Numerical approximation for fluids: Finite volume methods

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Conservation laws and numerical approximation

1. Fluid equations
2. Solutions of scalar conservation laws
3. Numerical approximation of scalar conservation laws

I. Fluid equations

Main variables:

- $\rho(t, \mathbf{x})$, density field,
- $\mathbf{u}(t, \mathbf{x})$, velocity field.
- $p(t, \mathbf{x})$, pressure field.
- $T(t, \mathbf{x})$, temperature field.
- $E(t, \mathbf{x})$, total energy field.

The continuity equation establishes the mass conservation,

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{1}$$

The conservation of momentum provides

$$\rho(\partial_t \mathbf{u} + \mathbf{u}\nabla\mathbf{u}) + \nabla p - \nabla \cdot \sigma = 0. \tag{2}$$

which is equivalent to the *momentum equation*

$$\partial_t(\rho\mathbf{u}) + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) + \nabla \cdot (pI - \sigma) = 0, \tag{3}$$

For Newtonian flows σ is assumed to be

$$\sigma = \mu \left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right) + (\xi - \frac{2}{3}\mu)I\nabla \cdot u, \tag{4}$$

where μ and ξ are the first and second viscosities of the fluid. For inviscid flows, $\mu = \xi = 0$,

$$\partial_t(\rho\mathbf{u}) + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) + \nabla p = 0. \tag{5}$$

Finally, we establish the conservation of energy,

$$\partial_t(\rho E) + \nabla \cdot (\rho\mathbf{u}H) = \mathbf{f} \cdot \mathbf{u}, \tag{6}$$

where H is the stagnation enthalpy,

$$H = E + \frac{p}{\rho}. \tag{7}$$

The system of equations is closed with the *equation of state* that can be written as

$$e = \frac{p}{\rho(\gamma - 1)}, \tag{8}$$

where γ is a physical constant and e is the internal energy. The energy E and the internal energy e are related by

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

Euler system for compressible flows in 2-D.

In the two dimensional case without external forces, if we write $\mathbf{u} = (u, v)$ and $\mathbf{x} = (x, y)$, the Euler system for compressible flows can be written as

$$\partial_t U + \nabla \cdot F = \partial_t U + \partial_x F_x + \partial_y F_y = 0, \text{ in } \Omega \tag{9}$$

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}, \qquad F_x = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{pmatrix}, \quad F_y = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v H \end{pmatrix} \tag{10}$$

where

$$p = (\gamma - 1)\rho \left(E - \frac{1}{2}(u^2 + v^2) \right), \quad H = E + \frac{p}{\rho}. \tag{11}$$

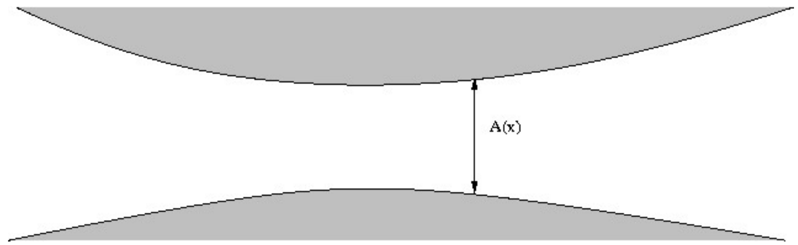


Figure 1: Duct with variable cross area.

Equations of a perfect gas on a duct with variable cross sectional area.

We consider the one-dimensional version of the Euler equations for a flow in a duct of variable cross sectional area A.

$$\partial_t(AU) + \partial_x(AF) = \frac{dA}{dx}P, \quad x \in (0, x_e), \tag{12}$$

where,

$$F = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{pmatrix}, \quad P = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix}, \quad U = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \tag{13}$$

$$H = e + \frac{p}{\rho} = \frac{\gamma}{\gamma - 1}\frac{p}{\rho} + \frac{1}{2}u^2. \tag{14}$$

The inviscid Burgers equation

The simplest model that contains some of the main features of the above systems is the Burgers equation,

$$\partial_t u + \partial_x (u^2/2) = 0, \qquad x \in \Omega \subset \mathbb{R}.$$

This is a particular case of a general conservation law

$$\partial_t u + \partial_x f(u) = 0, \qquad x \in \Omega \subset \mathbb{R},$$

with $f(u) = u^2/2$.

