

# FYS-GEO 4500

## Lecture Notes #7

### Finite Volume Methods for Nonlinear Systems

# Where we are today

	date	Topic	Chapter in LeVeque
<b>1</b>	1.Sep 2011	introduction to conservation laws, Clawpack	1 & 2
<b>2</b>	15.Sep 2011	the Riemann problem, characteristics	3 & 5
<b>3</b>	22.Sep 2011	finite volume methods for linear systems, high resolution	4 & 6
<b>4</b>	29.Sep 2011	boundary conditions, accuracy, variable coeff.	7,8, part 9
<b>5</b>	6.Oct 2011	nonlinear conservation laws, finite volume methods	11 & 12
<b>6</b>	13.Oct 2011	nonlinear equations & systems	13 & 14
	20.Oct 2011	no lecture	
<b>7</b>	27.Oct 2011	finite volume methods for nonlinear systems	15,16,17
<b>8</b>	3.Nov 2011	multidimensional systems and source terms, etc.	18, 19, 20, 21
	10.Nov 2011	no lecture	
<b>9</b>	17.Nov 2011	waves in elastic media	22
<b>10</b>	24.Nov 2011	unfinished business: capacity functions, source terms, project plans	
<b>11</b>	1.Dec 2011	student presentations	
	8.Dec 2011	no lecture	
<b>12</b>	15.Dec 2011	FINAL REPORTS DUE	



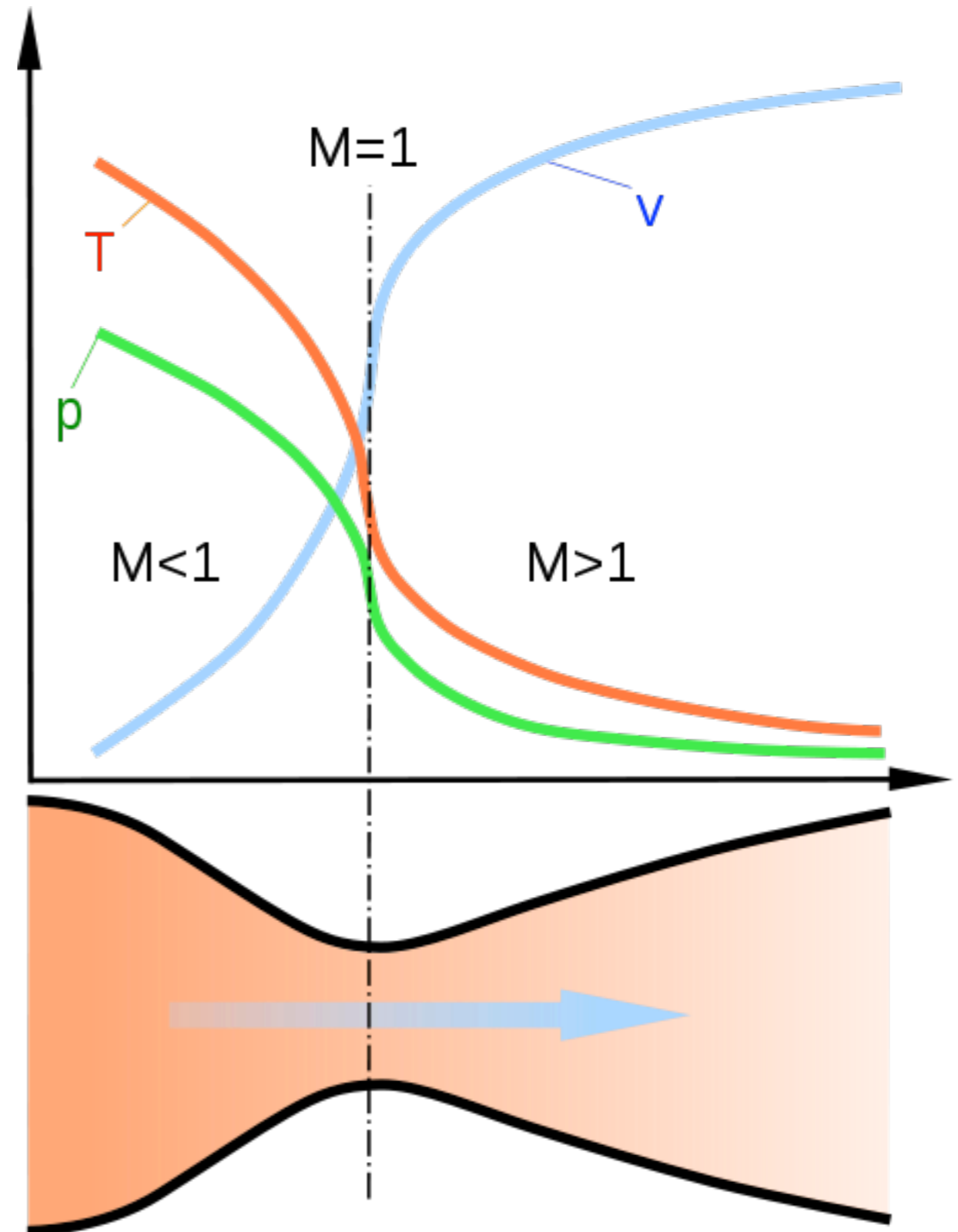
# Other topics in Gas Dynamics

# De Laval Nozzle

Invented by the Swedish engineer Gustaf de Laval in 1897.

This nozzle is the basis of how jet engines and rocket engines work.

The converging-diverging profile, with a sufficient difference in pressure between the reservoir and the exhaust, results in a smooth transition from subsonic to supersonic flow.




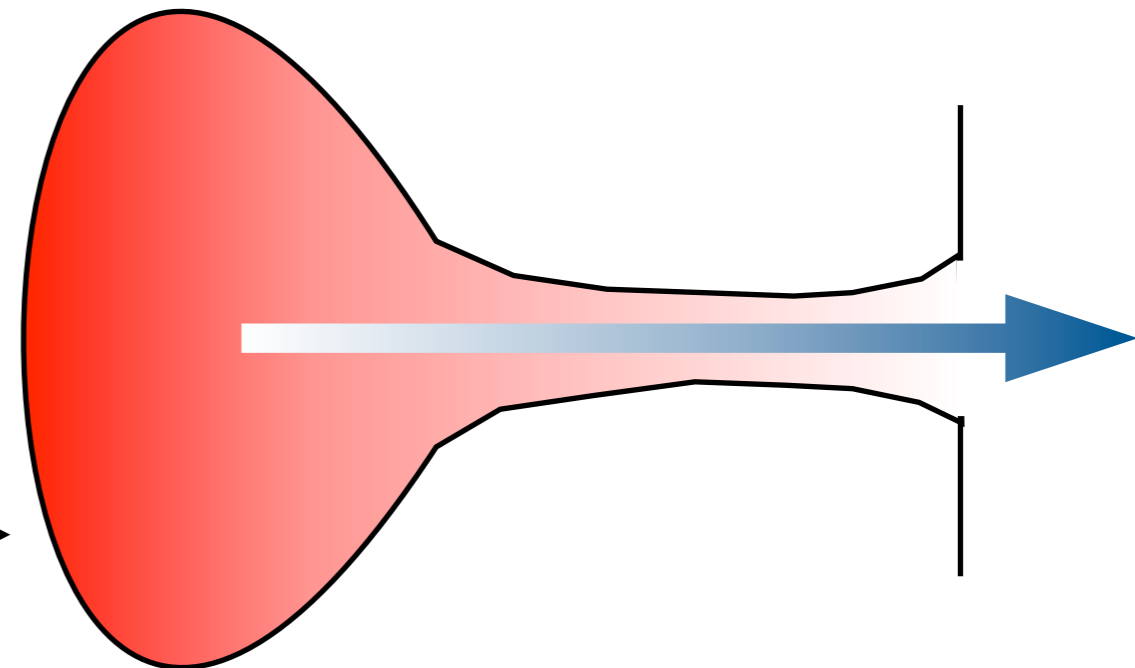
# How does a deLaval nozzle work?

Bernoulli's equation says that, for steady flow of a gas (ignoring gravity),

$$\frac{v^2}{2} + \left( \frac{\gamma}{\gamma-1} \right) \frac{p}{\rho} = \text{constant along a streamline,}$$

$$= \frac{v^2}{2} + \frac{c_s^2}{\gamma-1} \text{ for an ideal gas.}$$

Suppose we have a reservoir at high pressure connected via a pipe to a medium at much lower pressure. 



Then there is a maximum velocity at steady flow given by:

$$v_{\max} = c_0 \sqrt{\frac{2}{\gamma_0 - 1}}$$

where  $c_0$  and  $\gamma_0$  refer to the thermodynamic conditions in the reservoir (where  $v=0$ ), and this maximum value is obtained when the gas flows out into a vacuum ( $p=0$ ).

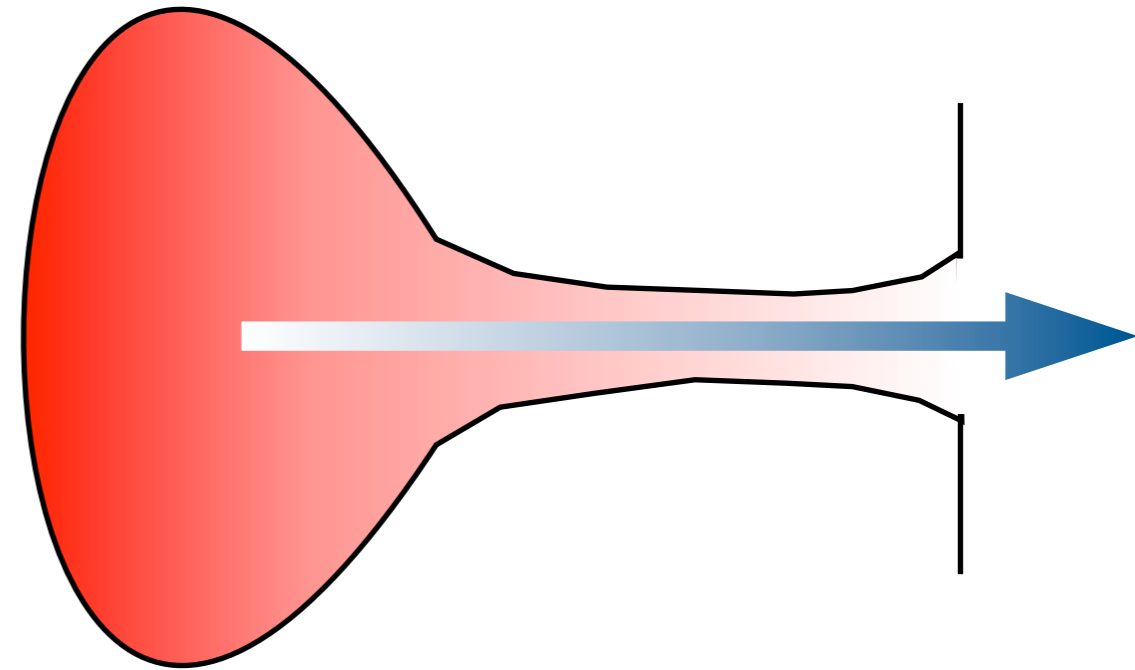
# How does a deLaval nozzle work?

Euler's equation gives us the relation between  $v$  and  $\rho$  along a streamline:

$$v dv = \frac{dp}{\rho}.$$

Using  $dp = c^2 \rho$ , where  $c$  is the *local* sound speed throughout the system, we get

$$\frac{d(\rho v)}{dv} = \rho \left( 1 - \frac{v^2}{c^2} \right),$$



indicating that the maximum possible mass flux  $\rho v$  obtains when  $v$  is equal to the local sound speed. By continuity, the flux is constant throughout the pipe, including the narrowest point.

For the ideal gas, the flux is

$$\rho v = \left( \frac{p}{p_0} \right)^{1/\gamma} \sqrt{\frac{2\gamma}{\gamma-1} p_0 \rho_0 \left[ 1 - \left( \frac{p}{p_0} \right)^{(\gamma-1)/\gamma} \right]}$$

# Velocity increases throughout the nozzle

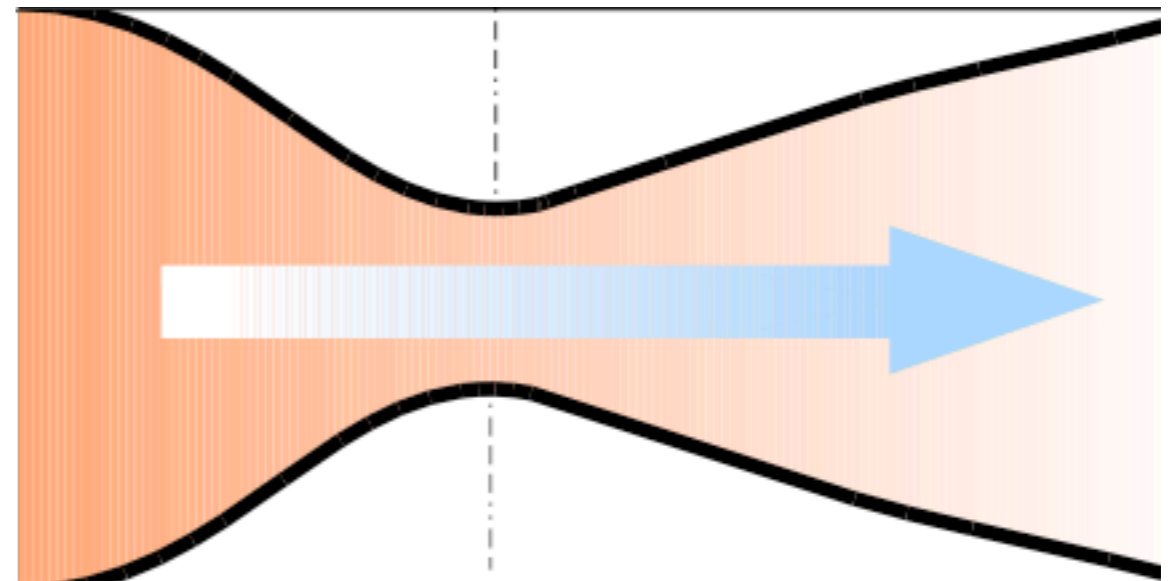
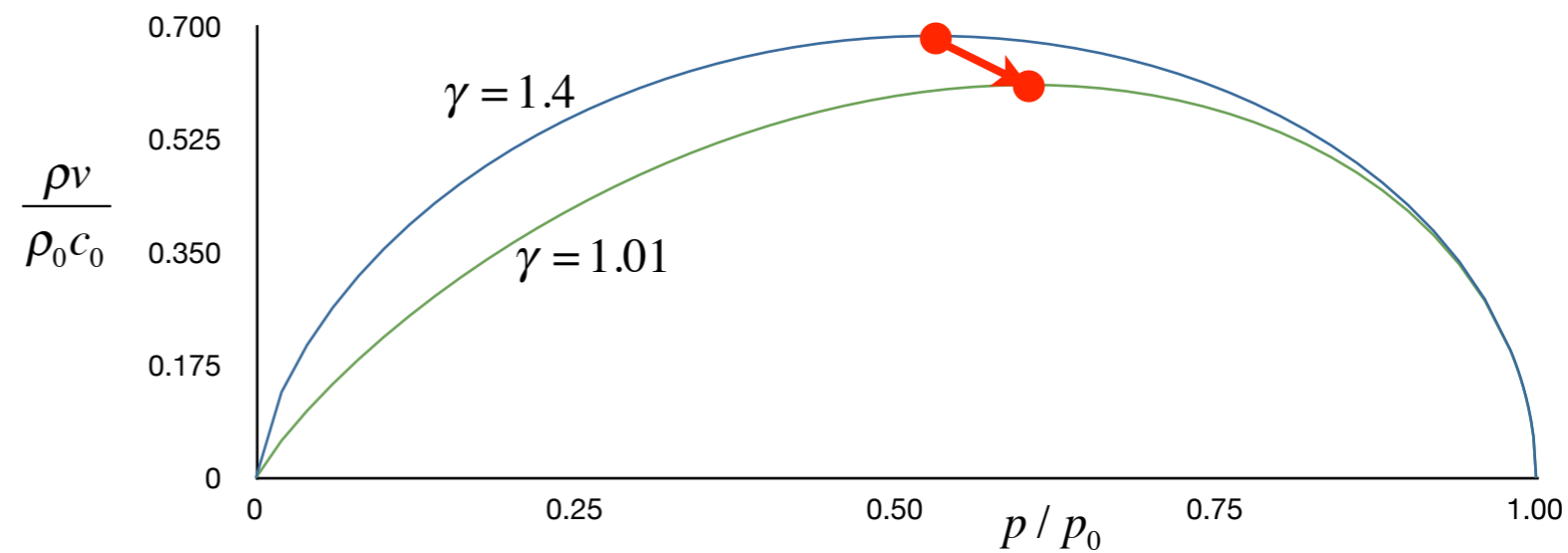
The maximum discharge rate is reached, if ever, at the narrowest point of a nozzle.

If the pressure at this point is less than  $0.53 p_0$  (in air) or less than  $0.6 p_0$  (in a nearly isothermal gas), the flow speed equals the sound speed at that point. The nozzle throat is the transition from subsonic to supersonic flow.

The velocity continues to increase through the diverging part of the nozzle, by continuity:

$$\frac{d(\rho v)}{dv} = \rho \left( 1 - \frac{v^2}{c^2} \right),$$

$$\rho v = \left( \frac{p}{p_0} \right)^{1/\gamma} \sqrt{\frac{2\gamma}{\gamma-1} p_0 \rho_0 \left[ 1 - \left( \frac{p}{p_0} \right)^{(\gamma-1)/\gamma} \right]},$$



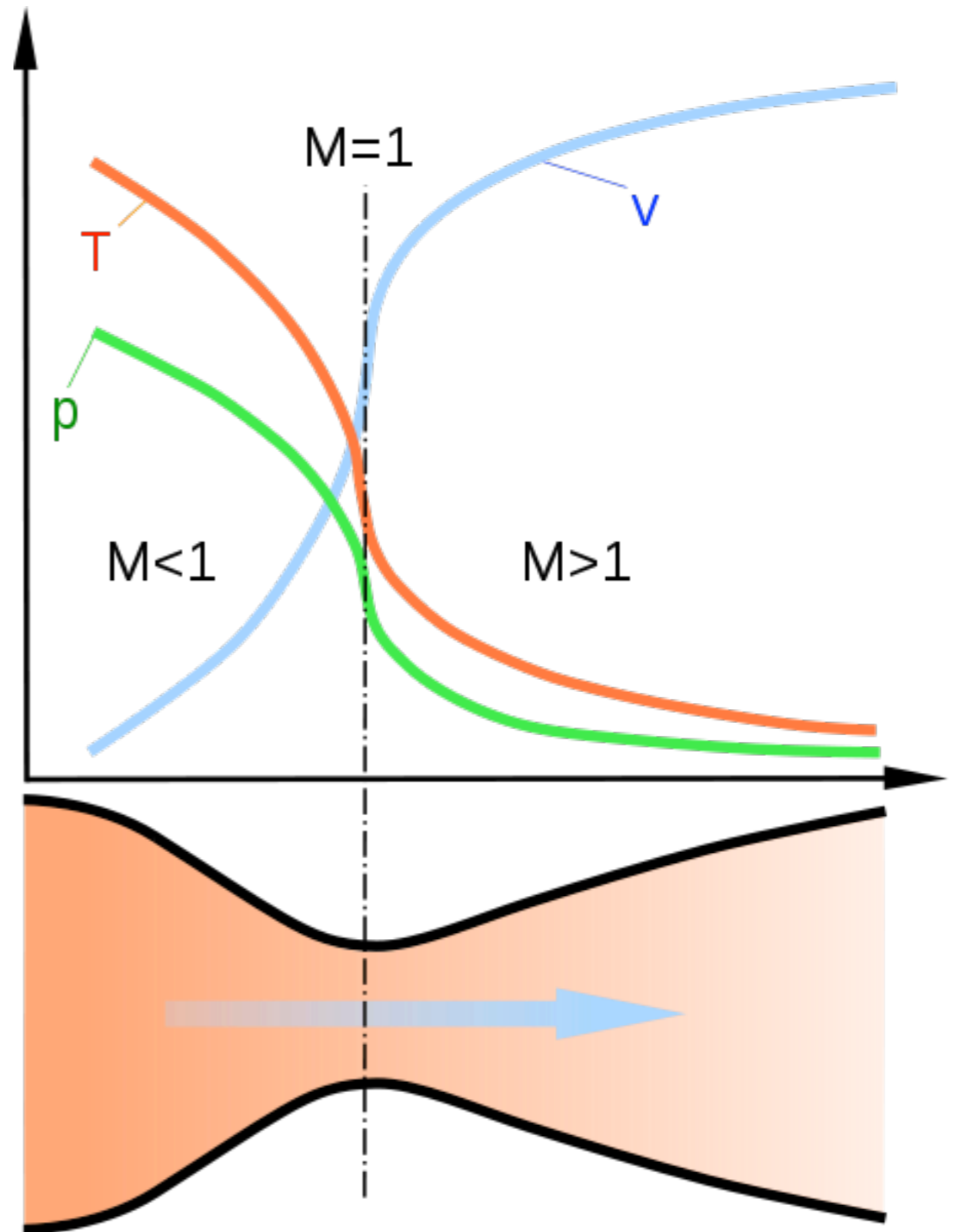
# De Laval Nozzle

Invented by the Swedish engineer Gustaf de Laval in 1897.

