On a numerical method for solving the equations of hydrodynamics and of ideal magnetohydrodynamics

Christian Klingenberg

Mathematics Dept., Würzburg University, Germany

presently visiting DMA, ENS, Rue d'Ulm

joint work with: Francois Bouchut, Ecole Normale Supérieure, Paris

Wolfram Schmidt, Astronomy Dept., Würzburg University, Germany

Knut Waagan, National Center for Atmospheric Research, Boulder, Colorado, USA

Entropy condition and conservation laws

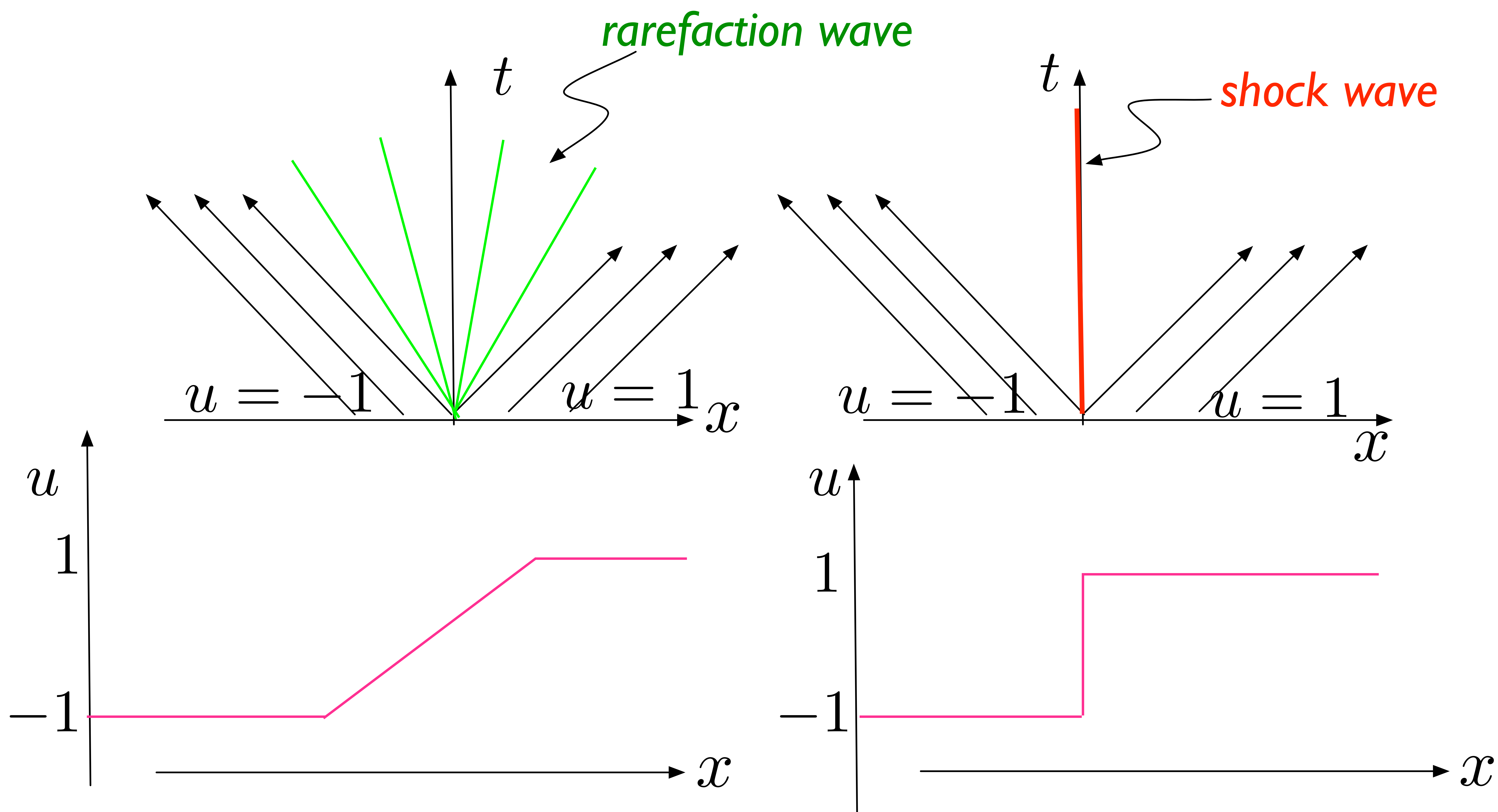
Many phenomena in continuum mechanics may be modelled as systems of hyperbolic conservation laws:

$$\frac{\partial U(x,t)}{\partial t} + \nabla F\big(U(x,t)\big) = 0$$

Their solutions need to be considered together with some *admissibility* condition,
also called *entropy* condition.

One initial data for the following scalar equation may allow for two solutions:

$$u_t + \left(\frac{u^2}{2}\right)_x = 0$$



Or consider equations of ideal magnetohydrodtynamics:

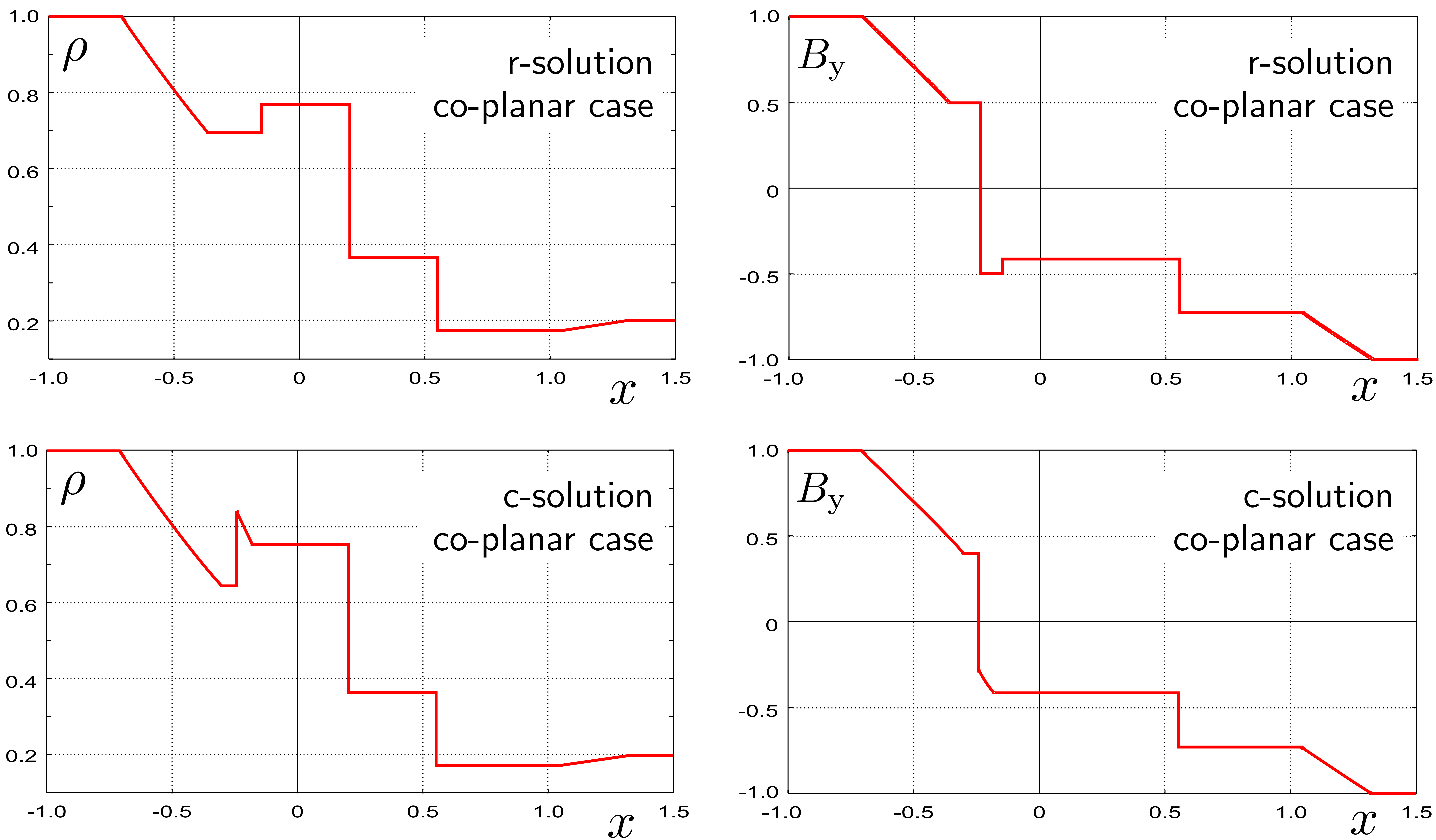
$$\partial_t \rho + \partial_x(\rho v_n) = 0,$$
$$\partial_t \rho v_n + \partial_x\left(\rho v_n^2 + p + \tfrac{1}{2}\mathbf{B}_t^2\right) = 0,$$
$$\partial_t \rho \mathbf{v}_t + \partial_x(\rho v_n \mathbf{v}_t - B_n \mathbf{B}_t) = 0,$$
$$\partial_t \mathbf{B}_t + \partial_x(v_n \mathbf{B}_t - B_n \mathbf{v}_t) = 0,$$
$$\partial_t E + \partial_x\left(\left(E + p + \tfrac{1}{2}\mathbf{B}_t^2\right) v_n - B_n \mathbf{B}_t \cdot \mathbf{v}_t\right) = 0.$$

with initial conditions:

$$\left(\rho_1, v_n^{(1)}, \mathbf{v}_t^{(1)}, B_n, \mathbf{B}_t^{(1)}, p_1\right) = \left(1, 0, \mathbf{0}, 1, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, 1\right),$$

$$\left(\rho_0, v_n^{(0)}, \mathbf{v}_t^{(0)}, B_n, \mathbf{B}_t^{(0)}, p_0\right) = \left(0.2, 0, \mathbf{0}, 1, \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}, 0.2\right)$$

Again the equations allows for two solutions:



Candidates for admissibility:

- *second law of thermodynamics*: the solution should satisfy an additional differential inequality, *entropy inequality*
- take into account *viscous effects:* take limit of vanishing viscosity

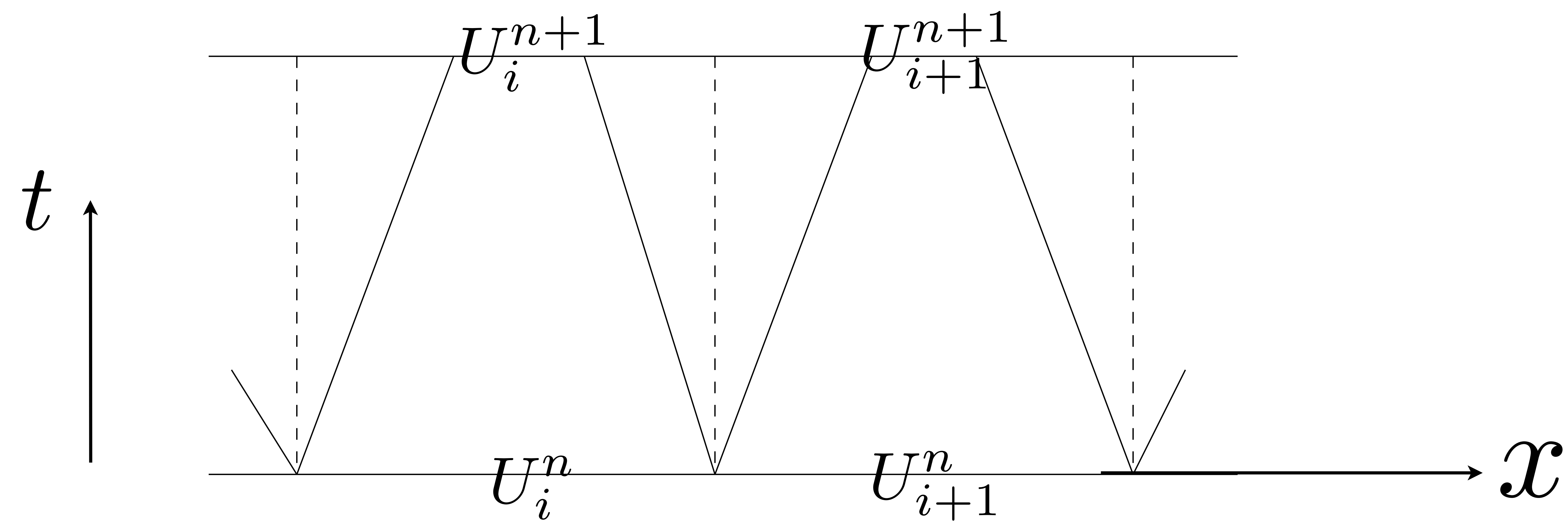
We shall use the following admissibility (or entropy) condition:

$$(\rho\phi(s))_t + \operatorname{div}(\rho\mathbf{u}\phi(s)) \le 0$$

where ϕ, is an appropriately chosen convex functional.

In particular an entropy condition should imply stability.
For gas dynamics it should be able to preserve nonnegative density and internal energy.

Thus we approximate our PDE by a Godunov-type scheme



$$U_i^{n+1} - U_i^n + \frac{\Delta t}{h_i}[F^c(U_i^n, U_{i+1}^n) - F^c(U_{i-1}^n, U_i^n)] = 0, \quad h_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$$

where the discrete solution satisfies

$$\eta(U_i^{n+1}) - \eta(U_i^n) + \frac{\Delta t}{h_i}[G^c(U_i^n, U_{i+1}^n) - G^c(U_{i-1}^n, U_i^n)] \leq 0$$

discrete entropy inequality

Such an a priori bound ensures that we compute physically relevant shocks.

For gas dynamics entropy consistency should give:

$$\text{if } \rho^n > 0 \text{ and } e^n > 0, \text{ then } \rho^{n+1} > 0 \text{ and } e^{n+1} > 0.$$

POSITIVITY

Brief history of approximate Riemann solvers

In the

1. **Reconstruct**
2. **Evolve**
3. **Average**

slide 10

Algorithm

Phil Roe in 1981 noticed that it is not necessary to do the evolution step (2.)(the Riemann solution) exact, because we loose quite a bit of information in the averaging step (3.).

He thus suggested to introduced an ***approximate Riemann solver***.

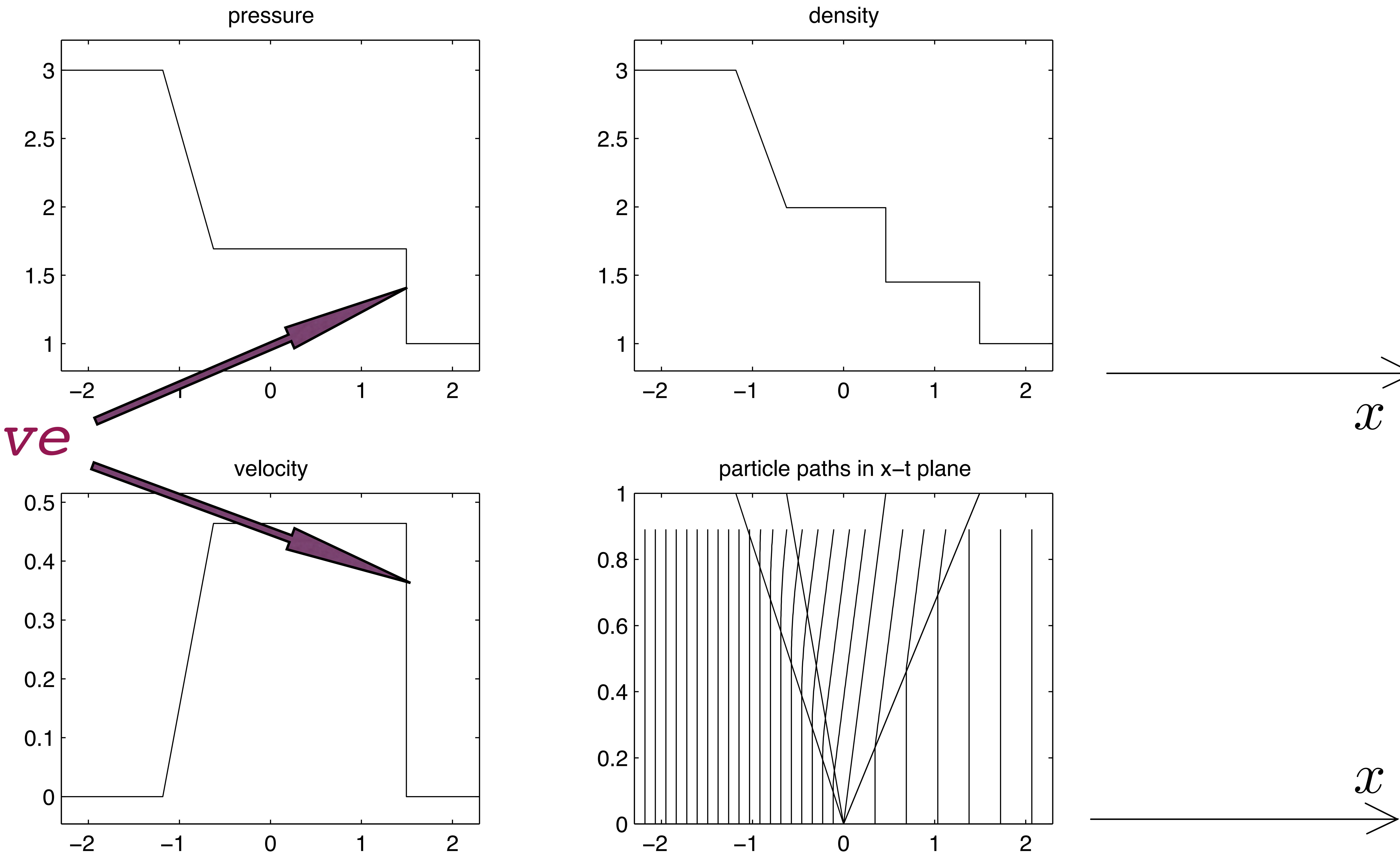
He introduced a local linearization of the flux which is consistent and conservative.

