Entropy stable schemes for hyperbolic conservation laws

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Non-linear hyperbolic PDE

Scalar conservation law

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

with initial condition

$$u(x,0) = u_0(x)$$

Even if u_0 is infinitely smooth, we may not have smooth solutions at future times. We need to allow discontinuous solutions. In this case, the PDE is not satisfied in a classical, pointwise sense. We need to use the notion of weak solutions .
Multiply the conservation law by a smooth, compactly supported test function $\phi(x,t)$

$$\int_0^\infty \int_{\mathbb{R}} (u_t + f(u)_x)\phi \mathrm{d}x \mathrm{d}t = 0$$

and perform integration by parts in both x and t variable

$$\int_0^\infty \int_{\mathbb{R}} (u\phi_t + f(u)\phi_x) \mathrm{d}x \mathrm{d}t + \int_{\mathbb{R}} u_0(x)\phi(x,0) \mathrm{d}x = 0 \qquad (1)$$

Non-linear hyperbolic PDE

Note that there are no derivatives on u and hence this equation makes sense even if u is not differentiable.

Definition: Weak solution I

A locally integrable function which satisfies equation (1) for all smooth test functions is called a weak solution.

Suppose the solution has a discontinuity across the curve $x = X(t)$. Then using the definition of weak solution, we can show that the solution must satisfy the *Rankine-Hugoniot condition* at every discontinuity point

$$f(u^+) - f(u^-) = s(u^+ - u^-), \qquad s = \dot{X}(t)$$

where s is the speed of propagation of the discontinuity.

Definition: Weak solution II

A piecewise smooth solution which satifies the Rankine-Hugoniot solution at points where solution is not smooth is a weak solution.

Solution by method of characteristics

Define the characteristic curve $X(t)$

$$\frac{\mathrm{d}X}{\mathrm{d}t} = f'(u(X(t),t)) = a(u(X(t),t))$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}t}u(X(t),t) = \frac{\partial u}{\partial t} + \frac{\mathrm{d}X}{\mathrm{d}t}\frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

Hence the solution is constant along the characteristics; since the slope depends on u, the characteristics are straight lines. Draw the characteristic passing through (x,t) backward in time to $(x_0,0)$, then

$$\frac{x - x_0}{t} = a(u_0(x_0))$$

Solve this to get $x_0 = x_0(x,t)$. Hence, a smooth solution is given by

$$u(x,t) = u_0(x_0(x,t))$$

Burgers equation: Rarefaction solution

Initial condition

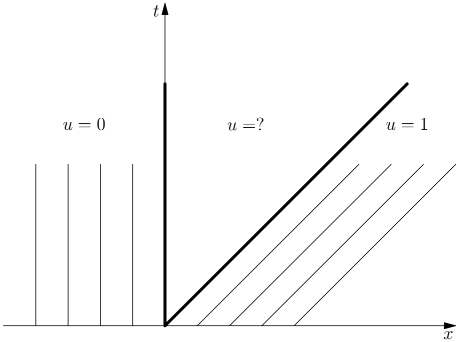
$$u_0(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0 \end{cases}$$

Foot of characteristic

$$x_0 = \begin{cases} x & \text{if } x < 0 \\ x - t & \text{if } x > t \end{cases}$$

so that

$$u(x,t) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > t \end{cases}$$



For $x \in (0, t)$, the characteristic can be drawn such that the foot is at $x_0 = 0$

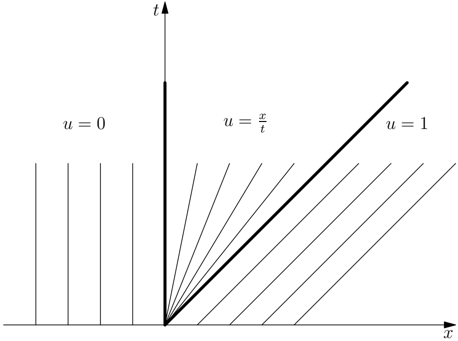
$$u(x,t) = \frac{x - x_0}{t}, \quad \text{and} \quad x_0 = 0, \quad \Longrightarrow \quad u(x,t) = \frac{x}{t}$$

This satisfies the PDE, $u_t + uu_x = -\frac{x}{t^2} + \frac{x}{t} \cdot \frac{1}{t} = 0$

Burgers equation: Rarefaction solution

Thus the solution can be completed as

$$u(x,t) = \begin{cases} 0 & \text{if } x < 0 \\ \frac{x}{t} & \text{if } 0 \le x \le t \\ 1 & \text{if } x > t \end{cases}$$



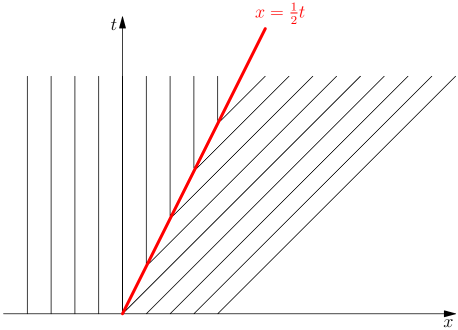
Plot the solution at any time $t > 0$. This solution is continuous but has some corners where derivatives are not defined. So this is still a weak solution of the conservation law.

Burgers equation: Non-uniqueness

We can introduce a discontinuous solution satisfying the RH condition

$$u(x,t) = \begin{cases} 0 & \text{if } x < \frac{1}{2}t \\ 1 & \text{if } x > \frac{1}{2}t \end{cases}$$

This is also a weak solution. Thus we can have **multiple weak solutions**, and this is a general feature of non-linear conservation laws.



- The characteristics show that causality is violated by this solution; characteristics are emanating from the shock line but they do not determine the future solution since we do not have data on the shock line.

Burgers equation: Non-uniqueness

- The shock solution is also unstable as is clear by smoothening the initial condition. Consider a smoothened initial condition and draw characteristics. (Draw this on board)

Entropy condition I

An admissible shock should have characteristics going into the shock curve as time advances. A discontinuity propagating with speed s given by the RH condition satisfies the entropy condition if

$$f'(u_l) > s > f'(u_r)$$

For a convex flux $f(u)$, $f''(u) > 0$, so that $f'(u)$ is an increasing function. Hence the entropy condition becomes

$$f'(u_l) > f'(u_r) \quad \Longrightarrow \quad u_l > u_r$$

There is always viscosity

Any real fluid has some viscosity. The inviscid Burger's equation

$$u_t + u u_x = 0$$

does not have any dissipative mechanism which is the reason we get non-uniqueness. We have neglected the viscosity thinking it is small and hence insignificant. But we lose some essential information about the solution when we do this simplification.

So let us consider the viscous Burgers equation

$$u_t^\epsilon + u^\epsilon u_x^\epsilon = \epsilon u_{xx}^\epsilon, \qquad \epsilon > 0$$

which has smooth solutions for all time. These solutions can be obtained using Cole-Hopf transformation [1].

One can take the limit of the viscous solution u^ϵ by letting $\epsilon \to 0$. The limiting solution is the unique entropy solution.

$$u = \lim_{\epsilon \to 0} u^\epsilon$$

Entropy function

Consider a convex scalar conservation law

$$u_t + f(u)_x = 0$$

Assume that there exists a convex function $\eta(u)$ and another function $\theta(u)$ such that

$$\eta'(u) f'(u) = \theta'(u)$$

Such a pair (η, θ) is called an entropy-entropy flux pair .

For Burgers equation, we can choose

$$\eta(u) = u^2, \qquad \theta(u) = \frac{2}{3} u^3$$

For smooth solutions

$$u_t + f'(u) u_x = 0, \qquad \eta'(u) u_t + \eta'(u) f'(u) u_x = 0,$$

Entropy function

leads to another conservation law

$$\eta_t + \theta_x = 0$$

This equality cannot hold for discontinuous solutions; if it did, then we would get a RH-type condition

$$\theta(u_r) - \theta(u_l) = s \cdot (\eta(u_r) - \eta(u_l))$$

However this is in general incompatible with the RH condition for the original conservation law.

In reality, the conservation law includes some dissipation

$$u_t + f_x = \epsilon u_{xx}, \quad \epsilon > 0 \quad \Longrightarrow \quad \eta'(u) u_t + \eta'(u) f'(u) u_x = \epsilon \eta'(u) u_{xx}$$

leads to the entropy equation

$$\eta_t + \theta_x = \epsilon(\eta(u) u_x)_x - \epsilon \eta''(u) u_x^2 \le \epsilon(\eta(u) u_x)_x \quad \text{since} \quad \eta''(u) > 0$$

Entropy function

In the limit of $\epsilon \to 0$, we get the entropy inequality

$$\eta_t + \theta_x \leq 0$$

This condition must be satisfied in weak sense for all $\phi \in C_0^1(\mathbb{R} \times \mathbb{R}^+)$, $\phi \geq 0$

$$\int_0^\infty \int_{\mathbb{R}} (\eta(u)\phi_t + \theta(u)\phi_x)\mathrm{d}x\mathrm{d}t + \int_{\mathbb{R}} \eta(u_0(x))\phi(x,0)\mathrm{d}t \geq 0$$

Entropy condition IV

A weak solution $u(x,t)$ is the entropy solution if for all convex entropy functions η and corresponding entropy fluxes θ, the inequality

$$\eta_t + \theta_x \leq 0$$

is satisfied in the weak sense.

Entropy function

Across a discontinuity, this is equivalent to

$$\theta(u_r) - \theta(u_l) \leq s \cdot (\eta(u_r) - \eta(u_l))$$

For the Burgers equation, taking $\eta(u) = u^2$, we get

$$\frac{2}{3}(u_r^3 - u_l^3) \leq \frac{1}{2}(u_r + u_l)(u_r^2 - u_l^2) \implies \frac{1}{6}(u_r - u_l)^3 \leq 0$$

and we recover the entropy condition for a admissible shock as $u_l > u_r$.

GR1, Theorem 3.4

If $u(x,t)$ satisfies entropy condition for one strictly convex entropy η, then it satisfies the entropy condition for all convex entropies.

Remark Kruzkov used the entropy pair

$$\eta(u) = |u - k|, \qquad \theta(u) = \mathrm{sign}(u - k)[f(u) - f(k)], \qquad k \in \mathbb{R}$$

Entropy function

Remark Scalar conservation laws have an infinite set of entropy pairs. For any convex function $\eta(u)$, define

$$\theta(u) = \int^u \eta'(s) f'(s) \mathsf{d}s \qquad \Longrightarrow \qquad \theta'(u) = \eta'(u) f'(u)$$

Remark To check entropy condition for numerical scheme, we will verify a discrete approximation of the condition

$$\frac{\mathsf{d}}{\mathsf{d}t} \int_a^b \eta(u(x,t)) \mathsf{d}x + \theta(u(b,t)) - \theta(u(a,t)) \leq 0$$

for the finite volume method.

Finite volume method

In the FVM, the basic unknown is the **cell average value** and this is evolved forward in time by using the conservation law applied to each finite volume. The basic scheme is of the form

$$u_j^{n+1} = u_j^n - \lambda[g_{j+\frac{1}{2}}^n - g_{j-\frac{1}{2}}^n], \qquad \lambda = \frac{\Delta t}{\Delta x}$$

where

$$g_{j+\frac{1}{2}} = g(u_j, u_{j+1})$$

is the **numerical flux** function. We will demand that the numerical flux is **consistent** in the sense that

$$g(u, u) = f(u)$$

The major task in the finite volume method is to find a suitable numerical flux function that leads to a stable and accurate scheme.

Godunov scheme

At any time t_n, the finite volume solution is made up of piecewise constant states. This naturally defines a Riemann problem at each cell face. Godunov's revolutionary idea was to solve these Riemann problems exactly for a short time period, and then average the solution onto piecewise constant states to obtain the cell averages at the next time $t_{n+1} = t_n + \Delta t$. The time step Δt should be small enough that neighbouring Riemann solutions do not interact with one another.

At face $j + \frac{1}{2}$ which separates the states u_j^n and u_{j+1}^n, the Riemann solution is self similar and may be written as

$$w_R(\xi; u_j^n, u_{j+1}^n), \qquad \xi = \frac{x - x_{j+\frac{1}{2}}}{t - t_n}, \qquad t > t_n$$

Godunov scheme can be written as a finite volume scheme with numerical flux

$$g_{j+\frac{1}{2}}^G = f(w_R(0; u_j^n, u_{j+1}^n))$$

Being based on exact solution, Godunov scheme satisfies all desirable properties like entropy condition, TVD property, maximum stability, etc.

Murman-Roe scheme

The idea introduced by Roe for Euler equations was to solve the Riemann problem approximately. In case of scalar problem, the idea is to replace non-linear PDE $u_t + f'(u)u_x = 0$ with a linear PDE

$$w_t + a_{j+\frac{1}{2}} w_x = 0$$

and solve this exactly. We must choose $a_{j+\frac{1}{2}} \approx f'(u(x_{j+\frac{1}{2}}, t_n))$

$$a_{j+\frac{1}{2}} = \begin{cases} \frac{f_{j+1}-f_j}{u_{j+1}-u_j} & u_j \neq u_{j+1} \\ f'(u_j) & \text{otherwise} \end{cases}$$

Solving the Riemann problem and evaluating the solution on $\xi = 0$ gives the Roe flux

$$g^R_{j+\frac{1}{2}} = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2}|a_{j+\frac{1}{2}}|(u_{j+1} - u_j) = \begin{cases} f_j & a_{j+\frac{1}{2}} > 0 \\ f_{j+1} & \text{otherwise} \end{cases}$$

Murman-Roe scheme

Being based on shocks only, the approximate solution is not good at modeling rarefactions. This can lead to entropy violating solutions. Consider the initial data

$$u_j^0 = \begin{cases} -1 & j \le -1 \\ +1 & j \ge 0 \end{cases}$$

The Roe scheme gives the solution

$$u_j^n = u_j^0$$

which is a stationary shock and hence a weak solution. But the correct solution is a rarefaction.

