FYS-GEO 4500 12 Oct 2009

Before we start:
Questions over the reading?

The problem set

Our schedule

	date		Topic	Chapter in LeVeque
1	17 Aug 2009	Monday 13.15-15.00	introduction to conservation laws, Clawpack	1 & 2 & 5
2	24 Aug 2009	Monday 13.15-15.00	the Riemann problem, characteristics	3
3	**28 Aug 2009**	**Friday 13.15-15.00**	finite volume methods for linear systems	4
4	**8 Sep 2009**	**Tuesday 13.15-15.00**	high resolution methods	6
5	21 Sep 2009	Monday 13.15-15.00	boundary conditions, accuracy, variable coeff.	7,8, part of 9
6	**29 Sep 2009**	**Tuesday 13.15-15.00**	nonlinear conservation laws, finite volume methods	11 & 12
7	5 Oct 2009	Monday 13.15-15.00	nonlinear equations & systems	13, part of 14
8	12 Oct 2009	Monday 13.15-15.00	finite volume methods for nonlinear systems	part of 14, 15
9	19 Oct 2009	Monday 13.15-15.00	varying flux functions, source terms	part of 16, 17
10	26 Oct 2009	Monday 13.15-15.00	multidimensional hyperbolic problems & methods	18 & 19
11	2 Nov 2009	Monday 13.15-15.00	systems & applications; project planning	20 & 21
12	16 Nov 2009	Monday 13.15-15.00	applications: tsunamis, pockmarks, venting, impacts	
13	23 Nov 2009	Monday 13.15-15.00	applications: volcanic jets, pyroclastic flows, lahars	
14	30 Nov 2009	Monday 13.15-15.00	review; progress, problems & projects	
16	7 Dec 2009	Monday 13.15-15.00	FINAL PROJECT REPORTS DUE	

Gas Dynamics (Chapter 14 in Leveque)

The barotropic equations and the shallow-water equations

$$\rho_t + (\rho u)_x = 0$$
$$(\rho u)_t + \left(\rho u^2 + p\right)_x = 0$$

The conservation laws for the barotropic system (i.e. with $p = P(\rho)$)

are exactly like the shallow water equations if we identify ρ with h and use

the equation of state
$$p = P(\rho) = \frac{1}{2} g \rho^2$$

Other barotropic forms include the isothermal equation of state

$$p = P(\rho) = a^2 \rho,$$

and the polytropic (or gamma-law) equation of state

$$p = P(\rho) = K\rho^\gamma$$

But next we add the energy equation…

The Euler equations of gas dynamics

This is the full system of three conservation laws, for mass, momentum, and energy, for fully compressible gas dynamics:

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

where
$$q = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, f(q) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{bmatrix}.$$

The total energy is composed of internal energy plus kinetic energy,

$$E = \rho e + \frac{1}{2}\rho u^2$$

and the system is completed by an equation of state $e = e(p,\rho)$.

The Jacobian $f'(q)$ has eigenvalues $u–c$, c, $u+c$ where the speed of sound is $c = \sqrt{\dfrac{dp}{d\rho}}$ at constant entropy.

The equation of state and associated relations for a polytropic gas

The ideal gas law: $\dfrac{p}{\rho} = nkT$

The internal energy: $e = c_v T = \dfrac{\alpha}{2} nkT = \dfrac{p}{(\gamma-1)\rho}$

The *enthalpy*: $h = e + \dfrac{p}{\rho} = c_p T = \left(1 + \dfrac{\alpha}{2}\right) nkT$

Relations between the specific heats: $\begin{cases} c_p - c_v = nk \\ \gamma = \dfrac{c_p}{c_v} = \left(\dfrac{\alpha+2}{\alpha}\right) \end{cases}$

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n : number of molecules per unit mass

k : Boltzmann's constant

c_v : specific heat at constant volume

α : number of degrees of freedom

c_p : specific heat at constant pressure

γ : adiabatic exponent

Entropy

In the system of Euler equations for gas dynamics, we have the advantage of having an explicit formula for entropy that we can use as an entropy condition.

The specific entropy s (i.e. entropy per unit mass) is given by the formula:

$$s = c_v \log\left(\frac{p}{\rho^\gamma}\right) + \text{constant}$$

The additive constant is unimportant and may be omitted, since the important thing to keep track of is changes in entropy. In smooth flow, entropy is constant; at shocks it jumps to a higher value.

Primitive variables

It is often useful to examine the equivalent equations in directly observable "primitive" variables, rather than the conserved variables.

The Euler equations in primitive form for a polytropic gas:

$$\rho_t + u\rho_x + \rho u_x = 0$$
$$u_t + uu_x + \frac{1}{\rho} p_x = 0$$
$$p_t + \gamma p u_x + u p_x = 0$$

in matrix notation:

$$\begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_x + \begin{bmatrix} u & \rho & 0 \\ 0 & u & \frac{1}{\rho} \\ 0 & \gamma p & u \end{bmatrix} \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_t = 0$$

Then the eigenvalues and eigenvectors are:

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

$$r^1 = \begin{bmatrix} -\rho/c \\ 1 \\ -\rho c \end{bmatrix} \quad r^2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad r^3 = \begin{bmatrix} \rho/c \\ 1 \\ \rho c \end{bmatrix}$$

where

$$c = \sqrt{\frac{\gamma\, \rho}{p}}$$

is the speed of sound in the polytropic gas.