Shock tube problem for the Euler equations of compressible gas dynamics:

at time $t = 0$

membrane at $x = 0$

at time $t = 1$



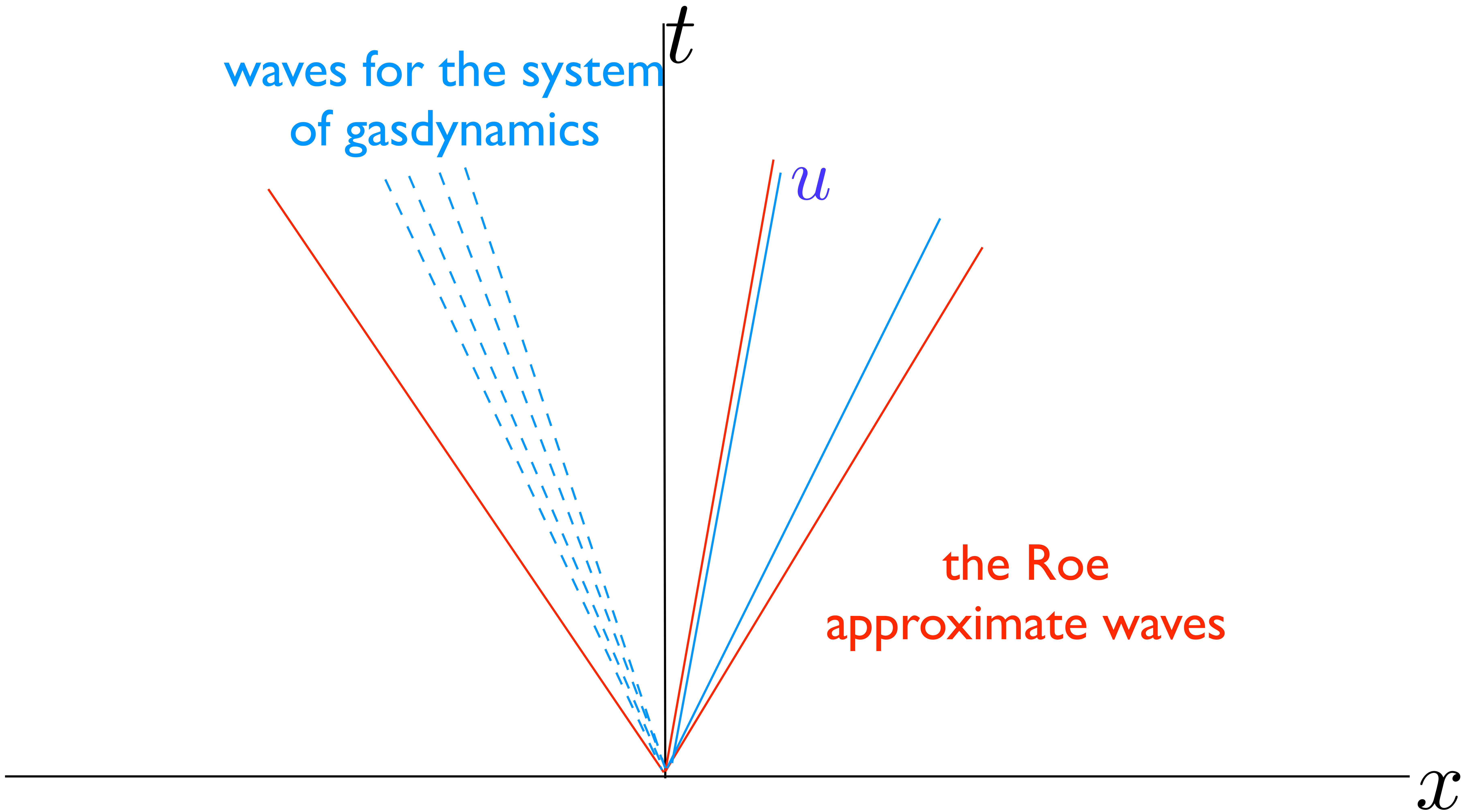
shock wave

x - axis

x - axis

This is the exact solution of the Riemann problem.

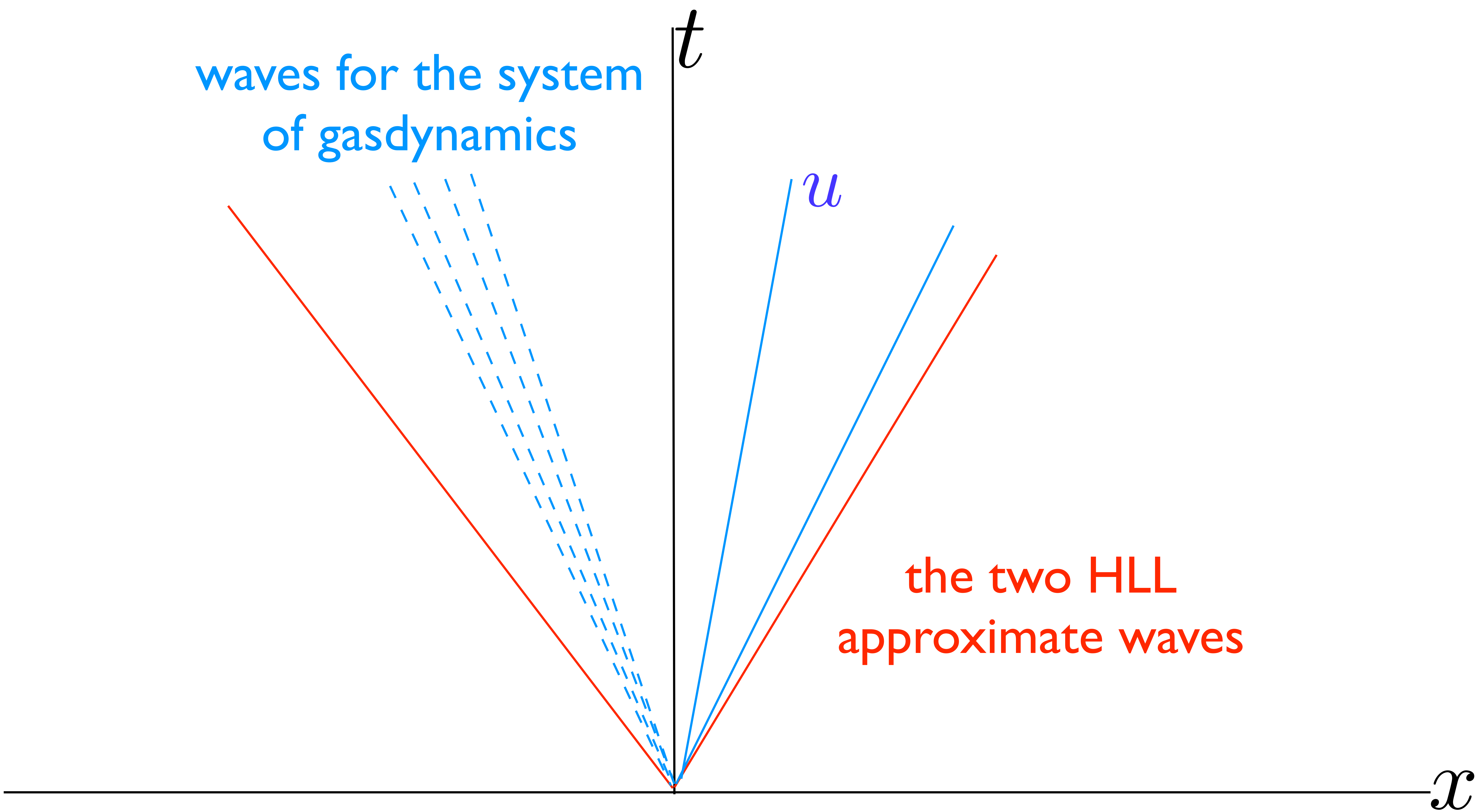
For the Euler equations Roe's approximate Riemann solver consists of three constant states separated by jumps.



advantage: can be made quite accurate

disadvantage: poor stability

Harten, Lax, van Leer 1983: even simpler approximate Riemann solver
with only two waves, called the "HLL" solver.



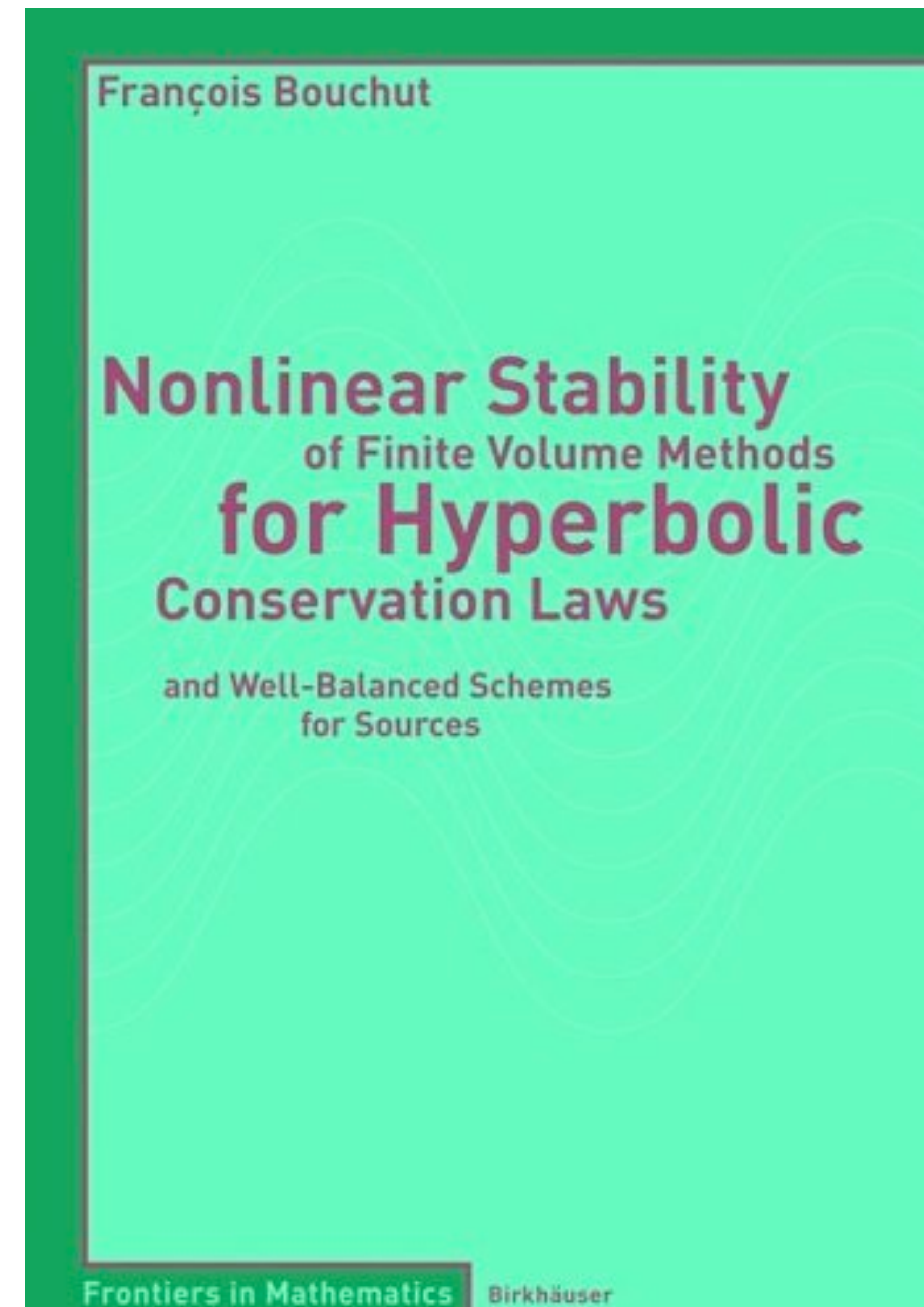
advantage: good stability, entropy consistent

disadvantage: poor accuracy

Toro et. al. (1994) for gas dynamics improved the HLL solver by introducing a middle wave, the "HLLC" solver.

Siliciu (1990), Tzavaras (1999) Coquel (1999), Coquel & Kl. (1999) and others noticed that the HLLC solver could be improved by a relaxation approach.

This opened the way for precise tools to analyze these schemes, see book by Bouchut (2004):



- relaxation solvers -

which are entropy consistent (stable), accurate and allow for rigorous analysis

The idea of relaxation solvers (using gas dynamics)

We embed system of compressible gas dynamics into a more "complete model".

For smooth solutions of the Euler equations

$$\begin{aligned} \rho_t + (\rho u)_x &= 0 \\ (\rho u)_t + (\rho u^2 + p)_x &= 0 \\ E_t + \big(u(E+p)\big)_x &= 0 \end{aligned}$$

we can write an evolution equation for the pressure:

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

Replace p by a new dependant variable π and let c replace the soundspeed $\rho\sqrt{p'(\rho)}$

$$(\rho\pi)_t + (\rho\pi u + c^2 u)_x = \rho\frac{p-\pi}{\epsilon}$$

Siliciu (1990), Coquel, et.al. (1999)

the enlarged system has a small parameter $\epsilon > 0$ s.th.

