A stochastic scheme for front tracking on unstructured meshes.

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Many physical problems involve physical fronts, which are thin interface between two physical domains with different properties, for instance: multi-phase flows or reacting flows.

In a numerical point of view, dealing with these fronts is a challenging task because numerical diffusion tends to smear the sharp fronts and then to create "non-physical mixing layers".

Many efficient and sophisticated methods have been proposed in order to deal with front propagation.

- Level set, VOF, front discretization/lagrangian;
- High-order methods;
- **Compressive/sharpening methods**.

In this talk, a new sharpening technique is presented. It involves a **fractional step approach** and a **random choice**.

Two references are on the basis of the present work:

"Solutions in the large for nonlinear hyperbolic systems of equations", Glimm, 1965.

"Probabilistic analysis of the upwind scheme for transport equations", Delarue&Lagoutière, 2011.

"Solutions in the large for nonlinear hyperbolic systems of equations", James Glimm, Communications on pure and applied mathematics, 1965.

- 1st order FV scheme without spatial average process
  $\rightarrow$ Fronts remain perfectly sharp.
- Effective convergence rate of 1, even on the LD fields ! (1/2 for classical 1st order FV schemes)
- Restricted to 1D.

"Probabilistic analysis of the upwind scheme for transport equations", Francois Delarue, Frédéric Lagoutière, Archive for rational mechanics and analysis, 2011.

- Analysis of the Upwind scheme in terms of the expectation of a stochastic process, even for unstructured multi-D meshes.
- Proof of convergence with order 1/2 for the Upwind scheme.
- The latter arises from the statistical average.

We present here a scheme that is based on these ideas and which has been proposed in the three following references.

• *"On the use of Glimm-like schemes for transport equations on multi-dimensional domain"*, O. Hurisse, Int. Journal for Numerical Methods in Fluids, Vol 93(4), 2020, (https://hal.archives-ouvertes.fr/hal-02462202).
$\Longrightarrow$ Numerical studies: robustness, rate of convergence, accuracy, ...

• *"Convergence of a multidimensional Glimm-like scheme for the transport of fronts"*, T. Gallouët, O. Hurisse, IMA Journal of Numerical Analysis, Vol. 42(4), 2022, (https://hal.archives-ouvertes.fr/hal-02940407).
$\Longrightarrow$ Theoretical analysis: proof of convergence for a simple situation

• *"A random choice scheme for scalar advection"*, T. Gallouët, O. Hurisse, S. Kokh, Int. Journal for Numerical Methods in Fluids, 2023.
$\Longrightarrow$ Extension of the scheme to the advection of any scalar quantity.

Outline of the talk:

- **Description of the scheme**
- **Numerical examples**

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Front propagation problem.

Let us consider the two-dimensional advection problem of the quantity ϕ:

$$\begin{cases} \frac{\partial}{\partial t}\phi(t,x,y) + \mathscr{U}(t,x,y)\cdot\nabla\phi(t,x,y) = 0, \\ \phi(t=0,x) \in \{0,1\}, \end{cases} \tag{1}$$

where $\mathscr{U}$ is a given smooth velocity field.

For the sake of simplicity, we restrict here to divergence-free velocity fields:

$$\nabla\cdot\mathscr{U} = 0.$$

But the scheme can be applied for more general compressible models.

System (1) then reads in conservative form:

$$\begin{cases} \frac{\partial}{\partial t}\phi(t,x,y) + \nabla\cdot(\mathscr{U}(t,x,y)\phi(t,x,y)) = 0, \\ \phi(t=0,x) \in \{0,1\}. \end{cases} \tag{2}$$

Definition of the scheme

We assume that: $\forall i\ \phi_i^n \in \{0,1\}$ at time t^n. We set $t^{n+1} = t^n + \Delta t$.

The overall scheme is based on a fractional step approach:

- Prediction step = an Upwind scheme (convection step), $(\phi_i^n)_i \rightarrow (\phi_i^{n+1,*})_i$

$$\frac{|\Omega_i|}{\Delta t}\left(\phi_i^{n+1,*} - \phi_i^n\right) + \sum_{\Omega_j \ neigh.\ \Omega_i} \phi_{ij}^n \mathscr{U}(t^n, \bar{x}_{ij}) \cdot n_{ij} S_{ij} = 0,$$

  where:

$$\phi_{ij}^n = \phi_i^n, \text{ if } \mathscr{U}(t^n, \bar{x}_{ij}) \cdot n_{ij} > 0,\ \phi_{ij}^n = \phi_j^n \text{ otherwise.}$$

  Explicit scheme $\rightarrow$ a classical CFL constraint on Δt has to be fulfilled.