The Jacobian for the conservation laws

This (for the polytropic gas) is slightly more complex, though equivalent:

$$f'(q) = \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2}(\gamma-3)u^2 & (3-\gamma)u & \gamma-1 \\ \frac{1}{2}(\gamma-1)u^3 - uH & H-(\gamma-1)u^2 & \gamma u \end{bmatrix}$$

where $H = \dfrac{E+p}{\rho} = h + \dfrac{1}{2}u^2$ is the total specific enthalpy.

And the eigenvalues and eigenvectors are:

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

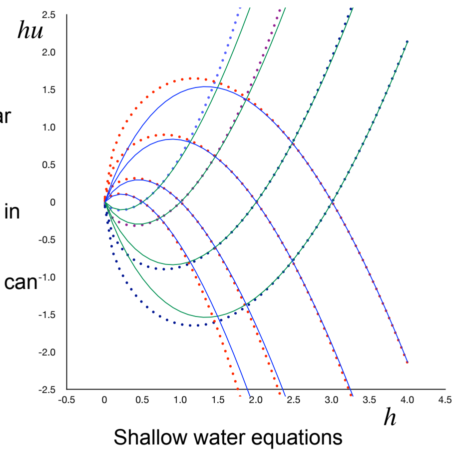
$$r^1 = \begin{bmatrix} 1 \\ u-c \\ H-uc \end{bmatrix} \quad r^2 = \begin{bmatrix} 1 \\ u \\ \frac{1}{2}u^2 \end{bmatrix} \quad r^3 = \begin{bmatrix} 1 \\ u+c \\ H+uc \end{bmatrix}$$

Genuine nonlinearity, linear degeneracy

Nonlinear systems of hyperbolic equations produce shocks and rarefaction waves; linear systems do not.

Nonlinear systems have integral curves and Hugoniot loci that diverge from one another; in linear systems these curves are identical.

But even in nonlinear systems, some waves can in fact act like linear waves in this sense.



Shallow water equations

Genuine nonlinearity, linear degeneracy

A wave (or field, we may say, referring to the collection of waves of the same family in all accessible space) is *genuinely nonlinear* if

$$\nabla\lambda^p \bullet r^p(q) \neq 0 \text{ for all } q$$

Physically this means that the characteristics are either compressing or expanding.

The opposite case is linear degeneracy,

$$\nabla\lambda^p \bullet r^p(q) = 0 \text{ for all } q$$

in this case the characteristics are parallel to one another.

The Euler equations have one linearly degenerate field

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

$$r^1 = \begin{bmatrix} -\rho/c \\ 1 \\ -\rho c \end{bmatrix} \quad r^2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad r^3 = \begin{bmatrix} \rho/c \\ 1 \\ \rho c \end{bmatrix}$$

This is easiest to see in the eigensystem for the primitive equations. In this case the gradient operator is defined by

$$\nabla \equiv \begin{bmatrix} \frac{\partial}{\partial\rho} \\ \frac{\partial}{\partial u} \\ \frac{\partial}{\partial p} \end{bmatrix}, \quad \text{so we find} \quad \nabla\lambda^1 = \begin{bmatrix} +\frac{c}{2\rho} \\ 1 \\ -\frac{c}{2\rho} \end{bmatrix}; \nabla\lambda^2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}; \nabla\lambda^1 = \begin{bmatrix} -\frac{c}{2\rho} \\ 1 \\ +\frac{c}{2\rho} \end{bmatrix}$$

And therefore

$$\nabla\lambda^1 \bullet r^1 = \tfrac{1}{2}(\gamma+1)$$
$$\nabla\lambda^2 \bullet r^2 = 0$$
$$\nabla\lambda^3 \bullet r^3 = \tfrac{1}{2}(\gamma+1)$$

The Riemann invariants for the polytropic gas

Thus, of the three eigenvectors, 1 and 3 represent waves that can become either rarefactions or shocks, while 2 is linearly degenerate and can only be a *contact discontinuity*.

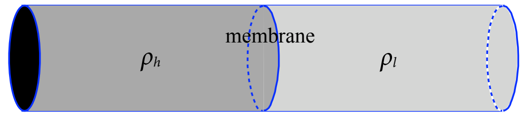
For any *simple wave* (not a rarefaction or a shock), the Riemann invariants are constant along particle paths through the wave. These are, for the 3 waves:

$$\text{1-wave: } s, \quad u + \frac{2c}{\gamma - 1}$$

$$\text{2-wave: } u, \ p$$

$$\text{3-wave: } s, \quad u - \frac{2c}{\gamma - 1}$$

Now we can make more sense of the shock tube!

