leading order terms (l.o.t.)}} + \underbrace{\textit{higher order terms}}_{\textit{(h.o.t.)}}$$

Equivalent Equation

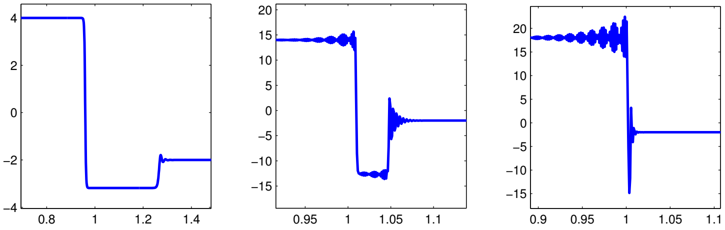
Cubic conservation law:

$$u_t + \left(u^3\right)_x = \varepsilon u_{xx} + \delta\varepsilon^2 u_{xxx}$$

Equivalent equation:

$$u_t = \underbrace{-(u^3)_x + \overbrace{c\Delta x u_{xx}}^{\varepsilon u_{xx}} + \overbrace{\delta c^2 \Delta x^2 u_{xxx}}^{\delta\varepsilon^2 u_{xxx}}}_{\textit{leading order terms (l.o.t.)}} + \underbrace{\textit{higher order terms}}_{\textit{(h.o.t.)}}$$

Recall: Failure at Strong Shocks



(a) $u_L = 4$ (b) $u_L = 14$ (c) $u_L = 18$

- Scheme performs well for small shocks but fails for large shocks.

Equivalent Equation

Equivalent equation:

$$u_t = \underbrace{-(u^3)_x + c\Delta x u_{xx} + \delta c^2 \Delta x^2 u_{xxx}}_{\textit{leading order terms (l.o.t.)}} + \underbrace{\textit{higher order terms}}_{\textit{(h.o.t.)}}$$

- For large shocks the higher-order terms (h.o.t.) in the equivalent equation start to influence the approximation.

Schemes with Well-Controlled Dissipation

Idea 2:

Impose a balance between leading-order and higher-order terms of the equivalent equation. Want:

$$|h.o.t.| < \tau \, |l.o.t.| \qquad \text{for } \tau << 1.$$

- Ensures that the nonclassical behaviour in approximation mostly comes from the correct small-scale mechanisms

Derivation of the WCD Condition

Scheme:

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p} \alpha_j f_{i+j}\right) + \frac{c}{\Delta x}\left(\sum_{j=-p}^{j=p} \beta_j u_{i+j}\right) + \frac{\delta c^2}{\Delta x}\left(\sum_{j=-p}^{j=p} \gamma_j u_{i+j}\right)$$

Equivalent equation:

$$\begin{aligned} u_t =& - f(u)_x + c\Delta x u_{xx} + \delta c^2 \Delta x^2 u_{xxx} \\ & - \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} A_k^p f^{[k]} + c \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} B_k^p u^{[k]} + \delta c^2 \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} C_k^p u^{[k]} \end{aligned}$$

with

$$A_k^p = \sum_{j=-p}^{p} \alpha_j j^k, \qquad B_k^p = \sum_{j=-p}^{p} \beta_j j^k, \qquad C_k^p = \sum_{j=-p}^{p} \gamma_j j^k$$

Derivation of the WCD Condition

Scheme:

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p} \alpha_j f_{i+j}\right) + \frac{c}{\Delta x}\left(\sum_{j=-p}^{j=p} \beta_j u_{i+j}\right) + \frac{\delta c^2}{\Delta x}\left(\sum_{j=-p}^{j=p} \gamma_j u_{i+j}\right)$$

Equivalent equation:

$$\begin{aligned} u_t =& -f(u)_x + c\Delta x u_{xx} + \delta c^2 \Delta x^2 u_{xxx} \\ & - \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} A_k^p f^{[k]} + c \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} B_k^p u^{[k]} + \delta c^2 \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} C_k^p u^{[k]} \end{aligned}$$

with

$$A_k^p = \sum_{j=-p}^{p} \alpha_j j^k, \qquad B_k^p = \sum_{j=-p}^{p} \beta_j j^k, \qquad C_k^p = \sum_{j=-p}^{p} \gamma_j j^k$$

Derivation of the WCD Condition

Scheme:

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left(\sum_{j=-p}^{j=p} \alpha_j f_{i+j}\right) + \frac{c}{\Delta x}\left(\sum_{j=-p}^{j=p} \beta_j u_{i+j}\right) + \frac{\delta c^2}{\Delta x}\left(\sum_{j=-p}^{j=p} \gamma_j u_{i+j}\right)$$

Equivalent equation:

$$u_t = -f(u)_x + c\Delta x u_{xx} + \delta c^2 \Delta x^2 u_{xxx}$$
$$-\sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} A_k^p f^{[k]} + c \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} B_k^p u^{[k]} + \delta c^2 \sum_{k=2p+1}^{\infty} \frac{\Delta x^{k-1}}{k!} C_k^p u^{[k]}$$

with

$$A_k^p = \sum_{j=-p}^{p} \alpha_j j^k, \qquad B_k^p = \sum_{j=-p}^{p} \beta_j j^k, \qquad C_k^p = \sum_{j=-p}^{p} \gamma_j j^k$$

Derivation of the WCD Condition

Analysis at an isolated discontinuity connecting u_L and u_R.
We assume $[\![u]\!] := u_L - u_R > 0$.

Formally,

$$u^{[k]} = \frac{[\![u]\!]}{\Delta x^k}, \qquad f^{[k]} = \frac{[\![f]\!]}{\Delta x^k} = \frac{[\![u^3]\!]}{\Delta x^k}.$$

Derivation of the WCD Condition

Analysis at an isolated discontinuity connecting u_L and u_R.
We assume $[\![u]\!] := u_L - u_R > 0$.

Formally,

$$u^{[k]} = \frac{[\![u]\!]}{\Delta x^k}, \qquad f^{[k]} = \frac{[\![f]\!]}{\Delta x^k} = \frac{[\![u^3]\!]}{\Delta x^k}.$$

Equivalent equation at isolated discontinuity

$$\frac{du}{dt} + \underbrace{\frac{[\![u^3]\!]}{\Delta x} - \frac{c[\![u]\!]}{\Delta x} - \frac{\delta c^2[\![u]\!]}{\Delta x}}_{l.o.t} = \underbrace{\frac{S_p^D c[\![u]\!]}{\Delta x} + \frac{S_p^C \delta c^2[\![u]\!]}{\Delta x} - \frac{S_p^f[\![u^3]\!]}{\Delta x}}_{h.o.t}$$

with

$$S_p^f = \sum_{k=2p+1}^{\infty} \frac{A_k^p}{k!} \qquad S_p^D = \sum_{k=2p+1}^{\infty} \frac{B_k^p}{k!} \qquad S_p^C = \sum_{k=2p+1}^{\infty} \frac{C_k^p}{k!}.$$

Derivation of the WCD Condition

Bounds on the h.o.t. and l.o.t. from above and below respectively.

$$|l.o.t| \geq \left(|\delta|c^2 + c - \sigma\right) \frac{|[\![u]\!]|}{\Delta x}.$$

and

$$|h.o.t| \leq \left(\hat{S}_p^D c + \hat{S}_p^C |\delta| c^2 + \hat{S}_p^f \sigma\right) \frac{|[\![u]\!]|}{\Delta x},$$

$\hat{S}_p^D$, $\hat{S}_p^C$ and $\hat{S}_p^f$ **only** depend on the order p and can be precomputed before any simulations.

WCD Condition

Want:

$$|h.o.t| < \tau\,|l.o.t| \qquad \text{for } \tau << 1$$

$\rightarrow$ WCD condition

$$\left(|\delta| - \frac{\hat{S}_p^C |\delta|}{\tau}\right) c^2 + \left(1 - \frac{\hat{S}_p^D}{\tau}\right) c - \left(1 + \frac{\hat{S}_p^f}{\tau}\right) \sigma > 0$$

- Quadratic inequality for scheme parameter c
- The smaller we choose τ the larger the order p ($\hat{S}_p^C$ decreases in p)