II. Solutions of scalar conservation laws

The linear advection equation

$$\partial_t u + a\partial_x u = 0, \quad x \in \mathbb{R},\ t > 0 \tag{15}$$

where a is a given constant. For a given initial datum

$$u(0,x) = u^0(x), \quad x \in \mathbb{R},$$

the Cauchy problem is well-defined and the solution is simply

$$u(t,x) = u^0(x - at),\ t \geq 0.$$

The solution u at time $t = t_0$ is a pure translation of the initial datum u^0. In fact, if we define the *characteristic lines* of (16) as

$$x'(t) = a,\ x(0) = x_0 \in \mathbb{R},$$

the solution u satisfies

$$\frac{d}{dt}u(t, x(t)) = 0,$$

i.e., it is constant along each characteristic line.

A similar situation occurs for the linear advection equation with a smooth variable coefficient $a(x)$,

$$\partial_t u + \partial_x (a(x) u) = 0, \quad x \in \mathbb{R},\ t > 0. \tag{16}$$

If we define the *characteristics lines* by

$$x'(t) = a(x(t)),\ x(0) = x_0,$$

then the solution u can be obtained solving an ordinary differential equation along these characterístics, namely

$$\frac{d}{dt} u(t, x(t)) = -a'(x(t)) u(t, x(t)).$$

Two important properties:

1. Finite speed of propagation.
2. Characteristics allow to define a natural notion of weak solution for such cases.

The inviscid Burgers equation

$$\begin{cases} \partial_t u + \partial_x(\frac{u^2}{2}) = 0, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), \end{cases}$$

Our main objective is to study the main properties of the solutions of this problem and their numerical approximation.

Characteristics

Let $u(x,t)$ be a smooth solution of the Burgers equation

$$\partial_t u + \partial_x(\frac{u^2}{2}) = 0$$

Then,

$$\partial_t u + u\partial_x u = 0.$$

We introduce the characteristics as the integral curves $x(t)$ of the differential equation

$$\frac{dx}{dt} = u(x,t).$$

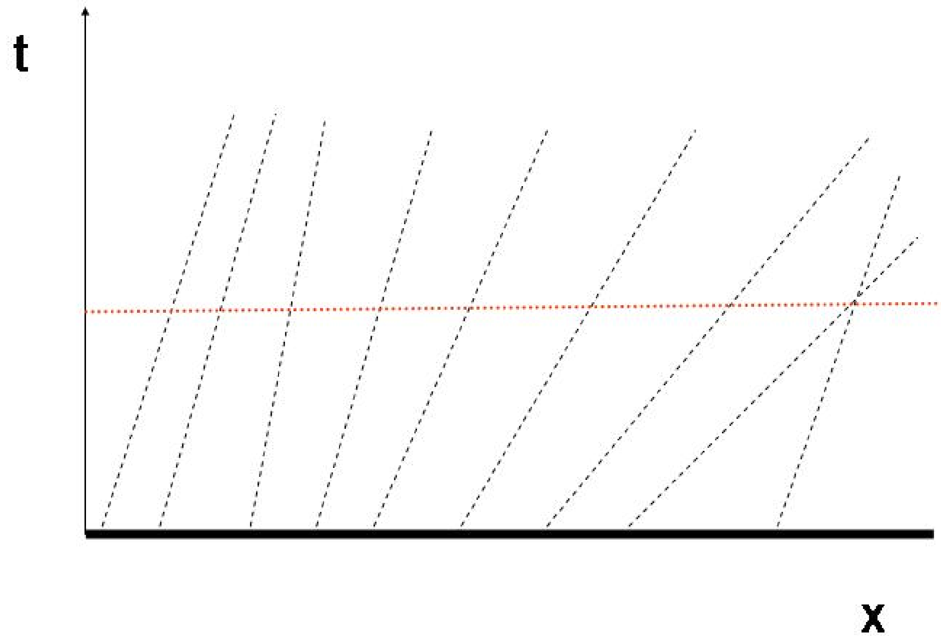
Along these curves the solution is constant since