Note that the numerical viscosity vanishes at the initial discontinuity, which is the cause of the unphysical solution.

Monotone scheme

The exact solutions have the property that if $u(x,0) \geq v(x,0)$, then $u(x,t) \geq v(x,t)$ a.e in x and t. This motivates the notion of monotone schemes. Write a general finite volume scheme in the form

$$u_j^{n+1} = H(u_{j-k}^n, \ldots, u_{j+k}^n)$$

We say that **the scheme is monotone if H is an increasing function of all its arguments**.

A 3-point scheme is of the form

$$u_j^{n+1} = H(u_{j-1}^n, u_j^n, u_{j+1}^n) = u_j^n - \lambda[g(u_j^n, u_{j+1}^n) - g(u_{j-1}^n, u_j^n)]$$

This is monotone if $g(\cdot,\cdot)$ is an increasing function of its first argument and a decreasing function of its second argument, and provided a CFL condition is satisfied. (Exercise: Check this for the Lax-Friedrich flux)

A monotone scheme is consistent with any entropy condition. This would make monotone schemes to be the ideal choice but unfortunately, **monotone schemes are atmost first order accurate**. Hence the notion of monotone schemes is not very useful if we want to construct high order schemes.

TVD schemes

The total variation of a grid function u_h is defined as

$$TV(u_h) = \sum_j |u_{j+1} - u_j|$$

The exact solutions of conservation laws have the property that their total variation does not increase with time. Hence we demand the same from the numerical solutions.

A numerical scheme is said to be total variation diminishing if

$$TV(u_h^{n+1}) \leq TV(u_h^n)$$

Practically this helps to prevent the appearance of spurious oscillations in the case of discontinuous numerical solutions.

To check if a scheme is TVD, we write it in **incremental form**

$$u_j^{n+1} = u_j^n + C_{j+\frac{1}{2}}^n \Delta u_{j+\frac{1}{2}}^n - D_{j-\frac{1}{2}}^n \Delta u_{j-\frac{1}{2}}^n, \qquad \Delta u_{j+\frac{1}{2}} = u_{j+1} - u_j$$

TVD schemes

Theorem (Harten)

If

$$C_{j+\frac{1}{2}} \geq 0, \quad D_{j+\frac{1}{2}} \geq 0, \quad C_{j+\frac{1}{2}} + D_{j+\frac{1}{2}} \leq 1$$

then the scheme is TVD.

Unfortunately, TVD schemes need not be entropy consistent. So we have to additionally check this property.

Viscosity form

We write the numerical flux in the viscosity form

$$g_{j+\frac{1}{2}} = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2\lambda} Q_{j+\frac{1}{2}} \Delta u_{j+\frac{1}{2}}$$

where Q is called the viscosity coefficient[1]. If the finite volume scheme satisfies

$$\lambda \left| \frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right| \le Q_{j+\frac{1}{2}} \le 1$$

then it is TVD. If we further restrict the viscosity coefficient to

$$\lambda \left| \frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right| \le Q_{j+\frac{1}{2}} \le \frac{1}{2}$$

then the scheme is TVD and stable in maximum norm.

[1] Such schemes are said to be essentially 3-point.

Example: Lax-Friedrichs scheme
The numerical flux is given by

$$g(u,v) = \frac{1}{2}(f(u) + f(v)) - \frac{1}{2\lambda}(v-u)$$

for which the viscosity coefficient is

$$Q^{LF}_{j+\frac{1}{2}} = 1$$

This corresponds to the upper bound in the TVD condition. Hence the scheme is TVD provided the CFL condition

$$\lambda \max_j \left| \frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right| \leq 1$$

is satisfied.

Example: Murman-Roe scheme
The numerical flux is given by

$$g^R(u,v) = \frac{1}{2}(f(u)+f(v)) - \frac{1}{2}|a(u,v)|(v-u)$$

and its numerical viscosity coefficient is

$$Q^R_{j+\frac{1}{2}} = \lambda |a(v_j, v_{j+1})| = \lambda \left| \frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right|$$

This corresponds to the lower bound in the TVD condition. The scheme is TVD provided the CFL condition

$$\lambda \max_j \left| \frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right| \leq 1$$

is satisfied. However, we know that this scheme admits entropy violating shocks.

Example: Lax-Wendroff scheme
The numerical flux is given by

$$g^{LW}(u,v) = \frac{1}{2}(f(u)+f(v)) - \frac{1}{2}\lambda a(u,v)(f(v)-f(u))$$

Hence its numerical viscosity coefficient is

$$Q^{LW}_{j+\frac{1}{2}} = (\lambda a_{j+\frac{1}{2}})^2 = \lambda^2 \left(\frac{\Delta f_{j+\frac{1}{2}}}{\Delta v_{j+\frac{1}{2}}} \right)^2$$

which *does not satisfy the TVD condition*. This also implies that it does not preserve monotonicity.

Entropy consistent scheme

Consider a general finite volume scheme

$$u_j^{n+1} = u_j^n - \lambda[g_{j+\frac{1}{2}}^n - g_{j-\frac{1}{2}}^n], \qquad g_{j+\frac{1}{2}} = g(u_{j-k+1}, \ldots, u_{j+1})$$

We say that the scheme is consistent with an entropy pair (U, F) if there exists a **numerical entropy flux** $G_{j+\frac{1}{2}} = G(u_{j-k+1}, \ldots, u_{j+1})$ which is consistent with the entropy flux $F(u)$ in the sense

$$G(u, \ldots, u) = F(u), \qquad \forall u$$

and the numerical solutions satisfy

$$\frac{U(u_j^{n+1}) - U(u_j^n)}{\Delta t} + \frac{G_{j+\frac{1}{2}}^n - G_{j-\frac{1}{2}}^n}{\Delta x} \leq 0$$

This is a discrete approximation to the entropy inequality

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} \leq 0$$

Definition (E-scheme)

A consistent, conservative scheme is called an E-scheme if its numerical flux satisfies

$$\operatorname{sign}(v_{j+1} - v_j)(g_{j+\frac{1}{2}} - f(u)) \leq 0$$

for all u between v_j and v_{j+1}.

Remark Note that an E-scheme is essentially 3-point. Indeed letting $v_{j+1} \to v_j$ with first $v_{j+1} \geq v_j$ and then with $v_{j+1} \leq v_j$ shows that g is essentially 3-point.

Remark A 3-point monotone scheme is an E-scheme. Since $g(u, v)$ is non-decreasing in u and non-increasing in v, we obtain

$$\begin{aligned} g(u,v) \leq g(u,w) \leq g(w,w) = f(w) \quad &\text{if} \quad u \leq w \leq v \\ g(u,v) \geq g(w,v) \geq g(w,w) = f(w) \quad &\text{if} \quad u \geq w \geq v \end{aligned}$$

and therefore

$$\operatorname{sign}(v - u)(g(u,v) - f(w)) \leq 0, \qquad \text{for all } w \text{ between } u \text{ and } v$$

In particular, the Godunov scheme is an E-scheme under CFL ≤ 1.

Lemma

Assume that CFL ≤ 1. Then E-fluxes are characterized by

$$\begin{cases} g_{j+\frac{1}{2}} \leq g^G_{j+\frac{1}{2}} & \text{if } v_j < v_{j+1} \\ g_{j+\frac{1}{2}} \geq g^G_{j+\frac{1}{2}} & \text{if } v_j > v_{j+1} \end{cases}$$

where g^G stands for Godunov numerical flux.

Lemma

Assume that CFL ≤ 1. E-schemes are characterized by

$$0 \leq Q^G_{j+\frac{1}{2}} \leq Q_{j+\frac{1}{2}}, \qquad \forall j \in \mathbb{Z}$$

Theorem (Viscous form and entropy condition)

Assume that the CFL condition

$$\lambda \max |a(u)| \le \frac{1}{2}$$

holds. An E-scheme whose coefficient of numerical viscosity satisfies

$$Q^G_{j+\frac{1}{2}} \le Q_{j+\frac{1}{2}} \le \frac{1}{2}$$

is consistent with any entropy condition.

The basic idea is to write any E-scheme as a convex combination of the Godunov scheme and a modified Lax-Friedrichs scheme, both of which satisfy entropy condition.

Godunov scheme

The finite volume solution is made of piecewise constant states

$$v_\Delta(x,t) = v_j^n, \quad x \in (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}), \quad t \in [t_n, t_{n+1})$$

which defines a Riemann problem at each cell face $x = x_{j+\frac{1}{2}}$

$$\frac{\partial w_R}{\partial t} + \frac{\partial}{\partial x} f(w_R) = 0, \quad x \in (x_j, x_{j+1}), \quad t \in [t_n, t_{n+1})$$

$$w_R(x,0) = \begin{cases} v_j^n, & x < x_{j+\frac{1}{2}} \\ v_{j+1}^n, & x > x_{j+\frac{1}{2}} \end{cases}$$

Under the CFL condition

$$\lambda \max |a(u)| \le \frac{1}{2}$$

the solution at next time level is given by projecting the Riemann solution onto piecewise constant states

$$v_j^{n+1} = \frac{1}{\Delta x} \int_0^{\frac{\Delta x}{2}} w_R(x/\Delta t; v_{j-1}^n, v_j^n) \mathsf{d}x + \frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^0 w_R(x/\Delta t; v_j^n, v_{j+1}^n) \mathsf{d}x$$

Godunov scheme

We can rewrite the above formula as a finite volume scheme with numerical flux

$$g^G_{j+\frac{1}{2}} = f(w_R(0; v_j, v_{j+1}))$$

Approximate Riemann solver

Let $w(x/t; u_l, u_r)$ be an approximation of the exact entropy solution $w_R(x/t; u_l, u_r)$ of the Riemann problem

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$
$$u(x,0) = \begin{cases} u_l, & x < 0 \\ u_r, & x > 0 \end{cases}$$

We will require that the approximate solution be consistent with the exact one in two respects

Conservation: Integrate over rectangle $(-\frac{\Delta x}{2}, +\frac{\Delta x}{2}) \times (0, \Delta t)$, and provided

$$\lambda |a(u)| \leq \frac{1}{2}, \qquad \text{for all } u \text{ between } u_l \text{ and } u_r$$

we get

$$\frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} w_R(x/\Delta t; u_l, u_r) \mathsf{d}x = \frac{1}{2}(u_l + u_r) + \lambda(f(u_l) - f(u_r))$$

Thus we require the approximate solution to satisfy

$$\frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} w(x/\Delta t; u_l, u_r)\mathsf{d}x = \frac{1}{2}(u_l + u_r) + \lambda(f(u_l) - f(u_r))$$

Entropy condition: Integrating the entropy inequality $U_t + F_x \leq 0$ yields

$$\frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} U(w_R(x/\Delta t; u_l, u_r))\mathsf{d}x \leq \frac{1}{2}(U(u_l) + U(u_r)) + \lambda(F(u_l) - F(u_r))$$

For consistency with the entropy condition, we require approximate solution to satisfy

$$\frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} U(w(x/\Delta t; u_l, u_r))\mathsf{d}x \leq \frac{1}{2}(U(u_l) + U(u_r)) + \lambda(F(u_l) - F(u_r))$$

Continuity: Finally, we require the solution to be continuous wrt the data

$$w(x/t; u, u) = u$$

Godunov-type scheme: With the help of such an approximate Riemann solution w, we define the Godunov-type scheme as follows

$$v_j^{n+1} = \frac{1}{\Delta x}\int_0^{\frac{\Delta x}{2}} w(x/\Delta t; v_{j-1}^n, v_j^n)\mathrm{d}x + \frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^0 w(x/\Delta t; v_j^n, v_{j+1}^n)\mathrm{d}x$$

Theorem

Let w be the approximate Riemann solver which satisfies (1) conservation, (2) consistency with entropy condition for an entropy pair (U, F) and is (3) continuous. Then the Godunov-type scheme can be put in conservation form, is consistent with the conservation law and is consistent with the entropy condition associated with (U, F) under the CFL condition CFL $\leq \frac{1}{2}$.

Roe scheme and its entropy modification

The Roe scheme is an approximate Riemann solver with

$$w(x/t; u_l, u_r) = \begin{cases} u_l, & x/t < a(u_l, u_r) \\ u_r, & x/t > a(u_l, u_r) \end{cases}$$

with numerical flux

$$g^R(u, v) = \frac{1}{2}(f(u) + f(v)) - \frac{1}{2}|a(u, v)|(v - u)$$

But we have seen that this admits entropy violating shocks. This solution has only shocks and hence there will be problem when the solution is a rarefaction. Harten and Hyman proposed the following approximate Riemann solver

$$w(x/t; u_l, u_r) = \begin{cases} u_l, & x/t < a_l \\ u^*, & a_l < x/t < a_r \\ u_r, & x/t > a_r \end{cases}$$

Here the intermediate state u^* and a_l, a_r are yet to be specified (See GR1).