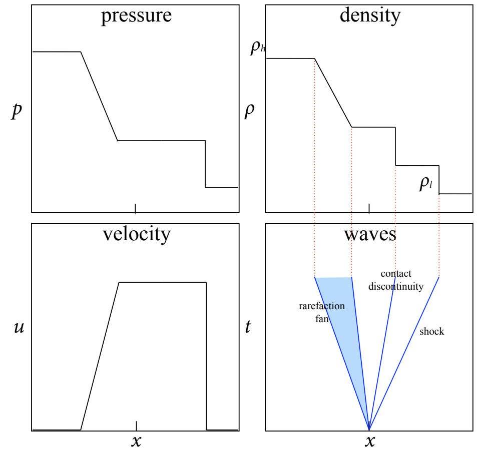


A closed tube filled with gas, separated by a membrane into sections with different densities.

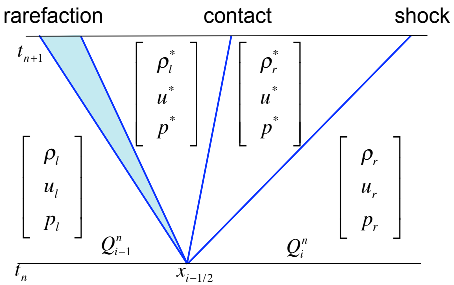
The membrane is suddenly removed, and the gas starts moving from the high-density region into the lower density region.

Three waves develop: a *shock wave*, a *contact discontinuity*, and a *rarefaction wave* (or *fan*). The first two travel to the right, the third to the left.

At the shock, velocity, pressure and density are all discontinuous. At the contact, only density is discontinuous. In the rarefaction fan, all variables are continuous, but their derivatives are not.



The Riemann problem for 3 waves:



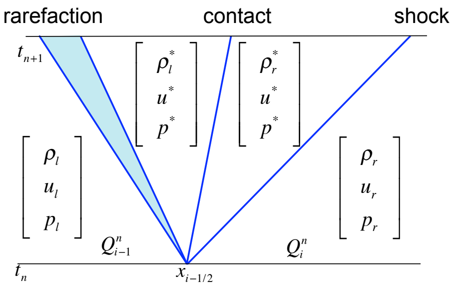
$$\begin{bmatrix} \rho_l \\ u_l \\ p_l \end{bmatrix} \quad \begin{bmatrix} \rho_l^* \\ u^* \\ p^* \end{bmatrix} \quad \begin{bmatrix} \rho_r^* \\ u^* \\ p^* \end{bmatrix} \quad \begin{bmatrix} \rho_r \\ u_r \\ p_r \end{bmatrix}$$

Now we have to solve for two intermediate states, not just one as before. And we have the rarefaction fan to deal with.

Note that only density changes across the contact discontinuity. This helps matters, in that we can use *almost* the same procedure as for the 2-equation shallow water set.

First we obtain (p^*, u^*) and then we use separate conditions to determine ρ_l^* and ρ_r^*.

The Riemann problem for 3 waves:



$$\begin{bmatrix} \rho_l \\ u_l \\ p_l \end{bmatrix} \quad \begin{bmatrix} \rho_l^* \\ u^* \\ p^* \end{bmatrix} \quad \begin{bmatrix} \rho_r^* \\ u^* \\ p^* \end{bmatrix} \quad \begin{bmatrix} \rho_r \\ u_r \\ p_r \end{bmatrix}$$

The 2-field is linearly degenerate. Across the contact u and p will be constant and only ϱ will jump.

The strategy for solving the problem is to use the Hugoniot loci and integral curves for the 1-field and 3-field, in the phase plane of u and p, in the same way as for the shallow-water equations to obtain (p^*, u^*). Then we calculate the densities on either side of the contact. Finally we solve for the solution within the rarefaction fan.

The general (exact) Riemann solver for the Euler equations for a polytropic gas

As before, we define functions

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

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

where $\beta = \dfrac{\gamma+1}{\gamma-1}$.

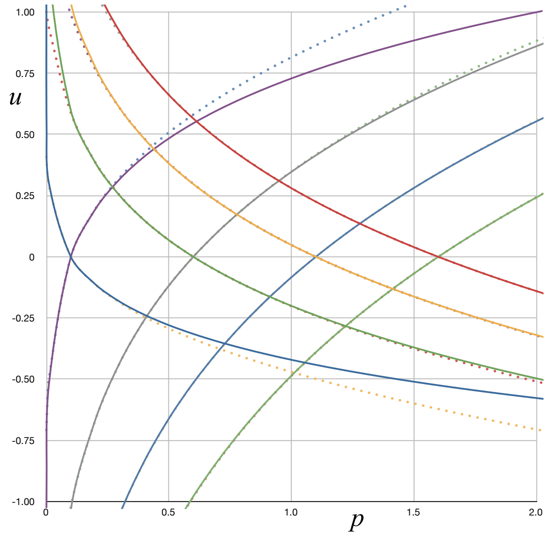
We then require that $\varphi_l(p_m) = \varphi_r(p_m)$, using an iterative procedure to find the intersection (p^*, u^*) of the curves. The densities on either side of the contact will then be given by

$$\rho_l^* = \left(\frac{1+\beta p^*/p_l}{p^*/p_l + \beta}\right)\rho_l; \quad \rho_r^* = \left(\frac{1+\beta p^*/p_r}{p^*/p_r + \beta}\right)\rho_r$$

Hugoniot loci and integral curves for the Euler Equations (polytropic gas)

Some integral curves (solid) and Hugoniot loci (dotted) for the Euler equations. Just as in the shallow water equations, these curves are close together in many places. An iterative solver can start from the intersection of the integral curves, which can be obtained explicitly.

