Asymptotic and invariant-domain preserving schemes for hyperbolic conservation laws with stiff reaction source term

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PDE study

PDE

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$$\partial_t u^\epsilon + \nabla\cdot\boldsymbol{f}(u^\epsilon) = \frac{1}{\epsilon}R(u^\epsilon), \qquad (\boldsymbol{x}, t) \in \Omega \times (0, T], \tag{1}$$

$$u^\epsilon(\cdot, 0) = u_0. \tag{2}$$

- Invariant-domain preserving: $u_0(\boldsymbol{x}) \in \mathcal{B} \implies u^\epsilon(\boldsymbol{x}, t) \in \mathcal{B}$.
- Entropy inequality: $\partial_t \eta(u^\epsilon) + \nabla\cdot\boldsymbol{q}(u^\epsilon) \leq \frac{1}{\epsilon}\eta'(u^\epsilon)R(u^\epsilon)$.
- There exists the unique limit $u^0 := \lim_{\epsilon\to 0} u^\epsilon$

Examples I

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Boltzmann equation

$$\partial_t f + v \cdot \nabla_{\boldsymbol{x}} f = \frac{1}{\epsilon} Q(f). \qquad \longrightarrow \text{local Maxwellian.}$$

shallow water equation

$$\begin{cases} \partial_t h + \partial_x (hv) = 0, \\ \partial_t (hv) + \partial_x \left(hv^2 + \frac{1}{2} g h^2 \right) = \frac{1}{\epsilon} (gh - |v| v). \end{cases} \qquad \longrightarrow \partial_t h + \partial_x \sqrt{g} h^{3/2} = 0.$$

Jin-Xin relaxation model

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + a \partial_x u = \frac{1}{\epsilon} (f(u) - v). \end{cases} \qquad \longrightarrow \partial_t u + \partial_x f(u) = 0.$$

(Simplified) examples II

$$\partial_t u^\epsilon + \nabla \cdot \boldsymbol{f}(u^\epsilon) = \frac{1}{\epsilon} R(u^\epsilon), \quad \mathcal{B} := [0,1].$$

single equilibrium point

$\Big(R(v) = 0 \Leftrightarrow v = 0\Big) \Rightarrow u^0 = 0.$ e.g. $R(v) = e^{-v} - 1.$

multiple (3) equilibrium points

$\Big(R(v) = 0 \Leftrightarrow v \in \{0, \alpha, 1\}\Big) \Rightarrow u^0 \in \{0, \alpha, 1\}.$ e.g. $R_\alpha(v) = v(1-v)(v-\alpha).$

How does u^0 distribute? How does u^0 look like?

Illustration of $R_\alpha(v) = v(1-v)(v-\alpha)$

Stable states: $\{0, 1\}$, unstable state: $\{\alpha\}$.

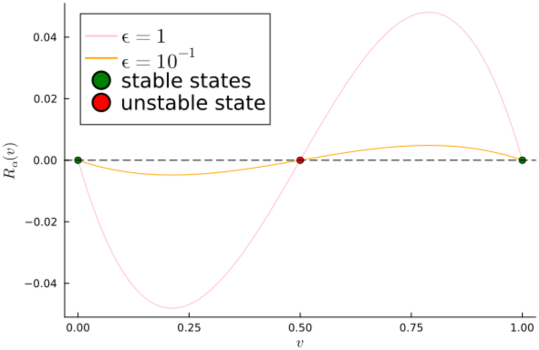


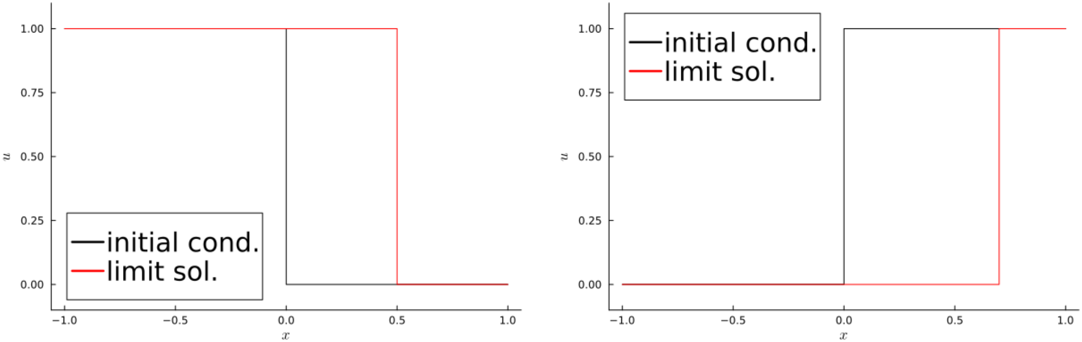
Figure: $\alpha = 0.5$

PDE study (convex flux)

H. Fan, S. Jin, and Z.-H. Teng (2000)

- For the shock-type initial condition, u^0 is a shock with speed $\frac{f(1)-f(0)}{1-0}$.
- For the rarefaction-type initial condition, u^0 is a shock with speed $f'(\alpha)$.