Entropy conservative schemes

Let (U, F) be an entropy pair and define the **entropy variable**

$$v = U'(u)$$

and **entropy potential**

$$\psi(v) = vf(u(v)) - F(u(v))$$

Consider the semi-discrete finite volume scheme

$$\frac{\mathrm{d}u_j}{\mathrm{d}t} + \frac{g^*_{j+\frac{1}{2}} - g^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

Assume that the flux satisfies the condition (Tadmor)

$$(v_{j+1} - v_j)g^*_{j+\frac{1}{2}} = \psi_{j+1} - \psi_j$$

Now multiply semi-discrete scheme by $v_j = U'(u_j)$

$$U'(u_j)\frac{\mathrm{d}u_j}{\mathrm{d}t} + v_j\frac{g^*_{j+\frac{1}{2}} - g^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

Entropy conservative schemes

We have the identity

$$v_j = \frac{1}{2}(v_j + v_{j+1}) - \frac{1}{2}(v_{j+1} - v_j) = \{\!\{v\}\!\}_{j+\frac{1}{2}} - \frac{1}{2}[\![v]\!]_{j+\frac{1}{2}}$$

so that

$$v_j g^*_{j+\frac{1}{2}} = \{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \frac{1}{2}[\![v]\!]_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} = \{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \frac{1}{2}[\![\psi]\!]_{j+\frac{1}{2}}$$

Similarly

$$v_j = \frac{1}{2}(v_j + v_{j-1}) - \frac{1}{2}(v_{j-1} - v_j) = \{\!\{v\}\!\}_{j-\frac{1}{2}} + \frac{1}{2}[\![v]\!]_{j-\frac{1}{2}}$$

so that

$$v_j g^*_{j-\frac{1}{2}} = \{\!\{v\}\!\}_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} + \frac{1}{2}[\![v]\!]_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} = \{\!\{v\}\!\}_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} + \frac{1}{2}[\![\psi]\!]_{j-\frac{1}{2}}$$

Entropy conservative schemes

Hence

$$
\begin{aligned}
v_j(g^*_{j+\frac{1}{2}} - g^*_{j-\frac{1}{2}}) &= \{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \frac{1}{2}(\psi_{j+1} - \psi_j) \\
&\quad - \{\!\{v\}\!\}_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} - \frac{1}{2}(\psi_j - \psi_{j-1}) \\
&= \left[\{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \frac{1}{2}(\psi_{j+1} + \psi_j)\right] \\
&\quad - \left[\{\!\{v\}\!\}_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} - \frac{1}{2}(\psi_j + \psi_{j-1})\right] \\
&= \left[\{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \{\!\{\psi\}\!\}_{j+\frac{1}{2}}\right] \\
&\quad - \left[\{\!\{v\}\!\}_{j-\frac{1}{2}} g^*_{j-\frac{1}{2}} - \{\!\{\psi\}\!\}_{j-\frac{1}{2}})\right]
\end{aligned}
$$

Define the numerical entropy flux

$$
G^*_{j+\frac{1}{2}} = \{\!\{v\}\!\}_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} - \{\!\{\psi\}\!\}_{j+\frac{1}{2}}
$$

Entropy conservative schemes

then we obtain the entropy equality

$$\frac{\mathsf{d}}{\mathsf{d}t}U(u_j) + \frac{G^*_{j+\frac{1}{2}} - G^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

Now, let us check the consistency of the flux. The numerical flux is

$$g^*_{j+\frac{1}{2}} = \frac{\psi_{j+1} - \psi_j}{v_{j+1} - v_j}$$

Firstly, this is a central flux since interchanging u_j, u_{j+1} gives the same value. Secondly, if $u_j = u_{j+1} = u$ and correspondingly $v_j = v_{j+1} = v = U'(u)$, the

$$\begin{aligned} g^*_{j+\frac{1}{2}} &= \psi'(v) = f(u(v)) + vf'(u(v))u'(v) - F'(u(v))u'(v) \\ &= f(u(v)) + [U'(u)f'(u(v)) - F'(u(v))]u'(v) \\ &= f(u) \end{aligned}$$

The numerical entropy flux is also a central flux and if $u_j = u_{j+1} = u$, we get

$$G^*_{j+\frac{1}{2}} = vf(u) - \psi(v) = F(u)$$

Entropy conservative schemes

and hence is consistent with the entropy flux.

Theorem

If the numerical flux $g^*_{j+\frac{1}{2}}$ satisfies the condition

$$[\![v]\!]_{j+\frac{1}{2}} g^*_{j+\frac{1}{2}} = [\![\psi]\!]_{j+\frac{1}{2}}$$

then the semi-discrete finite volume scheme satisfies entropy conservation associated to the entropy U.

Example: Burger's equation

Take $U(u) = \frac{1}{2}u^2$. Then

$$F(u) = \int^u U'(s)f'(s)\mathsf{d}s = \int^u (s)(s)\mathsf{d}s = \frac{1}{3}s^3$$

and

$$v = U'(u) = u, \qquad \psi = (u)(\frac{1}{2}u^2) - \frac{1}{3}u^3 = \frac{1}{6}u^3$$

The entropy conserving flux is

$$g^*_{j+\frac{1}{2}} = \frac{\psi_{j+1} - \psi_j}{v_{j+1} - v_j} = \frac{\frac{1}{6}u^3_{j+1} - \frac{1}{6}u^3_j}{u_{j+1} - u_j} = \frac{1}{6}(u_j^2 + u_j u_{j+1} + u^2_{j+1})$$

With this flux, the entropy equation is

$$\frac{\mathsf{d}}{\mathsf{d}t}(\frac{1}{2}u_j^2) + \frac{G^*_{j+\frac{1}{2}} - G^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

which implies that (assuming periodic bc)

$$\frac{\mathsf{d}}{\mathsf{d}t}\sum_j \frac{1}{2}u_j^2 = 0$$

i.e., the energy is conserved.

Viscosity form: $U(u) = \frac{1}{2}u^2$

In this case $v = U'(u) = u$. Define the straight line path

$$u_{j+\frac{1}{2}}(\xi) = \frac{1}{2}(u_j + u_{j+1}) + \xi [\![u]\!]_{j+\frac{1}{2}}$$

The entropy conservative flux is

$$g^*_{j+\frac{1}{2}} = \frac{\psi_{j+1} - \psi_j}{v_{j+1} - v_j} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \psi'(u_{j+\frac{1}{2}}(\xi))\mathsf{d}\xi = \int_{-\frac{1}{2}}^{\frac{1}{2}} f(u_{j+\frac{1}{2}}(\xi))\mathsf{d}\xi$$

Equating this to the viscosity form

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} f(u_{j+\frac{1}{2}}(\xi))\mathsf{d}\xi = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2}Q^*_{j+\frac{1}{2}} [\![u]\!]_{j+\frac{1}{2}}$$

we can write the viscosity coefficient as (Exercise)

$$Q^*_{j+\frac{1}{2}} = \int_{-\frac{1}{2}}^{\frac{1}{2}} 2\xi f'(u_{j+\frac{1}{2}}(\xi))\mathsf{d}\xi$$

Viscosity form: general case

In this case $v = U'(u)$. Define the straight line path

$$v_{j+\frac{1}{2}}(\xi) = \frac{1}{2}(v_j + v_{j+1}) + \xi [\![v]\!]_{j+\frac{1}{2}}$$

The entropy conservative flux is

$$g^*_{j+\frac{1}{2}} = \frac{\psi_{j+1} - \psi_j}{v_{j+1} - v_j} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \psi'(v_{j+\frac{1}{2}}(\xi)) \mathsf{d}\xi = \int_{-\frac{1}{2}}^{\frac{1}{2}} f(u(v_{j+\frac{1}{2}}(\xi))) \mathsf{d}\xi$$

Equating this to the viscosity form

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} f(u_{j+\frac{1}{2}}(\xi)) \mathsf{d}\xi = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2} P^*_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}}$$

we can write the viscosity coefficient as (Exercise)

$$P^*_{j+\frac{1}{2}} = \int_{-\frac{1}{2}}^{\frac{1}{2}} 2\xi f'(u(v_{j+\frac{1}{2}}(\xi))) \mathsf{d}\xi$$

Entropy consistent schemes

We must produce entropy at shock waves, which means that we need an entropy inequality. Consider the semi-discrete finite volume scheme

$$\frac{\mathrm{d}u_j}{\mathrm{d}t} + \frac{g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}}{\Delta x} = 0$$

Let us write the numerical flux in terms of viscosity form using jump in entropy variable

$$g_{j+\frac{1}{2}} = \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2} P_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}}$$

This can be re-written as

$$\begin{aligned}
g_{j+\frac{1}{2}} &= \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2} P^*_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} - \frac{1}{2}(P_{j+\frac{1}{2}} - P^*_{j+\frac{1}{2}}) [\![v]\!]_{j+\frac{1}{2}} \\
&= g^*_{j+\frac{1}{2}} - \frac{1}{2}(P_{j+\frac{1}{2}} - P^*_{j+\frac{1}{2}}) [\![v]\!]_{j+\frac{1}{2}} \\
&= g^*_{j+\frac{1}{2}} - \frac{1}{2} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}}, \qquad D_{j+\frac{1}{2}} = P_{j+\frac{1}{2}} - P^*_{j+\frac{1}{2}}
\end{aligned}$$

Entropy consistent schemes

where $g^*_{j+\frac{1}{2}}$ is the entropy conservative flux. Let us derive the entropy equation.

$$v_j(g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}) = v_j(g^*_{j+\frac{1}{2}} - g^*_{j-\frac{1}{2}}) - \frac{1}{2} v_j D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} + \frac{1}{2} v_j D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}}$$

Following steps as in the entropy conservative case

$$v_j D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} = \{\!\{v\}\!\}_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} - \frac{1}{2} [\![v]\!]_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}}$$

$$v_j D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}} = \{\!\{v\}\!\}_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}} + \frac{1}{2} [\![v]\!]_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}}$$

Hence

$$\begin{aligned} v_j(g_{j+\frac{1}{2}} - g_{j-\frac{1}{2}}) = & \quad \left[G^*_{j+\frac{1}{2}} - \frac{1}{2} \{\!\{v\}\!\}_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} \right] \\ & - \left[G^*_{j-\frac{1}{2}} - \frac{1}{2} \{\!\{v\}\!\}_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}} \right] \\ & + \frac{1}{4} [\![v]\!]_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} + \frac{1}{4} [\![v]\!]_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}} \end{aligned}$$

Entropy consistent schemes

Define the numerical entropy flux

$$G_{j+\frac{1}{2}} = G^*_{j+\frac{1}{2}} - \frac{1}{2}\{\!\{v\}\!\}_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}}$$

then the entropy equation is

$$\frac{\mathrm{d}}{\mathrm{d}t}U(u_j) + \frac{G_{j+\frac{1}{2}} - G_{j-\frac{1}{2}}}{\Delta x} = -\frac{1}{4}[\![v]\!]_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![v]\!]_{j+\frac{1}{2}} - \frac{1}{4}[\![v]\!]_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![v]\!]_{j-\frac{1}{2}} \leq 0$$

where the inequality follows provided

$$D_{j+\frac{1}{2}} \geq 0 \quad \forall j \quad \Longrightarrow \quad P_{j+\frac{1}{2}} \geq P^*_{j+\frac{1}{2}}$$

i.e., **the viscosity coefficient P must be larger than the viscosity coefficient P^* in the entropy conservative scheme**.

Hyperbolic Systems

Consider a system of hyperbolic conservation laws

$$\frac{\partial \boldsymbol{u}}{\partial t} + \sum_{j=1}^{d} \frac{\partial \boldsymbol{f}_j}{\partial x_j} = 0, \qquad \boldsymbol{f}_j = \boldsymbol{f}_j(\boldsymbol{u})$$

We say that (U, F) is an entropy pair for the above system if $U(\boldsymbol{u})$ is strictly convex and

$$F_j'(\boldsymbol{u}) = U'(\boldsymbol{u})\boldsymbol{f}_j'(\boldsymbol{u}), \qquad 1 \le j \le d$$

Smooth solutions satisfy the additional equation

$$\frac{\partial U}{\partial t} + \sum_{j=1}^{d} \frac{\partial F_j}{\partial x_j} = 0$$

while in general we can only demand the inequality

$$\frac{\partial U}{\partial t} + \sum_{j=1}^{d} \frac{\partial F_j}{\partial x_j} \le 0$$

to hold in the sense of distributions which can be motivated from vanishing viscosity approach. The existence of such pairs is not guaranteed in general.

