Quelques remarques sur le choix des schémas numériques (et des équations)

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Objectif de nombreux simulateurs actuels

Développer des simulateurs numériques capables de simuler des écoulements fluides dans une large gamme de régimes.
Examples de phénomènes :

- Simulation d'incendies (écoulements lents)
- Accident dans un centrale nucléaire (écoulements rapides. . .)

Examples d'équations :

- Navier Stokes incompressible
- Euler compressible

Ecoulements incompressibles, exemple : NS incomp.

- Equations souvent sous forme non conservative
- Discrétisation est faite sur maillages décalés (schéma MAC)
- Systèmes dont la partie convective est parfois non hyperbolique

Ecoulements compressibles, exemple : Euler comp.

- Utiliser la (bonne) forme conservative des équations (C1–)
- Inconnues discrètes sont colocalisées (C2–)
- Systèmes hyperboliques (C3–)

Essentiellement lié au fait que l'on s'attend à avoir des solutions discontinues.

Question: Peut on se libérer de ces trois “contraintes” ?

C1– Burgers, "equivalent equation"

$$\partial_t \rho + \partial_x(\rho^2) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$
$$\rho(x,0) = \begin{cases} 2, & x < 0 \\ 1, & x > 0 \end{cases}$$

For positive and regular solution, an equivalent equation is

$$\partial_t \rho^2 + \frac{4}{3}\partial_x(\rho^3) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

The classical upwind scheme on this latter equation leads to a solution which does not have the good localization of the discontinuity

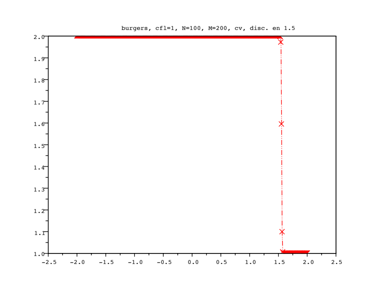
The speed of the discontinuity is 3 for burgers and $28/9$ for the equivalent equation

Burgers, "equivalent" equation

$$(h/k)((\rho_i^{n+1})^2 - (\rho_i^n)^2) + \frac{4}{3}((\rho_i^n)^3 - (\rho_{i-1}^n)^3) = 0,$$

Upwind scheme on the "equivalent" equation, CFL=1, solution for T=1/2 ($N = 100$, $M = 200$)

Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/4$



Bad localization of the discontinuity (1.555 instead of 1.5), bounds on the solution, no convergence

Burgers, numerical diffusion

$$\partial_t \rho + \partial_x(f(\rho)) = 0$$

On this equation, if $f' \geq 0$, upwinding is “similar” to add a numerical diffusion. Namely, is similar to

$$\partial_t \rho + \partial_x(f(\rho)) - \partial_x(\frac{hf'(\rho) - kf'^2(\rho)}{2}\partial_x \rho) = 0$$

The CFL condition is for $hf'(\rho) - kf'^2(\rho) \geq 0$ (i.e. $kf'(\rho) \leq h$)

In the case of the Burgers equation it gives

$$\partial_t \rho + \partial_x(\rho^2) - \partial_x((h\rho - 2k\rho^2)\partial_x \rho) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

Burgers, non conservative numerical diffusion

In the case of the “equivalent” equation

$$\partial_t \rho^2 + (4/3)\partial_x(\rho^3) = 0,$$

upwinding is similar to (since $\rho > 0$)

$$\partial_t \rho^2 + \frac{4}{3}\partial_x(\rho^3) - \partial_x((2h\rho^2 - 4k\rho^3)\partial_x \rho) = 0,$$

Turning back to the Burgers equation, this leads to

$$\partial_t \rho + \partial_x(\rho^2) - \frac{1}{\rho}\partial_x((h\rho^2 - 2k\rho^3)\partial_x \rho) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

This is a numerical diffusion (thanks to the CFL condition) but not on a conservative form.

The consequence is that a non conservative diffusion may lead to wrong discontinuities

Burgers, non conservative numerical diffusion on an equivalent equation

The discretization of a non conservative diffusion on the burgers equation lead to wrong discontinuities

But

Using a non conservative diffusion on an equivalent equation may gives the good discontinuities for the initial equation?

The answer is yes. . .

Compressible Euler Equations

$$\begin{aligned} \partial_t \rho + \mathrm{div}(\rho u) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+ \\ \partial_t(\rho u) + \mathrm{div}(\rho u \otimes u) + \nabla p = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+ \\ \partial_t E + \mathrm{div}(u(E+p)) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+ \end{aligned}$$

$E = \frac{1}{2}\rho|u|^2 + \rho e$
$p = \varphi(\rho, e)$ (perfect gaz : $p = (\gamma - 1)\rho e$)
Initial condition on ρ, u, p

Hyperbolic system on conservative form.

