Numerical methods for Partial Differential Equations

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Many laws in Physics are stated under the form of **conservation law**, namely

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} = 0 \, ,$$

where $u = u(\boldsymbol{x}, t)$ is a scalar unknown defined, for $t \geq 0$, in a domain $\Omega \subseteq \mathbb{R}^d$ and on its boundary $\Gamma = \partial\Omega$, $\mathbf{F} = \mathbf{F}(u, \boldsymbol{x}, t)$ is a vector-valued function in $\mathbb{R}^d$, depending upon u and possibly upon $\boldsymbol{x}$ and t, which is termed *flux* of u (at the point $\boldsymbol{x}$ and at time t); the symbol ∇ indicates the divergence operator, taken with respect to the spatial variables x_j.

Example: The convection-diffusion equation

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u - \nu \Delta u = 0$$

is a conservation law if $\nabla \cdot \mathbf{a} = 0$ in Ω at any time; its flux is given by

$$\mathbf{F} = \mathbf{F}(u, \boldsymbol{x}, t) = \mathbf{a}(\boldsymbol{x}, t) u - \nu \nabla u \, .$$

Indeed,

$$\nabla \cdot \mathbf{F} = \nabla \cdot (\mathbf{a} u) - \nu \nabla \cdot \nabla u = (\nabla \cdot \mathbf{a})\, u + \mathbf{a} \cdot \nabla u - \nu \Delta u = \mathbf{a} \cdot \nabla u - \nu \Delta u \, .$$

Conservation property

Let us choose an arbitrary region $\mathcal{V}$ contained in Ω, whose boundary $\partial\mathcal{V}$ is smooth enough so that the Divergence Theorem holds in $\mathcal{V}$.

Integrating the equation on $\mathcal{V}$ and applying this theorem, we get

$$\begin{aligned} 0 &= \int_{\mathcal{V}} \left(\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} \right) d\boldsymbol{x} = \frac{d}{dt} \int_{\mathcal{V}} u \, d\boldsymbol{x} + \int_{\mathcal{V}} \nabla \cdot \mathbf{F} \, d\boldsymbol{x} \\ &= \frac{d}{dt} \int_{\mathcal{V}} u \, d\boldsymbol{x} + \int_{\partial\mathcal{V}} \mathbf{F} \cdot \mathbf{n} \, d\gamma \, , \end{aligned}$$

where $\mathbf{n}$ denotes the unit vector normal to $\partial\mathcal{V}$, pointing outward $\mathcal{V}$.

The last integral represents the flux of u across the boundary of $\mathcal{V}$. Integrating over a time interval $[t', t'']$ and recalling that $\int_{t'}^{t''} \frac{d\varphi}{dt} \, dt = \varphi(t'') - \varphi(t')$, we have

$$\int_{\mathcal{V}} u(\boldsymbol{x}, t'') \, d\boldsymbol{x} = \int_{\mathcal{V}} u(\boldsymbol{x}, t') \, d\boldsymbol{x} - \int_{t'}^{t''} \int_{\partial\mathcal{V}} \mathbf{F} \cdot \mathbf{n} \, d\gamma \, dt \, .$$

This shows that if the flux of u across $\mathcal{V}$ vanishes, then the quantity $\int_{\mathcal{V}} u(\boldsymbol{x}, t) \, d\boldsymbol{x}$ is conserved. If not, its variation equals the balance between incoming flux and outcoming flux across $\partial\mathcal{V}$.

Idea of the Finite Volume Method

Let us fix a decomposition of the spatial domain Ω in *volumes*, o *cells* $\mathcal{V}_j$, having finite measure $|\mathcal{V}_j|$, which intersect only through their boundaries $\partial\mathcal{V}_j$.
Next, let us fix a time step $\Delta t > 0$, and the time instants $t_n = n\Delta t$, $n = 0, 1, ...$

Let us write the previous conservation property in the cell $\mathcal{V}_j$ and in the time interval $[t_n, t_{n+1}]$:

$$\int_{\mathcal{V}_j} u(\boldsymbol{x}, t_{n+1})\, d\boldsymbol{x} = \int_{\mathcal{V}_j} u(\boldsymbol{x}, t_n)\, d\boldsymbol{x} - \int_{t_n}^{t_{n+1}} \int_{\partial\mathcal{V}_j} \mathbf{F}\cdot\mathbf{n}_j \; d\gamma \; dt \; .$$