Strict convexity

The function $U(\boldsymbol{u})$ being strictly convex means that

$$U((1-\xi)\boldsymbol{u}_1 + \xi\boldsymbol{u}_2) < (1-\xi)U(\boldsymbol{u}_1) + \xi U(\boldsymbol{u}_2), \qquad 0 < \xi < 1$$

If $U(\boldsymbol{u})$ is differentiable, this means the symmetric matrix $U''(\boldsymbol{u})$

$$[U''(\boldsymbol{u})]_{ij} = \frac{\partial^2 U}{\partial u_i \partial u_j}$$

is positive definite, i.e.,

$$\boldsymbol{s}^\top U''(\boldsymbol{u})\boldsymbol{s} > 0, \qquad \forall \boldsymbol{s} \neq 0$$

and hence all eigenvalues of $U''(\boldsymbol{u})$ are strictly positive.

Symmetric Hyperbolic Systems

Suppose we do a change of variable from $\boldsymbol{u}$ to $\boldsymbol{v}$

$$\boldsymbol{u}'(\boldsymbol{v})\frac{\partial \boldsymbol{v}}{\partial t} + \sum_{j=1}^{d} \boldsymbol{f}_j'(\boldsymbol{u}(\boldsymbol{v}))\boldsymbol{u}'(\boldsymbol{v})\frac{\partial \boldsymbol{v}}{\partial x_j} = 0$$

and we write this as

$$A_0 \frac{\partial \boldsymbol{v}}{\partial t} + \sum_{j=1}^{d} A_j A_0 \frac{\partial \boldsymbol{v}}{\partial x_j} = 0$$

where

$$A_0 = \boldsymbol{u}'(\boldsymbol{v}), \qquad A_j = \boldsymbol{f}_j'(\boldsymbol{u})$$

If A_0 is symmetric, positive definite and $A_j A_0$ is symmetric, then we call this as a symmetric, hyperbolic form. The conservation law is said to be symmetrizable if such a change of variable exists.

Theorem (Godunov, Mock), ([2], Thm 3.2, page 25)

A necessary and sufficient condition for the conservation law to posses a strictly convex entropy U is that there exists a change of dependent variables $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{v})$ that symmetrizes it.

Given a strictly convex function, the following theorem tell us when it will be an entropy function.

Theorem ([2], Thm 3.1, page 24)

Let U be a strictly convex function. A necessary and sufficient condition for U to be an entropy is that the matrices $U''(\boldsymbol{u})\boldsymbol{f}_j'(\boldsymbol{u})$, $1 \leq j \leq d$ are symmetric.

Let U be a strictly convex entropy function. Define the entropy variables

$$\boldsymbol{v}^\top = U'(\boldsymbol{u})$$

Since $U''(\boldsymbol{u})$ is positive definite, we can uniquely convert from $\boldsymbol{u} \to \boldsymbol{v}$ and $\boldsymbol{v} \to \boldsymbol{u}$.

If we transform the PDE from conserved variables to entropy variables, we obtain a symmetric, hyperbolic form.

Given some conservation law, there is no general method to find an entropy function.

Usually, for systems coming from Physics, we already know the existence of an entropy condition from the second law of Thermodynamics.

For an entropy pair (U, F), define the **entropy potential**

$$\psi(\boldsymbol{v}) = \boldsymbol{v} \cdot \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{v})) - F(\boldsymbol{u}(\boldsymbol{v}))$$

Entropy conservative scheme

Consider the semi-discrete finite volume scheme

$$\frac{\partial \boldsymbol{u}_j}{\partial t} + \frac{\boldsymbol{f}^*_{j+\frac{1}{2}} - \boldsymbol{f}^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

and assume that the numerical flux $\boldsymbol{f}^*_{j+\frac{1}{2}} = \boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_{j+1})$ satisfies

$$[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} \cdot \boldsymbol{f}^*_{j+\frac{1}{2}} = [\![\psi]\!]_{j+\frac{1}{2}}$$

Taking the dot product of the scheme with $\boldsymbol{v}_j = U(\boldsymbol{u}_j)$ gives

$$\frac{\mathsf{d}}{\mathsf{d}t} U(\boldsymbol{u}_j) + \frac{F^*_{j+\frac{1}{2}} - F^*_{j-\frac{1}{2}}}{\Delta x} = 0$$

where

$$F^*_{j+\frac{1}{2}} = F^*(\boldsymbol{u}_j, \boldsymbol{u}_{j+1}) := \{\!\{\boldsymbol{v}\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}^*_{j+\frac{1}{2}} - \{\!\{\psi\}\!\}_{j+\frac{1}{2}}$$

is a consistent numerical entropy flux, i.e., $F^*(\boldsymbol{u}, \boldsymbol{u}) = F(\boldsymbol{u})$.

Higher order entropy conservative scheme

The entropy conservative flux $\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_{j+1})$ leads to a second order scheme. This flux can be used as a building block to construct higher order schemes (LeFloch et al. [3]).

Choose an integer $p \geq 1$ and let $\alpha_1, \alpha_2, \ldots, \alpha_p$ be numbers which satisfy

$$2\sum_{r=1}^{p} r\alpha_r = 1, \qquad \sum_{l=1}^{p} l^{2s-1}\alpha_r = 0, \quad s = 2, 3, \ldots, p$$

Define the numerical flux

$$\boldsymbol{f}^{*,2p}_{j+\frac{1}{2}} = \boldsymbol{f}^{*,2p}(\boldsymbol{u}_{j-p+1}, \ldots, \boldsymbol{u}_{j+p}) = \sum_{r=1}^{p} \alpha_r \sum_{s=0}^{r-1} \boldsymbol{f}^*(\boldsymbol{u}_{j-s}, \boldsymbol{u}_{j-s+r})$$

Then the semi-discrete FV scheme is $2p$'th order accurate

$$\frac{\boldsymbol{f}^{*,2p}_{j+\frac{1}{2}} - \boldsymbol{f}^{*,2p}_{j-\frac{1}{2}}}{\Delta x} = \frac{\partial \boldsymbol{f}}{\partial x}(x_j) + O(\Delta x)^{2p}$$

Higher order entropy conservative scheme

and satisfies the entropy equation

$$\frac{\mathsf{d}U_j}{\mathsf{d}t} + \frac{F^{*,2p}_{j+\frac{1}{2}} - F^{*,2p}_{j-\frac{1}{2}}}{\Delta x} = 0$$

where

$$F^{*,2p}_{j+\frac{1}{2}} = \sum_{r=1}^{p} \alpha_r \sum_{s=0}^{r-1} F^*(\boldsymbol{u}_{j-s}, \boldsymbol{u}_{j-s+r})$$

is a consistent entropy flux.

Example: For $p = 2$ we get the fourth order accurate entropy conservative flux

$$\boldsymbol{f}^{*,4}_{j+\frac{1}{2}} = \frac{4}{3}\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_{j+1}) - \frac{1}{6}\boldsymbol{f}^*(\boldsymbol{u}_{j-1}, \boldsymbol{u}_{j+1}) - \frac{1}{6}\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_{j+2})$$

Entropy consistent scheme

Consider the semi-discrete finite volume scheme

$$\frac{\partial \boldsymbol{u}_j}{\partial t} + \frac{\boldsymbol{f}_{j+\frac{1}{2}} - \boldsymbol{f}_{j-\frac{1}{2}}}{\Delta x} = 0$$

where the numerical flux is

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2} D_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}, \qquad D_{j+\frac{1}{2}} = D^\top_{j+\frac{1}{2}} \ge 0$$

Then we get the entropy inequality

$$\frac{\mathrm{d}}{\mathrm{d}t} U(\boldsymbol{u}_j) + \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} = -\frac{1}{4} [\![\boldsymbol{v}]\!]^\top_{j-\frac{1}{2}} D_{j-\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j-\frac{1}{2}} - \frac{1}{4} [\![\boldsymbol{v}]\!]^\top_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} \le 0$$

where

$$F_{j+\frac{1}{2}} = F^*_{j+\frac{1}{2}} - \frac{1}{2} \{\!\{\boldsymbol{v}\}\!\}^\top_{j+\frac{1}{2}} D_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

is a consistent numerical entropy flux.

The flux $\boldsymbol{f}_{j+\frac{1}{2}}$ is first order accurate since $[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} = O(\Delta x)$.

Dissipation matrix

Let us first write the entropy conservative flux in viscosity form

$$\boldsymbol{f}^*_{j+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2} P^*_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

Define the symmetric matrix

$$B(\boldsymbol{v}) = \frac{\partial}{\partial \boldsymbol{v}} \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{v}))$$

then (Exercise)

$$P^*_{j+\frac{1}{2}} = \int_{-\frac{1}{2}}^{\frac{1}{2}} 2\xi B(\boldsymbol{v}_{j+\frac{1}{2}}(\xi)) \mathrm{d}\xi$$

where $\boldsymbol{v}_{j+\frac{1}{2}}(\xi)$ is the linear path connecting $\boldsymbol{v}_j$, $\boldsymbol{v}_{j+1}$

$$\boldsymbol{v}_{j+\frac{1}{2}}(\xi) = \{\!\{\boldsymbol{v}\}\!\}_{j+\frac{1}{2}} + \frac{1}{2}\xi [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

Dissipation matrix

Let us write the entropy consistent flux also in viscosity form

$$\boldsymbol{f}_{j+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2} P_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

This can be rewritten as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2} \underbrace{(P_{j+\frac{1}{2}} - P^*_{j+\frac{1}{2}})}_{D_{j+\frac{1}{2}}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

Hence for entropy stability, we need to satisfy

$$P_{j+\frac{1}{2}} \geq P^*_{j+\frac{1}{2}} \quad \text{in the sense of SPD matrix ordering}$$

Using a linearization

$$[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} = H_{j+\frac{1}{2}} [\![\boldsymbol{u}]\!]_{j+\frac{1}{2}}, \qquad H_{j+\frac{1}{2}} = \boldsymbol{v}'(\boldsymbol{u})_{j+\frac{1}{2}} := \int_{-\frac{1}{2}}^{\frac{1}{2}} U''(\boldsymbol{u}(\boldsymbol{v}_{j+\frac{1}{2}}(\xi)))\mathsf{d}\xi$$

Dissipation matrix

we can write the flux as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2} P_{j+\frac{1}{2}} H_{j+\frac{1}{2}} [\![\boldsymbol{u}]\!]_{j+\frac{1}{2}}$$

If we match the above flux to the **Rusanov flux**,

$$P_{j+\frac{1}{2}} H_{j+\frac{1}{2}} = \lambda_m I \quad \Longrightarrow \quad P_{j+\frac{1}{2}} = \lambda_m H_{j+\frac{1}{2}}^{-1}$$

where λ_m is the maximum wavespeed at $j + \frac{1}{2}$. Tadmor shows that

$$\lambda_m H_{j+\frac{1}{2}}^{-1} \ge P_{j+\frac{1}{2}}^* \tag{2}$$

and hence the Rusanov flux is entropy consistent. We can write the Rusanov flux in terms of entropy variable jump as

$$\boldsymbol{f}_{j+\frac{1}{2}}^{Rus} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2} \lambda_m H_{j+\frac{1}{2}}^{-1} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

Dissipation matrix

Remark: It is usually not possible to find explicit formula for $H_{j+\frac{1}{2}}$. We can find an approximation to $H_{j+\frac{1}{2}}$ by performing a numerical integration, but we have to check that (2) is satisfied.

Rusanov-type dissipation matrix: An easier scheme is to first approximate

$$[\![\boldsymbol{u}]\!]_{j+\frac{1}{2}} \approx \boldsymbol{u}'(\boldsymbol{v})_{j+\frac{1}{2}}[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}, \qquad \boldsymbol{u}'(\boldsymbol{v})_{j+\frac{1}{2}} = \boldsymbol{u}'(\{\!\{\boldsymbol{v}\}\!\}_{j+\frac{1}{2}})$$

and then add the Rusanov dissipation to the entropy conservative flux

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2}\lambda_m \boldsymbol{u}'(\boldsymbol{v})_{j+\frac{1}{2}}[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

We discuss a similar approach later in the context of Euler equations, see also [4].

Roe-type dissipation matrix: Barth [5] shows that we can scale the eigenvectors in such a way that they satisfy the relation

$$RR^\top = \boldsymbol{u}'(\boldsymbol{v})$$

Dissipation matrix

The Roe flux is given by

$$\boldsymbol{f}^{Roe}_{j+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2} R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^{-1}_{j+\frac{1}{2}} [\![\boldsymbol{u}]\!]_{j+\frac{1}{2}}$$

Converting jump in $\boldsymbol{u}$ to $\boldsymbol{v}$

$$[\![\boldsymbol{u}]\!]_{j+\frac{1}{2}} \approx \boldsymbol{u}'(\boldsymbol{v})_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} = R_{j+\frac{1}{2}} R^{\top}_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

the dissipation in Roe flux can be written as

$$\begin{aligned} R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^{-1}_{j+\frac{1}{2}} [\![\boldsymbol{u}]\!]_{j+\frac{1}{2}} &= R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^{-1}_{j+\frac{1}{2}} R_{j+\frac{1}{2}} R^{\top}_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} \\ &= R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^{\top}_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}} \end{aligned}$$

We have an SPD dissipation matrix

$$D_{j+\frac{1}{2}} = R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^{\top}_{j+\frac{1}{2}}$$

Dissipation matrix

which can be used in combination with the entropy conservative flux

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2} R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^\top_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

The above flux leads to an entropy consistent scheme (but the dissipation is probably not optimal).

Remark: It is possible to carefully compute the dissipation matrix so that we get exact resolution of stationary contact waves, see [6].