This nozzle is the basis of how jet engines and rocket engines work.

The converging-diverging profile, with a sufficient difference in pressure between the reservoir and the exhaust, results in a smooth transition from subsonic to supersonic flow.

$$\frac{d(\rho v)}{dv} = \rho \left( 1 - \frac{v^2}{c^2} \right),$$






# Simulation of an erupting column using the Sage multi-material code

600 m ice 

3.2 km basalt 

Magma column, 98%  
basalt, 2% water (by mass) 

1500 K, 1 kbar

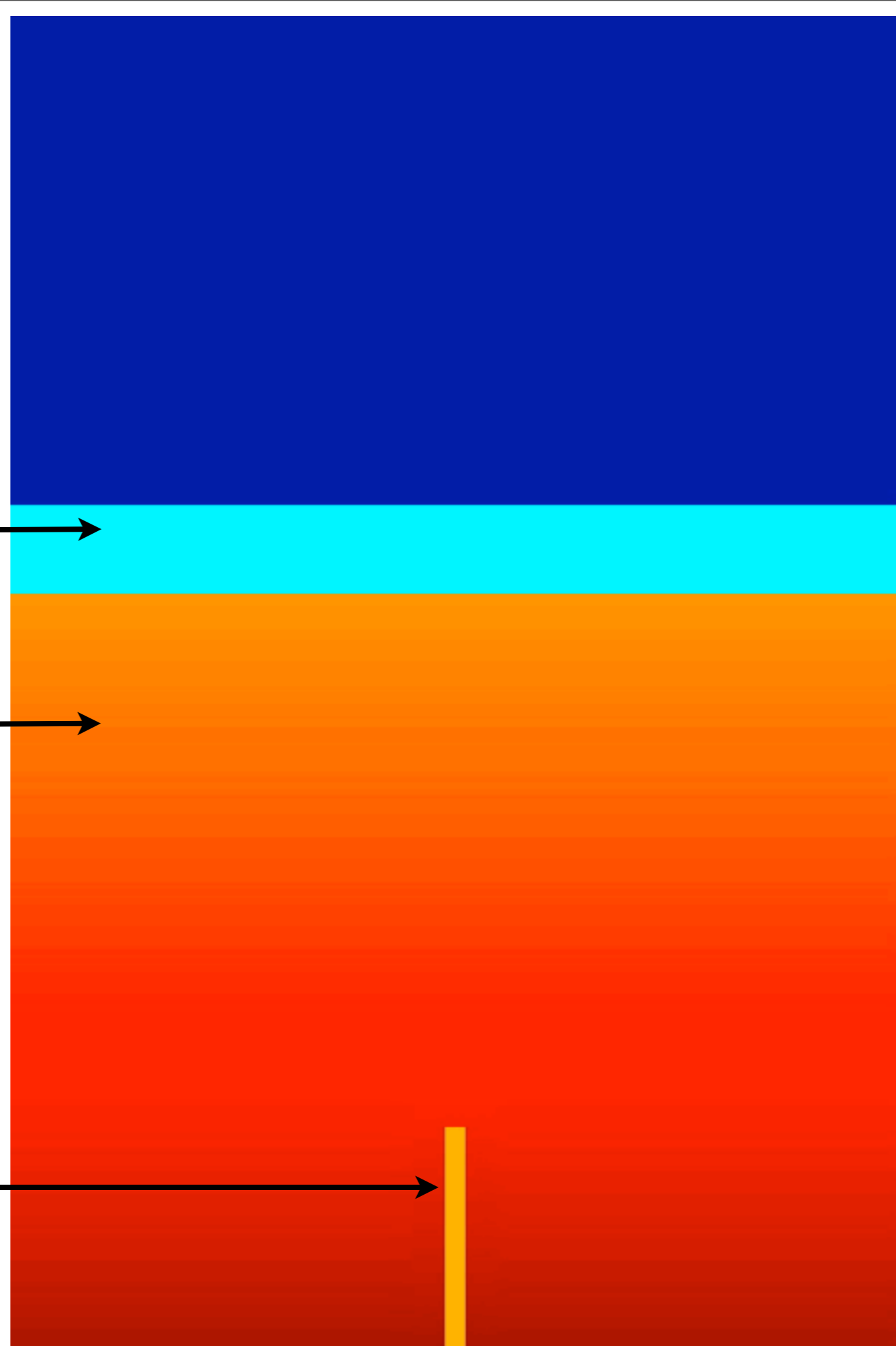
# Simulation of an erupting column using the Sage multi-material code

600 m ice →

3.2 km basalt →

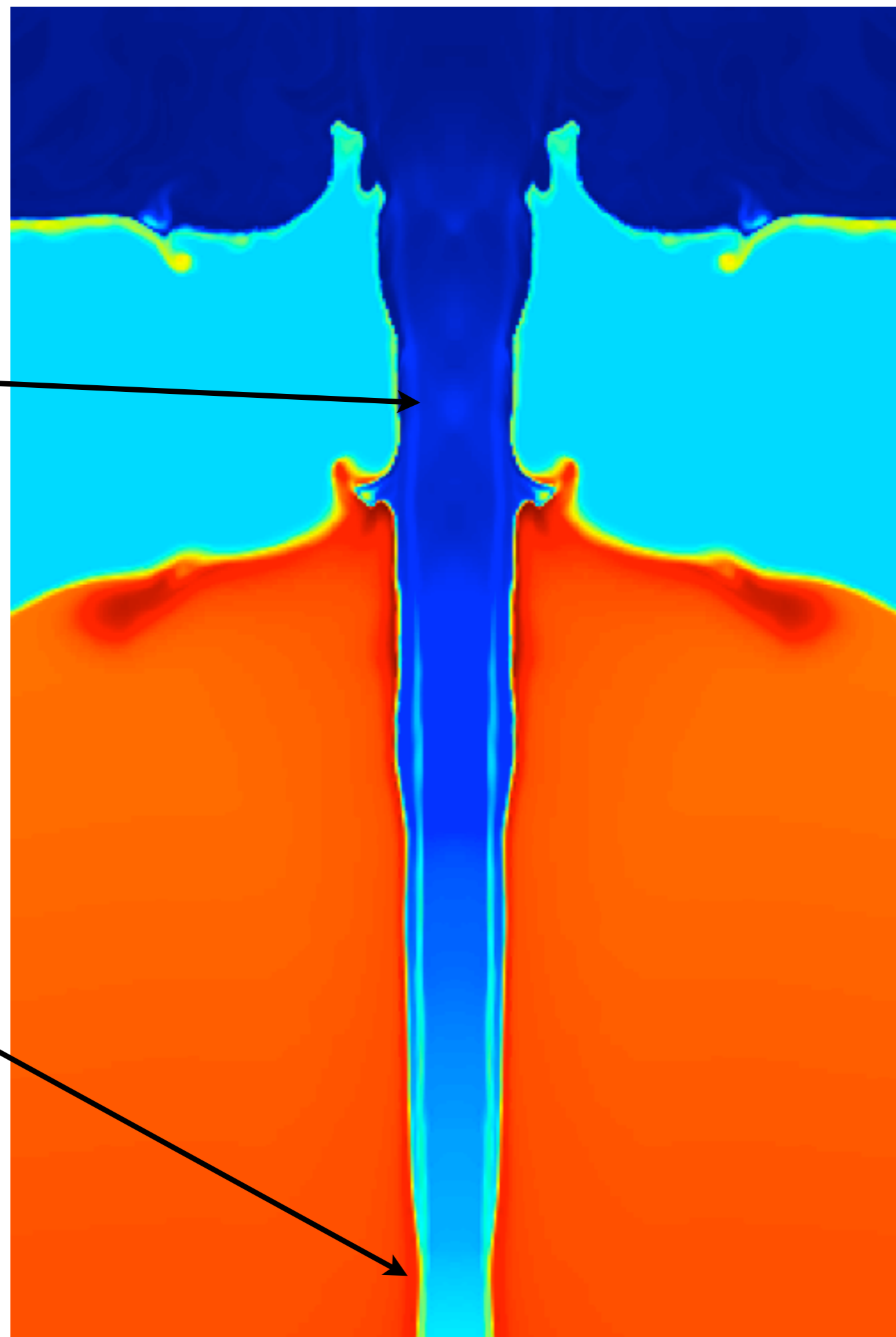
Magma column, 98%  
basalt, 2% water (by mass) →

1500 K, 1 kbar



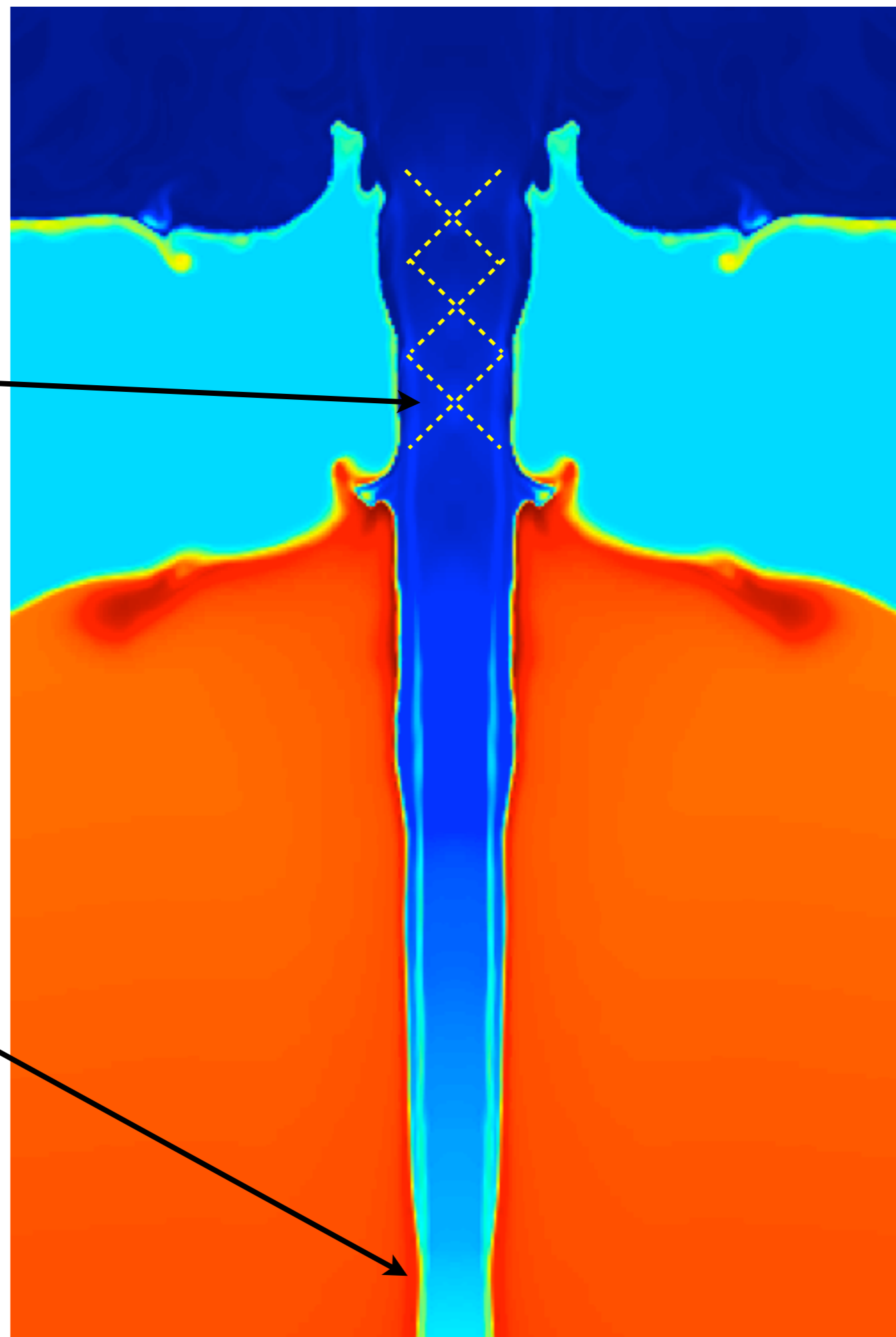
Shock waves and Mach disks (“shock diamonds”) in the supersonic nozzle flow

DeLaval nozzle



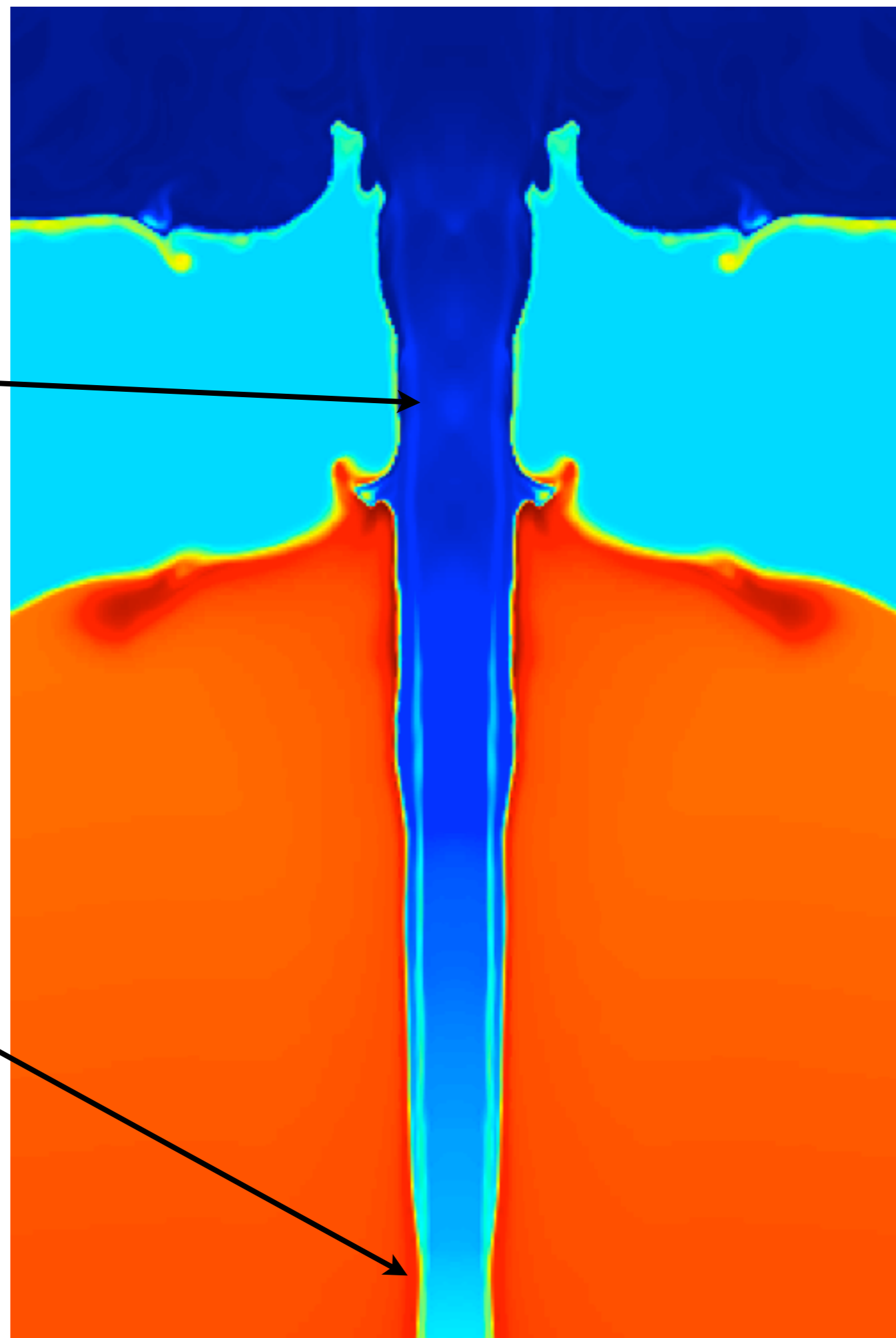
Shock waves and Mach disks (“shock diamonds”) in the supersonic nozzle flow

DeLaval nozzle



Shock waves and Mach disks (“shock diamonds”) in the supersonic nozzle flow

DeLaval nozzle



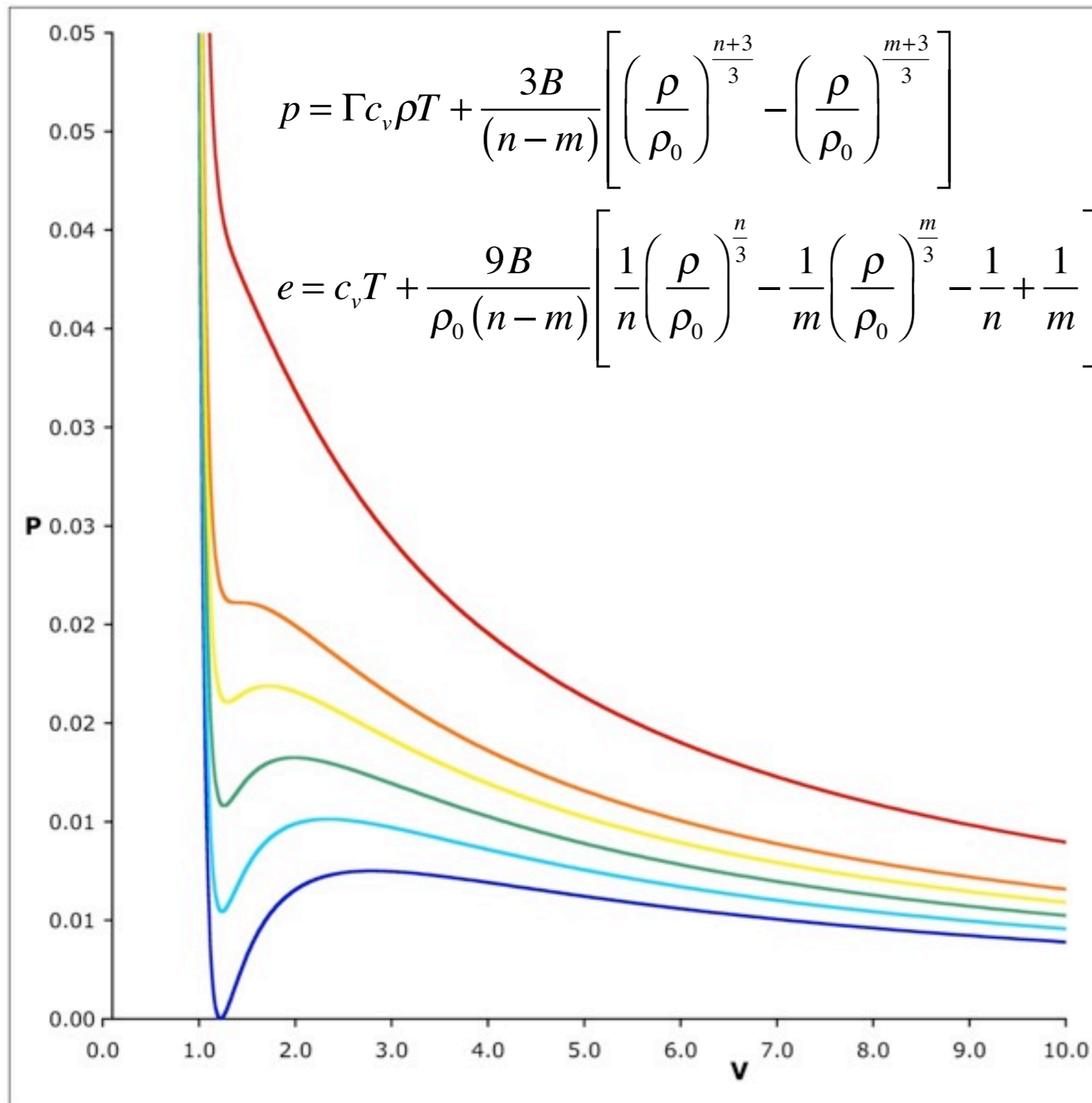
# Multifluid problems and other equations of state: How to do in Clawpack?