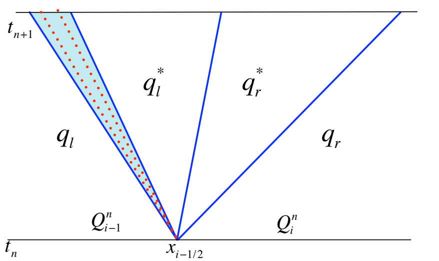
These curves are computed for γ=1.4 and densities ϱ_l= 3 and ϱ_r=1. For lower γ and higher density contrasts, the curves spread further apart.



We now have everything except the rarefaction:

The 1-rarefaction to connect the states q_l and q_l^*. Again we take advantage of the fact that the solution is a similarity solution, constant along the rays $\xi = x/t$. And we also know that the 1-Riemann invariant is constant through a rarefaction wave:

$$u + \frac{2c}{\gamma-1} = u_l + \frac{2c_l}{\gamma-1}$$



Then we have that $\xi = \lambda^1 = u - c$ within the rarefaction wave, so we can rewrite the Riemann invariant as

$$u + \frac{2(u-\xi)}{\gamma-1} = u_l + \frac{2c_l}{\gamma-1},$$

and solve for u as a function of ξ.

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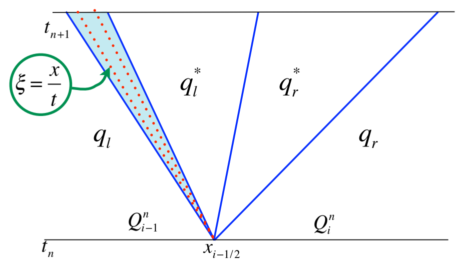

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Continuing the solution within the rarefaction

With the Riemann invariant

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we solve for u as a function of ξ:

$$u(\xi)=\frac{(\gamma-1)u_l+2(c_l+\xi)}{\gamma+1}.$$

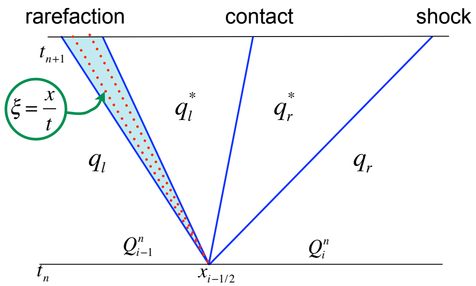
Then since p/ρ^γ is constant,

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

and

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

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



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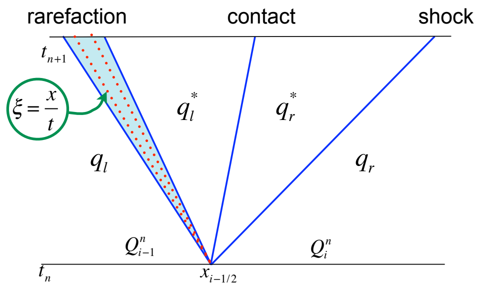

The exact solution is a perfect and complete structure and can be solved using iterative methods.

Continuing the solution within the rarefaction

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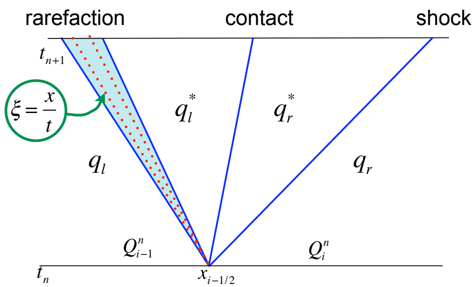

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However, in practical computation all of this is **not** used; instead we will use approximate Riemann solvers.

Continuing the solution within the rarefaction

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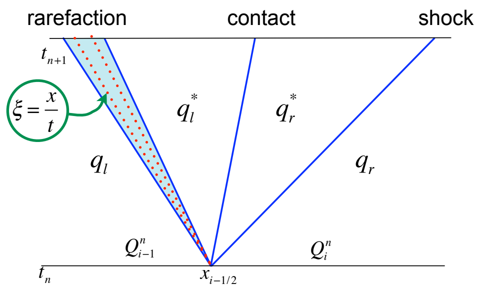


The exact solution is a perfect and complete structure and can be solved using iterative methods.

However, in practical computation all of this is **not** used; instead we will use approximate Riemann solvers.

The exact solution is useful for verification, however.

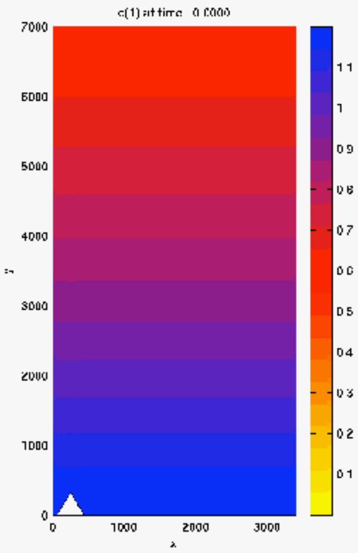
Multifluid problems and other equations of state

The easiest multi-fluid case is when you have two ideal gases with different values of γ. Then you set up the Riemann problem at the interface between the two fluids with right and left values for γ. 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.