- Projection step = Glimm Random Update / GRU, $\phi_i^{n+1,*} \rightarrow \phi_i^{n+1}$

$$\phi_i^{n+1} = \begin{cases} 1, & \text{if } \omega^n \in [0, \phi_i^{n+1,*}], \\ 0, & \text{otherwise,} \end{cases} \quad (3)$$

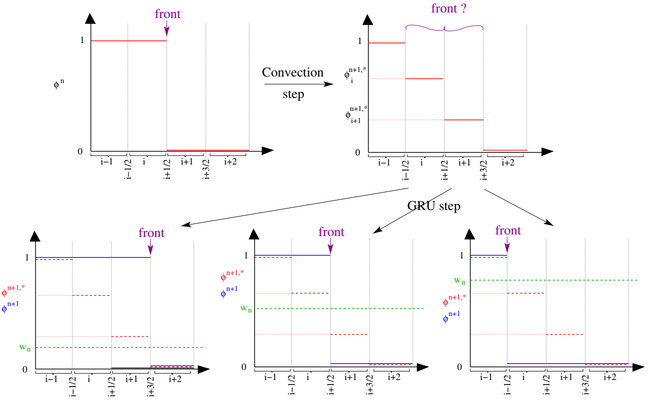
  where ω^n follows a uniform dist. on $(0,1)$. *This is a cell-wise update.*

In the following, Upwind step + GRU step $\longrightarrow$ Upwind-GRU.

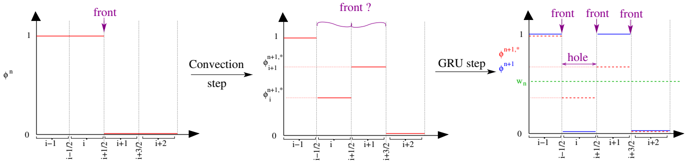
Illustration for a 1st order FV scheme with 2-point flux and MP

Prediction step:
After the convection step, the *front is smeared*. If the convection step is consistent, *the front is located somewhere inside this "smeared region"*. Where could the new front be located ?

Projection step/GRU:
Several positions are possible depending on the value of ω^n *which is the same for all cells*. There are three possible locations on this example.



- Choosing the **same** ω^n for all the cells with a **monotonicity preserving (MP) convection scheme** $\Rightarrow$ **no hole is introduced**.
- Counterexample with a non-MP scheme:



- Convection step $\Rightarrow$ $\phi_i^{n+1,*}$ may be $\neq$ from $\{0,1\}$ in the cells near the front.
- But if the convection scheme is consistent, the exact front is somewhere in the domain where $\phi_i^{n+1,*} \in]0,1[$.
- Projection step/GRU $\Rightarrow$ ϕ_i^{n+1} belongs to $\{0,1\}$ for all the cells.
- **Hence, the approximated front is perfectly sharp...**
- **... but not exactly at the location of the exact front. This is true but only statistically (thanks to the statistical consistency).**
- On regular cartesian meshes, the approximated front is simply translated (with MP convection scheme).

Additional remarks

- The overall scheme is not conservative (only statistically conservative).
- The method can be applied to compressible flows, $\nabla \cdot \mathscr{U} = 0$ is not mandatory. This choice just renders the first part of the talk more easy, but numerical tests for compressible flows are presented in the next sections.
- The velocity field can also be an approximated solution (for instance when coupling ϕ with the velocity field arising from the Euler system).
- Many other schemes may be used instead of the Upwind scheme, for instance high order schemes (MUSCL/RK2/Minmod has been tested).
- In fact, it seems that the main requirement for the convection scheme is to be "monotonicity preserving" (see next point).
- No hole is created when using the same ω^n for all the cells at a given iteration n (with a "monotonicity preserving" scheme).
- In a practical point of view, uniform distribution is replaced by low-discrepancy sequences (see below).
- Implementation of the GRU step is (very) easy on multi-D unstructured meshes and for multi-processor computers.
- CPU-time: GRU-step is almost free (can be restricted to the cells near the front).
- **Pathological cases for "thin shapes"/fronts collapse** (see example in the section presenting some numerical results).