The easiest multi-fluid case is when you have two ideal gases with different values of  $\gamma$ . Then you set up the Riemann problem at the interface between the two fluids with right and left values for  $\gamma$ . Things get complicated when mixing occurs.

Other analytical or tabular equations of state can also be incorporated into a finite volume conservative scheme. Sage, for example, uses the Sesame library of tabular equations of state for lots of materials. The Sesame library, developed at Los Alamos National Laboratory, contains mostly industrial materials, with a few materials of geological interest.

Leveque gives lots of references to papers in which Riemann solvers are developed for other equations of state in his section 14.15. Some of these will be worth looking into for geological applications.

# The Mie-Grüneisen-Lemons Multiphase EOS

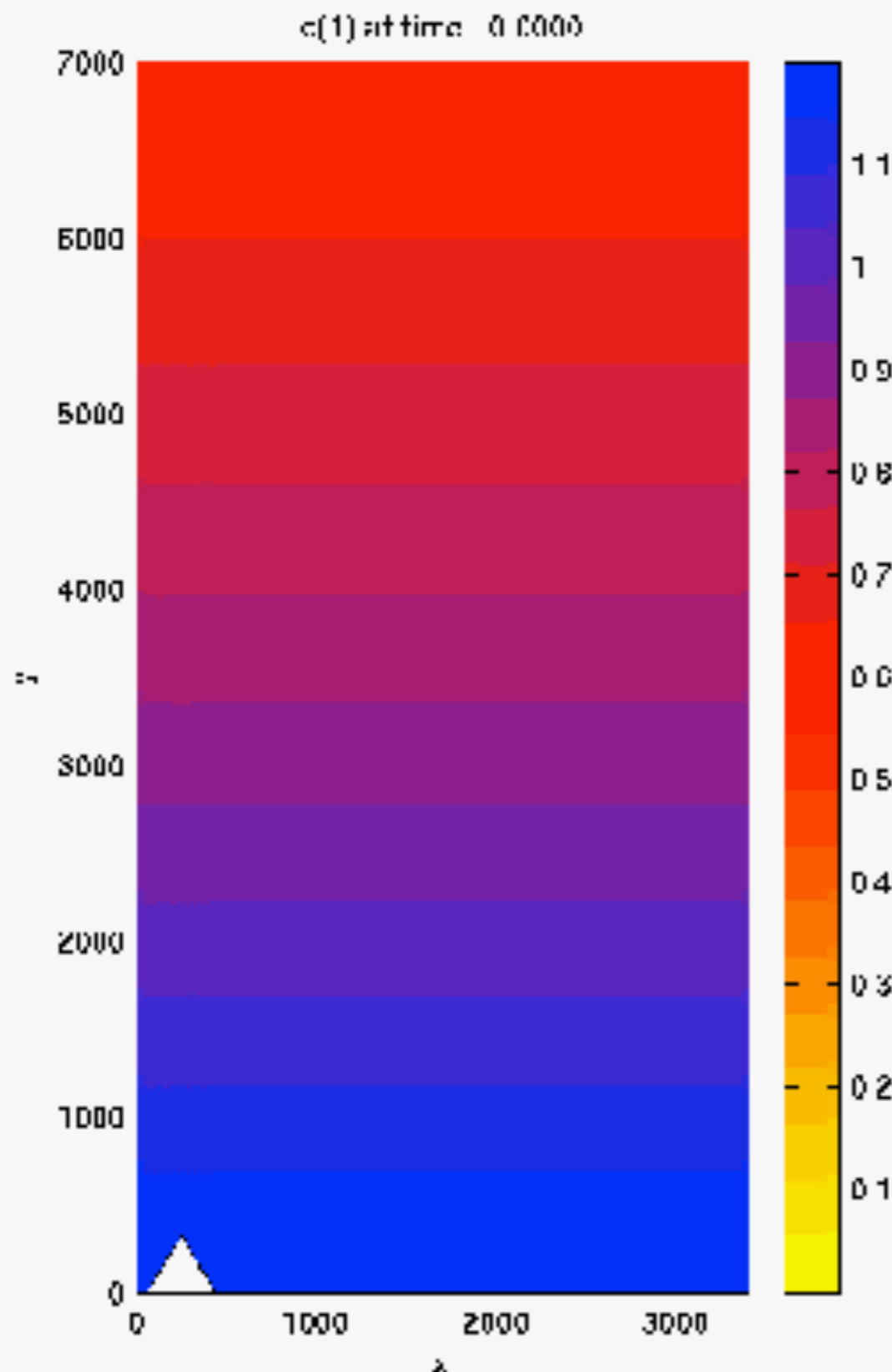


This is an equation of state proposed by Don Lemons based on Mie-Grüneisen theory for substances that undergo relatively simple phase transitions from solid to liquid to gas.

In common with the van der Waals EOS (see Leveque, ch 14.15 and 16.3.2), this EOS results in loss of hyperbolicity unless Maxwell constructions are used.

This EOS has substance-specific constants  $n, m, \rho_0, B, \Gamma$

# Dusty Gases, Anyone?



Marica Pelanti, a student of Randy Leveque, developed a code based on Clawpack for volcanic jets using a dusty gas model.

See\*: Pelanti & Leveque, "High-Resolution Finite Volume Methods for Dusty Gas Jets and Plumes", *SIAM J. Sci. Comput.* **28** (2006) 1335-1360.

Their model was multifluid: Euler equations for the gas, and a pressureless fluid for the dust, coupled together by drag and heat transfer.

Or... we could try a single-fluid dusty gas equation of state.

\* <http://www-roc.inria.fr/bang/Pelanti/>



# What happens when we add dust to gas?

The speed of acoustic waves in a general medium is,  $c_s = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_{\text{isentropic}}}$

which for an ideal gas is  $c_s = \sqrt{\frac{\gamma P}{\rho}}$

Assuming the dust remains coupled to the gas (via *Stokes drag*), for a little loading the density increases without the pressure changing much.

Thus the speed of sound *decreases*. In fact, it does so *dramatically*.

# An equation of state for a dusty gas\*

One version of a dusty-gas equation of state is: 
$$p = \frac{(1-K)}{(1-Z)} \rho RT,$$

where  $K$  is the mass concentration and  $Z$  is the volume fraction of solid particles.

These are related through  $K = \frac{Z\rho_s}{\rho}$ , where  $\rho_s$  is the particle solid density.

The speed of sound is then 
$$c_{ds} = \sqrt{\frac{\Gamma p}{\rho(1-Z)}}$$

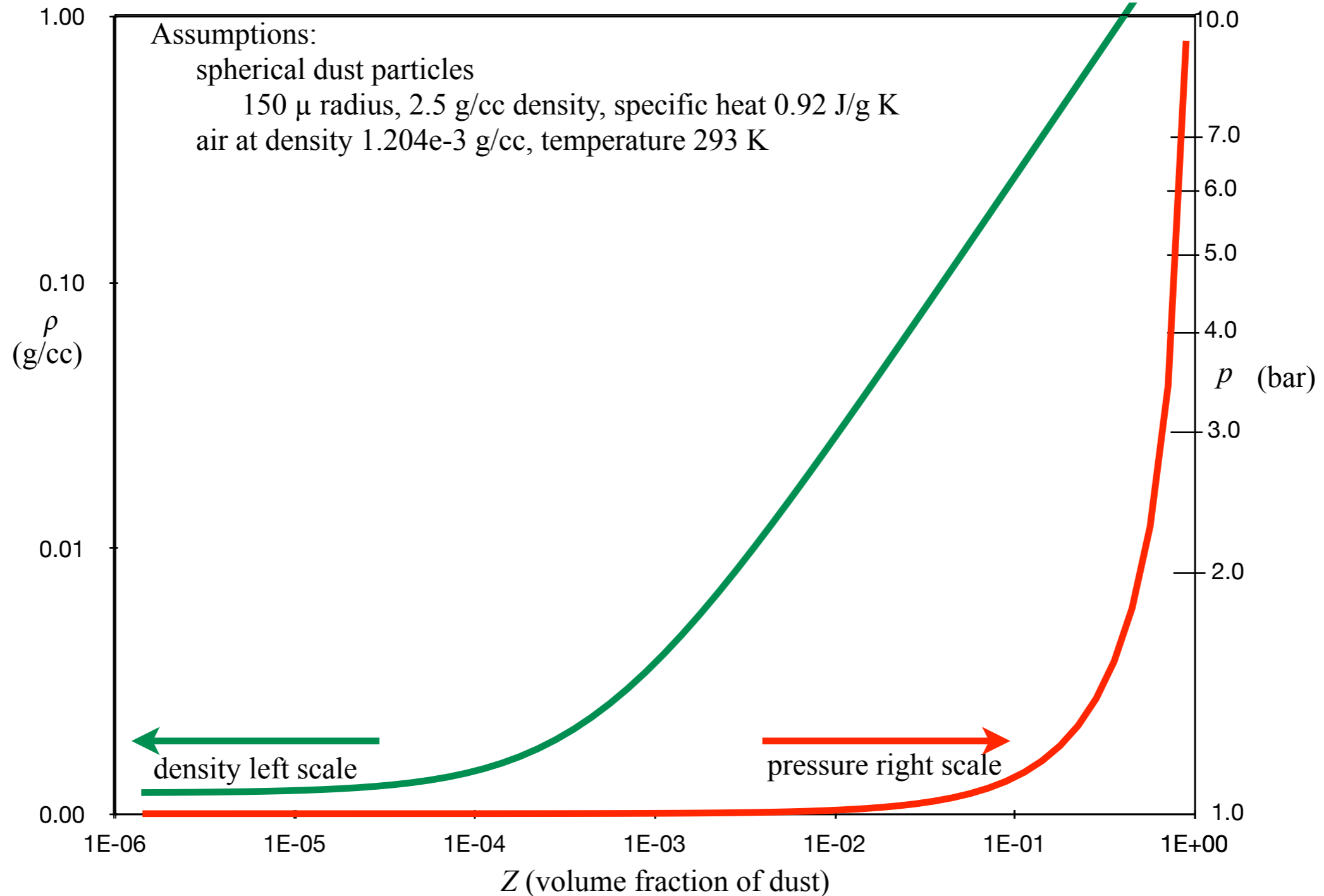
where the ratio of specific heats for the mixture is 
$$\Gamma = \frac{\gamma C_v(1-K) + C_{sp}K}{C_v(1-K) + C_{sp}K}.$$

The specific heat of the dust particles is  $C_{sp}$  and  $C_v$  is the specific heat at constant volume of the gas.

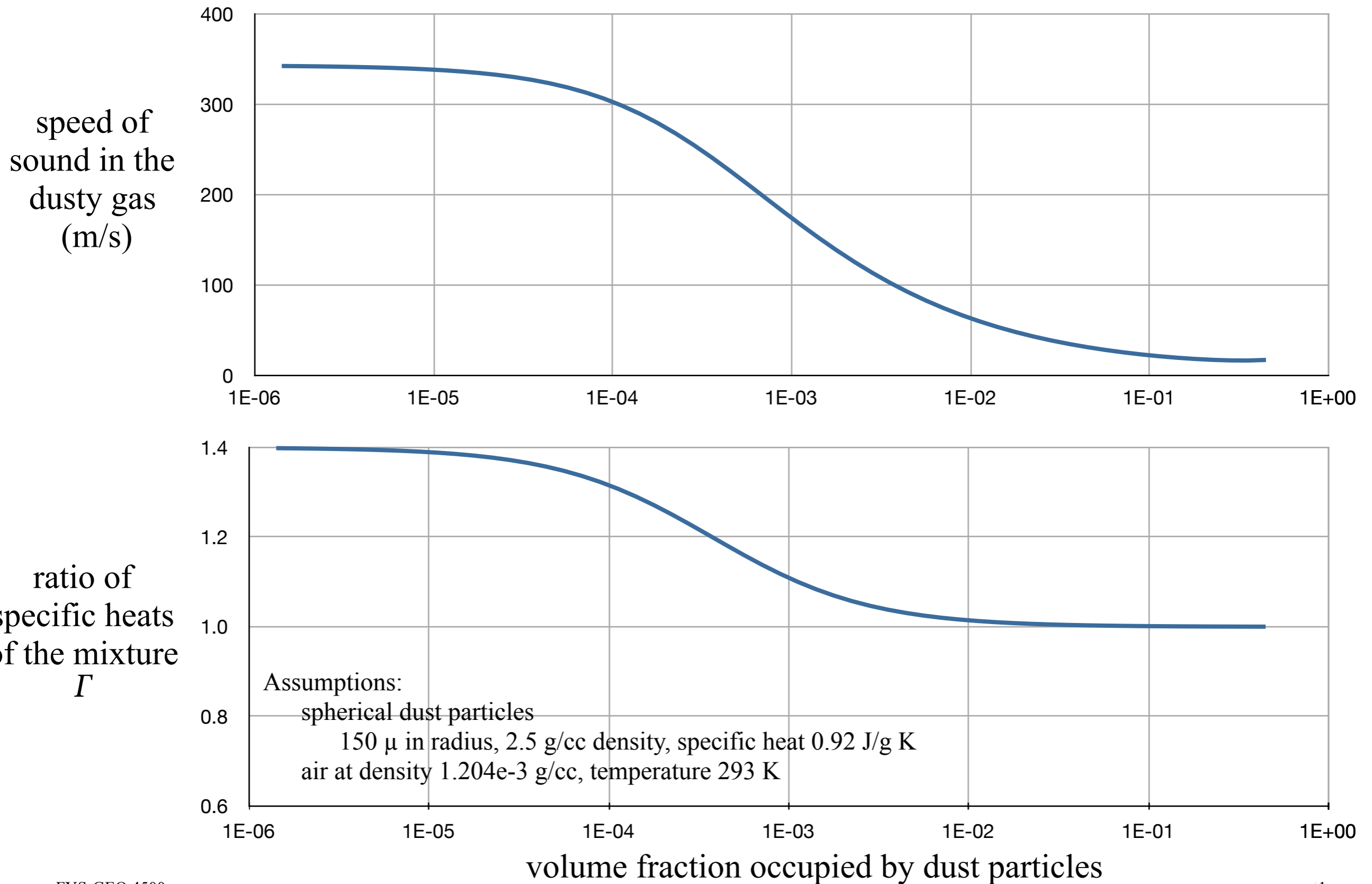
\*from Vishwakarma, Nath, & Singh (2008), *Physica Scripta* **78** 035402.

<http://stacks.iop.org/PhysScr/78/035402>

# Density increases more rapidly than pressure as the dust content increases



# Adding 0.1% dust (by volume) to air cuts the speed of sound in half, and the mixture approaches isothermal



# Shocks can be stronger in dusty gases

The maximum ratio of upstream to downstream densities across a shock is (see Landau & Lifshitz, *Fluid Dynamics*)

$$\frac{\rho_u}{\rho_d} = \frac{\gamma + 1}{\gamma - 1}.$$

For a diatomic gas (like air),  $\gamma = 1.4$ , so  $\frac{\rho_u}{\rho_d} = 6$ .

For a dusty gas,  $\gamma \Rightarrow 1$ , so  $\frac{\rho_u}{\rho_d}$  can be arbitrarily large. At  $\gamma = 1.01$ ,  $\frac{\rho_u}{\rho_d} = 201$ .