$$\frac{d}{dt}u(x(t),t) = \partial_t u(x(t),t)) + \partial_x(u(x(t),t))\frac{dx}{dt} = \partial_t u(x(t),t)) + \partial_x(u(x(t),t))u(x(t),t) = 0.$$

Therefore

$$\frac{dx}{dt} = u(x,t) = u^0(x(0),0),$$

and the characteristics are straight lines whose slopes depend on the initial data.



Note that, for some initial data (even for smooth ones) two different characteristics lines may possibly meet at some time $t = t_0$. In this case, the solution cannot be continuous for $t > t_0$ and classical solutions will not exist.

Weak solutions

Let u be a smooth solution of Burgers equation and let $\varphi \in C_0^1(\mathbb{R} \times [0,T))$ be a test function. Multiplying the equation of u by φ and integrating we obtain

$$\begin{aligned} 0 &= \int_0^\infty \int_{\mathbb{R}} \left(\partial_t u + \partial_x (\frac{u^2}{2}) \right) \varphi \\ &= -\int_0^\infty \int_{\mathbb{R}} \left(\partial_t \varphi + \frac{u^2}{2} \partial_x \varphi \right) - \int_{\mathbb{R}} u(x,0)\varphi(x,0). \end{aligned}$$

We adopt this identity as the definition of **weak solution**.

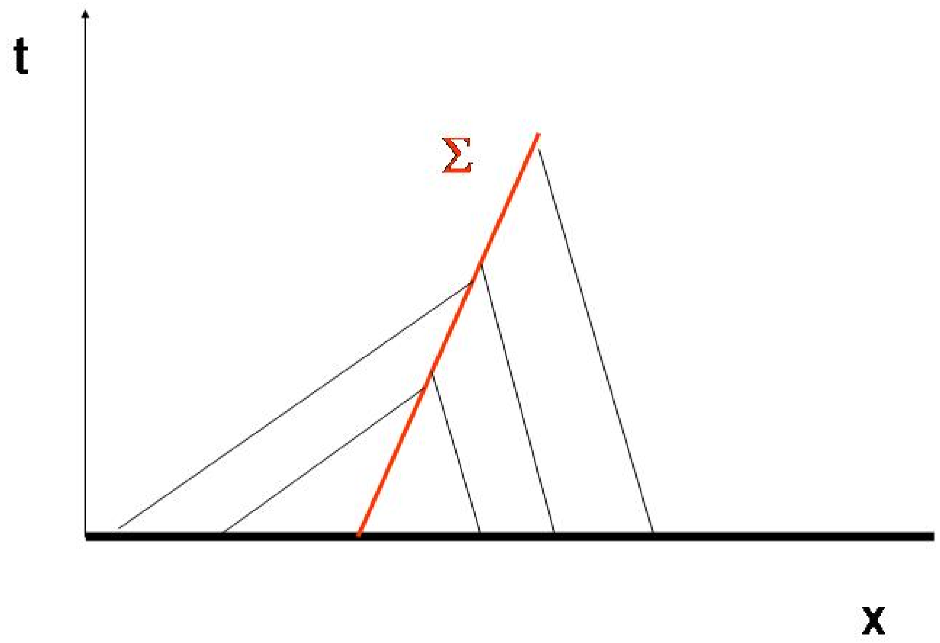
The following characterization of weak solutions is easily proved:

1. u is a classical solution when smooth (C^1).