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Quasi-random generator/Low-discrepancy sequences

The random number ω^n is generated thanks to a uniform distribution $\mathscr{U}(0,1)$.

But from a practical point of view, ω^n is chosen in quasi-random low-discrepancy sequences.

In the following, results are obtained using two famillies of sequences.

- **The Halton-Van der Corput low-discrepancy familly of sequences.** It is parametrized by two integers K_1 and K_2, relatively prime and such that $K_1 > K_2 > 0$. It is the most classical familly of sequences used for this kind of algorithm.
- **The Linear Congruential Generator**. It defined by a seed ω^0, and then by $\omega^{n+1} = modulo\left(\omega^n + \frac{\sqrt{5}-1}{2}, 1\right)$. It is very simple to implement.

Other possible sequences: Hammersley sequences, Sobol Sequences, ...

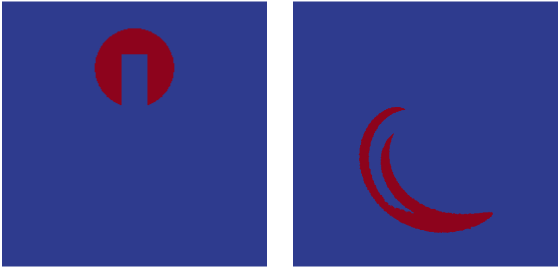
Non-solid rotation of a Zalesak shape.

- Velocity field: $U_x = a\ r\ (0.5 - y)$ and $U_y = a\ r\ (x - 0.5)$

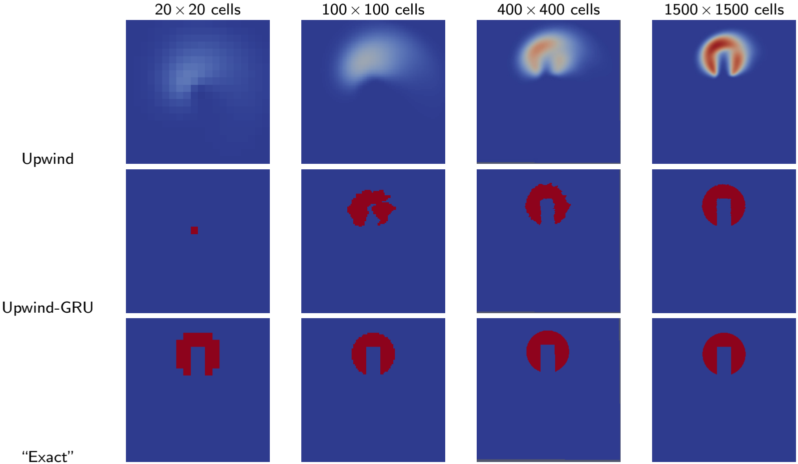
$$\text{with } r^2 = (0.5 - y)^2 + (x - 0.5)^2,$$

$$a = \begin{cases} 1, & \text{if } 0 < t \leq t_{end}/2, \\ -1, & \text{if } t_{end}/2 < t \leq t_{end}. \end{cases}$$

- Initial condition: Zalesak shape.
- Final exact solution at $t_{end} = 6\Pi\ s$ → approx. one half rotation and back.



Non-solid rotation of a Zalesak shape. Cartesian mesh. Van der Corput $K_1 = 5$ and $K_2 = 3$.



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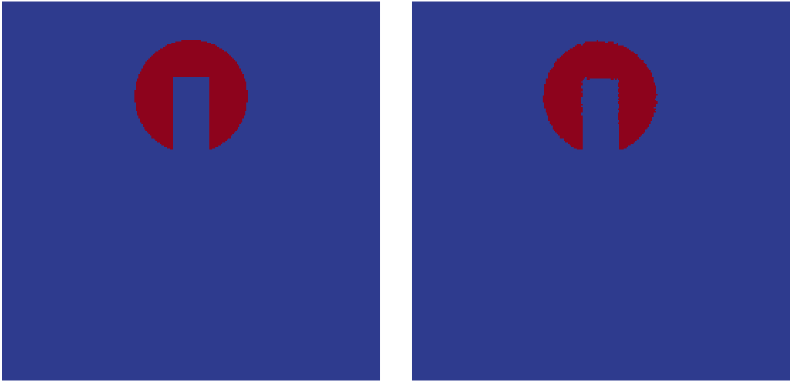

Figure: Non-solid rotation of a Zalesak shape. Cartesian mesh 1500×1500 cells. Exact (Left) and Upwind-GRU (Right).