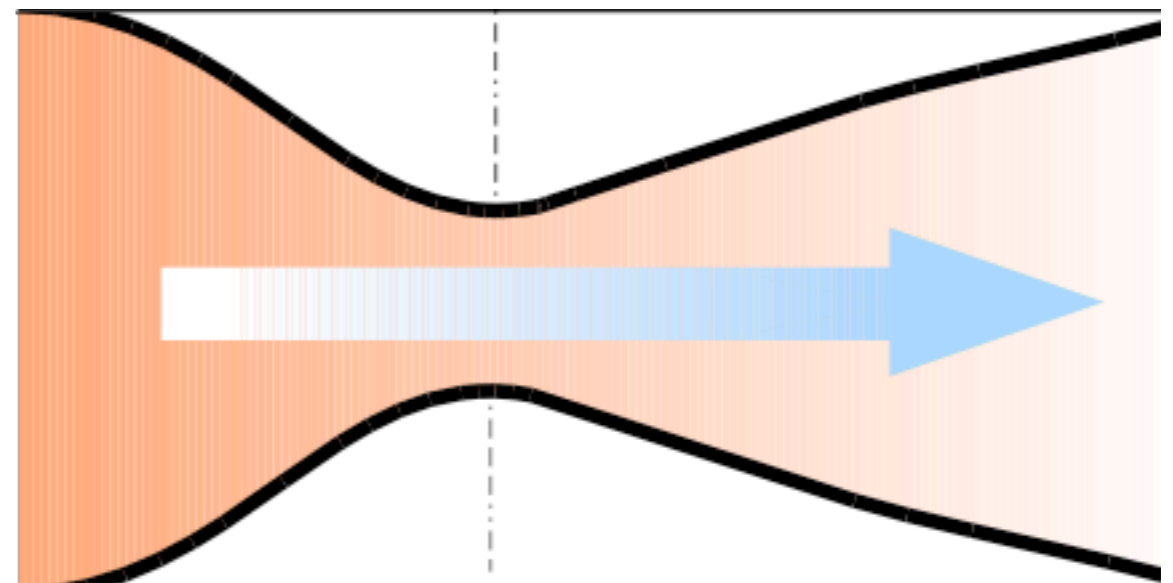
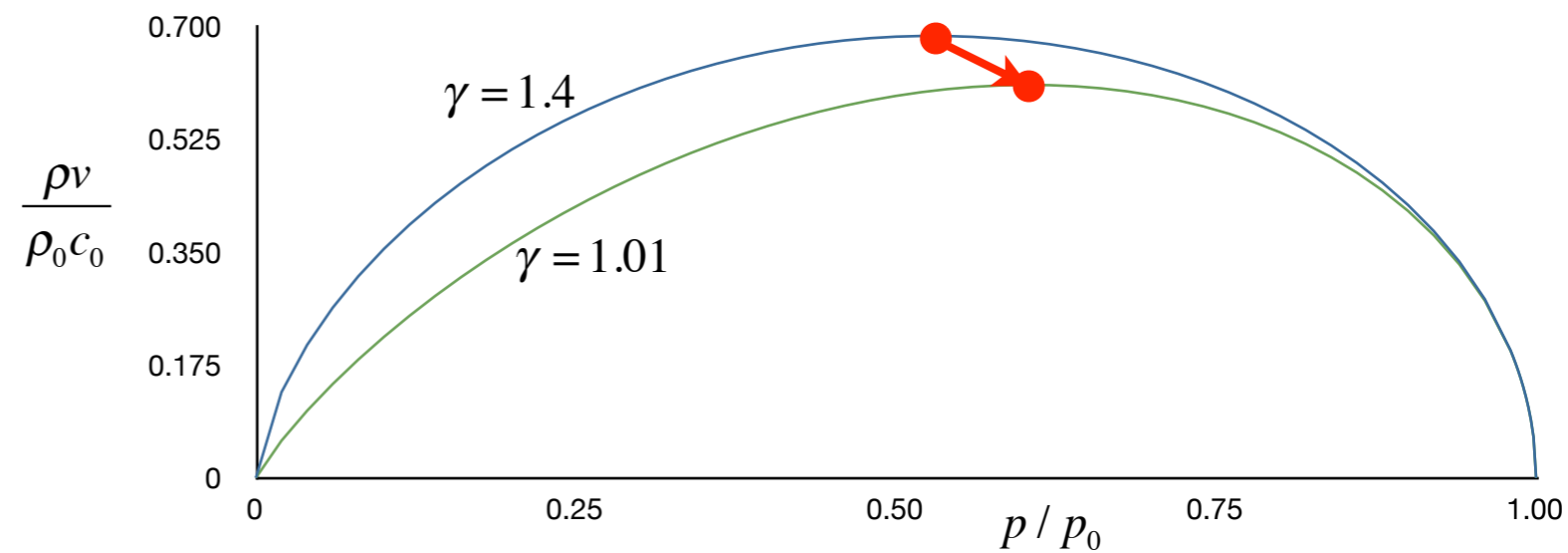
# The deLaval nozzle in a dusty gas

The maximum discharge rate is reached, if ever, at the narrowest point of a nozzle.

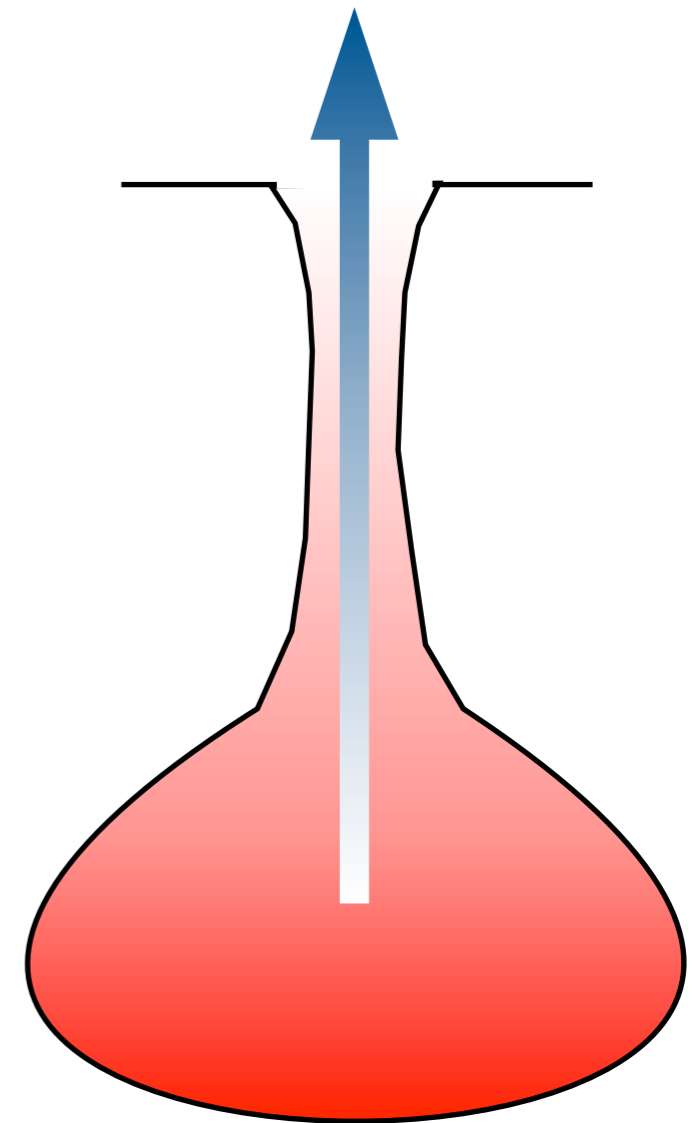
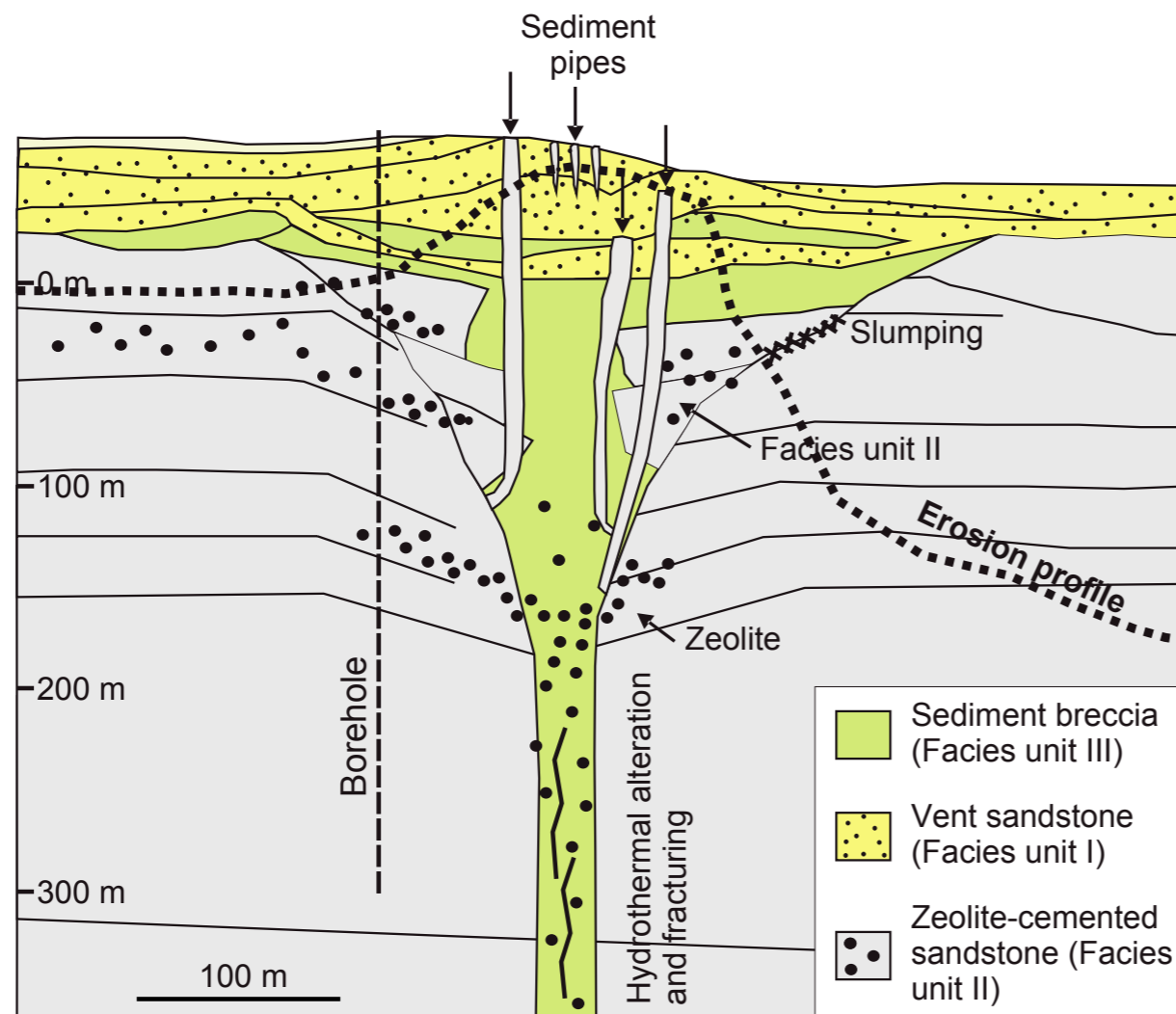
If the pressure at this point is less than  $0.53 p_0$  (in air) or less than  $0.6 p_0$  (in a 2% dusty gas), the flow speed equals the sound speed at that point. In the diverging portion, it becomes supersonic without passing through a shock.

In a dusty gas it is easier to get to supersonic flow both *because the local sound speed is lower* and *because the maximum discharge is reached with a lower pressure drop*.

$$\rho v = \left( \frac{p}{p_0} \right)^{1/\gamma} \sqrt{\frac{2\gamma}{\gamma-1} p_0 \rho_0 \left[ 1 - \left( \frac{p}{p_0} \right)^{(\gamma-1)/\gamma} \right]},$$



# Vents, kimberlite pipes, volcanos, and geysers may be natural deLaval nozzles for a dusty gas



# Finite Volume Methods for Nonlinear Systems (Chapter 15 in Leveque)



# Once again, we extend from what we've learned for linear systems of equations

We intend to solve the nonlinear conservation law  $q_t + f(q)_x = 0$

using a method that is in conservative form:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n)$$

and yielding a *weak solution* to this conservation law. To get the *correct* weak solution we must use an appropriate entropy condition.

# Recall Godunov's method:

Given a set of cell quantities  $Q_i^n$  at time  $n$ :

1. Solve the Riemann problem at  $x_{i-1/2}$  to obtain  $Q_{i-1/2}^\downarrow = q^\downarrow(Q_{i-1}^n, Q_i^n)$

2. Define the flux:  $F_{i-1/2}^n = f(Q_{i-1/2}^\downarrow)$

3. Apply the flux differencing formula:  $Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n)$

This will work for any general system of conservation laws. Only the formulation of the Riemann problem itself changes with the system.

# In terms of the REA scheme we have discussed

1. **Reconstruct** a piece-wise **linear** function from the cell averages.

$$q^n(x, t_n) = Q_i^n + \sigma_i^n(x - x_i) \text{ for } x \text{ in cell } i$$

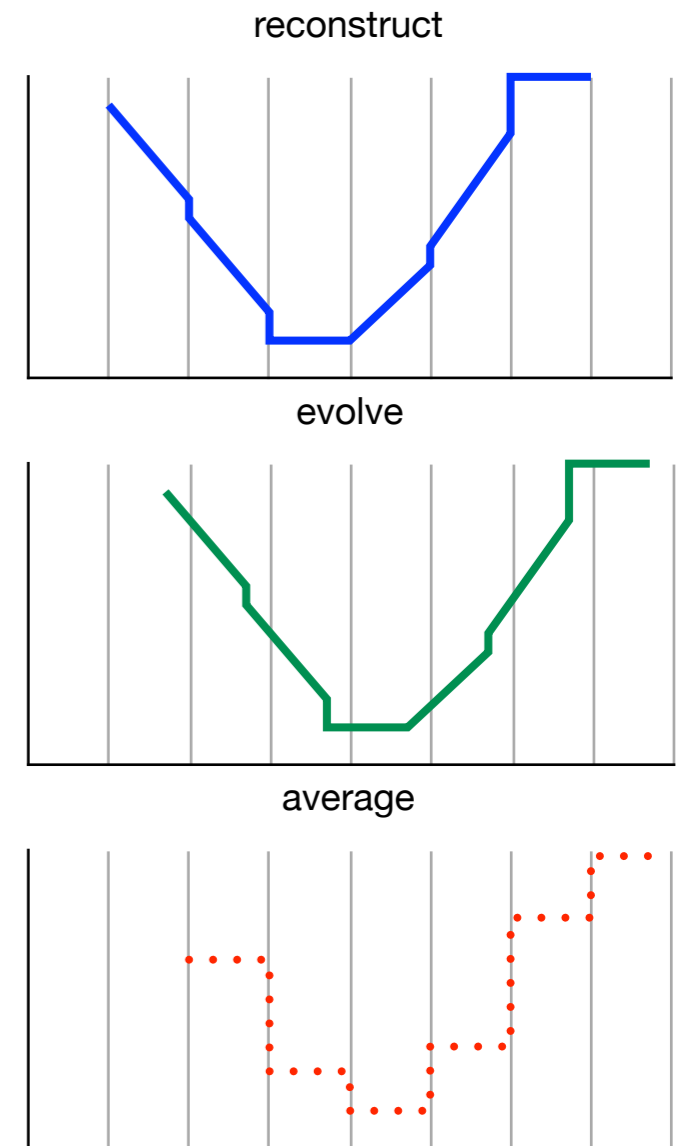
with the property that  $\text{TV}(q) \leq \text{TV}(Q)$

2. **Evolve** the hyperbolic equation (*approximately*) with this function to obtain a later-time function, by solving Riemann problems at the interfaces.

$$\tilde{q}^n(x, t_{n+1})$$

3. **Average** this function over each grid cell to obtain new cell averages.

$$Q_i^{n+1} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{q}^n(x, t_{n+1}) dx$$



The reconstruction step depends on the slope limiter that is chosen, and should be subject to TVD constraints. The other two steps do not affect TVD.

# Recall what TVD means:

Monotonicity preserving methods:

If a grid function that is initially monotone, i.e.  $Q_i^n \geq Q_{i-1}^n$  for all  $i$  at step  $n$

remains monotone at the next time:  $Q_i^{n+1} \geq Q_{i-1}^{n+1}$  for all  $i$  at step  $n + 1$

then the method is monotonicity preserving.

Total Variation Diminishing (TVD) methods:

Define the total variation of a grid function  $Q$  as: 
$$\text{TV}(Q) = \sum_{\text{grid}} |Q_i - Q_{i-1}|$$

A method is Total Variation Diminishing if 
$$\text{TV}(Q^{n+1}) \leq \text{TV}(Q^n)$$

If  $Q^n$  is monotone, then so is  $Q^{n+1}$ , and no spurious oscillations are generated.

This gives a form of stability necessary for proving convergence, also for nonlinear conservation laws.

# For advection, the REA algorithm gives us:

We update the advection equation by

$$Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x} (Q_i^n - Q_{i-1}^n) - \frac{1}{2} \frac{u\Delta t}{\Delta x} (\Delta x - u\Delta t) (\sigma_i^n - \sigma_{i-1}^n)$$

where the slope is given by

$$\sigma_i^n = \left( \frac{Q_{i+1}^n - Q_i^n}{\Delta x} \right) \phi_i^n$$

where  $\phi$  is the *flux limiter function*.

Choices for the flux limiter are:

upwind:  $\phi(\theta) = 0$

minmod:  $\phi(\theta) = \text{minmod}(1, \theta)$

Lax-Wendroff:  $\phi(\theta) = 1$

superbee:  $\phi(\theta) = \max(0, \min(1, 2\theta), \min(2, \theta))$

Beam-Warming:  $\phi(\theta) = \theta$

MC:  $\phi(\theta) = \max(0, \min((1 + \theta) / 2, 2, 2\theta))$

Fromm:  $\phi(\theta) = \frac{1}{2} (1 + \theta)$

van Leer:  $\phi(\theta) = \frac{(\theta + |\theta|)}{(1 + |\theta|)}$

$$\theta_i^n = \frac{Q_i^n - Q_{i-1}^n}{Q_{i+1}^n - Q_i^n}$$

# Slope limiters and flux limiters

The slope limiter formula for advection is:

$$Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x} (Q_i^n - Q_{i-1}^n) - \frac{1}{2} \frac{u\Delta t}{\Delta x} (\Delta x - u\Delta t) (\sigma_i^n - \sigma_{i-1}^n)$$

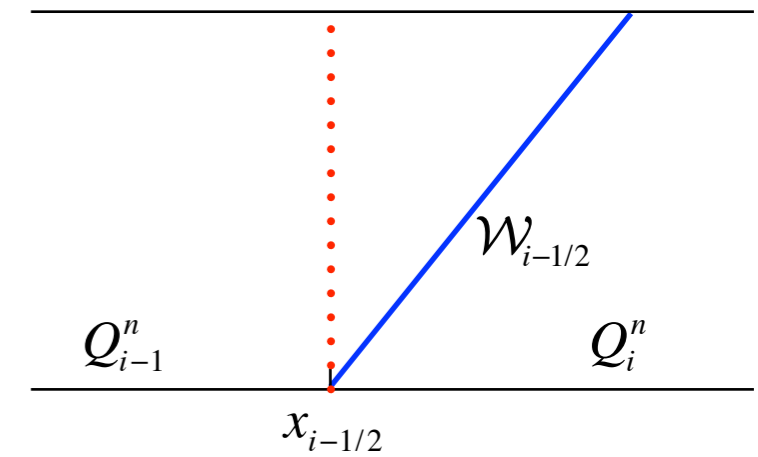
The flux limiter formulation for advection is:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n)$$

with the flux:

$$F_{i-1/2}^n = uQ_{i-1}^n + \frac{1}{2} u(\Delta x - u\Delta t) \sigma_{i-1}^n$$

# Wave limiters:



Let:  $\mathcal{W}_{i-1/2} = Q_i^n - Q_{i-1}^n$

Upwind formula:  $Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x} \mathcal{W}_{i-1/2}$

Lax-Wendroff formula:

$$Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x} \mathcal{W}_{i-1/2} - \frac{\Delta t}{\Delta x} (F_{i+1/2} - F_{i-1/2})$$

$$F_{i-1/2} = \frac{1}{2} \left( 1 - \left| \frac{u\Delta t}{\Delta x} \right| \right) |u| \mathcal{W}_{i-1/2}$$

High-resolution method:

$$\tilde{F}_{i-1/2} = \frac{1}{2} \left( 1 - \left| u \frac{\Delta t}{\Delta x} \right| \right) |u| \tilde{\mathcal{W}}_{i-1/2},$$

where

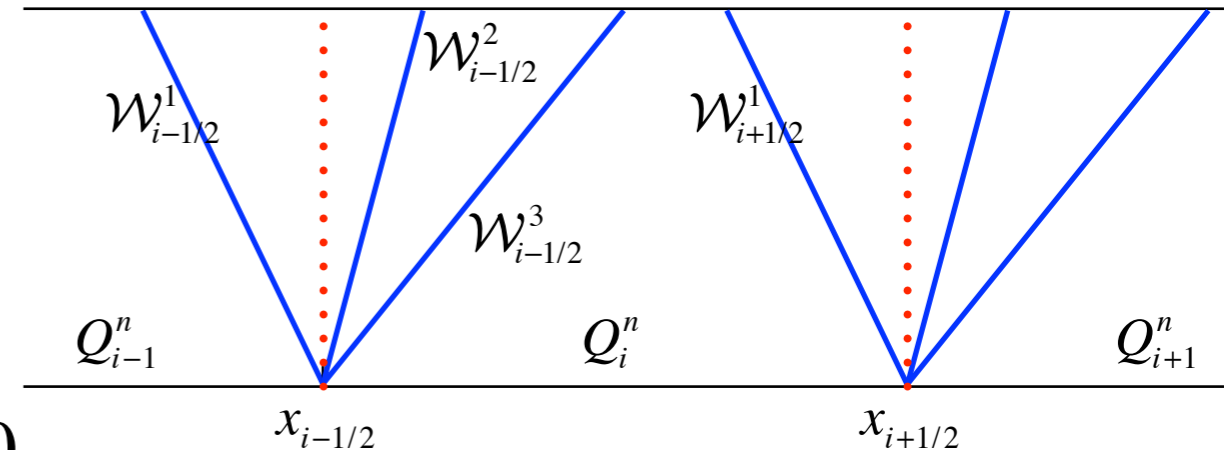
$$\tilde{\mathcal{W}}_{i-1/2} = \phi_{i-1/2} \mathcal{W}_{i-1/2}.$$

# Extension to linear systems

## Approach 1:

Diagonalise the system to  $q_t + \Lambda q_x = 0$

Apply the scalar algorithm to each component separately.