Denoting by $\partial\mathcal{V}_{j,\ell} = \partial\mathcal{V}_j \cap \partial\mathcal{V}_\ell$ the common interface between cells $\mathcal{V}_j$ and $\mathcal{V}_\ell$, we have

$$\int_{\mathcal{V}_j} u(\boldsymbol{x}, t_{n+1})\, d\boldsymbol{x} = \int_{\mathcal{V}_j} u(\boldsymbol{x}, t_n)\, d\boldsymbol{x} - \sum_{|\partial\mathcal{V}_{j,\ell}|>0} \int_{t_n}^{t_{n+1}} \int_{\partial\mathcal{V}_{j,\ell}} \mathbf{F}\cdot\mathbf{n}_j \; d\gamma \; dt \; .$$

Let us introduce the *cell averages* of the exact solution, as well as the *average flux* on each cell interface:

$$U_j^n = \frac{1}{|\mathcal{V}_j|}\int_{\mathcal{V}_j} u(\boldsymbol{x}, t_n)\, d\boldsymbol{x} \; , \qquad F_{j,\ell}^n = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \frac{1}{|\partial\mathcal{V}_{j,\ell}|}\int_{\partial\mathcal{V}_{j,\ell}} \mathbf{F}\cdot\mathbf{n}_j \; d\gamma \; dt \; .$$

Then, the previous relation becomes

$$|\mathcal{V}_j|\, U_j^{n+1} = |\mathcal{V}_j|\, U_j^n - \Delta t \sum_{|\partial\mathcal{V}_{j,\ell}|>0} |\partial\mathcal{V}_{j,\ell}|\, F_{j,\ell}^n \ .$$

Dividing by $|\mathcal{V}_j|$ and setting

$$\lambda_{j,\ell} = \Delta t \frac{|\partial\mathcal{V}_{j,\ell}|}{|\mathcal{V}_j|} \ ,$$

we obtain the relation

$$U_j^{n+1} = U_j^n - \sum_{|\partial\mathcal{V}_{j,\ell}|>0} \lambda_{j,\ell}\, F_{j,\ell}^n \ .$$

Such a formula suggests to define a numerical scheme, which updates the values of the cell averages from one time instant to the next one, by means of suitably defined *numerical fluxes*; each of them should be easily computable using only the information on the averages in the nearby cells.

- To be precise, let

$$u_j^n \simeq U_j^n$$

be a *discrete cell average*, namely the approximation of the exact cell average of the cell $\mathcal{V}_j$ at the time t_n, defined by the numerical scheme.

- Next, let

$$f_{j,\ell}^n = f(u_j^n, u_\ell^n) \simeq F_{j,\ell}^n$$

be a *numerical flux*, namely the approximation of the average flux between two contiguous cells $\mathcal{V}_j$ e $\mathcal{V}_\ell$, defined in terms of the corresponding discrete cell averages.

The numerical flux is determined by the choice of the function

$$f(u, v) = f(u, v; \mathbf{a}, \mathbf{n})$$

which appears in the previous formula.

- Then, the corresponding finite-volume numerical scheme is given by:

$$u_j^{n+1} = u_j^n - \sum_{|\partial\mathcal{V}_{j,\ell}|>0} \lambda_{j,\ell}\, f_{j,\ell}^n \ .$$

The model equation in one dimension

The simplest example of conservation law is the transport equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(au) = \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \,, \qquad \text{with constant } a \neq 0 \,.$$

The flux is given by $F(u) = au$.

The equation states that u is constant on the **characteristic** lines, i.e., the straight lines in the plane (x, t) defined by the equation