Non-solid rotation of a Zalesak shape. Cartesian mesh. Van der Corput $K_1 = 23$ and $K_2 = 5$.

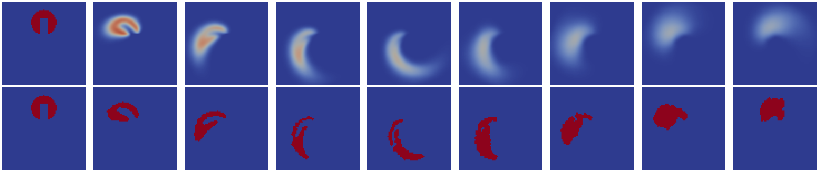

Figure: Non-solid rotation of the Zalesak's "C" shape for the structured mesh containing 75×75 cells at different times, $K_1 = 23$ and $K_2 = 5$. First row: Upwind scheme, second row: Upwind-GRU scheme.

Non-solid rotation of a Zalesak shape. Cartesian mesh. Van der Corput $K_1 = 23$ and $K_2 = 5$.

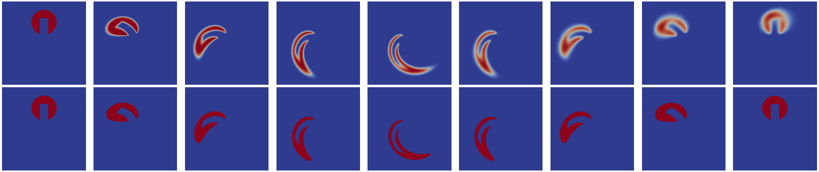

Figure: Non-solid rotation of the Zalesak's "C" shape for the structured mesh containing 1500×1500 cells at different times, $K_1 = 23$ and $K_2 = 5$. First row: Upwind scheme, second row: Upwind-GRU scheme.

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Model

- Model: the single-material Euler system,

$$\begin{cases} \frac{\partial}{\partial t}(\rho\alpha) + \nabla_x \cdot (\rho U \alpha) = 0, \\ \frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho U) = 0, \\ \frac{\partial}{\partial t}(\rho U) + \nabla_x \cdot \left(\rho U^2\right) + \nabla_x P(\rho, e) = 0, \\ \frac{\partial}{\partial t}(\rho E) + \nabla_x \cdot (U(\rho E + P(\rho, e))) = 0, \end{cases} \tag{4}$$

  with the specific total energy $E = e + U^2/2$ and the specific internal energy e.

- **Important: The pressure law does not depend on $\alpha \rightarrow P = P(\rho, e)$!**
- **We have a single material and only one EOS. The difference of density is reproduced through the temperature.**
- **$\Rightarrow$ The setting is different than for classical RMI simulations.**

Numerical aspects

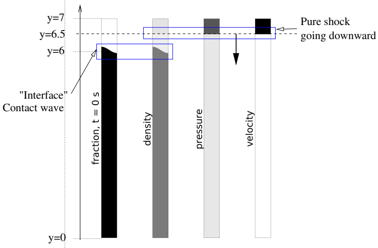
- Numerical scheme for prediction step:
  - First order Finite Volumes scheme is used (second order scheme available).
  - Interfacial fluxes are computed using the relaxation scheme proposed in [1].
  - This prediction step is conservative and it preserves monotonicity.
  - The CFL constraint is associated with the pressure waves $\Rightarrow$ contact waves are not accurately approximated for low Mach flows.
- Projection step: GRU is applied to the fraction α.
- Code: PATAPON, which is a GPU based solver developed by P. Helluy (IRMA, University of Strasbourg) using OpenCL/python libraries.
- Meshes: 2D Cartesian meshes are used (GPU efficiency).

[1] *Relaxation approximation of the Euler equations*, C. Chalons and J.-F. Coulombel, J. of Math. Anal. and App., Vol 348(2), 2008.