## Approach 2:

Solve the linear Riemann problem to decompose  $Q_i^n - Q_{i-1}^n$  into a number of waves.

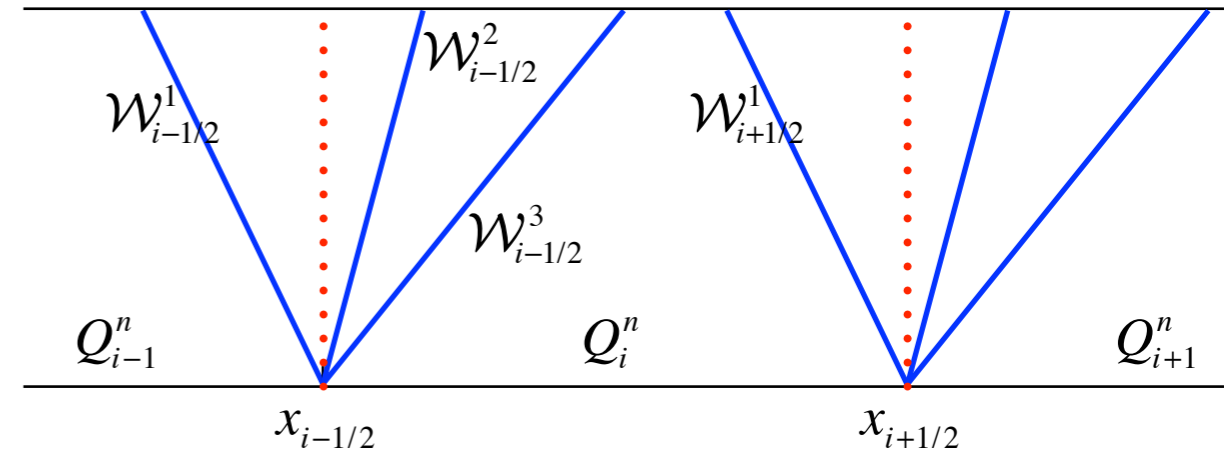
Apply a wave limiter to each wave.

**These approaches are equivalent.**

But note that it is important to apply the limiters to the waves rather than to the original variables.



# Wave propagation methods



Solving the Riemann problem between cells  $i$  and  $i+1$  gives the waves

$$Q_i - Q_{i-1} = \sum_{p=1}^m \mathcal{W}_{i-1/2}^p,$$

and speeds  $s_{i-1/2}^p$ . In the **nonlinear** case, an approximate solution is used.

These waves update the neighbouring cell averages via fluctuations, depending on sign of  $s_{i-1/2}^p$ .

The waves also give the decomposition of the slopes

$$\frac{Q_i - Q_{i-1}}{\Delta x} = \frac{1}{\Delta x} \sum_{p=1}^m \mathcal{W}_{i-1/2}^p,$$

Apply the limiter to each wave to obtain  $\tilde{\mathcal{W}}_{i-1/2} = \phi_{i-1/2} \mathcal{W}_{i-1/2}$ .

Use the limited waves in the second-order correction terms.

# High-resolution wave-propagation scheme

The fluctuation notation is more useful in the nonlinear case:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( \mathcal{A}^- \Delta Q_{i+1/2} + \mathcal{A}^+ \Delta Q_{i-1/2} \right) - \frac{\Delta t}{\Delta x} \left( F_{i+1/2} - F_{i-1/2} \right)$$

where

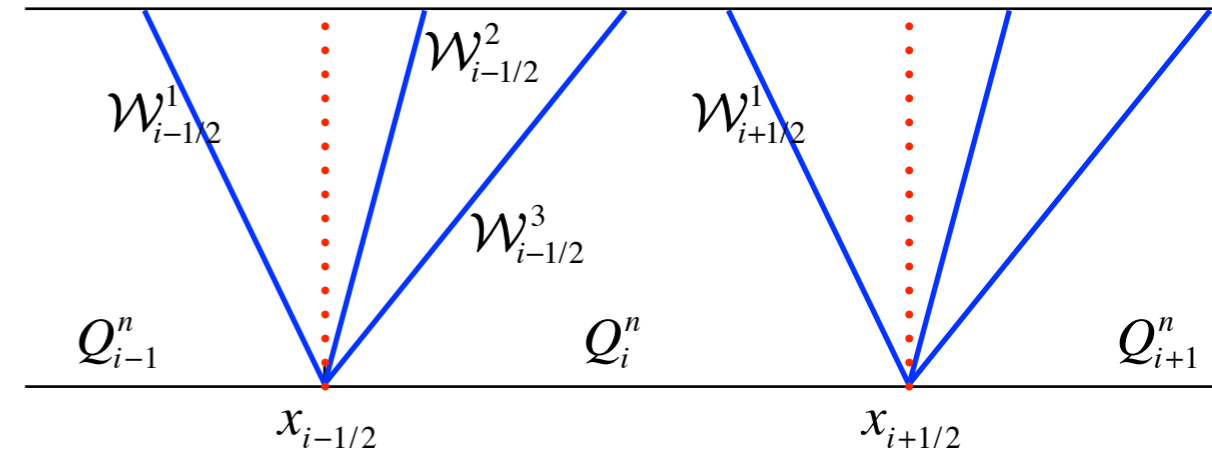
$$F_{i-1/2}^n = \frac{1}{2} \sum_{p=1}^m |s_{i-1/2}^p| \left( 1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^p| \right) \widetilde{\mathcal{W}}_{i-1/2}^p$$

$\widetilde{\mathcal{W}}_{i-1/2}^p$  represents the limited version of  $\mathcal{W}_{i-1/2}^p$ .

This is obtained by comparing  $\mathcal{W}_{i-1/2}^p$  with  $\mathcal{W}_{l-1/2}^p$  where

$$l = \begin{cases} i - 1 & \text{if } s_{i-1/2}^p > 0 \\ i + 1 & \text{if } s_{i-1/2}^p < 0 \end{cases}$$

# Wave limiters for a system



$Q_i - Q_{i-1}$  is split into waves  $\mathcal{W}_{i-1/2}^p = \alpha_{i-1/2}^p r_{i-1/2}^p$ ,

We replace these waves with the limited versions  $\tilde{\mathcal{W}}_{i-1/2}^p = \phi(\theta_{i-1/2}^p) \mathcal{W}_{i-1/2}^p$ .

where  $\theta_{i-1/2}^p = \frac{\mathcal{W}_{i-1/2}^p \cdot \mathcal{W}_{l-1/2}^p}{\mathcal{W}_{i-1/2}^p \cdot \mathcal{W}_{i-1/2}^p}$ , and  $l = \begin{cases} i-1 & \text{if } s_{i-1/2}^p > 0 \\ i+1 & \text{if } s_{i-1/2}^p < 0 \end{cases}$ .

Note that if  $r_{i-1/2}^p = r_{l-1/2}^p$  then  $\theta_{i-1/2}^p = \frac{\alpha_{l-1/2}^p}{\alpha_{i-1/2}^p}$ .

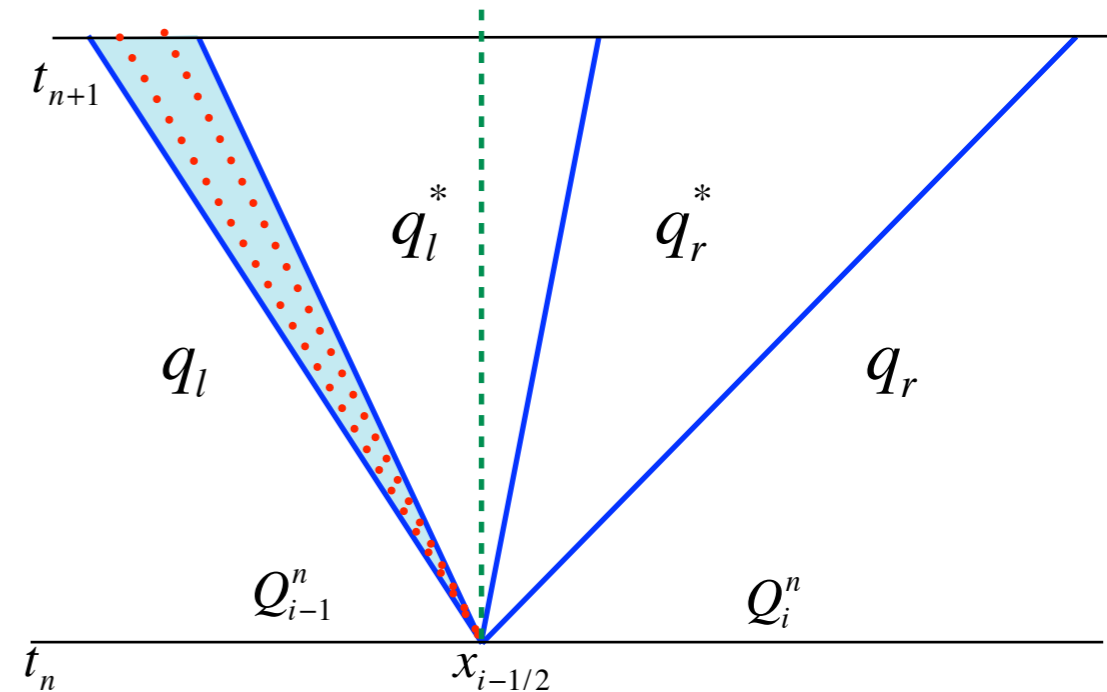
In the scalar case this reduces to

$$\theta_{i-1/2}^p = \frac{\mathcal{W}_{l-1/2}^p}{\mathcal{W}_{i-1/2}^p} = \frac{Q_l - Q_{l-1}}{Q_i - Q_{i-1}}$$

The exact Riemann solver for the nonlinear problem is expensive, and requires an iterative solver...

$$u = \varphi_l(p) = \begin{cases} u_l + \frac{2c_l}{\gamma-1} \left[ 1 - (p/p_l)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_l \\ u_l + \frac{2c_l}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_l}{\sqrt{1+\beta p/p_l}} \right] & \text{if } p \geq p_l \end{cases}$$

$$u = \varphi_r(p) = \begin{cases} u_r - \frac{2c_r}{\gamma-1} \left[ 1 - (p/p_r)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_r \\ u_r - \frac{2c_r}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_r}{\sqrt{1+\beta p/p_r}} \right] & \text{if } p \geq p_r \end{cases}$$



Solving  $\varphi_l(p_m) = \varphi_r(p_m)$  yields  $(p^*, u^*)$ , then  $\rho_l^* = \left( \frac{1 + \beta p^* / p_l}{p^* / p_l + \beta} \right) \rho_l$ ;  $\rho_r^* = \left( \frac{1 + \beta p^* / p_r}{p^* / p_r + \beta} \right) \rho_r$

In the rarefaction fan,  $u(\xi) = \frac{(\gamma-1)u_l + 2(c_l + \xi)}{\gamma+1}$ .

$$\rho(\xi) = \left( \frac{\rho_l^\gamma}{\gamma p_l} (u(\xi) - \xi)^2 \right)^{1/(\gamma-1)}$$

$$p(\xi) = \left( \frac{p_l}{\rho_l^\gamma} \right) \rho(\xi)^\gamma$$

# Newton's Method for finding a root of a function

Newton's method aims at finding a root by extrapolating from the function's slope at the point where each successive guess is taken. This is very robust, provided there are no intervening extrema.

Each successive guess is given by

$$x_{n+1} = x_n - \frac{f(x_n)}{k}$$

where the slope  $k$  is chosen from

(a)  $k = f'(x_n)$

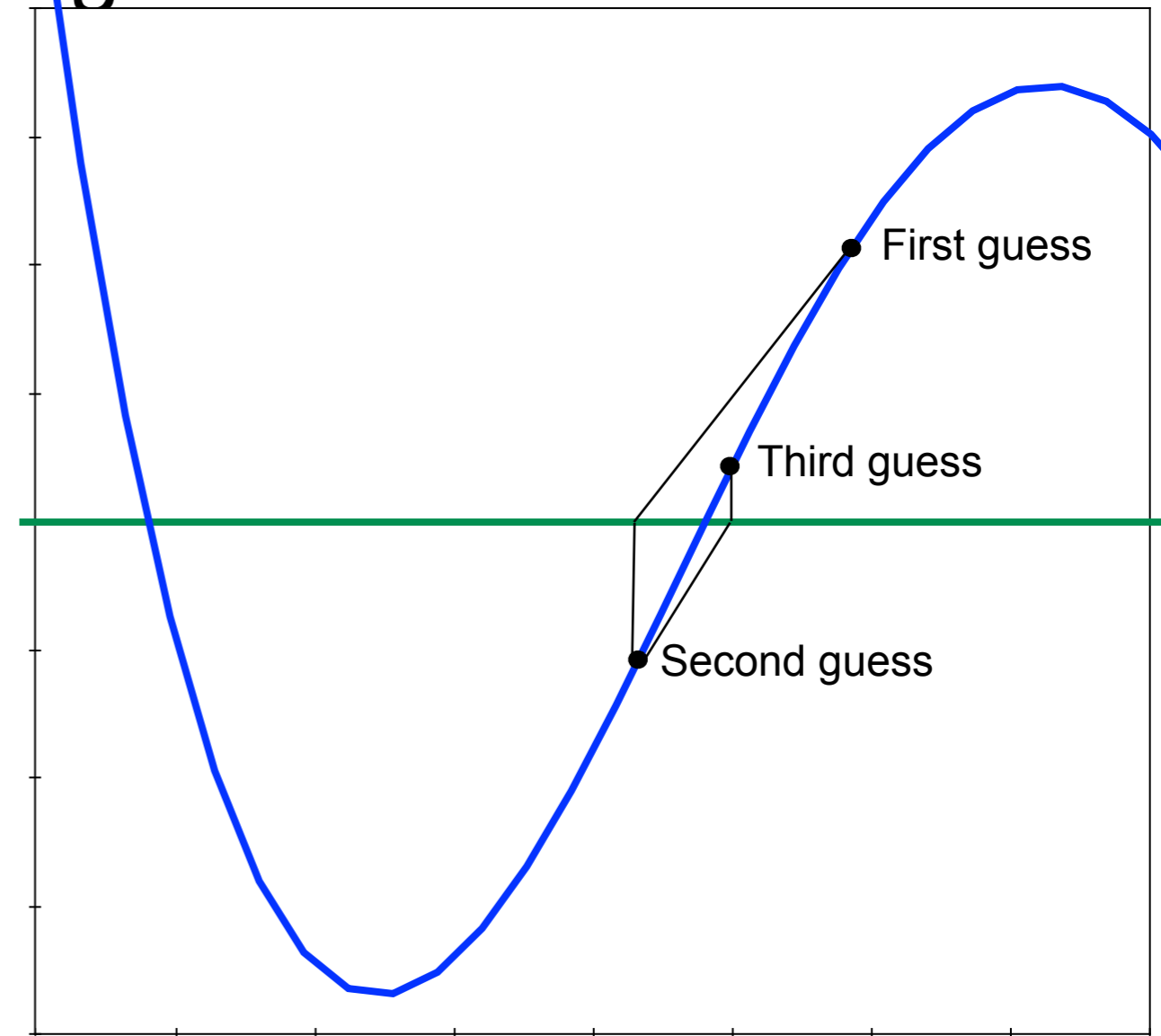
*tangent method*

(b)  $k = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$

*secant method*; more convenient than the tangent method when the derivative is unavailable or difficult to compute.

(c)  $k = \frac{f(x_n) - f(x_m)}{x_n - x_m}$

*regula falsi*;  $m$  is the most recent guess in which the function has the opposite sign. This method always brackets the root and is therefore most robust, but generally a bit slower.