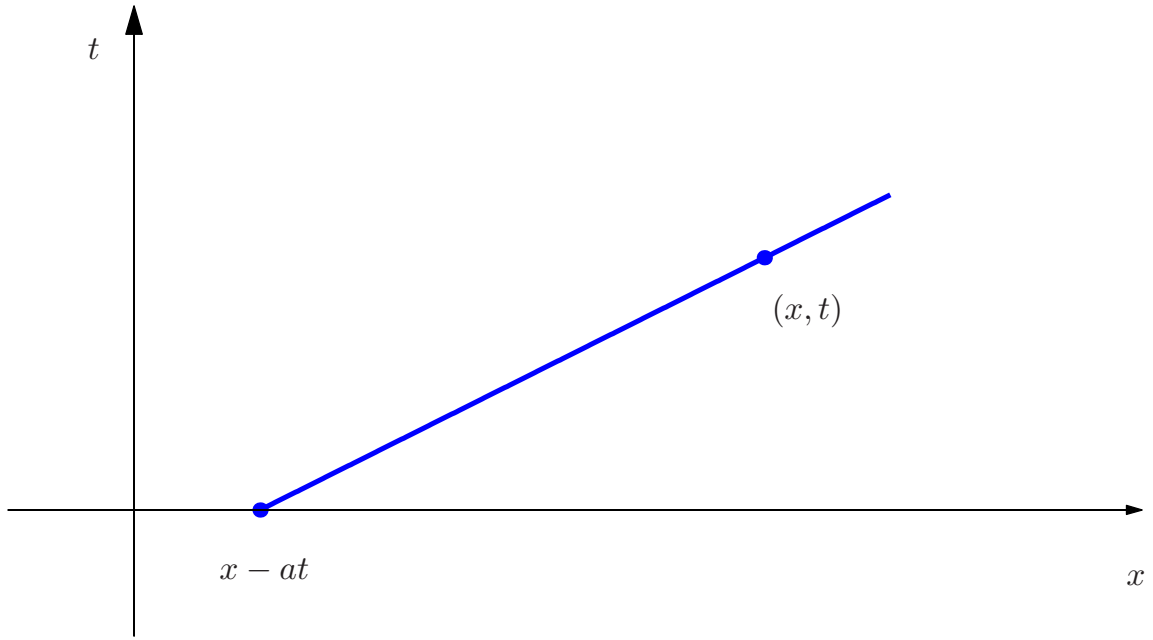
$$\frac{dx}{dt} = a \,;$$

they are the lines of equation $x = x(t) = at + b$ with constant b.

Indeed, the general solution has the form

$$u(x, t) = g(x - at)$$

where $g : \mathbb{R} \to \mathbb{R}$ is an arbitrary (differentiable) function.



In particular, the initial-vaalue problem

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0\,, \quad x \in \mathbb{R},\ t > 0\,,$$
$$u(x,0) = u_0(x)\,, \quad x \in \mathbb{R}\,,$$

has the unique solution

$$u(x,t) = u_0(x-at)\,, \qquad x \in \mathbb{R},\ t \geq 0\,.$$

Let us introduce a space discretization step $\Delta x > 0$ and the equally spaced nodes $x_j = j\Delta x$, $j \in \mathbb{Z}$. The intermediate points $x_{j+1/2} = (j + \frac{1}{2})\Delta x$ define the cells $\mathcal{V}_j = [x_{j-1/2}, x_{j+1/2}]$, having the nodes x_j as centers.

The conservation relation in the cell $\mathcal{V}_j$ and in the time interval $[t_n, t_{n+1}]$ takes the form

$$\begin{aligned}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t_{n+1})\, dx \quad &= \quad \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t_n)\, dx \\ &\quad - \left(\int_{t_n}^{t_{n+1}} F(u(x_{j+1/2}, t))\, dt - \int_{t_n}^{t_{n+1}} F(u(x_{j-1/2}, t))\, dt \right) .\end{aligned}$$

Setting

$$U_j^n = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t_n)\, dx \qquad \text{e} \qquad F_{j+1/2}^n = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} F(u(x_{j+1/2}, t))\, dt \ ,$$

the previous relation becomes

$$\Delta x\, U_j^{n+1} = \Delta x\, U_j^n - (\Delta t\, F_{j+1/2}^n - \Delta t\, F_{j-1/2}^n) \ .$$

If we introduce the constant (having the dimension of a velocity^{-1})

$$\lambda = \frac{\Delta t}{\Delta x} > 0 \, ,$$

we obtain

$$U_j^{n+1} = U_j^n - \lambda (F_{j+1/2}^n - F_{j-1/2}^n) \, .$$

A *finite-volume discretization scheme* is thus written as

$$u_j^{n+1} = u_j^n - \lambda (f_{j+1/2}^n - f_{j-1/2}^n) \, ,$$

with *numerical fluxes*

$$f_{j+1/2}^n = f(u_j^n, u_{j+1}^n) \, ,$$

where $f(u, v)$ is a suitable function depending upon two real variables u e v (and upon a, too).
In order to guarantee the *consistency* of the discretization scheme with respect to the exact equation, the function f is required to satisfy the property

$$f(u, u) = au \qquad \text{for any value of } u \in \mathbb{R} \, .$$

In the sequel, we consider some relevant examples of numerical fluxes, and the corresponding finite-volume schemes.