- Computational domain:
  - rectangular domain $L_x = 0.5\ m$ and $L_y = 7\ m$,
  - regular square cells, N cells along L_x and $14 \times N$ along L_y,
  - gravity is not accounted for.
- Perfect gas EOS:

  $P = \rho e(\gamma - 1)$ and $e = C_v T$ with $\gamma = 1.4$ and $C_v = 720\ J/K$.
- Boundary conditions:

  Left / right = symmetry/wall - top / bottom = outlet.
- Initial conditions:



- above the shock: $\alpha = 0$, $P = 1.68\ bar$
- light fluid zone: $\alpha = 0$, $P = 1.0\ bar$ and $T = 293\ K$
- heavy fluid zone: $\alpha = 1$, $P = 1.0\ bar$ and $T = 58\ K$
- separation between light/heavy fluids: $y = 0.6 + 0.1\ \cos(2\Pi x)$

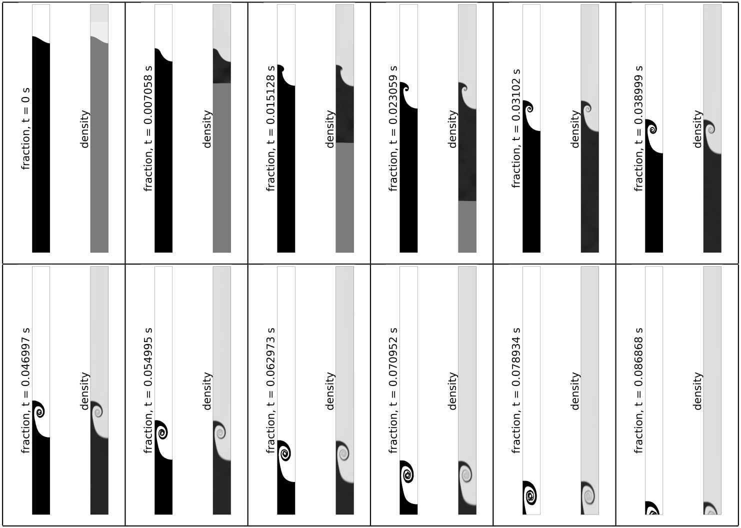


Figure: RMI, 2048x28672 cells, first order FV scheme + GRU.

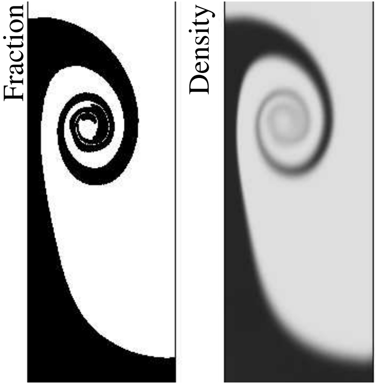


Figure: RMI, 2048 cells along x, first order FV scheme + GRU, zoom at time $t = 0.062973$ s.

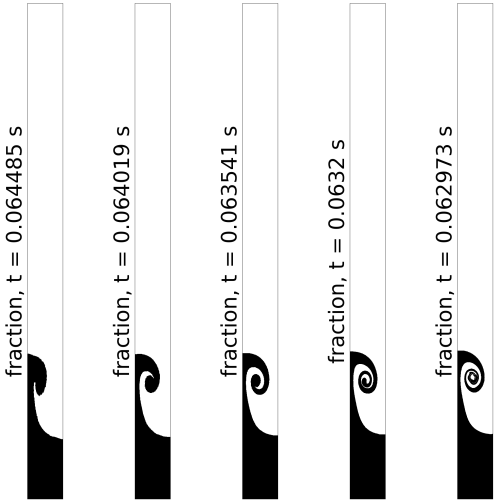


Figure: RMI, $\{128, 256, 512, 1024, 2048\}$ cells along x, first order FV scheme + GRU.

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Conclusion

- The GRU step has been applied here to front propagation (it applies to compressible or incompressible flows)...
- ... but it has recently been extended to the transport of any scalar functions (joint work with T. Gallouët and S. Kokh).
- It can be applied with a lot of existing schemes (fractional step approach).
- It is efficient/accurate and remains very simple and robust.
- It performs as well on unstructured meshes (not shown here).
- A proof of convergence has been proposed for simple cases with the Upwind-GRU scheme (joint work with T. Gallouët).

Perspectives: numerical aspects

- More tests should be performed $\rightarrow$ comparisons with other schemes (error/accuracy *versus* cpu-time).
- Proposition for handling the pathological behavior/front collapse.
- For RMI simulations : a two-phase flow model with a pressure law $P(\alpha, \rho, e)$ with an EOS depending on α + GRU step applied to α (work in progress with P. Helluy).

Thank you.