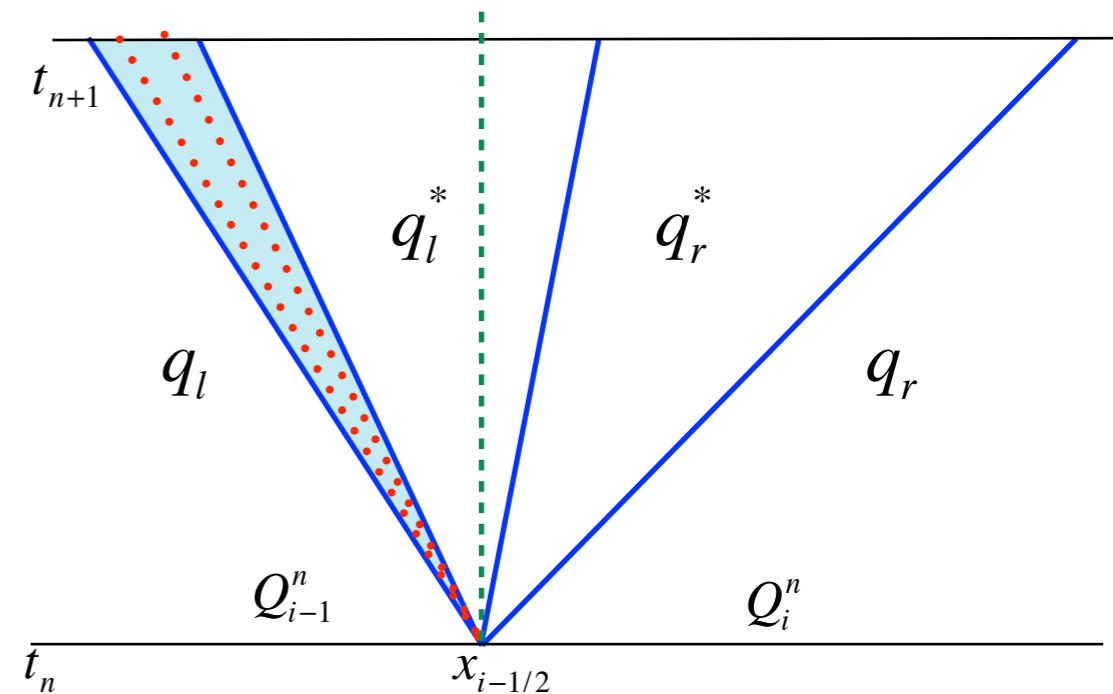




The exact Riemann solver for the nonlinear problem is expensive, and most of it is not necessary!

$$u = \varphi_l(p) = \begin{cases} u_l + \frac{2c_l}{\gamma-1} \left[ 1 - (p/p_l)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_l \\ u_l + \frac{2c_l}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_l}{\sqrt{1+\beta p/p_l}} \right] & \text{if } p \geq p_l \end{cases}$$

$$u = \varphi_r(p) = \begin{cases} u_r - \frac{2c_r}{\gamma-1} \left[ 1 - (p/p_r)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_r \\ u_r - \frac{2c_r}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_r}{\sqrt{1+\beta p/p_r}} \right] & \text{if } p \geq p_r \end{cases}$$



Solving  $\varphi_l(p_m) = \varphi_r(p_m)$  yields  $(p^*, u^*)$ , then  $\rho_l^* = \left( \frac{1 + \beta p^* / p_l}{p^* / p_l + \beta} \right) \rho_l$ ;  $\rho_r^* = \left( \frac{1 + \beta p^* / p_r}{p^* / p_r + \beta} \right) \rho_r$

In the rarefaction fan,  $u(\xi) = \frac{(\gamma-1)u_l + 2(c_l + \xi)}{\gamma+1}$ .

$$\rho(\xi) = \left( \frac{\rho_l^\gamma}{\gamma p_l} (u(\xi) - \xi)^2 \right)^{1/(\gamma-1)}$$

$$p(\xi) = \left( \frac{p_l}{\rho_l^\gamma} \right) \rho(\xi)^\gamma$$

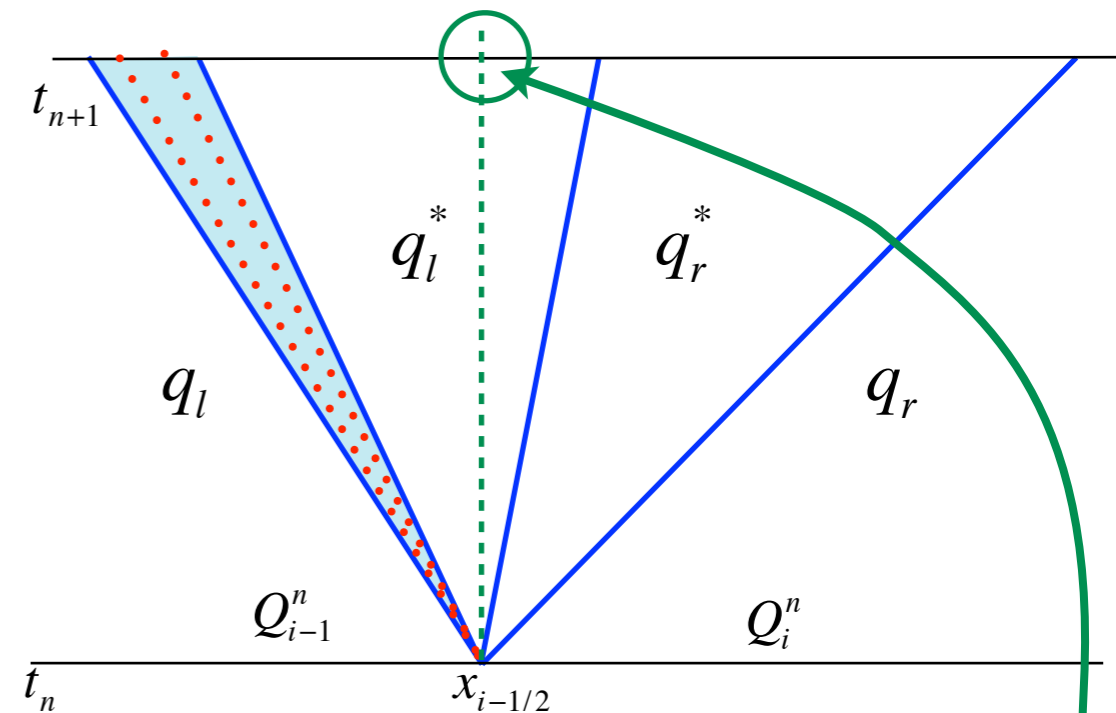
These are useful for exact solutions of certain problems.

But in simulations we only need the solution at the cell interface!

The exact Riemann solver for the nonlinear problem is expensive, and most of it is not necessary!

$$u = \varphi_l(p) = \begin{cases} u_l + \frac{2c_l}{\gamma-1} \left[ 1 - (p/p_l)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_l \\ u_l + \frac{2c_l}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_l}{\sqrt{1+\beta p/p_l}} \right] & \text{if } p \geq p_l \end{cases}$$

$$u = \varphi_r(p) = \begin{cases} u_r - \frac{2c_r}{\gamma-1} \left[ 1 - (p/p_r)^{\frac{\gamma-1}{2\gamma}} \right] & \text{if } p \leq p_r \\ u_r - \frac{2c_r}{\sqrt{2\gamma(\gamma-1)}} \left[ \frac{1-p/p_r}{\sqrt{1+\beta p/p_r}} \right] & \text{if } p \geq p_r \end{cases}$$



Solving  $\varphi_l(p_m) = \varphi_r(p_m)$  yields  $(p^*, u^*)$ , then  $\rho_l^* = \left( \frac{1 + \beta p^* / p_l}{p^* / p_l + \beta} \right) \rho_l$ ;  $\rho_r^* = \left( \frac{1 + \beta p^* / p_r}{p^* / p_r + \beta} \right) \rho_r$

In the rarefaction fan,  $u(\xi) = \frac{(\gamma-1)u_l + 2(c_l + \xi)}{\gamma+1}$ .

$$\rho(\xi) = \left( \frac{\rho_l^\gamma}{\gamma p_l} (u(\xi) - \xi)^2 \right)^{1/(\gamma-1)}$$

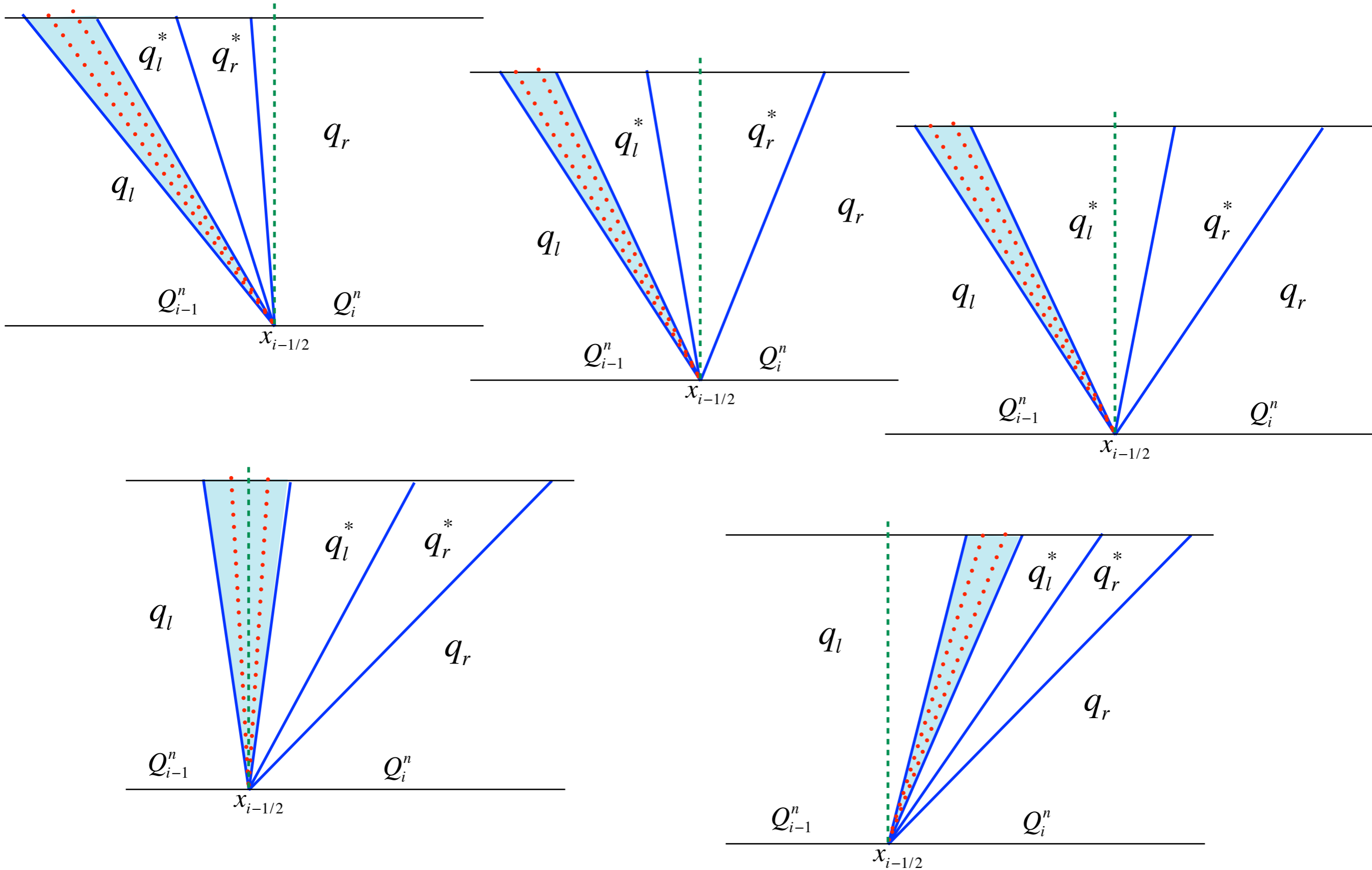
$$p(\xi) = \left( \frac{p_l}{\rho_l^\gamma} \right) \rho(\xi)^\gamma$$

These are useful for exact solutions of certain problems.

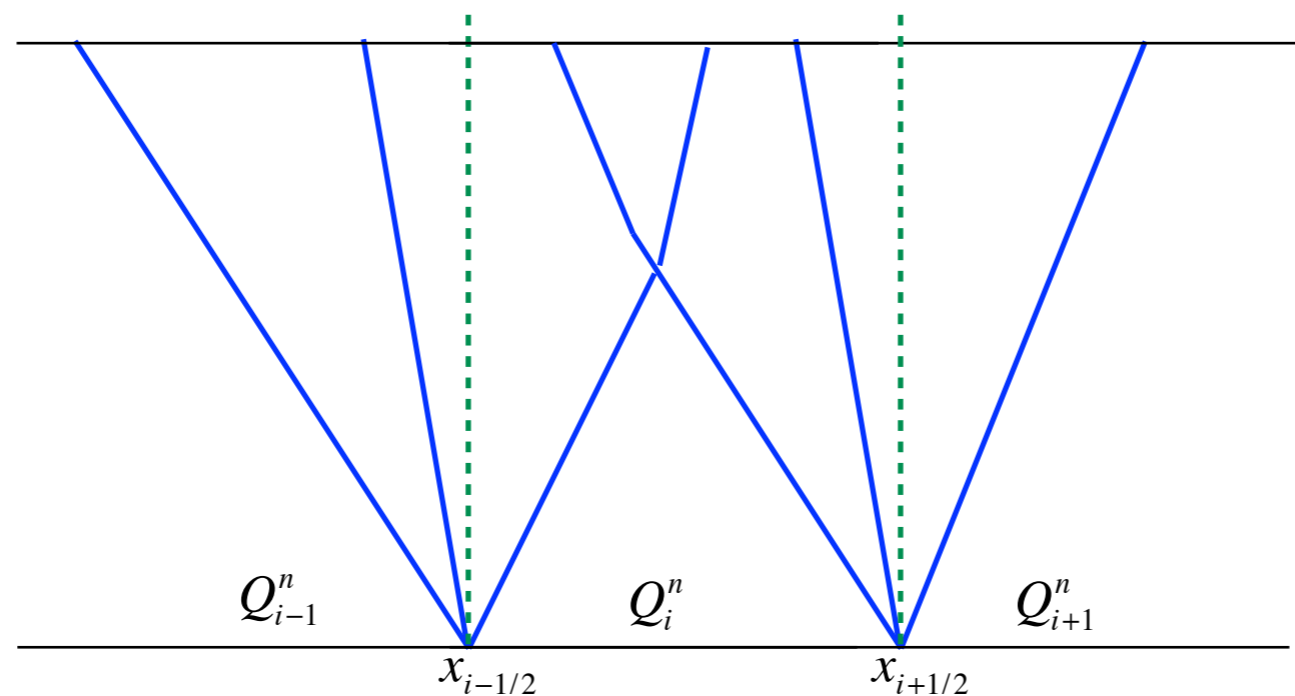
But in simulations we only need the solution at the cell interface!



But we do need to know where the cell interface lies with respect to the waves, and compute accordingly



# Wave interactions



Waves that interact with each other within a cell will not change the cell-interface values on the next time step provided the Courant number is less than 1.

# Riemann solvers in CLAWPACK

In CLAWPACK, the hyperbolic problem is specified by providing a **Riemann solver** with

**Input:** the value of  $q$  in each grid cell

**Output:** the solution to the Riemann problem *at each cell interface*:

The Waves  $\mathcal{W}^p$ ,  $p = 1, 2, \dots, m$  for a system of  $m$  equations

The Speeds  $s^p$ ,  $p = 1, 2, \dots, m$

The Fluctuations  $\mathcal{A}^\pm \Delta Q$ , for high-resolution corrections

Because the problem is solved entirely using Riemann solvers, you won't see anything in the code that resembles the original system of partial differential equations.

# Wave propagation for nonlinear systems

An **approximate** Riemann solver is typically used to get the wave decomposition

$$Q_i - Q_{i-1} = \sum_{p=1}^m \mathcal{W}_{i-1/2}^p,$$

where the wave  $\mathcal{W}_{i-1/2}^p$  propagates at a speed  $s_{i-1/2}^p$ .

If we define  $\hat{A}_{i-1/2} = \hat{A}(Q_i^n, Q_{i-1}^n)$  as a linearised approximation to  $f'(q)$  valid in the neighbourhood of  $(Q_i, Q_{i-1})$ ,

then we can solve the simpler linear Riemann problem at that cell interface for the linearised equation:

$$q_t + \hat{A}_{i-1/2} q_x = 0,$$

to obtain

$$\mathcal{W}_{i-1/2}^p = \alpha_{i-1/2}^p \hat{r}_{i-1/2}^p, \quad s_{i-1/2}^p = \hat{\lambda}_{i-1/2}^p.$$

# Approximate Riemann Solvers

Approximate the true Riemann solution by a set of waves consisting of finite jumps propagating at *constant* speeds (as in the linear case).

Use a *local linearisation*: replace  $q_t + f(q)_x = 0$  by  $q_t + \hat{A}_{i-1/2} q_x = 0$ , where  $\hat{A} = \hat{A}(q_l, q_r) \approx f'(q_{ave})$ .

Then decompose

$$q_l - q_r = \sum_{p=1}^m \alpha^p \hat{r}^p$$

to obtain the waves  $\mathcal{W}^p = \alpha^p \hat{r}^p$  with speeds  $s^p = \hat{\lambda}^p$ .

But how do we chose  $\hat{A}$ ?

# The Roe solver

The most widely used approximate Riemann solver is the one developed by Phil Roe at the Royal Aircraft Establishment. The approach is to solve the linearised equation

$$q_t + \hat{A}q_x = 0,$$

where  $\hat{A}$  is an average matrix such that  $\hat{A}(q_r, q_l) \equiv \hat{A}_{rl} \approx f'(q_{ave})$ .

and  $\hat{A}_{rl}(q_r - q_l) = f(q_r) - f(q_l) = s(q_r - q_l)$

The Roe-average matrix can be determined analytically for many important nonlinear systems, including the shallow-water equations and the Euler equations.

# Roe's approximate Riemann solver

Roe suggested these constraints for  $\hat{A}$  :

1.  $\hat{A}_{rl}(q_r - q_l) = f(q_r) - f(q_l)$  Cf. Rankine-Hugoniot condition.
2.  $\hat{A}$  is diagonalisable with real eigenvalues.
3.  $\hat{A}_{rl} \rightarrow f'(\bar{q})$  smoothly as  $q_l, q_r \rightarrow \bar{q}$

A single shock is captured exactly because (1.) is essentially the Rankine-Hugoniot jump condition.

$f(q_r) - f(q_l) = s(q_r - q_l)$  implies that  $q_r - q_l$  is an eigenvector of  $\hat{A}$  .

It is a good approximation for weak waves, or smooth flow.

The wave-propagation algorithm is also conservative since

$$\mathcal{A}^- \Delta Q_{i-1/2} + \mathcal{A}^+ \Delta Q_{i-1/2} = \sum_p s_{i-1/2}^p \mathcal{W}_{i-1/2}^p = \hat{A} \sum_p \mathcal{W}_{i-1/2}^p .$$

# How to use an approximate Riemann solver

Since we only need the solution at the cell interface, we determine the state along  $x/t = 0$ , calling it  $Q^*$ . Thus with

$$Q^* = Q_{i-1} + \sum_{p:s^p < 0} \mathcal{W}_{i-1/2}^p, \quad F_{i-1/2} = f(Q^*),$$

we form the fluctuations as

$$\mathcal{A}^- \Delta Q = F_{i-1/2} - f(Q_{i-1}), \quad \mathcal{A}^+ \Delta Q = f(Q_i) - F_{i-1/2}.$$

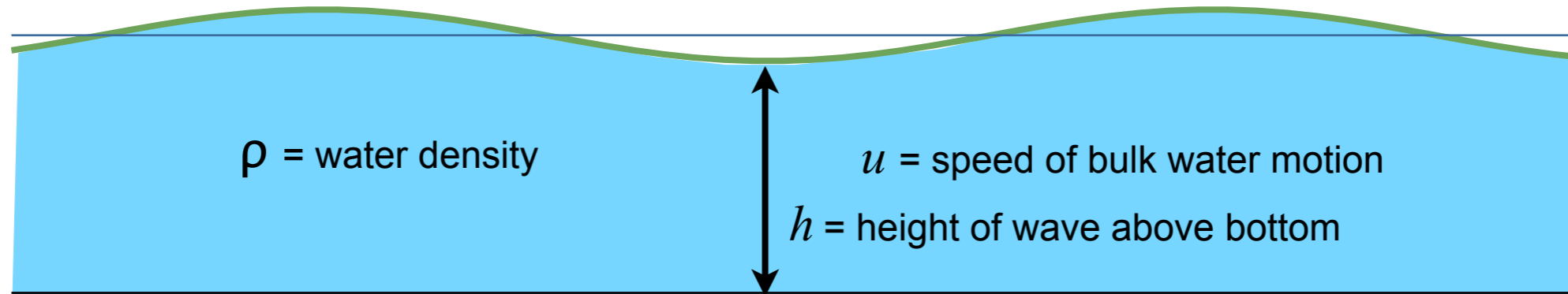
You can sometimes use  $\mathcal{A}^- \Delta Q = \sum_{p:s^p < 0} s^p \mathcal{W}^p$ ,  $\mathcal{A}^+ \Delta Q = \sum_{p:s^p > 0} s^p \mathcal{W}^p$ ,

which is conservative if  $\mathcal{A}^- \Delta Q + \mathcal{A}^+ \Delta Q = f(Q_i) - f(Q_{i-1})$ ,

as is true for the Roe solver.



# Example: Roe solver for shallow-water equations



$$h(x,t) = \text{depth}$$

$$u(x,t) = \text{bulk speed, varies only with } x$$

Conservation of mass and momentum gives the system:

$$q_t + f(q)_x = \begin{bmatrix} h \\ hu \end{bmatrix}_t + \begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{bmatrix}_x = 0.$$

which has the Jacobian matrix:

$$f'(q) = \begin{bmatrix} 0 & 1 \\ -u^2 + gh & 2u \end{bmatrix}, \quad \lambda = u \pm \sqrt{gh}.$$

# Roe solver for Shallow Water

Given  $h_l, u_l, h_r, u_r$ , define  $\bar{h} = \frac{h_l + h_r}{2}$ ,  $\hat{u} = \frac{\sqrt{h_l}u_l + \sqrt{h_r}u_r}{\sqrt{h_l} + \sqrt{h_r}}$ .