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 pressure-less 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 ρ_s is the particle solid density.

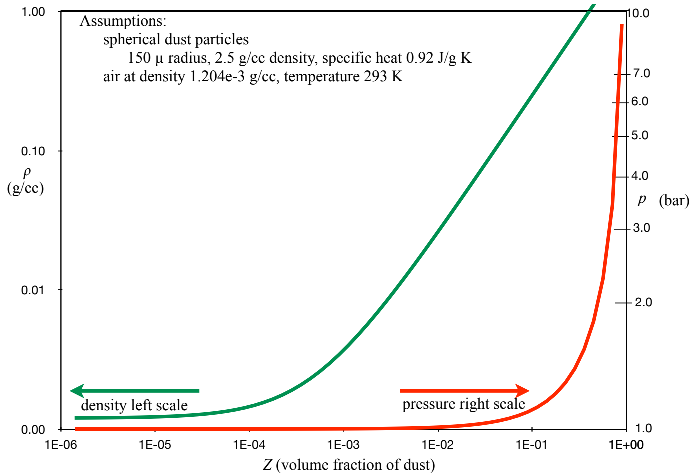
The speed of sound is then $c_{ds} = \sqrt{\frac{\Gamma p}{\rho(1-Z)}}$

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

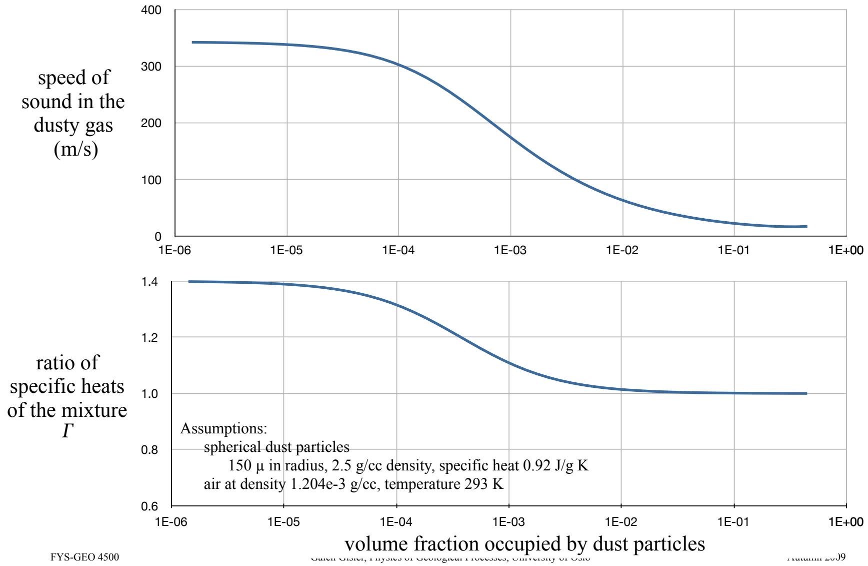
The specific heat of the dust particles is C_{sp} and C_v is the specific heat at constant volume of the gas.

*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 2% dust (by volume) to air reduces the speed of sound to 50 m/s, and the mixture becomes nearly isothermal

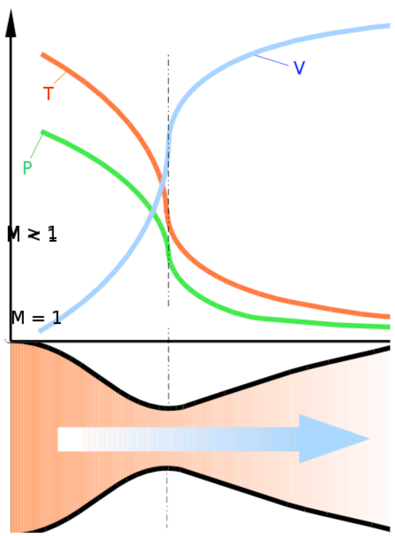


De Laval Nozzle

Invented by the Swedish inventor 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.



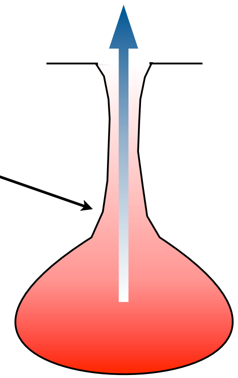
How does a deLaval nozzle work?

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

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

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

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 γ_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 ϱ along a streamline:

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

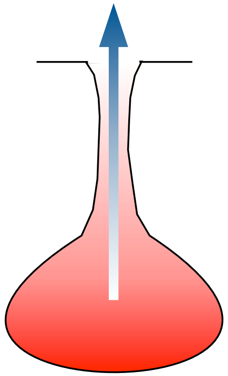
Using $dp = c^2 \rho$, where c is the *local* sound speed throughout the system, we get

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

indicating that the mass flux ϱv has a maximum where v is equal to the local sound speed. By continuity, this maximum holds at the narrowest point of the pipe, where v itself is equal to its maximum.