2. u satisfies the Rankine-Hugoniot conditions

$$[u]_\Sigma n_t + [u^2/2]_\Sigma n_x = 0$$

along discontinuities Σ.



If we parametrize the discontinuity Σ with a function $s(t)$ by

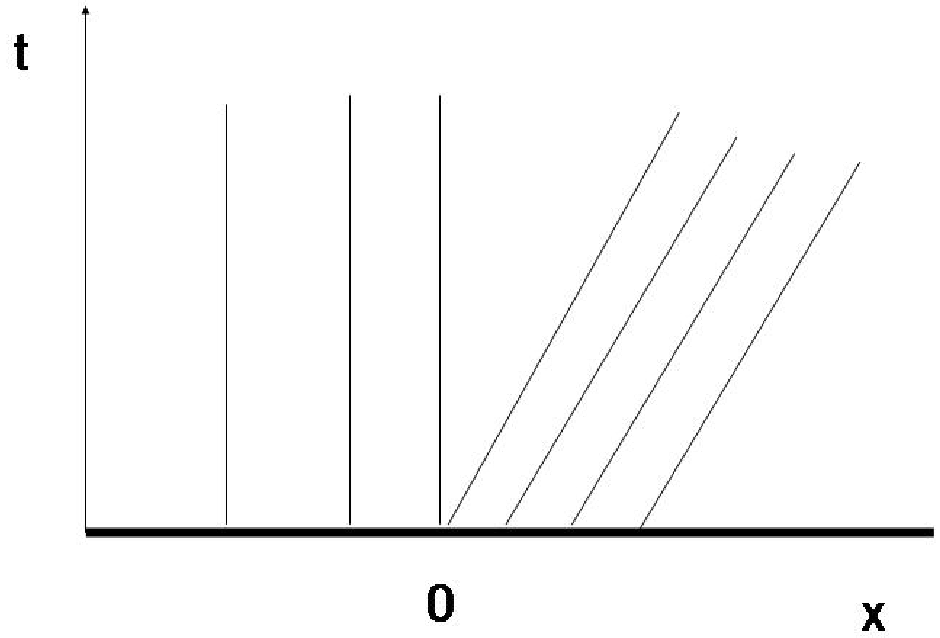
$$\Sigma = \{(t, s(t)),\ t \in (0, T)\}$$

then $s(t)$ must satisfy

$$s'(t) = \frac{[u^2/2]_{(t,s(t))}}{[u]_{(t,s(t))}}.$$

Weak solutions allows us to determine the physically relevant solution when characteristics intersect. However, this definition does not provide unicity for some initial data.

A situation where characteristics do not fill the domain



In general, the physical relevant solution is obtained by defining a new class of solutions, known as *entropy solutions*, for which unicity holds. Entropy solutions can also be characterized as limits, as $\varepsilon \to 0$, of solutions of the Burgers equations with viscosity:

$$\begin{cases} \partial_t u + \partial_x(\frac{u^2}{2}) = \varepsilon \partial_{xx} u, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), \end{cases}$$

III Numerical approximation of scalar conservation laws

A first example

Consider the advection equation

$$\begin{cases} \partial_t u + a\partial_x u = 0, & \text{in } \mathbb{R}\times(0,T), \\ u(x,0) = u^0(x). \end{cases}$$

We introduce a uniform discretization in space and time. We take $\Delta t, \Delta x > 0$.