Then if  $\hat{A}$  is defined as the Jacobian matrix evaluated at the special state

$$\hat{q} = (\bar{h}, \bar{h}\hat{u}),$$

we find that:

the Roe conditions are satisfied,

an isolated shock is modelled well,

and the wave propagation algorithm is conservative.

If we use limited waves, we obtain high-resolution methods as before.

# Roe solver for Shallow Water

Given  $h_l, u_l, h_r, u_r$ , define  $\bar{h} = \frac{h_l + h_r}{2}$ ,  $\hat{u} = \frac{\sqrt{h_l} u_l + \sqrt{h_r} u_r}{\sqrt{h_l} + \sqrt{h_r}}$ .

“Roe average”

Then if  $\hat{A}$  is defined as the Jacobian matrix evaluated at the special state

$$\hat{q} = (\bar{h}, \bar{h}\hat{u}),$$

we find that:

the Roe conditions are satisfied,

an isolated shock is modelled well,

and the wave propagation algorithm is conservative.

If we use limited waves, we obtain high-resolution methods as before.

# Roe solver for Shallow Water

Given  $h_l, u_l, h_r, u_r$ , define  $\bar{h} = \frac{h_l + h_r}{2}$ ,  $\hat{u} = \frac{\sqrt{h_l}u_l + \sqrt{h_r}u_r}{\sqrt{h_l} + \sqrt{h_r}}$ .

Then if  $\hat{A}$  is defined as the Jacobian matrix evaluated at the special state

$$\hat{q} = (\bar{h}, \bar{h}\hat{u}),$$

the eigenvalues of  $\hat{A} = f'(\hat{q})$  are:

$$\hat{\lambda}^1 = \hat{u} - \hat{c}, \quad \hat{\lambda}^2 = \hat{u} + \hat{c}, \quad \hat{c} = \sqrt{g\bar{h}},$$

and the eigenvectors are:

$$\hat{r}^1 = \begin{bmatrix} 1 \\ \hat{u} - \hat{c} \end{bmatrix}, \quad \hat{r}^2 = \begin{bmatrix} 1 \\ \hat{u} + \hat{c} \end{bmatrix},$$



# Roe solver for the Euler equations

The eigensystem of the Euler equations for a polytropic gas is:

$$\lambda^1 = u - c \quad \lambda^2 = u \quad \lambda^3 = u + c$$

$$r^1 = \begin{bmatrix} 1 \\ u - c \\ H - uc \end{bmatrix} \quad r^2 = \begin{bmatrix} 1 \\ u \\ \frac{1}{2}u^2 \end{bmatrix} \quad r^3 = \begin{bmatrix} 1 \\ u + c \\ H + uc \end{bmatrix}$$

These need to be evaluated at the Roe-averaged state, so we need the Roe averages for  $u$ ,  $H$ ,  $c$ . These are:

$$\hat{u} = \frac{\sqrt{\rho_{i-1}}u_{i-1} + \sqrt{\rho_i}u_i}{\sqrt{\rho_{i-1}} + \sqrt{\rho_i}}$$

$$\hat{H} = \frac{\sqrt{\rho_{i-1}}H_{i-1} + \sqrt{\rho_i}H_i}{\sqrt{\rho_{i-1}} + \sqrt{\rho_i}}$$

$$\hat{c} = \sqrt{(\gamma - 1) \left( \hat{H} - \frac{1}{2}\hat{u}^2 \right)}$$

# Roe solver for the Euler equations

Then the wave decomposition between the left and right states is

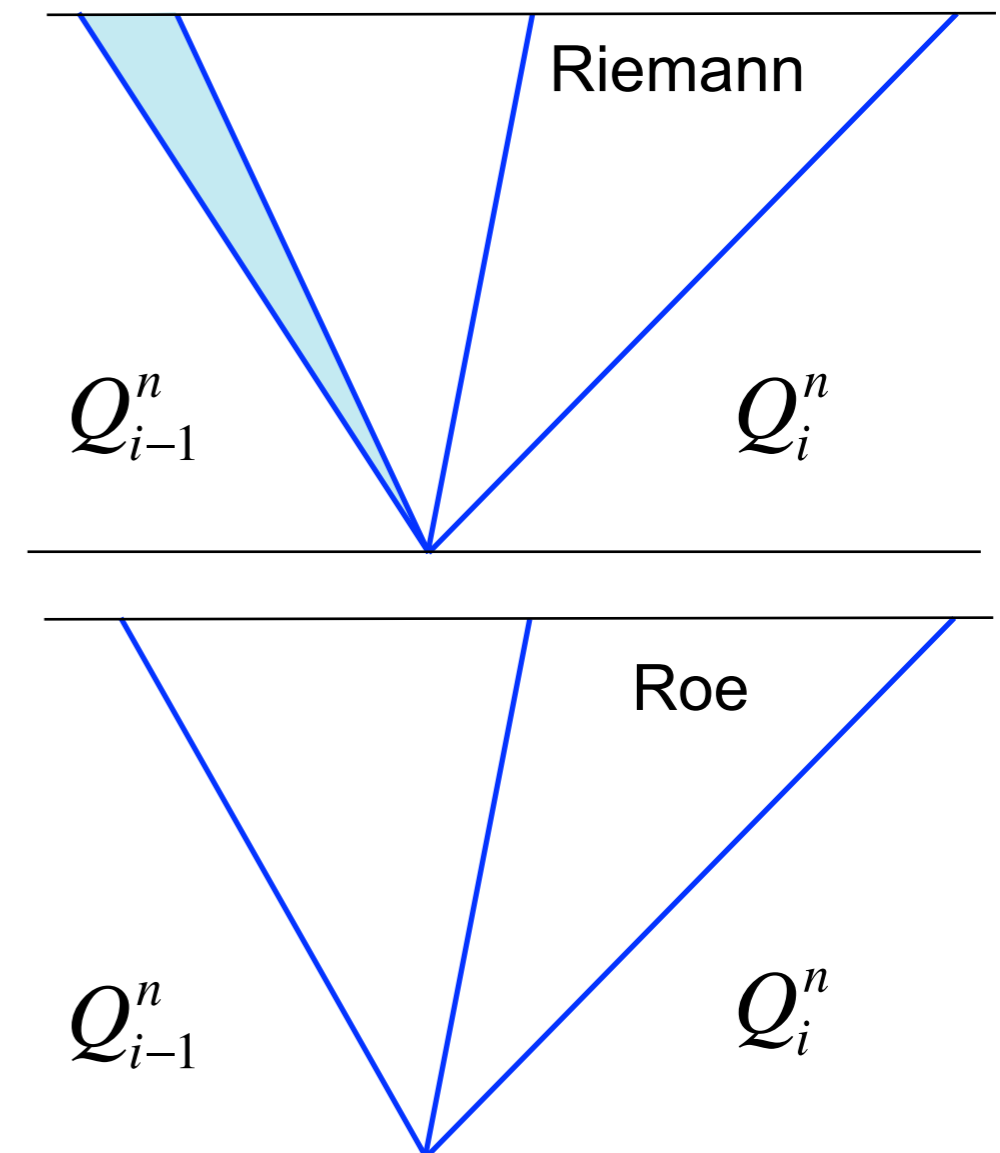
$$\delta \equiv Q_i - Q_{i-1} = \alpha^1 \hat{r}^1 + \alpha^2 \hat{r}^2 + \alpha^3 \hat{r}^3$$

where

$$\alpha^2 = (\gamma - 1) \frac{(\hat{H} - \hat{u}^2) \delta^1 + \hat{u} \delta^2 - \delta^3}{\hat{c}^2}$$

$$\alpha^3 = \frac{\delta^2 + (\hat{c} - \hat{u}) \delta^1 - \hat{c} \alpha^2}{2\hat{c}}$$

$$\alpha^1 = \delta^1 - \alpha^2 - \alpha^3$$



But note that, while the Riemann solution consists of three waves, one of which is a rarefaction fan, the Roe solution only consists of three waves. In most cases this does not matter, since the desired solution at  $x/t=0$  will be the same intermediate state. In the case of a transonic rarefaction a modification (in the form of an entropy fix) is necessary.

# Roe solver for the Euler equations

Then the wave decomposition between the left and right states is

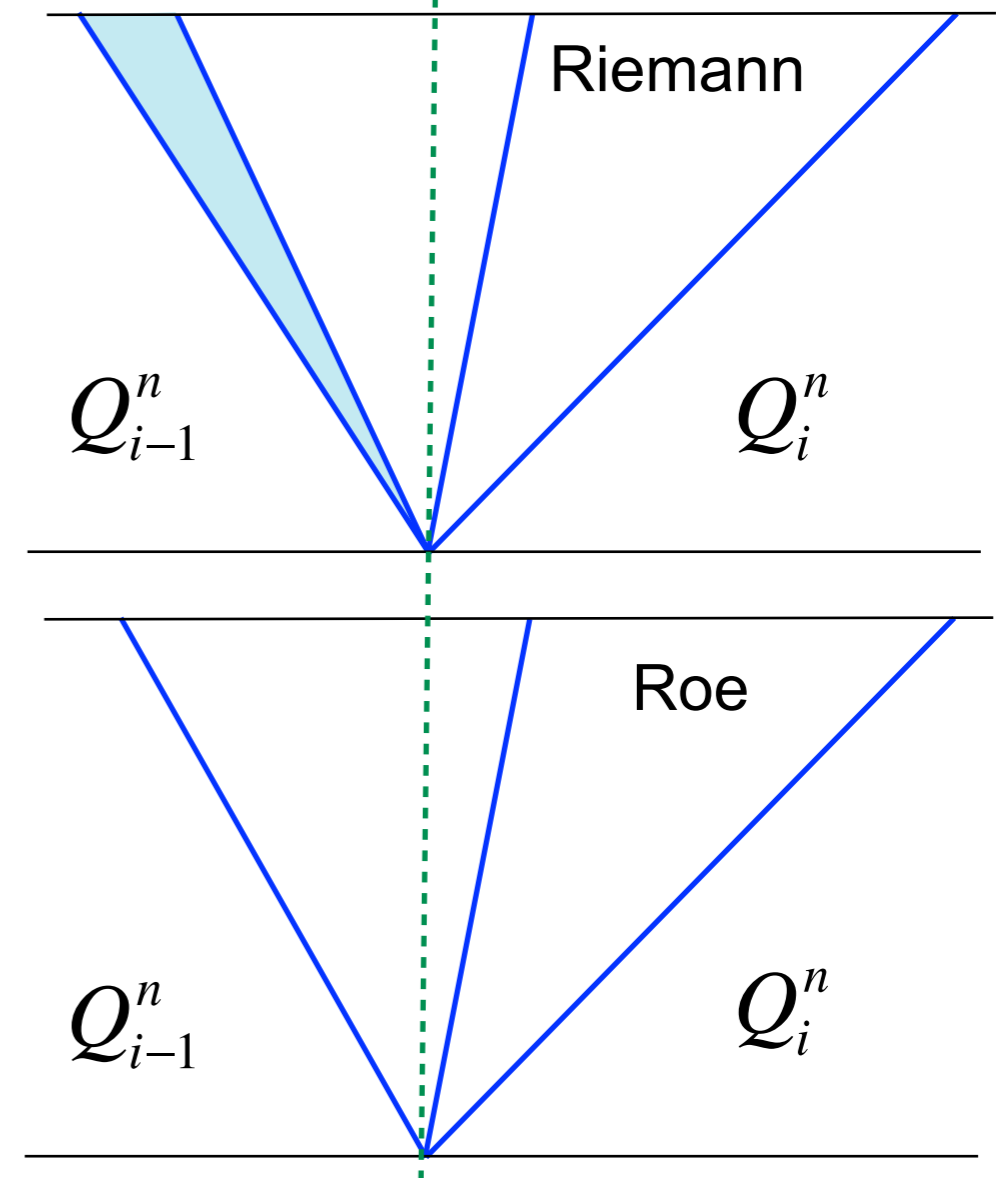
$$\delta \equiv Q_i - Q_{i-1} = \alpha^1 \hat{r}^1 + \alpha^2 \hat{r}^2 + \alpha^3 \hat{r}^3$$

where

$$\alpha^2 = (\gamma - 1) \frac{(\hat{H} - \hat{u}^2) \delta^1 + \hat{u} \delta^2 - \delta^3}{\hat{c}^2}$$

$$\alpha^3 = \frac{\delta^2 + (\hat{c} - \hat{u}) \delta^1 - \hat{c} \alpha^2}{2\hat{c}}$$

$$\alpha^1 = \delta^1 - \alpha^2 - \alpha^3$$



But note that, while the Riemann solution consists of three waves, one of which is a rarefaction fan, the Roe solution only consists of three waves. In most cases this does not matter, since the desired solution at  $x/t=0$  will be the same intermediate state. In the case of a transonic rarefaction a modification (in the form of an entropy fix) is necessary.



# Entropy fix for transonic rarefactions

Suppose there is a transonic rarefaction in the  $k$  wave:

$$\lambda_l^k < 0 < \lambda_r^k, \quad q_l^k = Q_{i-1} + \sum_{p=1}^{k-1} \mathcal{W}^p, \quad q_r^k = q_l^k + \mathcal{W}^k$$

The method proposed by Harten and Hyman, modified slightly by Leveque, and implemented in Clawpack, is the following. Define

$$\beta = \frac{\lambda_k^r - \hat{\lambda}_k}{\lambda_k^r - \lambda_k^l}$$

where  $\hat{\lambda}_k$  is the Roe-averaged eigenvalue for this wave. Then in computing the fluctuations

$$\mathcal{A}^- \Delta Q_{i-1/2} = \sum_p \left( s_{i-1/2}^p \right)^- \mathcal{W}_{i-1/2}^p, \quad \mathcal{A}^+ \Delta Q_{i-1/2} = \sum_p \left( s_{i-1/2}^p \right)^+ \mathcal{W}_{i-1/2}^p$$

for the speed of the  $k$  wave use

$$\left( \hat{\lambda}^k \right)^- = \beta \lambda_l^k, \quad \left( \hat{\lambda}^k \right)^+ = (1 - \beta) \lambda_r^k$$

# The Harten-Lax-van Leer (HLL) Solver

This solver uses only 2 waves with

$s^1$  = minimum characteristic speed

$s^2$  = maximum characteristic speed

Write

$$\mathcal{W}^1 = Q^* - q_l, \quad \mathcal{W}^2 = q_r - Q^*$$

where the middle state  $Q^*$  is uniquely determined by the conservation requirement:

$$s^1 \mathcal{W}^1 + s^2 \mathcal{W}^2 = f(q_r) - f(q_l)$$

$$\Rightarrow Q^* = \frac{f(q_r) - f(q_l) - s^2 q_r + s^1 q_l}{s^1 - s^2}$$

Modifications of this include positivity constraints and the addition of a third wave.

# Riemann solvers: exact vs approximate?

Whether to use a Roe solver, or other approximate Riemann solver, as opposed to an iterative exact solver is debatable.

Exact solvers are typically costly in time and storage

You don't need all the information generated

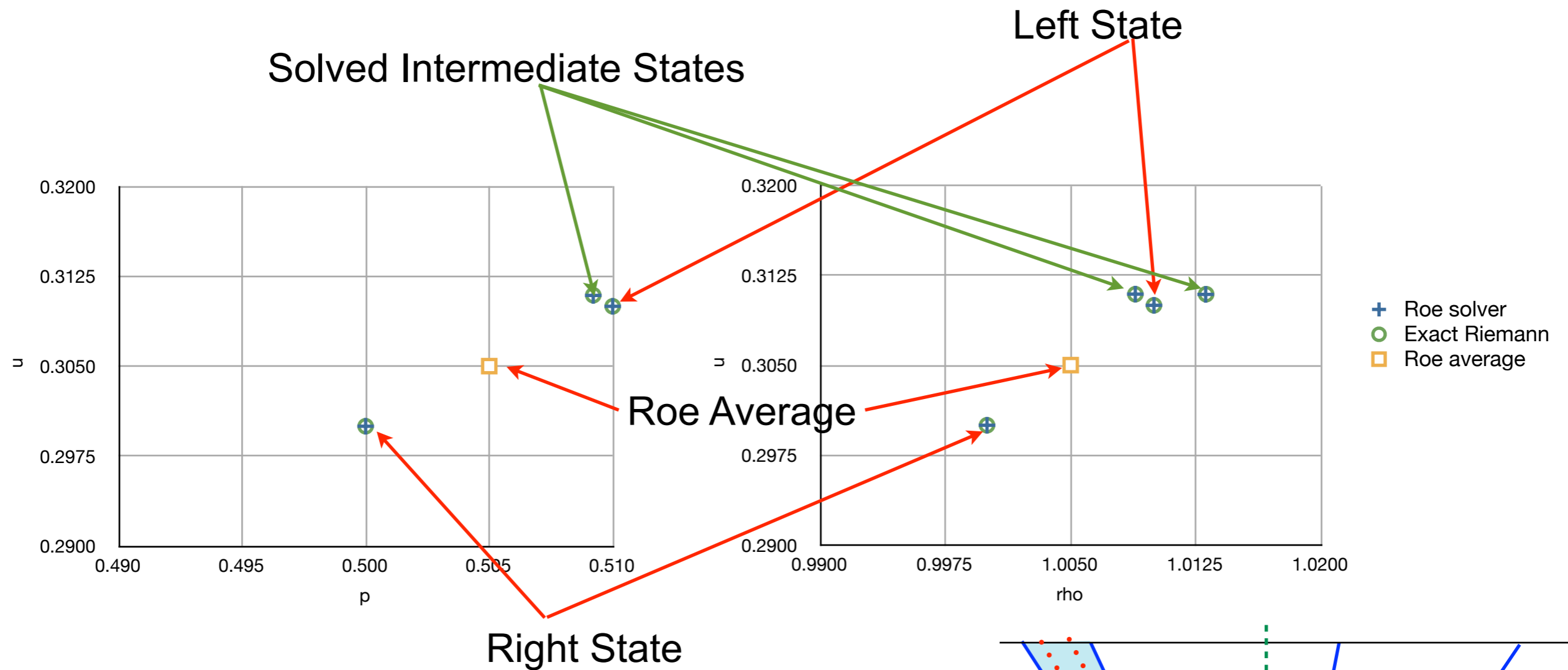
However, if you use a Roe solver:

You don't get the full structure of the rarefaction wave

In certain circumstances, the approximation may be poor

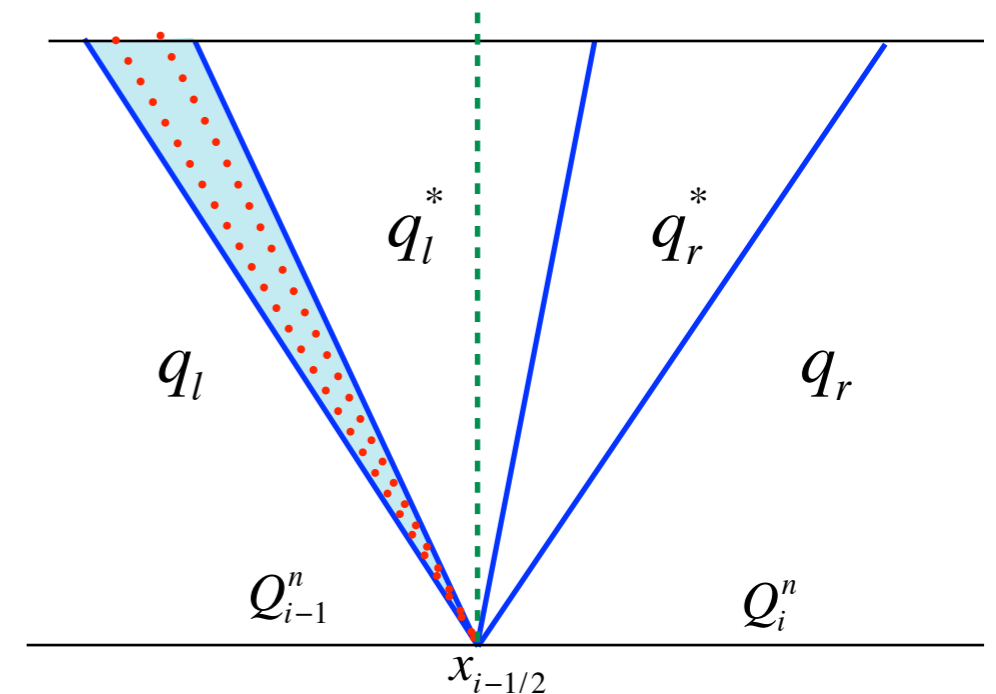
As computers and methods improve, more people may prefer exact iterative solvers.