The forward/centered Euler method

The numerical flux $f(u, v)$ is given by

$$f_E(u, v) = \frac{a}{2}(u + v)$$

and the resulting scheme is

$$u_j^{n+1} = u_j^n - \frac{1}{2}\lambda a(u_{j+1}^n - u_{j-1}^n) \, .$$

It can be equivalently written as

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

thus, it corresponds to a *centered approximation* of the spatial derivative.

This method gives very poor results; hence, it is never used in practice!

The numerical flux $f(u, v)$ is given by

$$f_{LF}(u, v) = \frac{a}{2}(u + v) + \frac{1}{2\lambda}(u - v)$$

and the resulting scheme is

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{1}{2}\lambda a(u_{j+1}^n - u_{j-1}^n) \ .$$

It can be equivalently written as

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

thus, it corresponds to adding an **artificial diffusion** term (or **numerical diffusion** term) proportional to Δx (and independent of a).

The Upwind method

The numerical flux $f(u,v)$ is given by

$$f_U(u,v) = \frac{a}{2}(u+v) + \frac{|a|}{2}(u-v) = \begin{cases} au & \text{if} \quad a > 0\,, \\ av & \text{if} \quad a < 0\,. \end{cases}$$

and the resulting scheme is

$$u_j^{n+1} = \begin{cases} u_j^n - \lambda a(u_j^n - u_{j-1}^n) & \text{if} \quad a > 0\,, \\ u_j^n - \lambda a(u_{j+1}^n - u_j^n) & \text{if} \quad a < 0\,. \end{cases}$$

It can be equivalently written as

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0 \qquad \text{if} \quad a > 0\,,$$

or

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_j^n}{\Delta x} = 0 \qquad \text{if} \quad a < 0\,.$$

Thus, the spatial derivative is discretized by a backward incremental quotient if $a > 0$, by a forward incremental quotient if $a < 0$.

Recalling that information propagates from left to right if $a > 0$ and from right to left if $a < 0$, we can say that the scheme defines the new values of the cell averages coherently with the propagation of information.

Equivalently, the Upwind scheme can be written as

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

hence, again it corresponds to adding a *numerical diffusion* term proportional to Δx, but now depending upon a.

The method is *first order* accurate both in space and in time, i.e,

$$\text{discretization error } \sim \; c_1 \Delta x + c_2 \Delta t \,.$$

The Lax-Wendroff method

The numerical flux $f(u, v)$ is given by

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

and the resulting scheme is

$$u_j^{n+1} = u_j^n - \frac{1}{2}\lambda a(u_{j+1}^n - u_{j-1}^n) + \frac{1}{2}(\lambda a)^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \, .$$

It can be equivalently written as

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

(the *numerical diffusion* term now depends upon both a and λ).

The method is *second order* accurate both in space and in time, i.e,

$$\text{discretization error } \sim \; c_1(\Delta x)^2 + c_2(\Delta t)^2 \, .$$

The Courant number and the CFL stability condition

An important quantity in the study of the numerical stability of the previous schemes is given by the **Courant number**

$$\text{Cour} = |a|\lambda = |a|\frac{\Delta t}{\Delta x} \ .$$

Indeed, the numerical solution is asymptotically stable (i.e., the numerical cell averages all remain bounded as the number of time steps increases) if and only if the following **CFL (Courant, Friedrichs e Lewy) condition** is fulfilled:

$$\text{Cour} \leq 1 \ , \qquad \text{namely,} \qquad \Delta t \leq \frac{\Delta x}{|a|} \ .$$

This condition guarantees that the exact solution at time t_{n+1} in the cell $\mathcal{V}_j$ depends upon its values at time t_n in the cells $\mathcal{V}_{j-1}$, $\mathcal{V}_j$ e $\mathcal{V}_{j+1}$ only, as indeed it occurs for the numerical cell averages.

The case Cour $= 1$

The case Cour $= 1$ deserves a particular attention.

- The exact cell averages evolve according to the law

$$U_j^{n+1} = \begin{cases} U_{j-1}^n & \text{if } \ a > 0 \ , \\ U_{j+1}^n & \text{if } \ a < 0 \ . \end{cases}$$

- The Lax-Friedrichs, Upwind and Lax-Wendroff methods all give the same solution; precisely, the numerical cell averages evolve according to the law

$$u_j^{n+1} = \begin{cases} u_{j-1}^n & \text{if } \ a > 0 \ , \\ u_{j+1}^n & \text{if } \ a < 0 \ . \end{cases}$$

- We conclude that the numerical cell averages coincide with the exact ones at each time advancing step, provided they coincide at the initial time.