For the isentropic case, the flux is

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



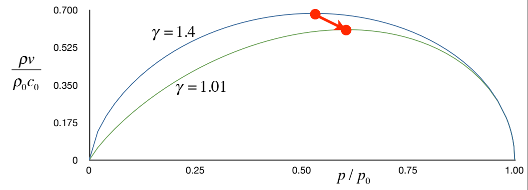
How does a deLaval nozzle work?

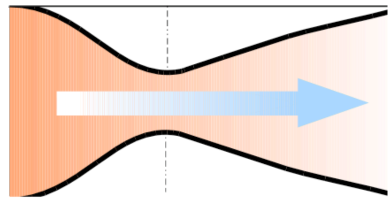
$$\rho v = \left(\frac{p}{p_0}\right)^{1/\gamma} \sqrt{\frac{2\gamma}{\gamma - 1} p_0 \rho_0 \left[1 - \left(\frac{p}{p_0}\right)^{(\gamma-1)/\gamma}\right]},$$

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

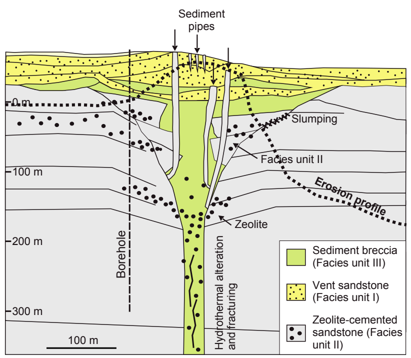
If the pressure at this point is less than 0.53 p_0 (in air) or less than 0.6 p_0 (in a 2% dusty gas), the flow speed equals the sound speed at that point. In the diverging portion, it becomes supersonic without passing through a shock.

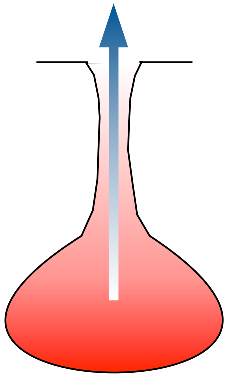
In a dusty gas it is easier to get to supersonic flow both *because the local sound speed is lower* and because the *maximum discharge is reached with a lower pressure drop*.





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





Shocks can be stronger in dusty gases

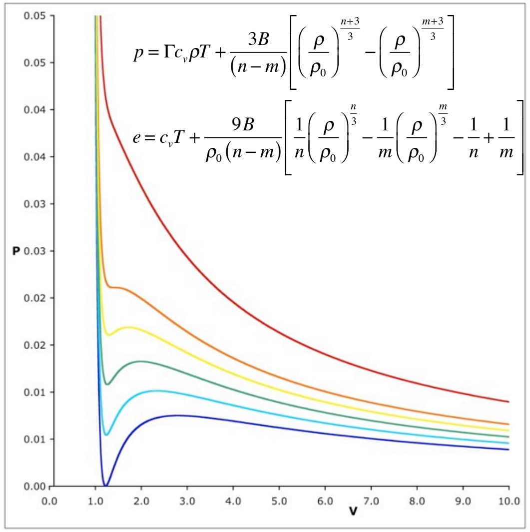
The maximum ratio of upstream to downstream densities across a shock is (see Landau & Lifshitz, *Fluid Dynamics*)

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

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 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, ρ_0, B, Γ

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:

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

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

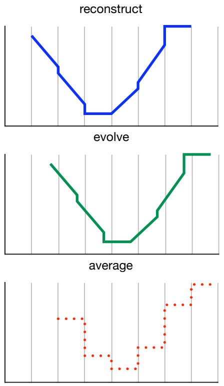
Recall Godunov's method:

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

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 $\mathrm{TV}(q) \le \mathrm{TV}(Q)$

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. $Q_i^n \ge Q_{i-1}^n$ for all i at step n

remains monotone at the next time: $Q_i^{n+1} \ge Q_{i-1}^{n+1}$ 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: $\mathrm{TV}(Q) = \sum_{\text{grid}} |Q_i - Q_{i-1}|$

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

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
$$Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x}\left(Q_i^n - Q_{i-1}^n\right) - \frac{1}{2}\frac{u\Delta t}{\Delta x}(\Delta x - u\Delta t)\left(\sigma_i^n - \sigma_{i-1}^n\right)$$
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 ϕ is the *flux limiter function*.