Illustration of u^0



(a) shock-type initial condition

(b) rarefaction-type initial condition

Figure: $f(v) = \frac{1}{2}v^2$, $T = 1$, $\alpha = 0.7$

General case?

Unfortunately, we did not find any study for general flux and multi-dimensional cases.

Numerical study

1. How to numerically reproduce the PDE behavior?
2. How to numerically preserve the physical features (invariant-domain preserving, entropy inequalities...)?
3. asymptotic preserving:

$$\boxed{\lim_{\epsilon \to 0} \lim_{h \to 0} u_h^\epsilon = u^0 = \lim_{h \to 0} \lim_{\epsilon \to 0} u_h^\epsilon \qquad (3)}$$

$\Rightarrow$ stiff case can be efficiently solved:

$$|u^\epsilon - u_h^\epsilon| \leq |u^\epsilon - u^0| + |u^0 - u_h^0| + |u_h^0 - u_h^\epsilon|$$

4. How to generalize to general flux and in multi-dimension?

Trivial idea (Implicit-explicit method)

$$\frac{U^{n+1} - U^n}{\Delta t} + \nabla \cdot \boldsymbol{f}(U^n) = \frac{1}{\epsilon} R(U^{n+1}).$$

- Transport part is treated explicitly with the hyperbolic CFL condition $\Delta t \leq Ch$.
- Reaction part is treated implicitly to avoid the stability issue.

Numerical attempts

R. J. LeVeque and H. C. Yee (1990)

Classical ideas cannot correctly reproduce the correct shock location.

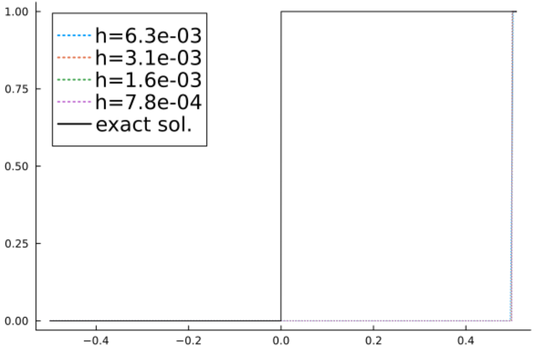


Figure: Implicit-explicit method

Attempts in the literature

W. Bao and S. Jin (2002)

- Advantages: $O(h \log h)$ convergence rate
- Disadvantages: 1D, convex flux, shock-type initial condition

M. Svärd and S. Mishra (2011)

- Advantages: Convergence is observed for both shock- and rarefaction-type initial conditions
- Disadvantages: 1D, convex flux, no interaction between rarefaction and shock.

What if we take a less stiff source term?

$$\boxed{\frac{1}{\epsilon} \to \frac{1}{\Phi_{\epsilon,h}}, \quad \Phi_{\epsilon,h} = \max(h^{\theta}, \epsilon).}$$

Concrete scheme (operator splitting)

$$(\mathsf{U}_i^n)_i \xrightarrow{\text{transport}} (\mathsf{W}_i^{n+1})_i \xrightarrow{\text{reaction}} (\mathsf{U}_i^{n+1})_i \tag{4}$$

Reaction step

Solving

$$\begin{cases} \dfrac{d}{ds}v = \dfrac{1}{\Phi_{\epsilon,h}} v(1-v)(\mathsf{W}_i^{n+1}-\alpha), \quad s \geq 0, \\ v(0) = \mathsf{W}_i^{n+1} \in \mathcal{B}. \end{cases} \tag{5}$$

$$\Rightarrow \mathsf{U}_i^{n+1} = v(\Delta t) = \frac{\mathsf{W}_i^{n+1}\exp\left(\tau_{\epsilon,\theta}(\mathsf{W}_i^{n+1}-\alpha)\right)}{1+\mathsf{W}_i^{n+1}\left(\exp\left(\tau_{\epsilon,\theta}(\mathsf{W}_i^{n+1}-\alpha)\right)-1\right)} \in \mathcal{B},$$

with $\tau_{\epsilon,\theta} = \frac{\tau}{\Phi_{\epsilon,h}}$.