Equivalent system

Euler system is equivalent, for regular solutions, to the following one

$$
\begin{aligned}
\partial_t \rho + \mathrm{div}(\rho u) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+ \\
\partial_t (\rho u) + \mathrm{div}(\rho u \otimes u) + \nabla p = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+ \\
\partial_t \rho e + \mathrm{div}(\rho u e) + p\,\mathrm{div}\, u = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+
\end{aligned}
$$

and there are some reasons to prefer (in particular with staggered grids) to work with this system instead of the initial system

But, this system is not equivalent to the initial system when the solution contains shocks

Working with internal energy in Euler Equations

when the solution contains a shock wave, the initial Euler Equations are not equivalent to the following ones

$$\partial_t \rho + \mathrm{div}(\rho u) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$
$$\partial_t(\rho u) + \mathrm{div}(\rho u \otimes u) + \nabla p = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$
$$\partial_t \rho e + \mathrm{div}(\rho u e) + p\,\mathrm{div}\, u = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$

But, discretizing the third equation by adding a convenient source term gives an approximate solution which converges, as the mesh size and the time step go to 0 (with a *CFL* condition in the case of an explicit scheme), to a weak entropy solution of the Euler Equations (assuming some estimates on the approximate solution).

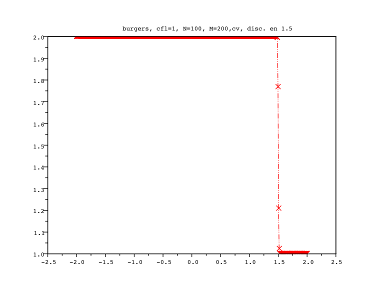
Papers of R. Herbin, W. Kheriji, J.-C. Latché and T. T. Trung, C. Zaza

Indeed, the source term converge to 0 except in the shocks waves.

C2– Burgers viewed as a coupled system, classical upwind

$$\partial_t \rho + \partial_x (u\rho) = 0, \quad u = \rho, \quad x \in \mathbb{R}, \; t \in \mathbb{R}_+$$
$$\rho(x,0) = \begin{cases} 2, & x < 0 \\ 1, & x > 0 \end{cases}$$

Upwind scheme, CFL=1, solution for T=1/2 ($N = 100$, $M = 200$)
Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/4$



Good localization of the discontinuity, few numerical diffusion, bounds on the solution, convergence.

Burgers viewed as a coupled system, upwind-ncv

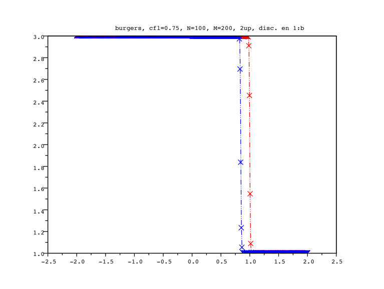
Upwind on $u\partial_x\rho + \rho\partial_x u$. Since $u = \rho$ (collocated), it gives

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + 2u_i^n(\rho_i^n - \rho_{i-1}^n) = 0, \quad u_i^n = \rho_i^n$$

Initial condition : 3 for $x < 0$ and 1 for $x > 0$

Upwind-ncv scheme, CFL=1/4, solution for T=1/4 ($N = 100$, $M = 200$)

Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/2$



Wrong localization of the discontinuity, bounds on the solution, no convergence.

Burgers viewed as a coupled system, upwind-ncv

$\partial_x(\rho u) = u\partial_x \rho + \rho \partial_x u$.

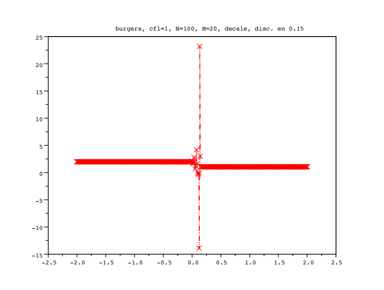
Upwind-ncv=upwind + discretization of $h(\partial_x u)^2$.

No problem for a regular solution. A problem might arise if $\partial_x u$ not in L^2.