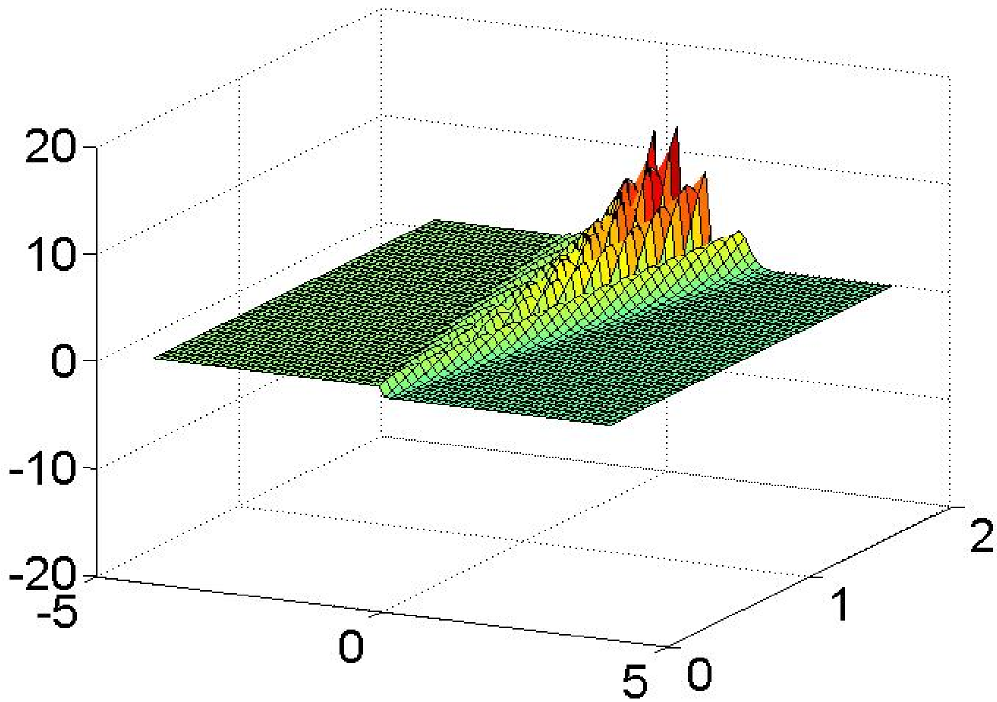
$$\begin{cases} t^n = n\Delta t, & n \in \mathbb{N} \\ x_j = j\Delta x, & j \in \mathbb{Z} \end{cases}$$

Our objective is to compute $u_j^n \sim u(x_j, t^n)$.

The simplest scheme:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0,$$

does not converge!!



Teorema (Lax) A consistent and stable numerical scheme is convergent.

Consistent schemes

The order of accuracy of a difference scheme is the largest number $p \geq 1$ such that any smooth solution u and for $\lambda = \Delta t/\Delta x$ constant, the numerical scheme evaluated on it provides a rest of the order

$$\mathcal{O}(\Delta t^{p+1}), \quad \text{as } \Delta t \to 0.$$

A numerical scheme is **consistent** if its order of accuracy is at lest 1.

The above scheme is consistent.

Stability

A numerical scheme is stable if it satisfies a discrete maximum principle: If $m \leq u_j^0 \leq M$ for all $j \in \mathbb{Z}$ then $m \leq u_j^n \leq M$ for all $n \in \mathbb{N}$ y $j \in \mathbb{Z}$

The above numerical scheme is not stable. To see that we can perform the von Neumann analysis. We consider solutions of the type

$$u_j^n = A^n e^{ikj\Delta x}$$

and we see that the amplification factor is $|A| > 1$.

Conservative schemes

$$\partial_t u + \partial_x f(u) = 0,\ x \in \mathbb{R},\ t > 0,$$
$$u(x,0) = u^0(x).$$

We assume that f is a C^2 function, $u^0 \in L^\infty(\mathbb{R})$ and we set

$$a(u) = f'(u).$$

We set

$$\lambda = \frac{\Delta t}{\Delta x}.$$

General 3-point explicit difference scheme:

$$v_j^{n+1} = H(v_{j-1}^n, v_j^n, v_{j+1}^n),\ \forall n \geq 0, j \in \mathbb{Z}, \tag{17}$$

where $H : \mathbb{R}^3 \to \mathbb{R}$ is a continuous function and v_j^n denotes an approximation of the exact solution u at the grid point $(x_j = j\Delta x, t_n = n\Delta t)$.