Numerical Experiments

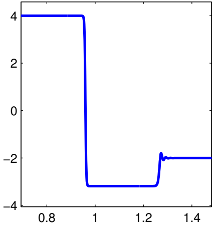
Cubic Conservation Law

$$u_t + (u^3)_x = \varepsilon u_{xx} + \delta \varepsilon^2 u_{xxx}$$

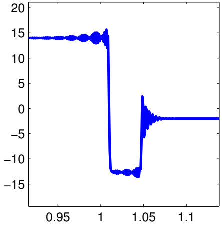
Riemann problems

$$u(x,0) = \begin{cases} u_L & x \leq 0.4 \\ -2 & x > 0.4 \end{cases}$$

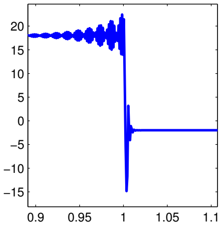
Recall: Failure at Strong Shocks



(a) $u_L = 4$



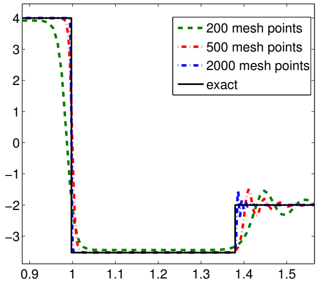
(b) $u_L = 14$



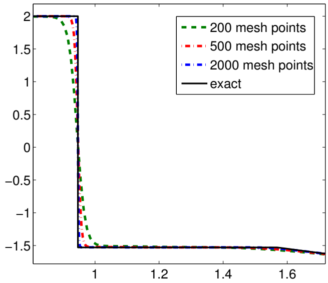
(c) $u_L = 18$

- Scheme with controlled dissipation performs well for small shocks but fails for large shocks.

Numerical Experiments: Small Shocks

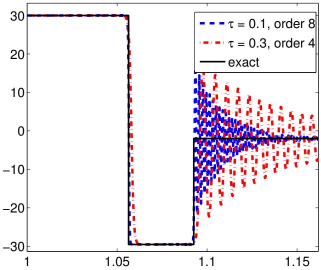


(a) $u_L = 4$: Double shock

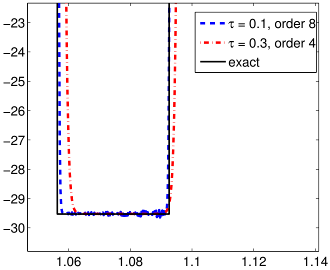


(b) $u_L = 2$: Shock-rarefaction

Numerical Experiments: Moderate Shocks

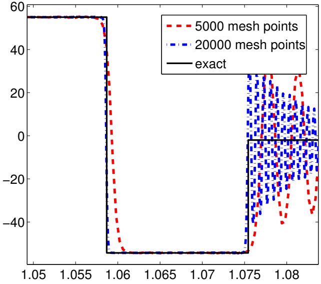


(a) $u_L = 30$

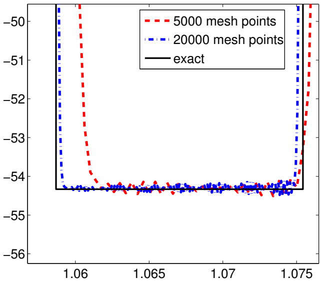


(b) Zoom at nonclassical state

Numerical Experiments: Large Shocks



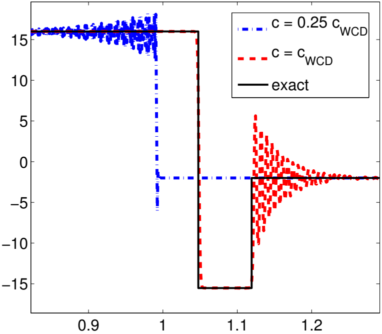
(a) $u_L = 55$



(b) Zoom at nonclassical state

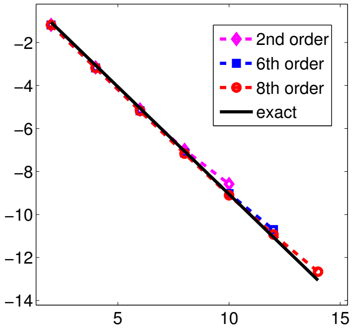
Violating WCD condition

Scheme parameter c is chosen such that it does satisfy (red) and it does not satisfy (blue) the WCD condition.

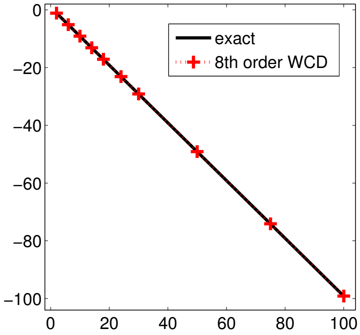


Kinetic Relation

Hayes & LeFloch (1997): Concept of kinetic relations as selection principle for physically meaningful nonclassical solution.