Choices for the flux limiter are:

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

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

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

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

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

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

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

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

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

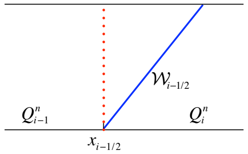
Slope limiters and flux limiters

The slope limiter formula for advection is:
$$Q_i^{n+1} = Q_i^n - \frac{u\Delta t}{\Delta x}\left(Q_i^n - Q_{i-1}^n\right) - \frac{1}{2}\frac{u\Delta t}{\Delta x}(\Delta x - u\Delta t)\left(\sigma_i^n - \sigma_{i-1}^n\right)$$

The flux limiter formulation for advection is:
$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1/2}^n - F_{i-1/2}^n\right)$$

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

Lax-Wendroff formula:

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

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

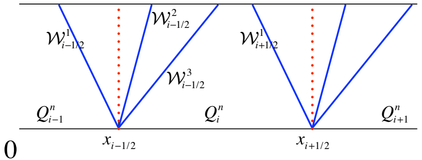
High-resolution method:

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

where

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

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:

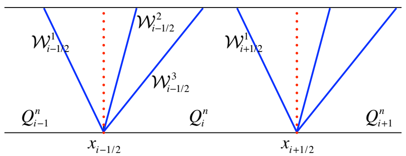
Solve the linear Riemann problem to decompose $Q_i^n - Q_{i-1}^n$ into a number of waves.

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

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

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

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

The waves also give the decomposition of the slopes

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

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

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:

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

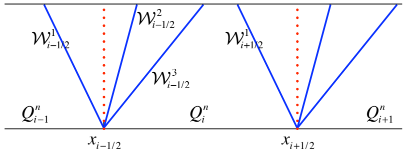
where $$F^n_{i-1/2} = \frac{1}{2}\sum_{p=1}^{m}\left|s^p_{i-1/2}\right|\left(1 - \frac{\Delta t}{\Delta x}\left|s^p_{i-1/2}\right|\right)\widetilde{\mathcal{W}}^p_{i-1/2}$$

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

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

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

Wave limiters for a system



$Q_i - Q_{i-1}$ is split into waves $\mathcal{W}^p_{i-1/2} = \alpha^p_{i-1/2} r^p_{i-1/2}$,

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

where $\theta^p_{i-1/2} = \dfrac{\mathcal{W}^p_{i-1/2} \cdot \mathcal{W}^p_{I-1/2}}{\mathcal{W}^p_{i-1/2} \cdot \mathcal{W}^p_{i-1/2}}$, and $I = \begin{cases} i-1 \text{ if } s^p_{i-1/2} > 0 \\ i+1 \text{ if } s^p_{i-1/2} < 0 \end{cases}$.

Note that if $r^p_{i-1/2} = r^p_{I-1/2}$ then $\theta^p_{i-1/2} = \dfrac{\alpha^p_{I-1/2}}{\alpha^p_{i-1/2}}$.

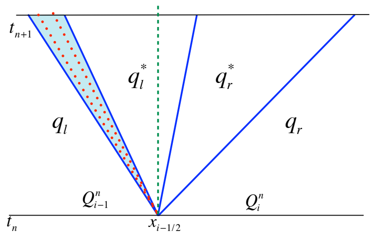
In the scalar case this reduces to

$$\theta^p_{i-1/2} = \frac{\mathcal{W}^p_{I-1/2}}{\mathcal{W}^p_{i-1/2}} = \frac{Q_I - Q_{I-1}}{Q_i - Q_{i-1}}$$

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

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

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



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

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

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

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

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!

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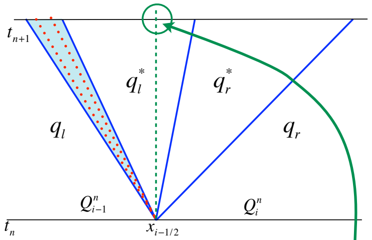

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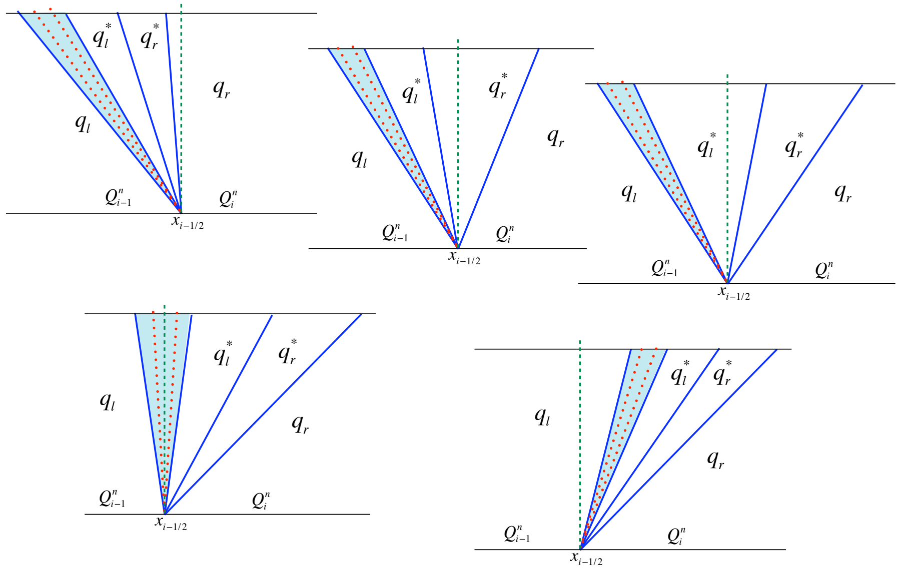
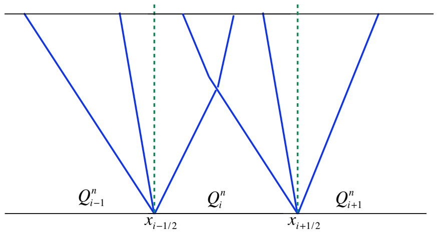
These are useful for exact solutions of certain problems.