Higher order entropy consistent scheme

To construct higher order scheme, we will follow the reconstruction approach. At each face $j + \frac{1}{2}$, we obtain a left and right value of entropy variables $\boldsymbol{v}^L_{j+\frac{1}{2}}$, $\boldsymbol{v}^R_{j+\frac{1}{2}}$ and define the numerical flux as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^{*,2p}_{j+\frac{1}{2}} - \frac{1}{2} D_{j+\frac{1}{2}} (\boldsymbol{v}^R_{j+\frac{1}{2}} - \boldsymbol{v}^L_{j+\frac{1}{2}})$$

Note that we use the higher order entropy conservative flux, and use the reconstructed values to define the dissipative flux. Then we get the entropy equation

$$\begin{aligned} \frac{\mathsf{d}}{\mathsf{d}t} U(\boldsymbol{u}_j) + \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} \quad = \quad & -\frac{1}{4} (\boldsymbol{v}_j - \boldsymbol{v}_{j-1})^\top D_{j-\frac{1}{2}} (\boldsymbol{v}^R_{j-\frac{1}{2}} - \boldsymbol{v}^L_{j-\frac{1}{2}}) \\ & -\frac{1}{4} (\boldsymbol{v}_{j+1} - \boldsymbol{v}_j)^\top D_{j+\frac{1}{2}} (\boldsymbol{v}^R_{j+\frac{1}{2}} - \boldsymbol{v}^L_{j+\frac{1}{2}}) \end{aligned}$$

where

$$F_{j+\frac{1}{2}} = F^{*,2p}_{j+\frac{1}{2}} - \frac{1}{2} \{\!\{\boldsymbol{v}\}\!\}^\top_{j+\frac{1}{2}} D_{j+\frac{1}{2}} (\boldsymbol{v}^R_{j+\frac{1}{2}} - \boldsymbol{v}^L_{j+\frac{1}{2}})$$

We do not know the sign of the right hand side. We have to design a reconstruction scheme that allows us to fix the sign of the terms on the right.

Sign preserving reconstruction

Recall that the dissipation matrix can be written as

$$D_{j+\frac{1}{2}} = R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R_{j+\frac{1}{2}}^\top$$

Define the new variables

$$\boldsymbol{w}_k = R_{j+\frac{1}{2}}^\top \boldsymbol{v}_k, \qquad k = \ldots, j-1, j, j+1, \ldots$$

We will use the ENO reconstruction scheme to obtain $\boldsymbol{w}_{j+\frac{1}{2}}^L$, $\boldsymbol{w}_{j+\frac{1}{2}}^R$. We can then compute

$$\boldsymbol{v}_{j+\frac{1}{2}}^L = R_{j+\frac{1}{2}}^{-1} \boldsymbol{w}_{j+\frac{1}{2}}^L, \qquad \boldsymbol{v}_{j+\frac{1}{2}}^R = R_{j+\frac{1}{2}}^{-1} \boldsymbol{w}_{j+\frac{1}{2}}^R$$

But it is not necessary to compute $\boldsymbol{v}_{j+\frac{1}{2}}^L$, $\boldsymbol{v}_{j+\frac{1}{2}}^R$ since we can write the flux as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}_{j+\frac{1}{2}}^{*,2p} - \frac{1}{2} R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| (\boldsymbol{w}_{j+\frac{1}{2}}^R - \boldsymbol{w}_{j+\frac{1}{2}}^L)$$

Sign preserving reconstruction

Fjordholm and Mishra [7] have shown that the ENO scheme preserves the sign of the jump, i.e.,

$$\mathrm{sign}(\boldsymbol{w}_{j+1} - \boldsymbol{w}_j) = \mathrm{sign}(\boldsymbol{w}^R_{j+\frac{1}{2}} - \boldsymbol{w}^L_{j+\frac{1}{2}})$$

On the right of the entropy equation, we have terms like

$$\begin{aligned}
& (\boldsymbol{v}_{j+1} - \boldsymbol{v}_j)^\top D_{j+\frac{1}{2}} (\boldsymbol{v}^R_{j+\frac{1}{2}} - \boldsymbol{v}^L_{j+\frac{1}{2}}) \\
= \quad & (\boldsymbol{v}_{j+1} - \boldsymbol{v}_j)^\top R_{j+\frac{1}{2}} |\Lambda_{j+\frac{1}{2}}| R^\top_{j+\frac{1}{2}} (\boldsymbol{v}^R_{j+\frac{1}{2}} - \boldsymbol{v}^L_{j+\frac{1}{2}}) \\
= \quad & (R^\top_{j+\frac{1}{2}} \boldsymbol{v}_{j+1} - R^\top_{j+\frac{1}{2}} \boldsymbol{v}_j)^\top |\Lambda_{j+\frac{1}{2}}| (R^\top_{j+\frac{1}{2}} \boldsymbol{v}^R_{j+\frac{1}{2}} - R^\top_{j+\frac{1}{2}} \boldsymbol{v}^L_{j+\frac{1}{2}}) \\
= \quad & (\boldsymbol{w}_{j+1} - \boldsymbol{w}_j)^\top |\Lambda_{j+\frac{1}{2}}| (\boldsymbol{w}^R_{j+\frac{1}{2}} - \boldsymbol{w}^L_{j+\frac{1}{2}}) \\
\geq \quad & 0
\end{aligned}$$

This shows that scheme satisfies entropy inequality.

For second order scheme, the ENO scheme is same as reconstruction using minmod limiter.

Euler equations

We will consider Euler equations in 1-D, which model friction-less fluids and can be written as

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} = 0$$

where

$$\boldsymbol{u} = \begin{bmatrix} \rho \\ \rho v \\ \rho e \end{bmatrix}, \qquad \boldsymbol{f} = \begin{bmatrix} \rho v \\ p + \rho v^2 \\ (\rho e + p) v \end{bmatrix}$$

and

$$\rho = \text{mass density}, \quad \rho v = \text{momentum density}, \quad \rho e = \text{energy density}$$

and p is the pressure. The energy is made up of internal energy and kinetic energy

$$\rho e = \rho \varepsilon + \frac{1}{2} \rho v^2$$

where $\varepsilon =$ internal energy per unit mass.

Thermodynamic considerations

We have four unknowns but only three equations. We need a way to relate the internal energy to the thermodynamics variable ρ, p, T where T is the absolute temperature.

For a system in equilibrium, the thermodynamic variables satisfy an **equation of state**

$$f(\rho, p, T) = 0$$

which may be solved for one of the variables, e.g., $p = p(\rho, T)$. The equation of state for an **ideal gas** can be written as

$$p = \rho R T$$

where R is the **gas constant**.

The specific heats at constant volume and constant pressure are defined as

$$C_v = \left(\frac{\partial \varepsilon}{\partial T}\right)_\tau, \qquad C_p = \left(\frac{\partial h}{\partial T}\right)_p, \qquad \text{where} \qquad \tau = \frac{1}{\rho}, \qquad h = \varepsilon + p\tau$$

Thermodynamic considerations

For an ideal gas

$$\varepsilon = \varepsilon(T), \qquad h = h(T)$$

If we assume that C_v, C_p are independent of temperature (calorically and thermally perfect gas), which is a good assumption for air under normal conditions, we get

$$\varepsilon = C_v T, \qquad h = C_p T, \qquad C_p - C_v = R$$

Define the ratio of specific heats

$$\gamma = \frac{C_p}{C_v} \quad \Longrightarrow \quad C_v = \frac{R}{\gamma - 1}, \quad C_p = \frac{\gamma R}{\gamma - 1}$$

Now we can close the model by using

$$\varepsilon = C_v T = \frac{RT}{\gamma - 1} = \frac{p}{(\gamma - 1)\rho}$$

Some authors/books refer to this model as a **polytropic ideal gas**.

Thermodynamic considerations

The second law of thermodynamics introduces a new state variable called **entropy** and denoted s. Under a quasi-static process

$$T\mathsf{d}s = \mathsf{d}\varepsilon + p\mathsf{d}\tau$$

For a polytropic ideal gas

$$s = s_0 + C_v \ln(\varepsilon/\rho^{\gamma-1})$$

Euler equation: Entropy function

For our purpose, we can drop the constants and define the physical entropy function as

$$s = \ln(p/\rho^\gamma)$$

From the Euler equations, we can derive an additional equation

$$\frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial x}(\rho v s) = 0$$

This motivates us to define the mathematical entropy function and entropy flux as

$$U = -\frac{\rho s}{\gamma - 1}, \qquad F = -\frac{\rho v s}{\gamma - 1} \tag{3}$$

We can check that $U(\boldsymbol{u})$ is a strictly convex function and $F'(\boldsymbol{u}) = U'(\boldsymbol{u})\boldsymbol{f}'(\boldsymbol{u})$ is satisfied.

In fact, we have many entropy functions of the form

$$U = -\frac{\rho \eta(s)}{\gamma - 1}, \qquad F = -\frac{\rho v \eta(s)}{\gamma - 1}$$

Euler equation: Entropy function

where $\eta(s)$ is any function that satisfies

$$\gamma\eta''(s) < \eta'(s)$$

The entropy condition for Navier-Stokes equations with Fourier law of heat condition requires that $\eta(s)$ must be an affine function [8, 9]. Hence we will use the linear function $\eta(s) = s$ from now onwards.

For the entropy pair (3), the entropy variable is

$$\boldsymbol{v} = U'(\boldsymbol{u}) = \begin{bmatrix} \frac{\gamma - s}{\gamma - 1} - \beta v^2 \\ 2\beta v \\ -2\beta \end{bmatrix}, \qquad \beta = \frac{\rho}{2p} = \frac{1}{2RT}$$

and the entropy potential is

$$\psi = \boldsymbol{v} \cdot \boldsymbol{f} - F = \rho v$$

Euler equation: Entropy conservative flux [6]

An entropy conservative flux must satisfy the condition

$$(\boldsymbol{v}_{j+1} - \boldsymbol{v}_j) \cdot \boldsymbol{f}^*_{j+\frac{1}{2}} = \psi_{j+1} - \psi_j$$

This is one equation for the three components of the flux and is clearly under-determined. There are many possible solutions and we discuss one of them.

Let $\boldsymbol{f}^* = [f^*_\rho, f^*_m, f^*_e]^\top$ and let us choose ρ, v, β as independent variables. For any two grid functions a, b we have the identity

$$[\![ab]\!]_{j+\frac{1}{2}} = a_{j+1}b_{j+1} - a_j b_j = \frac{a_j + a_{j+1}}{2}(b_{j+1} - b_j) + \frac{b_j + b_{j+1}}{2}(a_{j+1} - a_j)$$

To keep the notation concise, we will drop the subscripts

$$[\![ab]\!] = \{\!\{a\}\!\}[\![b]\!] + \{\!\{b\}\!\}[\![a]\!]$$

Using this relation, we can write

$$[\![\psi]\!] = [\![\rho v]\!] = \{\!\{\rho\}\!\}[\![v]\!] + \{\!\{v\}\!\}[\![\rho]\!]$$

Euler equation: Entropy conservative flux [6]

The jump in entropy variables is

$$\begin{aligned}
[\![v_1]\!] &= -\frac{[\![s]\!]}{\gamma - 1} - \{\!\{v^2\}\!\}[\![\beta]\!] - \{\!\{\beta\}\!\}[\![v^2]\!] \\
&= -\frac{[\![s]\!]}{\gamma - 1} - \{\!\{v^2\}\!\}[\![\beta]\!] - 2\{\!\{\beta\}\!\}\{\!\{v\}\!\}[\![v]\!] \\
[\![v_2]\!] &= 2\{\!\{\beta\}\!\}[\![v]\!] + 2\{\!\{v\}\!\}[\![\beta]\!] \\
[\![v_3]\!] &= -2[\![\beta]\!]
\end{aligned}$$

We try to write $[\![s]\!]$ in terms of jumps in ρ, β

$$\begin{aligned}
s &= \ln(p/\rho^\gamma) = -(\gamma - 1)\ln\rho - \ln\beta - \ln 2 \\
[\![s]\!] &= -(\gamma - 1)[\![\ln\rho]\!] - [\![\ln\beta]\!]
\end{aligned}$$

For a positive quantity, define the **logarithmic average**

$$\langle a \rangle = \frac{[\![a]\!]}{[\![\ln a]\!]}$$

Euler equation: Entropy conservative flux [6]

Then

$$[\![s]\!] = -(\gamma-1)\frac{[\![\rho]\!]}{\langle\rho\rangle} - \frac{[\![\beta]\!]}{\langle\beta\rangle}$$

and hence

$$[\![v_1]\!] = \frac{[\![\rho]\!]}{\langle\rho\rangle} + \left[\frac{1}{(\gamma-1)\langle\beta\rangle} - \{\!\{v^2\}\!\}\right][\![\beta]\!] - 2\{\!\{\beta\}\!\}\{\!\{v\}\!\}[\![v]\!]$$

The condition for entropy conservative flux is

$$[\![v_1]\!]f_\rho^* + [\![v_2]\!]f_m^* + [\![v_3]\!]f_e^* = [\![\rho v]\!]$$

Plugging in all the jump terms and collecting them together, we get

$$\begin{aligned} & \frac{f_\rho^*}{\langle\rho\rangle}[\![\rho]\!] + \left[-2\{\!\{\beta\}\!\}\{\!\{v\}\!\}f_\rho^* + 2\{\!\{\beta\}\!\}f_m^*\right][\![v]\!] \\ & + \left[\left(\frac{1}{(\gamma-1)\langle\beta\rangle} - \{\!\{v^2\}\!\}\right)f_\rho^* + 2\{\!\{v\}\!\}f_m^* - 2f_e^*\right][\![\beta]\!] \\ = \quad & \{\!\{v\}\!\}[\![\rho]\!] + \{\!\{\rho\}\!\}[\![v]\!] \end{aligned}$$

Euler equation: Entropy conservative flux [6]

This equation must hold for all possible left and right states. Take the states such that $[\![\rho]\!] \neq 0$, $[\![v]\!] = [\![\beta]\!] = 0$ which yields the mass flux

$$f_\rho^* = \langle \rho \rangle \{\!\{v\}\!\}$$

Similarly, the other fluxes are obtained as

$$f_m^* = \frac{\{\!\{\rho\}\!\}}{2\{\!\{\beta\}\!\}} + \{\!\{v\}\!\} f_\rho^*$$

and

$$f_e^* = \left[\frac{1}{2(\gamma-1)\langle \beta \rangle} - \frac{1}{2}\{\!\{v^2\}\!\} \right] f_\rho^* + \{\!\{v\}\!\} f_m^*$$

It is easy to check that these are consistent fluxes (Exercise).