Definition 1 *The above difference scheme can be put in conservation form if there exists a continuous function* $g : \mathbb{R}^2 \to \mathbb{R}$ *such that*

$$H(v_{-1}, v_0, v_1) = v^0 - \lambda[g(v_{-1}, v_0) - g(v_0, v_1)]. \tag{18}$$

The function g *is called the numerical flux.*

If we define

$$g^n_{j+1/2} = g(v^n_j, v^n_{j+1})$$

then, the numerical scheme (17) reads

$$v^{n+1}_j = v^n_j - \lambda(g^n_{j+1/2} - g^n_{j-1/2}). \tag{19}$$

The difference scheme (19) is consistent with equation (17) if

$$g(v, v) = f(v), \ \forall v \in \mathbb{R}. \tag{20}$$

Concerning the initial datum (17) we will consider any *suitable* discretization. A common choice is to take

$$v_{j,0} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u^0(x)\, dx, \tag{21}$$

where $x_{j+1/2} = (x_j + x_{j+1})/2$.

Finally the approximation by a conservative scheme of (17)-(17) is

$$v_j^{n+1} = v_j^n - \lambda(g_{j+1/2}^n - g_{j-1/2}^n),\ j \in \mathbb{Z},\ n \geq 0 \tag{22}$$

$$v_j^0 = v_{j,0}. \tag{23}$$

The Lax-Wendroff theorem

For a given sequence (v_j^n) we introduce the piecewise constant function v_Δ defined in $(0,\infty)\times\mathbb{R}$ by

$$v_\Delta(t,x) = v_j^n,\ \ t\in[t_n,t_{n+1}),\ x\in(x_{j-1/2},x_{j+1/2}). \tag{24}$$

Theorem 2 *(Lax-Wendroff) Assume that the difference scheme (19) is consistent with (17) and let $v^0 = (v_{j,0})$ be given by (21). Assume that there exists a sequence $\Delta x\to 0$ such that if $\Delta t = \lambda\Delta x$ (with λ constant)*

$$\|v_\Delta\|_{L^\infty((0,\infty)\times\mathbb{R}))} \le C,$$
$$v_\Delta \text{ converges in } L^1_{loc}((0,\infty)\times\mathbb{R})) \text{ and a.e. to a function } u$$

Then u is a weak solution of (17)-(17).

The above theorem tell us that a difference scheme in conservation form which converges always converges to a weak solution.

The idea of the proof is that a conservative numerical scheme satisfies the weak discrete form

$$\Delta t \, \Delta x \sum_n \sum_j \left(u_j^{n+1} \frac{\varphi_j^{n+1} - \varphi_j^n}{\Delta t} + f_{j+1/2}^n \frac{\varphi_{j+1}^n - \varphi_j^n}{\Delta x} \right) + \Delta x \sum_j u_j^0 \varphi_j^0 = 0$$

and this is a natural discretization of the weak form

$$\int_0^T \int_{\mathbb{R}} \left(u \partial_t \varphi + f(u) \partial_x \varphi \right) \, dx \, dt + \int_{\mathbb{R}} u^0(x) \varphi(x,0) = 0.$$

The main questions now are:

- Find sufficient conditions to convergence.
- Find criteria which ensure that the limit is the unique entropy solution.
- Determine the order of accuracy of the difference scheme.

Stability

We focus on the linear advection equation

$$\partial_t u + a\partial_x u = 0.$$

Assume that we have a 3-points linear difference scheme of the form

$$v_j^{n+1} = c_{-1}v_{j-1}^n + c_0 v_j^n + c_1 v_{j+1}^n,\ n \geq 0. \tag{25}$$

It can be shown that the linear difference scheme (25) can be put in conservation form if and only if

$$c_{-1} + c_0 + c_1 = 1.$$

The numerical flux is then given by

$$g(u,v) = \frac{c_{-1}u - c_1 v}{\lambda},$$

and the consistency condition (20) reads

$$c_{-1} - c_1 = \lambda a.$$

Thus, setting

$$q = 1 - c_0,$$

the conservative and consistent schemes can be written in viscous form as

$$v_j^{n+1} = v_j^n - \lambda a(v_{j+1}^n - v_{j-1}^n)/2 + q(v_{j+1}^n - 2v_j^n + v_{j-1}^n)/2$$