(a) Controlled Dissipation



(b) Well-Controlled Dissipation

Extension to Systems of Conservation Laws

Extension to systems by applying the concepts componentwise.

Example:

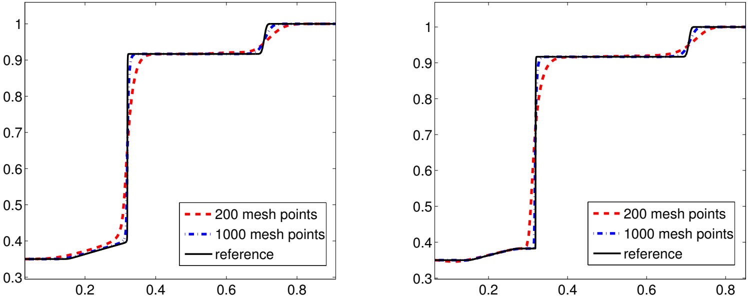
Van der Waals fluids with viscosity and capillarity

$$\begin{aligned} \tau_t - u_x &= 0 \\ u_t + p(\tau)_x &= \varepsilon u_{xx} - \delta\,\varepsilon^2 \tau_{xxx}. \end{aligned}$$

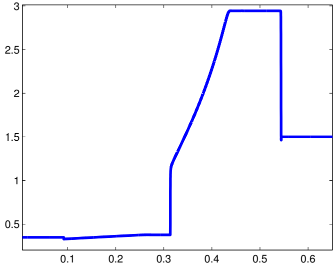
u: velocity of the fluid
τ: volume of the fluid

$$p(\tau) = \frac{R\,T}{(\tau - 1/3)} - \frac{3}{\tau^2}$$

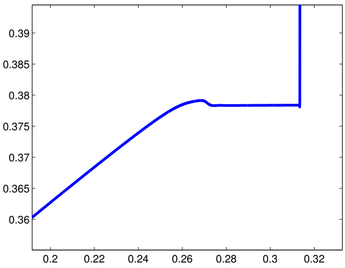
where $R = 8/3$ and $T = 1.005$.



(a) $\delta = 0$ (b) $\delta = 1$



(a) $\tau_R = 25$



(b) Zoom at nonclassical state

Extension to the Pseudo-Parabolic Regularization

Example: Regularized Buckley-Leverett equation

$$u_t + f(u)_x = \varepsilon u_{xx} + \delta \varepsilon^2 u_{xxt}$$

with

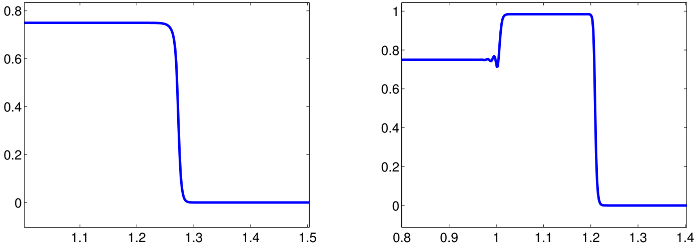
$$f(u) = \frac{u^2}{u^2 + \kappa (1 - u)^2}, \qquad 0 \leq u \leq 1, \qquad \kappa > 0$$

Example: Regularized Buckley-Leverett equation

$$u_t + f(u)_x = \varepsilon u_{xx} + \delta \varepsilon^2 u_{xxt}$$

with

$$f(u) = \frac{u^2}{u^2 + \kappa (1-u)^2}, \qquad 0 \le u \le 1, \qquad \kappa > 0$$



(a) $\delta = 0$ (b) $\delta = 5$

References

- Jacobs, McKinney, Shearer (1995)
  Traveling wave solutions of the modified Korteweg-deVries-Burgers equation. *Journal of Differential Equations*, 116(2):448-467, 1995.
- Kissling, Rohde (2010)
  The computation of nonclassical shock waves with a heterogeneous multiscale method. *NHM*, 5(3):661-674, 2010.
- LeFloch, Mohammadian (2008)
  Why many theories of shock waves are necessary: Kinetic functions, equivalent equations, and fourth-order models. *Journal of Computational Physics*, 227(8):4162-4189, 2008.