The Vofire (Reconstructed Finite Volume) method for the tracking of interfaces on unstructured meshes

Emmanuel Labourasse
Bruno Després & Frédéric Lagoutière (P6)

CEA DIF
Outline

- Motivations
- Geometric formulation for pure advection
- Application in the ALE framework
- Results in 3D
- Conclusions
Motivations

- Physical constraints (for instance for the hohlraum calculation)
  - Several materials and phases (for instance four for an ICF target and four for the surrounding cavity)
  - Very different properties for the materials (equation of states, opacity, reaction,...)

- Numerical features
  - Millions of cells in 3D
  - Million(s) of mixed cells
  - Unstructured meshes
  - Parallel Calculation

- Need: a robust, quick and efficient reconstruction method
Subjective review of interface tracking

<table>
<thead>
<tr>
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<th>locally conservative in mass</th>
<th>interface geometry</th>
<th>cheap</th>
<th>robust</th>
<th>parallel</th>
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<td>Front-T. (^a)</td>
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\(^d\) Controled by the Newton convergency
Initial observation

We observe the numerical diffusion in elementary advection test cases is made up of two distinct phenomena in the case of a transport velocity unaligned with the mesh main directions.

Therefore, we must distinguish between the diffusion parallel to the transport direction (1D), and the transversal diffusion (multi-D).
How to deal with this issue?

An anti-diffusive process must act

- in the direction normal to the velocity field,
- then in the direction of the velocity field.

![Diagram showing sharp interface reconstruction in each cell and velocity field reconstruction methods]
Geometric formulation (1/3)

We focus on the pure advection equation: \( \partial_t c + a.\nabla c = 0 \).

First stage: the transversal reconstruction

![Diagram](image)

Notations

We call \( s_j \) the surface of \( T_j \). \( T_j \) is geometrically split into two subgrid triangles \( T_{jk} \) and \( T_{jl} \) of surface \( s_{jk} \) and \( s_{jl} \), with \( s_{jk} + s_{jl} = s_j \).

How to reconstruct \( c_{jk} \) and \( c_{jl} \) (subgrid values of \( c \) in \( T_{jk} \) and \( T_{jl} \))?

**Goal:** \( c_{jk} \) has to be as close as possible of \( c_k \), \( c_{jl} \) has to be as close as possible of \( c_l \).

**Constraints:** conservative reconstruction, maximum principle preservation.
Geometric formulation (2/3)

Assuming for instance $c_k \leq c_l$, 4 configurations can occur:

a) transport

\[ c_{jk} = c_k \]

\[ c_{jl} = \frac{c_j s_{jk} - c_k s_{jk}}{s_{jl}} \]

\[ c_j \notin ]c_k, c_l[ \]

no transversal reconstruction

b) sharp, conservative reconstruction

\[ |c_k - c_j| s_{jk} \leq |c_l - c_j| s_{jl} \]

\[ c_j \in ]c_k, c_l[ \]

c) The other cases are similar.
Example of reconstruction (1/2)

Diffusion occurs

No reconstruction: the advection phase is diffusive,

No diffusion

With transversal reconstruction: no more diffusion.
We can not reconstruct (in cell \( j \))

No transversal reconstruction possible, but no “transversal” diffusion anyway, because there is only one downwind cell.
Second stage: transport direction
After the transversal reconstruction, 1D problems remain.

To be as anti-diffusive as possible, these problems are solved using the downwind scheme under stability constraint.
This geometrical formulation can be recast as an algebraic formulation on 3D and on any cells, in minimizing functionals (not presented here). For the case a), the algebraic formulation is equivalent to the geometric formulation.
The scheme is made up of three stages:

- **the transversal reconstruction stage** - The constant by cell, discontinuous at faces field is recast as a discontinuous in cell, as continuous as possible at faces field,

- **the transport direction stage** - Using the previous field, compute the fluxes with the UltraBee calculation,

- **the projection stage** - Compute the resulting constant by cell, discontinuous at faces field.
Advection test case

Pure advection in the diagonal direction (on tetraedra: 2D solution, 3D mesh).

mesh & extruded initial value

extruded solution for section $z = z_{ave}$
Issues in lagrangian framework

Lagrangian: the mesh follows the material interfaces

+ interfaces match the mesh
- the mesh is deformed with the interfaces

Eulerian: the mesh is fixed

+ mesh is free from the interfaces
- interfaces are diffused
ALE method

- **Lagrangian phase**

\[
\frac{d}{dt} \int_{V_{lag}(t)} \rho dV = 0 \\
\frac{d}{dt} \int_{V_{lag}(t)} \rho u dV + \int_{S(t)} P dS = 0 \\
\frac{d}{dt} \int_{V_{lag}(t)} \rho e dV + \int_{S(t)} P u. n dS = 0
\]

- **EOS** : \((p, T) = f(\rho, e)\)

- smoothing of the resulting mesh

- **Projection phase**

\[
\frac{D}{Dt} \int_{V_{ale}(t)} \rho_i dV + \int_{S(t)} \rho_i (u - u_g). n dS = 0 \\
\frac{D}{Dt} \int_{V_{ale}(t)} \rho u dV + \int_{S(t)} \rho u (u - u_g). n dS = 0 \\
\frac{D}{Dt} \int_{V_{ale}(t)} \rho e u (u - u_g). n dS = 0
\]

with \(i\) the material, \(\rho_i = \rho c_i\)

and \(\sum_i c_i = 1\)

- **EOS** : \((p, T) = f(\rho, e)\)

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Results: two-phase shock tube

Sod’s shock tube on distorted mesh: 1D solution on a 3D mesh

Initial conditions:
- Order 1 advection:
  - 113 mixed cells
- Order 2 advection:
  - 47 mixed cells

Vofire advection:
- 6 mixed cells
Three materials instability

A shock hits a triple line: difficult benchmark for interface reconstruction (3 interfaces, 1 triple line).

2D

3D

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Results: 3 materials instability

- Equipotential smoother (Tipton-Jun), explicit (Jacobi),
- Metrics: intersection of gradient lengthscales (internal energy, concentrations),
- Swept advection extended at the 2nd order with MUSCL,
- Vofire reconstruction for the concentrations.
Limitations

Low level numerical diffusion remains (but the interfaces are compact),

Interface reconstruction can initiate a Rayleigh-Taylor (or Richtmyer-Meshkov) instability.
## Subjective comparison in 3D

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\(^a\text{cf. previous slide : limitations}\)

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Conclusion and futur works

- We have presented the Vofire method applied to the material interfaces in 3D configuration on unstructured meshes,

- We obtain a very favourable ratio cost/efficiency: 
  \[ \text{Vofire cost} < 0.5 \text{ advection step cost} \]
  whereas 
  \[ \text{Youngs-PLIC cost} > 10 \text{ advection step cost} \],

- Discontinuities remain compact (the diffusion zone is finite),

- Parallel implementation is not difficult,

- A paper is in preparation for publication.