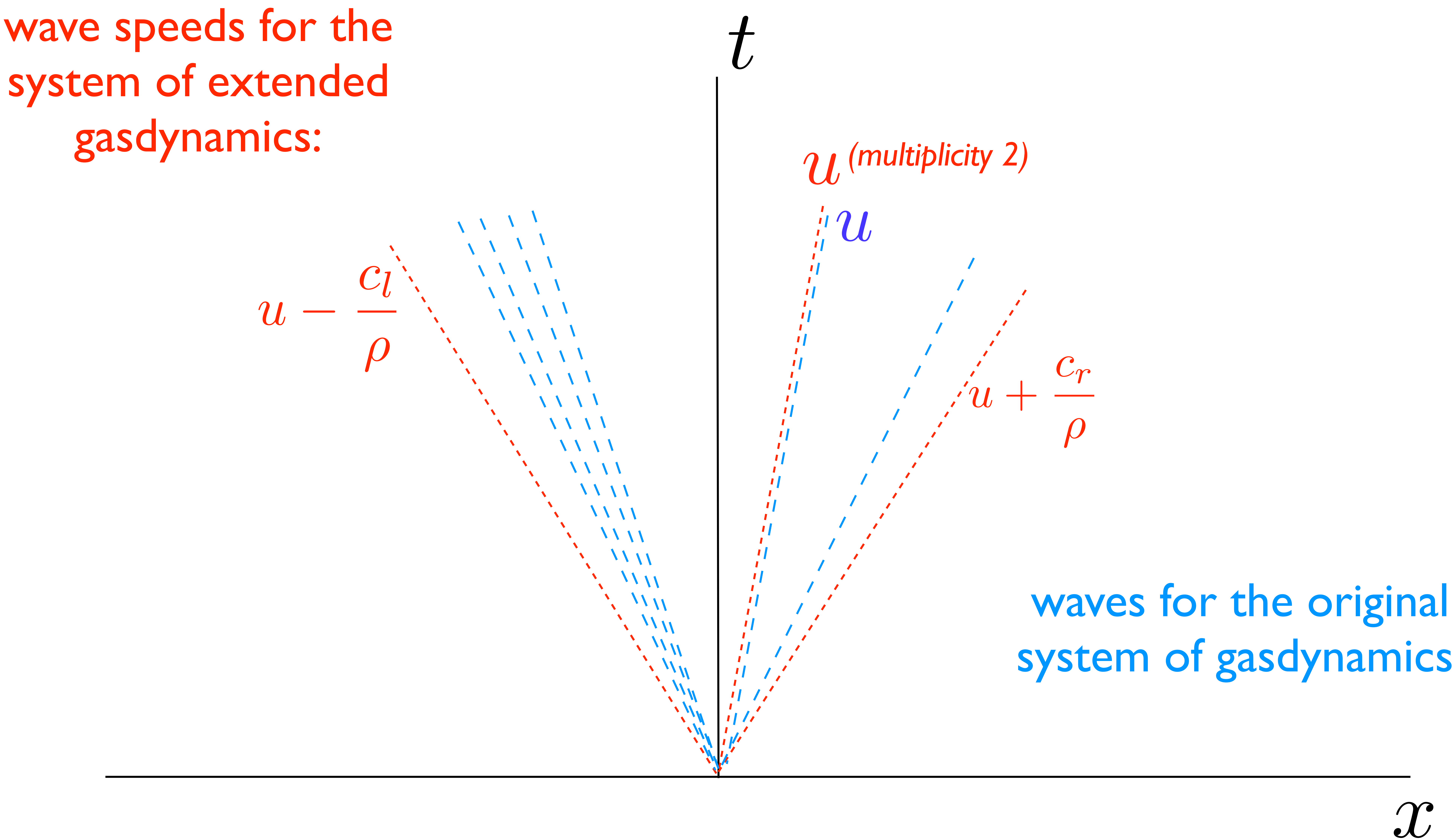
$\epsilon > 0$ enlarged system

$\epsilon = 0$ original system

$$\rho_t + (\rho u)_x = 0$$
$$(\rho u)_t + (\rho u^2 + \pi)_x = 0$$
$$E_t + [(E + \pi)u]_x = 0$$
$$(\rho\pi)_t + (\rho\pi u + c^2 u)_x = \rho\frac{p - \pi}{\epsilon}$$

The constant c replaces the sound speed, which is a nonlinear function.

The advantage of the extended system is that by making the pressure a new dependent variable it easy to solve the Riemann problem for the homogeneous part of the extended system (all eigenvalues are degenerate).


wave speeds for the system of extended gasdynamics:
t
u (multiplicity 2)
u
$u - \frac{c_l}{\rho}$
$u + \frac{c_r}{\rho}$
waves for the original system of gasdynamics:
x

Absolutely essential is the choice of the constant c (replacing the sound speed).

$$c > \rho\sqrt{p'(\rho)}$$

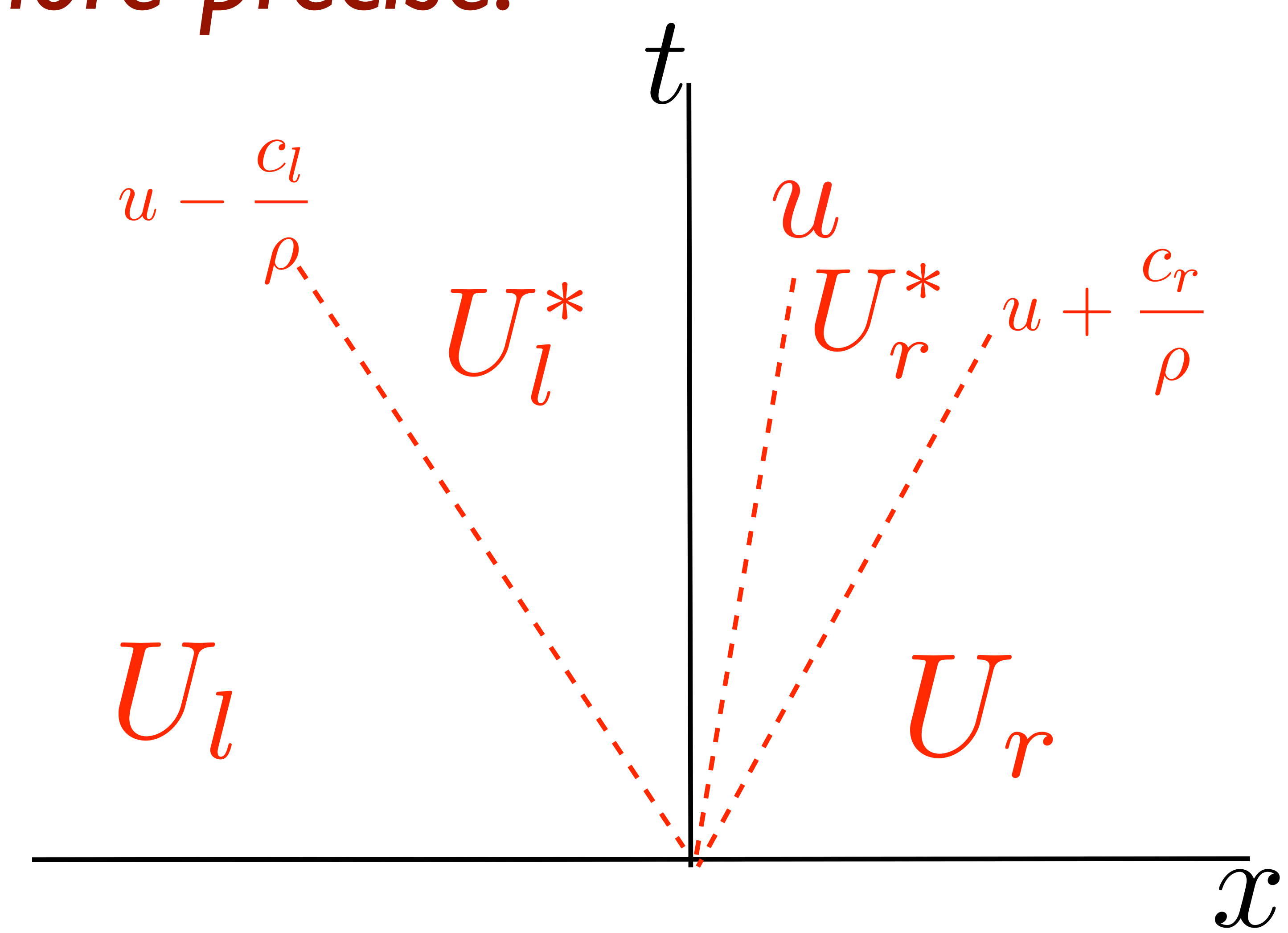
"subcharacteristic condition"

The choice of c determines the "stability' of this relaxation.

It ensures an entropy inequality.

This is analyzed à la Chen, Levermore, Liu (1994) allowing for rigorous justification.

more precise:



$$\forall \rho \in [\rho_l, \rho_l^*], \quad \rho^2 \left(\frac{\partial p}{\partial \rho}\right)_s \leq c_l^2$$

$$\forall \rho \in [\rho_r, \rho_r^*], \quad \rho^2 \left(\frac{\partial p}{\partial \rho}\right)_s \leq c_r^2$$

For practical purposes, in order to devise a formula for a numerical scheme, one has to choose a particular value for c out of the possible values the inequality allows for.

$$
\text{if } p_r - p_l \geq 0, \quad \begin{cases} \dfrac{c_l}{\rho_l} = \sqrt{p'(\rho_l)} + \alpha \left(\dfrac{p_r - p_l}{\rho_r \sqrt{p'(\rho_r)}} + u_l - u_r \right)_+, \\ \dfrac{c_r}{\rho_r} = \sqrt{p'(\rho_r)} + \alpha \left(\dfrac{p_l - p_r}{c_l} + u_l - u_r \right)_+, \end{cases}
$$

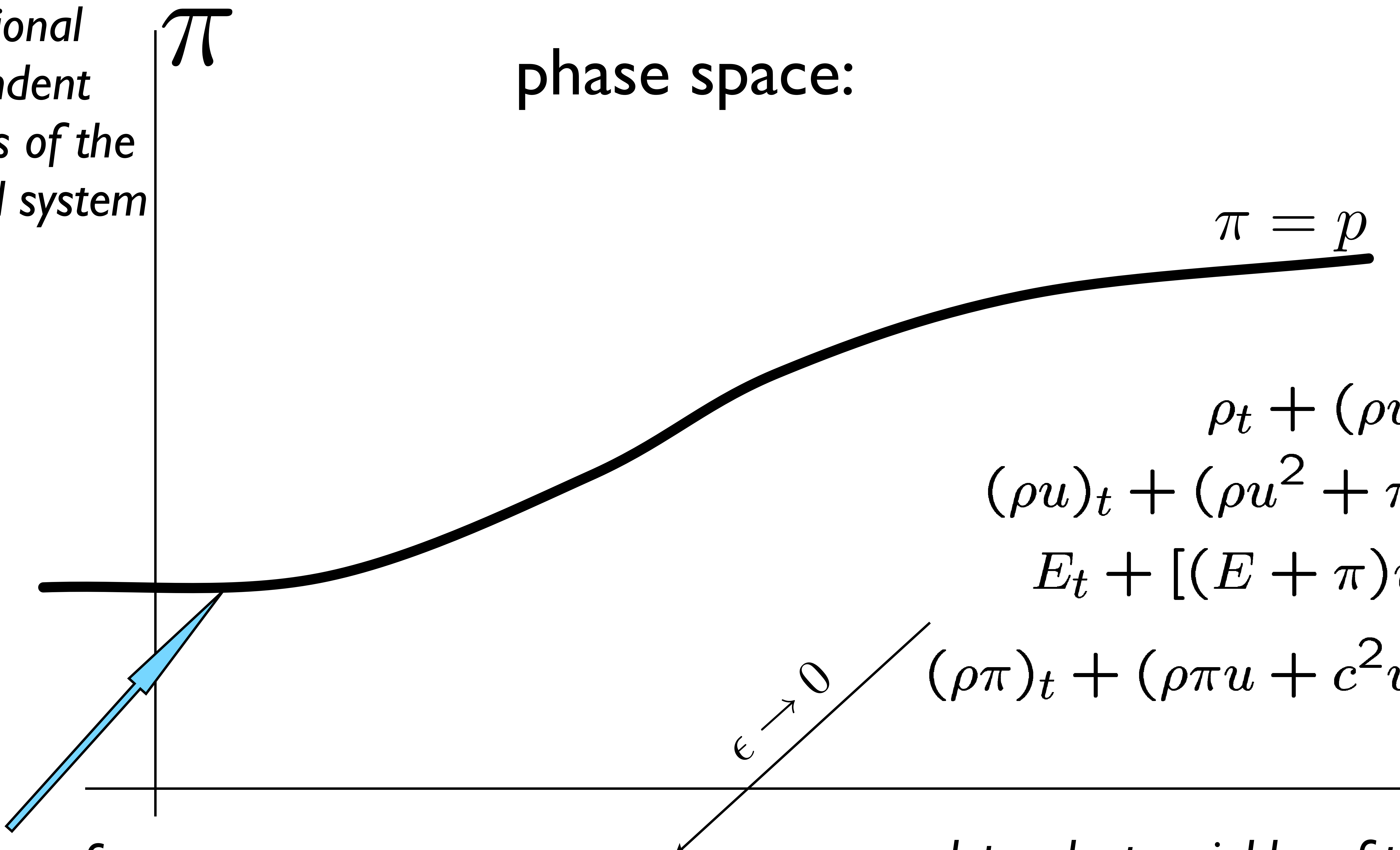
$$
\text{if } p_r - p_l \leq 0, \quad \begin{cases} \dfrac{c_r}{\rho_r} = \sqrt{p'(\rho_r)} + \alpha \left(\dfrac{p_l - p_r}{\rho_l \sqrt{p'(\rho_l)}} + u_l - u_r \right)_+, \\ \dfrac{c_l}{\rho_l} = \sqrt{p'(\rho_l)} + \alpha \left(\dfrac{p_r - p_l}{c_r} + u_l - u_r \right)_+. \end{cases}
$$

Bouchut (2004)

This ensures the optimal properties of this approximate Riemann solver.

Illustrate relaxation solver in phase space

additional dependent variables of the extended system



equilibrium manifold

$$\rho_t + (\rho u)_x = 0$$
$$(\rho u)_t + (\rho u^2 + \pi)_x = 0$$
$$E_t + [(E + \pi)u]_x = 0$$
$$(\rho\pi)_t + (\rho\pi u + c^2 u)_x = \rho\frac{p - \pi}{\epsilon}$$

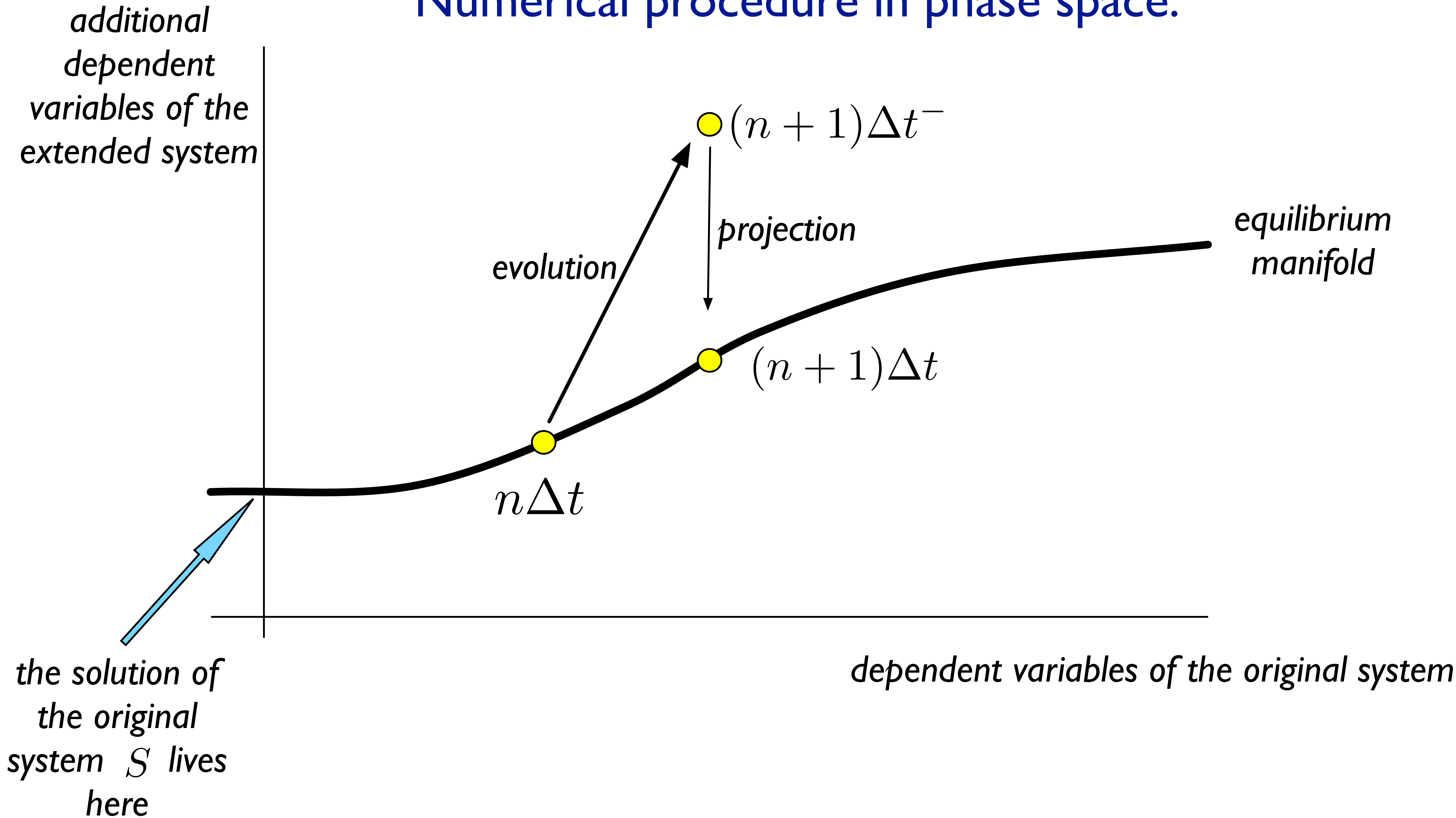
the solution of the original system lives here