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

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

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

Because the problem is solve 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

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

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

If we define $\hat{A}_{i-1/2} = \hat{A}(Q^n_i, Q^n_{i-1})$ 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

$$\mathcal{W}^p_{i-1/2} = \alpha^p_{i-1/2}\hat{r}^p_{i-1/2}, \quad s^p_{i-1/2} = \hat{\lambda}^p_{i-1/2}.$$

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 $\hat{A}$?

Approximate Riemann Solvers

Properties desired for $\hat{A}$:

$\hat{A}$ must be diagonalisable with real eigenvalues

$\hat{A}_{i-1/2} \to f'(q)$ as $Q_{i-1}, Q_i \to q$

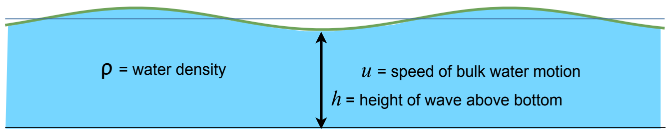
$\hat{A}_{i-1/2}(Q_i - Q_{i-1}) = s(Q_i - Q_{i-1}) = f(Q_i) - f(Q_{i-1})$

With these properties, the method will be conservative, it will give the right answer across shocks (why?), and it is a good approximation for smooth flow.

We could take $\hat{A}_{i-1/2} = f'(\hat{Q}_{i-1/2})$ where $\hat{Q}_{i-1/2}$ is a suitable average of (Q_{i-1}, Q_i) . We'll use basically this approach.

Or we could take $\hat{A}_{i-1/2} = \frac{1}{2}\left[f'(Q_{i-1}) + f'(Q_i)\right]$.

Example: Roe solver for shallow-water equations



$h(x,t)$ = depth

$u(x,t)$ = 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

"Roe average"

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

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Roe solver for Shallow Water

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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:

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

The Shallow-water Riemann solver in Clawpack is a Roe solver

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

"Roe average"

```
      do 30 i=2-mbc,mx+mbc¬
c¬
c         ¬
c     # compute  Roe-averaged quantities: ¬
         ubar = (qr(i-1,2)/dsqrt(qr(i-1,1)) + ql(i,2)/dsqrt(ql(i,1)))/¬
     .       ( dsqrt(qr(i-1,1)) + dsqrt(ql(i,1)) )¬
         cbar=dsqrt(0.5d0*grav*(qr(i-1,1) + ql(i,1)))¬
         ¬
c     # delta(1)=h(i)-h(i-1) and  delta(2)=hu(i)-hu(i-1)¬
      delta(1) = ql(i,1) - qr(i-1,1)¬
      delta(2) = ql(i,2) - qr(i-1,2)¬
¬
c # compute coeffs in the evector expansion of delta(1),delta(2)¬
      a1 = 0.5d0*(-delta(2) + (ubar + cbar) * delta(1))/cbar¬
      a2 = 0.5d0*( delta(2) - (ubar - cbar) * delta(1))/cbar¬
¬
c     # finally, compute the waves.¬
         wave(i,1,1) = a1¬
         wave(i,2,1) = a1*(ubar - cbar)
         s(i,1) = ubar - cbar¬
         ¬
         wave(i,1,2) = a2¬
         wave(i,2,2) = a2*(ubar + cbar)
         s(i,2) = ubar + cbar¬
         ¬
   30 continue¬
```

```
      do 100 m=1,2¬
         do 100 i=2-mbc, mx+mbc¬
            amdq(i,m) = 0.d0¬
            apdq(i,m) = 0.d0¬
            do 90 mw=1,mwaves¬
               if (s(i,mw) .lt. 0.d0) then¬
                  amdq(i,m) = amdq(i,m) + s(i,mw)*wave(i,m,mw)¬
                else¬
                  apdq(i,m) = apdq(i,m) + s(i,mw)*wave(i,m,mw)¬
                endif¬
   90       continue¬
  100    continue¬
```

from: $CLAW/book/chap13/swhump1/rp1sw.f

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.

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,

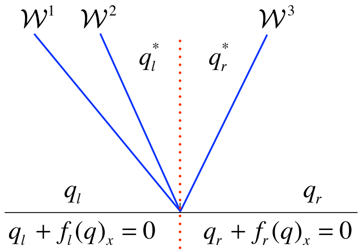
and certain kinds of source terms.

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

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

f-wave approximate Riemann solver

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

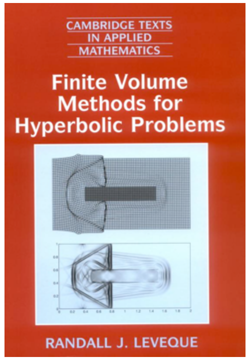
$$\hat{A} = f'\left(\frac{q_l + q_r}{2}\right)$$

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

Hand in your code and results to me by Monday 19 October.