Burgers viewed as a coupled system, upwind-staggered

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + (u^n_{i+\frac{1}{2}}\rho_i^n - u^n_{i-\frac{1}{2}}\rho^n_{i-1}) = 0,$$
$$u_{i+\frac{1}{2}} = (1/2)(\rho_i^n + \rho^n_{i+1})$$

Upwind-staggered scheme, CFL=1, solution for T=1/20 ($N = 100$, $M = 20$)
Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/4$

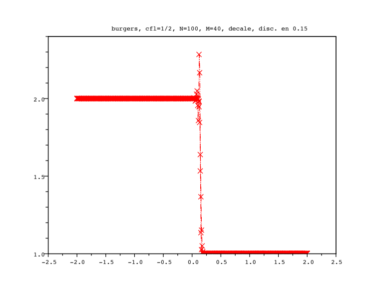


Pretty good localization of the discontinuity (0.15), but no bound of the solution ⇝ time step too large

Burgers viewed as a coupled system, upwind-staggered

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + (u^n_{i+\frac{1}{2}}\rho_i^n - u^n_{i-\frac{1}{2}}\rho^n_{i-1}) = 0,$$
$$u_{i+\frac{1}{2}} = (1/2)(\rho_i^n + \rho^n_{i+1})$$

Upwind-staggered scheme, CFL=1/2 (reduced CFL), solution for T=1/20 ($N = 100$, $M = 40$)
Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/4$

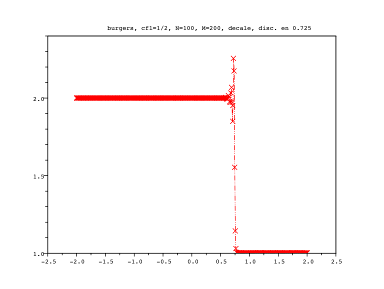


Good localization of the discontinuity (0.15), positivity but no upper bound on the solution.

Burgers viewed as a coupled system, upwind-staggered

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + (u^n_{i+\frac{1}{2}}\rho_i^n - u^n_{i-\frac{1}{2}}\rho^n_{i-1}) = 0,$$
$$u_{i+\frac{1}{2}} = (1/2)(\rho_i^n + \rho^n_{i+1})$$

Upwind-staggered scheme, CFL=1/2 (reduced CFL), solution for T=1/4 ($N = 100$, $M = 200$)
Space step: $h = 1/N$, $M =$ number of time steps, $k = (CFL)h/4$



Good localization of the discontinuity (0.75), positivity but no upper bound on the solution.

Burgers viewed as a coupled system, upwind-staggered

Consistency in the sense of Lax

If the numerical solution is bounded (independently of the mesh size and the time step) it converges (as mesh size goes to 0, under appropriate CFL condition) to the weak entropy solution of Burgers (D. Doyen and R. Eymard)

Staggered schemes for coupled conservation laws

$$\partial_t \rho + \mathrm{div}(\rho u) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$

and

$$\partial_t z + u \cdot \nabla z = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$

More precisely, the second equation is rather (for possible discontinuity of u and z)

$$\partial_t (\rho z) + \mathrm{div}(\rho u z) = 0,\ x \in \mathbb{R}^3,\ t \in \mathbb{R}_+$$

For instance, a constant z is solution of this equation, we espect the numerical scheme to have the same property (it is related to the stability of the scheme).

Collocated for ρ and z, upwind scheme, 1d

u is given on a dual grid

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + (F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}) = 0,$$

$$F^n_{i+\frac{1}{2}} = u^n_{i+\frac{1}{2}}\rho_i^n, \text{ if } u^n_{i+\frac{1}{2}} > 0$$
$$F^n_{i+\frac{1}{2}} = u^n_{i+\frac{1}{2}}\rho_{i+1}^n, \text{ if } u^n_{i+\frac{1}{2}} < 0$$

Then, a convenient discretization for z is

$$(h/k)(\rho_i^{n+1} z_i^{n+1} - \rho_i^n z_i^n) + (G^n_{i+\frac{1}{2}} - G^n_{i-\frac{1}{2}}) = 0$$

$$G^n_{i+\frac{1}{2}} = F^n_{i+\frac{1}{2}} z_i^n, \text{ if } u^n_{i+\frac{1}{2}} > 0 \qquad (\rho > 0)$$
$$G_{i+\frac{1}{2}} = F^n_{i+\frac{1}{2}} z_{i+1}^n, \text{ if } u^n_{i+\frac{1}{2}} < 0$$

A constant z is solution of the scheme

Staggered for ρ and z, 1d

The unknowns are ρ_i, $z_{i+1/2}$ (example : $z = u$, qdm)

$$(h/k)(\rho_i^{n+1} - \rho_i^n) + (F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}) = 0$$

- Define ρ on the dual mesh (with mass conservation) $\rho_{i+1/2} = \frac{1}{2}(\rho_i + \rho_{i+1})$
- Discrete conservation law on the dual mesh

$$(h/k)(\rho^{n+1}_{i+1/2} - \rho^n_{i+1/2}) + (F^n_{i+1} - F^n_i) = 0$$

$F^n_i = (1/2)(F^n_{i+1/2} + F^n_{i-1/2})$

- Then, a convenient discretization for z is

$$(h/k)(\rho^{n+1}_{i+\frac{1}{2}} z^{n+1}_{i+\frac{1}{2}} - \rho^n_{i+\frac{1}{2}} z^n_{i+\frac{1}{2}} + (G^n_{i+1} - G^n_i) = 0$$

$$G^n_i = F^n_i z^n_{i-\frac{1}{2}}, \text{ if } F^n_i > 0$$
$$G^n_i = F^n_i z^n_{i+\frac{1}{2}}, \text{ if } F^n_i < 0$$