$$\rho_t + (\rho u)_x = 0$$
$$(\rho u)_t + (\rho u^2 + p)_x = 0$$
$$E_t + \big(u(E + p)\big)_x = 0$$

dependent variables of the original system

ρ, u, E

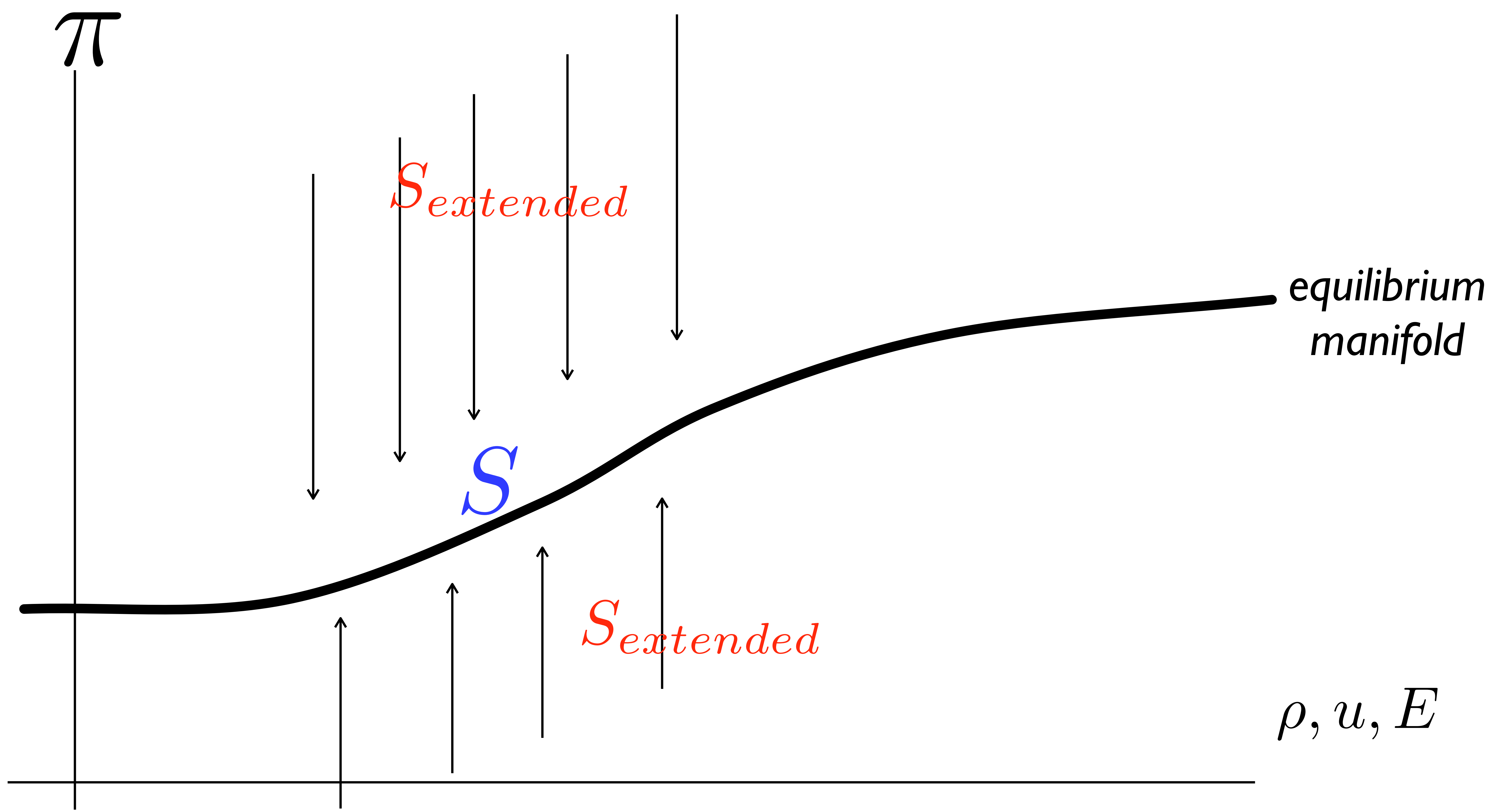
Numerical procedure in phase space:



This results in a numerical method for the original system.

It is possible to extend the entropy S of the original system of gas dynamics to an entropy $S_{extended}$ of the system of extended gas dynamics

such that for $\epsilon \longrightarrow 0$ the extended entropy converges to the original entropy.



this procedure translates Riemann solvers for the extended system to Riemann solvers for the original system

- preserves $\rho \geq 0$
- can handle vacuum
- this ensures that the "second law of thermodynamics" is staisfied by the numerical solution of our original system

A relaxation solver for magnetohydrodynamics

Bouchut, Klingenberg, Waagan: *A multi-wave approximate Riemann solver for ideal MHD based on relaxation I - theoretical framework*, Numerische Mathematik (2007)

Brief introduction into magnetohydrodynamics (MHD)

- ionized compressible gas subject to magnetic fields
- couple the Euler equations of compressible gas dynamics to equations for magnetic fields

Ideal MHD: Ignore resistivity ("viscous effect") $\Longrightarrow$ hyperbolic system.

New issues:

- Coupled with elliptic constraint $\nabla \cdot \vec{B} = 0$.
- Nonstrictly hyperbolic
- Nonconvex (not strictly hyperbolic) $\Longrightarrow$ compound waves

Conservation laws of MHD

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho\vec{u}\\ \vec{B}\\ E\end{bmatrix}+\nabla\cdot\begin{bmatrix}\rho\vec{u}\\ \rho\vec{u}\vec{u}+I\left(\left(p+\frac{1}{2}B^2\right)-\vec{B}\vec{B}\right)\\ \vec{u}\vec{B}-\vec{B}\vec{u}\\ \left(E+p+\frac{1}{2}B^2\right)\vec{u}-\vec{B}(\vec{u}\cdot\vec{B})\end{bmatrix}=0.$$

go to
page 41

In components:

$$q=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ B^{(x)}\\ B^{(y)}\\ B^{(z)}\\ E\end{bmatrix},\qquad f(q)=\begin{bmatrix}\rho u\\ \rho u^2+p+\frac{1}{2}B^2-(B^{(x)})^2\\ \rho uv-B^{(x)}B^{(y)}\\ \rho uw-B^{(x)}B^{(z)}\\ 0\\ vB^{(x)}-B^{(y)}u\\ wB^{(x)}-B^{(z)}u\\ u\left(E+p+\frac{1}{2}B^2\right)-B^{(x)}(uB^{(x)}+vB^{(y)}+wB^{(z)})\end{bmatrix}$$

One-dimensional MHD

$$q_t + f(q)_x = 0$$

Note that

$$\frac{\partial}{\partial t} B^{(x)} = 0$$

In 1-D, $\nabla \cdot \vec{B} = 0$ means $B^{(x)} =$ constant.

Variations in $B^{(x)}$ remain stationary.

1-D equations reduce to **7-wave system** for

$$\tilde{q} = (\rho, \rho u, \rho v, \rho w, B^{(y)}, B^{(z)}, E).$$

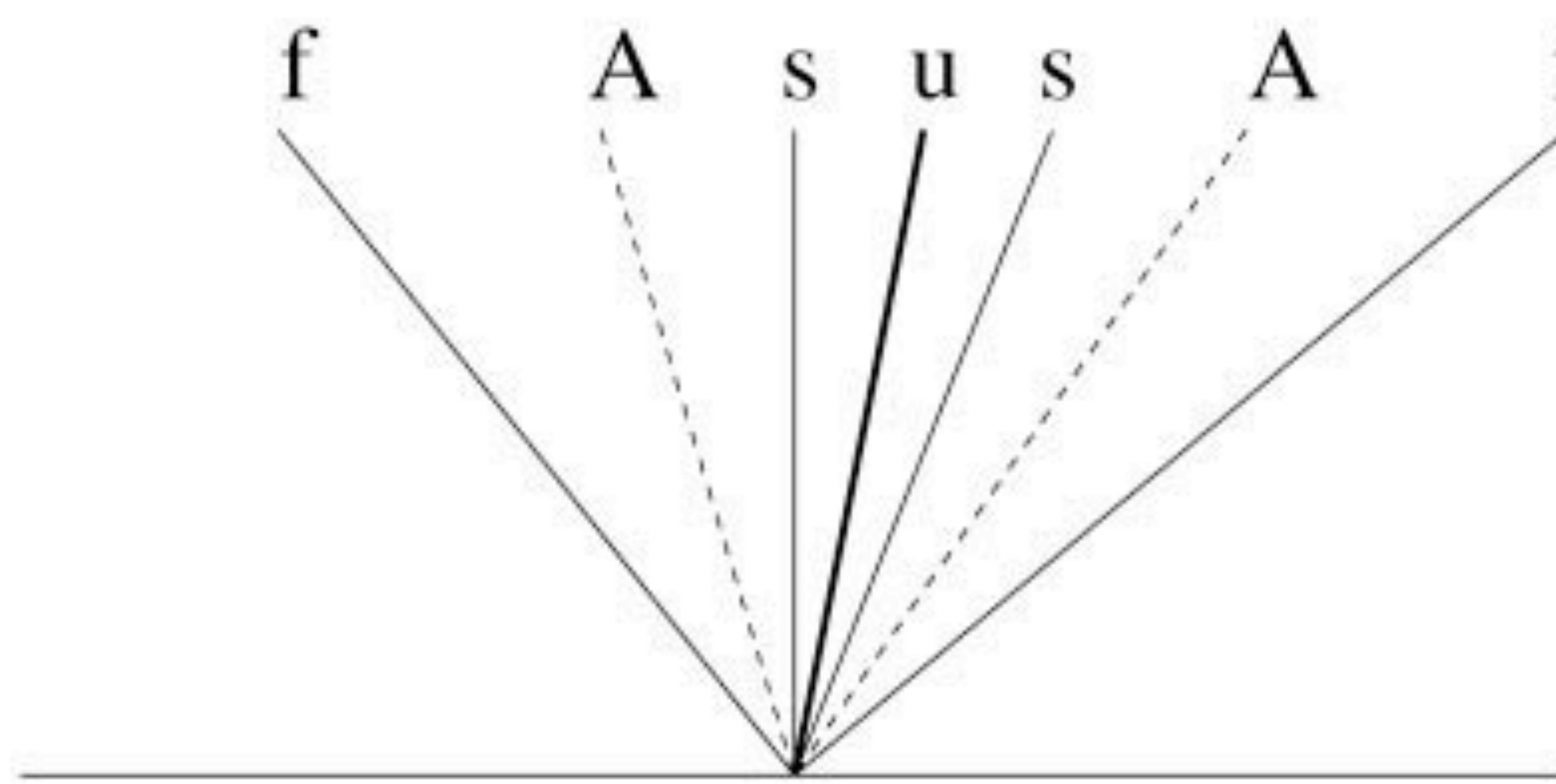
$$\boxed{\begin{aligned} \text{also write } (v, w) &= u_\perp \\ (B_y, B_z) &= B_\perp \end{aligned}}$$

Jacobian matrix has 7 eigenvalues (wave speeds)

$$u, \quad u \pm c_s, \quad u \pm c_A, \quad u \pm c_f$$

Waves in one-dimensional MHD

u	entropy waves — contact discontinuities
$u \pm c_s$	slow magnetosonic waves
$u \pm c_A$	Alfvén waves
$u \pm c_f$	fast magnetosonic waves



Magnetosonic waves are genuinely nonlinear

The divergence of B

In theory $\nabla \cdot \vec{B} \equiv 0$.

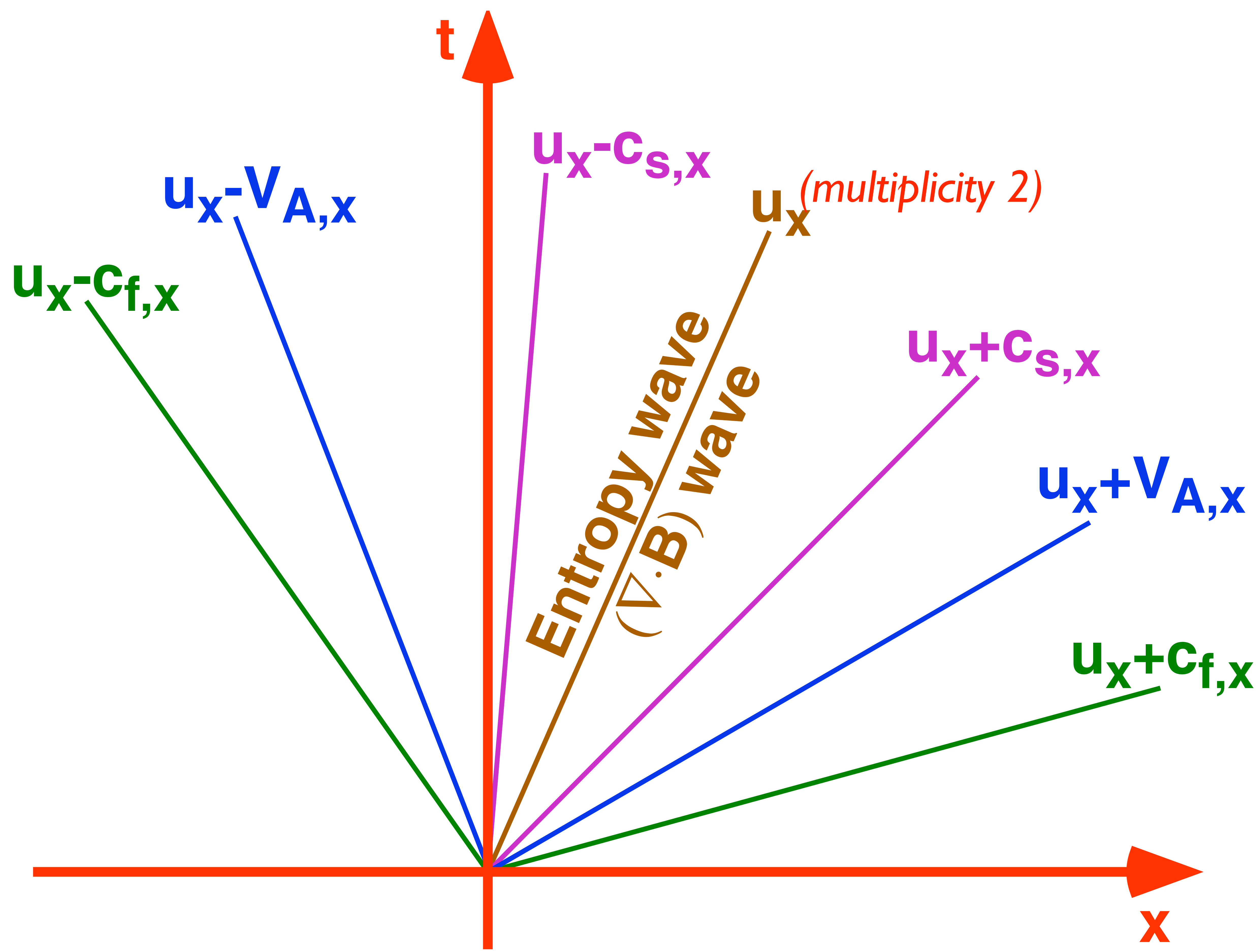
True at $t = 0 \implies$ true for all time.

Numerical methods may not preserve this.