Entropy residual

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Theorem

For any convex entropy $\eta \in C^2(\mathcal{B};\mathbb{R})$ with associated flux $\boldsymbol{q}$, and for any test function $\psi \in W_0^{1,\infty}(\Omega \times [0,T];\mathbb{R}_+)$, we have

$$
\begin{aligned}
&\int_\Omega \mathcal{I}_h\big(\eta(u_h^N)\big)(\boldsymbol{x})\psi(\boldsymbol{x},T) - \int_\Omega \mathcal{I}_h\big(\eta(u_h^0)\big)(\boldsymbol{x})\psi(\boldsymbol{x},0) \\
&- \int\int \left\{\eta(u_h^\epsilon)\partial_t\psi + \boldsymbol{q}(u_h^\epsilon)\cdot\nabla\psi + \frac{1}{\Phi_{\epsilon,h}}\eta'(u_h^\epsilon)R(u_h^\epsilon)\psi\right\} \le C\Lambda(h),
\end{aligned} \tag{6}
$$

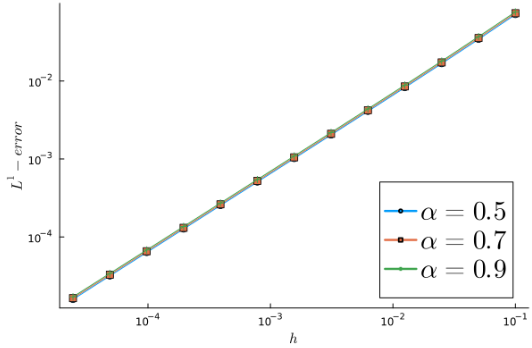
where

$$
\Lambda(h) = \frac{h}{\Phi_{\epsilon,h}^2}\|u_h^\epsilon\|_{L^1(L^1)} + \left(\frac{h}{\Phi_{\epsilon,h}} + \frac{h^2}{\Phi_{\epsilon,h}^2}\right)\|\nabla u_h^\epsilon\|_{L^1(L^1)}, \tag{7}
$$

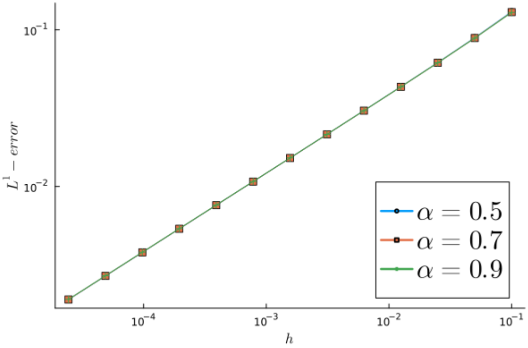
$\Phi_{\epsilon,h} = \max(h^\theta, \epsilon)$.

Numerical tests (Gridap.jl)

Numerical test I



(a) Smooth IC



(b) Rough IC

Figure: 1D linear transport with smooth and rough IC: $\epsilon = 1$ (nonstiff case).

Numerical test II

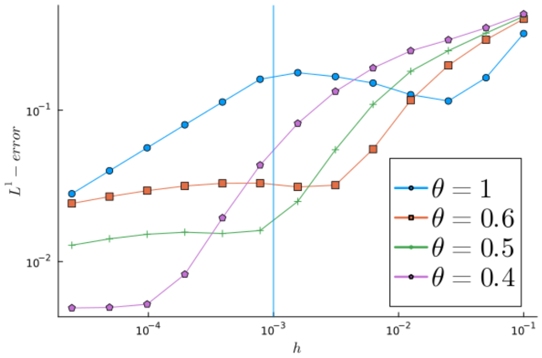


Figure: 1D linear transport with smooth IC: $\alpha = 0.7$, $\epsilon = 10^{-3}$.

Numerical test III

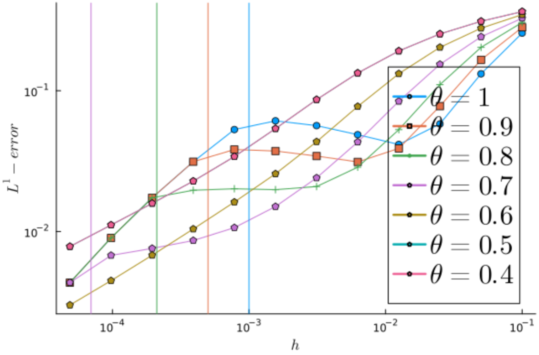
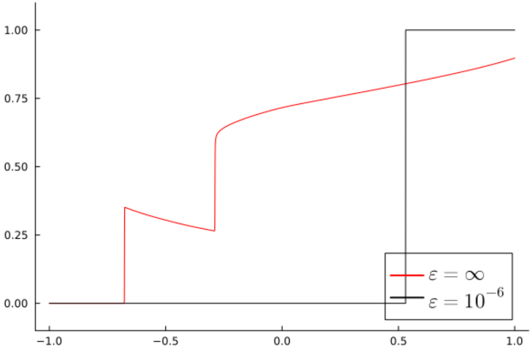
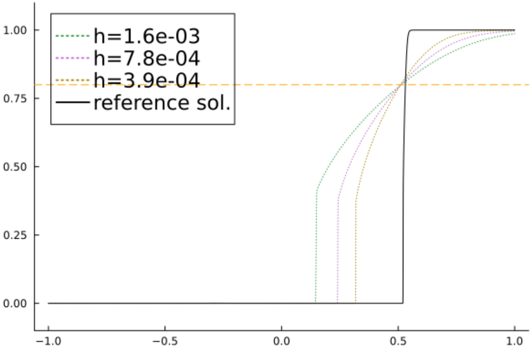


Figure: 1D Burgers equation with smooth IC: $\alpha = 0.7$, $\epsilon = 10^{-3}$.