A constant z is solution of the scheme (R. Herbin and J. C. Latché)

C3– Resonant system

$U : \mathbb{R} \times \mathbb{R}_+ \to D \subset \mathbb{R}^p$
$f \in C^1(\mathbb{R}^p, \mathbb{R}^p)$

$$\partial_t U + \partial_x f(U) = 0, \; x \in \mathbb{R}, \; t \in \mathbb{R}_+$$

- hyperbolic : $Df(U)$ diagonalizable in $\mathbb{R}$ for all $U \in D$.
- weakly hyperbolic : $Df(U)$ has real eigenvalues only
- resonant : weakly hyperbolic but not hyperbolic

Linear resonant system

$f(u) = Au$, A $p \times p$-matrix with real eigenvalues but not diagonalizable

$$\partial_t U + A\partial_x U = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

$$U(\cdot, 0) = U_0$$

- Well posed in C^∞
- not well posed in L^p

Example 1

$$\partial_t u + \partial_x(au) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

$a = a_g$ on $\mathbb{R}_-$, $a = a_d$ on $\mathbb{R}_+$
$a_g a_d < 0$

$$\partial_t U + A\partial_x U = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

$$U = \begin{bmatrix} u \\ a \end{bmatrix}, A = \begin{bmatrix} a & u \\ 0 & 0 \end{bmatrix}$$

If $a_g > 0$ and $a_d < 0$, no solution in the class of functions

If $a_d > 0$ and $a_g < 0$, infinity of solutions

Example 2, fluid flows in porous media

Fluid flows in porous media under gravity effects

$$\partial_t u + \partial_x (kf(u)) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

$k = k_g$ on $\mathbb{R}_-$, $k = k_d$ on $\mathbb{R}_+$ ($k > 0$)
$f(0) = f(1) = 0$, $f \in C^1([0,1], \mathbb{R})$.
It can be written as a non linear resonant system
(resonant for u such that $f'(u) = 0$).

$$U = \begin{bmatrix} u \\ k \end{bmatrix}, F(U) = \begin{bmatrix} k(f(u)) \\ 0 \end{bmatrix}, DF(U) = \begin{bmatrix} kf'(u) & f(u) \\ 0 & 0 \end{bmatrix}$$

This problem has a unique entropy weak solution for any initial datum u_0 taking values between 0 and 1 and one has convergence of all "monotone" FV schemes (Seguin-Vovelle-Bachmann)

Example 3, solid mechanics

$v = (v_1, v_2) \in C^1(\mathbb{R}^2, \mathbb{R}^2)$ is given
unknown : $e : \mathbb{R}^2 \times \mathbb{R}_+ \to \mathbb{R}^2$, $e = (e_1, e_2)$

$$\partial_t e + \nabla(v \cdot e) = 0$$

It is a linear resonant system in direction n such that $v \cdot n = 0$
It is interesting in the case of the inital data satisfies $\mathrm{curl}(e_0) = 0$
It is expected to have also at any time $\mathrm{curl}(e) = 0$
Then, the system is equivalent to the following one

$$\partial_t e_1 + \mathrm{div}(v e_1) - e_1 \partial_y v_1 + e_2 \partial_x v_2 = 0$$
$$\partial_t e_2 + \mathrm{div}(v e_2) - e_2 \partial_x v_2 + e_1 \partial_y v_1 = 0$$

which is non resonant (and more adapted to numerical simulation)
We have existence and uniqueness for the IVP if v is regular

Example 3

Convection part of $\partial_t e + \nabla(v \cdot e) = 0$, $v = (v_1, v_2)$

$$\partial_t e + A_1 \partial_1 e + A_2 \partial_2 e = 0$$

$$A_1 = \begin{bmatrix} v_1 & v_2 \\ 0 & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 0 & 0 \\ v_1 & v_2 \end{bmatrix}$$

For a normal vector $n = (n_1, n_2)$,

$$n_1 A_1 + n_2 A_2 = \begin{bmatrix} n_1 v_1 & n_1 v_2 \\ n_2 v_1 & n_2 v_2 \end{bmatrix}$$

is resonant if $v \cdot n = 0$, $v \neq 0$
(0 is a double eigenvalue and $n_1 A_1 + n_2 A_2 \neq 0$)