Various approaches:

- Don't worry about it
  (ok for smooth solutions to order of method)
- Divergence-cleaning — projection onto $\nabla \cdot \vec{B} = 0$
- Constrained transport:
  Staggered grids and updating formula that preserves
  $\nabla \cdot \vec{B} = 0$
- 8-wave solver — advect $\nabla \cdot \vec{B}$ away

wave speeds for the original system of MHD:



the Powell 8-wave structure

comparing wave structure for hydrodynamics (HD) and MHD:

- HD (Euler): $(n = 5)$
  - $\lambda = u, u, u, u + c, u - c$
  - one nonlinear wave mode
  - one type of shock

- MHD: $(n = 8)$
  - $\lambda = u, u, u + c_f, u - c_f,$
    $u + c_A, u - c_A, u + c_s, u - c_s$
  - three wave modes: fast, Alfven, slow
  - three types of shocks

Designing the relaxation solver for MHD

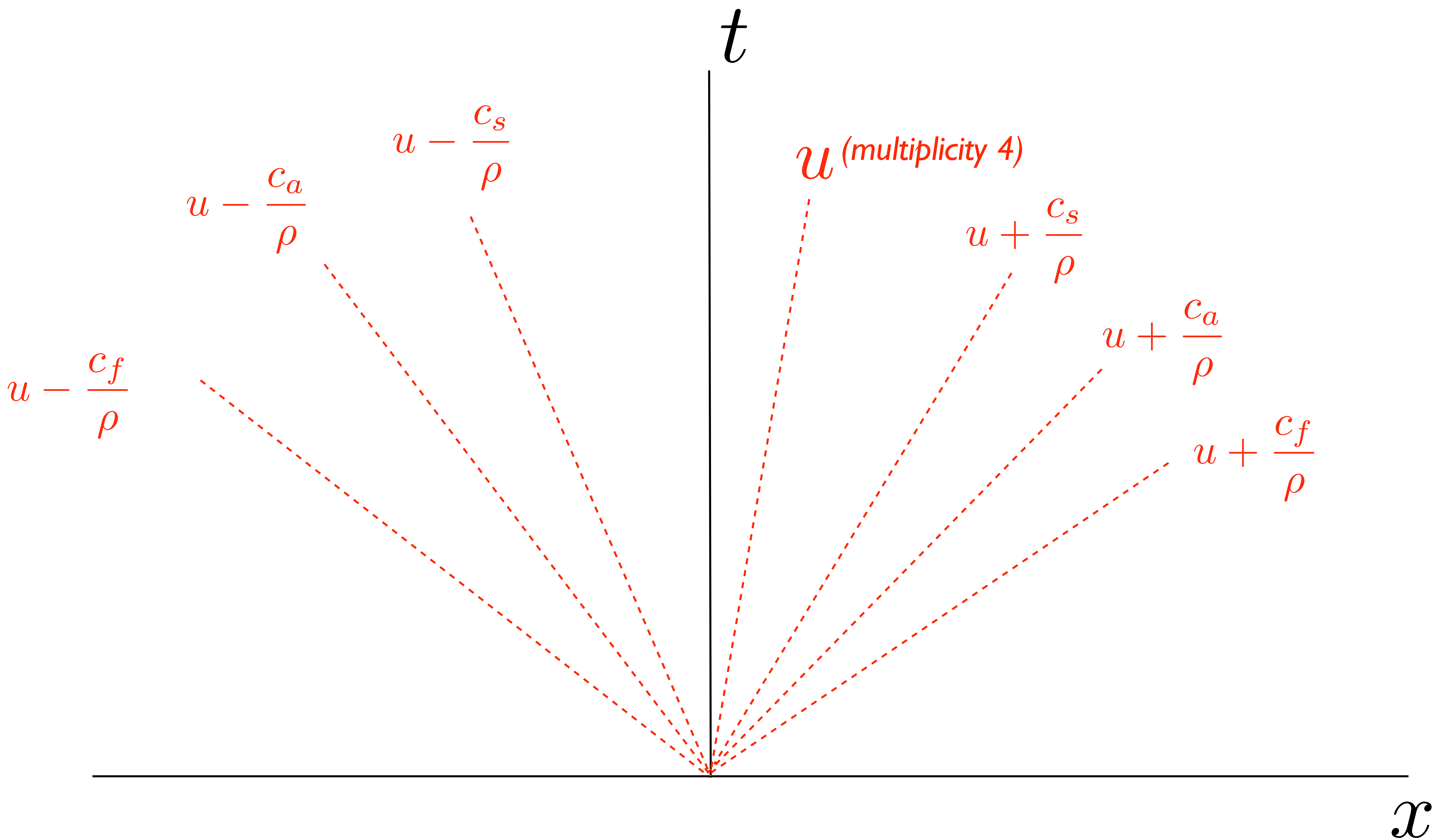
The extended system for MHD:

$$
\begin{aligned}
\rho_t + (\rho u)_x &= 0 \\
(\rho u)_t + (\rho u^2 + \pi)_x &= 0 \\
(\rho u_\perp)_t + (\rho u v + \pi_\perp)_x &= 0 \\
E_t + [(E + \pi)u + \pi_\perp \cdot u_\perp]_x &= 0 \\
(B_\perp)_t + (B_\perp u - B_x u_\perp)_x &= 0 \\
(\rho\pi)_t + [\rho\pi u + (c_s^2 + c_f^2 - c_a^2)u - c_a b \cdot u_\perp]_x &= \rho \frac{p + \frac{1}{2}B_\perp^2 - \frac{1}{2}B_x^2 - \pi}{\epsilon} \\
(\rho\pi_\perp)_t + (\rho\pi_\perp u + c_a^2 u - c_a b u)_x &= \rho \frac{-B_x B_\perp - \pi_\perp}{\epsilon}
\end{aligned}
$$

go to page 35

with:
$$
\begin{aligned}
\pi &= p + |B|^2/2 - B_x^2 \\
\pi_\perp &= -B_x B_\perp
\end{aligned}
$$

wave speeds for the system of extended magnetohydrodynamics:



A three wave approximate Riemann solver is obtained by:

$$\text{Set } c_s = c_a = c_f$$

Theorem

The approximate Riemann solver defined by this 3-wave relaxation is positive and defines a discrete entropy inequality if for all intermediate states we have:

$$\frac{1}{\rho_2} - \frac{B_x^2}{c_a^2} \geq 0$$

$$\left| \frac{B_\perp^1 + B_\perp^2}{2} - \frac{B_x b}{c_a} \right|^2 \leq \left(\frac{c_s^2 c_f^2}{c_a^2} - (\rho^2 p')_{1,2} \right) \left(\frac{1}{\rho_2} - \frac{B_x^2}{c_a^2} \right)$$

The proof of the discrete entropy inequality

$$\rho_i^{n+1}\phi(s(\rho_i^{n+1},e_i^{n+1}))-\rho_i^n\phi(s(\rho_i^n,e_i^n))+\frac{\Delta t}{h}\left(G^s_{i+\frac{1}{2}}-G^s_{i-\frac{1}{2}}\right)\leq 0$$

is given in Bouchut, Kl., Waagan (2007).

A formal derivation of this for smooth solutions is available by a Chapman-Enscog expansion.

Write $\pi = p+\frac{1}{2}B_\perp^2 - \frac{1}{2}B_x^2 + g(\epsilon) + O(\epsilon^2)$ $\qquad \pi_\perp = -B_x B_x + +g_\perp \epsilon + O(\epsilon^2)$

Insert this into the extended system

$$\begin{aligned}
\rho_t + (\rho u)_x &= 0\\
(\rho u)_t + (\rho u^2+\pi)_x &= 0\\
(\rho u_\perp)_t + (\rho u v + \pi_\perp)_x &= 0\\
E_t + [(E+\pi)u + \pi_\perp\cdot u_\perp]_x &= 0\\
(B_\perp)_t + (B_\perp u - B_x u_\perp)_x &= 0\\
(\rho\pi)_t + [\rho\pi u + (c_s^2+c_f^2-c_a^2)u - c_a b\cdot u_\perp]_x &= \rho\frac{p+\frac{1}{2}B_\perp^2-\frac{1}{2}B_x^2-\pi}{\epsilon}\\
(\rho\pi_\perp)_t + (\rho\pi_\perp u + c_a^2 u - c_a b u)_x &= \rho\frac{-B_x B_\perp - \pi_\perp}{\epsilon}
\end{aligned}$$

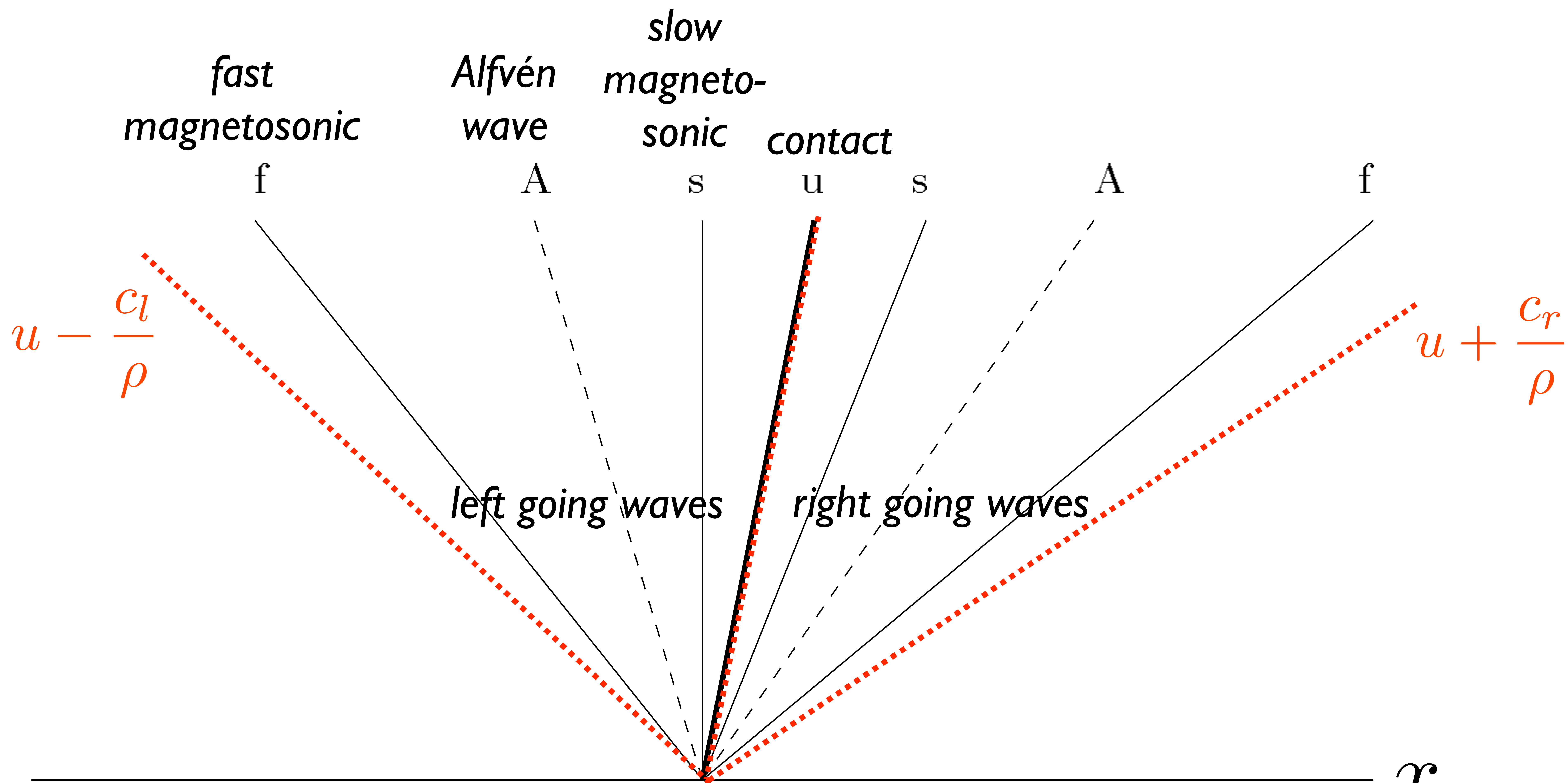
This gives

$$
\begin{aligned}
\rho_t + (\rho u)_x &= 0 \\
(\rho u)_t + (\rho u^2 + \pi)_x &= \epsilon \left[\left(\frac{c_s^2 + c_f^2 - c_a^2}{\rho} - (\rho p' + B_\perp^2) \right) u_x + (B_x B_\perp - \frac{B_x b}{c_a})(u_\perp)_x \right]_x + O(\epsilon^2) \\
(\rho u_\perp)_t + (\rho u v + \pi_\perp)_x &= \epsilon \left[(B_x B_\perp - \frac{B_x b}{c_a}) u_x + (\frac{c_a^2}{\rho} - B_x^2)(u_\perp)_x \right]_x + O(\epsilon^2) \\
E_t + [(E+\pi)u + \pi_\perp \cdot u_\perp]_x &= \epsilon \Bigg[u \left(\frac{c_s^2 + c_f^2 - c_a^2}{\rho} - (\rho p' + B_\perp^2) \right) u_x + u(B_x B_\perp - \frac{B_x b}{c_a}) \cdot (u_n)_x \\
&\quad + u_\perp \cdot (B_x B_\perp - \frac{B_x b}{c_a}) u_x + u_\perp \cdot (\frac{c_a^2}{\rho} - B_x^2)(u_\perp)_x \Bigg]_x + O(\epsilon^2) \\
(B_\perp)_t + (B_\perp u - B_x u_\perp)_x &= 0
\end{aligned}
$$

The entropy is evolved by an equation of the type

$$\eta(U)_t + G(U)_x - \epsilon[\eta'(U) D(U) U_x]_x = -\epsilon D(U)^t \eta''(U) U_x \cdot U_x$$

The conditions of the theorem then ensure entropy dissipation.



the three wave solver superimposed onto the exact 8-wave solution

When devising a numerical scheme we need to get concrete speeds of the waves out of the inequality in the theorem.

Bouchut, Klingenberg, Waagan: *A multiwave approximate Riemann solver for ideal MHD based on relaxation II - numerical aspects*, manuscript (2007)

Theorem:

For the three wave solver the following relaxation speeds are sufficient to guarantee positivity and entropy stability:

$$c_l = \rho_l a_l^0 + \alpha \rho_l \left((u_l - u_r)_+ + \frac{(\pi_r - \pi_l)_+}{\rho_l \sqrt{p_l'} + \rho_r a_{qr}} \right)$$

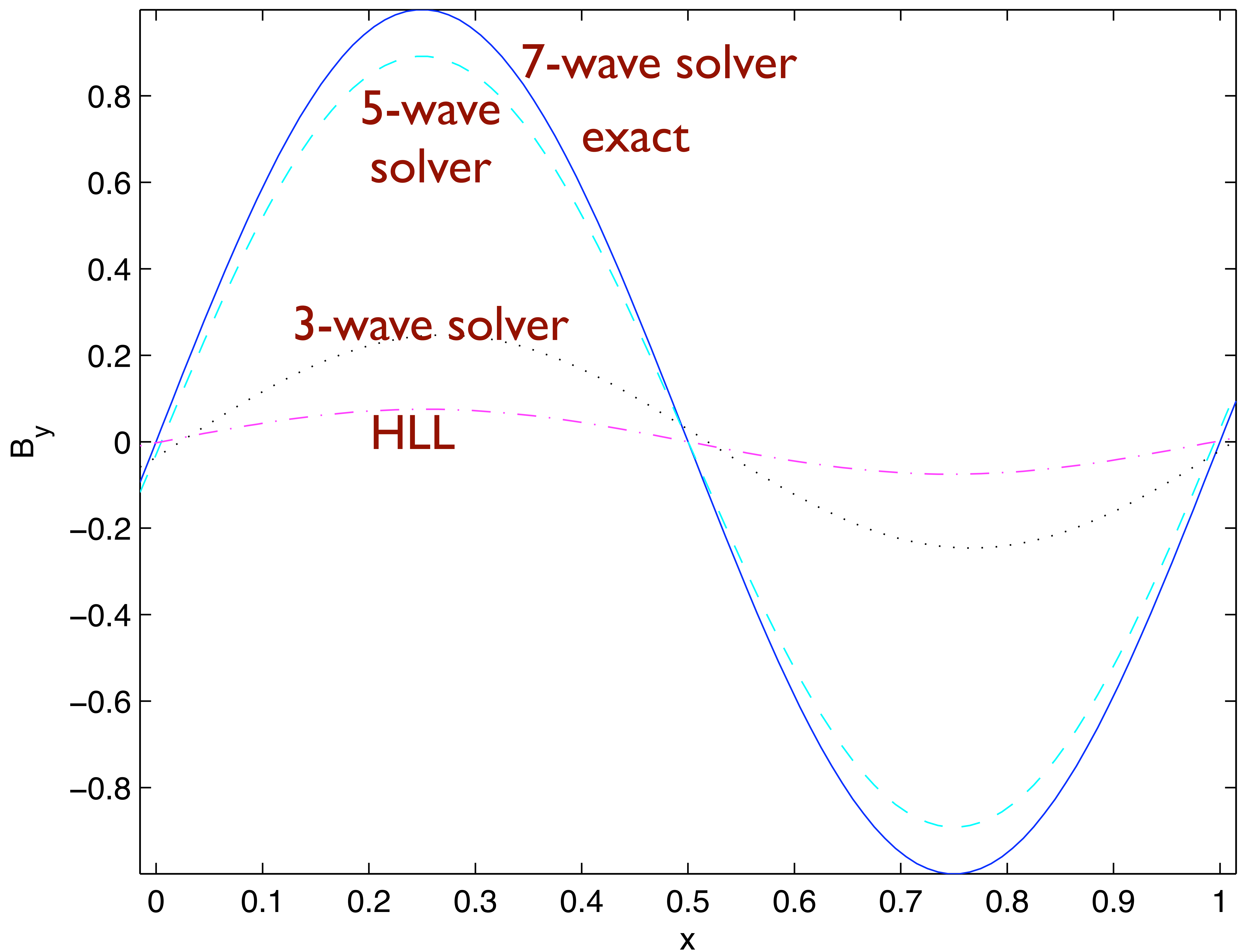
$$c_r = \rho_r a_r^0 + \alpha \rho_r \left((u_l - u_r)_+ + \frac{(\pi_l - \pi_r)_+}{\rho_r \sqrt{p_r'} + \rho_l a_{ql}} \right)$$

where $\alpha = \frac{\gamma + 1}{2}$ and α_l^0 α_r^0 are given by a complicated formula.