For some more numerical fluxes, see [10], [11].

Kinetic energy consistency

Kinetic energy per unit volume

$$K = \frac{1}{2}\rho v^2$$

satisfies the following equation

$$\frac{\mathsf{d}}{\mathsf{d}t}\int_\Omega K \mathsf{d}x = \int_\Omega p \frac{\partial v}{\partial x} \mathsf{d}x - \frac{4}{3}\int_\Omega \mu \left(\frac{\partial v}{\partial x}\right)^2 \mathsf{d}x \le \int_\Omega p \frac{\partial v}{\partial x} \mathsf{d}x \tag{4}$$

Work done by pressure forces, absent in incompressible flows
Irreversible destruction due to molecular diffusion

Note: Convection contributes to only flux of KE across $\partial\Omega$. It does not change the total amount of KE inside the domain (except for boundary fluxes).

The correct KE budget is important for simulation of turbulence since the KE cascade from large scales to small scales is a very important characteristic of turbulent flows.

KE preserving FVM

$$\begin{aligned}
\frac{\partial K}{\partial t} &= -\frac{1}{2}v^2\frac{\partial \rho}{\partial t} + v\frac{\partial(\rho v)}{\partial t} \\
&= -\frac{\partial}{\partial x}(p + \rho v^2/2 - \frac{4}{3}\mu\frac{\partial v}{\partial x})v + p\frac{\partial v}{\partial x} - \frac{4}{3}\mu\left(\frac{\partial v}{\partial x}\right)^2
\end{aligned}$$

Centered numerical flux

$$\boldsymbol{f}_{j+\frac{1}{2}} = \begin{bmatrix} f^\rho \\ f^m \\ f^e \end{bmatrix}_{j+\frac{1}{2}} = \begin{bmatrix} f^\rho \\ \tilde{p} + \{\!\{v\}\!\} f^\rho \\ f^e \end{bmatrix}_{j+\frac{1}{2}}, \qquad g_{j+\frac{1}{2}} = \begin{bmatrix} 0 \\ \tau \\ \tilde{v}\tau - q \end{bmatrix}_{j+\frac{1}{2}}$$

where

$$\{\!\{v\}\!\}_{j+\frac{1}{2}} = \frac{1}{2}(v_j + v_{j+1}), \quad \tau_{j+\frac{1}{2}} = \frac{4}{3}\mu\frac{v_{j+1} - v_j}{\Delta x}, \quad q_{j+\frac{1}{2}} = -\kappa\frac{T_{j+1} - T_j}{\Delta x}$$

KE preserving FVM

Discrete KE equation

$$\sum_j \Delta x \frac{\mathsf{d}K_j}{\mathsf{d}t} = \sum_j \left[\frac{\Delta v_{j+\frac{1}{2}}}{\Delta x} \tilde{p}_{j+\frac{1}{2}} - \frac{4}{3}\mu \left(\frac{\Delta v_{j+\frac{1}{2}}}{\Delta x} \right)^2 \right] \Delta x$$

This is consistent with (4) and hence we refer to such a scheme as being KE consistent.

Jameson's KEP flux

$$\boldsymbol{f}_{j+\frac{1}{2}} = \begin{bmatrix} \{\!\{\rho\}\!\} \ \{\!\{u\}\!\} \\ \{\!\{p\}\!\} + \{\!\{v\}\!\} f^\rho \\ \{\!\{H\}\!\} f^\rho \end{bmatrix}_{j+\frac{1}{2}}, \qquad \text{compare with} \quad \boldsymbol{f}_{j+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1})$$

We are free to choose $\tilde{p}$ and the mass and energy fluxes in other ways. The entropy conservative flux also satisfies the KE consistency, since the momentum flux is of the correct form.

Euler equation: Rusanov-type dissipation

The Rusanov flux is given by

$$\boldsymbol{f}_{j+\frac{1}{2}}^{Rus} = \frac{1}{2}(\boldsymbol{f}_j + \boldsymbol{f}_{j+1}) - \frac{1}{2}\lambda_m [\![\boldsymbol{u}]\!]_{j+\frac{1}{2}}$$

Derigs et al. [4] derive the exact relation

$$[\![\boldsymbol{u}]\!] = \mathcal{H}[\![\boldsymbol{v}]\!], \qquad \mathcal{H} = \begin{bmatrix} \langle\rho\rangle & \langle\rho\rangle\{\!\{v\}\!\} & \tilde{E} \\ \langle\rho\rangle\{\!\{v\}\!\} & \langle\rho\rangle\{\!\{v\}\!\}^2 + \tilde{p} & (\tilde{E}+\tilde{p})\{\!\{v\}\!\} \\ \tilde{E} & (\tilde{E}+\tilde{p})\{\!\{v\}\!\} & \frac{1}{\langle\rho\rangle}\left[\frac{\hat{p}^2}{\gamma-1} + \tilde{E}^2\right] + \tilde{p}\{\!\{v\}\!\}^2 \end{bmatrix}$$

$$\tilde{p} = \frac{\{\!\{\rho\}\!\}}{2\{\!\{\beta\}\!\}}, \quad \hat{p} = \frac{\langle\rho\rangle}{2\langle\beta\rangle}, \quad \tilde{E} = \frac{\hat{p}}{\gamma-1} + \frac{1}{2}\langle\rho\rangle\{\!\{v^2\}\!\}$$

The matrix $\mathcal{H}$ is obviously symmetric and can also be shown to be positive definite. Then the entropy consistent flux can be taken as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2}\lambda_m \mathcal{H}_{j+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

Euler equation: Roe-type dissipation

The Jacobian matrix is

$$\boldsymbol{u}'(\boldsymbol{v}) = \begin{bmatrix} \rho & \rho v & E \\ \rho v & p + \rho v^2 & \rho H v \\ E & \rho H v & \frac{\gamma p E}{(\gamma-1)\rho} + \frac{1}{4}\rho v^4 \end{bmatrix}, \qquad H = h + \frac{1}{2}v^2 = (\rho e + p)/\rho$$

The eigenvectors are usually written as

$$R = \begin{bmatrix} 1 & 1 & 1 \\ v - a & v & v + a \\ H - va & \frac{1}{2}v^2 & H + va \end{bmatrix}, \qquad a^2 = \frac{\gamma p}{\rho}$$

But this does not satisfy the condition $RR^\top = \boldsymbol{u}'(\boldsymbol{v})$. Define the diagonal matrix

$$S = \operatorname{diag}\left[\frac{\rho}{2\gamma}, \frac{(\gamma-1)\rho}{\gamma}, \frac{\rho}{2\gamma}\right]$$

and the scaled eigenvector matrix

$$\tilde{R} = RS^{\frac{1}{2}}$$

Euler equation: Roe-type dissipation

Then we can check that $\tilde{R}\tilde{R}^\top = \boldsymbol{u}'(\boldsymbol{v})$, so that the dissipation in Roe flux can be written as

$$[\![\boldsymbol{u}]\!] \approx \tilde{R}\tilde{R}^\top [\![\boldsymbol{v}]\!], \quad -\frac{1}{2}\tilde{R}|\Lambda|\tilde{R}^{-1}[\![\boldsymbol{u}]\!] \approx -\frac{1}{2}\tilde{R}|\Lambda|\tilde{R}^{-1}\tilde{R}\tilde{R}^\top [\![\boldsymbol{v}]\!] = -\frac{1}{2}\tilde{R}|\Lambda|\tilde{R}^\top [\![\boldsymbol{v}]\!]$$

and hence the entropy consistent flux can be taken as

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2}\tilde{R}_{j+\frac{1}{2}}|\Lambda_{j+\frac{1}{2}}|\tilde{R}^\top_{j+\frac{1}{2}}[\![\boldsymbol{v}]\!]_{j+\frac{1}{2}}$$

The dissipation matrix

$$D_{j+\frac{1}{2}} = \tilde{R}_{j+\frac{1}{2}}|\Lambda_{j+\frac{1}{2}}|\tilde{R}^\top_{j+\frac{1}{2}}$$

is symmetric and positive definite.

Entropy stable DG scheme

Divide the domain into disjoint cells $I_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$ and inside each cell, we approximate the solution by a polynomial

$$\boldsymbol{v}_h(x) = \text{polynomial of degree } k \text{ for } x \in I_j$$

and $\boldsymbol{v}_h(x)$ may be discontinuous at the cell faces $x_{j+\frac{1}{2}}$. Note that we **expand the entropy variable in terms of polynomials**. The semi-discrete DG scheme is

$$\int_{I_j} \boldsymbol{\phi}_h \cdot \partial_t \boldsymbol{u}(\boldsymbol{v}_h) \mathrm{d}x - \int_{I_j} \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{v}_h)) \cdot \partial_x \boldsymbol{\phi}_h \mathrm{d}x + \boldsymbol{f}_{j+\frac{1}{2}} \cdot \boldsymbol{\phi}_h(x_{j+\frac{1}{2}}^-) - \boldsymbol{f}_{j-\frac{1}{2}} \cdot \boldsymbol{\phi}_h(x_{j-\frac{1}{2}}^+) = 0$$

where the test functions $\boldsymbol{\phi}_h$ are also piecewise polynomials of degree k. The numerical flux is given by

$$\boldsymbol{f}_{j+\frac{1}{2}} = \boldsymbol{f}^*_{j+\frac{1}{2}} - \frac{1}{2} D_{j+\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}}, \qquad [\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}} = \boldsymbol{v}_h(x_{j+\frac{1}{2}}^+) - \boldsymbol{v}_h(x_{j+\frac{1}{2}}^-)$$

Let us take $\boldsymbol{\phi}_h = \boldsymbol{v}_h$ in the DG scheme.

$$\int_{I_j} \boldsymbol{v}_h \cdot \partial_t \boldsymbol{u}(\boldsymbol{v}_h) \mathrm{d}x - \int_{I_j} \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{v}_h)) \cdot \partial_x \boldsymbol{v}_h \mathrm{d}x + \boldsymbol{f}_{j+\frac{1}{2}} \cdot \boldsymbol{v}_h(x_{j+\frac{1}{2}}^-) - \boldsymbol{f}_{j-\frac{1}{2}} \cdot \boldsymbol{v}_h(x_{j-\frac{1}{2}}^+) = 0$$

Entropy stable DG scheme

Since $\boldsymbol{v}_h = U'(\boldsymbol{u}(\boldsymbol{v}_h))$

$$\int_{I_j} \boldsymbol{v}_h \cdot \partial_t \boldsymbol{u}(\boldsymbol{v}_h) \mathrm{d}x = \int_{I_j} \partial_t U(\boldsymbol{u}(\boldsymbol{v}_h)) \mathrm{d}x$$

The integrand in the second term can be written as

$$\begin{aligned} \boldsymbol{f} \cdot \partial_x \boldsymbol{v} &= \partial_x(\boldsymbol{f} \cdot \boldsymbol{v}) - \boldsymbol{v} \cdot \partial_x \boldsymbol{f} \\ &= \partial_x(\boldsymbol{f} \cdot \boldsymbol{v}) - U'(\boldsymbol{u}) \boldsymbol{f}'(\boldsymbol{u}) \partial_x \boldsymbol{u} \\ &= \partial_x(\boldsymbol{f} \cdot \boldsymbol{v}) - F'(\boldsymbol{u}) \partial_x \boldsymbol{u} \\ &= \partial_x(\boldsymbol{f} \cdot \boldsymbol{v}) - \partial_x F \\ &= \partial_x(\boldsymbol{f} \cdot \boldsymbol{v} - F) \\ &= \partial_x \psi \end{aligned}$$

Hence the second term becomes

$$-\int_{I_j} \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{v}_h)) \cdot \partial_x \boldsymbol{v}_h \mathrm{d}x = \psi(\boldsymbol{v}_h(x_{j-\frac{1}{2}}^+)) - \psi(\boldsymbol{v}_h(x_{j+\frac{1}{2}}^-))$$