Define the ℓ^2-norm of a sequence $v = (v_j)$ as

$$\|v\|_2 = (\Delta x \sum_j v_j^2)^{1/2}.$$

Then, the difference scheme is L^2-stable if there exists a constant $C > 0$, independent of Δt such that

$$\|v^n\|_2 \leq C\|v^0\|_2, \ \forall n \geq 0.$$

The coefficient $\mu = \lambda a$ is called the Courant number and it can be shown that the differential scheme above is L^2-stable if q satisfies

$$(\lambda a)^2 \leq q \leq 1.$$

In the particular case $q = (\lambda a)^2$ we obtain a second order accurate differential scheme known as Lax-Wendroff scheme which is L^2-stable under the condition

$$\lambda |a| \leq 1.$$

This condition can be interpreted geometrically in terms of the domain of dependence of the numerical difference scheme. This interpretation is known as the Courant-Friedrichs-Levy (CFL) condition.

Some examples

Lax-Friedrichs scheme

$$\frac{u_j^{n+1} - \frac{1}{2}(u_{j+1}^n + u_{j-1}^n)}{\Delta t} + \frac{f(u_{j+1}^n) - f(u_{j-1}^n)}{\Delta x} = 0,$$

which can be put in conservation form with the numerical flux

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

In the linear case, $q = 1$ and this scheme is L^2-stable under the CFL condition

$$\max_{j,n} |f'(u_j^n)| \frac{\Delta t}{\Delta x} \leq 1.$$

Upwind scheme Assume f monotone

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{f(u_{j+1}^n)-f(u_j^n)}{\Delta x}=0, \qquad \text{si } f'<0,$$

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{f(u_j^n)-f(u_{j-1}^n)}{\Delta x}=0, \qquad \text{si } f'>0,$$

In the linear case, $q=|a\lambda|=|\nu|$ and the scheme is L^2-stable under the CFL condition.

Godunov scheme

The Godunov scheme is based on the exact solution of local Riemann problems. The numerical flux is given by

$$g(u,v)=\begin{cases} \min_{w\in[u,v]} f(w), & \text{if } u\le v \\ \max_{w\in[u,v]} f(w), & \text{if } v\le u \end{cases}$$

In the linear case, it coincides with the upwind difference scheme.

Murman-Roe

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

where

$$a(u,v) = \begin{cases} \frac{f(v)-f(u)}{v-u} & \text{if } u \neq v \\ f'(u) & \text{if } u = v \end{cases},$$

Lax-Wendroff

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

where

$$a(u,v) = \begin{cases} \frac{f(v)-f(u)}{v-u} & \text{if } u \neq v \\ f'(u) & \text{if } u = v \end{cases},$$

Definition 3 *A numerical scheme* $v_j^{n+1} = H(v_{j-1}^n, v_j^n, v_{j+1}^n)$ *is monotone if* H *is increasing in each variable.*

Definition 4 *A numerical scheme* $v_j^{n+1} = H(v_{j-1}^n, v_j^n, v_{j+1}^n)$ *is TVD if*

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

where $TV(v_j^n) = \sum_j |v_{j+1}^n - v_j^n|$.

Definition 5 *A numerical scheme* $v_j^{n+1} = H(v_{j-1}^n, v_j^n, v_{j+1}^n)$ *is* L^∞*-stable if there exists a constant* $C > 0$ *such that*

$$\sup_j |v_j^n| \leq C$$

for all $n \geq 0$.

A numerical scheme TVD and L^∞-stable is convergent.

Monotone schemes are TVD, L^∞-stable and consistent with the entropy condition.

Lax-Friedrichs, upwind and Godunov are monotone.