Numerical test IV



(a) Reference sol.



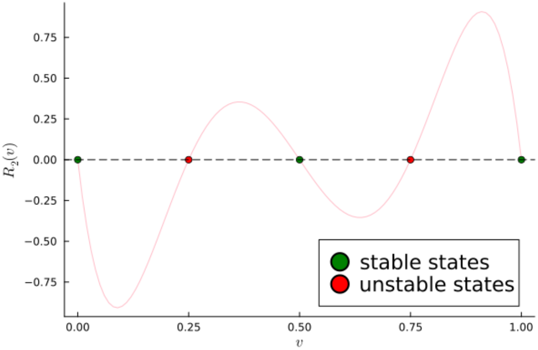
(b) Numerical sol.

Figure: 1D nonlinear transport with nonconvex flux ($f(v) = \frac{\sin(2\pi v)}{2\pi}$) and rough IC: $T = 1$, $\alpha = 0.8$, $\epsilon = 10^{-6}$, $\theta = \frac{1}{2}$

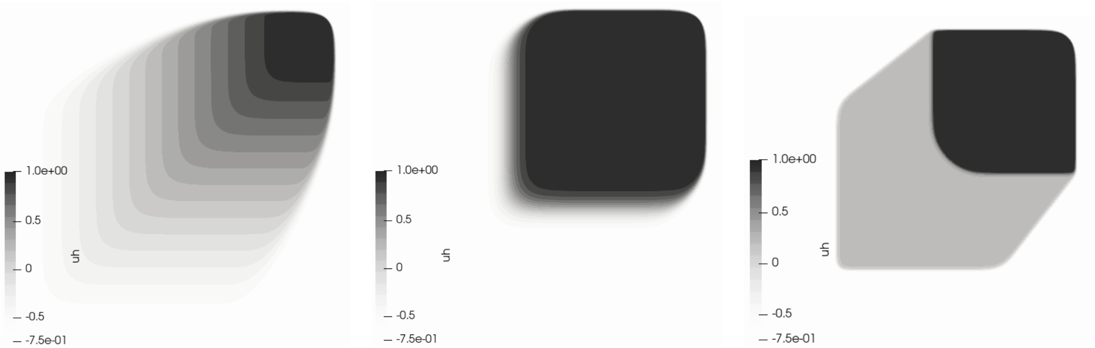
Numerical test V

$\boldsymbol{f}(u) = (\frac{1}{2}u^2, \frac{1}{2}u^2)$, $\mathcal{B} = [a, b] = [-0.75, 1]$.
For the reaction term, we introduce
$z = \varphi(v) = \frac{v-a}{b-a}$.

- $R_1(v) = z(1-z)(z-\varphi(0))$
- $R_2(v) = 4^4 z(z-\frac{1}{4})(z-\frac{1}{2})(z-\frac{3}{4})(1-z)$



Numerical test V



(a) $\epsilon = \infty$ (b) $\epsilon = 10^{-3}, R_1$ (c) $\epsilon = 10^{-3}, R_2$

Figure: 2D Burgers equation with rough IC, $\theta = \frac{1}{2}$, $\alpha = \varphi(0) = \frac{3}{7}$ in panel (b).

That's all

Thank you!

Back up

AP?

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$$\Phi_{\epsilon,h} = \max(h^\theta, \epsilon)$$

$\lim_{\epsilon\to0}\lim_{h\to0} u_h^\epsilon = u^0$

1. For fixed $\epsilon > 0$, $\lim_h \Phi_{\epsilon,h} = \epsilon \Rightarrow \lim_h u_h^\epsilon = u^\epsilon$.
2. $\lim_\epsilon \lim_h u_h^\epsilon = \lim_\epsilon u^\epsilon = u^0$.

$u^0 = \lim_{h\to0}\lim_{\epsilon\to0} u_h^\epsilon$

1. $\lim_\epsilon \Phi_{\epsilon,h} = h^\theta \Rightarrow \lim_\epsilon u_h^\epsilon = u_h^{h^\theta}$.
2. $|u_h^{h^\theta} - u^0| \leq |u_h^{h^\theta} - u^{h^\theta}| + |u^{h^\theta} - u^0| \to 0 \Rightarrow \lim_h \lim_\epsilon u_h^\epsilon = \lim_h u^{h^\theta} = u^0$.