# How good is the Roe solver?

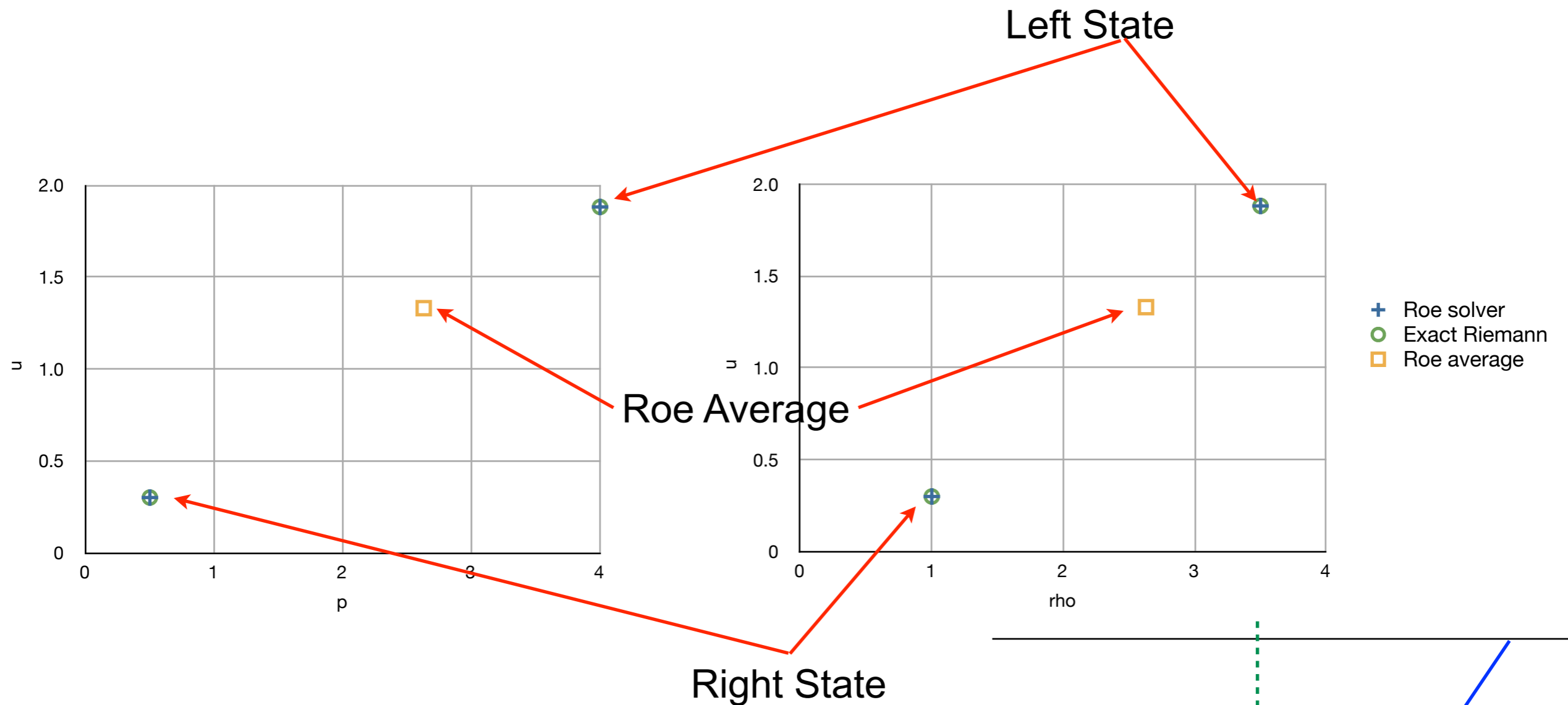


Example for the Euler equations, comparing iterative exact and approximate Roe solvers.

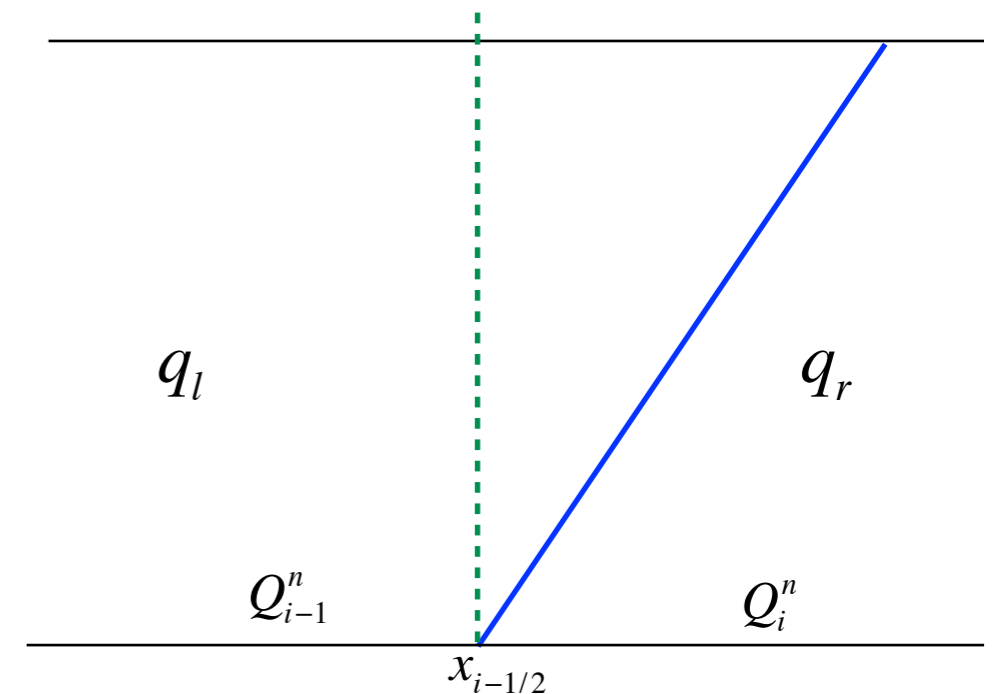
When the left and right states are close together, the Roe solver is very good.



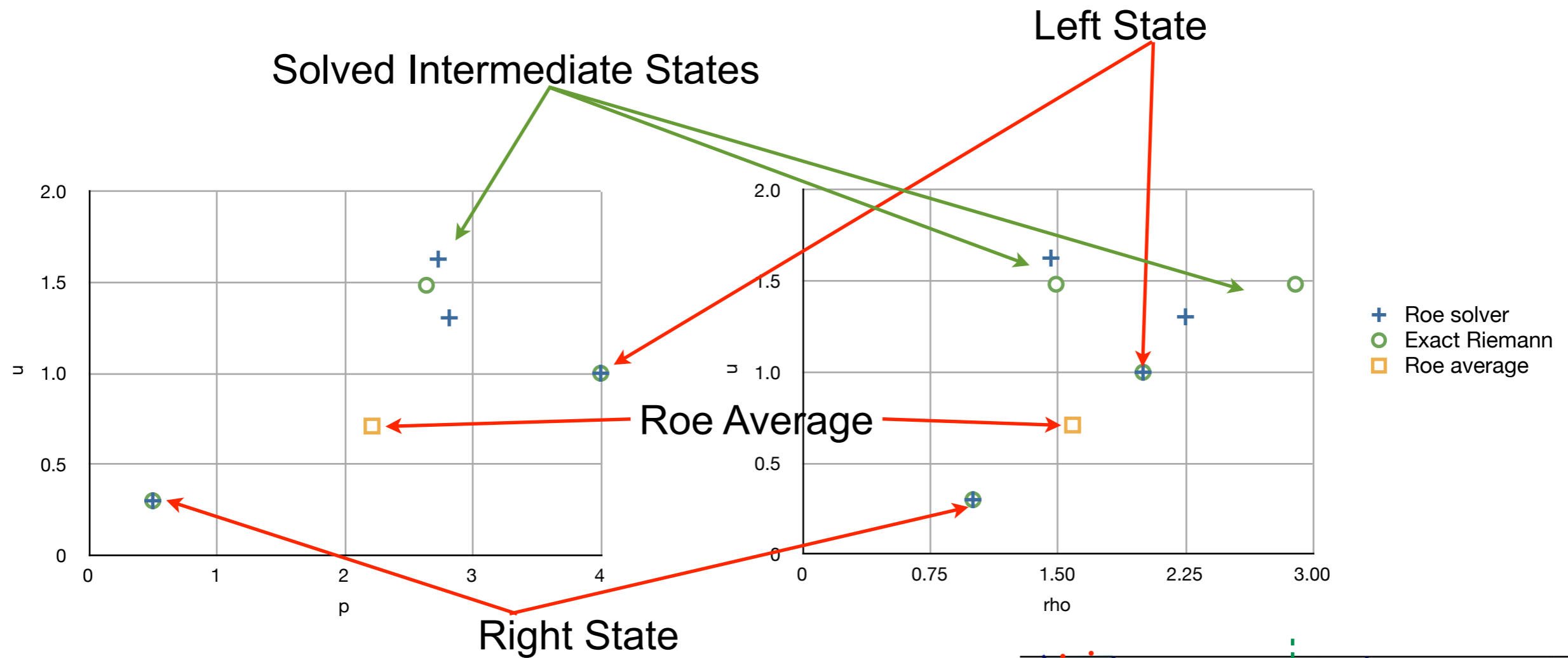
# How good is the Roe solver?



When the left and right states are connected by a single shock, there are no intermediate states, and the Roe solver is exact



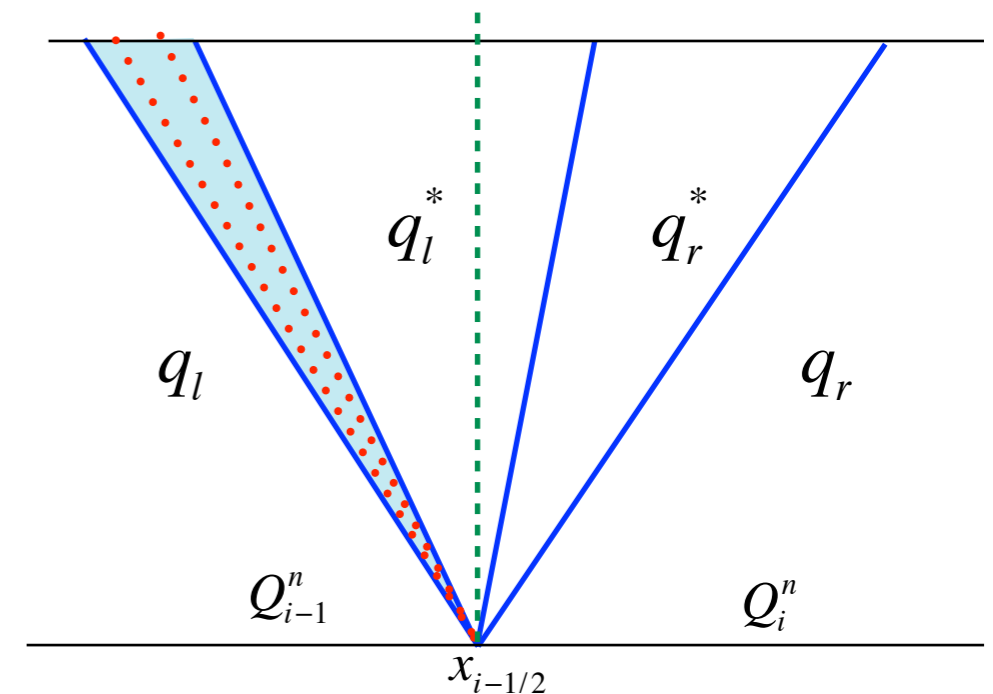
# How good is the Roe solver?



For arbitrary right and left states, the Roe solver is definitely inaccurate.

If the resolution is sufficiently good, this circumstance should not occur in practice.

But in the other two cases, one or two iterations in the exact solve may be enough.



# $f$ -wave approximate Riemann solver

Instead of splitting  $Q$  into waves, we might consider splitting the flux  $f$  into  $M_w$  “waves” ( $M_w \leq w$ ):

$$f(Q_i) - f(Q_{i-1}) = \sum_{p=1}^{M_w} \mathcal{Z}_{i-1/2}^p$$

It turns out this is useful for spatially varying flux functions, i.e.

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

with applications, for example, in:

wave propagation in heterogeneous nonlinear media,

flow in heterogeneous porous media,

traffic flow with varying road conditions,

conservation laws on curved manifolds,

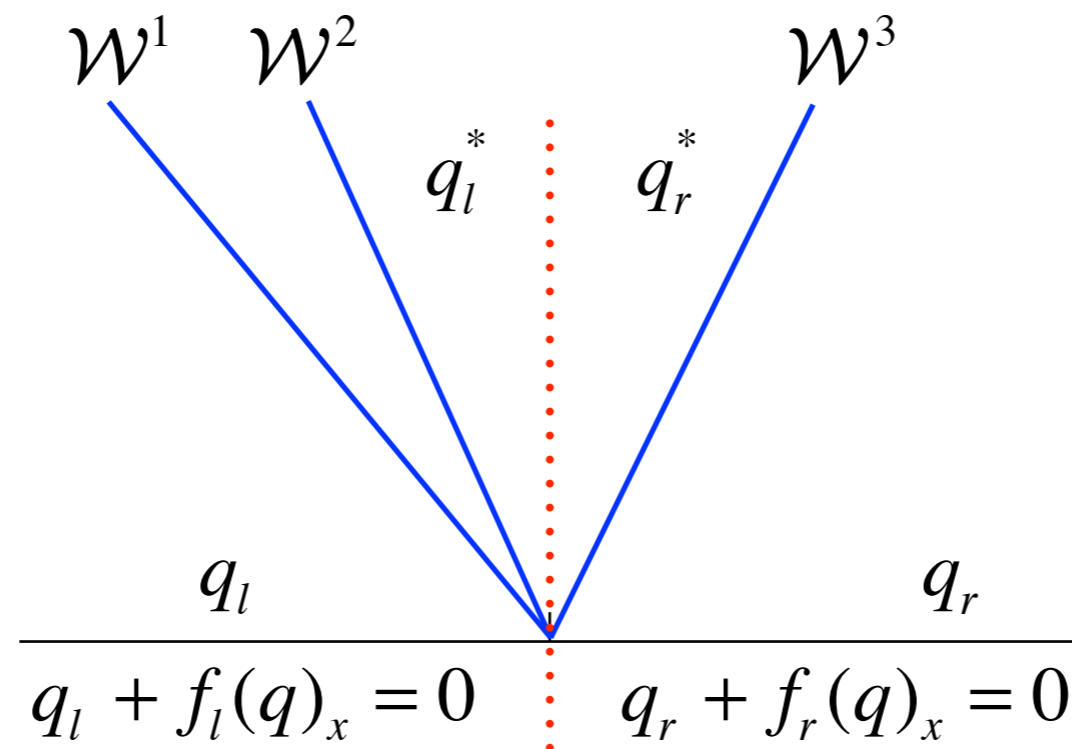
and certain kinds of source terms.

# Flux-based wave decomposition ( $f$ -waves)

Choose wave forms  $r^p$  (for example, eigenvectors of the Jacobian on each side).

Then decompose the flux difference:

$$f_r(q_r) - f_l(q_l) = \sum_{p=1}^m \beta^p r^p = \sum_{p=1}^m \mathcal{Z}^p$$





# Wave propagation algorithm using waves

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( \mathcal{A}^- \Delta Q_{i+1/2} + \mathcal{A}^+ \Delta Q_{i-1/2} \right) - \frac{\Delta t}{\Delta x} \left( F_{i+1/2} - F_{i-1/2} \right)$$

In the standard version:

$$\left\{ \begin{array}{l} Q_i - Q_{i-1} = \sum_{p=1}^m \mathcal{W}_{i-1/2}^p \\ \mathcal{A}^- \Delta Q_{i+1/2} = \sum_p \left( s_{i+1/2}^p \right)^- \mathcal{W}_{i+1/2}^p \\ \mathcal{A}^+ \Delta Q_{i-1/2} = \sum_p \left( s_{i-1/2}^p \right)^+ \mathcal{W}_{i-1/2}^p \\ \tilde{F}_{i-1/2} = \frac{1}{2} \sum_{p=1}^m |s_{i-1/2}^p| \left( 1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^p| \right) \tilde{\mathcal{W}}_{i-1/2}^p \end{array} \right.$$

# Wave propagation algorithm using $f$ -waves

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( \mathcal{A}^- \Delta Q_{i+1/2} + \mathcal{A}^+ \Delta Q_{i-1/2} \right) - \frac{\Delta t}{\Delta x} \left( F_{i+1/2} - F_{i-1/2} \right)$$

Using  $f$ -waves:

$$\left\{ \begin{array}{l} f_i(Q_i) - f_{i-1}(Q_{i-1}) = \sum_{p=1}^m \mathcal{Z}_{i-1/2}^p \\ \mathcal{A}^- \Delta Q_{i+1/2} = \sum_{p:s_{i-1/2}^p < 0} \mathcal{Z}_{i+1/2}^p \\ \mathcal{A}^+ \Delta Q_{i-1/2} = \sum_{p:s_{i-1/2}^p > 0} \mathcal{Z}_{i-1/2}^p \\ \tilde{F}_{i-1/2} = \frac{1}{2} \sum_{p=1}^m \text{sgn}(s_{i-1/2}^p) \left( 1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^p| \right) \tilde{\mathcal{Z}}_{i-1/2}^p \end{array} \right.$$

# $f$ -wave approximate Riemann solver

Let  $\hat{A}$  be any averaged Jacobian matrix, for example:

$$\hat{A} = f' \left( \frac{q_l + q_r}{2} \right)$$

Use eigenvectors of  $\hat{A}$  to do  $f$ -wave splitting.

Then  $\mathcal{A}^- \Delta Q_{i+1/2} + \mathcal{A}^+ \Delta Q_{i-1/2} = f(Q_i) - f(Q_{i-1})$ , so the method is conservative.

If  $\hat{A}$  is the Roe average, then this is equivalent to the normal Roe Riemann solver, and

$$\mathcal{Z}^p = s^p \mathcal{W}^p.$$

# Assignment for next time

**Read Chapter 14 and Chapter 15.**

**Write** (in Fortran or Python) an approximate Riemann solver for the Euler equations using the Roe average. Test it on the shock tube problem, or (optionally) on the Woodward-Colella blast-wave problem. Use the shallow-water Riemann solver as a guide.