Entropy stable DG scheme

The boundary flux terms can be written as

$$\boldsymbol{f}_{j+\frac{1}{2}} \cdot \boldsymbol{v}_h(x_{j+\frac{1}{2}}^-) = \{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}} - \frac{1}{2}[\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}}$$

where

$$\{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} = \frac{1}{2}[\boldsymbol{v}_h(x_{j+\frac{1}{2}}^-) + \boldsymbol{v}_h(x_{j+\frac{1}{2}}^+)]$$

Using the definition of the numerical flux

$$\begin{aligned}
\boldsymbol{f}_{j+\frac{1}{2}} \cdot \boldsymbol{v}_h(x_{j+\frac{1}{2}}^-) \quad &= \quad \{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}} - \frac{1}{2}[\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}} \cdot \boldsymbol{f}^*_{j+\frac{1}{2}} \\
&\quad\quad + \frac{1}{4}[\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}}^\top D_{j+\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}} \\
&= \quad \{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}} - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j+\frac{1}{2}}^+)) + \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j+\frac{1}{2}}^-)) \\
&\quad\quad + \frac{1}{4}[\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}}^\top D_{j+\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}}
\end{aligned}$$

Entropy stable DG scheme

Similarly

$$\begin{aligned}
\boldsymbol{f}_{j-\frac{1}{2}} \cdot \boldsymbol{v}_h(x_{j-\frac{1}{2}}^-) &= \{\!\{\boldsymbol{v}_h\}\!\}_{j-\frac{1}{2}} \cdot \boldsymbol{f}_{j-\frac{1}{2}} + \frac{1}{2}[\![\boldsymbol{v}_h]\!]_{j-\frac{1}{2}} \cdot \boldsymbol{f}_{j-\frac{1}{2}} \\
&= \{\!\{\boldsymbol{v}_h\}\!\}_{j-\frac{1}{2}} \cdot \boldsymbol{f}_{j-\frac{1}{2}} + \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j-\frac{1}{2}}^+)) - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j-\frac{1}{2}}^-)) \\
&\quad -\frac{1}{4}[\![\boldsymbol{v}_h]\!]_{j-\frac{1}{2}}^\top D_{j-\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j-\frac{1}{2}}
\end{aligned}$$

Adding all terms we get

$$\begin{aligned}
\int_{I_j} \partial_t U(\boldsymbol{v}_h) \mathrm{d}x &+ \left[\{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}} - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j+\frac{1}{2}}^+)) - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j+\frac{1}{2}}^-))\right] \\
&- \left[\{\!\{\boldsymbol{v}_h\}\!\}_{j-\frac{1}{2}} \cdot \boldsymbol{f}_{j-\frac{1}{2}} - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j-\frac{1}{2}}^+)) - \frac{1}{2}\psi(\boldsymbol{v}_h(x_{j-\frac{1}{2}}^-))\right] \\
&= -\frac{1}{4}[\![\boldsymbol{v}_h]\!]_{j-\frac{1}{2}}^\top D_{j-\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j-\frac{1}{2}} - \frac{1}{4}[\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}}^\top D_{j+\frac{1}{2}} [\![\boldsymbol{v}_h]\!]_{j+\frac{1}{2}} \\
&\leq 0
\end{aligned}$$

Entropy stable DG scheme

Defining the numerical entropy flux

$$F_{j+\frac{1}{2}} = \{\!\{\boldsymbol{v}_h\}\!\}_{j+\frac{1}{2}} \cdot \boldsymbol{f}_{j+\frac{1}{2}} - \{\!\{\psi(\boldsymbol{v}_h)\}\!\}_{j+\frac{1}{2}}$$

we get the **cell entropy inequality**

$$\frac{\mathsf{d}}{\mathsf{d}t} \int_{I_j} U(\boldsymbol{v}_h)\mathsf{d}x + F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} \leq 0$$

Remark: We have shown entropy stability of DG scheme of arbitrary order of accuracy.

Remark: We use integration by parts to prove the entropy stability. In practice we use quadrature to approximate the integrals but due to non-linearity, the quadratures are not exact. This inexact integration spoils the entropy stabililty property, which can lead to inaccurate solutions on coarse meshes.

DG scheme with SBP property

The goal is to construct a DG scheme which satisfies the entropy condition even if the numerical integration is not exact. The two main ingredients are

1. **summation by parts** or **SBP** property
2. the use of entropy conservative/consistent fluxes

For more details see [12], [13], [14], [15].

The DG scheme is based on nodal Lagrange basis functions. So we map each cell I_i to the reference cell $I = [-1, +1]$. We choose $k + 1$ Gauss-Lobatto-Legendre (GLL) quadrature nodes

$$-1 = \xi_0 < \xi_1 < \ldots < \xi_k = 1$$

Define the Lagrange basis polynomials each of degree k

$$L_j(\xi) = \prod_{l=0, l\neq j}^{k} \frac{\xi - \xi_l}{\xi_j - \xi_l}, \qquad L_j(\xi_l) = \delta_{jl}$$

DG scheme with SBP property

Define the continuous and discrete inner products

$$(u, v) := \int_I uv \mathsf{d}\xi, \qquad (u, v)_h := \sum_{j=0}^{k} \omega_j u(\xi_j) v(\xi_j)$$

Recall that this GLL quadrature is exact for polynomials of degree upto $2k - 1$.

We want to approximate the first derivative of a grid function at the GLL nodes. The interpolation is given by

$$u_h(\xi) = \sum_{l=0}^{k} L_l(\xi) u_l$$

We differentiate the interpolant and evaluate at GLL nodes

$$u_h'(\xi_j) = \sum_{l=0}^{k} L_l'(\xi_j) u_l = \sum_{l=0}^{k} D_{jl} u_l, \quad 0 \le j \le k$$

DG scheme with SBP property

where we defined the differentiation matrix

$$D_{jl} = L_l'(\xi_j), \qquad 0 \le j, l \le k$$

Define the **mass** and **stiffness** matrices

$$M_{jl} = (L_j, L_l)_h \neq (L_j, L_l), \qquad S_{jl} = (L_j, L_l')_h = (L_j, L_l')$$

The mass matrix is approximate and diagonal,

$$M_{jl} = \sum_{r=0}^{k} \omega_r L_j(\xi_r) L_l(\xi_r) = \sum_{r=0}^{k} \omega_r \delta_{jr} \delta_{lr} = \omega_j \delta_{jl}$$

$$M = \mathrm{diag}\{\omega_0, \omega_1, \ldots, \omega_k\}$$

also known as **lumped mass matrix**, while the stiffness matrix is exact.

Theorem (SBP property)

Define

$$B = \mathrm{diag}\{-1, 0, \ldots, +1\}$$

Then

$$S = MD, \qquad MD + D^\top M = S + S^\top = B$$

which is a discrete analogue of integration by parts.

Proof: By definition

$$\begin{aligned}
S_{jl} &= (L_j, L_l')_h \\
&= \sum_{r=0}^{k} \omega_r L_j(\xi_r) L_l'(\xi_r) = \sum_{r=0}^{k} \omega_r \delta_{jr} L_l'(\xi_r) \\
&= \omega_j L_l'(\xi_j) = M_{jj} D_{jl} \\
&= \sum_{r=0}^{k} M_{jr} D_{rl} \quad \Longrightarrow \quad S = MD
\end{aligned}$$

Next

$$
\begin{aligned}
S_{jl} + S_{lj} &= (L_j, L_l') + \big(L_l, L_j'\big) \\
&= \int_{-1}^{1} (L_j L_l' + L_l L_j') \mathsf{d}\xi \\
&= \int_{-1}^{1} \frac{\mathsf{d}}{\mathsf{d}\xi}(L_j L_l) \mathsf{d}\xi \\
&= L_j(1) L_l(1) - L_j(-1) L_l(-1) \\
&= L_j(\xi_k) L_l(\xi_k) - L_j(\xi_0) L_l(\xi_0) \\
&= \delta_{jk}\delta_{lk} - \delta_{j0}\delta_{l0} \\
&= B_{jl}
\end{aligned}
$$

and hence $S + S^{\top} = B$ is proved. $\square$

Theorem

For each $j = 0, 1, \ldots, k$, we have

$$\sum_{l=0}^{k} D_{jl} = \sum_{l=0}^{k} S_{jl} = 0, \qquad \sum_{l=0}^{k} S_{lj} = \tau_j = \begin{cases} -1 & j = 0 \\ 0 & 1 \leq j \leq k-1 \\ +1 & j = k \end{cases}$$

Note: $B = \mathrm{diag}(\tau_0, \tau_1, \ldots, \tau_k)$

Proof: (1) The Lagrange polynomials form a partition of unity

$$\sum_{l=0}^{k} L_l(\xi) = 1 \qquad \forall \xi$$

Hence

$$\sum_{l=0}^{k} D_{jl} = \sum_{l=0}^{k} L_l'(\xi_j) = 0$$

(2) Next, using previous Theorem and result from (1)

$$\sum_{l=0}^{k} S_{jl} = \omega_j \sum_{l=0}^{k} D_{jl} = 0$$

(3) Finally, using $S^\top = B - S$

$$\sum_{l=0}^{k} S_{lj} = \sum_{l=0}^{k} B_{jl} - \sum_{l=0}^{k} S_{jl} = \sum_{l=0}^{k} B_{jl} = B_{jj} = \tau_j$$

Semi-discrete DG scheme: Scalar case

Find $u_h = \sum_{l=0}^{k} u_l^i L_l(\xi)$ such that for all test functions ϕ_h of degree k

$$\int_{I_i} \frac{\partial u_h}{\partial t} \phi_h \mathsf{d}x - \int_{I_i} f(u_h) \frac{\partial \phi_h}{\partial x} \mathsf{d}x + f_{i+\frac{1}{2}} \phi_h(x_{i+\frac{1}{2}}^-) - f_{i-\frac{1}{2}} \phi_h(x_{i-\frac{1}{2}}^+) = 0$$

The boundary flux is given by some numerical flux formula

$$f_{i+\frac{1}{2}} = f(u_h(x_{i+\frac{1}{2}}^-), u_h(x_{i+\frac{1}{2}}^+)) = f(u_k^i, u_0^{i+1})$$

and couples the solution in the two cells i and $i+1$.

We map to reference cell $I = [-1, +1]$

$$x = x_i(\xi) = \frac{1}{2}(x_{i-\frac{1}{2}} + x_{i+\frac{1}{2}}) + \frac{1}{2}\xi \Delta x_i$$

The DG scheme becomes

$$\frac{\Delta x_i}{2} \int_I \frac{\partial u_h}{\partial t} \phi_h \mathsf{d}\xi - \int_I f(u_h) \frac{\partial \phi_h}{\partial \xi} \mathsf{d}\xi + f_{i+\frac{1}{2}} \phi_h(1) - f_{i-\frac{1}{2}} \phi_h(-1) = 0$$

Semi-discrete DG scheme: Scalar case

We will approximate the integrals by GLL quadrature, and also approximate the flux

$$f(u_h) \approx f_h(\xi) := \sum_{j=0}^{k} f(u_j^i) L_j(\xi) = \sum_{j=0}^{k} f_j^i L_j(\xi)$$

Taking the test functions $\phi_h = L_j$

$$\frac{\Delta x_i}{2} \frac{\mathrm{d}}{\mathrm{d}t} (u_h, L_j)_h - \left(f_h, L_j'\right)_h + f_{i+\frac{1}{2}} L_j(1) - f_{i-\frac{1}{2}} L_j(-1) = 0$$

$$\frac{\Delta x_i}{2} \sum_{l=0}^{k} \frac{\mathrm{d}u_l^i}{\mathrm{d}t} (L_j, L_l)_h - \sum_{l=0}^{k} f_l^i \left(L_l, L_j'\right)_h + f_{i+\frac{1}{2}} \delta_{jk} - f_{i-\frac{1}{2}} \delta_{j0} = 0$$

Define

$$u^i = \begin{bmatrix} u_0^i \\ u_1^i \\ \vdots \\ u_{k-1}^i \\ u_k^i \end{bmatrix}, \quad f^i = \begin{bmatrix} f_0^i \\ f_1^i \\ \vdots \\ f_{k-1}^i \\ f_k^i \end{bmatrix}, \quad \hat{f}^i = \begin{bmatrix} f_{i-\frac{1}{2}} \\ 0 \\ \vdots \\ 0 \\ f_{i+\frac{1}{2}} \end{bmatrix}$$

Semi-discrete DG scheme: Scalar case

Then we can write the DG scheme as

$$\frac{\Delta x_i}{2} M \frac{\mathsf{d}u^i}{\mathsf{d}t} - S^\top f^i = -B\hat{f}^i$$

Using $S^\top = B - S$, we rewrite this as

$$\frac{\Delta x_i}{2} M \frac{\mathsf{d}u^i}{\mathsf{d}t} + S f^i = B(f^i - \hat{f}^i)$$

or using $S = MD$

$$\frac{\Delta x_i}{2} \frac{\mathsf{d}u^i}{\mathsf{d}t} + D f^i = M^{-1} B(f^i - \hat{f}^i)$$

Note that

$$\frac{2}{\Delta x_i}(Df^i)_j = \frac{\partial f}{\partial x}(x_j) + O(\Delta x)^k$$

The last equation shows that we have a collocation method, i.e., we are collocating the PDE at the GLL nodes, together with a penalty term for the end nodes.