We have also found a seven wave approximate solver.

again we can prove entropy consistency under some complicated "subcharacteristic" condition

We have explicit formulas for the speeds.



$$\rho = 1.0, \quad p = 1.0$$

$$B_y = -\sin(2\pi x) \quad B_z = -\cos(2\pi x)$$

$$v = \sin(2\pi x) \quad w = \cos(2\pi x)$$

$$B_x = 1.0, \quad \gamma = 5/3.$$

stationary left-going Alfven wave

How do relaxation solvers compare to other solvers in applications?

We tested such a new approximate Riemann solver in an astrophysics code:

PROMETHEUS

developed in Max Planck Institute Astronomy (in Munich) since 1989 (Müller)
ported to FLASH (in Chicago) and still used today.

This code solves the hydrodynamic equations and has additional physical effects implemented.

Klingenberg, Schmidt, Waagan: *Numerical comparison of Riemann solvers for astrophysical hydrodynamics*, Journal of Computational Physics (2007)

PROMETHEUS	***PROMETHEUS - modified (preliminary)***
PPM *(piecewise parabolic method)*	PPM with our Riemann solver
This uses an “exact” Riemann solver. It is higher order accurate.	This uses our approximate Riemann solver.

Our approximate Riemann solver satisfies the entropy condition
and it also ensures that density will not become negative.

The PPM method in PROMETHEUS can not guarantee this.

Thus PPM with our Riemann solver can not guarantee this.

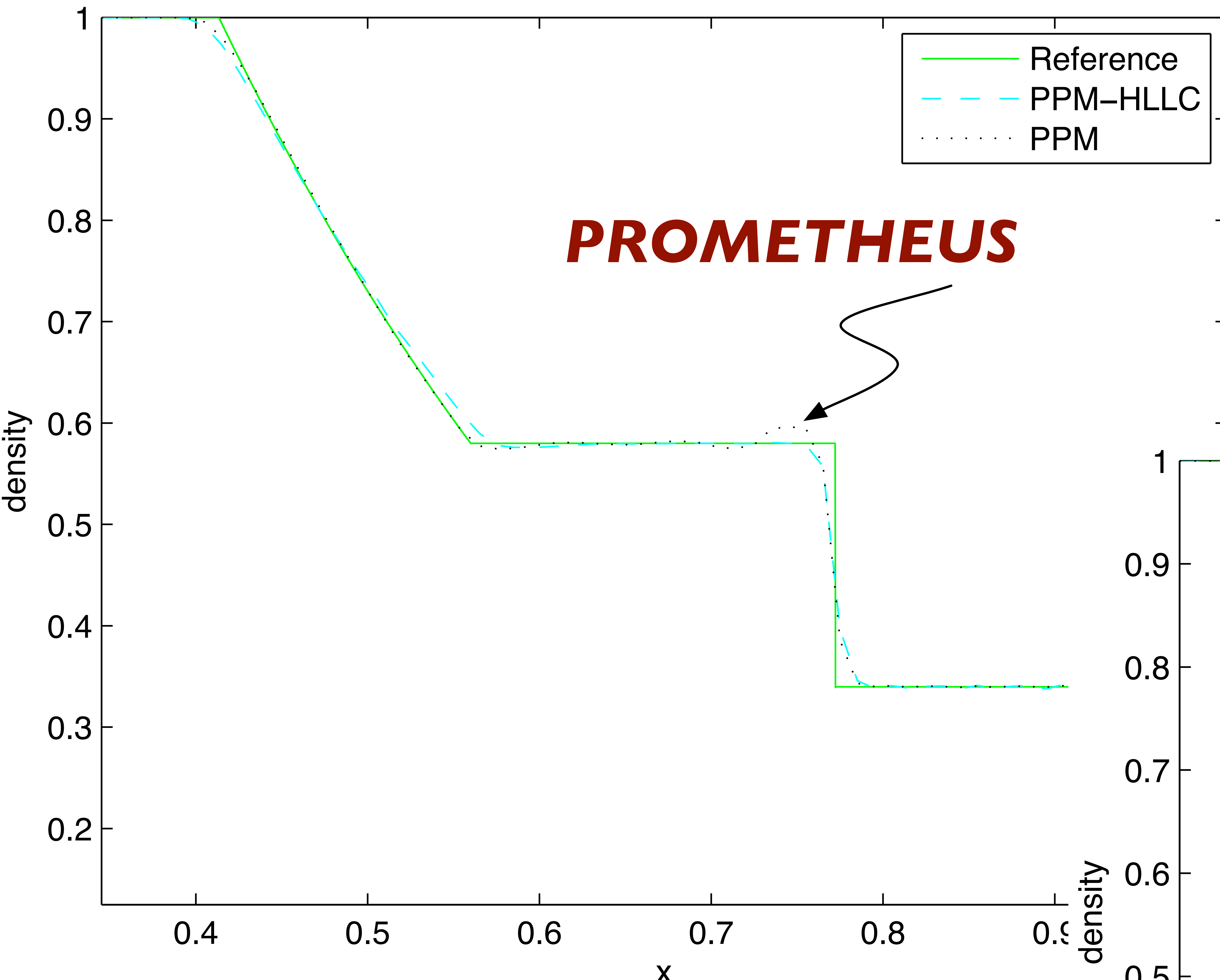
Hence we have also changed the numerical method in PROMETHEUS which makes the method higher order accurate.

PROMETHEUS - modified:

- our Riemann solver, made higher order such that positivity is preserved
- a new time integration was implemented (Runge-Kutta)

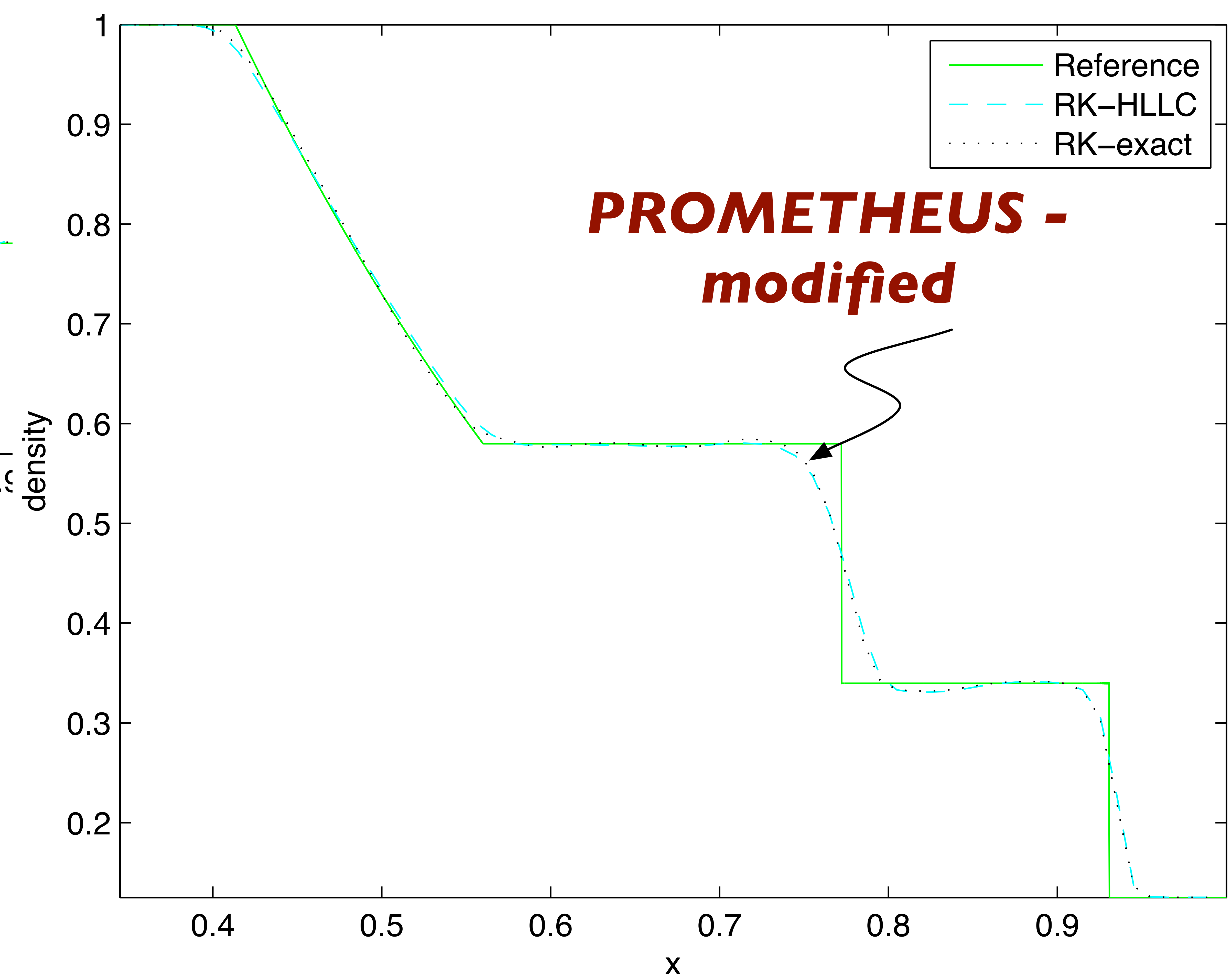
we compared these two codes:

- in one space dimension: particular Riemann problems
- in two space dimensons: mixing layers
- in three space dimensions: driven fully developed turbulence



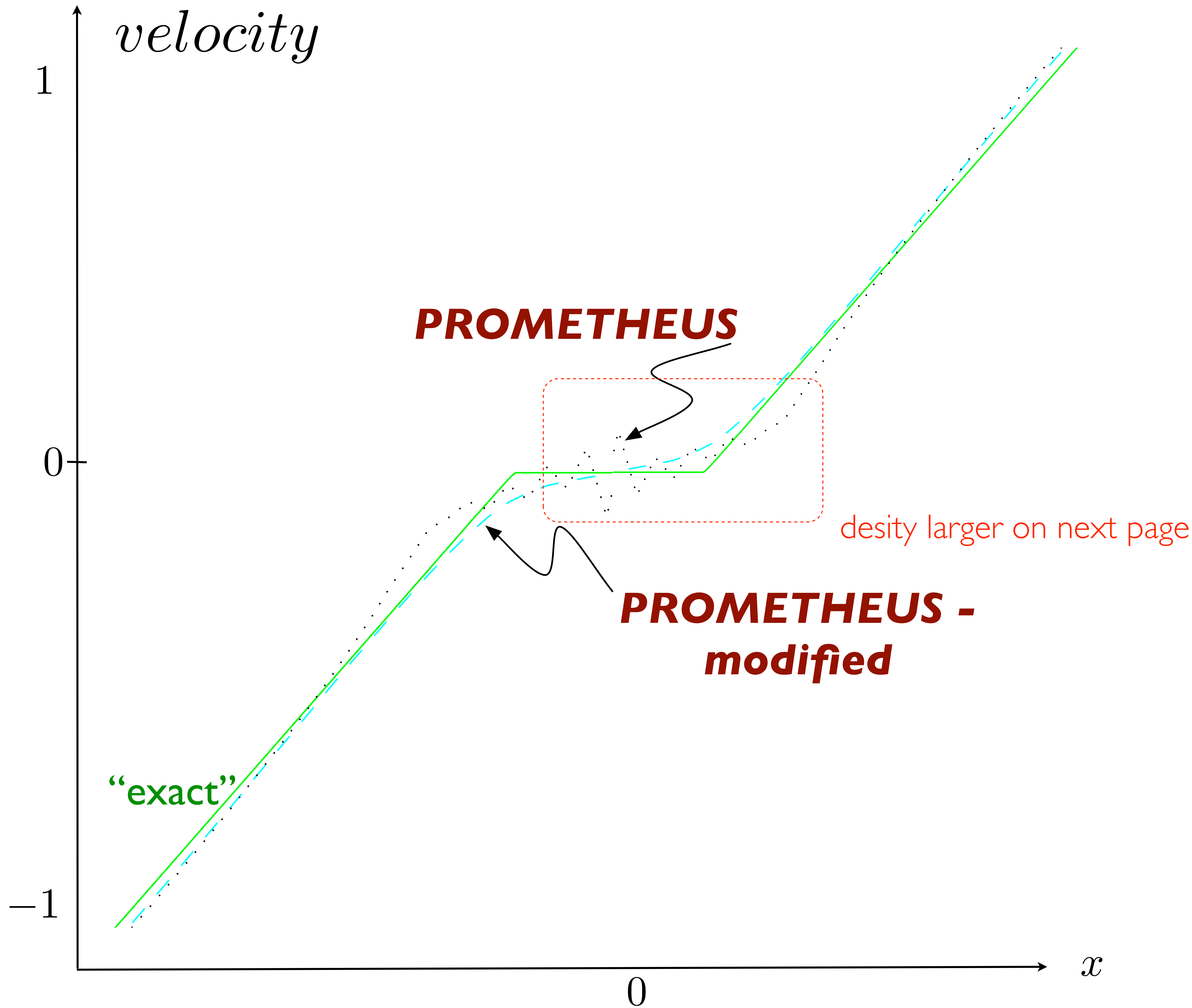
one space dimension:

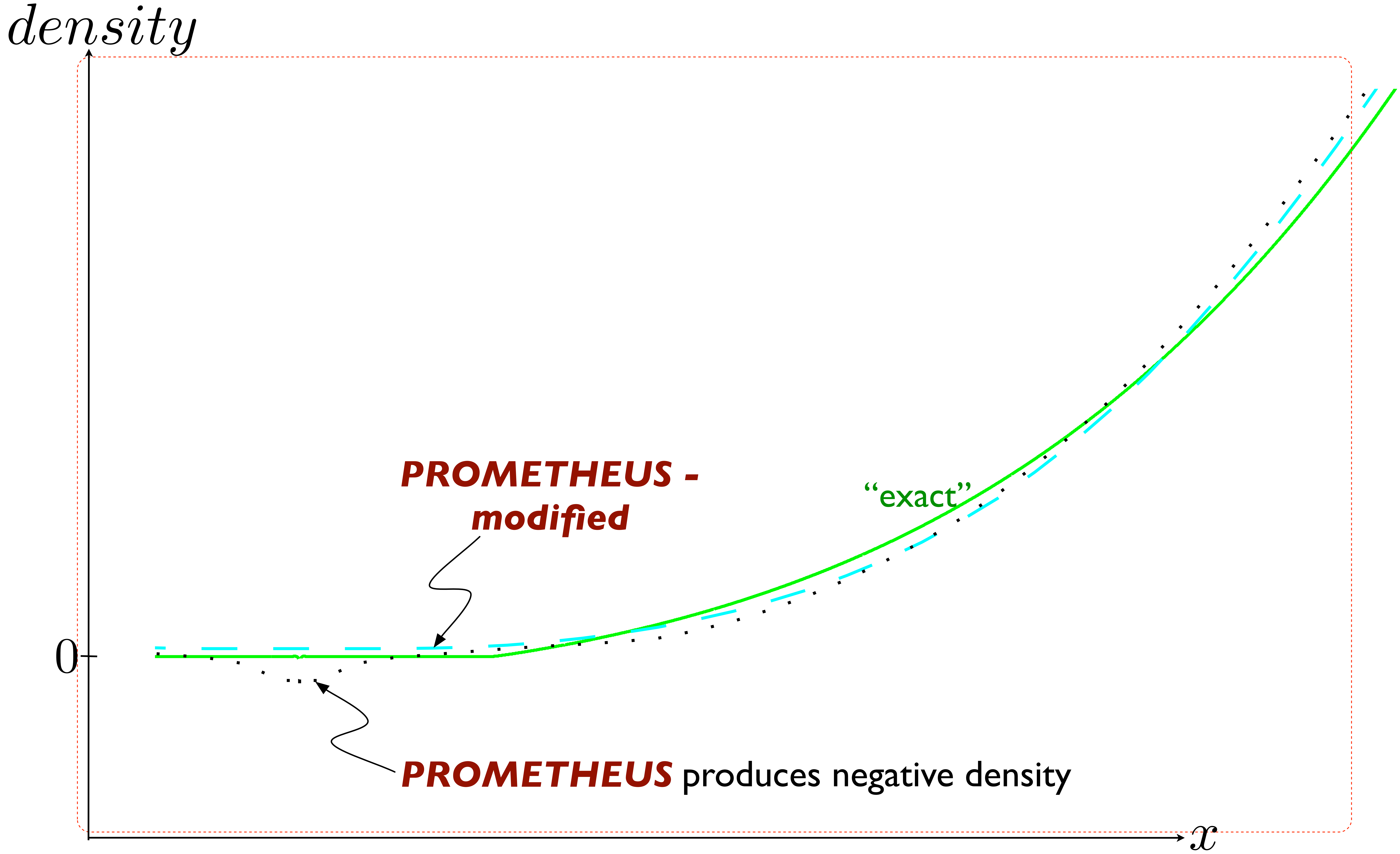
Riemann problems



the modified code smears out a little more

This Riemann problem has two strong rarefaction waves going apart creating a low density region.

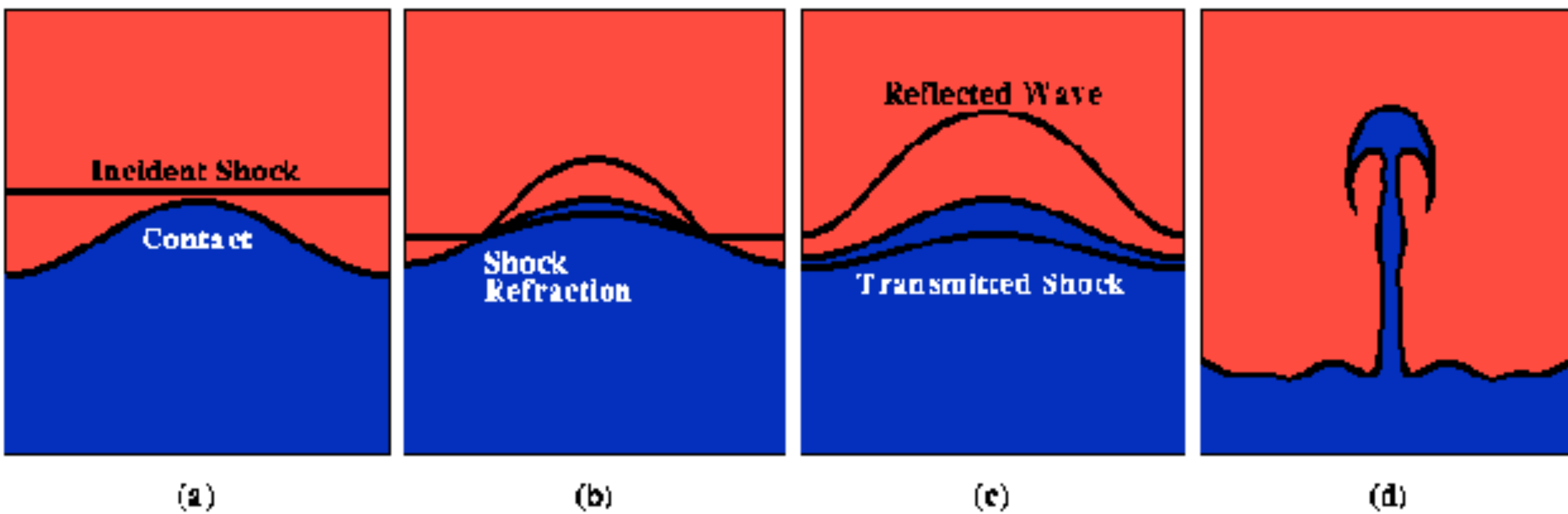


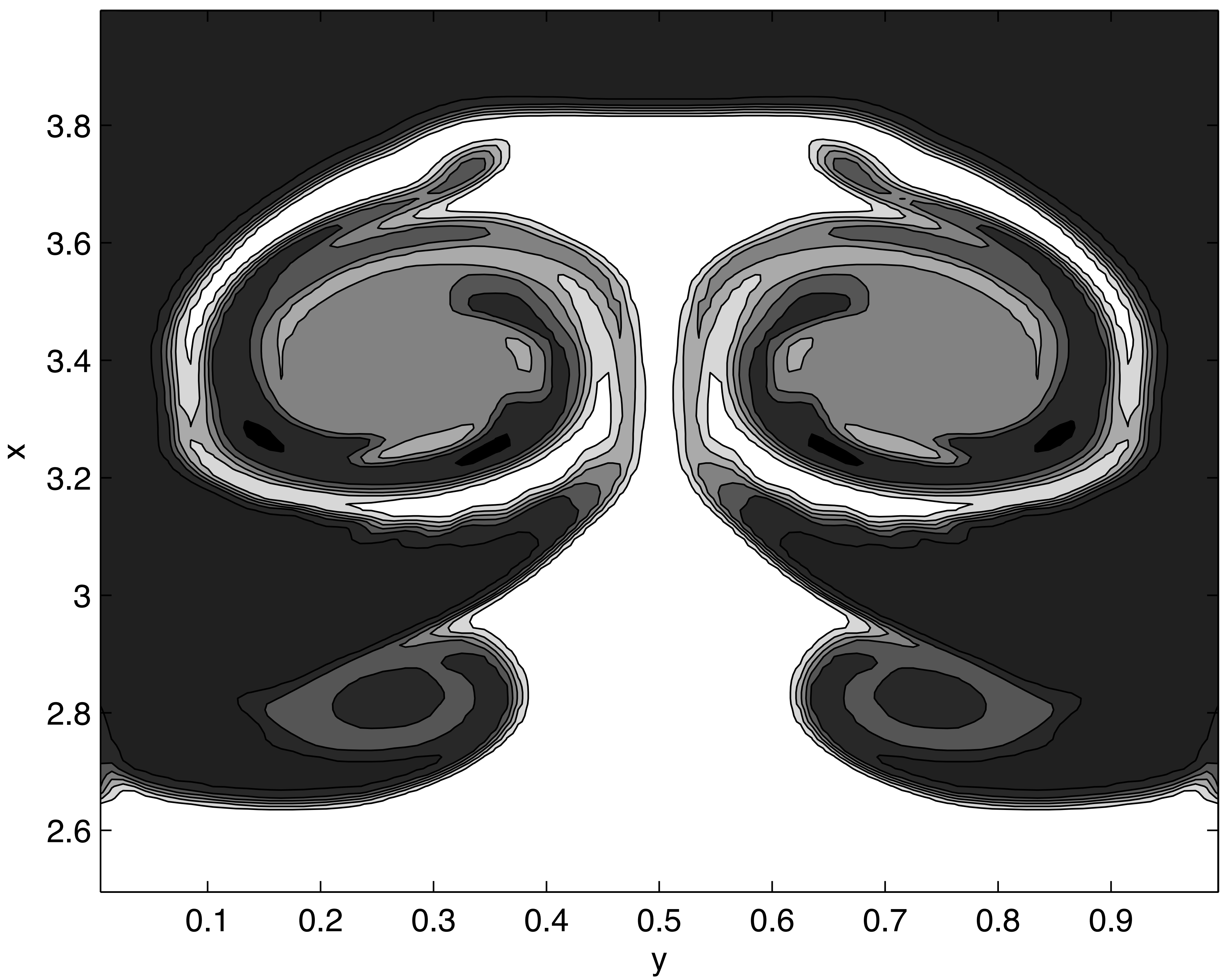


density
0
x
PROMETHEUS - modified
"exact"
PROMETHEUS produces negative density

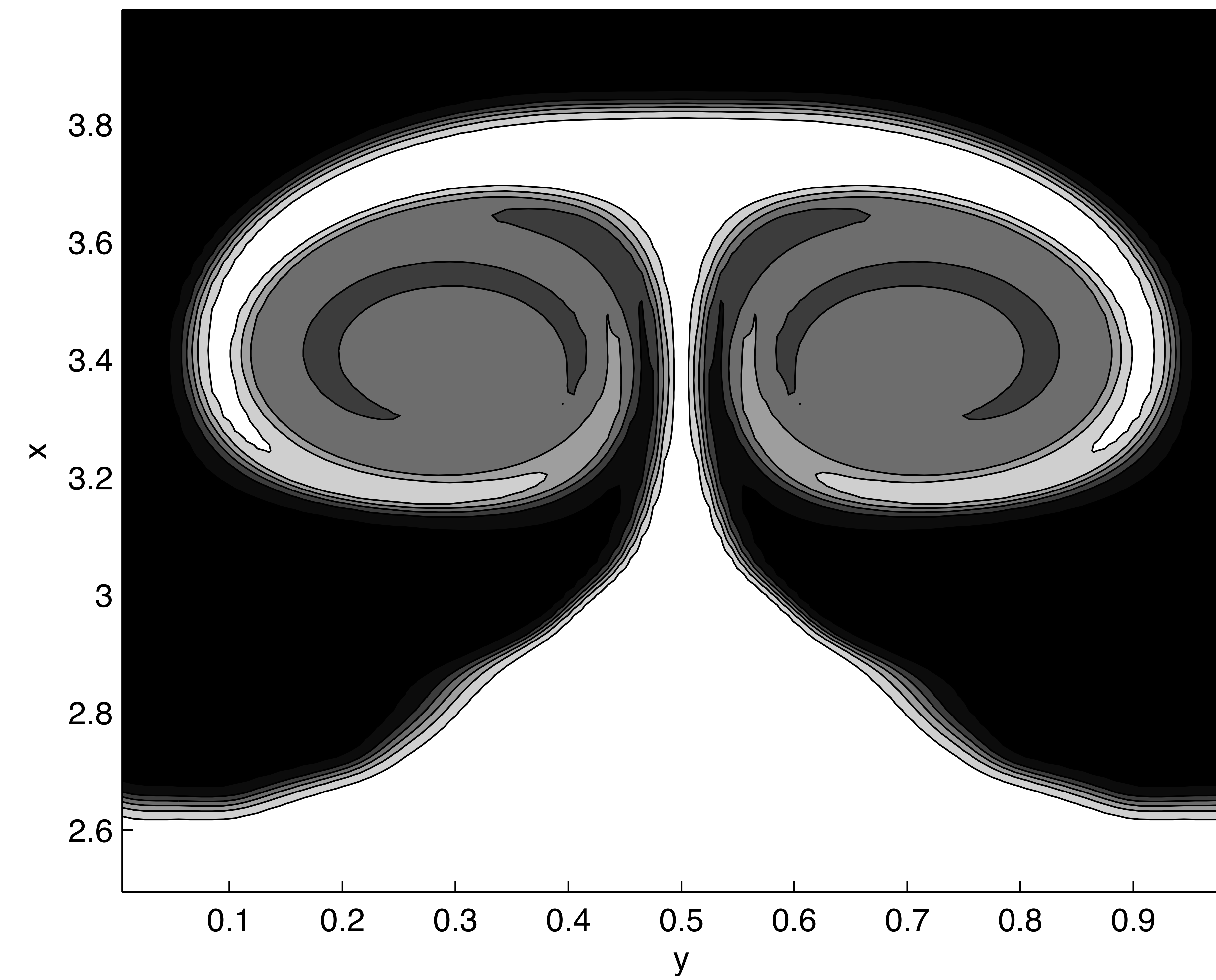
two space dimensions:

Richtmeyer-Meshkov instability

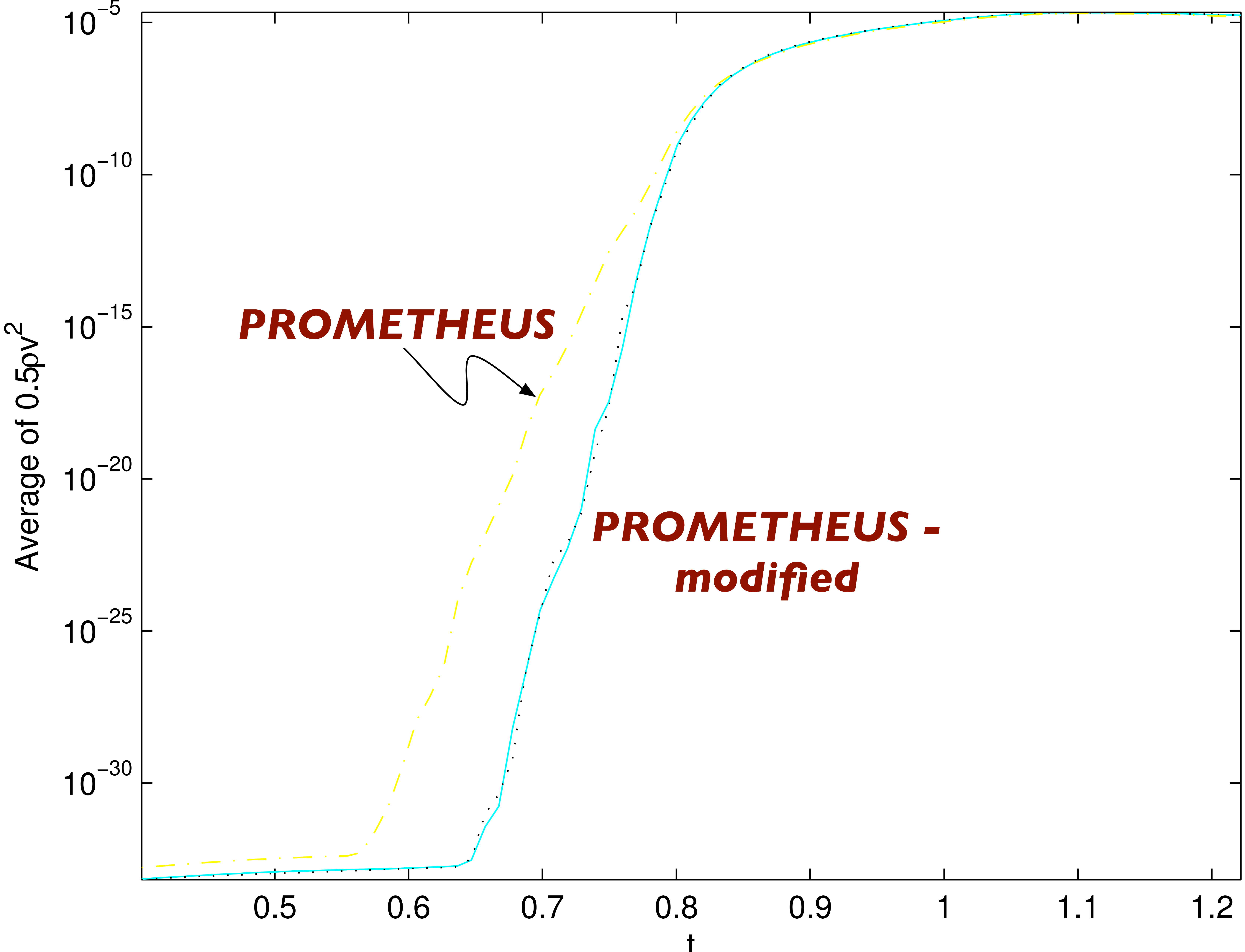




PROMETHEUS



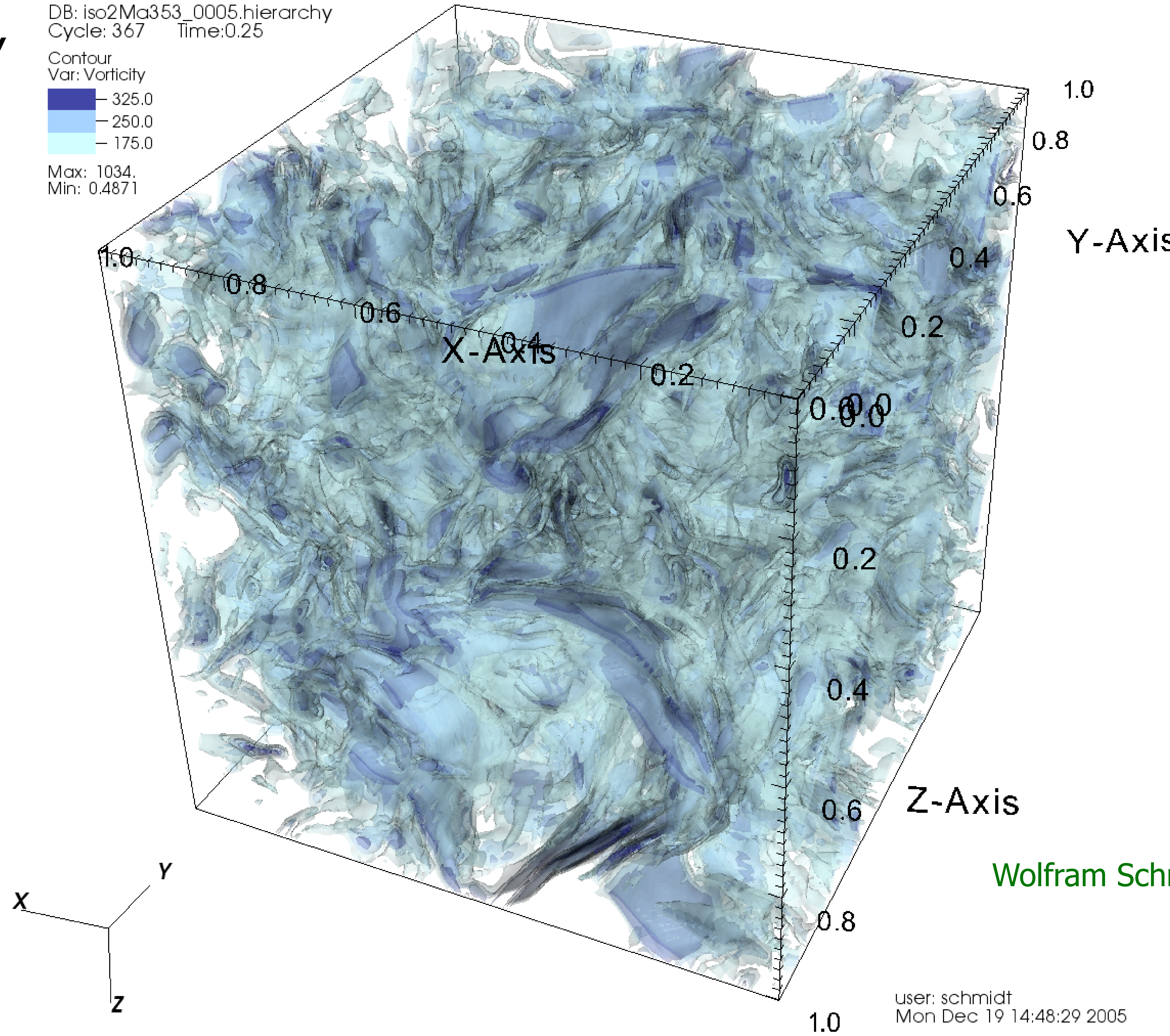
PROMETHEUS - modified:



The growth of instability is similar for both codes
as seen here by transversal component of kinetic energy.

three space dimensions, turbulence simulations:

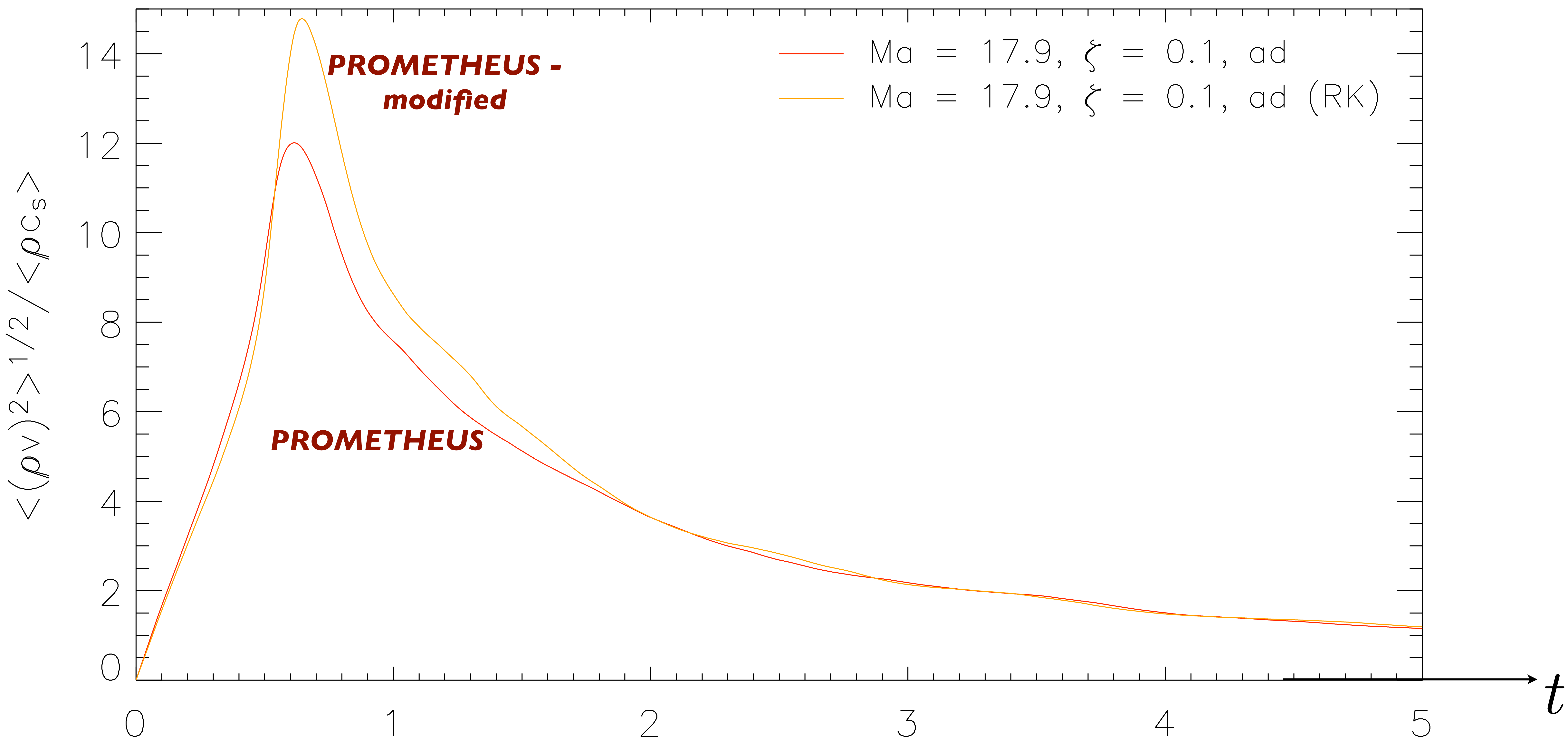
vorticity



Wolfram Schmidt, J. Niemeyer (2006)

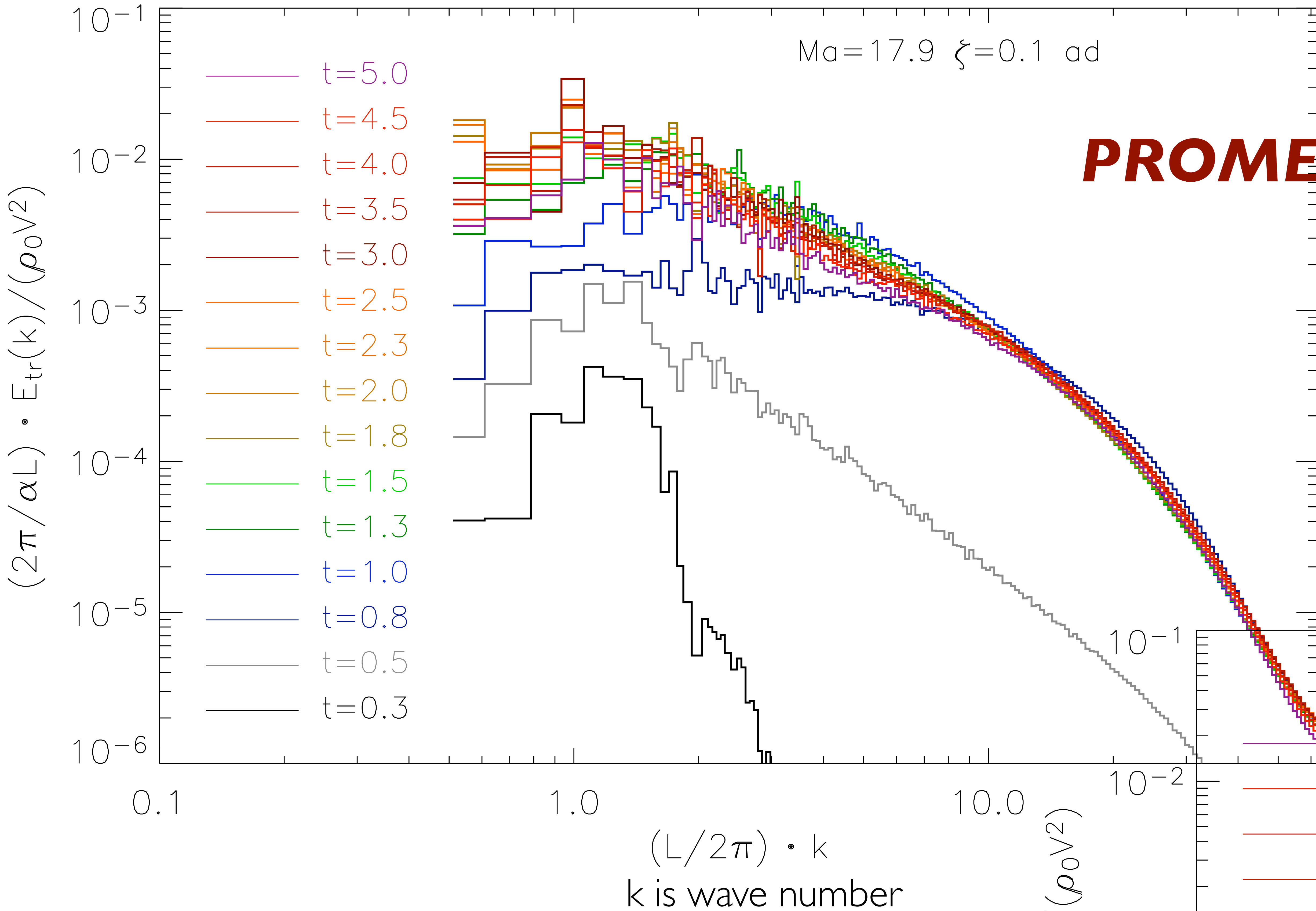
These simulations elucidate the intermittent structure of turbulent flow

- Vorticity is concentrated in regions of fractal dimension $D < 3$
- Subsonic turbulence: Vortex filaments (eddies)
- Supersonic turbulence: Sheets of high vorticity (shocks)

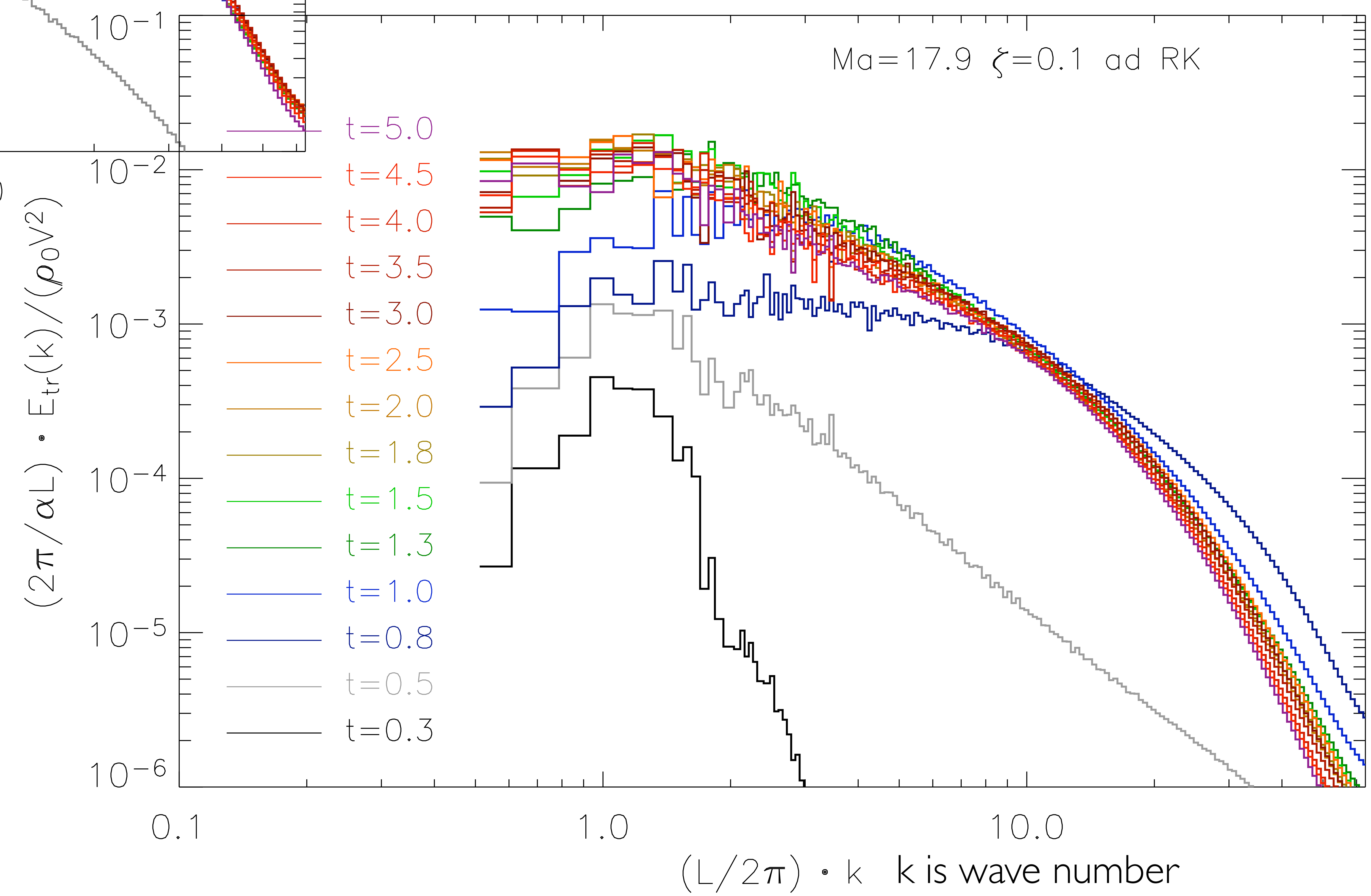


time evolution of root mean squared Mach number

PROMETHEUS



PROMETHEUS - *modified*



time histories of transversal energy spectra conclusion:

dissipativity of ***PROMETHEUS*** is independent of Mach number

dissipativity of ***PROMETHEUS-modified*** is less for higher than for lower Mach numbers

The PPM method is widely used in the astrophysics community. Thus there was a concern on how much their results depend on this algorithm

We conclude that PPM is accurate with respect to the Riemann solver.

PROMETHEUS-modified is at least 20% faster than ***PROMETHEUS***.