Semi-discrete DG scheme: System case

We skip the detailed derivation in system case and directly give the equations. Consider a system of p equations and define the matrices and vectors

$$\boldsymbol{M} = M \otimes I_p, \quad \boldsymbol{D} = D \otimes I_p, \quad \boldsymbol{S} = S \otimes I_p, \quad \boldsymbol{B} = B \otimes I_p$$

$$\boldsymbol{u}^i = \begin{bmatrix} \boldsymbol{u}_0^i \\ \boldsymbol{u}_1^i \\ \vdots \\ \boldsymbol{u}_k^i \end{bmatrix}, \quad \boldsymbol{f}^i = \begin{bmatrix} \boldsymbol{f}_0^i \\ \boldsymbol{f}_1^i \\ \vdots \\ \boldsymbol{f}_k^i \end{bmatrix}, \quad \hat{\boldsymbol{f}}^i = \begin{bmatrix} \boldsymbol{f}_{i-\frac{1}{2}} \\ 0 \\ \vdots \\ 0 \\ \boldsymbol{f}_{i+\frac{1}{2}} \end{bmatrix}$$

Then the semi-discrete scheme can be written as

$$\frac{\Delta x_i}{2} \boldsymbol{M} \frac{\mathsf{d}\boldsymbol{u}^i}{\mathsf{d}t} - \boldsymbol{S}^\top \boldsymbol{f}^i = -\boldsymbol{B} \hat{\boldsymbol{f}}^i$$

$$\frac{\Delta x_i}{2} \frac{\mathsf{d}\boldsymbol{u}^i}{\mathsf{d}t} + \boldsymbol{D} \boldsymbol{f}^i = \boldsymbol{M}^{-1} \boldsymbol{B} (\boldsymbol{f}^i - \hat{\boldsymbol{f}}^i)$$

Entropy conservative scheme

We consider a single element, so we will omit the superscript i. The collocation scheme can be written as

$$\frac{\Delta x_i}{2}\frac{\mathrm{d}\boldsymbol{u}_j}{\mathrm{d}t} + \sum_{l=0}^{k} D_{jl}\boldsymbol{f}(\boldsymbol{u}_l) = \frac{\tau_j}{\omega_j}(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j)$$

We modify this scheme by introducing a **symmetric** flux $\boldsymbol{f}^*$ in the interior and boundary terms

$$\frac{\Delta x_i}{2}\frac{\mathrm{d}\boldsymbol{u}_j}{\mathrm{d}t} + 2\sum_{l=0}^{k} D_{jl}\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l) = \frac{\tau_j}{\omega_j}(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) \tag{5}$$

E.g., if $\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l) = \frac{1}{2}(\boldsymbol{f}(\boldsymbol{u}_j) + \boldsymbol{f}(\boldsymbol{u}_l))$, we get

$$2\sum_{l=0}^{k} D_{jl}\boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l) = \sum_{l=0}^{k} D_{jl}\boldsymbol{f}(\boldsymbol{u}_j) + \sum_{l=0}^{k} D_{jl}\boldsymbol{f}(\boldsymbol{u}_l) = \sum_{l=0}^{k} D_{jl}\boldsymbol{f}(\boldsymbol{u}_l)$$

Theorem (Entropy conservative scheme)

If $\boldsymbol{f}^*$ is consistent and symmetric, then (5) is conservative and high order accurate. If $\boldsymbol{f}^*$ is entropy conservative, then (5) is also entropy conservative.

<u>Proof</u>: (1) Conservation property: The mean value changes as

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=0}^{k}\frac{\Delta x}{2}\omega_j \boldsymbol{u}_j &= \sum_{j=0}^{k}\tau_j(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) - 2\sum_{j=0}^{k}\sum_{l=0}^{k} S_{jl}\boldsymbol{f}^*(\boldsymbol{u}_j,\boldsymbol{u}_l) \\
&= \sum_{j=0}^{k}\tau_j(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) - \sum_{j=0}^{k}\sum_{l=0}^{k}(S_{jl}+S_{lj})\boldsymbol{f}^*(\boldsymbol{u}_j,\boldsymbol{u}_l) \\
&= \sum_{j=0}^{k}\tau_j(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) - \sum_{j=0}^{k}\sum_{l=0}^{k} B_{jl}\boldsymbol{f}^*(\boldsymbol{u}_j,\boldsymbol{u}_l) \\
&= \sum_{j=0}^{k}\tau_j(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) - \sum_{j=0}^{k}\tau_j\boldsymbol{f}(\boldsymbol{u}_j) \\
&= -(\boldsymbol{f}_{i+\frac{1}{2}}^* - \boldsymbol{f}_{i-\frac{1}{2}}^*)
\end{aligned}
$$

The mean value in the cell changes only due to boundary fluxes.

(2) Accuracy property: Define

$$\boldsymbol{f}^*(x,y) = \boldsymbol{f}^*(\boldsymbol{u}(x), \boldsymbol{u}(y)), \qquad \boldsymbol{f}(x) = \boldsymbol{f}(\boldsymbol{u}(x))$$

Then $\boldsymbol{f}^*(x,y)$ is also symmetric and consistent

$$\boldsymbol{f}^*(x,y) = \boldsymbol{f}^*(y,x), \qquad \boldsymbol{f}^*(x,x) = \boldsymbol{f}(x)$$

Hence

$$\frac{\partial \boldsymbol{f}}{\partial x}(x) = \frac{\partial \boldsymbol{f}^*}{\partial x}(x,x) + \frac{\partial \boldsymbol{f}^*}{\partial y}(x,x) = 2\frac{\partial \boldsymbol{f}^*}{\partial y}(x,x)$$

The difference matrix D is exact for polynomials of degree upto k

$$\frac{4}{\Delta x}\sum_{l=0}^{k} D_{jl}\boldsymbol{f}^*(x(\xi_j), x(\xi_l)) = 2\frac{\partial \boldsymbol{f}}{\partial y}(x(\xi_j), x(\xi_j)) + O(\Delta x^k) = \frac{\partial \boldsymbol{f}}{\partial x}(x(\xi_j)) + O(\Delta x^k)$$

Hence the scheme has high order of accuracy.

(3) Entropy conservation: We compute the rate of change of total entropy in cell

$$
\begin{aligned}
\frac{\mathsf{d}}{\mathsf{d}t}\sum_{j=0}^{k}\frac{\Delta x}{2}\omega_j U_j &= \sum_{j=0}^{k}\frac{\Delta x}{2}\omega_j \boldsymbol{v}_j^\top \frac{\mathsf{d}\boldsymbol{u}_j}{\mathsf{d}t} \\
&= \sum_{j=0}^{k}\tau_j \boldsymbol{v}_j^\top(\boldsymbol{f}_j - \hat{\boldsymbol{f}}_j^*) - 2\sum_{j=0}^{k}\sum_{l=0}^{k} S_{jl}\boldsymbol{v}_j^\top \boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l)
\end{aligned}
$$

The second term can be written as

$$
\begin{aligned}
& \sum_{j=0}^{k}\sum_{l=0}^{k}(B_{jl} + S_{jl} - S_{lj})\boldsymbol{v}_j^\top \boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l) \\
=\ & \sum_{j=0}^{k}\tau_j \boldsymbol{v}_j^\top \boldsymbol{f}_j + \sum_{j=0}^{k}\sum_{l=0}^{k} S_{jl}(\boldsymbol{v}_j - \boldsymbol{v}_l)^\top \boldsymbol{f}^*(\boldsymbol{u}_j, \boldsymbol{u}_l) \\
=\ & \sum_{j=0}^{k}\tau_j \boldsymbol{v}_j^\top \boldsymbol{f}_j + \sum_{j=0}^{k}\sum_{l=0}^{k} S_{jl}(\psi_j - \psi_l) \\
=\ & \sum_{j=0}^{k}\tau_j(\boldsymbol{v}_j^\top \boldsymbol{f}_j - \psi_j)
\end{aligned}
$$

Then

$$\frac{\mathsf{d}}{\mathsf{d}t}\sum_{j=0}^{k}\frac{\Delta x}{2}\omega_j U_j = \sum_{j=0}^{k}\tau_j(\psi_j - \boldsymbol{v}_j^\top \hat{\boldsymbol{f}}_j^*) = (\psi_k - \boldsymbol{v}_k^\top \boldsymbol{f}_{i+\frac{1}{2}}^*) - (\psi_0 - \boldsymbol{v}_0^\top \boldsymbol{f}_{i-\frac{1}{2}}^*)$$

All quantities on right are from element i, so the rhs is

$$(\psi_k^i - (\boldsymbol{v}_k^i)^\top \boldsymbol{f}_{i+\frac{1}{2}}^*) - (\psi_0^i - (\boldsymbol{v}_0^i)^\top \boldsymbol{f}_{i-\frac{1}{2}}^*)$$

We can rewrite

$$\psi_k^i = \frac{1}{2}\psi_k^i + \frac{1}{2}\psi_k^i + \frac{1}{2}\psi_0^{i+1} - \frac{1}{2}\psi_0^{i+1} = \{\!\{\psi\}\!\}_{i+\frac{1}{2}} - \frac{1}{2}[\![\psi]\!]_{i+\frac{1}{2}}$$

$$\boldsymbol{v}_k^i = \{\!\{\boldsymbol{v}\}\!\}_{i+\frac{1}{2}} - \frac{1}{2}[\![\boldsymbol{v}]\!]_{i+\frac{1}{2}}$$

Hence

$$\begin{aligned}
\psi_k^i - (\boldsymbol{v}_k^i)^\top \boldsymbol{f}_{i+\frac{1}{2}}^* &= \{\!\{\psi\}\!\}_{i+\frac{1}{2}} - \frac{1}{2}[\![\psi]\!]_{i+\frac{1}{2}} - \{\!\{\boldsymbol{v}\}\!\}_{i+\frac{1}{2}}^\top \boldsymbol{f}_{i+\frac{1}{2}}^* + \frac{1}{2}[\![\boldsymbol{v}]\!]_{i+\frac{1}{2}}^\top \boldsymbol{f}_{i+\frac{1}{2}}^* \\
&= \{\!\{\psi\}\!\}_{i+\frac{1}{2}} - \{\!\{\boldsymbol{v}\}\!\}_{i+\frac{1}{2}}^\top \boldsymbol{f}_{i+\frac{1}{2}}^* =: -F_{i+\frac{1}{2}}^*
\end{aligned}$$

so that we have entropy equation

$$\frac{\mathsf{d}}{\mathsf{d}t}\sum_{j=0}^{k}\frac{\Delta x}{2}\omega_j U_j + (F^*_{i+\frac{1}{2}} - F^*_{i-\frac{1}{2}}) = 0$$

Entropy consistent scheme

Now we take a numerical flux that satisfies

$$[\![\boldsymbol{v}]\!]_{i+\frac{1}{2}} \cdot \boldsymbol{f}_{i+\frac{1}{2}} \leq [\![\psi]\!]_{i+\frac{1}{2}}$$

An example of such a flux is

$$\boldsymbol{f}_{i+\frac{1}{2}} = \boldsymbol{f}^*_{i+\frac{1}{2}} - \frac{1}{2} D_{i+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{i+\frac{1}{2}}, \qquad D_{i+\frac{1}{2}} = D^\top_{i+\frac{1}{2}} \geq 0$$

From the previous theorem, we have seen we get only some boundary terms which can be can written as

$$\psi^i_k - (\boldsymbol{v}^i_k)^\top \boldsymbol{f}_{i+\frac{1}{2}} = \underbrace{\{\!\{\psi\}\!\}_{i+\frac{1}{2}} - \{\!\{\boldsymbol{v}\}\!\}^\top_{i+\frac{1}{2}} \boldsymbol{f}_{i+\frac{1}{2}}}_{-F_{i+\frac{1}{2}}} - \frac{1}{4} [\![\boldsymbol{v}]\!]^\top_{i+\frac{1}{2}} D_{i+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{i+\frac{1}{2}}$$

so that we get the entropy inequality

$$\begin{aligned} \frac{\mathsf{d}}{\mathsf{d}t} \sum_{j=0}^{k} \frac{\Delta x}{2} \omega_j U_j + (F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}) &= -\frac{1}{4} [\![\boldsymbol{v}]\!]^\top_{i-\frac{1}{2}} D_{i-\frac{1}{2}} [\![\boldsymbol{v}]\!]_{i-\frac{1}{2}} - \frac{1}{4} [\![\boldsymbol{v}]\!]^\top_{i+\frac{1}{2}} D_{i+\frac{1}{2}} [\![\boldsymbol{v}]\!]_{i+\frac{1}{2}} \\ &\leq 0 \end{aligned}$$

Summary

Entropy stability concept allows to construct non-linearly stable schemes.

Semi-discrete entropy stable finite volume and DG schemes of arbitrary high order of accuracy can be constructed.

The entropy conservative schemes are non-dissipative, and hence useful for compressible flow LES and DNS.

Kinetic energy consistent schemes [16] have been shown to be useful for low Mach LES [17].

Entropy stable schemes have also been constructed for MHD, see [18], [19], [15]

For recent review, see Chapters 18 and 19 in [20]

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